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Sumit Patil

Sathiskumar Ponnusami

Ahmed Kovacevic

Neeraj Asati

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Sumit Patil[1*], Sathiskumar Ponnusami[2], Ahmed Kovacevic[3], Neeraj Asati [4]

[1] Doctoral Student, Centre for Compressor Technology,
City, University of London, UK
Email: sumit.patil@city.ac.uk

[2] Lecturer in Structural Mechanics (Aeronautics),
City, University of London, UK
Email: sathiskumar.ponnusami@city.ac.uk

[4] Professor, Howden/RAEng Chair in Compressor Technology,
City, University of London, UK
Email: a.kovacevic@city.ac.uk

[5] Head of Design & Development,
Kirloskar Pneumatic Company Ltd.,Pune, India
Email: neeraj.asati@kirloskar.com

* Corresponding Author

ABSTRACT

Artificial Neural Networks (ANN) are emerging as promising tools for advancements in state of the art design and optimization techniques. Twin screw compressor technology is matured in all aspects of design and manufacturing. But the potential application of Artificial Intelligence (AI) or Machine Learning (ML) has not yet been explored in this domain. This paper attempts at training an ANN, which is a class of AI/ML techniques, to predict the energy efficiencies of twin screw compressors for different rotor profile shapes. The N profile by N. R. Stosic (1997) is chosen as the profile system to generate multiple retrofitted profiles by varying only five curve parameters. Generally, the energy efficiency of a screw compressor with a certain rotor profile is calculated by solving the chamber model which is a thermodynamic simulation of the compression process. The objective of this study is to check if an ANN can be successfully trained with large enough data of different profiles and their respective energy efficiencies to capture the physics of the compression process and predict the energy efficiencies for given profiles with reasonable accuracy. It has been found that the ANN is able to learn the pattern associated with profile shapes and their energy efficiency to a fair degree. But increasingly large data-sets are required for training the ANN to achieve a higher accuracy of prediction. This work stands as a pilot study to explore further possibilities for use of these techniques in rotor profiling and/or screw compressor design and optimization.

1. INTRODUCTION

Twin screw compressor rotor profiles influence the energy efficiency and reliability of these machines to a large extent. Rotor profiles for twin screw compressors have evolved over the years along with the advances in the helical rotor manufacturing technology. This evolution has led to energy efficient and reliable modern twin screw compressors. But the rising concerns over carbon emissions and a highly competitive market demand for even more energy efficient machines. Hence research efforts are directed at exploring new techniques that may lead to further advancements in the state of the art screw compressor technology, rotor profiling being an essential element of it.

Artificial Intelligence (AI) and Machine Learning (ML) have been successfully applied to solve several engineering problems. Artificial Neural Networks (ANN) are a class of these techniques with a potential to be useful in screw compressor design and optimization. Neural networks are capable of learning from data to identify complex or non-linear underlying patterns between inputs and outputs arising from the physics of the process. Such a capability can be useful in many ways such as- designing robust design and optimization frameworks, automating parts of the design process flows and getting deeper insights into the physics of compression process.

A rotor profile is a system of particular mathematical curves serving a purpose to define the geometry or shape of a screw rotor. As put very aptly by Edstrom (1992)- “rotor profiles are some kind of ‘recipe’, wherein lines, points and mathematical curves serve as ‘ingredients’ which are mixed in suitable proportions”. Even in the domain of a specific profile system such as N-profile (N. R. Stosic, 1997) (N. Stosic & Hanjalic, 1997) or SRM-D profile (Astberg, 1984), a wide range of rotor shapes can be generated by varying individual constituent curve parameters. The definitions of each curve with associated curve parameters (radii, angles, eccentricity, lengths, etc.) form a set of input values that fully determine the profile shape. The performance of these profiles can be evaluated by a detailed thermodynamic simulation of the compression process (Hanjalic & Stosic, 1997) with rotors having the defined profile. The SCORPATH thermodynamic solver (N. Stosic, 2005) was used in this study to calculate the effect of different profile shapes on specific power which is a measure of compressor’s energy efficiency. It is one of the quickest and versatile chamber models, hence used to most effectively generate vast data-sets required for the training of ANN.

This paper attempts to train an ANN on the generated SCORPATH data which has profiles as inputs and their specific powers as output. The objective is to evaluate if the ANN can learn the associations between inputs and output to predict the specific powers for unseen profiles (test-data) with a reasonable accuracy. It is found that The trained ANN is capable of predicting the energy efficiency of unseen rotor profiles with more than 99% accuracy if trained with a large enough data-set. It indicates that the learning in the domain of rotor profiling is possible. Still there are some limitations of the proposed approach which are also discussed.

The paper starts by outlining the objective and methodology adopted to train a neural network to predict the energy efficiency of rotor profile based on the profile input parameters. The neural network framework is then explained in detail starting with the data generation, training algorithm and testing of the model. The accuracy of the trained model w.r.t. the chamber model is presented in the results section. The paper ends with a conclusion and discussion of the limitations as well as further scope for application of AI/ML techniques in screw compressor rotor profiling.

2. OUTLINE

Machine learning algorithms and their application is a vast topic on its own. Setting up a neural network (NN) for certain task has 3 steps- data generation, training and testing. Choice of a right training algorithm, choosing just the right size of the data-set for training, fine-tuning of the model itself, etc require an in depth technical attention and analysis. For the purpose of this pilot study, the most commonly used NN training algorithm and training model parameters were chosen from literature. A comprehensive analysis of the nuances of NN training and their effect on performance of NN is out of the scope of this paper.

The objective of this study is to train a NN to predict the energy efficiency of a rotor profile based on the profile input parameters. The profile input parameters in this case are 4 radii- *R1, R2, R3* & *R4* and a polynomial exponent- n necessary to define a complete N-Profile (N. R. Stosic, 1997) for a rotor pair with fixed lobe combination, centre distance as well as main and gate rotor addendum. The 3-D characteristics of rotors such as length, wrap angle and other design parameters such as port positions are also not varied. For the purpose of thermodynamic evaluation of a screw compressor, additional inputs are required such as speed of the rotors, pressure ratio, inlet temperature, oil injection parameters, etc. These inputs too are kept constant for all the profiles. Hence this NN is tasked to predict the energy efficiency for different screw compressor rotors with no change except their rotor profile shape in the end plane. Figure 1 depicts an example of different profile shapes generated in end plane of rotors with same inner and outer diameters as well as rest of the design and operational parameters. Such are the different profiles for which the NN needs to predict the energy efficiencies.

As specified earlier, the energy efficiency of a screw compressor is expressed as specific power which signifies

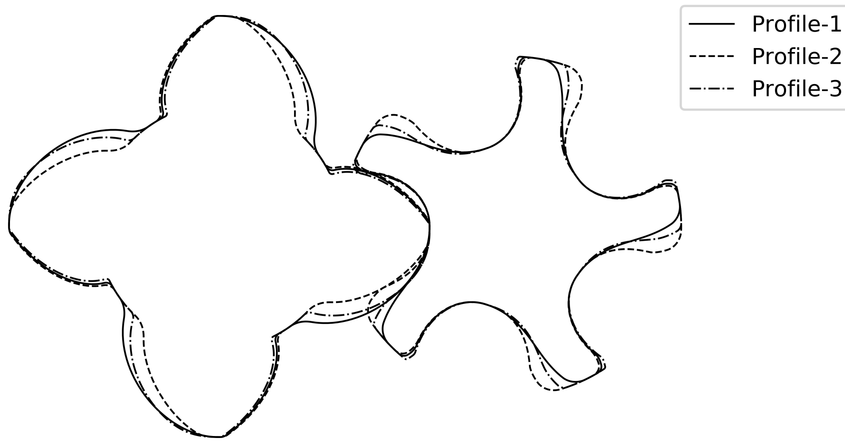

Figure 1: Three retrofitted 4/5 N-rotor profiles with different set of profile input parameters (*R1, R2, R3, R4* & *n*)

the power consumed by the compressor to deliver a unit of compressed air. It can be calculated using software tools like SCOPRATH or SCORG (Kovacevic, Stosic, Mujic, & Smith, 2005).

The following section goes through specifics of the NN framework for the intended objective hereby outlined.

3. FRAMEWORK

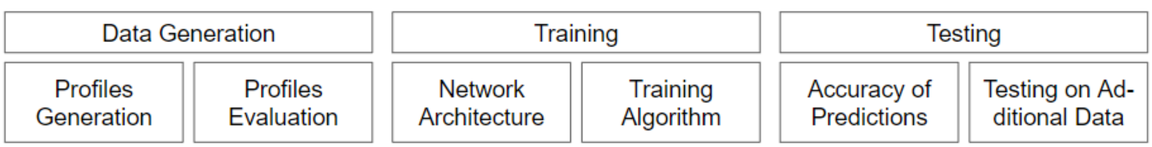

Figure 2: The general framework and steps of setting up a neural network model

3.1 Data Generation

For training the NN, a huge data-set of profile input parameters (*R1, R2, R3, R4* & *n*) and the corresponding specific powers for these profiles calculated through chamber model is required. The size of this data-set should be enough to capture as many variations in shapes of the profiles as possible for the NN to be better at predicting specific powers for a wide range of shapes. For this, a reasonable range of each input parameter is decided through experience with rotor profile generation. In these five ranges for five input parameters, 8 to 10 uniformly spaced values of each parameter were picked. For every possible combination of these 8 to 10 values for 5 different input parameters, a total of ~50000 N-Profiles were designed using a computer code. Not all of these 50000 profiles were valid, since for some combinations of these parameters reversals or non-tangency at nodes may arise in profiles. Such invalid profiles were filtered out using a computer code that automatically checks for reversals and other discrepancies in the generated profiles. Upon these rejections, a data-set of ~30000 valid profiles was fed to SCORPATH's chamber model with the same operating conditions for all profiles. The resulting specific powers for each profile were saved against respective set of input parameters. This pretty much completes the data generation part for setting up the NN model.

This data of 30000 profiles and their respective specific powers calculated through thermodynamic simulations can be readily used to train and test the NN.

3.2 Training

The neural networks are inspired by the way neurons fire in a human brain during any neurological activity. A NN basically consists of a network structure also known as network architecture which mimics the arrangement of neurons tasked to learn from the data fed to it. An in depth treatment of all the technical aspects of NN is not possible in this paper; interested readers are hence advised to refer standard texts on these techniques such as Géron (2019) for more details. A neuron in the context of NN is a node which can take on numerical values. A typical NN consists of multiple interconnected layers of neurons which are individually fired or not fired fired based on the associated activation function with the network. The first layer of the network is an input layer which passes input parameters to the network which might have several hidden layers. In figure 3, a typical neural network with two hidden layers, an input layer and an output layer for the problem under discussion is depicted as an example.

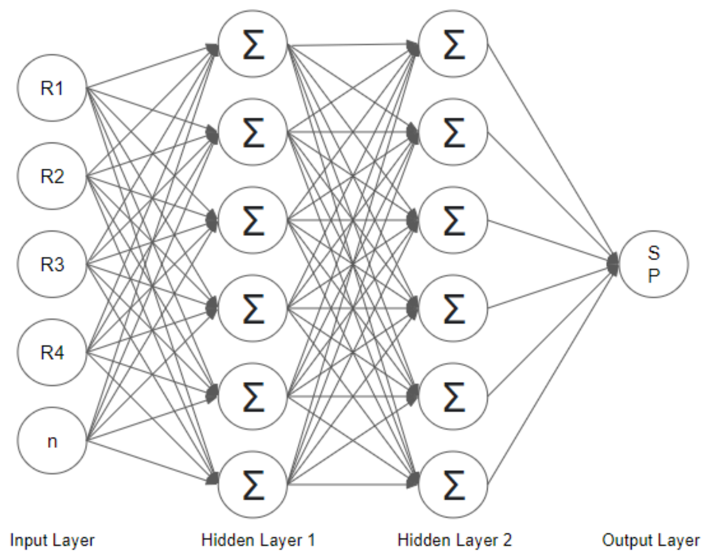

Figure 3: An exemplary neural network architecture with one input layer, two fully connected hidden layers and a single output

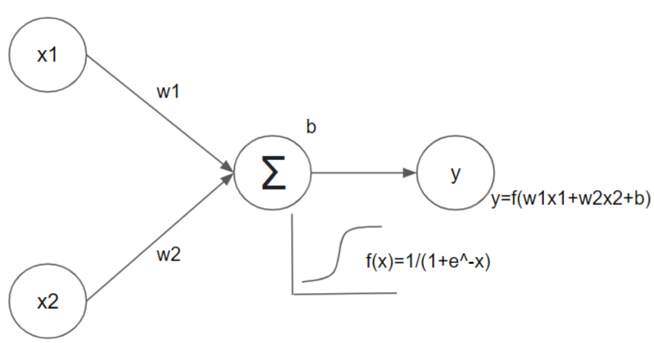

Figure 4: Working of a neuron in an artificial neural network with two inputs and single output

The connections in the network fundamentally act as weights on the inputs and each neuron also has a bias which is added to the multiplication of input value and weight. Figure 4 depicts the working of a single neuron which has two input connections and a single output. The connection weights $w1$ and $w2$ are multiplied with inputs $x1$, $x2$ and added to the bias b. The final output though is obtained by applying the activation function on $w1x1 + w2x2 + b$. The activation function simply converts the numerical output of the function into neuron output; an indication for the triggering of the neuron. Mathematical functions like Sigmoid, Rectified linear unit, etc are used as activation functions.

During training process, based on the training data, a training algorithm tries to find the set of weights and biases for each neuron and its connections such that the error between target value (fed with the training data) and the neural network prediction is minimized. This is an iterative process and a good quality of data ensures good training of the model.

The NN developed for the purpose of predicting specific powers for the rotor profiles has an input layer with five neurons which take on the values of the five input parameters. There is only one hidden layer with ten neurons fully connected to the input layer. And finally there is a single output neuron which is specific power (SP). The Sigmoid function is chosen as the activation function. This level of complexity of the network is deemed enough to capture the essence of this learning problem. In case of more number of input parameters or inclusion of non-geometric parameters in optimization (such as speed of rotors, pressure ratio, etc.), a network architecture with more than one hidden layer might be required. In case of the inclusion of more input parameters, the size of training data would also grow multiplicatively. This is one of the challenges in scaling the learning of NN to a wider range of input parameters.

As for the choice of training algorithm, 'Bayesian Regularization' was a preferred choice due to its better generalization outside the training data than other algorithms.

3.3 Testing

Testing serves the purpose of checking how well the trained model performs outside the trained data. Since the model is trained to minimize the error between known targets and model predictions, model performance is always good in training data. For testing purpose, the NN must only be given the input values (profile parameters) and its prediction must be compared with the expected/known output (which in this case is the specific power). Hence, for testing the NN, additional data is required. This problem can be solved by keeping aside some small portion of the data from the originally generated data-set before feeding it to the model for training. This kept aside data can serve as the testing data-set post training. Hence out of the close to 30000 profile data points, only $\sim$24000 randomly chosen data profiles were used for training the model and the remaining were later used for testing the performance of the trained model.

An additional testing data can always be generated separate from the originally generated data-set. Keeping aside a chunk of the original data may lead to gaps in the fed data for training. This could affect the model's performance due to a reduced quality of data for training. In this study, an additional data-set of 100 randomly chosen valid retrofit profile shapes was generated for an additional testing. Results of both the testing are presented in the following section.

4. RESULTS

The NN is tasked to predict the specific power for given profile as closely as possible to the specific power for the same profile calculated by solving chamber model. To evaluate how well does the trained NN do this job, the specific power predictions and the calculated specific powers can be plotted on a graph. Ideally, there will be a perfect correlation between these two quantities marked by 100% accuracy of NN prediction. But in reality the predictions by NN don't perfectly match with target values. Instead they fall within certain close range around the target value. The correlation hence established can be measured by the correlation coefficient R. R=1 signifies a perfect correlation and a 100% accuracy of the NN. R value of such a correlation plot for testing data-set serves as a good indicator of the NN's accuracy. Another way to evaluate the performance of NN is by looking at the %errors between predicted and target specific powers for the testing data points.

For the NN under discussion, as stated earlier, a data-set of $\sim$30000 profiles was generated. Out of these, $\sim$24000 (80%) data points were randomly picked up for training and the remaining $\sim$6000 (20%) were used for testing. During training, the training algorithm had to pass over the entire training data-set approximately 600 times (epochs) to find the best combination of weights and biases for constituent neurons in the network. This takes only about a minute's time. At the end of the training, the model could predict the specific powers with more than 99% accuracy for the maximum number of data points in the training data-set. A R value of 0.9930 was achieved for the training data-set which indicates that the NN was able to fit well over the training data.

Whatsoever might be the NN performance in training, it is not considered a good model unless it predicts well outside the training data. A good model generalizes well outside the training data. Hence the NN is evaluated on the testing data-set of ~6000 data-points. The NN is asked to predict the specific powers for the profile input parameters in testing data. The predictions are then compared against the specific powers calculated through thermodynamic simulation. Similar correlation plot is generated in figure 5 which shows that the NN works very well within the testing data too, with a correlation factor of R=0.9932.

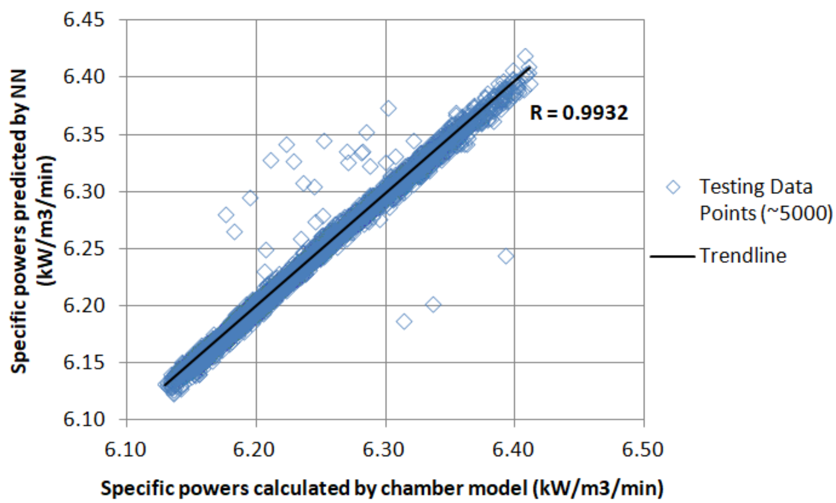

Figure 5: Plot of the specific powers predicted by NN against those calculated by solving the chamber model for all the profiles in testing data-set

Mind that the data in testing data-set is previously unseen by NN and it still is able to predict the specific powers for these profiles with tremendous accuracy. If the %error between predicted specific powers and target specific powers is calculated, only 30 out of the ~6000 profiles have prediction errors greater than 0.3%. That is, more than 99.5% profiles in the test data had their specific powers predicted by the NN within 0.3% accuracy. More so, more than 90% profiles had their specific power predictions within 0.1% of the thermodynamically calculated specific power.

In order to further validate this model, an additional set of 100 valid profiles was generated by randomly selecting the five profile parameters. These 100 profiles are completely separate from the training or testing data-set. Once again, the %errors between specific power predictions by NN and the target specific powers calculated through thermodynamic simulation were looked at. The graph in figure 6 shows the absolute %errors for these 100 profiles. The maximum error between predictions and targets does not exceed 0.3% even in the additional randomly generated data-set.

The trained NN is able to predict the specific power based on input values relatively quickly than the physics based solver. This is possible because the NN is essentially working with linear expressions of the form $wx + b$ at each neuron whereas the physics based solver works with differential equations and their numerical solutions. The SCORPATH solver used in this study is one of the fastest chamber models which does one thermodynamic calculations in approximately 0.3 seconds. The NN trained on the data from SCORPATH can predict the specific powers as quickly as 12 millisecond. Obviously, the speed is gained but at the cost of versatility; since data-based NN model can not predict for anything outside its own scope whereas the physics based model can adapt.

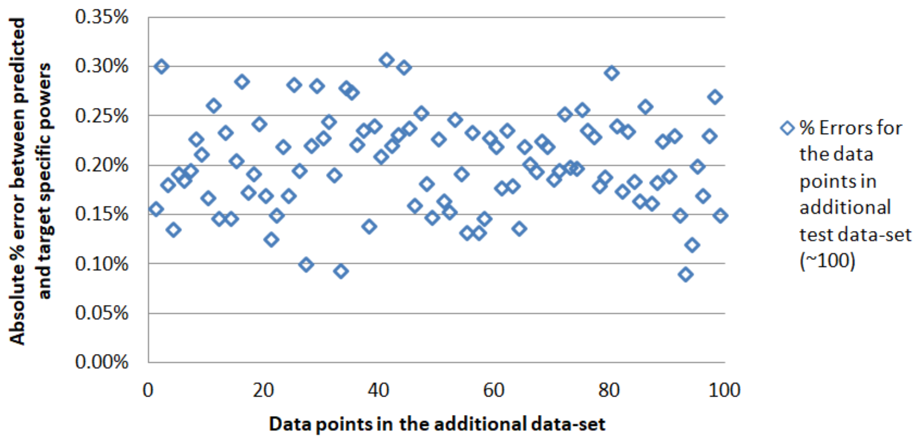

Figure 6: Absolute %errors between specific powers predicted by NN and those calculated by solving the chamber model for all the profiles in the additional testing data-set

5. CONCLUSIONS AND FUTURE SCOPE

Conclusions of this research can be summarized as following-

- ANN are capable of predicting the specific powers for different rotor profile shapes with an accuracy of more than 99%
- The higher accuracy of prediction is linked with size of the data-set. Scaling the model to include more input parameters would inflate the required training data-set by multiple orders.
- The trained NN can predict the specific power (data-based prediction) 25000 times faster than it takes for the actual calculation of the specific power in a solver (physics based calculation).
- The trained NN only mimics the physics based solver over the range of training data. It needs to be updated in case of any fundamental change in the physics based model or the range of inputs.

Rotor profiling as referred earlier is a ‘recipe’ of mathematical curves mixed in ‘suitable proportions’. It is hereby demonstrated in a limiting sense that a computer program could learn the nuances of this ‘recipe’ through rigorous virtual experimenting with different profile shapes. This approach however is computationally very extensive in its current form. The data-set of 50000 profiles used in this study has relatively very few variables (only 5); still it takes several hours to generate and calculate performances of all these profiles. On top of that, the chamber model for simulating a compression process might be frequently updated based on experiments or a better understanding of the physics of the process. In such cases, the knowledge base for training would need to be updated too.

However, in light of these promising results, neural networks and artificial intelligence on the large pose as promising candidates for a further application in screw compressor design and optimization. If the challenges such as data-set scaling and accuracy are properly addressed in near future, the ‘machine intelligence’ developed by NN may be used backwards for generating profiles with desired energy efficiency and other criteria. Scope of the current research can also be expanded by application of another class of AI algorithms, namely Conditional Generative Adversarial Networks (CGAN) to rotor profiling. These class of algorithms use deep convolutional neural networks (CNN) which generate images based on certain conditional parameters. If these models are trained on images of different rotor profiles and the conditional parameter are set to the desirable parameters associated with these profiles, such algorithms should in theory be able to generate rotor profiles on their own based on the desirable parameters which could be energy efficiency or manufacturability. This would be a radically different approach to rotor profile generation and optimization. The initial research presented hereby builds confidence in the potential of these class of techniques in compressor technology.

REFERENCES

Astberg, A. (1984, March 6). *Screw rotor machine and rotor profile therefor.* Google Patents. (US Patent 4,435,139)

Edstrom, S. E. (1992). A modern way to good screw rotors. *Proc. of the 1992 International Compressor Engineering Conference at Purdue*.

Géron, A. (2019). *Hands-on machine learning with scikit-learn, keras, and tensorflow: Concepts, tools, and techniques to build intelligent systems.* " O'Reilly Media, Inc.".

Hanjalic, K., & Stosic, N. (1997). Development and optimization of screw machines with a simulation model-part ii: Thermodynamic performance simulation and design optimization. *Journal of Fluids Engineering*, *119*, 664–668.

Kovacevic, A., Stosic, N., Mujic, E., & Smith, I. K. (2005). Design integration for screw compressors. *ASME International Mechanical Engineering Congress and Exposition*, *42118*, 29–33.

Stosic, N. (2005). *Scorpath - screw compressor optimal rotor profiles and thermodynamics.* Software Package for Screw Compressor Design. Retrieved from `http://www.staff.city.ac.uk/~ra600/DISCO/DISCO\%20SCORPATH.htm`

Stosic, N., & Hanjalic, K. (1997). Development and optimization of screw machines with a simulation model-part i: Profile generation. *Journal of fluids engineering*, *119*(3), 659–663.

Stosic, N. R. (1997, November 20). *Plural screw positive displacement machines.* Google Patents. (International Patent WO1997043550A1)

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