TESIS DOCTORAL

HYBRIDIZATION OF MACHINE LEARNING FOR ADVANCED MANUFACTURING

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Por los que están y por los que se fueron pero están

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Formato de la Tesis

El formato en el que ha sido elaborada la tesis se corresponde con el de **compendio de publicaciones** dado que corresponde a un compendio de trabajos previamente publicados. De acuerdo con lo contemplado en el artículo 14.1 del Capítulo II del Reglamento de Doctorado de la Universidad de Salamanca aprobado por la Comisión de Doctorado y Posgrado el 15 de febrero de 2013 que indica: "*los estudios de doctorado concluyen con la elaboración y defensa de una tesis doctoral, que consistirá en un trabajo original de investigación, elaborado por el doctorando, en cualquier campo del conocimiento, siguiendo el formato determinado por la Comisión Académica del Programa de Doctorado, entre los posibles formatos establecidos por la Comisión de Doctorado*".

El presente apartado da cumplimiento al artículo 4.1 del Procedimiento para la Presentación de la Tesis Doctoral en la Universidad de Salamanca en el formato de Compendio de Artículos/Publicaciones, aprobado por la Comisión de Doctorado y Posgrado el 15 de febrero de 2013.

Las publicaciones que forman este compendio y que han sido publicadas en revistas científicas, del ámbito de la especialidad del trabajo desarrollado en la tesis, e indexadas en el *Journal Citation Reports* son:

- Vicente Vera[1], Emilio Corchado[2], Raquel Redondo[3], Javier Sedano[4], Álvaro E.García[1], **'Applying Soft Computing Techniques to Optimise a Dental Milling Process'**, Neurocomputing, New trends on Soft Computing Models in Industrial and Environmental Applications, 109 (2013): 94–104, https://doi.org/10.1016/j.neucom.2012.04.033 - Factor de Impacto Publicado JCR: 2.005, Cuartil mayor: Q1, Área: Computer Science, Artificial Intelligence Cuartil: Q1 Posición en el área: 28/121.
- Raquel Redondo[3], Javier Sedano[4], Vicente Vera[1], Beatriz Hernando[1], Emilio Corchado[2], **'A Novel Hybrid Intelligent System for Multi-Objective Machine Parameter Optimization'**, Pattern Analysis and Applications 18, no. 1 (2015): 31–44, https://doi.org/10.1007/s10044-013-0345-7 - Factor de Impacto Publicado JCR: 1.104, Cuartil mayor: Q3, Área: Computer Science, Artificial Intelligence Cuartil: Q3 Posición en el área: 80/130.

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Asimismo, con la presente tesis se opta a la mención de "**Doctor internacional**", por lo tanto cumple con las indicaciones señaladas en el Procedimiento para la Obtención de la Mención de "Doctor Internacional" en el Título de Doctor por la Universidad de Salamanca, aprobado por la Comisión Ejecutiva de la Escuela de Doctorado, en su sesión de fecha 28 de mayo de 2018.

Adicionalmente, se pretende obtener la mención "**Doctorado industrial**", al cumplir con lo indicado en el artículo 15.bis del Real Decreto 99/2011, de 28 de enero, por el que se regulan las enseñanzas oficiales de Doctorado.

Resumen

En el contexto de la industria, hoy por hoy, los términos “Fabricación Avanzada”, “Industria 4.0” y “Fábrica Inteligente” están convirtiéndose en una realidad. Las empresas industriales buscan ser más competitivas, ya sea en costes, tiempo, consumo de materias primas, energía, etc. Se busca ser eficiente en todos los ámbitos y además ser sostenible. El futuro de muchas compañías depende de su grado de adaptación a los cambios y su capacidad de innovación. Los consumidores son cada vez más exigentes, buscando productos personalizados y específicos con alta calidad, a un bajo coste y no contaminantes. Por todo ello, las empresas industriales implantan innovaciones tecnológicas para conseguirlo.

Entre estas innovaciones tecnológicas están la ya mencionada Fabricación Avanzada (*Advanced Manufacturing*) y el *Machine Learning* (ML). En estos campos se enmarca el presente trabajo de investigación, en el que se han concebido y aplicado soluciones inteligentes híbridas que combinan diversas técnicas de ML para resolver problemas en el campo de la industria manufacturera. Se han aplicado técnicas inteligentes tales como Redes Neuronales Artificiales (RNA), algoritmos genéticos multiobjetivo, métodos proyeccionistas para la reducción de la dimensionalidad, técnicas de agrupamiento o *clustering*, etc. También se han utilizado técnicas de Identificación de Sistemas con el propósito de obtener el modelo matemático que representa mejor el sistema real bajo estudio.

Se han hibridado diversas técnicas con el propósito de construir soluciones más robustas y fiables. Combinando técnicas de ML específicas se crean sistemas más complejos y con una mayor capacidad de representación/solución. Estos sistemas utilizan datos y el conocimiento sobre estos para resolver problemas. Las soluciones propuestas buscan solucionar problemas complejos del mundo real y de un amplio espectro, manejando aspectos como la incertidumbre, la falta de precisión, la alta dimensionalidad, etc.

La presente tesis cubre varios casos de estudio reales, en los que se han aplicado diversas técnicas de ML a distintas problemáticas del campo de la industria manufacturera. Los casos de estudio reales de la industria en los que se ha trabajado, con cuatro conjuntos de datos diferentes, se corresponden con:

- Proceso de fresado dental de alta precisión, de la empresa Estudio Previo SL.
- Análisis de datos para el mantenimiento predictivo de una empresa del sector de la automoción, como es la multinacional Grupo Antolin.

Adicionalmente se ha colaborado con el grupo de investigación GICAP de la Universidad de Burgos y con el centro tecnológico ITCL en los casos de estudio que forman parte de esta tesis y otros relacionados.

Las diferentes hibridaciones de técnicas de ML desarrolladas han sido aplicadas y validadas con conjuntos de datos reales y originales, en colaboración con empresas

industriales o centros de fresado, permitiendo resolver problemas actuales y complejos. De esta manera, el trabajo realizado no ha tenido sólo un enfoque teórico, sino que se ha aplicado de modo práctico permitiendo que las empresas industriales puedan mejorar sus procesos, ahorrar en costes y tiempo, contaminar menos, etc. Los satisfactorios resultados obtenidos apuntan hacia la utilidad y aportación que las técnicas de ML pueden realizar en el campo de la Fabricación Avanzada.

Abstract

In the industry context, nowadays the terms "Advanced Manufacturing", "Industry 4.0" and "Smart Factory" are becoming real. Industrial companies seek to be more competitive, whether in costs, time, consumption of raw materials, energy, etc. Companies seek to be efficient in all areas and also to be sustainable. The future of many companies depends on their degree of adaptation to changes and their innovation capacity. Consumers are increasingly demanding, looking for personalized and specific products with high quality, at low cost and non-polluting. In order to meet these requirements, industrial companies implement technological innovations.

These technological innovations include the previously mentioned Advanced Manufacturing and Machine Learning (ML). The present research work is focused in these fields, hybrid intelligent solutions have been designed and applied, combining several ML techniques in order to solve problems in the field of manufacturing industry. Intelligent techniques have been applied, including Artificial Neural Networks (ANN), multiobjective genetic algorithms, projection methods for the reduction of dimensionality, clustering techniques, etc. In order to obtain the mathematical model that best represents the real system under study, Systems Identification techniques have also been used.

Several techniques have been hybridized with the purpose of building more robust and reliable solutions. By combining specific ML techniques, more complex systems are created with a greater representation / solution capacity. To solve such problems, these systems use data and knowledge about them. The proposed solutions search for solving ad wide spectrum of real-world complex problems, handling aspects such as uncertainty, lack of precision, high dimensionality, etc.

This doctoral thesis includes several real case studies, in which various ML techniques have been applied to different problems in the field of manufacturing industry. The real case studies of the industry that are addressed, with four different data sets, correspond to:

- Dental high-precision milling process, by the company Estudio Previo SL.
- Data analysis for predictive maintenance purposes in a company from the automotive sector, as it is the multinational Grupo Antolin.

Furthermore, in the case studies that are part of this thesis and other related ones, collaboration with the GICAP research group at the University of Burgos and with the ITCL technological centre has been carried out.

The different developed hybridizations of ML techniques have been applied and validated with real and original data sets, in collaboration with industrial companies or milling centres, allowing to solve current and complex problems. Thus, the work carried

out has not only had a theoretical approach, but it has also been applied in an empirical way, allowing industrial companies to improve their processes, reducing costs and time, polluting less, etc. The satisfactory results that have been achieved indicate the helpfulness and contribution that ML techniques can make in the field of Advanced Manufacturing.

Parte I. Introducción y objetivos

En esta primera parte se incluye una introducción con los antecedentes del tema objeto de estudio de esta tesis, la solución propuesta, la metodología utilizada, los objetivos, el listado de las publicaciones generadas en torno al objeto de estudio y las principales conclusiones.

1 Antecedentes

En el mundo actual, el sector industrial y sus empresas, deben abordar una serie de cambios para ser cada vez más competitivos. Las empresas del sector industrial en países HCC (*High-cost Countries*) deben competir con las de países considerados LCC (*Low-cost Countries*).

El futuro de muchas de estas empresas está ligado a su adaptabilidad a un entorno cada vez más estricto. Por ello, para conseguir la evolución de sus productos, cobra especial importancia la innovación, mediante el uso de nuevos materiales, nuevas tecnologías de fabricación, la digitalización, el internet de las cosas industrial (IIoT - *Industrial Internet of Things*), etc. Adicionalmente, los clientes son cada vez más exigentes; existe una tendencia en alza a la personalización de los productos, sin perder calidad, a la vez que una gran preocupación por la sostenibilidad.

Las empresas pueden utilizar la fabricación avanzada para ofrecer productos diferentes a los de sus competidores, con un valor añadido y diferenciador del resto, y/o cambiar cómo son fabricados, siendo más competitivas tanto en entornos desarrollados como con empresas localizadas en LCC.

Las compañías buscan ser más competitivas, ágiles y eficientes, mejorando sus procesos para maximizar la producción garantizando la calidad, por supuesto, reduciendo costes, y a su vez con consumos sostenibles de energía y materias primas. Muchas de las tecnologías de Fabricación Avanzada no son nuevas, pero sí lo son las recientes formas de integración y mejoras de uso que se consiguen con la digitalización y las tecnologías habilitadoras de la Industria 4.0 [1]. La aplicación conjunta de tecnologías es lo que puede marcar la diferencia creando nuevos retos y oportunidades. En el futuro se considera clave, tanto en la investigación como en la práctica, la fabricación inteligente, porque aporta valor añadido a los sistemas y productos mediante la aplicación de tecnologías punteras [2].

La presente Tesis Doctoral se centra en el estudio y validez de la hibridación de distintas técnicas de ML [3] aplicadas a varios casos de estudio de fabricación avanzada en la industria, con sus correspondientes conjuntos de datos multidimensionales. Se presentan cuatro casos de estudio: dos de ellos están relacionados con el fresado de alta precisión para la obtención de piezas dentales, y los otros dos con la industria del sector de componentes de la automoción.

En cuanto a los primeros casos de estudio, cabe indicar que en los últimos años la industria dental ha experimentado grandes cambios gracias a la digitalización y el uso de nuevos materiales para la creación de prótesis dentales. El uso de tecnologías CAD/CAM [4, 5], junto con las máquinas de fresado de alta precisión, en el campo de la Terapéutica Médica (Odonto-Estomatología), es una industria en continuo auge y que se espera que crezca aún más [6], por lo que es muy interesante la aplicación de procesos de optimización en dicho campo.

El fresado de las piezas dentales es un paso crucial en un proceso de restauración dental. Dichas piezas deben tener gran exactitud, veracidad y precisión, debiendo ajustar perfectamente con el resto de piezas dentales del paciente, generando una correcta respuesta biológica y mecánica [5]. Existen estudios que se centran en medir la precisión obtenida en las piezas dentales mediante el proceso de fresado [7, 8], pero hay muy poco trabajo previo en cuanto a la optimización del propio proceso de fabricación mediante fresado.

El uso de ML es cada vez más común en todo el campo médico, pero en el ámbito de la odontología todavía está en sus primeros pasos [9, 10], aunque avanza rápidamente más allá de la práctica dental basada en texto e imágenes [11]. La mayoría de los estudios previos en este campo son sobre el diagnóstico dental, por ejemplo, en la detección de caries [12] y su tratamiento [13] o incluso sobre la detección de fallos en el tratamiento [14]. Los estudios están centrados principalmente en la creación de sistemas que ayuden a los profesionales dentales a tomar decisiones [15].

Igualmente existen estudios en los que sus autores hibridan técnicas de ML en el ámbito de la odontología. Entre estos trabajos se encuentra [16], sin embargo, este trabajo tiene una finalidad completamente diferente a la optimización del propio proceso de fabricación, como se presenta en esta tesis, sino que se centra en el ámbito médico/biológico, en concreto en la recuperación de tejidos. En este estudio se han implementado dos tipos de algoritmos genéticos difusos híbridos, que incluyen el método Mogul y el método Thrift, con el propósito de estimar el efecto de los concentrados de plaquetas en la proliferación de células madre derivadas del diente humano. El enfoque que se propone con algoritmos genéticos difusos da como resultado un mejor sistema para la predicción de la edad en células vivas cultivadas en plasma rico en plaquetas y lisado de plaquetas.

Gracias al uso de tecnologías CAD/CAM en el ámbito de la Odonto-Estomatología para la rehabilitación y restauración oral-dental, se mejora el procesamiento y optimización de parámetros relacionados con la manufactura de las prótesis, tales como el tiempo de procesamiento, precisión, etc. en el desarrollo de piezas (tales como prótesis dentales-orales para realizar coronas parciales, *inlays*, *onlays*, etc.). Esta industria manufacturera, además de estar en continuo auge, es económicamente ventajosa, por lo que diversos estudios se centran en ella [17-19].

El proceso de optimización de los parámetros de la máquina, por ejemplo el parámetro de tiempo, permite importantes ahorros económicos debido al elevado número de piezas dentales producidas diariamente por el mismo centro de fresado dental de alta precisión. Esto puede ayudar significativamente a aumentar la eficiencia de una empresa y contribuir sustancialmente a la reducción de costes en la preparación y configuración de los procesos de las máquinas. Otro ejemplo es el ajuste marginal de una prótesis dental a la estructura dental remanente (dentina y esmalte), evitando así la invasión de tejidos y / o zonas anatómicas no preparadas. Este es el objetivo de cualquier tratamiento dental, ya que el éxito ahora radica en el ajuste de aproximadamente 15-25 micrómetros entre la prótesis y el resto de estructuras. Esto potenciaría y evitaría el filtrado de gérmenes y fluidos orales que en el corto o mediano plazo conducirán al fracaso del tratamiento.

Durante muchos años, el proceso tradicional de hacer y preparar estructuras dentales ha implicado el uso de cera, seguido de un proceso llamado "*Lost Wax*" [20]. Es una metodología válida, pero menos precisa. De hecho, se han dado casos en los que la prótesis no se ha ajustado correctamente a la estructura dental, lo que ha provocado caries a corto o medio plazo y el fracaso del tratamiento. El resultado óptimo sería el llamado ajuste pasivo, es decir, un ajuste entre 15-25 micrómetros que conduciría al éxito en el tratamiento de restauración dental.

Por estas y otras razones, actualmente es de gran interés optimizar los procesos [21, 22] relacionados con la preparación de prótesis dentales (estructuras dentales de materiales como cobalto-cromo, titanio, cerámica y / o resina) caracterizados por una alta precisión de ajuste en micrómetros.

El uso de algoritmos de optimización e identificación [23] hibridados junto a otras técnicas de ML, es una tecnología muy apropiada para abordar el desarrollo de este tipo de herramientas inteligentes. Sin embargo, los procesos de configuración de variables y parámetros son un problema bien conocido no resuelto por completo. En la literatura se han propuesto varias técnicas diferentes. En [24] se utiliza una matriz ortogonal de Taguchi para optimizar el efecto de los parámetros de inyección; en [25] se estudia la influencia de los parámetros operativos del mecanizado ultrasónico utilizando Taguchi y el método F-test; en [26] se exploran diferentes formas de mejorar la calidad del micromecanizado de metales con láser excimer KrF, utilizando el método de diseño experimental basado en matrices ortogonales. Los métodos convencionales pueden mejorarse en gran medida mediante la aplicación de técnicas de *Soft Computing* [27].

El novedoso método propuesto en esta tesis, para optimizar un proceso de fabricación en este ámbito, consiste en combinar distintas técnicas de ML tales como las redes neuronales artificiales (RNA) [28] y los algoritmos genéticos [29, 30].

Dos de los casos de estudio expuestos en esta tesis, versan sobre la optimización de la fabricación de piezas dentales metálicas en un centro de mecanizado de alta precisión de 5 ejes. La producción por fresado con estas máquinas sólo permite fabricar un modelo dental al mismo tiempo, por eso es importante optimizar este proceso de fabricación, optimizar los parámetros de la máquina puede suponer una reducción del tiempo necesario de fabricación además de ganar en precisión, ahorrar en materias primas y herramientas, etc. Al cabo del día se fabrican un alto número de piezas dentales, por lo que optimizar este proceso permite conseguir un gran ahorro económico.

Por otro lado, en la industria no solo se busca mejorar ciertos procesos de fabricación sino cualquier circunstancia que haga las compañías más competitivas. Por ello, las compañías industriales están desarrollando proyectos para converger al concepto de "Fabrica Inteligente" [31]. Con este tipo de proyectos las fábricas quieren ser capaces de aprender y adaptarse a los cambios en tiempo real y para poder conseguirlo deben tener información y datos constantes sobre los elementos involucrados en la fábrica. Para poder capturar toda esta información, es necesario instalar sensores y dispositivos IoT [32]. Gracias a la IIoT es posible tener millones de datos relacionados con las fábricas y sus máquinas. Pero todos estos datos no sirven de nada y resultan caros a no ser que se puedan analizar y es aquí donde las propuestas de Big Data [33] y Analítica Visual aparecen.

En la presente tesis se propone también extender un trabajo previo de hibridación de aprendizaje no supervisado para visualización (HUEP – *Hybrid Unsupervised Exploratory Plots*) [34] y aplicarlo por primera vez a dos casos reales de estudio. Dichos modelos son aplicados para el análisis de datos provenientes de varias máquinas industriales relacionadas con la fabricación de componentes de la automoción mediante técnicas de corte por agua a altas presiones.

Como sugieren algunos estudios [35], la computación visual juega un papel vital en la Industria 4.0 y la Fabricación Avanzada. En [36] se muestra cómo la aplicación de computación visual permite empoderar a los trabajadores en el marco de la Industria 4.0. En [37] los autores se focalizan en cómo la fusión de gráficos, la visión y las tecnologías multimedia pueden enriquecer el papel del nuevo operario 4.0. Otros estudios presentan una metodología para implementar mantenimiento predictivo basado en datos, no solo para tomar decisiones en la máquina, sino en la adquisición de datos y procesado con un análisis visual de la vida útil restante de una máquina de mecanizado [38].

Pero las empresas no deben olvidar el balance coste-beneficio alrededor de la Industria 4.0, como se explica en [39], donde se propone una metodología basada en la analítica de datos para monitorizar en la Industria 4.0, de un modo eficiente en cuanto a costes, con un caso real del sector de la automoción.

Existen estudios que investigan la aplicación de ML para mantenimiento predictivo y detección de fallos con un enfoque de clasificación, pero están basados en aprendizaje supervisado. En cambio, se ha dedicado menos esfuerzo a investigar la aplicación en este campo del aprendizaje no supervisado, aunque existe algún trabajo previo. Por ejemplo, en [40] se propone la aplicación de *k-means* combinado con lógica difusa para propósitos de mantenimiento predictivo. En [41], se ha aplicado una combinación de *clustering* con *k-means* restringido, modelado difuso y puntuación basada en "*Local Outlier Factor*" para detectar anomalías en un motor diesel marino auxiliar. Otra investigación [42] aplicó cinco métodos de agrupamiento (jerárquico, *k-medoids*, *k-means*, DBSCAN y OPTICS) para un modelo de monitoreo del estado de operación en un proceso de deposición de vapor químico en una empresa de semiconductores.

Otros estudios que buscan la detección de fallos o el mantenimiento predictivo analizan conjuntos de datos que han sido muy utilizados y probados en la literatura: conjunto de datos de cojinetes de motor [43-45], conjunto de datos de caja de cambios [43, 46, 47] y el conocido conjunto de datos *Tennessee Eastman Process* (TEP) [48]. En [49] se ha utilizado otro popular conjunto de datos sobre rodamientos. En la literatura se encuentran frecuentemente estudios de detección de fallos con conjuntos de datos de rodamientos; este tipo de conjuntos de datos se utilizan a menudo debido a la importancia de los fallos en estos dispositivos. Pero en la industria existen otros procesos, máquinas y dispositivos que también son importantes y que pueden requerir realizar una detección de fallos en ellos.

Con todo, la mayoría de los conjuntos de datos mencionados anteriormente están desactualizados y no están directamente relacionados con las máquinas que se encuentran en una fábrica del sector de la automoción. Una de las principales novedades de la presente investigación es el análisis de un caso de estudio novedoso y real que comprende dos máquinas habituales en la industria del automóvil. Los fallos que afectan a estas máquinas no están relacionados con los motores o sus rodamientos, sino con otro tipo de problemas.

Por otra parte, en cuanto a los métodos, previamente algunos autores han aplicado *Principal Component Analysis* (PCA) y RNA a máquinas de rotación [50] pero no con un propósito de visualización como se aborda en el presente trabajo. En otros estudios, también se han propuesto métodos de PCA extendidos: WPD-PCA [51], FPCA [52], FDKPCA [53] y DWRPCA [54] para detección de fallos pero no desde una perspectiva de visualización.

En esta tesis doctoral se proponen combinaciones novedosas en el marco de los HUEPs, que incorporan técnicas de *Exploratory Projection Pursuit* (EPP) adicionales por primera vez. Más específicamente, este estudio propone el uso de HUEPs como herramienta visual que sirve para analizar si los datos recolectados de los sensores instalados en diferentes máquinas son correctos y están bien seleccionados. Por otro lado, los HUEPs contribuyen en gran medida a la monitorización de estas máquinas y, en consecuencia, a la toma de decisiones para anticiparse a los fallos asociados.

A diferencia de otros trabajos previos existentes en la literatura, en esta tesis se utilizan e hibridan técnicas de ML que no se habían usado conjuntamente con anterioridad y se demuestra la viabilidad de esta hibridación empíricamente con casos de uso reales que tampoco han sido utilizados previamente.

La aplicación de ML en la fabricación avanzada tiene un gran potencial. En estas tesis, se aspira a demostrar cómo la hibridación de ciertas técnicas de ML es útil en la optimización de los parámetros de máquinas de procesos industriales, como es el caso de la fabricación de piezas dentales en un centro de mecanizado de alta precisión con cinco ejes. De la misma manera, se demuestra la validez de estos sistemas inteligentes en la ayuda visual para la toma de decisiones en las empresas, con respecto a la detección de fallos o el mantenimiento predictivo, mediante la aplicación a casos de estudio en una empresa del sector de la automoción. Con dichos objetivos alcanzados, entre otros, se permite a las empresas ahorrar en tiempo y costes.

2 Solución propuesta

Como ya se ha expuesto previamente, esta tesis propone la hibridación de técnicas de ML [3] para aplicarse en casos de uso de la industria manufacturera, exactamente bajo el paradigma de Fabricación Avanzada. En todos los casos de uso se propone la aplicación de técnicas de *Soft Computing* [55], más específicamente técnicas de reducción de dimensionalidad de los datos. Con dichas técnicas se pueden obtener patrones, relaciones o revelar la estructura interna en los datos. El propósito es extraer la información más representativa del conjunto de datos de una alta dimensional original, permitiendo la visualización de los mismos y utilizar dicha información representativa en un segundo paso hibridando con otras técnicas de ML.

Las técnicas de reducción de dimensionalidad aplicadas en las publicaciones que integran esta tesis son:

- Análisis de componentes principales (ACP) o *Principal Component Analysis* (PCA) [56]
- *Maximum Likelihood Hebbian Learning* (MLHL) [57]
- *Cooperative Maximum Likelihood Hebbian Learning* (CMLHL) [58]
- *Classical Multidimensional Scaling* (CMDS) [59]
- *Sammon Mapping* (SM) [60]
- *Factor Analysis* (FA) [61]

Una vez aplicadas estás técnicas se obtiene un nuevo conjunto de datos más reducido, que contiene la información más relevante del conjunto original, que se puede analizar gráficamente, pero que además se puede utilizar en un siguiente paso, hibridando con otras técnicas de ML.

Para los casos de uso en los que se busca optimizar los parámetros de configuración de una máquina, como es el caso del centro de mecanizado para fabricar piezas dentales, se utilizan posteriormente las siguientes técnicas:

- RNA con aprendizaje supervisado: se emplea el Perceptron Multicapa (PM), entrenado para modelar (identificación de sistemas [62]), las características más relevantes obtenidas con las primeras técnicas.
- Algoritmos genéticos, como son NSGA-II [63] y MOSA [64], a los que se les aplica como función de adaptación los modelos neuronales (PM) indicados anteriormente.

Para los casos de uso en los que se busca ayudar en la toma de decisiones con visualizaciones que permiten detectar y anticipar fallos en el funcionamiento de máquinas, se aplican en un segundo paso técnicas de agrupamiento o *clustering.* Dichas técnicas dividen un conjunto de datos en grupos de características afines aplicando distintas medidas de similitud. El agrupamiento obtenido con estas técnicas se combina con el obtenido en un primer paso con las técnicas de reducción de dimensionalidad. En concreto las técnicas de agrupamiento utilizadas son:

- k-means [65], técnica de agrupamiento particional. Se aplica con distintas métricas de distancia: *Squared Euclidean* / *Cityblock* / *Cosine* / *Correlation*.
- Agrupamiento aglomerativo (*Agglomerative clustering*). Se aplica con distintas métricas de distancia: *Euclidean* / *Chebyshev* / *Minkowski* / *Correlation* / *Seuclidean*/ *Squared Euclidean* / *Cityblock* / *Mahalanobis* / *Cosine* / *Spearman* / *Hamming* / *Jaccard*; y varios criterios de enlace (*linkage*): *average* / *centroid* / *complete* / *median* / *single* / *ward* / *weighted*.

Las técnicas de agrupamiento permiten utilizar varios criterios de distancia, tal y como se ha indicado. Esto implica que se puede llevar a cabo una adaptación, llegando a aplicar diferentes soluciones al conjunto de datos obtenido con las técnicas proyeccionistas, consiguiendo resultados diferentes en cada caso.

La novedosa propuesta que hibrida técnicas de reducción de dimensionalidad con técnicas de agrupamiento se denomina HUEP [34].

3 Metodología

La metodología utilizada en las publicaciones que forman parte de esta tesis está reflejada en la Parte II. En cada una de las publicaciones se enumeran, entre otros, los siguientes apartados:

- Introducción y/u objetivos: donde se explican brevemente los casos de estudio y cuáles son los objetivos a alcanzar.
- Metodología y/o técnicas utilizadas: en cada publicación se explican en varios apartados todas las técnicas utilizadas de ML hibridadas, y por tanto, la metodología que se va a aplicar al objeto de estudio.
- Caso de estudio: se explican detalladamente cada caso de estudio al que se aplican las técnicas a evaluar.
- Resultados: se detallan los resultados obtenidos.
- Conclusiones: se expresa en ese apartado las principales conclusiones obtenidas con la aplicación de las técnicas seleccionadas para cada caso de estudio.

Se ha seguido la siguiente metodología común en cada uno de los trabajos llevados a cabo:

- El primer paso es establecer el objeto de estudio a analizar, siempre de acuerdo con los objetivos del plan de investigación. Por lo que el caso de estudio debe ser del ámbito de la industria manufacturera.
- Se recopilan los datos que serán utilizados. Para poder aplicar las metodologías seleccionadas a cada objeto de estudio es preciso disponer de datos con los que trabajar. Dichos conjuntos de datos son pre-procesados y deben poseer las siguientes características:
  - Deben ser datos del sector industrial, sobre todo un conjunto de datos que corresponda con el concepto de Fabricación Avanzada y que permita a la empresa mejorar en sus procesos.
  - Deben tener un tamaño lo suficientemente grande, de alta dimensionalidad y con una alta cantidad de muestras.
  - Es imprescindible que contengan las variables que se considera que definen el objeto de estudio, de modo que se pueda optimizar y/o mejorar el proceso analizado.
  - La calidad de los datos debe estar presente. Si es necesario se normalizan las variables, o se tratan los datos nulos o corruptos. Al igual que, si es preciso, se restringen a un periodo de tiempo en el cuál han sucedido los eventos a analizar.
- Aplicación de técnicas de ML hibridadas. Como primer paso en todos los casos de estudio se aplican diversas técnicas de reducción de dimensionalidad y posteriormente dependiendo del caso de estudio, se aplican sistemas de identificación y algoritmos genéticos para la optimización del proceso estudiado,

o bien técnicas de *clustering* para detección y anticipación de fallos en los procesos analizados.

- Todas las publicaciones muestran sólo los mejores resultados obtenidos, por las limitaciones de longitud en las mismas. Pero en todos los objetos de estudio se realiza una exhaustiva experimentación, con la utilización de diferentes parámetros en cada una de las técnicas aplicadas, para conseguir resultados coherentes.
- En cada objeto de estudio se realiza un examen detallado de los resultados obtenidos con cada una de las técnicas aplicadas, obteniendo las conclusiones relativas tanto al caso de estudio analizado como a las técnicas utilizadas. Una vez se tienen las conclusiones se valoran cuáles serían las líneas de trabajo futuras.

4 Objetivos

El objetivo principal de esta tesis es avanzar en la aplicación de técnicas de ML a la industria manufacturera, dentro del campo de la Fabricación Avanzada, con el objetivo de conseguir mejorar/optimizar algunos de sus procesos significativamente. Como consecuencia, se contribuirá a hacer a las compañías más competitivas y sostenibles.

Se pretende demostrar que hibridando estas técnicas de manera innovadora se consigue un mayor potencial que aplicándolas de manera independiente.

En los siguientes puntos se desglosa este objetivo principal enumerando los diferentes propósitos buscados:

- Identificar las carencias de los trabajos previos enmarcados en el problema objeto de estudio. Se revisará la base teórica y los últimos avances en ML aplicados en la industria en el ámbito de la fabricación avanzada. Especialmente los trabajos existentes que utilizan las mismas técnicas de ML que se van a aplicar en los casos de estudio de esta tesis.
- Conocer los casos de estudio en profundidad. Analizar los conjuntos de datos que se van a utilizar para identificar las variables más importantes. El objetivo es que los resultados se ajusten a las problemáticas reales de las industrias estudiadas.
- Emplear e hibridar técnicas de ML a los conjuntos de datos, identificando las que aporten mejores resultados en cada caso.
- Validar que aplicando técnicas hibridadas de ML se consigue optimizar los parámetros de las máquinas para mejorar los procesos industriales y también verificar que es posible anticiparse a fallos en las máquinas; y por lo tanto ayudar en la toma de decisiones a las empresas.
- Demostrar que se pueden aplicar estas técnicas hibridadas a distintos casos de estudio; de esto modo, se consigue que las empresas puedan aplicarlas en un futuro a nuevos casos de estudio y ser por lo tanto más competitivas y poseer una mayor capacidad de adaptación e innovación.

5 Listado de publicaciones

A continuación se incluye una lista completa de las publicaciones originales en las que la doctoranda ha participado durante sus estudios de doctorado y que están relacionadas con el trabajo de investigación de esta tesis. Todas ellas son publicaciones internacionales. Se listan clasificadas según el tipo (revista científica, congreso internacional o capítulo de libro).

Revistas científicas indexadas en *Journal Citation Reports*:

1. Vicente Vera, Emilio Corchado, Raquel Redondo, Javier Sedano, Álvaro E. García. **Applying Soft Computing Techniques to Optimise a Dental Milling Process.** Neurocomputing, New trends on Soft Computing Models in Industrial and Environmental Applications, 109 (2013): 94–104, https://doi.org/10.1016/j.neucom.2012.04.033 - Factor de Impacto Publicado JCR: 2.005, Cuartil mayor: Q1, Área: Computer Science, Artificial Intelligence Cuartil: Q1 Posición en el área: 28/121

2. Raquel Redondo, Javier Sedano, Vicente Vera, Beatriz Hernando, Emilio Corchado. **A Novel Hybrid Intelligent System for Multi-Objective Machine Parameter Optimization.** Pattern Analysis and Applications 18, no. 1 (2015): 31–44, https://doi.org/10.1007/s10044-013-0345-7 - Factor de Impacto Publicado JCR: 1.104, Cuartil mayor: Q3, Área: Computer Science, Artificial Intelligence Cuartil: Q3 Posición en el área: 80/130

3. Raquel Redondo, Álvaro Herrero, Emilio Corchado, Javier Sedano. **A Decision-Making Tool Based on Exploratory Visualization for the Automotive Industry.** Applied Sciences 10, no. 12 (2020): 4355, https://doi.org/10.3390/app10124355 - Factor de Impacto Publicado JCR: 2.474, Cuartil mayor: Q2, Área: Engineering, Multidisciplinary Cuartil: Q2 Posición en el área: 32/91

Publicaciones en congresos internacionales:

1. Raquel Redondo, Pedro Santos, Andres Bustillo, Javier Sedano, José Ramón Villar, Maritza Correa, José Ramón Alique, Emilio Corchado, **A Soft Computing System to Perform Face Milling Operations**, International Work-Conference on Artificial Neural Networks - IWANN, (2009): 1282-1291, Distributed Computing, Artificial Intelligence, Bioinformatics, Soft Computing, and Ambient Assisted Living. https://dx.doi.org/10.1007/978-3-642-02481-8_190

2. Vicente Vera, Alvaro Enrique Garcia, María Jesús Suarez, Beatriz Hernando, Raquel Redondo, Emilio Corchado, María Araceli Sánchez, Ana Belén Gil and Javier Sedano. **Optimizing a dental milling process by means of Soft Computing Techniques**. 10th International Conference on Intelligent Systems

Design and Applications - ISDA, (2010): 1430-1435. Cairo. IEEE Catalog Number: CFP10394-CDR. ISBN 978-1-4244-8135-4. http://dx.doi.org/10.1109/ISDA.2010.5687111

3. Vicente Vera, Álvaro Enrique García, María Jesús Suarez, Beatriz Hernando, Raquel Redondo, Emilio Corchado, María Araceli Sánchez, Ana Gil and Javier Sedano. **A bio-inspired computational high-precision dental milling System**. IEEE Proceedings of the World Congress on Nature and Biologically Inspired Computing –NaBIC, (2010): 423-429. Kytakyushu, Japan. ISBN: 978-1-4244-7375-5. http://dx.doi.org/10.1109/NABIC.2010.5716341

4. Vicente Vera, Javier Sedano, Emilio Corchado, Raquel Redondo, Beatriz Hernando, Mónica Cámara and Álvaro Enrique García. **Machine Parameters Optimisation Using Soft Computing Techniques for a Dental Milling Process**. Soft Computing Models in Industrial and Environmental Applications, 6th International Conference SOCO 2011. Springer - Advances in Intelligent and Soft Computing Volume 87, (2011): 599-609. ISBN: 978-3-642-19643-0 https://doi.org/10.1007/978-3-642-19644-7_63

5. Vicente Vera, Javier Sedano, Emilio Corchado, Raquel Redondo, Beatriz Hernando, Mónica Cámara, Amer Laham, Alvaro Enrique García. **A Hybrid System for Dental Milling parameters optimisation**. 6th International Conference on Hybrid Artificial Intelligence Systems - HAIS 2011. Wroclaw, Poland, Part II, LNAI 6679, (2011): 437–446. ISBN 978-3-642-21218-5, Hybrid Artificial Intelligent Systems, Lecture Notes in Computer Science, 2011, Volume 6679/2011, 437-446, https://doi.org/10.1007/978-3-642-21222-2_53

6. J.R. Villar, Javier Sedano, Emilio Corchado, Vicente Vera, Beatriz Hernando, Raquel Redondo. **Intelligent operating conditions design by means of bio-inspired models**. Third World Congress on Nature and Biologically Inspired Computing - NaBIC 2011. (2011): 608 - 613, ISBN: 978-1-4577-1122-0 https://doi.org/10.1109/NaBIC.2011.6089731

7. Pavel Krömer, Tomás Novosad, Václav Snásel, Vicente Vera, Beatriz Hernando, Laura García-Hernández, Héctor Quintián-Pardo, Emilio Corchado, Raquel Redondo, Javier Sedano, Alvaro Enrique García. **Prediction of Dental Milling Time-Error by Flexible Neural Trees and Fuzzy Rules**. 13th International Conference Intelligent Data Engineering and Automated Learning - IDEAL 2012. Lecture Notes in Computer Science Volume 7435, (2012): 842-849. Proceedings. Print ISBN 978-3-642-32638-7 Online ISBN 978-3-642-32639-4 https://doi.org/10.1007/978-3-642-32639-4_100

8. Pavel Krömer, Tomás Novosad, Václav Snásel, Vicente Vera, Beatriz Hernando, Laura García-Hernández, Héctor Quintián-Pardo, Emilio Corchado, Raquel Redondo, Javier Sedano, Alvaro Enrique García: **Evaluation of Novel Soft Computing Methods for the Prediction of the Dental Milling Time-Error Parameter**. 7th International Conference Soft Computing Models in Industrial and Environmental Applications - SOCO 2012, (2012): 163-172. Online ISBN.978-3-642-32922-7 https://doi.org/10.1007/978-3-642-32922-7_17

9. Bruno Baruque, Raquel Redondo, Álvaro Herrero, Vicente Vera, Beatriz Hernando, Álvaro E. García, Javier Sedano, José Luis Calvo-Rolle, Hector Quintián, Emilio Corchado. **Soft computing models for feature selection of an industrial dental milling case study**. 13th International Symposium on Manufacturing and Systems Engineering. ISOMA 2012

10. Raquel Redondo, Álvaro Herrero, Emilio Corchado, Javier Sedano. **Neural visualization for the analysis of energy and water consumptions in the automotive industry**. The 13th International Conference on Soft Computing Models in Industrial and Environmental Applications, Advances in Intelligent Systems and Computing, Volume 771. (2019): 167-176, Springer, https://doi.org/10.1007/978-3-319-94120-2_16

Capítulo de libro:

1. Álvaro Herrero, Bruno Baruque, Raquel Redondo, Emilio Corchado, Lourdes Sáiz, Ana Lara, Colin Fyfe. A cooperative unsupervised architecture to develop a business management model. Tendencias de la minería de datos en España. (2004): 253-262. ISBN 84-688-8492-1

Las tres publicaciones que constituyen esta tesis doctoral cumplen con los requerimientos para presentarla en formato de compendio de publicaciones y todas ellas tratan sobre el objeto de estudio representado en el título de la presente tesis.

En la primera de las publicaciones, titulada "**Applying Soft Computing Techniques to Optimise a Dental Milling Process**", se presenta la aplicación de varias técnicas de *Soft Computing* para la optimización de un proceso de fresado de alta precisión para la fabricación de piezas dentales.

La publicación titulada "**A Novel Hybrid Intelligent System for Multi-Objective Machine Parameter Optimization**" aporta una contribución significativa, presentando una optimización multiobjetivo del proceso de fabricación de distintos tipos de piezas dentales en el centro de mecanizado de alta precisión de cinco ejes.

Estas dos primeras publicaciones hibridan técnicas de reducción de dimensionalidad con técnicas de identificación de sistemas y con algoritmos genéticos.

La tercera de las publicaciones "**A Decision-Making Tool Based on Exploratory Visualization for the Automotive Industry**", presenta dos casos de estudio de fabricación avanzada de la industria de la automoción, pero en este caso hibridando técnicas de reducción de dimensionalidad con técnicas de *clustering*, con el objetivo de ayudar en la toma de decisiones respecto a la detección de fallos y el mantenimiento predictivo.

Todas las publicaciones se complementan al presentar distintos casos de uso de fabricación avanzada en la industria, con hibridación de técnicas de ML, que en todos los casos aplican técnicas de reducción de dimensionalidad, de manera novedosa en las problemáticas analizadas.

6 Conclusiones y trabajo futuro

El trabajo de investigación desarrollado en esta Tesis Doctoral ha consistido, principalmente, en hibridar diversas técnicas de ML para aplicar en casos de uso reales de fabricación avanzada y de este modo demostrar su validez empíricamente. La principal conclusión es que dicha validez ha sido demostrada para las problemáticas analizadas.

Con los resultados obtenidos se ha conseguido comprobar la contribución de las hibridaciones propuestas, demostrando que la aportación de las técnicas de ML cuando son adecuadamente combinadas es superior a cuando se hace por separado.

Se ha conseguido contribuir a resolver los problemas planteados en los casos de estudio mediante el uso de las hibridaciones planteadas. Por un lado, se ha conseguido optimizar el proceso de fabricación de piezas dentales, lo que supone un ahorro en tiempo y costes para las empresas que apliquen estas técnicas. Por otro lado, se ha demostrado que la técnica de HUEP permite la monitorización de sensores y máquinas para anticipar fallos en maquinaria del campo de la automoción. Esta contribución a la analítica visual de datos puede ayudar a las empresas en la toma de decisiones en proyectos de detección de fallos y mantenimiento predictivo.

El uso de estas técnicas, aplicadas a la industria, permite mejorar/optimizar ciertos procesos, y por lo tanto, hacer a las compañías más competitivas y sostenibles. De acuerdo con esto, la principal línea de trabajo futuro que se propone consistiría en aplicar estas técnicas en otros casos de estudio de la industria, relacionados con otros sectores u otros tipos de máquinas.

De manera más específica, para el caso del fresado de piezas dentales, las líneas de investigación futuras incluyen modelar la diferencia de erosión (diferencia entre los diámetros de la herramienta antes y después de la fabricación), lo que ayuda a medir la precisión del proceso de fresado dental. Además, el modelo resultante se aplicaría a diferentes metales utilizados en las prótesis dentales y en otros procesos industriales, como por ejemplo, del sector aeroespacial.

En el caso del mantenimiento preventivo en el sector de la automoción, ya se están aplicando HUEPs a algunos otros componentes / máquinas para validar su capacidad de monitoreo de operaciones y detección de fallos. Como línea de trabajo futuro, también se explorará el uso de HUEPs con fines orientados a la calidad, por ejemplo, con el fin de mejorar la detección de defectos en piezas. También se propone aplicar técnicas de ML similares en una herramienta que genera visualizaciones específicas para operadores de máquinas y personal de mantenimiento. Esto ayudaría a supervisar la fabricación y en el mantenimiento de la máquina. Por último otra línea de trabajo futuro prometedora sería la combinación en los HUEPs de resultados obtenidos a partir de modelos de ML con aprendizaje supervisado para conseguir una herramienta holística.

Conclusions and future work

The research work developed in this Doctoral Thesis has consisted of, mainly, hybridizing various ML techniques to be applied in real use cases of advanced manufacturing and, therefore, demonstrate their empirical validity. The main conclusion is that such validity has been demonstrated for the set of problems under analysis.

In view of the obtained results, it has been possible to verify the contribution of the proposed hybridizations, proving that the benefits of ML techniques when they are properly combined is greater than when they are used in isolation.

It has been also possible to contribute to solving the problems associated to the case studies through the use of the proposed hybridizations. On the one hand, the manufacturing process of dental pieces has been optimized, which means time and cost savings for companies applying these techniques. On the other one, it has been demonstrated that the HUEPs technique allows the monitoring of sensors and machines in order to anticipate failures in machinery that is commonly used in the automotive industry. This contribution to visual data analytics can help companies in decision making about failure detection and predictive maintenance projects.

The usage of these techniques, applied in industry, allows to improve/optimize certain processes and, therefore, boost the competitiveness and sustainability of companies. According to this, the main work line of future work would be applying these techniques in other industrial case studies, related to other manufacturing sectors or machine types.

More specifically, for the dental milling case, future research lines may include modelling differences in erosion (difference between tool diameters before and after manufacturing), which helps to measure accuracy in the dental milling process. In addition, the resulting model could be applied to diverse metals used in dental prostheses and in other industrial processes such as in the aerospace sector.

For preventive maintenance in the automotive sector, HUEPs are already being applied to some other components/machinery to validate its operation monitoring and failure detection capabilities. As a proposal for future work, the use of HUEPs for quality-oriented purposes will also be explored, for example in order to improve defect detection in produced parts.

It is also proposed to apply similar ML techniques in a tool generating specific visualizations for machine operators and maintenance personnel. This would be useful for production supervision and machine maintenance. Finally, another promising future-work line would be to combine the results obtained from ML models with supervised learning in HUEPs, in order to obtain a holistic tool.

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Parte II. Publicaciones seleccionadas

A continuación se incluye una copia completa de las publicaciones originales que constituyen esta Tesis Doctoral. Al estar redactadas en inglés se añade para cada una de ellas un resumen en castellano.

Applying Soft Computing Techniques to Optimise a Dental Milling Process

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Índice

Resumen

Este estudio presenta un novedoso procedimiento que hibrida técnicas de *Soft Computing*, como son: Redes Neuronales Artificiales (RNA), sistemas de identificación y algoritmos genéticos.

El objetivo es optimizar las condiciones de configuración de un centro de mecanizado. Más específicamente se trata de optimizar el proceso de fabricación de piezas de alta precisión, incluida la precisión de acabado, ahorrando tiempo y costes financieros y / o energéticos.

La metodología aplicada hibrida técnicas de ML basándose en las siguientes fases:

- En primer lugar, se aplican técnicas de reducción de dimensionalidad. Un modelo neuronal no supervisado extrae la estructura interna y las características relevantes del conjunto de datos original que representa el sistema. Las técnicas utilizadas son Análisis de Componentes Principales o *Principal Component Analysis* (PCA) y *Cooperative Maximum-Likelihood Hebbian Learning* (CMLHL).
- En segundo lugar, utilizando las características relevantes del conjunto de datos obtenidas en el paso previo, se modela específicamente el rendimiento del sistema dinámico con las diferentes variables. Para ello se utiliza un modelo neuronal supervisado (Perceptron multicapa) y técnicas de identificación. En este paso se obtiene el modelo capaz de adaptarse al proceso de fabricación.
- Finalmente, se utiliza un algoritmo genético para optimizar los parámetros de la máquina a partir de una función de adaptación o *fitness* no paramétrica. Se utiliza el modelo obtenido en el paso previo como función de *fitness*.

Esta hibridación de técnicas se aplica a un caso de estudio real. En concreto, el novedoso enfoque propuesto se ha probado en un proceso real de fresado dental, utilizando un centro de mecanizado de alta precisión con cinco ejes, lo que requiere una alta precisión de acabado de medidas en micrómetros. Existen en dicho proceso una gran cantidad de factores del proceso a analizar.

El objetivo buscado, con el caso real de estudio al que se aplica el método propuesto, es la reducción del tiempo necesario para la fabricación. En el momento de configuración de los parámetros de la máquina se tiene un tiempo estimado de fabricación, pero una vez finaliza la fabricación se observa habitualmente que el tiempo requerido es mayor del previsto. Lo que se pretende es optimizar los parámetros de la máquina, para reducir este tiempo real de fabricación y así reducir el error en su predicción. Optimizar el tiempo requerido para la fabricación de piezas dentales, permite, entre otras cosas, fabricar un mayor número de piezas al disponer de más tiempo.

El conjunto de datos cuenta con 98 muestras con 8 variables de entrada y una de salida. Después de aplicar PCA y CMHL a los datos, se concluye que ambos métodos encuentran una estructura interna clara en el conjunto de datos al identificar varios grupos. Ambos identifican las revoluciones y el radio como variables relevantes.

CMLHL proporciona una representación más dispersa que PCA y por lo tanto las proyecciones de CMLHL proporcionan una información más relevante, dado que identifica adicionalmente como variables importantes la temperatura y el error de tiempo. Analizando los resultados obtenidos con CMLHL se concluye que este método identifica varios grupos ordenados por radio, revoluciones y temperatura y que dentro de cada grupo existen clasificaciones por "error de tiempo". Por lo tanto, en la primera fase se concluye que el conjunto de datos tiene una estructura interna interesante basada en los grupos identificados.

En el siguiente paso, se modelan las relaciones entre las entradas y los errores de tiempo de producción. Se inicia aplicando varios sistemas de modelado basados en RNA. Se utiliza un Perceptron multicapa (*Multilayer Perceptron* - MLP) para monitorizar la detección de errores de tiempo en la fabricación de piezas dentales. Esta RNA se entrena a partir de los algoritmos de entrenamiento más utilizados; como son el algoritmo de Lenvenberg-Marquardt, los métodos cuasi-Newton, el algoritmo de retropropagación resistente y el algoritmo de gradiente conjugado escalado, utilizando como criterios las técnicas de regularización bayesiana y parada temprana. El modelo final elegido por su reducido error es una red *feedforward* entrenada con el algoritmo de Lenvenberg-Marquardt y con criterio regularizado bayesiano. Se puede concluir que la RNA seleccionada es capaz de simular y predecir correctamente el tiempo para la fabricación de piezas dentales (como consecuencia del proceso de producción). Esta RNA es capaz de modelar más del 86% de las medidas reales.

Con el modelo obtenido, no sólo se puede predecir el error en los tiempos de fabricación, sino que se puede usar como función de *fitness* en el siguiente paso propuesto en este estudio, utilizándolo en un algoritmo genético. De este modo, se pueden determinar las mejores condiciones operativas del proceso de fresado. En el último paso, se utiliza el modelo obtenido previamente y se prueban distintos rangos de variables de entrada no normalizadas. Tras los experimentos ejecutados, se obtienen como resultado que el error de tiempo se puede optimizar para diferentes valores de radio, temperatura y RPM; es decir, es posible lograr un error en la predicción del tiempo cercano a cero.

Después de aplicar la hibridación de las tres técnicas propuestas al conjunto de datos real, se ha evaluado la validez del método propuesto. En base a los resultados obtenidos, el método descrito en este estudio se puede utilizar para optimizar los parámetros de máquinas usadas en procesos industriales. Este método aumenta la eficiencia de las empresas y reduce sustancialmente el coste de preparar y configurar los procesos de la máquina. También ayuda en el proceso de producción utilizando nuevos materiales. El proceso de fresado dental presenta una importante tasa de error en el tiempo de fabricación de alrededor del 29%. Esto se debe a la diferencia entre el tiempo estimado de la propia máquina y el tiempo real de producción. El modelo obtenido es capaz de modelar más del 86% de las medidas reales en relación al error de tiempo (modelando más del 96,8% del trabajo en tiempo real). Esto ayuda a reducir el error y la tasa de variabilidad de los procesos de fabricación hasta un 4%, que es una tasa de error aceptable en la planificación del trabajo de fresado dental, en comparación con el 29% inicial.

Abstract

This study presents a novel soft computing procedure based on the application of artificial neural networks, genetic algorithms and identification systems, which makes it possible to optimise the implementation conditions in the manufacturing process of high precision parts, including finishing precision, while saving both time and financial costs and/or energy. This novel intelligent procedure is based on the following phases. Firstly, a neural model extracts the internal structure and the relevant features of the data set representing the system. Secondly, the dynamic system performance of different variables is specifically modelled using a supervised neural model and identification techniques. This constitutes the model for the fitness function of the production process, using relevant features of the data set. Finally, a genetic algorithm is used to optimise the machine parameters from a non parametric fitness function. The novel proposed approach was tested under real dental milling processes using a high-precision machining centre with five axes, requiring high finishing precision of measures in micrometers with a large number of process factors to analyse. The results of the experiment, which validate the performance of the proposed approach, are presented in this study.

1 Introduction

It is becoming increasingly necessary to have intelligent software tools to optimise tasks associated with modelling industrial processes, especially those associated with high precision finishing, such as the dental milling process.

The optimisation of machine parameters in the fabrication process could potentially improve the flexibility of the process, the adjustments of machine parameters, research in new materials, and its implementation in the fabrication process. It also improves some future designs. Presently, this is achieved with the help of experts (Research and development units in companies work to adjust parameters from the experimental design by carrying out a number of machine trials based on their own experiences). Machine parameter optimisation in the fabrication process includes the development of models to assess the behaviour of the variables in the process and to find the fitness function that can be optimised. The machine parameter optimisation should help the experts in better understanding the production process itself in order to produce products using new materials in a short period of time.

The application of the optimisation process in the field of Medical Therapeutics (Odonto-Stomatology), a booming industry, is both novel and economically advantageous [1, 2, 3, 4, 5, 6]. Improved processing and optimisation of parameters such as processing time, accuracy, etc., for the development of pieces (such as dental-oral prostheses to perform partial crowns, inlays, onlays, etc. with application for rehabilitation and oral-dental restoration) are to the focus of rigorous studies today. The optimisation process of machine parameters, for example the time parameter, permits significant economic savings due to the high number of dental pieces produced daily by the same high-precision dental milling machine centre. This could significantly help to increase a company's efficiency, and substantially contribute to cost reductions in the preparation and setting of the machines processes. Another example is the marginal adjustment of a dental prosthesis to the remaining tooth structure (dentine and enamel), thus avoiding tissue invasion and/or unprepared anatomical areas. This is the goal of any dental treatment, since the success now lies in the adjustment of approximately 15-25 micrometers between the prosthesis and the remaining structures. This would enhance and prevent the filtering of germs and oral fluids that within the short or medium term will lead to treatment failure.

For many years the traditional process of making and preparing dental structures has involved the use of wax, followed by a process called "Lost Wax" [7].

This is a valid methodology, but could interfere with the preparation of a series of variables that are not securely controlled. In fact, there have been cases in which the prosthesis has not fit the tooth structure correctly, resulting in short or medium term tooth decay and failure of the treatment. The optimal outcome would be the so-called passive adjustment, i.e. adjusted between 15-25 micrometers which would lead to success in dental restorative treatment.

Because of these and other reasons it is currently of great interest to optimise processes [8, 9] related to the preparation of dental prostheses (dental structures of materials such as cobalt chromium, titanium, ceramics and/or resin) characterised by a high precision of adjustment in micrometers.

Artificial Intelligence [10], in conjunction with optimisation and identification algorithms [11, 12], is a very appropriate technology for addressing the development of such intelligent tools. Nevertheless, the variable and parameter setting processes are a well-known problem that has not yet been fully resolved. Several different techniques have been proposed in literature. In [13] a Taguchi orthogonal array is used to optimise the effect of injection parameters; in [14] the influence of ultrasonic machining operating parameters is studied using Taguchi and the F-test method; [15] explores different ways of improving the quality of the KrF excimer laser micromachining of metal using the orthogonal array-based experimental design method. Conventional methods can be greatly improved through the application of soft computing techniques [16].

The novel method proposed in this research is a three-step procedure based on several soft computing techniques as artificial neural networks (ANN) [17, 18] and genetic algorithms (GA) [19, 20, 21]. Firstly, the dataset is analysed using statistical and projection methods such as Principal Component Analysis (PCA) [22, 23, 24] and Cooperative Maximum-Likelihood Hebbian Learning (CMLHL) [25] to extract the dataset structure and to perform feature selection to establish whether the data set is sufficiently informative. This means that if the initial collected data set, once analysed shows a certain degree of clustering, it can be seen as a sign of a representative data set (there are no problems related to any sensor when collecting the information, and the process is well defined by the data set).The subsequent steps of the process can then be applied, in which the most representative features are identified and used. A model is generated during the modelling stage to estimate, in this case, the production time errors by modelling techniques. As previously explained, this study is interested in decreasing the production time. Finally, the ANN model obtained in the last step is used as a fitness function to be optimised in the genetic algorithm.

This paper is organised as follows. Section 2 introduces the unsupervised neural models for analysing the datasets. Section 3 presents the system identification techniques used in the system modelling. Section 4 introduces the applied GA. Section 5 describes the case study: a real dental milling process. Section 6 presents the optimising of a dental milling process. The final section presents the different models that are used to solve the high precision dental milling optimisation case study. At the end, the conclusions are set out and some comments on future research lines are outlined.

2 Data Structure Analysis using Connectionist Techniques

Soft Computing [10, 26, 27, 28, 29, 30] is a set of several technologies whose aim is to solve inexact and complex problems [31, 32]. It investigates, simulates, and analyses very complex issues and phenomena in order to solve real-world problems [33, 34]. Soft Computing has been successfully applied in many different fields as, for example, feature selection [17, 18].

In this study, an extension of a neural PCA version [22, 23, 24] and other Exploratory Projection Pursuit [35, 36, 37, 38] extensions are used to select the most relevant input features in the data set and to study its internal structure.

Feature Selection [39, 40, 41] and extraction [42, 43, 44, 45] entails feature construction, space dimensionality reduction, sparse representations and feature selection among others. They are all commonly used pre-processing tools in machine learning tasks, which include pattern recognition. Although researchers have grappled with such problems for many years, renewed interest has recently surfaced in feature extraction.

The feature selection approach in this study is based on the issue of dimension reduction. Initially, some projection methods such as PCA [22, 23, 24], MLHL [36] and CMLHL [25, 46, 47] are applied. Their first step is to analyse the internal structure of a representative data set from a case study. If after applying these models, a clear internal structure can be identified, this means that the data recorded is informative enough. Otherwise, further data must be properly collected [8, 9].

2.1 Principal Component Analysis

Principal Component Analysis (PCA) originated in work by Pearson [22], and independently by Hotelling [23], is a statistical method describing multivariate data set variations in term of uncorrelated variables, each of which is a linear combination of the original variables. Its main goal is to derive new variables, in decreasing order of importance, which are linear combinations of the original variables and are uncorrelated with each other.

From a geometrical point of view, PCA can be defined as a rotation of the axes of the original coordinate system to a new set of orthogonal axes that are ordered in terms of the amount of variation of the original data that they account for. PCA aims to find that orthogonal basis which maximises the data's variance for a given dimensionality of basis.

Using PCA, it is possible to find a smaller group of underlying variables that describe the data. PCA has been the most frequently reported linear operation involving unsupervised learning for data compression and feature selection [24].

2.2 A Neural Implementation of Exploratory Projection Pursuit

The standard statistical method of EPP [25, 37, 38], provides a linear projection of a data set, but it projects the data onto a set of basic vectors which best reveal the interesting structure in data. Interestingness is usually defined in terms of how far the distribution is from the Gaussian distribution [48].

One neural implementation of EPP is Maximum Likelihood Hebbian Learning (MLHL) [36]. It identifies interestingness by maximizing the probability of the residuals under specific probability density functions that are non-Gaussian.

An extended version of this model is the Cooperative Maximum Likelihood Hebbian Learning (CMLHL) [25, 49] model. CMLHL is based on MLHL [36] adding lateral connections [25, 49], which have been derived from the Rectified Gaussian Distribution [48]. The resultant net can find the independent factors of a data set but does so in a way that captures some type of global ordering in the data set.

Considering an N-dimensional input vector ( ), and an M-dimensional output vector ( ), with Wij being the weight (linking input j to output i), then CMLHL can be expressed [49] as:

Feed-forward step:

$$y_i = \sum_{j=1}^{\mathbf{N}} W_{ij} x_j, \forall i \qquad (1)$$

Lateral activation passing:

$$y_i(t+1) = [y_i(t) + \tau(b - Ay)]^+ \qquad (2)$$

Feedback step:

$$e_j = x_j - \sum_{i=1}^{M} W_{ij} y_i, \forall j \qquad (3)$$

Weight change:

$$\Delta W_{ij} = \eta . y_i . sign(e_j) | e_j |^{p-1} \qquad (4)$$

Where: η is the learning rate, [ ]+ is a rectification necessary to ensure that the y -values remain within the positive quadrant, τ is the "strength" of the lateral connections, b is the bias parameter, p is a parameter related to the energy function [25, 36] and A is the symmetric matrix used to modify the response to the data [25]. The effect of this matrix is based on the relation between the distances separating the output neurons.

3 System Identification and Modelling

System identification (SI) [11, 26] aims to obtain mathematical models to estimate the behaviours of a physical process whose dynamic equations are unknown. The identification criterion consists in evaluating the group of candidate models that best describes the dataset gathered for the experiment; that is, given a certain model $M(\theta_*)$, its prediction error may be defined as in Eq. (5), where $y(t)$ is the real output and $\hat{y}(t \mid \theta_*)$ is the prediction of this. The goal is to obtain a model that meets the following premise [11]: a good model is one that makes good predictions and which produces small errors when the observed data is applied.

Classic SI refers to the parametrical literature, which has its origin in linear system analysis [12]. Nevertheless, increased computational capability and the availability of soft computing techniques have widened research into SI. ANNs are one of the most interesting soft computing paradigms used in SI. When using ANN, the purpose of an identification process is to determine the weight matrix based on the observations Z^t, so as to obtain the relationships between the network nodes. The supervised learning algorithm is then applied to find the estimator θ, so as to obtain the identification criterion. In this case, the minimization of the mean square error criterion as defined in Eq. (6) and Eq. (7) is used. The iterative minimization scheme is defined in Eq. (8), where $\theta(t)$ is the estimated parametrical vector, $f(t)$ represents the search direction and $\mu(t)$ the step size.

The SI procedure comprises several steps: the selection of the models and their structure, the learning methods, the identification and optimisation criteria and the validation method [11, 12, 50, 51, 52]. Validation ensures that the selected model meets the necessary conditions for estimation and prediction. Typically, validation is carried out using three different methods: the residual analysis $\varepsilon(t, \hat{\theta}(t))$ (by means of a correlation test between inputs, their residuals and their combinations); the mean squared error (MSE) and the generalization error value (normalised sum of squared errors (NSSE), and finally a graphical comparison between the desired outputs and the model outcomes through simulation [8, 9, 12].

$$\varepsilon(t, \theta_*) = y(t) - \hat{y}(t \mid \theta_*) \tag{5}$$

$$V_N(\theta, z^t) = \frac{1}{N} \sum_{t=1}^{N} \left[y(t) - \hat{y}(t \mid \theta)\right]^{\mathrm{T}} \left[y(t) - \hat{y}(t \mid \theta)\right] \tag{6}$$

$$\hat{\theta} = \arg\min_{\theta} V_N(\theta, Z^t) \tag{7}$$

$$\theta(t+1) = \theta(t) + \mu(t) f(t) \tag{8}$$

4 Genetic Algorithms for System Optimisation

Metaheuristic algorithms [53, 54] are considered a computational method that optimises a problem by iteratively trying to improve a candidate solution with regards to a given measure of quality. Metaheuristics are powerful strategies that can efficiently detect high-quality (near optimal) solutions to complex optimization problems within reasonable running time.

Metaheuristics make few or no assumptions about the problem being optimised and can search very large spaces of candidate solutions. Among these algorithms, there are two well-known types: the genetic algorithms [55, 56, 57], and the simulated annealing algorithm [58, 59]; other methods can be: Tabu search [60, 61] and ant colony optimisation [62].

GA [19, 20, 21, 63, 64] are a type heuristic search that mimics the process of natural evolution (Darwin's theory about evolution). This heuristic is routinely used to generate useful solutions to optimisation and search problems. It solves both constrained and unconstrained optimisation problems.

Genetic algorithms find $(x_i, \dots, x_n)$ such that $f(x_i, \dots, x_n)$ will be maximum or minimum. The functions are shown from Eq. (9) to Eq. (11), where $f(x)$ is the fitness function, $c(x)$ represents inequality constraints, $ceq(x)$ represents the equality constraints, m is the number of nonlinear inequality constraints and mt is the total number of nonlinear constraints:

$$Min\ \ or\ \ Max\ \ f(x) \tag{9}$$

$$c_i(x) \le a_i;\ \ i = 1,\dots,m \tag{10}$$

$$ceq_i(x) = b_i;\ \ i = m+1,\dots,mt \tag{11}$$

5 A Real Case Study: Optimising a Dental Milling Process

The acronym CAD/CAM (Computer Aided Design / Computer Aided Manufacturing) refers to a production technique that combines computer skills, which are then applied in both the design and manufacturing of pieces. Originally applied in the field of engineering, its use is now widespread, extending to many other areas.

In the field of dentistry, CAD/CAM systems are used primarily to manufacture fixed prosthetic restorations such as inlays, veneers and crowns. During the last decade, the technological evolution of these systems has provided restoration alternatives to rehabilitate teeth deficiencies, using different materials such as porcelain, composite and metal blocks, which previously could not be processed due to technical limitations [65].

There is currently an increased interest in manufacturing pillars and in making the structure of the prosthesis implant using CAD/CAM technology [1]. There are several reasons for this increase. First, the structure of the prosthetic implant is constructed from a solid block of material. With this specific production technique, the material is more homogeneous and contains high mechanical properties. Second, the inaccuracies are reduced since the processes of waxing, coating and casting no longer exist [66]. The prosthetic implants drawn up by CAD/CAM technology present more passive adjustment than the cast structures [2, 3, 4].

Since 1971 a marginal fit of less than 120 micrometers in tooth-supported restorations [67] has been regarded as clinically acceptable. In the prosthetic implant, the tolerable discrepancy between the implant abutment and the prosthetic supra-structure can be variable. A mismatch that does not exceed 30 micrometers can be tolerated [68], although Branemark et al. declare that the discrepancy must never exceed 10 micrometers [69]. However there is a consensus that the lack of passive adjustment acts as a causal factor in many technical complications such as loosening and/or fractures in the metal structure, retaining screws, abutments and ceramic or acrylic [70].

To perform any one of the many treatments allowed by this systematic approach, the CAD/CAM systems consist of the following stages of processing:

1. Digitization of the substrate that will make the restoration. It can be taken directly, optically in the patient's mouth, or extra-orally, after making a conventional impression, and emptied in a plaster cast.
2. Computer aided design. This is done by the specific software for each system, designing the prosthetic cap structure or the final restoration. This step is not done in those cases where the digitization is from the scanning of the structure to be obtained.
3. Once the design of the structure is finished, the next step is to manufacture the structure, which is achieved by applying the third stage of processing, the machining or CAM phase [5].

The operating system is accomplished through computer numerical control (CNC). The data obtained using the CAD-software are converted into "commands" which are “read” by the milling machine and then translated into drilling steps.

This multidisciplinary study uses a 5-axis milling (latest generation) device. In addition to controlling movement between the tool and the piece in three axes, this 5-axis machine can also control both the rotation of the piece in two axes, one perpendicular to the axis of the tool and the other parallel to it, and the rotation of the piece on a horizontal axis with the inclination of the tool around an axis perpendicular to the former. The advantages of 5-axis machines are numerous: it allows complete multilateral machining in a single cycle, which implies a reduction of non-productive time and eliminates the lack of precision arising from the multiple ties of the piece. It also allows better access to restricted areas difficult to reach. The angle adjustment can be freely defined. Another advantage is that it is possible to use shorter and more rigid tools, which results in improved surface finish.

This multidisciplinary research describes the way in which a soft computing system can be applied to optimise the data gathered by means of a Machining Milling Center of HERMLE type-C 20 U (iTNC 530), with swivelling rotary (280 mm), with a control system using high precision drills and bits (Fig. 4 to Fig. 6), by optimising the time error detection for manufacturing dental metal. Fig. 1 to Fig. 3 show the metal pieces manufacturing process using a dynamic high-precision machining centre with five axes.

Fig. 1 Metal milled cobalt-chromium consists of a bridge with two lower molars

Fig. 2 Occlusal view of milled cobalt-chromium consists of a bridge with two lower molars

Fig. 3 Finished metal-porcelain bridgework

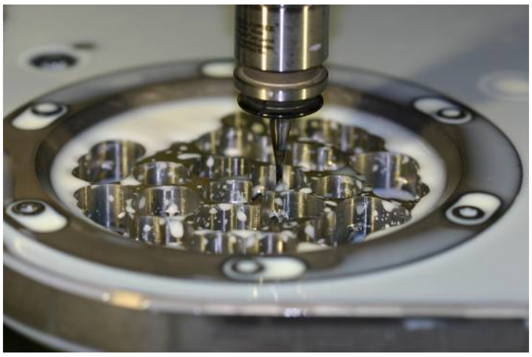

Fig. 4 Milling of cobalt-chromium specimens

Fig. 5 Machining/ Milling Center of HERMLE type-C 20 U (iTNC 530), with swivelling rotary (280 mm), with a control system using drills and bits of high precision

Fig. 6 Metal pieces manufactured by a dynamic high-precision machining centre with five axes

The case study is described by an initial data set of 98 samples obtained by the dental scanner in the manufacturing of dental pieces with different tool types (plane, toric, spherical and drill) and characterized by 8 input variables (Tool, Radius, Revolutions, Feed rate X, Y and Z, Thickness, Initial Temperature) and 1 output variable (Time Error for manufacturing) as shown in Table 1. Time error for manufacturing is the difference between the estimated time by the machine itself and real production time (negative values indicate that real time exceeds estimated time).

Variable (Units)	Range of values
Type of tool	Plane, toric, spherical and drill
Radius (mm.)	0.25 to 1.5
Revolutions per minute (RPM)	7,500 to 38,000
Feed rate X (mm. by minute)	0 to 3,000
Feed rate Y (mm. by minute)	0 to 3,000
Feed rate Z (mm. by minute)	50 to 2,000
Thickness (mm.)	10 to 18
Temperature (ºC)	24.1 to 31
Real time of work (s)	6 to 1,794
Time errors for manufacturing (s)	-28 to -255

Table 1 Values of each variable used in the process

6 A Novel Soft Computing Procedure to Optimise a Dental Milling Process

The manufacturing of dental pieces process optimisation in terms of time errors, based on the optimisation of the system behaviour, is carried out within the framework of this study by means of an ANN estimated model. The time error parameter is chosen as an important factor in this process (in terms of economical benefits for the company) as an example to show the potential of this novel soft computing proposal.

6.1 Identification of the Relevant Features

Firstly, the dental manufacturing process is parameterised and its dynamic performance in normal operation is obtained by the real process of manufacturing dental pieces. Then, the gathered data is processed using projection models based on the analysis of parameters as the variance [22, 23, 24] or the kurtosis as CMLHL [25, 46, 47, 49]. This is done to identify internal data set structures in order to analyse whether the data set is sufficiently representative and to identify the most relevant features in the second step.

6.2 Modelling and optimisation of a normal dental milling operation

Once the relevant variables and their transformations have been extracted from the production data, then a model capable of fitting the normal manufacturing operation must be obtained. This is done to identify bias in the estimated production time. The different model learning methods used in this study were implemented in Matlab© [71]. The model structures were analysed in order to obtain the models that best suited the dataset. Since the number of examples was somewhat small; a 10-fold cross-validation schema was selected. The number of samples is low as they were obtained during the real process, delaying the company timing. The final model is obtained using the entire data set.

Moreover, several different indexes were used to validate the models [8, 9] such as the percentage representation of the estimated model; the graphical representation for the

prediction ($\hat{y}_1(t \mid m)$) versus the measured output ($y_1(t)$); the loss function or error function (V) and the generalization error value.
The percentage representation of the estimated model is calculated as the normalised mean error for the prediction (FIT1, FIT) using the validation data set and the complete data set, respectively. The loss function or error function (V) is the numeric value of the mean square error (MSE) that is computed using the estimation data set; the generalisation error value is the numeric value of the normalised sum of square errors (NSSE) that is computed using the validation data set. Finally, is calculated the variance of the mean square errors (◎) [34, 72].
Once the model for the time error in the manufacturing of dental pieces is selected, this model is used as a fitness function in GA's in order to obtain the best optimisation of the time errors. This optimisation process begins with a set of solutions called population (chromosomes). Each individual in the population is then evaluated by the fitness function obtained in the last step (ANN model of the manufacturing system). GA and the different types of genetic operators (selection, crossover and mutation) used in this study were implemented in Matlab© [73]. The complete novel soft computing procedure is showed in Fig. 7.

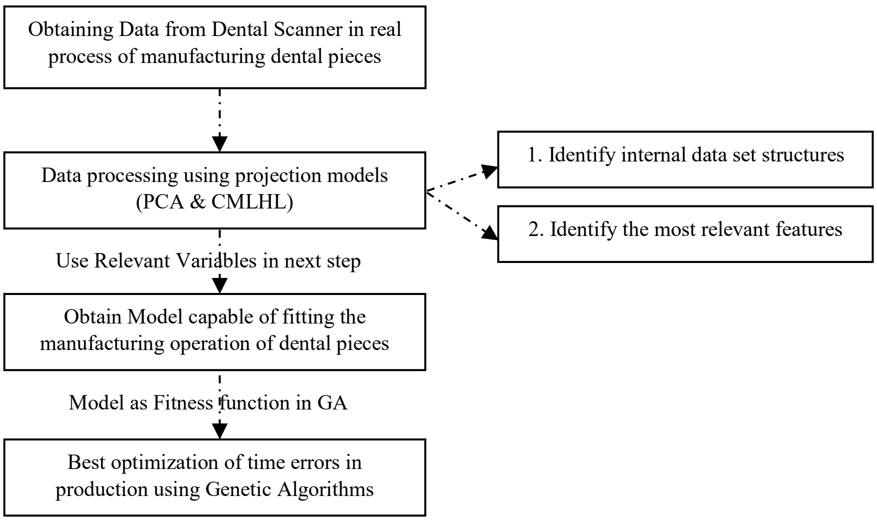

Fig. 7 A novel soft computing procedure to optimise a Dental Milling Process

7 Results

This case study initially analysed the data set in order to obtain the variables/characteristics that are most closely related to manufacturing time errors.
In the first step, several unsupervised models were applied for the sake of comparison. In this case a neural version of PCA and CMLHL were applied as powerful techniques for identifying internal dataset structures. The axes forming the projections (Fig. 8.a and Fig. 8.b) represent combinations of the variables contained in the original datasets. In the case of PCA, the model is looking for those directions with the biggest variance, while CMLHL is looking for the kurtosis (directions which are as little Gaussian as possible) [25, 36].
As may be seen in Fig. 8, PCA (Fig. 8.a) and CMLHL (Fig. 8.b), both methods found a clear internal structure in the dataset by identifying several clusters (see Table 2 and

Table 3). Both also identified revolutions and radius as relevant variables. It is clear that CMLHL provides a more sparse representation than the PCA, and that CMLHL projections provide more clear information identifying parameters such as temperature and time error as other important variables.
An analysis of the results obtained with the CMLHL model (Fig. 8.b) leads to the conclusion that this method has identified several different clusters ordered by radius, revolutions and temperature. Inside each cluster, there are further classifications by 'time error' and the dataset can be said to have an interesting internal structure based on the clusters identified.

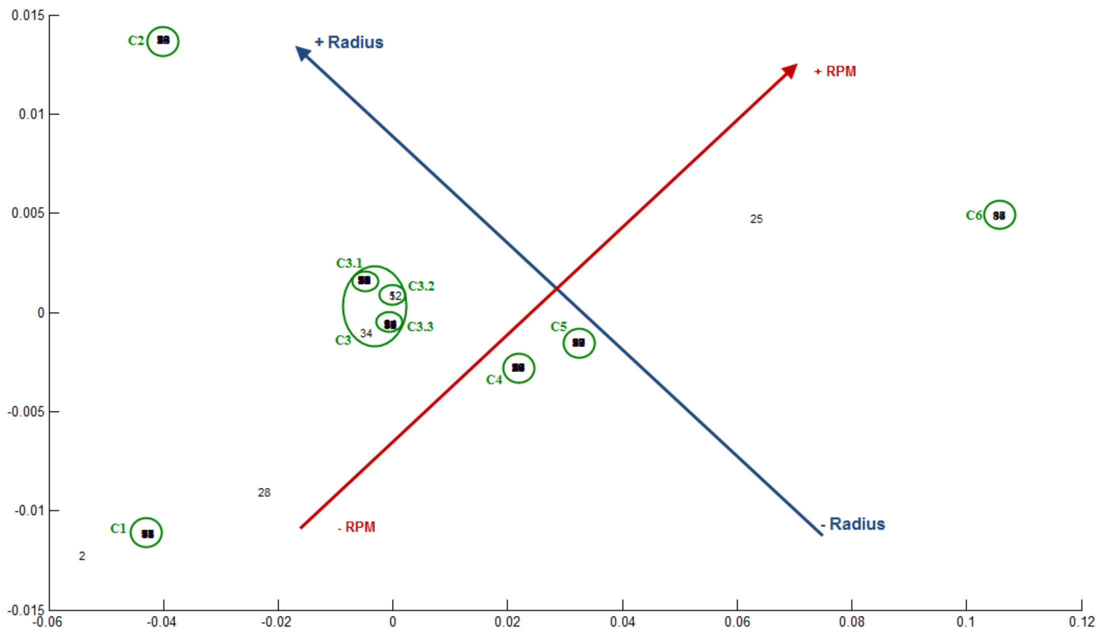

Fig. 8.a Projection of PCA

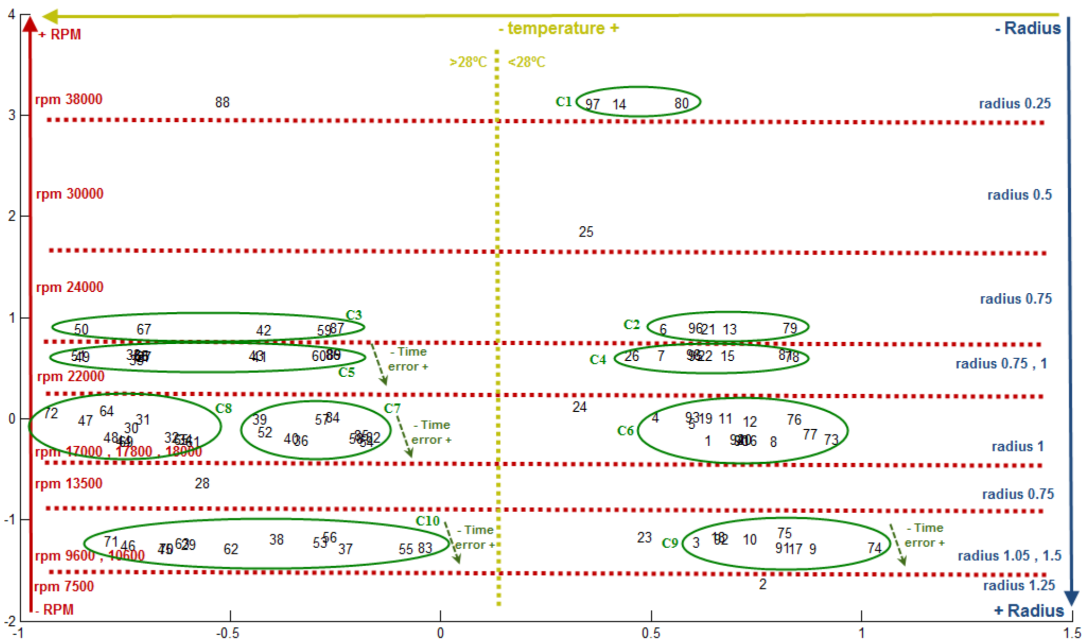

Fig. 8.b CMLHL projection after 100,000 iterations using a learning rate of 0.01, p=0.5 and τ=0.05

Fig. 8 PCA projection (Fig. 8.a) and CMLHL projection (Fig. 8.b)

Cluster		**Samples**	**RPM**	**Radius**
-		2	7,500	1.25
C1		9, 17, 37, 45, 53, 55, 62, 70, 74, 83, 91	9,600	1.05
C2		3, 10, 18, 23, 29, 38, 46, 56, 63, 71, 75, 92	10,600	1.5
-		28	13,500	0.75
C3	**C3.1**	1, 8, 16, 20, 30, 32, 36, 40, 44, 48, 52, 54, 58, 61, 65, 69, 73, 77, 82, 85, 90, 94	17,000	1
		34	17,000	
	C3.2	5, 12	18,000	
	C3.3	4, 11, 19, 24, 31, 39, 47, 57, 64, 72, 84, 93	17,800	
C4		7, 15, 22, 26, 27, 33, 41, 43, 49, 51, 60, 66, 68, 86, 89, 95, 98	22,000	0.75
		1		1
C5		6, 13, 21, 42, 50, 59, 67, 79, 87, 96	24,000	0.75
-		25	30,000	0.5
C6		14, 80, 88, 97	38,000	0.25

Table 2 Samples description and clusters obtained by using PCA method

Cluster	**Samples**	**RPM**	**Radius**	**Temperature**
C1	80, 14, 97	38,000	0.25	24.1 to 25.3
-	88	38,000	0.25	28.4
-	25	30,000	0.5	25.7
C2	79, 13, 21, 6, 96	24,000	0.75	24.1 to 25.3
C3	87, 59, 42, 67, 50	24,000	0.75	28.4 to 31
C4	78, 81, 15, 22, 7, 95, 98, 26	22,000	0.75	24.1 to 25.7
C5	86, 89, 60, 41, 43, 27, 33, 35, 66, 68, 49, 51	22,000	0.75, 1	28.4 to 31
C6	73, 77, 76, 8, 11, 12, 16, 20, 19, 90, 94, 1, 4, 93, 5	17,000, 17,800, 18,000	1	24.1 to 25.3
-	24	17,800	1	25.7
C7	82, 85, 84, 54, 58, 57, 52, 36, 40, 39	17,000, 17,800	1	28.4 to 29.3
C8	30, 32, 61, 65, 31, 64, 44, 48, 69, 47, 72	17,000, 17,800	1	30.4 , 31
-	28	13,500	0.75	30.4

C9	74, 75, 9, 10, 17, 18, 91, 3, 92	9,600, 10,600	1.05 , 1.5	24.1 to 25.3
-	23	10,600	1.5	25.7
C10	83, 55, 56, 53, 37, 38, 62, 29, 63, 45, 70, 46, 71	9,600, 10,600	1.05 , 1.5	28.4 to 31
-	2	7,500	1.25	

Table 3 Samples description and clusters obtained by using CMLHL method

When the dataset is considered sufficiently informative, as in this case, the next step is to model the relations between inputs and production time errors in the process, which is begun by applying several artificial neural network modelling systems.

A multilayer perceptron network (feedforward network) was used to monitor time error detection in the manufacturing of dental pieces. Data set is pre-processed from the input and output normalization step (normalizing the minimum and maximum values to [-1 1]), the reduction of the input vectors dimension (the data set gathered in the previous step). ANN is trained from the most widely used training algorithms such as the Lenvenberg-Marquardt algorithm [74], quasi-Newton methods [75], the resilient back-propagation algorithm [76] and the escalated conjugate gradient algorithm [77], using criteria from early stopping and Bayesian regularization techniques [78].
The graphic representations of the prediction ($\hat{y}_1(t \mid m)$) of time error detection in the manufacturing of dental pieces versus the real time measured ($y_1(t)$) for the model chosen are shown in Fig. 9. These figures were used to validate the models. In Fig. 9.a and Fig. 9.b the X-axis shows the total number of samples. In Fig. 9.a and Fig. 9.b the Y-axis represents the normalized output and unnormalised output variable range, respectively, which refers to the time errors for manufacturing.
Table 4 shows the features for the best ANN proposed: the characteristics and qualities for estimation and prediction, and its indexes (indicator values). The final model chosen is a Feedforward Network. The ANN structure has 30 hyperbolic tangent units (layer 1), 20 hidden hyperbolic tangent units (layer 2), 5 hidden hyperbolic tangent units (layer 3) and 1 linear output unit. The network is estimated by using the Lenvenberg-Marquardt algorithm with Bayesian regularized criterion. This model does not only present a lower loss function (V) and error values (NSSE), but also a higher system representation index value FIT1. Also a good FIT value and a small variance of the mean square errors (◎).
From Fig. 9, it may be concluded that the ANN selected is able to simulate and predict the behaviour of time errors for the manufacturing of dental pieces (as a consequence of the production process). They are capable of modelling more than 86% of the actual measurements.

Model	Indexes
The feedforward network has 30 hyperbolic tangent units (layer 1), 20 hidden hyperbolic tangent units (layer 2), 5 hidden hyperbolic tangent units (layer 3) and 1 linear output unit [30 20 5 1]. The network is estimated using the resilient back-propagation algorithm with early stopping criterion.	FIT1: 71.03%;V: 0.024; NSSE: 0.033; ◎: 0.00023; FIT: 85.19%
The feedforward network has 30 hyperbolic tangent units (layer 1), 25 hidden hyperbolic tangent units (layer 2), 25 hidden hyperbolic tangent units (layer 3), 4 hidden hyperbolic tangent units (layer 4) and 1 linear output unit [30 25 25 4 1]. The network is estimated using the resilient backpropagation algorithm with early stopping criterion.	FIT1: 73.00%;V: 0.017; NSSE: 0.038; ◎: 0.00007; FIT: 87.43%
The feedforward network has a structure [3 30 3 1]. The network is estimated using the Lenvenberg-Marquardt algorithm with Bayesian regularized criterion.	FIT1: 74.36%;V: 0.018; NSSE: 0.019; ◎: 0.00042; FIT: 86.45%
The feedforward network has a structure [30 20 5 1]. The network is estimated using the Lenvenberg-Marquardt algorithm with Bayesian regularized criterion.	FIT1: 78.57%;V: 0.0097; NSSE: 0.015; ◎: 0.000059; FIT: 86.87%
The feedforward network has a structure [30 25 25 4 1]. The network is estimated using the Lenvenberg-Marquardt algorithm with Bayesian regularized criterion.	FIT1: 75.31%;V: 0.015; NSSE: 0.0168; ◎: 0.00012; FIT: 85.03%
The feedforward network has a structure [30 20 5 1]. The network is estimated using the quasi-Newton algorithm with early stopping criterion.	FIT1: 71.17%;V: 0.023; NSSE: 0.028; ◎: 0.000054; FIT: 88.49%
The feedforward network has a structure [30 20 5 1]. The network is estimated using the escalated conjugate gradient algorithm with early stopping criterion.	FIT1: 71.37%;V: 0.018; NSSE: 0.042; ◎: 0.00012; FIT: 85.76%
The feedforward network has a structure [30 20 5 1]. The network is estimated using the Lenvenberg-Marquardt algorithm with early stopping criterion.	FIT1: 70.17%;V: 0.035; NSSE: 0.045; ◎: 0.0037; FIT: 89.39%
The feedforward network has a structure [30 25 25 4 1]. The network is estimated using the Lenvenberg-Marquardt algorithm with early stopping criterion.	FIT1: 77.67%;V: 0.0098; NSSE: 0.035; ◎: 0.000045; FIT: 89.39%

Table 4 Indicator values for several proposed models of time error for manufacturing under the Dental Milling process

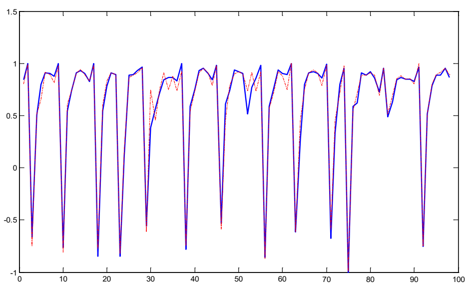

Fig. 9.a Normalized output response of the model

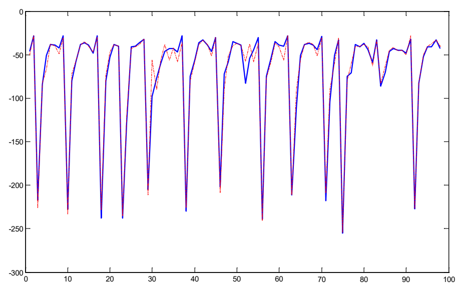

Fig. 9.b Unnormalized output response of the model

Fig. 9 Output response of the model: The feedforward network [30 20 5 1] is estimated using the Lenvenberg-Marquardt algorithm with Bayesian regularized criterion. The current output (solid line) is graphically presented with prediction (dash-dot line)

The model of the time error obtained may be used not only to predict time errors for the manufacture of dental pieces, but as a fitness function in the next step to determine the best operating conditions of dental milling processes. GA starts with a randomly generated initial population of size 100 individuals. Tournament selection is used to determine the parents for the next generation. Individuals from the current population are selected proportionally to their fitness, thus forming the basis for the next generation. Two-point crossover combines two parents to form a new individual for the next generation. And adaptive feasible mutation makes small changes in the individuals in the population. The population obtained by these genetic modifications is evaluated against the fitness function and enters a new search process in the next generation. The algorithm stops after it reaches a fixed number of generations and the best individual is returned as a solution to the given problem. Fig. 10 shows the output response of the time error for different unnormalised input variable ranges. In Fig. 10.a the X-axis shows the revolutions per minute (RPM), from 10,000 to 35,000 RPM. The Y-axis shows the temperature from 24ºC to 31ºC, and the Z-axis represents the unnormalised output variable range from -200 s to 200 s (seconds). The time error is also shown on the bar. In Fig. 10.b the X-axis shows the temperature from 24ºC to 31ºC, and the Y-axis represents the unnormalised output variable range, from -100 s to 60 s for a constant value of 20,000 RPM. In both figures the radius is fixed to a constant value of 0.75 mm. In Fig. 10.c the X-axis shows the radius, from 0.25 mm. to 1.5 mm. The Y-axis shows the temperature from 24ºC to 31 ºC and the Z-axis represents the unnormalised output variable range from -80 s to 20 s. The time error is shown on the bar, too. In Fig. 10.d the X-axis shows the temperature from 24ºC to 31ºC, and the Y-axis represents the unnormalised output variable range, from -30 s to 5 s for a constant radius value of 1 mm. In both figures the number of revolutions is fixed per minute to a constant value of 30,000 RPM.

Some results obtained in order to obtain the best optimisation of the time errors for different conditions of operation fixed are shown following. For example, the time error can be optimised for different values of radius, temperature and RPM; i.e., it is possible to achieve a time error close to zero for a radius of 1.45 mm, 22,834 RPM and a temperature of 27.69ºC. Furthermore, if the temperature is fixed to 26ºC and the time error is close to zero, the revolutions and the radius to optimise those variables are 37,592 RPM and 1 mm., respectively.

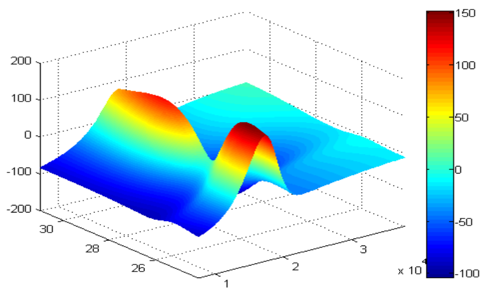

Fig. 10.a 3D graph, the X-axis represents the RPM, the Y-axis the temperature and the Z-axis the output (time error). The other variable radius is fixed to 0.75 mm

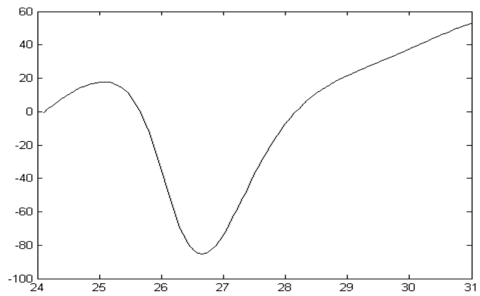

Fig. 10.b 2D graph, the X-axis represents the temperature and the Y-axis the output (time error). The others variables, RPM and radius are fixed to 20,000 RPM and 0,75 mm, respectively

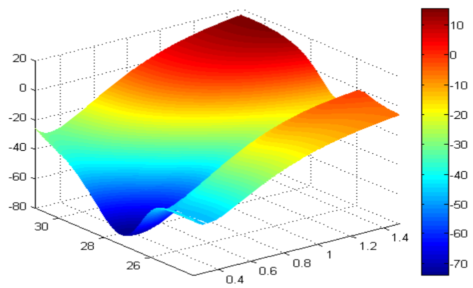

Fig. 10.c 3D graph, the X-axis represents de radius, de Y-axis the temperature and the Z-axis the output (time error). The other variable, RPM is fixed to 30,000 RPM

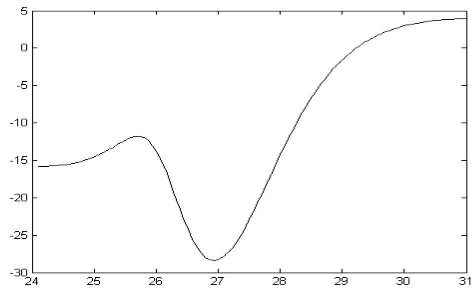

Fig. 10.d 2D graph, the X-axis represents the temperature and the Y-axis the output (time error).The others variables, radius and RPM are fixed to 1 mm and 30,000 RPM, respectively

Fig. 10 Output response of the time error for different unnormalised input variable ranges

8 Conclusions and future work

The novel soft computing optimisation process described in this study can be used to optimise machine parameters for industrial processes, based on the obtained results. This method increases the companies' efficiency and substantially reduces the cost of preparing and setting machine processes. It also helps in the production process using new materials. We have used this method for optimisation and adjustments during the manufacturing process of dental pieces such as implants according to medical specifications for precise mouldings.

The method proposed is based on the selection of the most important features in an initial step. ANN are then used for modelling the features. Finally, a GA tries to achieve the best conditions for manufacturing from the model. The ANN model is used as fitness function in the GA.

The dental milling process presents an important manufacturing time error rate of about 29%. This is due to the difference between the estimated time of the machine itself and the real production time. The obtained model is capable of modelling more than 86% of the actual measurements in relation to time error (modelling more than 96.8% of real time work). This helps to reduce the error and the variability rate of manufacturing processes down to 4%, compared to the initial 29%, which is an acceptable error rate in planning work for dental milling.

Future lines of research include modelling the temperature difference and the erosion difference (difference between diameters of the tool before and after the manufacturing), which helps to measure the accuracy of the dental milling process. Additionally, it will investigate the selection of the most suitable features using a wrapper feature selection method, in which genetic algorithms and neural networks are hybridized. Finally, an algorithm will be developed to automatically identify the best operating conditions: minor time errors for the manufacturing of dental pieces and minor erosion. The resulting model would moreover be applied to different metals used in prosthetic dentistry and in other industrial processes, such as the automotive sector.

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A Novel Hybrid Intelligent System for Multi-Objective Machine Parameter Optimization

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Índice

Resumen

En esta investigación multidisciplinar se presenta un sistema inteligente híbrido para realizar un proceso de optimización multiobjetivo de parámetros industriales. El sistema inteligente propuesto se basa en la aplicación de varias técnicas de ML: búsqueda exploratoria de proyecciones, computación evolutiva y neuronal además de sistemas de identificación.

La verificación empírica del sistema inteligente híbrido propuesto se realiza en un dominio industrial real, donde se define y analiza un caso de estudio. Los experimentos se llevan a cabo en base a procesos reales de fresado dental utilizando un centro de mecanizado de alta precisión con cinco ejes, requiriendo una alta precisión de acabado (medidas en micrómetros) con un gran número de factores de proceso a analizar. Las prótesis dentales deben ser precisas, teniendo un ajuste marginal alto. Un mal ajuste puede provocar fracturas, reducir la longevidad de la pieza, decoloración o irritación, lo que puede llevar a provocar caries y/o enfermedad periodontal, conduciendo al fracaso del tratamiento.

Este estudio busca un mejor procesamiento y la optimización de varios de los parámetros del centro de mecanizado, como son el tiempo de fabricación, la temperatura, precisión, etc. en la fabricación de prótesis dentales. El sistema obtenido es multiobjetivo ya que a partir de varios de valores de entrada se optimizan dos variables de salida.

Se presentan un modelo hibrido de ML basado en tres pasos:

- En el primer paso se aplican técnicas de búsqueda exploratoria de proyecciones (PCA y CMLHL), comprobando que el conjunto de datos tiene estructura interna y obteniendo las variables más relevantes.
- En el segundo paso se consiguen dos modelos, para optimizar el error de tiempo y la diferencia de temperatura en el proceso de fabricación. Estos se obtienen mediante RNA supervisadas junto con algoritmos de identificación.
- En el tercer paso se usan técnicas de computación evolutiva, como son los algoritmos genéticos NSGA-II y MOSA. Se utilizan en estos, como función de *fitness*, los dos modelos obtenidos en el paso previo para conseguir una optimización multiobjetivo.

Se busca conseguir la mejor optimización de las variables de configuración de la máquina de fresado como son la velocidad de alimentación (X) y velocidad de alimentación (Y). El objetivo final es minimizar el error de tiempo y la diferencia de temperatura en el proceso de fabricación.

Con la optimización del tiempo de fabricación se consigue ahorrar tiempo y energía. Con la optimización de la diferencia de temperatura se consigue, por un lado, evitar la rotura del útil de fresado o fresa, que al ser de alta precisión tiene un coste elevado, y por otro, evitar una fabricación incorrecta de la pieza y por lo tanto pérdida de material. Optimizando estos valores se consigue un ahorro económico.

El conjunto de datos cuenta con 114 muestras con 15 variables de entrada y 2 de salida.

En el primer paso se analiza el conjunto de datos con el fin de obtener las variables/características que están más relacionadas con los errores de tiempo de fabricación y la diferencia de temperatura en la máquina. Como técnicas para identificar estructuras de conjuntos de datos internos se aplican versiones neuronales de PCA y CMLHL. Dado que hay dos parámetros principales a optimizar, el conjunto de datos se divide en dos conjuntos: uno con el error de tiempo y otro con la diferencia de temperatura. Con ambos métodos y en ambos subconjuntos se encuentra una clara estructura interna en los datos. En ambos casos CMLHL proporciona una información más clara que PCA al estar más dispersa la proyección. En ambos conjuntos de datos se identifican las velocidades de alimentación X e Y como variable relevantes, al igual que el error de tiempo y las variables de temperatura en cada conjunto correspondiente. Con CMLHL se pueden observar más variables relevantes que con PCA.

Cuando el conjunto de datos se considera suficientemente informativo, como en este caso, el siguiente paso es modelar la relación entre las entradas y los errores de tiempo de producción, y entre las entradas y la diferencia de temperatura en el proceso, lo cual se logra aplicando varios modelos de RNA. Se utilizan dos MLP para monitorizar el error de tiempo y la diferencia de temperatura en la fabricación de piezas dentales. Los MLP se entrenan a partir de los algoritmos de entrenamiento más utilizados, como son el algoritmo de Lenvenberg-Marquardt, los métodos cuasi-Newton, el algoritmo de retropropagación resiliente y el algoritmo de gradiente conjugado escalado, utilizando los criterios de parada normal, parada temprana y técnicas de regularización bayesiana.

Los modelos de error de tiempo y diferencia de temperatura obtenidos se utilizan en el tercer paso como dos funciones de adaptación o *fitness*, de los algoritmos genéticos MOSA y NSGA-II, para determinar las mejores condiciones operativas para los procesos de fresado dental. Es decir, se trata de elegir los valores de la velocidad de avance X y velocidad de alimentación Y con el menor error de tiempo posible y el menor cambio de temperatura. Tanto MOSA como NSGA-II son válidos para encontrar los modelos buscados. Sin embargo, NSGA-II presenta un peor comportamiento teniendo en cuenta el MSE del error de tiempo en algunos experimentos.

El conjunto de datos recopilados en este proceso de fresado dental real presenta una importante tasa de error en el tiempo de fabricación de aproximadamente el 26,8%. Esto se debe a la diferencia entre el tiempo estimado de la propia máquina y el tiempo real de producción. El modelo obtenido es capaz de modelar más del 82% de las medidas reales en relación al error de tiempo (modelando más del 96,1% del trabajo en tiempo real). Esto ayuda a reducir el error y la tasa de variabilidad de los procesos de fabricación hasta un 4%, que es una tasa de error aceptable en la planificación del trabajo de fresado dental, en comparación con el 26,8% inicial. Además, la diferencia de temperatura entre el inicio y el final del proceso de fabricación dental tiene un aumento de aproximadamente un 10,2%. El modelo obtenido es capaz de modelar más del 99% de las medidas reales en relación a la diferencia de temperatura (modelando más del 99%

del trabajo de temperatura final real). La optimización multiobjetivo es capaz de encontrar los mejores valores para las velocidades de avance X e Y, a partir de algunos parámetros fijos como son las condiciones normales de fabricación y la minimización multiobjetivo de errores de tiempo y la diferencia de temperatura. Si bien, tanto el MOSA como el NSGA-II son válidos para aprender los modelos, los mejores resultados se obtienen en menos tiempo con NSGA-II. Es decir, la solución se puede obtener con un coste computacional menor. Por lo tanto, el proceso de fresado podrá minimizar los errores de tiempo y la diferencia de temperatura a un valor lo más cercano a cero posible.

Se puede afirmar que el sistema inteligente híbrido para una optimización multiobjetivo descrito en esta investigación se puede utilizar con éxito para optimizar los parámetros de máquinas en procesos industriales. Esto puede aumentar la eficiencia de una empresa, reduciendo sustancialmente el tiempo de preparar y configurar la máquina, además de ahorrar en costes y energía al optimizar los tiempos de fabricación, y además evitar la rotura de fresas y la pérdida de materia prima al optimizar la temperatura de funcionamiento.

Abstract

This multidisciplinary research presents a novel hybrid intelligent system to perform a multi-objective industrial parameter optimization process. The intelligent system is based on the application of evolutionary and neural computation in conjunction with identification systems, which makes it possible to optimize the implementation conditions in the manufacturing process of high precision parts, including finishing precision, while saving time, financial costs and/or energy. Empirical verification of the proposed hybrid intelligent system is performed in a real industrial domain, where a case study is defined and analyzed. The experiments are carried out based on real dental milling processes using a high-precision machining centre with five axes, requiring high finishing precision of measures in micrometers with a large number of process factors to analyze. The results of the experiments which validate the performance of the proposed approach are presented in this study.

1 Introduction

Intelligent systems have been widely used for industrial process modelling. Recently, different paradigms of Artificial Intelligence have been applied to different industrial problems [1, 2, 3].

System identification [4, 5, 6] has made it possible to model, simulate and predict the behavior of many industrial applications successfully and in different areas such as: control, robotics [7], energy processes [8], milling machine [9], high precision [1], power system security [10], etc. A novel and economically advantageous application is the optimization process in the field of Medical Therapeutics (Odonto-Stomatology), a booming industry [9, 11, 12, 13].

Prosthetic restorations must have a high marginal fit [14]. A bad marginal fit [15] affects fracture resistance and reduces the longevity of the restoration, resulting in higher risk of recurrent carious lesions and periodontal disease, as well as the dissolution of the cement [16] which allows entry of fluid and microorganisms between the tooth and the restoration, causing discoloration, pulpal irritation, secondary carious lesions and treatment failure [17].

Disturbances or marginal discrepancies between 50 and 120 micrometers are considered clinically acceptable in relation to the longevity of the restorations [18, 19]. Improved processing and optimization of parameters such as processing time, temperature, accuracy, etc., for the development of pieces (such as dental-oral prostheses for partial crowns, inlays, onlays, etc. with application for rehabilitation and oral-dental restoration) are the focus of rigorous studies today [9]. The optimization process of machine parameters, such as the time parameter [20], permits significant economic savings due to the high number of dental pieces produced daily by the same high-precision dental milling machine centre. Another important factor in the milling process is the temperature of the tools, which can be expanded or fractured by an inappropriate feed rate or by the heating of the coolant. Maintaining a constant temperature during the manufacturing process will make it possible to produce dental pieces with suitable quality. This could significantly help to increase a company's efficiency, and substantially contribute to cost reductions in the preparation and setting of the machines processes.

One way to achieve this optimization is based on the hybridization [9, 21, 22, 23, 24, 25] of emerging and active techniques such as neural [5, 25] and evolutionary computation [26, 27], nature-inspired smart systems [28], data mining and decision support systems [29], information fusion [30], ensemble models, visualization techniques [31], cognitive and reactive distributed AI systems [32], case- based reasoning [33], among others.

This study is organized as follows. Section 2 describes hybrid intelligent systems. Section 3 introduces the unsupervised neural models applied for analyzing the datasets. Section 4 presents the system identification techniques used in the system modelling. Section 5 introduces the applied multi-objective genetic algorithm. Section 6 presents the hybrid intelligent system for the optimization of the process. Section 7 describes the industrial case study: a real dental milling process. The final section presents the different models that are used to solve the high precision dental milling optimization case study. At the end, the conclusions are set out and some comments on future research lines are presented.

2 Hybrid Intelligent Systems

The hybridization of intelligent techniques [9, 21, 22, 23, 24, 25] from different computational intelligence fields is becoming more and more popular due the growing awareness that such combinations frequently perform better than the individual techniques from computational intelligence (evolutionary [26, 27] and neurocomputing [5, 25], fuzzy systems [4], and so on).

Practical experience has indicated that hybrid intelligence techniques might be helpful to solve some of the challenging real world problems. In a hybrid intelligence system, a synergistic combination of multiple techniques is used to build an efficient solution of a specific problem.

3 Exploratory Projection Pursuit

In this study, an extension of a neural Principal Component Analysis (PCA) version [34, 35, 36] and other Exploratory Projection Pursuit (EPP) [37, 38, 39] versions are used initially to select the most relevant input features in the data set, and secondly to study its internal structure.

Feature Selection [40, 41] describes the tools and techniques available for reducing inputs to a manageable size for processing and analysis.

The feature selection approach in this study is based on the issue of dimension reduction. Initially, some projection methods such as PCA [34, 35, 36], MLHL [38] and CMLHL [31, 42] are applied. Their first step is to analyze the internal structure of a representative data set from a case study. If after applying these models, a clear internal structure can be identified, this means that the data recorded is informative enough. Otherwise, further data must be properly collected [20].

PCA is a statistical model [34, 35] which describes the variation in a set of multivariate data in terms of a set of uncorrelated variables, each of which is a linear combination of the original variables.

Its goal is to derive new variables, in decreasing order of importance, that are linear combinations of the original variables and are uncorrelated with each other.

Using PCA, it is possible to find a smaller group of underlying variables that describe the data. PCA has been the most frequently reported linear operation involving unsupervised learning for data compression and feature selection [36].

3.1 A Connectionist Implementation of Exploratory Projection Pursuit

Exploratory Projection Pursuit (EPP) [37, 38, 39] is a more recent statistical method aimed at solving the difficult problem of identifying structure in high dimensional data. It does this by projecting the data onto a low dimensional subspace in which the data structure is searched by eye. However, not all projections will reveal this structure equally well. It therefore defines an index that measures how "interesting" a given projection is, and then represents the data in terms of projections that maximize the index.

The first step for EPP is to define which indexes represent interesting directions. "Interestingness" is usually defined with respect to the fact that most projections of high-dimensional data give almost Gaussian distributions [37]. Thus, in order to identify "interesting" features in data, it is appropriate to look for those directions in which the data-projections are as far from the Gaussian as possible.

Kurtosis is based on the normalized fourth moment and measures the heaviness of the tails of a distribution. A bimodal distribution will often have a negative kurtosis, which will therefore signal that a particular distribution shows evidence of clustering.

If a Gaussian distribution with mean a and variance x is as interesting as a Gaussian distribution with mean b and variance y, then such information may be removed from the data (sphering). In effect, the second order structure can obscure structures of a higher order that are more interesting.

Cooperative Maximum Likelihood Hebbian Learning (CMLHL) [42] is based on Maximum Likelihood Hebbian Learning (MLHL) [43], an EPP connectionist model. CMLHL includes lateral connections [42, 44] derived from the Rectified Gaussian Distribution (RGD) [45]. The RGD is a modification of the standard Gaussian distribution in which the variables are constrained to be non-negative, enabling the use of non-convex energy functions. The CMLHL architecture is depicted in Fig. 1, where lateral connections are highlighted.

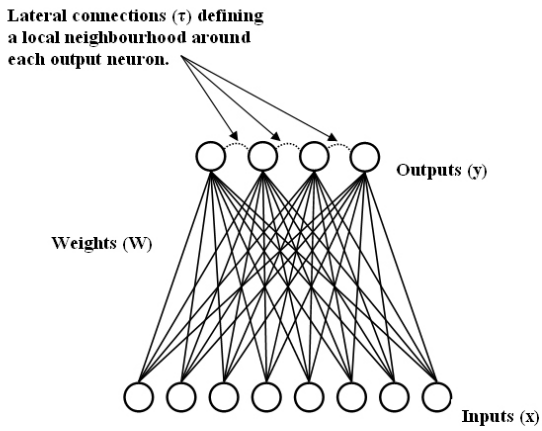


Fig.1 CMLHL: lateral connections between neighboring output neurons

The lateral connections used by CMLHL are based on the cooperative distribution mode that is closely spaced along a non-linear continuous manifold. Consequently, the resultant net can find the independent factors of a dataset in a way that captures some type of global ordering.

Considering an N-dimensional input vector (*x*), an M-dimensional output vector (*y*) and with W_{ij} being the weight (linking input *j* to output *i*), CMLHL can be expressed as:

Feed-forward step:

$$y_i = \sum_{j=1}^{N} W_{ij} x_j , \forall i \qquad (1)$$

Lateral activation passing:

$$y_i(t+1) = \left[y_i(t) + \tau(b - Ay) \right]^{+} \qquad (2)$$

Feedback step:

$$e_j = x_j - \sum_{i=1}^{M} W_{ij} y_i , \forall j \qquad (3)$$

Weight change:

$$\Delta W_{ij} = \eta . y_i . sign(e_j) | e_j |^p \qquad (4)$$

Where: η is the learning rate, τ is the "strength" of the lateral connections, *b* the bias parameter and p is a parameter related to the energy function [42, 43].

A is a symmetric matrix used to modify the response to the data, the effect of which is based on the relation between the distances between the output neurons. It is based on Cooperative Distribution, but to speed up the learning process, it can be simplified to:

$$A(i, j) = \delta_{ij} - \cos\left(2\pi(i - j)/ M\right) \qquad (5)$$

where, δ_{ij} is the Kronecker delta.

4 System Modelling Using Identification Algorithms

System identification (SI) [4, 5, 6] aims to obtain mathematical models to estimate the behaviors of a physical process whose dynamic equations are unknown. The identification criterion consists of evaluating the group of candidate models that best describes the dataset gathered for the experiment. The goal is to obtain a model that meets the following premise [6]: a good model is one that makes good predictions and produces small errors when the observed data is applied.

Classic SI refers to the parametrical literature, which has its origin in linear system analysis [7]. Nevertheless, increased computational capability and the availability of soft computing techniques have widened research into SI. Artificial Neural Networks (ANN) are one of the paradigms used in SI [46]. When using ANN, the purpose of an identification process is to determine the weight matrix based on the observations Z^t, so as to obtain the relationships between the network nodes. The SI procedure comprises several steps: the selection of the models and their structure, the learning methods, the identification and optimization criteria and the validation method [6, 7, 46, 47]. Validation ensures that the selected model meets the necessary conditions for estimation and prediction. Typically, validation is carried out using three different methods: the residual analysis $\varepsilon(t,\hat{\theta}(t))$ (by means of a correlation test between inputs, their residuals and their combinations); the mean squared error (MSE) and the generalization error value (normalized sum of squared errors (NSSE)), and finally a graphical comparison between the desired outputs and the model outcomes through simulation [7, 20].

5 Multi-objective optimization

Multi-objective optimization [48, 49] deals with solving optimization problems which involve multiple objectives, there is usually no single solution which is optimum with respect to all objectives. The resulting problem usually has a set of optimal solutions, known as Pareto-optimal solutions, non-inferior solutions, or effective solutions [49]. Since there exists more than one optimal solution and since without further information no one solution can be said to be better than any other Pareto-optimal solution, one of the goals of multi-objective optimization is to find as many Pareto-optimal solutions as possible. Within these multi-objective algorithms, there are two well-known types among others, such as (i) the non-dominated sorting genetic algorithm (NSGA-II) [50]. This algorithm sorts the population in different surfaces according to the Pareto dominance operator, but also using the so-called crowding distance and (ii) the multi-objective simulated annealing (MOSA) [51]. This algorithm is able to elicit a set of non-dominated solutions and it has been shown as a good meta-heuristic technique to evolve the model learning when multi-objective problems arise. In this study, the NSGA-II and the MOSA are used as the multi-optimization strategy.

6 A Novel Hybrid Intelligent System for Multi-objective Machine Parameter Optimization in a Dental Milling Process

The process of optimizing the manufacturing dental pieces in terms of time errors, based on the optimization of the system behavior, is carried out within the framework of this study by means of a hybrid intelligent system. The potential of this novel system is exemplified by the time error parameter and the temperature. The first parameter is chosen as an important factor in this process in terms of the economic benefit for a company. In the second case, a proper temperature in the manufacturing process would make it possible to obtain better quality products.

6.1 Identification of the Relevant Features

Firstly, the dental manufacturing process is parameterized and its dynamic performance in normal operation is obtained by the real process of manufacturing dental pieces. The gathered data is then pre-processed using projection models based on the analysis of parameters as the variance [34, 35, 36] or the kurtosis as CMLHL [31, 42]. This is done to identify internal data set structures in order to analyze whether the data set is sufficiently representative and to identify the most relevant features.

6.2 Modelling and optimization of a normal dental milling operation

Once the relevant variables and their transformations have been extracted from the production data, a model capable of fitting the normal manufacturing operation must be obtained. This is done to identify bias in the time error for manufacturing and the difference of temperature in the machine. The different model learning methods used in this study were implemented in Matlab© [52]. The model structures were analyzed in order to obtain the models that best suited the dataset. Since the number of examples was small, a 10-fold cross-validation schema was selected. The final model is obtained using all the data set.

Moreover, several different indexes were used to validate the models [20] such as the percentage representation of the estimated model, the graphical representation for the prediction ($\hat{y}_1(t \mid m)$) versus the measured output ($y_1(t)$), the loss function or error function (V) and the generalization error value.

The loss function or error function (V) is the numeric value of the MSE that is computed using the estimation data set by means of Eq. (6), while the generalization error value is the numeric value of the NSSE that is computed using the validation data set by means of Eq. (6). The percentage representation of the estimated model is calculated as the normalized mean error for the prediction (FIT1, FIT) using the validation data set and the complete data set, respectively, Eq. (7), where N is the number of samples of the data set used. Finally, the variance of the mean square errors (λ) is calculated [8].

$$J_1(m) = \frac{1}{N} \sum_{t=1}^{N} \left| y(t) - \hat{y}_1(t \mid m) \right|^2 \qquad (6)$$

$$FIT(\%) = \left(1 - \frac{\sqrt{J_1(m)}}{\sqrt{\frac{1}{N}\sum_{t=1}^{N}|y(t)|^2}} \right) 100 \qquad (7)$$

Once the model of the time error and the difference of temperature parameter in the machine for manufacturing dental pieces is selected, these models are used as two fitness functions in a multi-objective optimization with NSAGII and MOSA in order to obtain the best optimization of the time errors and changes of temperature. Both algorithms used in this study were implemented in Matlab© [53]. The complete novel hybrid intelligent system is shown in Fig. 2.

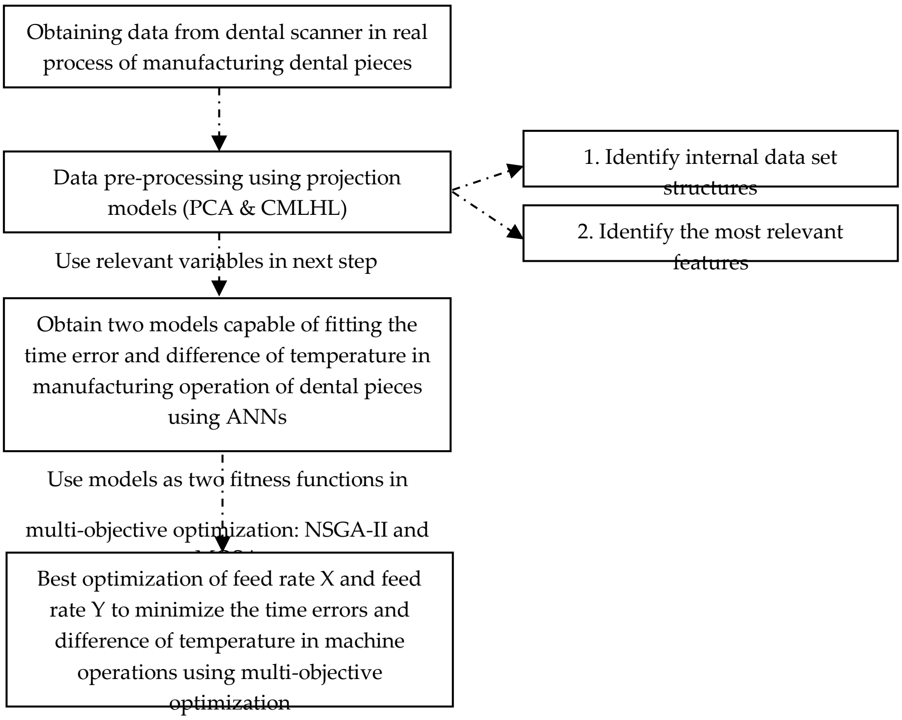


Fig. 2 A novel hybrid intelligent system to optimize a Dental Milling Process

7 A Real Case Scenario: a Dental Milling Process Optimization

Society demands aesthetics, biocompatibility and durability. This results in the need for fully adjusted dental treatments, with maximum strength and better appearance, but without limitation of materials or existing teeth situations (bridges, large structures, etc.).

The development of technology in dentistry is advancing with the application of both industrial tools and computer science in this field (dental science).

The milling process in the preparation of dental prostheses is currently the most modern processing prosthesis in existence. This technique involves a process in which the frame molds for crowns and bridges are milled or polished from different material blocks.

The material (Cr-Co, Ti), the tools and the feed rates affect the conformation times. Since the processing involves polishing/milling the piece, the time of conformation determines its size. It is important to obtain the optimum diameter of the material block for minimizing tool wear and the loss of material.

Another important factor is the temperature of the milling tools, which can be expanded or fractured because of an inappropriate feed rate or because of the heating of the coolant. This could result in the inappropriate conformation of prosthetic restorations (crowns, bridges).

The industrial case scenario is based on the real data gathered by means of a Machining Milling Center of HERMLE type-C 20 U (iTNC 530), with swiveling rotary (280 mm), with a control system using high precision drills and bits, by optimizing the time error detection for manufacturing dental metal.
The real case study is described by an initial data set of 114 samples obtained by the dental scanner in the manufacturing of dental pieces with different tool types (plane, toric, spherical and drill) characterized by 15 input variables (see Table 1). The input variables are the type of work, the thickness, the size of the tool, the radius of the tool, the tool, the number of pieces, the revolutions of the drill, the feed rate in each of the dimensions (X, Y and Z), the advance in the angle, the advance in the rotation, the initial tool diameter, the initial temperature and the estimated duration of the work.

Table 1 Different features from the process, their units and ranges

Variable (Units)	Range of values
Type of work (TW)	One Locator attachment of cobalt-chromium (1), single-implant crown of cobalt-chromium (2), four unit implant bridge of cobalt-chromium (3), single crown of cobalt-chromium (4), two unit implant bridge of cobalt-chromium (5) and four crowns bridge of cobalt-chromium (6).
Thickness (mm) (T)	8 to 15
Size of tool (mm) (ST)	T2 to T23
Radius (mm) (R)	0.25 to 1.5
Tool (To)	toric, spherical, plain, drill
Number of pieces (NP)	1 to 4
Revolutions per minute (RPM)	9,600 to 38,000
Feed rate X (mm. per minute) (FR X)	0 to 3,000
Feed rate Y (mm. per minute) (FR Y)	0 to 3,000
Feed rate Z (mm. per minute) (FR Z)	75 to 2,000
Advance in angle (mm. per minute) (AA)	0 to 550
Advance in rotation (mm. per minute) (AR)	0 to 550
Initial Diameter tool (mm) (ITD)	91.5035 to 110.4407
Initial Temperature (ºC) (IT)	24.8 to 30.4
Estimated work time (s) (EWT)	12 to 2,034
Time error for manufacturing (s) (TE)	-28 to -449
Difference of temperature in the machine (ºC) (DT)	0.9 to 6.7
Difference of diameter of the tool (mm) (DD)	0.00080 to 0.11950

There are two main parameters to estimate in this research: the time error for manufacturing and the difference of temperature in the machine. The time error for manufacturing is the difference between the estimated time by the machine itself and real work time (negative values indicate that real time exceeds estimated time). The difference of temperature in the machine is the difference between initial and final temperature in a dental milling process.

8 Results

This multidisciplinary research initially analyzed the data set in order to obtain the variables/characteristics that are most closely related to manufacturing time errors and difference of temperature in the machine.

In the first step, several unsupervised models were applied for the sake of comparison. In this case, neural versions of PCA and CMLHL were applied as powerful techniques for identifying internal dataset structures. In order to analyze the two main parameters to be estimated (the time error for manufacturing and the difference of temperature in the machine) the initial data set was divided into two data sets: one with the time error and another with the difference of temperature.

The axes forming the projections (Fig. 3.a, Fig. 3.b, Fig. 4.a and Fig. 4.b) represent combinations of the variables contained in the original datasets. In the case of PCA, the model is looking for those directions with the biggest variance, while CMLHL is looking for the kurtosis (directions which are as little Gaussian as possible) [38, 42].

In relation to time error, (see Fig. 3), both methods, PCA (Fig. 3.a) and CMLHL (Fig. 3.b), are able to find a clear internal structure in the dataset by identifying several clusters (see Table 2 and Table 3). Both methods also identified feed rate X and Y as relevant variables. It is clear that CMLHL provides a sparser representation than PCA, and that CMLHL projections provide more clear information identifying parameters such as type of work and time error as other important variables.

An analysis of the results obtained with the CMLHL model (Fig. 3.b) leads to the conclusion that this method has identified several different clusters ordered by feed rate X and Y and the type of work. Inside each cluster, there are further classifications by 'time error' and the dataset can be said to have an interesting internal structure based on the clusters identified.

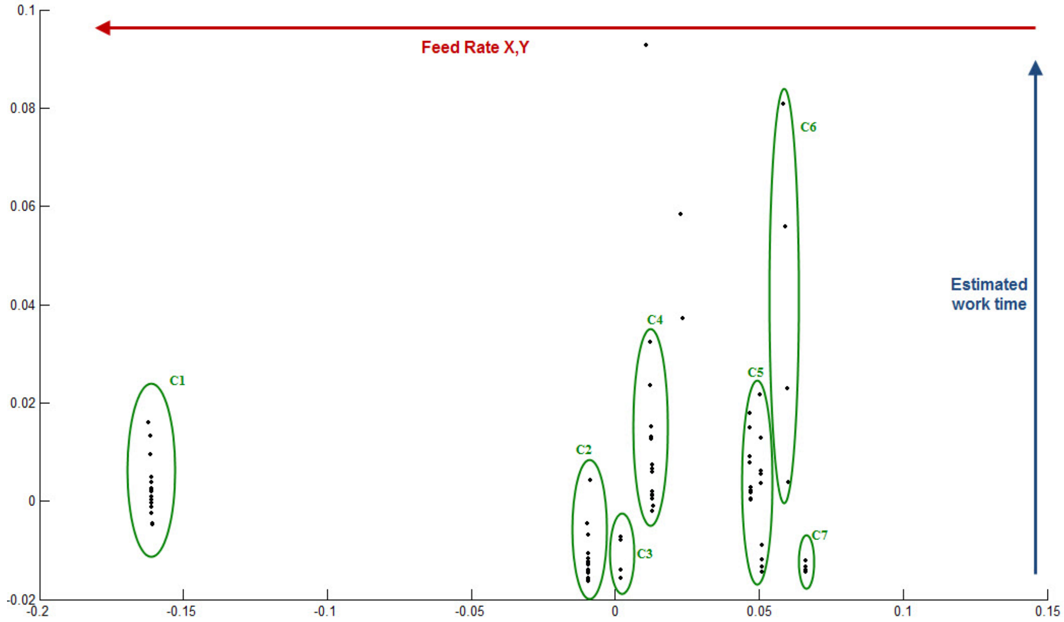


Fig.3.a Projection of PCA for data set with time error

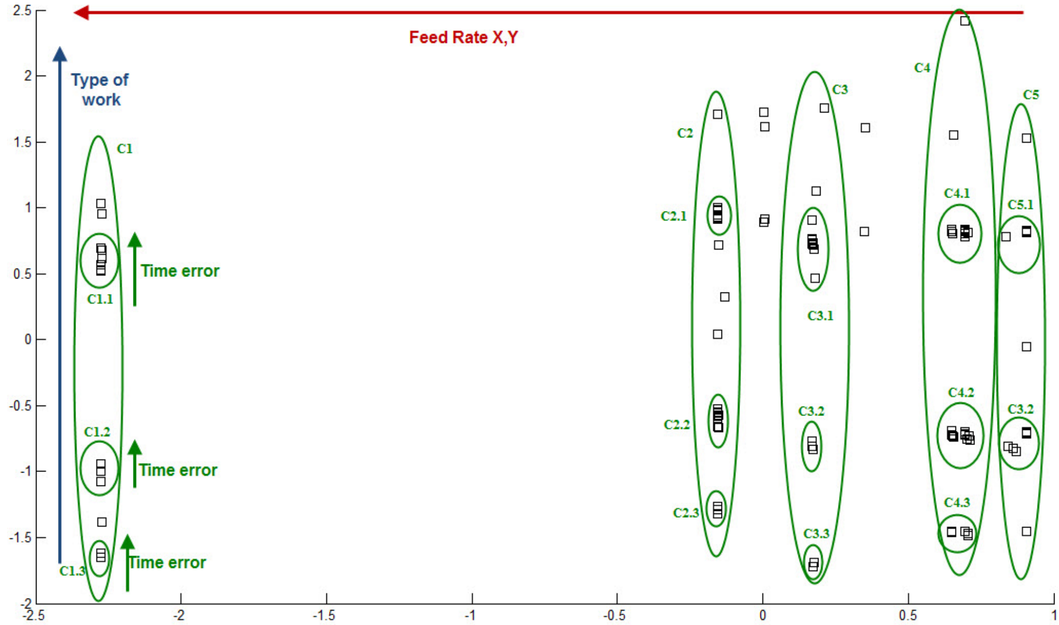


Fig.3.b CMLHL projection for data set with time error

Fig. 3 PCA projection (Fig. 3.a) and CMLHL projection (Fig. 3.b) for data set with time error

Table 2 Samples description and clusters obtained by using PCA method with time error.

Cluster	Feed Rate X, Feed Rate Y (mm per minute)	Estimated Work time (s)
C1	3,000	from 660 to 378
C2	1,000	from 408 to 6
C3	850	from 168 to 12
C4	700	from 900 to 258

C5	250 and 200	from 690 to 12
C6	75	from 1794 to 348
C7	0	from 48 to 6

Table 3 Samples description and clusters obtained by using CMLHL method with time error.

Cluster		**Type of work**	**Initial Temperature (ºC)**	**Feed Rate X,Y (mm per minute)**
C1	**C1.1**	4	from -238 to -202	3,000
	C1.2	2	from -317 to -227	
	C1.3	1	from -218 to -211	
C2	**C2.1**	4	from -98 to -42	1,000
	C2.2	2	from -44 to -71	
	C2.3	1	from -51 to 306	
C3	**C3.1**	4	from -128 to -43	700
	C3.2	2	from -86 to -75	
	C3.3	1	from -110 to -104	
C4	**C4.1**	4	from -46 to -33	250 and 200
	C4.2	2	from -46 to -35	
	C4.3	1	from -39 to -35	
C5	**C5.1**	4	from -36 to -28	75 and 0
	C5.2	2	from -45 to -30	

In relation to the difference of temperature, (see Fig. 4), both methods, PCA (Fig. 4.a) and CMLHL (Fig. 4.b), found a clear internal structure in the dataset by identifying several clusters (see Table 4 and Table 5). It is clear that CMLHL provides a sparser representation than that obtained by PCA, and that CMLHL projections provide more clear information identifying parameters such as the type of work, feed rate X and Y, initial temperature and difference of temperature as important variables.

An analysis of the results obtained with the CMLHL model (Fig. 4.b) leads to the conclusion that this method has identified several different clusters ordered by difference of temperature and type of work. Inside each cluster, there are further classifications by 'feed rate X,Y' and ‘initial temperature’ and the dataset can be said to have an interesting internal structure based on the clusters identified.

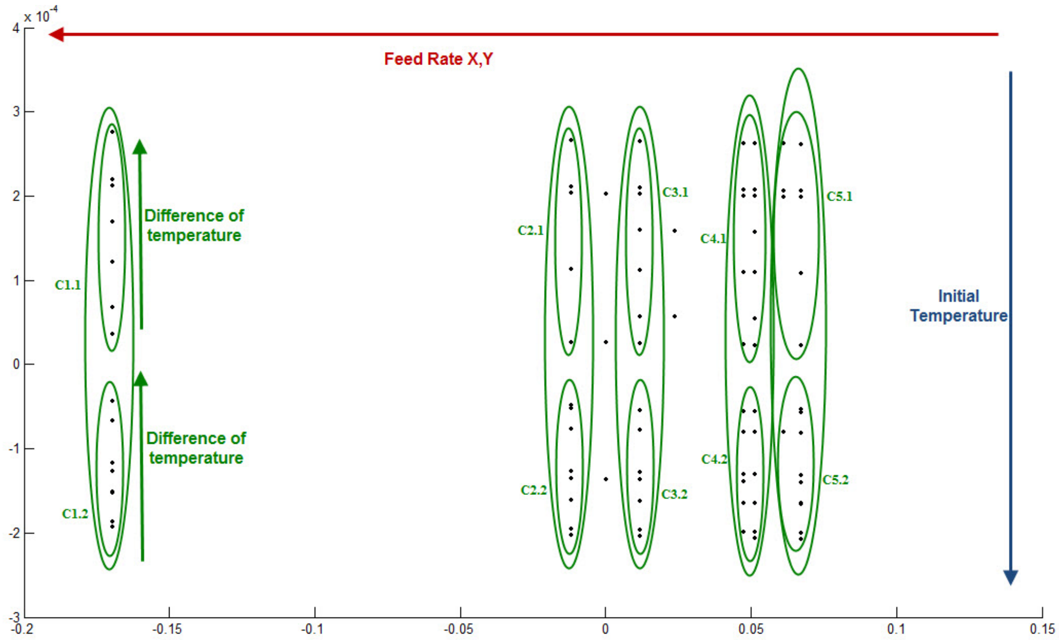


Fig.4.a Projection of PCA for data set with difference of temperature

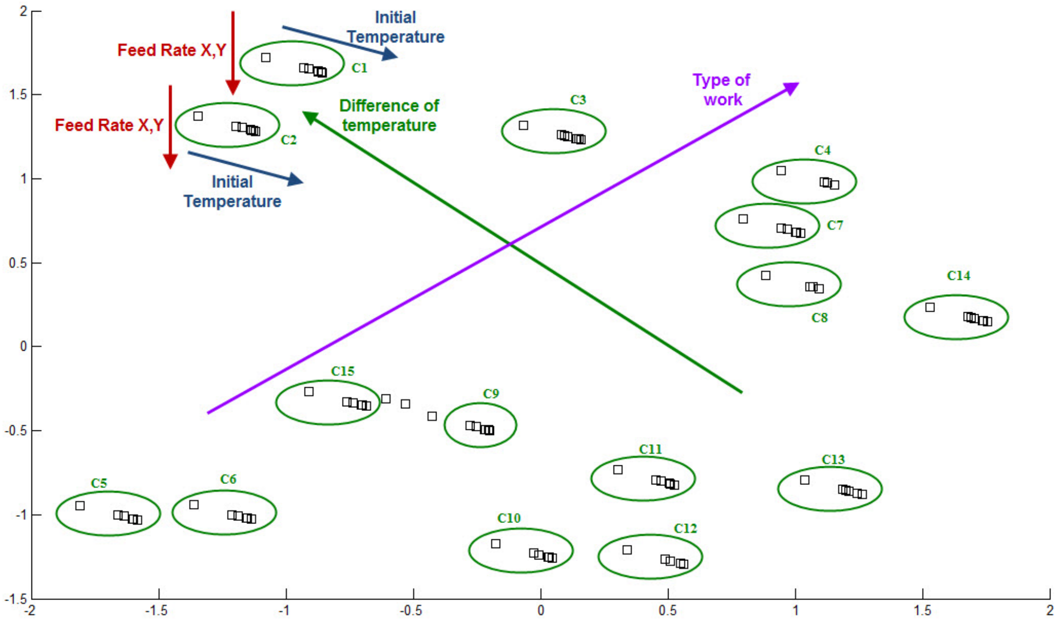


Fig.4.b CMLHL projection for data set with difference of temperature

Fig. 4 PCA projection (Fig. 4.a) and CMLHL projection (Fig. 4.b) for data set with difference of temperature

Table 4 Samples description and clusters obtained by using PCA method with difference of temperature.

Cluster		Difference of temperature (ºC)	Initial Temperature (ºC)	Feed Rate X,Y (mm per minute)
C1	C1.1	from 6.7 to 0.7	from 24.1 to 25.7	3,000
	C1.2	from 3.3 to 0.9	from 28.1 to 31	
C2	C2.1	from 6.7 to 0.7	from 24.1 to 25.3	1,000
	C2.2	from 3.8 to 0.9	from 28.4 to 31	

C3	**C3.1**	from 6.7 to 0.7	from 24.1 to 25.7	700
	C3.2	from 3.3 to 0.9	from 28.4 to 31	
C4	**C4.1**	from 6.7 to 0.7	from 24.1 to 25,7	250 and 200
	C4.2	from 3.3 to 0.9	from 28. 4 to 31	
C5	**C5.1**	from 6.7 to 0.7	from 24.1 to 25.3	75 and 0
	C5.2	from 3.8 to 0.9	from 28.4 to 31	

Table 5 Samples description and clusters obtained by using CMLHL method with difference of temperature.

Cluster	Difference of temperature (ºC)	Type of work	Initial temperature (ºC)
C1	6.7	2	24.1
C2	6.7	2	25.3
C3	5.6	4	24.8
C4	4.7	6	25.2
C5	3.3	1	31
C6	2.4	1	30.4
C7	3	4	25
C8	2.3	4	25.7
C9	2.7	2	28.4
C10	2	4	31
C11	1.7	4	29.3
C12	0.9	4	30.4
C13	0.9	5	29
C14	0.7	4	25.3
C15	3.3	2	28.7

When the dataset is considered sufficiently informative, as in this case, the next step is to model the relationship between inputs and production time errors, and between inputs and the difference of temperature in the process, which is accomplished by applying several artificial neural network modelling systems.

Two multilayer perceptron networks (MLP) (feedforward network) were used to monitor time error and the difference of temperature in the manufacturing of dental pieces. The data set is pre-processed from the input and output normalization step, and the reduction of the input vectors dimension (the data set gathered in the previous step). The MLP is trained from the most widely used training algorithms such as the Lenvenberg-Marquardt algorithm [54], quasi-Newton methods [55], resilient backpropagation algorithm [56] and escalated conjugate gradient algorithm [57], using the criteria of normal stopping, early stopping, and Bayesian regularization techniques [58].

The features for the two best MLP proposed and its indexes are stated below:

The feedforward network -called f1- to predict the time error has 30 hyperbolic tangent units (layer 1), 25 hidden hyperbolic tangent units (layer 2), 25 hidden hyperbolic tangent units (layer 3), 4 hidden hyperbolic tangent units (layer 4) and 1 linear output unit. The parameters in the network were estimated using the Lenvenberg-Marquardt algorithm with normal stopping criterion. Normalizing the minimum and maximum values of data set to [-1 1].

The feedforward network -called f2- to predict the difference of temperature has 30 hyperbolic tangent units (layer 1), 20 hidden hyperbolic tangent units (layer 2), 5 hidden hyperbolic tangent units (layer 3) and 1 linear output unit. The parameters in the network were estimated using the Lenvenberg-Marquardt algorithm with Bayesian regularized criterion. Normalizing the data set to media null and variance 1.

These models (f1 and f2) do not only present the lowest V (0.001 and 5.25E-5) and NSSE (0,013 and 0,12E-3), but also a higher system representation index value FIT1 (82,45% and 99,87%) and a small (0.1E-4 and 1.32E-9). From these indicators, it may be concluded that the ANNs selected are able to simulate and predict the behavior of time errors and the difference of temperature for manufacturing dental pieces (as a consequence of the production process).

The models of time error (f1) and difference of temperature (f2) obtained may be used as two fitness functions in the next step to determine the best operating conditions for the dental milling processes, i.e., to choose the values of feed rate X and feed rate Y with the least possible time error and the least change of temperature in the process.

In Fig. 5 is shown the representation of this optimization process. Where IT, TW and EWT are values fixed and FR X and FR Y are values obtained when TE and DT are close to zero.

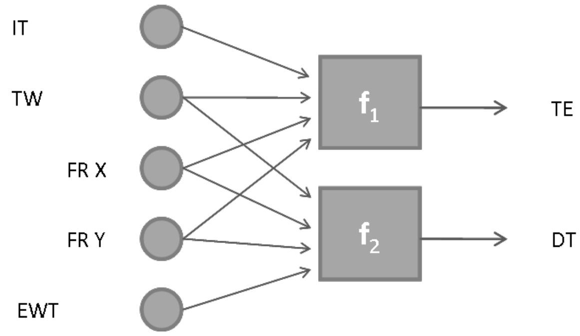


Fig. 5 Optimization multi-objective NSA-II and MOSA about the variables TE and DT. IT, TW and EWT are values fixed. The values FR X and FR Y are obtained.

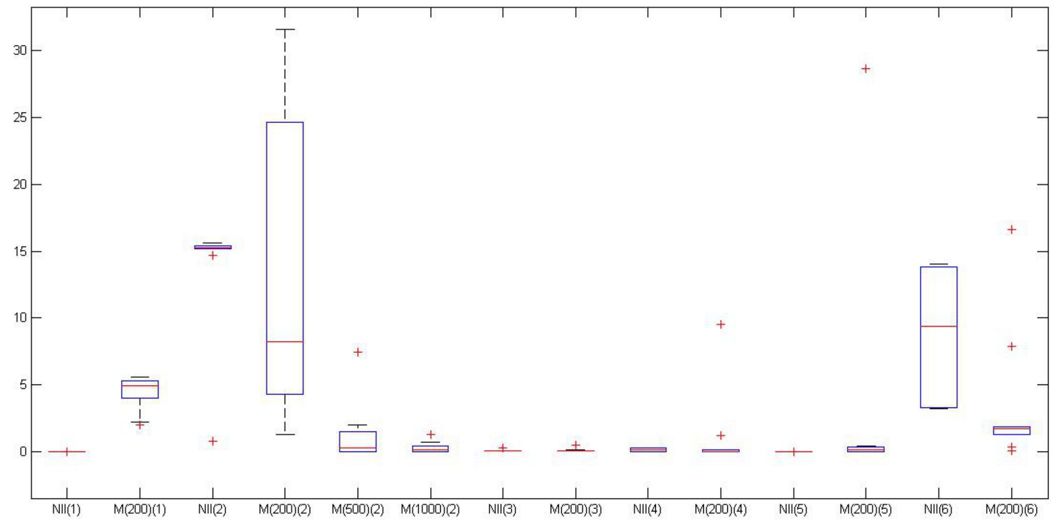
For the problem, 11 experiments have been designed and 10 runs of each experiment have been carried out for statistics purposes. The experiments use a population size of 100 individuals, 200 iterations for the NSGA-II (and a bigger number of iterations for the

MOSA [200, 500 and 1,000 in some experiments]). The crossover probabilities are 0.8 and mutation probabilities are 0.2. MOSA uses Δ=0.1, T_0=1 and T_1=0.01. The results are shown in Table 6 and in the boxplot of Fig. 6. In the Table, the 11 experiments are compared for the best individual error found and for the individual closest to the origin. Although some differences have been found, both the MOSA and the NSGA-II are valid to learn the models. Nevertheless, the NSGA-II presents a worst behavior in the MSE of time error in some experiments.

Besides, in Fig. 7 is depicted one of the multi-optimization experiments accomplished and shown in the Table 6, concretely the number five. The X-axis shows the feed rate X (mm. per minute) and the Y-axis represents feed rate Y (mm. per minute), for from 0 to 3,000. The features fixed are 29 ºC for initial temperature and 900 s for estimated work time. In Fig. 7.a the Z-axis represents the output variable range (time error) from -3,000 s to 1,000 s. This value is also shown on the vertical bar. In Fig. 7.c the Z-axis represents the output variable range (difference of temperature) from -8ºC to 4ºC. The difference in temperature is also shown on the vertical bar. Fig. 7.b and Fig. 7.d present the final value got for the feed rate X and Y with a value close to zero in the two outputs optimized (the black point in the interior of circle).

Table 6 Experimentation results for manufacturing under different condition in the Dental Milling process. MSE value of the mean central point of the MSE function for the individuals of lowest MSE value individual in the populations (MSE) and the closest to the origin individual in the populations, considering the 10 runs of each experiment. Capital letters M or NII refer to MOSA and NSGA-II.

Algorithm used		Execution	Values fixed			Value obtained for the closest to the origin				MSE	
Experiments		Time (m.)	TW	IT	EWT	FR X	FR Y	DT	TE	DT	TE
1	NII	**41**	1	31	12	**1,111.36**	**1,663.99**	**4.43E-09**	**2.31E-11**	2E-05	6.74E-11
	M(200)	229	1	31	12	419.31	718.48	2.217	-0.12	4.389	4.317
2	NII	**43**	2	28.7	12	**784.58**	**1,517.3**	**-0.883**	**-0.20**	13.822	1.778
	M(200)	141	2	28.7	12	803.13	1,633.81	-1.126	1.16	13.265	5.181
	M(500)	456	2	28.7	12	740.88	1,431.94	-0.903	-0.86	4.33	1.434
	M(1000)	4380	2	28.7	12	806.80	1,695.88	-1.33	-0.259	2.489	0.908
3	NII	**41**	3	25.7	366	**839.08**	**939.69**	**0.182**	**6.94E-06**	0.077	1.62E-03
	M(200)	119	3	25.7	366	874.71	788.15	0.366	0.184	0.107	9.539
4	NII	**46**	4	28.4	378	**449.29**	**1,305.34**	**-3.2E-05**	**7.03E-08**	0.131	54,859.73
	M(200)	66	4	28.4	378	453.11	646.09	0.0059	0.123	1.089	1.638
5	NII	**45**	5	29	900	**953.86**	**1,132.3**	**-4.4E-15**	**3.27E-13**	0.00015	1.05E-06
	M(200)	65	5	29	900	434.11	646.09	0.038	0.448	0.154	34.68
6	NII	**45**	6	25.2	1380	**498.13**	**1,711.1**	**1.784**	**0.0002**	8.703	23,273.33
	M(200)	88	6	25.2	1380	971.64	2,045.09	1.353	0.0065	4.734	12.229
7	NII	**45**	1	30.4	282	**192.96**	**475.59**	**1.265**	**0.021**	3.504	0.648
	M(200)	80	1	30.4	282	646.45	870.97	1.355	-0.103	2.133	0.114
8	NII	**44**	6	25.2	660	**117.39**	**1,709.47**	**0.0019**	**-0.00017**	11.263	11,141.42
	M(200)	54	6	25.2	660	142.19	1,671.5	0.412	-2.534	6.430	66.352
9	NII	**44**	2	28.7	66	**904.5**	**1436**	**4.88E-15**	**-1.14E-13**	6.3E-07	7.62E-12
	M(200)	49	2	28.7	66	763.53	1,245.88	-0.156	0.287	3.541	11.938
	M(500)	253	2	28.7	66	829.46	1,284.11	0.088	-0.181	0.254	6.290
10	NII	**45**	3	28.4	378	**66.78**	**1,266.11**	**0.173**	**0.029**	1.09	0.019
	M(200)	81	3	28.4	378	60	1,266.19	0.156	-1.602	4.34	6.103
	M(500)	240	3	28.4	378	749.68	1,011.99	2.627	0.136	7.37	2.47
11	NII	**45**	6	25.2	2034	**1,631.99**	**1,090.45**	**2.686**	**0.011**	7.506	0.041
	M(200)	117	6	25.2	2034	572.99	1,264.7	3.199	0.413	11,519	9.164



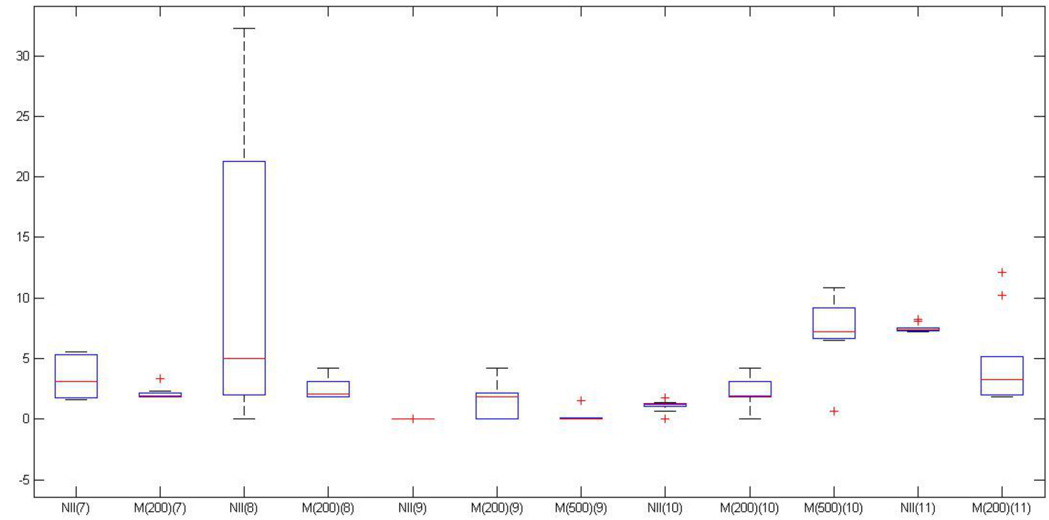


Fig. 6 Boxplot of the central points of the MSE for the best individuals considering only the MSE function in DT. Each box is identified using M for MOSA or N for NSGA-II and a number for the experiment.

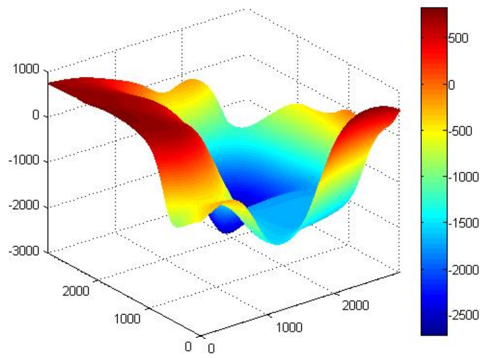


Fig. 7.a 3D graph, the X-axis represents feed rate X, the Y-axis is the feed rate Y and the Z-axis the output (time error)

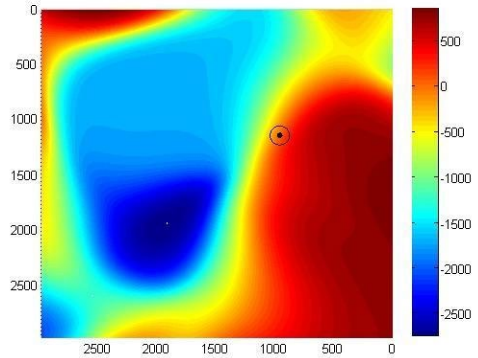


Fig. 7.b 2D graph, the X-axis represents feed rate X and the Y-axis is the feed rate Y. The black point is the chosen output (time error)

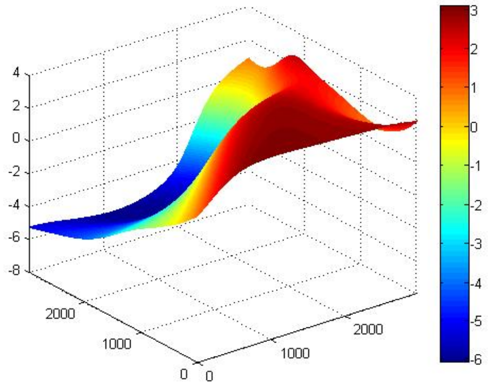


Fig. 7.c 3D graph, the X-axis represents feed rate X, the Y-axis is the feed rate Y and the Z-axis the output (difference of temperature)

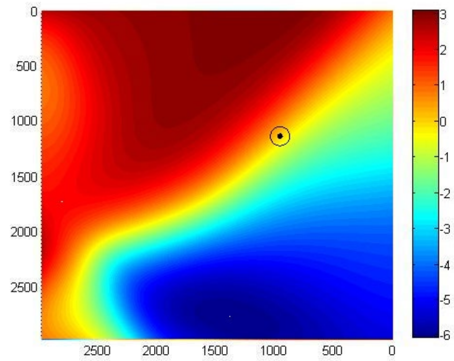


Fig. 7.d 2D graph, the X-axis represents feed rate X and the Y-axis is the feed rate Y. The black point is the chosen output (difference of temperature)

Fig. 7 Output response of the time error and the difference of temperature for different input variable ranges in the manufacturing of two unit implant bridges of cobalt-chromium

9 Conclusions and future work

The novel hybrid intelligent system with a multi-objective optimization process described in this research can be successfully used to optimize machine parameters for industrial processes, based on the obtained results. The optimization process may increase a company's efficiency and substantially reduces the cost of preparing and setting machine processes. We have used this method for multi-objective optimization and adjustments during the manufacturing process of dental pieces such as implants according to medical specifications for precise mouldings.

The method proposed is based on the selection of the most important features in an initial step. ANNs are then trained for modelling the features and these can thus be used as two fitness functions in the multi-objective optimization. Finally, a NGSA-II and MOSA try to achieve the best conditions for manufacturing from the model.

The data set collected in this real dental milling process presents an important manufacturing time error rate of about 26.8%. This is due to the difference between the estimated time of the machine itself and the real production time. The obtained model is capable of modelling more than 82% of the actual measurements in relation to the time error (modelling more than 96.1% of real time work). This helps to reduce the error and the variability rate of manufacturing processes down to 4%, compared to the initial 26.8%, which is an acceptable error rate in planning work for dental milling. Also, the difference of temperature between the beginning and the end of the dental manufacturing process has an increase of about 10.2%. The obtained model is capable of modelling more than 99% of the actual measurements in relation to the difference of temperature (modelling more than 99% of real final temperature work).

The multi-objective optimization is able to find the best values for the feed rate X and Y from some fixed parameters such as normal conditions of manufacturing and the multi-objective minimization of time errors, and the difference of temperature. Although, both the MOSA and the NSGA-II are valid to learn the models, the best results -considering the 10 runs- are obtained in less time with NSGA-II; i.e., the solution can be obtained with less computational cost. Therefore, the milling process will be able to minimize the time errors and the difference of temperature to a value as close to zero as possible.

Future lines of research will investigate the selection of the most suitable features using a wrapper feature selection method, in which Genetic Algorithms and ANNs are hybridized. Finally, an algorithm will be developed to automatically identify the best operating conditions: minor time errors for the manufacturing of dental pieces and minor differences of temperature. Moreover, the resulting model would be applied to different metals used in prosthetic dentistry and in other industrial processes, such as the automotive sector.

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A Decision-Making Tool Based on Exploratory Visualization for the Automotive Industry

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Índice

Resumen

En los últimos años, las empresas industriales están avanzando en la transformación digital apoyadas en las Tecnologías Habilitadoras (Big Data, IoT, etc.) de la Industria 4.0. Como consecuencia, las empresas cuentan con grandes volúmenes de datos e información que deben ser analizados para otorgarles ventajas competitivas. Esto es de suma importancia en campos como la detección de fallos y el mantenimiento predictivo. Sin embargo, encontrar patrones en dichos datos no es fácil, pero las tecnologías de vanguardia como ML pueden contribuir enormemente.

Las empresas, en su búsqueda de la fábrica inteligente, están sensorizando y haciendo uso de IoT y Big Data, lo que supone que están almacenando una cantidad ingente de información. Pero dicha información debe usarse de modo eficiente, se debe alcanzar un balance coste-beneficio. Además, no siempre es sencillo establecer qué datos hay que recoger y es complejo instrumentar y digitalizar ciertas variables. Por lo que se hace necesario validar que la información con la que se cuenta es suficiente o efectiva para el propósito buscado.

El presente estudio propone una extensión de la técnica HUEP (*Hybrid Unsupervised Exploratory Plots*) para ayudar a las empresas en la analítica visual de datos de cara a tomar decisiones en proyectos de detección de fallos o mantenimiento predictivo.

Los HUEPs son una técnica de visualización que combina la búsqueda exploratoria de proyecciones (EPP) con métodos de agrupación o *clustering*. En este estudio se propone una formulación extendida de HUEPs, agregando por primera vez los siguientes métodos de EPP:

- *Classical Multidimensional Scaling* (CMDS)
- *Sammon Mapping* (SM)
- *Factor Analysis* (FA)

Los HUEPs extendidos, junto con los existentes previamente, se validan empíricamente con dos casos de estudio asociados a una empresa multinacional del sector de la automoción. Se analizan dos conjuntos de datos de fabricación industrial real que contienen datos recopilados de máquinas de un proceso de fabricación de componentes mediante corte por chorro de agua. Los conjuntos de datos corresponden a los intensificadores y el ciclón de una máquina *waterjet*.

Se han generado muchas visualizaciones diferentes combinando varias técnicas EPP (PCA, MLHL, CMLHL, CMDS, SM y FA) junto con las técnicas de agrupamiento *(k-means* y aglomerativas), probando con diferentes valores en sus parámetros.

En los resultados obtenidos se observa que los HUEPs extendidos obtienen mejores visualizaciones que si se aplicasen sólo las técnicas EPP. Los datos que indican un fallo se agrupan en un mismo grupo aislado. Además, se observa que con CMDS se consigue

la mejor visualización. Para los dos conjuntos de datos se consigue mejores resultados combinando CMDS con agrupamiento aglomerativo en lugar de *k-means*.

Al visualizar los resultados obtenidos con los conjuntos de datos del presente estudio, se ha demostrado que la extensión propuesta de los HUEPs supera a la formulación original. Cabe mencionar que los HUEPs generados por CMDS son más útiles que los demás ya que las distintas anomalías se agrupan y visualizan de forma más clara. Asimismo, CMDS es una técnica de EPP interesante porque se puede aplicar con varias métricas de distancia que se ajustan al conjunto de datos bajo estudio. Por otro lado, para los conjuntos de datos analizados (donde las muestras "normales" son muchas más que las que fallan), el agrupamiento aglomerativo agrupa los datos de una manera más consistente que *k-means*.

También se ha demostrado que, dependiendo del conjunto de datos, podría ser mejor utilizar una combinación de métodos para generar un HUEP que otro. Es decir, las mejores visualizaciones para el intensificador no se generan con la misma combinación de parámetros que las del conjunto de datos del ciclón. Por tanto, es importante realizar una experimentación exhaustiva con cada combinación diferente para identificar la mejor visualización.

Se ha corroborado que los HUEPs son una técnica que se puede utilizar para ver de forma visual y sencilla que los datos que se han recopilado tienen una estructura y que pueden ser representativos e informativos. Los HUEPs pueden además mostrar grupos separados que diferencian los fallos del funcionamiento normal. La extensión a los HUEPs propuesta ayuda en la toma de decisiones ya que muestra los datos de una manera visual que apoya en esta tarea. Se ha probado y validado en un escenario industrial complejo con conjuntos de datos asociados que comprenden una gran cantidad de muestras y una gran cantidad de características. Los resultados obtenidos demuestran que HUEP es una técnica que soporta la monitorización de sensores y máquinas para anticipar fallos. Esta contribución a la analítica visual de datos puede ayudar a las empresas en la toma de decisiones en proyectos de detección de fallos y mantenimiento predictivo.

Abstract

In recent years, the digital transformation is advancing in industrial companies supported by the Key Enabling Technologies (Big Data, IoT, etc.) in Industry 4.0. As a consequence, companies have large volumes of data and information that must be analysed to give them competitive advantages. This is of the utmost importance in fields such as Failure Detection (FD) and Predictive Maintenance (PdM). However, finding patterns in such data is not easy, but cutting-edge technologies such as Machine Learning (ML) can greatly contribute. As a solution, this study extends Hybrid Unsupervised Exploratory Plots (HUEPs) as visualization techniques that combines Exploratory Projection Pursuit (EPP) and Clustering methods. An extended formulation of HUEPs is proposed, adding for the first time the following EPP methods: Classical Multidimensional Scaling, Sammon Mapping, and Factor Analysis. Extended HUEPs are validated in a case study associated to a multinational company in the automotive industry sector. Two real-life datasets containing data gathered from a Waterjet Cutting tool are visualised in an intuitive and informative way. The obtained results show that HUEPs is a technique that supports the continuous monitoring of machines in order to anticipate failures. This contribution to visual data analytics can help companies in decision-making regarding FD and PdM projects.

1 Introduction

In the industrial sector there are several issues that most corporations are trying to address. As far as technology advances, some of these problems could be solved or at least their negative impact could be reduced. Recently, the concept of Industry 4.0 [1] has been proposed, involving several cutting-edge technologies such as Robotics, Artificial Intelligence, Industrial Big Data [2], Industrial Internet of Things (IIoT) [3], deep learning and deep analytics, computer vision, visual data analytics, visual computing, and digital twins [4] among others. These resources are greatly contributing to solve many of the problems in industrial manufacturing and improving manufacturing processes.

Industrial companies are developing projects in order to converge to the “smart factory” [5, 6] concept. With such projects, factories want to be able to learn and adapt to changes in real time and, in order to do that, it is necessary to have permanent information and data about the elements involved in the plant. To be able to capture all this information, sensors and IoT devices need to be installed. Thanks to IIoT it is possible to have millions of data items related to factories and their machines. But all these datasets are useless and expensive unless they can be analysed; here it is where the proposals of Big Data and Visual Analytics appear.

In general terms, companies are not able to accomplish the implantation of the smart factory paradigm in all their plants. The costs of becoming a smart factory are potentially unaffordable; therefore, companies are not sensorizing all their machines or processes. The required storage resources (cloud) to keep this huge quantity of information is not for free. Normally, the data of a machine in a factory involves a great volume of information with a high-dimensionality. Additionally, as there are many different machines being permanently monitored, the produced data are heterogeneous and not complete (sensors and communications may fail).

When properly used, all these datasets could make a factory more efficient in several areas: resources savings, costs reduction, optimization of production times, increasing sustainability, minimizing failures and downtime, etc., but the investment in gathering, storing and analysing these datasets usually is very high. Because of that, it is very important to be sure that sensors, devices and related datasets are carefully chosen and with the proper features. These data would have a high dimensionality that should be in balance with the costs and requirements of the company. In order to overcome this well-known problem named "the curse of dimensionality", Machine Learning (ML) and interactive visualization for data exploration could greatly contribute. As a result, any department from industrial companies could benefit from the use of visual analytics in decision-making.

In keeping with this idea, present study proposes to extend Hybrid Unsupervised Exploratory Plots (HUEPs) [7] and apply them for sensor validation and condition monitoring as a decision-making tool based in a visual analysis for a subsequent predictive maintenance (PdM). HUEPs are a recently-proposed technique where Exploratory Projection Pursuit (EPP) [8] and clustering [9] methods could be combined to generate informative and intuitive 3D visualizations of high-dimensional data (see Section 2). When using different colours and the glyph metaphor, they can display more information than a standard 2D or 3D projection in a more intuitive way. HUEPs are validated and extended in the present paper by incorporating some additional EPP techniques, namely Classical Multidimensional Scaling (CMDS), Sammon Mapping (SM), and Factor Analysis (FA).

This study helps to analyse the datasets structure and clearly identify issues in machines, anticipating to potential failures. If the initial collected dataset, once analysed, reveals a defined structure including clusters "reporting" issues, this can be seen as a sign of a representative data set. The data used in this study have been provided by Grupo Antolin [10] (a multinational company in the automotive industry sector) and refer to several waterjet industrial tools (machines to perform industrial cutting using extremely-high pressure water) located in an automotive plant. This proposal advances previous work as hybridization of unsupervised learning for visualization is applied for the first time to this real case study. Datasets collected for PdM purposes have never been analysed before with HUEPs.

As it is stated before, it is necessary a balance between cost and benefits. Data visualization contributes to find such balance, especially in cases of high volumes of information with high-dimensionality. Exploratory analysis must be one of the first steps in industrial data analytics [11] and visualizations are advisable to know if the collected data make sense [12]. As some studies suggest [13], visual computing plays a vital role in both the Industry 4.0 and advanced manufacturing. In [14] it is shown how the application of visual computing can empower workers in the framework of Industry 4.0. A use case is presented, showing how visual analytics incorporated in a plant's Human-machine Interface can improve the cognitive process of supervising a production line and applying corrective maintenance. In [15] authors focus on how the fusion of graphics, vision and media technologies can enrich the role of the new operator 4.0. Other surveys present a methodology to implement a data-driven PdM not only in the machine decision making, but also in data acquisition and processing with a visual analysis of the Remaining Useful Life (RUL) of a machining tool [16]. As stated, companies should not forget the cost-improvement trade-off around the Industry 4.0, explained in [11], where a methodology based on data analytics has been proposed for cost-efficient monitoring the Industry 4.0 with a real use case within the automotive industry.

Some previous studies that researched on the application of ML to PdM and faults/anomalies detection have proposed a classification approach, based on supervised learning. Less effort has been devoted to investigate the contributions of unsupervised learning, although some previous work does exist. For instance, in [17] authors proposed the application of the k-means method combined with Fuzzy Logic for PdM purposes. In [18], a combination of "constrained k-means clustering, fuzzy modelling and LOF-Based score" has been applied in order to detect anomalies in an auxiliary marine diesel engine. Other research [19] applied five clustering methods (Hierarchical, k-medoids, k-means, DBSCAN, and OPTICS) for a health condition monitoring model at a chemical vapor deposition process in a semiconductor company.

Other studies on fault diagnosis or PdM analyse a kind of datasets that have been very widely used and tested in the literature: motor bearing dataset [20, 21, 22], gear-box dataset [20, 23, 24] and the Tennessee Eastman Process (TEP) dataset [25]. In [26] another popular rolling bearing dataset has been used for testing a deep distance metric learning method.

For fault diagnosis in locomotive roller bearings, some authors proposed [27] Fuzzy c-means (FCM). Another paper proposed a deep neural network named CatAAE for unsupervised fault diagnosis of rolling bearings [28]. There are also studies that propose supervised learning for bearing defect classification [29]. In [30] authors proposed a nearest and farthest distance preserving projection (NFDPP) algorithm to explore the relationships of a sample with its farthest and nearest neighbours at validated in identifying compound faults in locomotive bearings.

Some other studies have applied the well-known k-Nearest Neighbour (KNN) method; in [31] it was proposed a method based on the Evidential KNN with applications in a power plant; there are also studies that applied KNN to a motor gears dataset [32]. Some other authors have applied PCA and Artificial Neural Networks (ANN) to rotation machines [33] but not with a visualization purpose. In other studies, extended PCA methods have been also proposed: WPD-PCA [34], FPCA [35], FDKPCA [36], and DWRPCA [37] for fault detection purposes but not from a visualization perspective.

Extensive fault diagnosis studies are found in the literature with bearings dataset; this kind of datasets are frequently used because of the importance of the failures in this devices. There are also other processes, machines, and devices that are important in the industry too and that may require to perform fault diagnostics.

All in all, most of the above-mentioned datasets are outdated and are not directly related with the machines found in an automotive factory. One of the main novelties of the present research is the analysis of a novel and real-life case study comprising two usual machines in the automotive industry. The failures affecting these machines are not related with motors or their bearings but with a different kind of problems. Furthermore, novel combinations for HUEPs are proposed, incorporating additional EPP techniques for the first time. This study proposes the use of HUEPs as a visual tool in order to analyse if the collected data from the installed sensors in different machines are correct and well selected. HUEPs greatly contribute to the monitoring of these machines, and consequently to taking decisions in order to anticipate to the associated failures.

The remaining sections of this study are structured as follows: Section 2 presents the techniques and methods that are applied to analyse the data. Section 3 details the real-life case study and the analysed machines, while results are presented and discussed in Section 4. Finally, Section 5 sets out the conclusions and proposals for future work.

2 Hybrid Unsupervised Exploratory Plots

In order to extract knowledge from unlabelled datasets, many different methods could be applied. Among all of the ML methods, projection techniques are considered a viable approach for information seeking, as humans are able to recognize different features and to detect anomalies by inspecting graphs. Such patterns may convert perceptible if variations are made to the spatial coordinates of original datasets. Though, an a priori choice to identify which parameters will reveal most patterns requires prior knowledge of unidentified patterns and this is not an easy task. In order to do that, Exploratory Projection Pursuit (EPP) [8] is used for this purpose of data visualization. Contrasted with feature selection, EPP belongs to the feature extraction paradigm, as the resulting dimensions are combinations (could be linear or non-linear) of the original features in the dataset. Contrarily, clustering [9] is concerned with grouping together objects that are similar to each other and dissimilar to objects belonging to other clusters. Therefore, patterns within the same cluster are more similar to each other than they are to a pattern belonging to a different cluster.

Recent work [7] has proposed the independent application of EPP techniques on the one hand and clustering ones on the other. Complete results of the two of them are then combined, together with the glyph metaphor, in a novel and different way, called Hybrid Unsupervised Exploratory Plot (HUEP). HUEPs are a general-purpose approach where any EPP and clustering techniques could be combined to generate 3D visualizations from high-dimensional data. In Figure 1 it is shown the process to generate a HUEP. These depictions are informative and intuitive not only for data scientists but for all the company staff (not requiring previous knowledge about ML). Once a proper HUEP configuration has been selected by an expert, the other company staff will only need to analyse the obtained visualization. The HUEPs can be used by 'non-expert' professionals due to their simplicity as no further decisions and parameter tuning is required. Proposed HUEPs are hybrid as they combine both exploratory (dimensionality reduction) techniques as well as clustering ones. Besides, both types of techniques are unsupervised as they apply this kind of learning (no target class or value is provided to be reproduced for new data instances).

In the original formulation of HUEPs [7], k-means [38] and Hierarchical Methods were applied as clustering techniques. Complementarily, PCA [39], MLHL [40] and CMLHL [41] were applied as EPP techniques. A wide variety of EPP techniques exists but before this study, only the three previously-mentioned ones have been applied under the frame of HUEPs. Each EPP technique project the data in a different way, thus for the same dataset the obtained visualizations could be very different. As it happens for most of the Data Analysis problems, there is not a technique that always get the best results for different datasets. Thus, depending on the analysed data, one HUEP that uses a certain EPP method may be more suitable than other one. In keeping with this idea, it is proposed in this study to extend HUEPs with other EPP techniques for a certain dataset. The main purpose is to validate that HUEPs can be extended with other EPP methods, and to prove that certain EPP methods could be more suitable than other ones when analysing the present dataset.

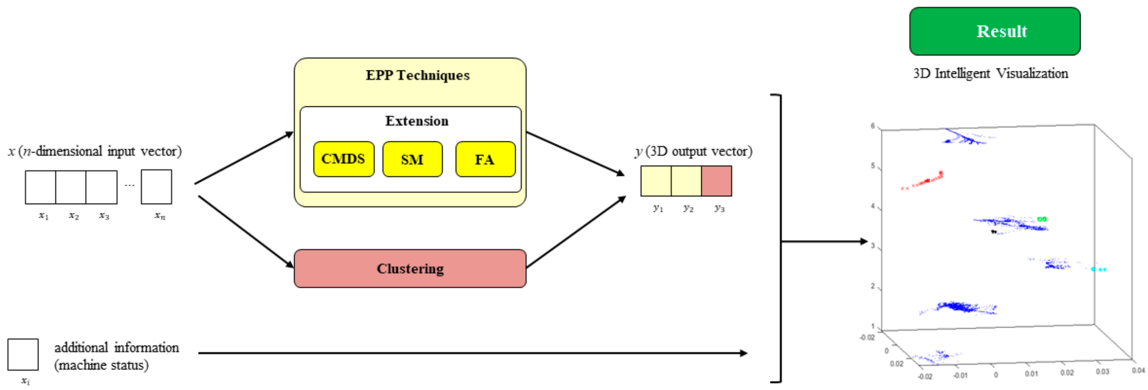


Figure 1. Process to obtain a HUEP.

The original HUEP formulation has been extended in the present study by incorporating and validating some additional EPP techniques, namely Classical Multidimensional Scaling (CMDS), Sammon Mapping (SM) and Factor Analysis (FA) – in yellow in Figure 1. They are described in the following subsections.

2.1. Classical Multidimensional Scaling

Multidimensional scaling (MDS) [42] is a set of methods that project high-dimensional data into a low-dimensional space using distances or dissimilarities. Classical MDS (CMDS) is a member MDS that shows the structure of distance-like data as a geometrical image [43]. Generally, MDS input is not a dataset but the similarities of a set of items instead. CMDS uses a single distance matrix of Euclidian type as input.

CMDS is also known as Principal Coordinates Analysis (PCoA) [44], Torgerson Scaling or Torgerson–Gower scaling. It is often used to visualize data when only their distances or dissimilarities are available but in this research, in order to extend and validate HUEPs with this family of methods, the original dataset has been reduced to a distance matrix. This matrix (pairwise distance between pairs of observations) creates a new configuration of points using the following metrics:

- Euclidean.
- Squared Euclidean.
- Standardized Euclidean (seuclidean): Each coordinate difference between observations is scaled by dividing by the corresponding element of the standard deviation.
- Cityblock.

- Minkowski.
- Chebyshev: maximum coordinate difference.
- Cosine: One minus the cosine of the included angle between points.
- Correlation: One minus the sample correlation between points.
- Hamming: which is the percentage of coordinates that differ.
- Jaccard: 'One minus the Jaccard coefficient, which is the percentage of non-zero coordinates that differ.
- Spearman: One minus the sample Spearman's rank correlation between observations.

2.2. Sammon Mapping

Sammon Mapping (SM) [45, 46] or Sammon Projection is a projection method for analysing multivariate data. It can be seen as a type of MDS method using a non-linear metric that is frequently used for EPP. SM maps a high-dimensional dataset to a lower dimensionality one conserving the intrinsic structure of the data when the patterns are projected.

Unlike standard PCA and other EPP techniques, SM is a non-linear approach as the result cannot be represented as a linear combination of the original variables. Nevertheless, SM minimise the differences between corresponding pairwise point distances in the two spaces. PCA applies the optimal mapping to the dataset, while SM tries to obtain a lower dimensional dataset that keeps the original structure as much as possible. Because of that, the SM algorithm has a high computational load O(n^2).

SM aims to minimize the following error function, which is often called as Sammon's stress or Sammon's error:

$$E = \frac{1}{\sum_{i<j} d^*_{ij}} \sum_{i<j}^{n} \frac{(d^*_{ij} - d_{ij})^2}{d^*_{ij}} \tag{1}$$

Where the source dataset are N vectors in L-dimensional space, given by X_i, $i = 1, \ldots, N$. It seeks to map these into d-dimensional space (with $d < L$), to give vectors Y_i, $i = 1, \ldots, N$; d_{ij} is the pairwise distance between Y_i and Y_j , and similarly d_{ij} for the distance between X_i and X_j:

As originally suggested [45], the minimization could be achieved by gradient searching techniques or by other methods, but frequently involving iterative procedures. Convergent results are not always reached and the number of iterations are decided experimentally [47].

2.3. Factor Analysis (FA)

Factor Analysis [48, 49] is a data analysis technique that could be used for dimensionality reduction. It is used to reduce a large number of variables into a smaller set of factors, where factors means the lower number of unobserved or underlying variables. FA objective is to discover independent latent variables. It is frequently used with datasets with a big number of observed variables that could reveal a smaller number of underlying variables.

FA differentiate from PCA as the former enforces a strict structure of a fixed number of common (latent) factors while the latter defines p factors in decreasing order of importance. The main factor in FA is the one that, after rotation, provides the maximal interpretation while the most significant factor in PCA is the one that maximises the variance. Frequently, the main factor in FA is different from the direction of the first principal component. PCA extracts factors based on the total variance of the factors but FA extracts factors based on the variance shared by the factors. PCA is used to find the fewest number of variables that explain the most variance, while FA is used to look for the latent underlying factors.

3 A Real Case Study: Waterjet Cutting

As previously stated, in order to validate the proposed HUEP extension, it has been applied to a case study involving a waterjet industrial tool. As a result, two datasets have been generated by collecting data from two different machines. HUEPs are generated in order to analyse these datasets, which comprise a great number of samples with a high number of features.

The machines under study are located in one factory from Grupo Antolin [10], a multinational company from the automotive industrial sector.

Waterjet cutting is used in various manufacturing industries (such as aerospace and automotive ones) for cutting, shaping, etc. [50]. This tool is used to cut several kinds of materials by means of an extremely high pressure jet of water, or a mixture of water and an abrasive substance. In the present work, the waterjet uses only water and is applied during the fabrication of some parts manufactured in the factory. Two of its independent components have been selected for analysis due to their critical role:

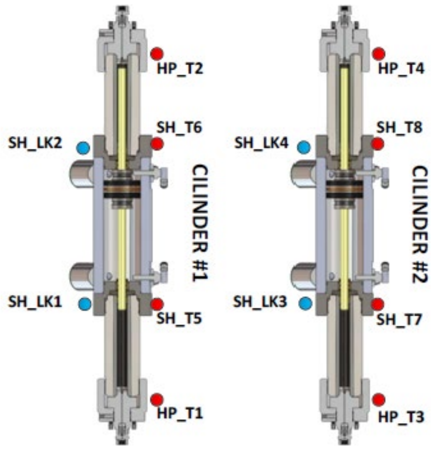
- Intensifier: the waterjet pumps or intensifiers [51] that supply water at extremely high pressure to waterjet machines.
- Cyclone: the vacuum cyclone unit located in a waterjet machine used for suctioning the waste generated towards a chute. It also holds the pieces during the cut.

To do this analysis, a time interval (February 2020) has been selected among all the available data as it includes samples of different anomalies/failures. As a consequence of the maintenance operations that are carried out, there are no anomalies most of the time and it is not easy to find a period containing examples of some different anomalies.

3.1. Intensifier

The function of a water pump or intensifier (Figure 2) is to raise the water pressure to the level needed in the waterjet machines for an optimal operation. Explained in a very simple manner, the intensifier works like this: it begins when the low pressure water enters in the intensifier (3-5 bar), after several filters the water reaches a pump that raises the pressure to 10 bar, then the water flows to the cylinders that will be compressed by a hydraulic group that using plunger/piston system will be able to reach an extremely high pressure (around 3000 bar) The intensifiers under study have two cylinders, as can be seen in Figure 2.

(a) Picture of the intensifier



(b) Sensors placement sketch

Figure 2. Example of intensifier and sketch of sensors (blue and red circles).

According to the experience of the workers in the plant, it is known that before a failure happens, an increase in temperature in different zones of the cylinder is observed. Another problem directly related with the increase of temperature is the water leaking, that is caused by the deterioration of the cylinder and that can be visually observed. As this could lead to a critical failure, specific sensors have been installed in order to measure the temperature in the seal head (SH) and the hydraulic piston (HP) of the intensifier. Additionally, leak sensors have been installed in each cylinder. With the installation of these sensors, as shown in Figure 2, a diagnosis of the status of the machine could be performed in order to prevent failures.

The dataset analysed in this research comprises 7,414 samples (from February 2020) and 36 parameters (features) described in Table 1, which were gathered every 5 minutes (except for the increase of water leak).

Table 1. Intensifier features. Variables gathered from each cylinder, SH and HP. XX in the feature name refers to the number of each sensor.

Feature Name	Description	Unit
HPXXTemp_oC_avg	HP average temperature	ºC
HPXXTemp_oC_max	HP maximum temperature	ºC
HPXXTemp_oC_min	HP minimum temperature	ºC
HPXXTemp_oC_std	HP standard deviation temperature	ºC
SHXXTemp_oC_avg	SH average temperature	ºC
SHXXTemp_oC_max	SH maximum temperature	ºC
SHXXTemp_oC_min	SH minimum temperature	ºC
SHXXTemp_oC_std	SH standard deviation temperature	ºC
SHXXLeak_mLm	SH increase leak of water since last period	1,5 ml / increase

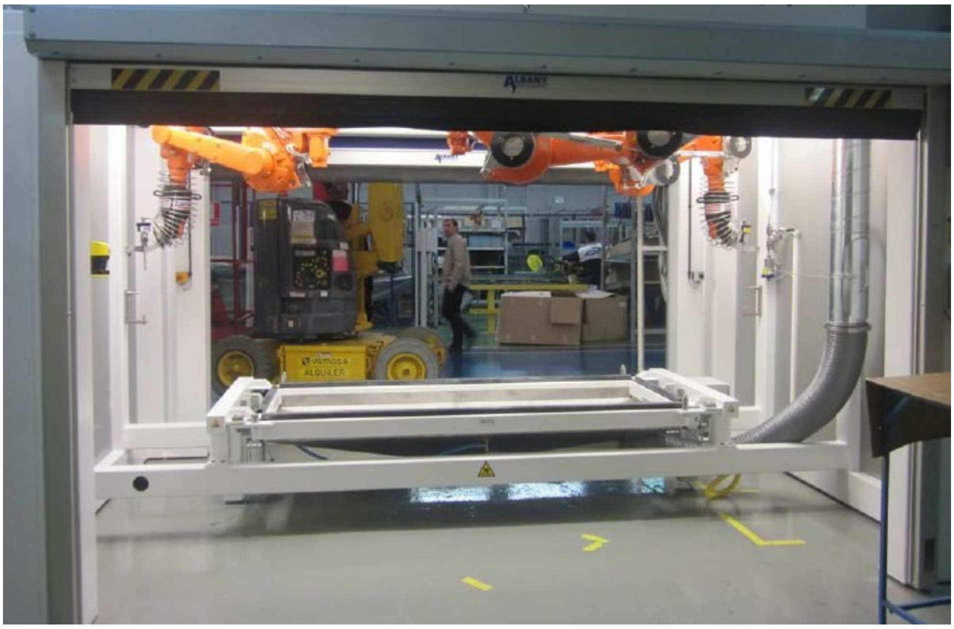
As the intensifier has two cylinders and each cylinder has two SH and two HP, the total features are 36: 4 temperature features per SH, 4 temperature features per HP, and 1 feature per SH for the leak problem. There is a temperature sensor per SH and HP and a leak sensor per SH. As the features are recorded for a given time period, the maximum, minimum, average, and standard deviation statistics are calculated during this period and stored. In the case of the leak sensor, the increment when compared to the previous period is stored.

There are 3 main problems or failures that affect the intensifier:

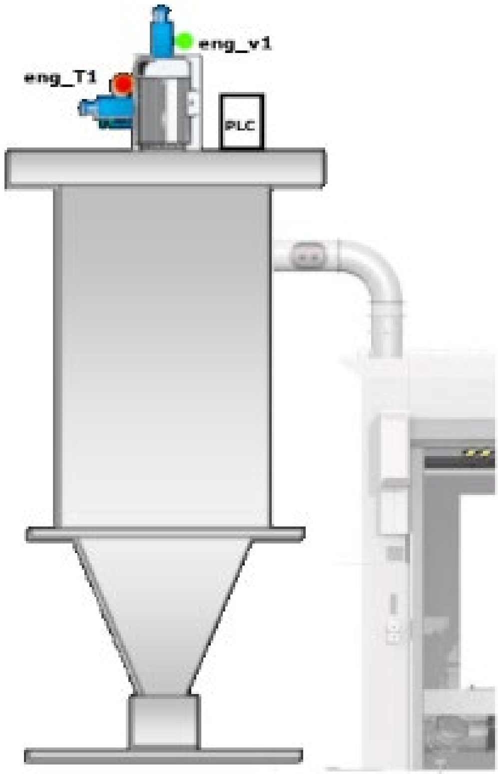
- Water leaks: the intensifier will stop working if there is a severe water leak. This is a critical failure with high associated costs as it stops production.
- High temperature in a cylinder: if high temperature lasts in time, it could lead to a break in the header.
- Detected SH malfunction: it means that it is necessary to repair the SH or otherwise, it will crash and stop the production. This malfunction/problem is perceived by the maintenance staff.

3.2. Cyclone

This is the normal process when manufacturing a piece in the waterjet machine: the worker places a part inside the machine and gives the start order, the cut operation is performed in a continuous way during the cycle. The water pressure generated by the intensifier reaches the level required by the robots in the waterjet for doing the complete cut of the piece. By means of a vacuum system, both the excess water and the cutting leftovers from the work are drained through a vacuum cyclone unit.



(a) Waterjet machine



(b) Sensors placement sketch.

Figure 3. Example of a waterjet machine with the cyclone and sketch of sensors (red and green circles).

Cyclone failures are usually related to the vacuum system that the cyclone motor itself runs. This suction is responsible for tying the piece to be cut in addition to absorbing the remains of water and cuttings leftovers of the piece. The generated waste from the waterjet is suctioned towards a garbage chute. The most representative failures in this area are usually related to blockages in the suction circuit and air outlets and vacuum malfunctioning. The data stored for detecting failures are related to the cyclone engine that are obtained from the PLC. Additionally, vibration and temperature sensors have been installed in this motor in order to obtain more information about its status.

The dataset for this component comprises 623 samples (February 2020) and 24 parameters (features) described in Table 2, gathered for each manufacturing cycle.

Table 2. Cyclone features. Variables gathered per manufacturing cycle.

Feature Name	Description	Unit
AccPeak_g_avg	Engine vibration average	G
AccPeak_g_max	Engine vibration maximum	G
AccPeak_g_min	Engine vibration minimum	G
AccPeak_g_std	Engine vibration standard deviation	G
CmdDutyEngineSpeed_Hz	Fan RPM setpoint	Hz
CmdRestEngineSpeed_percent	% RPM idle setpoint	%
CmdVacuumPressure_mBar	Vacuum pressure setpoint	mBar
EngineTemp_oC_avg	Engine temperature average	ºC
EngineTemp_oC_max	Engine temperature maximum	ºC
EngineTemp_oC_min	Engine temperature minimum	ºC
EngineTemp_oC_std	Engine temperature standard deviation	ºC
FanSpeed_Hz_avg	Fan speed average	Hz
FanSpeed_Hz_max	Fan speed maximum	Hz
FanSpeed_Hz_min	Fan speed minimum	Hz
FanSpeed_Hz_std	Fan speed standard deviation	Hz
VacuumPressure1_mBar_avg	Vacuum pressure sensor1 average	mBar
VacuumPressure1_mBar_max	Vacuum pressure sensor1 maximum	mBar
VacuumPressure1_mBar_min	Vacuum pressure sensor1 minimum	mBar
VacuumPressure1_mBar_std	Vacuum pressure sensor1 standard deviation	mBar
VacuumPressure2_mBar_avg	Vacuum pressure sensor2 average	mBar
VacuumPressure2_mBar_max	Vacuum pressure sensor2 maximum	mBar
VacuumPressure2_mBar_min	Vacuum pressure sensor2 minimum	mBar
VacuumPressure2_mBar_std	Vacuum pressure sensor2 standard deviation	mBar
Duration	Cycle time for part production	ms

Features are obtained from the machine PLC and from the device installed for detecting vibrations on the engine and the temperature sensor. Data are stored in the cloud for each production cycle, whose duration varies depending on the part that is being produce. The maximum, minimum, average, and standard deviation statistics are calculated during the period and stored.

There are two main problems or failures that affect the cyclone:

- Suction circuit is blocked: the waste absorbing system does not work properly. This is a critical failure as it stops production.
- Vacuum malfunctioning: the vacuum does not work properly. It is an infrequent failure that does not stop production but could lead to defective parts.

4 Results

The above-introduced HUEPs (see Section 2) have been applied to the real-world case study datasets described in previous section. Plenty of different visualizations have been generated by combining all the EPP (PCA, MLHL, CMLHL, CMDS, SM, and FA) together with the clustering (*k*-means and agglomerative) techniques, tuned with different parameter values. However, for the sake of brevity, in this section only the main results are presented for comparison purposes. As no quantitative indicators have been developed yet to compare the level of goodness in a certain visualization, obtained results are compared taking into account one main criterion: whether the visualization let users identify the anomalies by depicting them isolated from the other ("normal") data samples. That is, "similar" data samples are visualized as groups separated from "dissimilar" data samples.

Different values were tested during experimentation for each one of the parameters associated to the applied models:

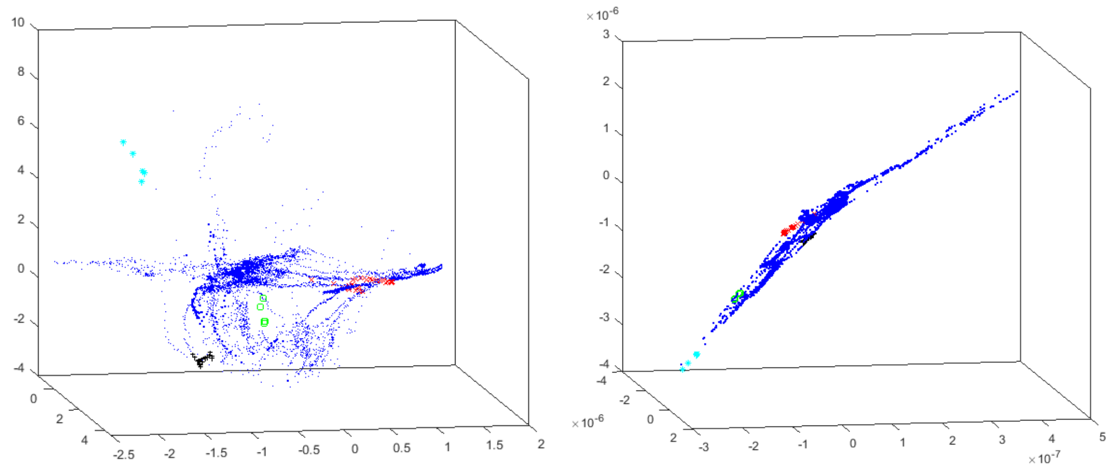
- PCA: number of output dimensions: 2/3.
- MLHL: number of output dimensions: 2/3; number of iterations: 1000/2000/3000; learning rate: 0.01/0.005/0.001; p: 0.1/0.5.
- CMLHL: number of output dimensions: 2/3; number of iterations: 1000/2000/3000; learning rate: 0.01/0.005/0.001; p: 0.1/0.5; τ: 0.05.
- CMDS: number of output dimensions: 2/3; distance metrics: Euclidean / Squared Euclidean / Standardized Euclidean / Cityblock / Minkowski / Chebyshev / Cosine / Correlation / Jaccard / Spearman.
- SM: number of output dimensions: 2/3; number of iterations: 100/200/500.
- FA: number of output dimensions: 2/3; 200 iterations maximum.
- *k*-means: distances: Squared Euclidean / Cityblock /Cosine / Correlation; *k*: 3/4/6/8.
- Agglomerative clustering: distances: Euclidean / Chebyshev / Minkowski / Correlation / Seuclidean / Squared Euclidean / Cityblock / Mahalanobis / Cosine / Spearman / Hamming / Jaccard; linkages: average / centroid / complete / median / single / ward / weighted; a cutoff value adjusted to obtain the same number of clusters as in the case of *k*-means (3/4/6/8).

4.1 Intensifiers Results

Results shown in this section include visualizations of all the data samples in the intensifier dataset. Each one of them is depicted by adding the following extra information (related to the machine status) through the glyph metaphor:

- x (red x): water leak.
- + (black +): high temperature in cylinder #1.
- * (cyan *): high temperature in cylinder #2.
- o (green o): detected SH malfunctioning.
- • (blue point): no problem reported (i.e. intensifier properly working).

Initially, the two best EPP 3D projections (CMLHL and FA) are shown in Figure 4. These simple visualizations (the right-straight output of the EPP methods) are shown for comparison purposes in order to contrast them with the obtained HUEP visualizations (see below).

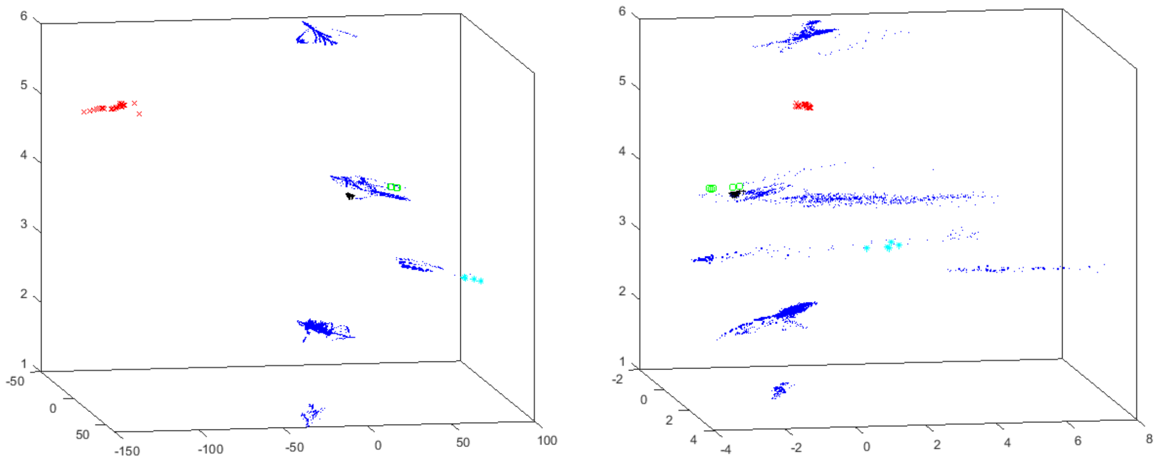


(a) CMLH 3D visualization (b) FA 3D visualization

Figure 4. 3D visualizations generated by the EPP methods on the intensifier dataset.

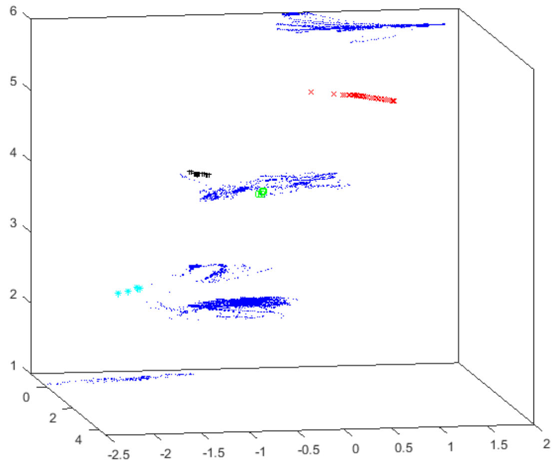
It can be observed that CMLHL (Figure 4.a) does not show the principal failure (red x) separated from the other data instances and that FA (Figure 4.b) does not show any data grouping and all samples are mixed. However, in the FA projection some of the anomalies are somehow grouped but not isolated from the other ones.

The best results generated by the HUEPs are presented in Figure 5. Each figure shows the result obtained by the corresponding HUEP as stated in the label; i.e. the combination of the EPP method-for example (a) PCA-, with the hierarchical clustering method tuned according to the given parameter values -for example (a) 6 clusters (k parameter) using Cityblock as distance metric and Complete as linkage method. In all HUEP figures, the cluster number assigned to each data instance is shown in the vertical (z) axis. For example, in Figure 5 as all the results are associated to 6 clusters, so values 1 to 6 are shown in the z axis of all the HUEPs.

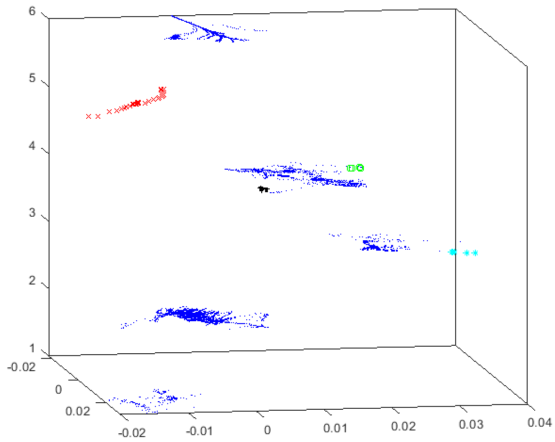


(a) HUEP: PCA + hierarchical clustering (*k*=6,Cityblock, and complete)

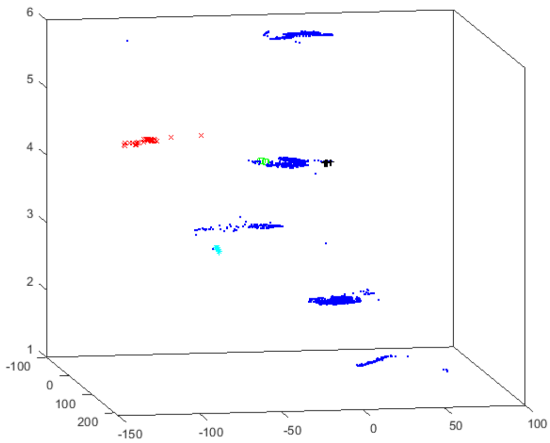
(b) HUEP: MLHL + hierarchical clustering (*k*=6, Cityblock, and complete)



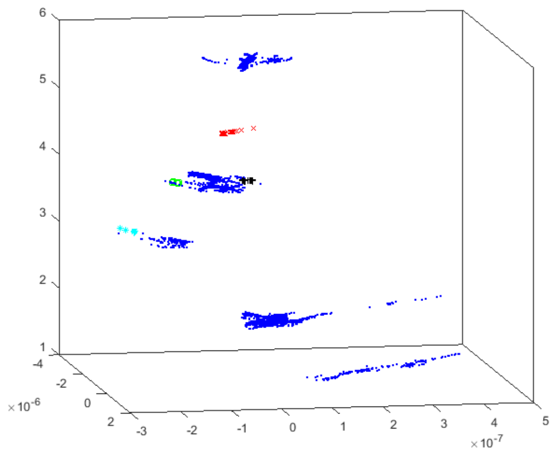
(c) HUEP: CMLHL+ hierarchical clustering (*k*=6, Cityblock, and complete)



(d) HUEP: CMDS - cityblock+ hierarchical clustering (*k*=6, Cityblock, and complete)



(f) HUEP: SM+ hierarchical clustering (*k*=6, Cityblock, and complete)



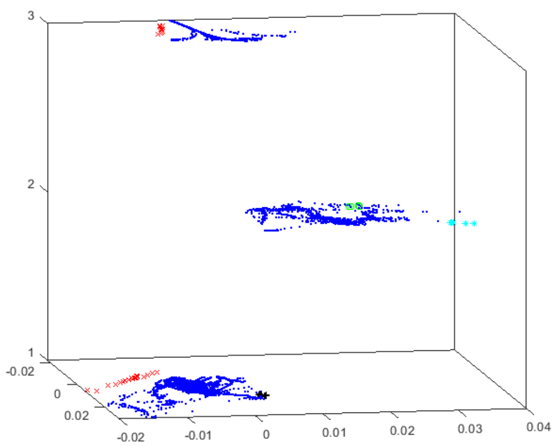
(g) HUEP: FA+ hierarchical clustering (*k*=6, Cityblock, and complete)

Figure 4. HUEP visualizations on the intensifier dataset. EPP + hierarchical clustering.

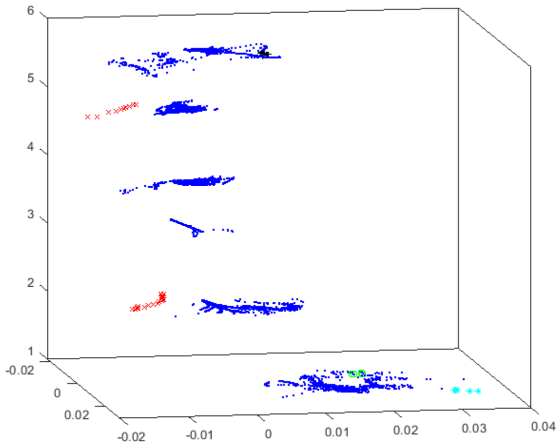
Regarding the results obtained with the extended HUEPs, it can be said that adding the clustering information to the EPP projection leads to a significant improvement in the visualization. This can be clearly seen in the case of the main failure (red x) as all these data samples are assigned to the same cluster (number 5) and hence isolated from the other ones.

When comparing the applied EPP methods, CMDS (Figure 5.d and Figure 6.e) outperforms the other ones as in this projection it can be observed that all the data samples associated to failures or problems are separated from the "normal" points (in blue). All in all, it can be concluded that the three novel EPP techniques (CMDS, SM, and FA), when combined with a clustering technique in a HUEP, bring more information than the EPP projection on its own. If the FA projection (Figure 4.b) is compared to the HUEP obtained from FA and hierarchical clustering -k=6, Cityblock, and complete- (Figure 5.g) it can be said that the visualization is much more informative.

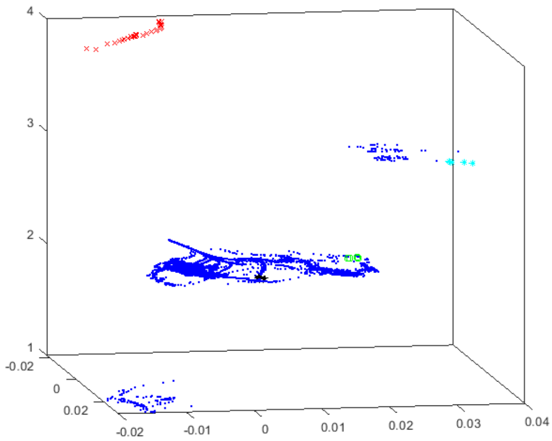
As CMDS is the EPP method generating the best HUEP for this dataset, additional results obtained with this method are shown in Figure 6. The main purpose of this figure is to compare the visualizations generated when varying clustering parameters.



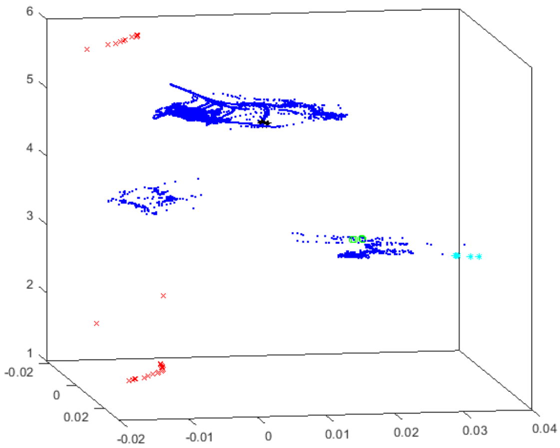
(a) HUEP: CMDS – Cityblock + *k*-means (*k*=3 and Cityblock)



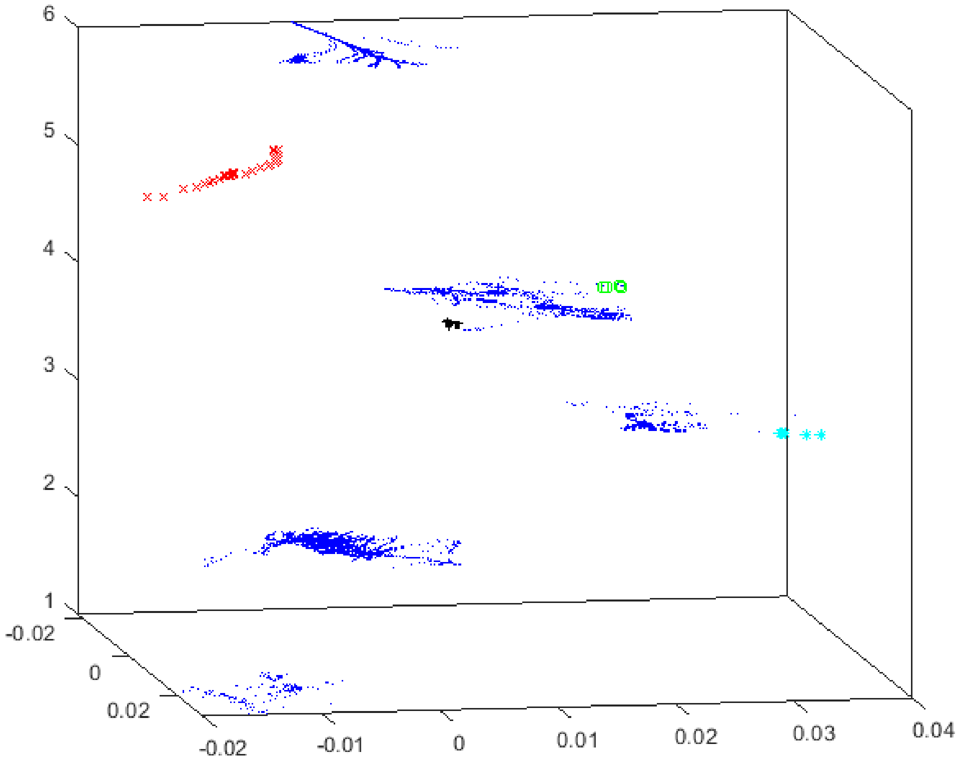
(b) HUEP: CMDS – Cityblock + *k*-means (*k*=6 and Cityblock)



(c) HUEP: CMDS – Cityblock + hierarchical clustering (*k*=4, Minkowski, and weighted)



(d) HUEP: CMDS – Cityblock + hierarchical clustering (*k*=6, Chebyshev, and complete)



(e) HUEP: CMDS – Cityblock + hierarchical clustering (*k*=6, Cityblock, and complete)

Figure 5. HUEP visualizations generated by CMDS – Cityblock and different clustering parameters on the intensifier dataset.

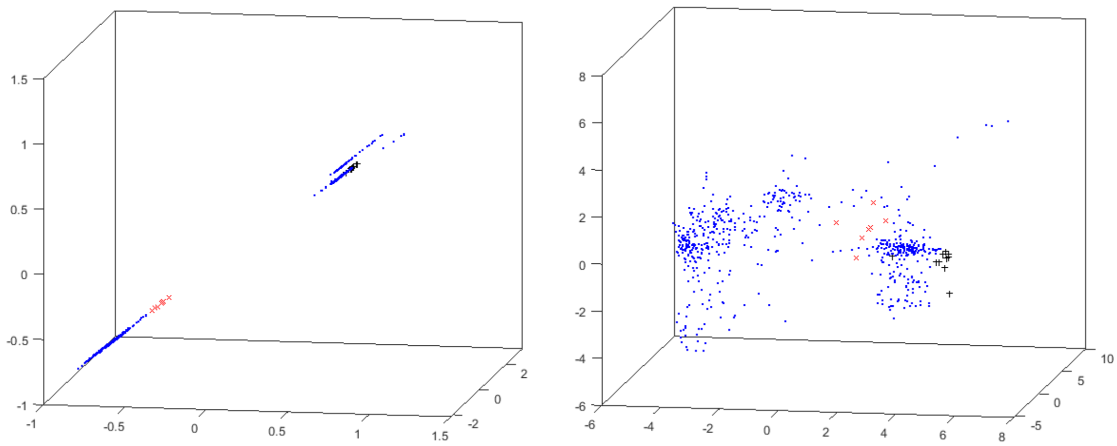
In Figure 6, the same CMDS – Cityblock projection is combined with k-means and hierarchical clustering outputs. As it can be seen, the hierarchical clustering can separate in independent groups the critical-failure data (red x). Oppositely, k-means does not separate this critical samples in a unique group, splitting these data in two different groups. When increasing the number of clusters (k), data are more separated and hence visualizations are more informative. It can be said that hierarchical clustering is the one generating better visualizations when combined with CMDS in a HUEP for the intensifier dataset. More precisely, Figure 6.e presents the best one of the HUEP visualizations generated on this dataset.

4.2. Cyclone Results

Results shown in this section include visualizations of all the data samples in the Cyclone dataset. Each one of them is depicted by adding the following extra information (related to the machine status) through the glyph metaphor:

- x (red x): suction circuit is blocked.
- + (black +): vacuum malfunctioning.
- • (blue point): no problem reported (i.e. cyclone properly working).

As for the previous dataset, the best EPP visualizations are shown in Figure 7. In this case, the selected ones are the CMLHL (Figure 7.a) and CMDS (Figure 7.b) projections.

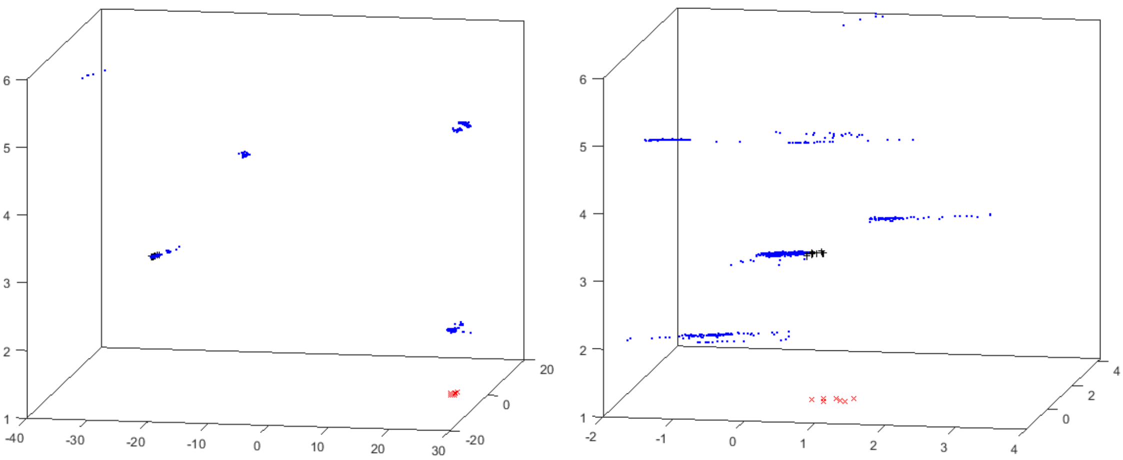


(a) CMLHL 3D visualization

(b) CMDS – Seuclidean 3D visualization

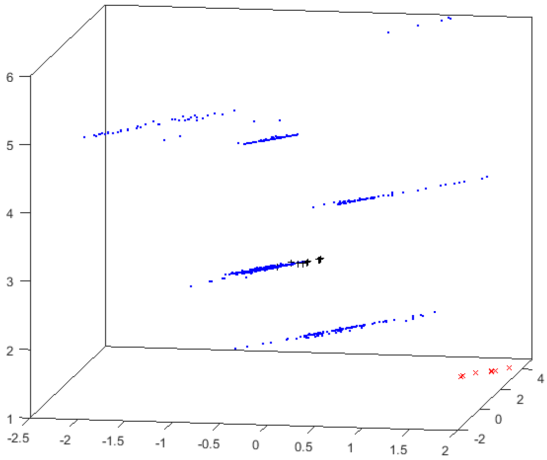
Figure 6. 3D visualizations generated by EPP methods on the cyclone dataset.

It can be observed that none of the EPP techniques generates a visualization clearly separating the data samples associated to anomalies. These projections are significantly enhanced when combined with clustering results in HUEPs, as shown in Figure 8.

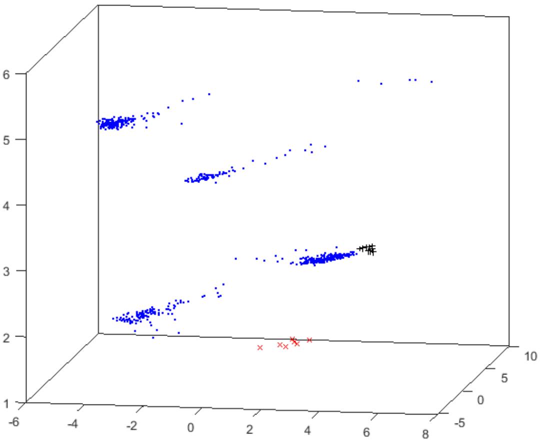


(a) HUEP: PCA + hierarchical clustering (*k*=6, Cityblock, and weighted)

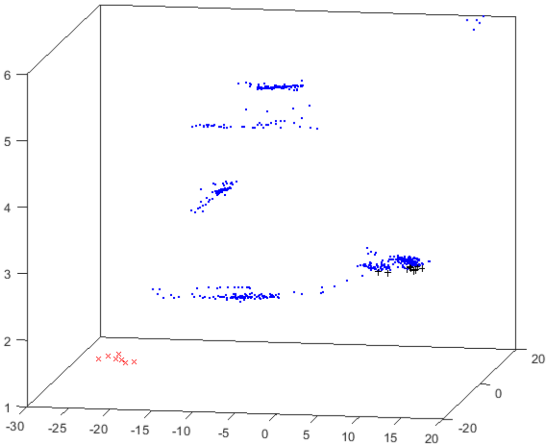
(b) HUEP: MLHL + hierarchical clustering (*k*=6, Cityblock, and weighted)



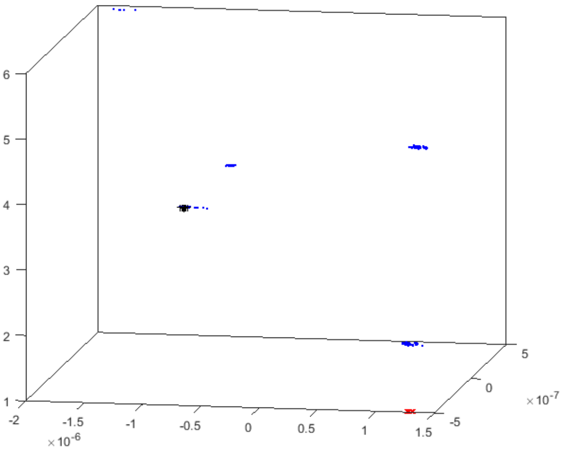
(c) HUEP: CMLHL + hierarchical clustering (*k*=6, Cityblock, and weighted)



(d) HUEP: CMDS – Seuclidean + hierarchical clustering (*k*=6, Cityblock, and weighted)



(e) HUEP: SM + hierarchical clustering (*k*=6, Cityblock, and weighted)

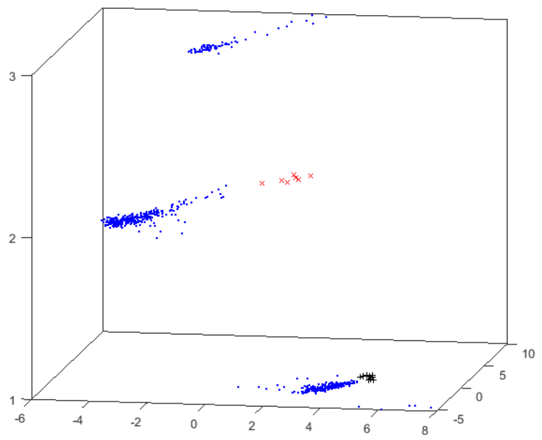


(f) HUEP: FA + hierarchical clustering (*k*=6, Cityblock, and weighted)

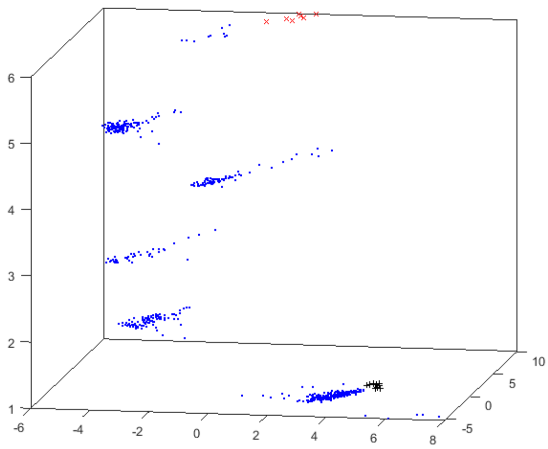
Figure 7. HUEP visualizations on the cyclone dataset. EPP + hierarchical.

As it has been shown for the previous dataset, it is worth mentioning that CMDS generates the best HUEPs for the cyclone dataset. The best result is obtained with CMDS Seuclidean + hierarchical clustering (k=6, Cityblock, and weighted), shown in Figure 8.d and Figure 9.c. In these visualizations, the critical failure (Suction circuit is blocked) samples (red x) are isolated in a unique group, as well as those samples associated to the other anomaly (black +), which are also depicted in a separated group. HUEPs generated on this dataset can clearly visualize the critical failure in a separate group. This is done thanks to the combination with clustering results; the samples associated to the main failure are grouped in the same cluster, clearly visualizing them in a separate group. Although the samples from the other anomaly (Vacuum malfunctioning) are clustered with many "normal" samples, the CMDS projection visualizes them in a separate way.

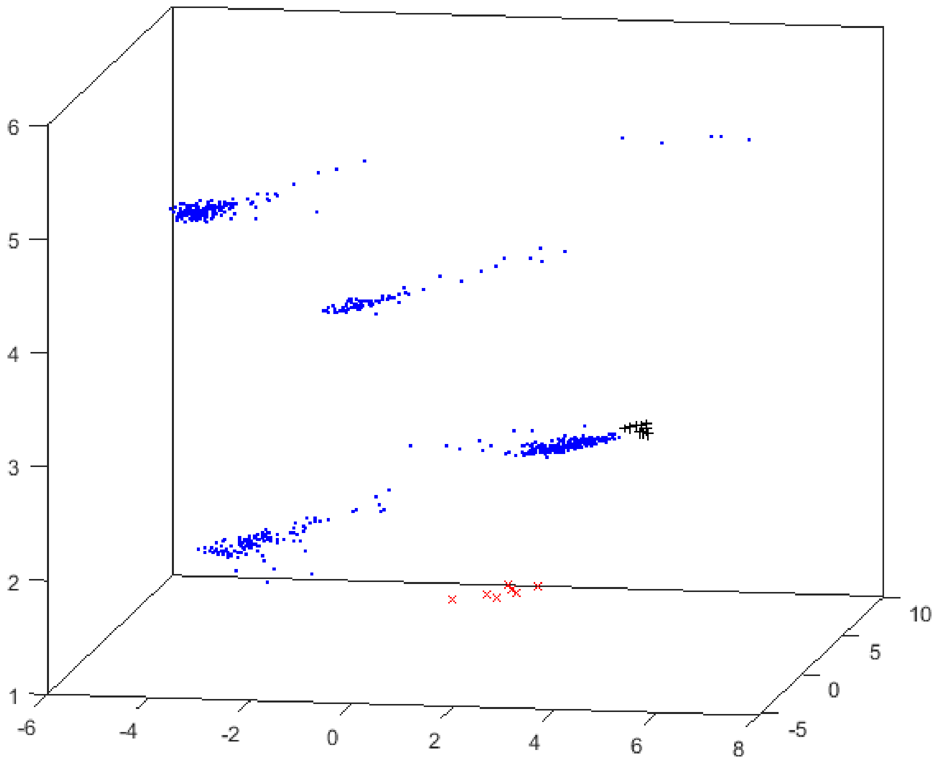
Once again CMDS is the EPP method generating the best HUEP and additional results obtained with this method are shown in Figure 9. The main purpose of this figure is to compare the visualizations generated when varying clustering parameters.



(a) HUEP: CMDS – Seuclidean + *k*-means (*k*=3 and Correlation)



(b) HUEP: CMDS – Seuclidean + *k*-means (*k*=6 and Correlation)



(c) HUEP: CMDS – Seuclidean + hierarchical clustering (*k*=6, Cityblock, and weighted)

Figure 8. HUEP visualizations generated by CMDS – Seuclidean and different clustering parameters on the cyclone dataset.

Figure 9 shows the results obtained by combining CMDS - Seuclidean with k-means and hierarchical clustering. The hierarchical clustering method can separate in cluster #1 the critical-failure samples (red x), but k-means groups these data together with "normal" samples. So, it can be said that, as in the case of the previous dataset, hierarchical clustering leads to better visualization results for the cyclone dataset.

In general terms, the HUEPs generated by agglomerative (hierarchical) clustering are more informative than those generated by k-means for the two datasets under analysis.

This is consistent with general heuristics [52], as agglomerative clustering is more appropriate if groups are expected to have different size. Oppositely, k-means is the best option when the expected groups have approximately similar size. In the two analysed datasets, there are many more data samples associated to the "normal" functioning of the components than those associated to failures. Consequently, HUEPs visualizations would be better using agglomerative clustering rather than k-means. The validation carried out with both datasets have shown that HUEPs generated by CMDS are the most useful ones, as they provide visualizations separating failures from "normal" samples in the clearest way.

5 Conclusions and Future Work

This study has shown that HUEPs are a technique that supports the monitoring of sensors and machines in order to anticipate to failures. Firstly, it can be used to visually and easily see that the data that has been gathered have a structure and that they could be representative and informative. Then, HUEPs can show separate groups differentiating failures from normal functioning. The proposed HUEP extension supports decision making as it depicts data in a visual way that assists on this task. This has been tested and validated in a complex industrial scenario with associated datasets comprising a great number of samples and a high number of features. As a result, PdM can be carried out in a complementary way to other tools, anticipating to deviations in operating conditions.

It has been proved that the proposed extension of HUEPs outperforms the original formulation when visualizing the datasets from the present case study. It is worth mentioning that HUEPs generated by CMDS are more useful than the other ones as the different anomalies are grouped and visualised in a clearer way. Additionally, CMDS is an interesting EPP technique because it can be applied with several distance metrics that adjust to the dataset under study. On the other hand, for the analysed datasets (where the "normal" samples are many more than the failure ones), agglomerative clustering groups data in a more consistent way than k-means.

It has been proved that, depending on the dataset, it could be better to use a combination of methods to generate a HUEP or another one. That is, the best visualizations for the intensifier are not generated with the same parameter combination than those for the cyclone dataset. Hence, it is important to carry out an exhaustive experimentation with every different combinations in order to identify the best visualization. Once it is performed, any person familiar with the manufacturing process (such as skilled operators and maintenance staff among others) would be qualified to analyse the visualization obtained and take decisions based on them.

As a future line of work, authors propose to combine HUEPs with the outputs of supervised models in order to implement a holistic tool. Furthermore, it is proposed a tool that generates specific visualizations for machine operators and maintenance staff. This would help them in supervising the manufacturing and aiding in the machine maintenance. Additionally, HUEPs are being applied to some other components/machines to validate their ability for operation monitoring and failure detection. The use of HUEPs for quality purposes will also be explored, in order to improve the detection of quality defects.

Author Contributions

Conceptualization, A.H., E.C. and J.S.; methodology, A.H.; software, R.R.; formal analysis, R.R. and A.H.; data curation R.R.; writing—original draft preparation, R.R. and A.H.; writing—review and editing, R.R., A.H., E.C. and J.S.; supervision, A.H., E.C. and J.S. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest

The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript, in alphabetic order:

ANN	Artificial Neural Networks
CMDS	Classical Multidimensional Scaling
CMLHL	Cooperative Maximum-Likelihood Hebbian Learning
EPP	Exploratory Projection Pursuit
FA	Factor Analysis
FD	Failure Detection
HP	Hydraulic Piston
HUEP	Hybrid Unsupervised Exploratory Plot
IoT	Internet of Things
KNN	k-Nearest Neighbour
MDS	Multidimensional scaling
ML	Machine Learning
MLHL	Maximum-Likelihood Hebbian Learning
PCA	Principal Component Analysis

PdM	Predictive Maintenance
SH	Seal Head
SM	Sammon Mapping

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