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Dynamic multistep uncertainty prediction in spatial geometry

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Abstract

Maintenance procedures for complex engineering systems are increasingly determined by predictive algorithms based on historic data, experience and knowledge. Such data and knowledge is accompanied by varying degrees of uncertainty which impact equipment availability, turnaround time and unforeseen costs throughout the system life cycle. Once quantified, these uncertainties call for robust forecasting to facilitate dependable maintenance costing and ensure equipment availability.

This paper builds on the theory of spatial geometry as a methodology to forecast uncertainty where available data is insufficient for the application of traditional statistical analysis. To ensure continuous forecast accuracy, a conceptual dynamic multistep prediction model is presented applying spatial geometry with long-short term memory (LSTM) neural networks. Based in MATLAB, this deep learning model predicts uncertainty for the in-service life of a given system. The further into the future the model predicts, the lower the confidence in the uncertainty prediction. Forecasts are therefore also made for a single time step ahead. When this single step is reached in real time, the next step is forecast and used to update the long range prediction. The uncertainty here is contributed by an aggregation of quantitative data and qualitative, subjective expert opinions and additional traits such as environmental conditions. It is therefore beneficial to indicate which of these factors prompts the greatest impact on the aggregated uncertainty for each forecast point. Future work will include the option to simulate and interpolate input data to enhance the accuracy of the LSTM and explore suitable approaches to mitigate, tolerate or exploit uncertainty through deep learning.

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1. Introduction

Modern proactive maintenance strategies are gradually utilising condition monitoring and deep learning to achieve optimum predictions in turnaround time, equipment availability and costing. However, many systems are maintained on a corrective or time-based basis, where maintenance data is often recorded sporadically [1–3]. This promotes varying degrees of uncertainty throughout the system life cycle. Once quantified, these uncertainties call for continuous and rigorous forecasting to facilitate dependable maintenance costing and ensure equipment availability. A forecast is a calculation or estimation using data from historic and new data to forecast a future

outcome (Bayesian), while a prediction is an indication of a future event with or without prior information [4,5].

An examination of the research background is made in Section 2, covering existing and emerging techniques in deep learning and forecasting concerning uncertainty. An overview of the proposed model structure and calculations is given in Section 3. The framework is applied to sample datasets in Section 4 with preliminary results to illustrate the multistep prediction. Section 5 discusses the strengths and limitations of the framework along with conclusions and future work in this area.

2. Research background

A deep learning platform is only as proficient as the quality and availability of the model data it is built on. The ability to make robust forecasts of unobserved data based on observed available data is a key indicator of model quality [6]. This quality is typically achieved through Bayesian reasoning, which applies Bayes' Theorem to update forecasts and predictions when presented with new data [7–13]. While ideally performed with large datasets, emerging methodologies are able to make predictions with limited data combined with qualitative opinions and experience with a degree of confidence [5]. Models must be flexible to make optimal predictions, though with a degree of uncertainty. A widely recognised and validated approach to optimise training of deep learning networks is Gaussian processes, which make use of non-parametric regression and classification models. These models grow in complexity as training data grows in dynamicity [6,7,14].

One of the most well-known applications of forecasting is in meteorology. To this end, Wang et al. [15] proposed a deep uncertainty quantification (DUQ) model to learn from historic data through a negative log-likelihood error (NLE) calculation to forecast weather patterns. Relationships between variables were predicted by regression algorithms. The combination of deep learning and UQ was shown to improve generalisation of point estimation compared to RMSE calculation to forecast multi-step meteorological time series. Extensions of this approach beyond meteorology may merit further research.

Bayesian deep learning (BDL) is one of the most popular techniques to learn from and forecast data trends [6–8,14,16]. However, BDL can require significant modification models, adopting variation inference instead of backpropagation. This makes implementation more complex and computationally slower, and can even reduce test accuracy [15,16]. This issue can be mitigated in part by dropout training, as proposed by Gal [16] in a method to approximate Bayesian inference in Gaussian processes in deep neural networks. Defined as a layer within the network structure, dropout randomly sets input sequences below a defined probability to 0. This alters the underlying network structure for each iteration to prevent overfitting [17]. Model uncertainty obtained from existing deep learning models showed improvement in predictive log-likelihood and RMSE [16]. The uncertainty assessed here was in the deep learning process itself, not the resulting uncertainty interval. It was highlighted that alternative distributions to normal in Gaussian processes will result in different uncertainty estimates, the use of which may trade-off uncertainty quality with computational complexity.

Long short-term memory (LSTM) networks are a form of recurrent neural network (RNN). Largely used in speech recognition, text recognition and sequential time-series forecasting, they are comprised of gates to selectively hold or forget information based on relevance and update predictions when new data is presented. This is determined by weights and biases applied to them. LSTMs have an advantage over other types of RNN, which use backpropagation, in their ability to use these gates to avoid vanishing or exploding gradients [16,18,19].

One of the greatest challenges of quantifying and forecasting uncertainty with confidence is the quality and availability of data [20–22]. Even if big data is available, parametrics and statistical assessments must be treated with caution without validation and established correlations. Spatial geometry is an uncertainty forecasting approach derived by Schwabe et al. [23] as an alternative to traditional parametric techniques where available data is not sufficient to fulfil the Central Limit Theorem [23–26]. Forecasts are determined by the geometric symmetry of cost variance data given as a 'point cloud' at the time of estimation. Uncertainty was represented by vectors through polar force-field analysis. The aggregated vectors for each time unit gave an indication of future cost variance, indicating shape change for the next time interval, represented in state space.

While a range of deep learning-based approaches exist to forecast data over time, there is limited literature that assesses variations in the uncertainty of such data. Given the sporadic nature of the availability and quality of corrective or time-based maintenance data, continuous and rigorous forecasts of their uncertainties is vital to facilitate dependable maintenance costing and ensure equipment availability. Spatial geometry enables uncertainty to be forecast where data is scarce, but is not able to extrapolate such forecasts with the introduction of new data over time. This is a feature of LSTMs, which, if combined with spatial geometry, can enable multistep prediction of uncertainties given by sporadic data.

3. Model overview

The proposed conceptual model combines spatial geometry with LSTM networks to enable covariant analysis of dynamic variables within state space. Adapted from the approach proposed by Schwabe et al. [23], the spatial geometry element of the model calculates the geometric symmetry between input variances for each time unit via polar force-field analysis in vector space. The aggregated vector length and degree are assumed to represent the source of greatest uncertainty. For each calculation, the radial degree between each input vector and their input order is kept constant.

To test the model and validate against the initial spatial geometry approach, US Department of Defense Air Force Selected Acquisition Report (SAR) summary tables were used [23,27]. This data detailed annual cost variances in US \$ Mil over the life cycle of a range of US Air Force military platforms over a 28 year time period from 1986-2013. This consisted of 1410 reports representing 49 unique programs, categorized into 6 cost variance factors and formatted as absolute integers by Schwabe et al. [23,27]:

- Quantity: Change in the number of units of an end item of equipment.
- Schedule: Change in procurement or delivery schedule, completion date, development or production milestone.
- Engineering: Alterations to physical or functional characteristics of a system.
- Estimating: Correction of previous estimating errors or to refinements of current estimates.

- Other: Unforeseeable events not covered in any other category (e.g. natural disaster or strike).
- Support: Cost changes for support equipment of major hardware item not included in other costs.

The vector space coordinates of each time unit are calculated by scaling the full dataset according to Eq. 1, where n is the number of inputs (6 for the sample data). The X and Y end vector coordinates for each dimension, i over the time period, j are obtained by Eq. 2, iterated through each θ of the radial degree around the unit circle. The aggregate vectors are the sum of these points, given by Eq. 3, and the magnitude is given by Eq. 4. The coordinate end points are stacked to represent the dynamic change in uncertainty of each input and aggregated vectors over time, illustrated in Fig. 1 using the test sample data with 6 input dimensions.

$$dataScaled_{i,j} = \frac{data_{i,j} - data_{minValue}}{data_{range}} \times \left(1 - \frac{1}{n}\right) + \frac{1}{n} \quad (1)$$

$$absEndX_{i,j} = \cos(\theta) \times dataScaled_{i,j} \quad (2)$$

$$absEndY_{i,j} = \sin(\theta) \times dataScaled_{i,j}$$

$$aggVectX_j = \sum_{i=1}^n absEndX_{i,j} \quad (3)$$

$$aggVectY_j = \sum_{i=1}^n absEndY_{i,j}$$

$$aggVectMagnitude_j = \sqrt{aggVectX_j^2 + aggVectY_j^2} \quad (4)$$

The symmetry and vector length of individual factors as well as the aggregated vector magnitude and direction is forecasted using the LSTM. For each time step of the input sequence, the network learns to predict the value of the next time step. This process uses and adapts built-in MATLAB functions to generate and train the network, make predictions and update future time steps [28].

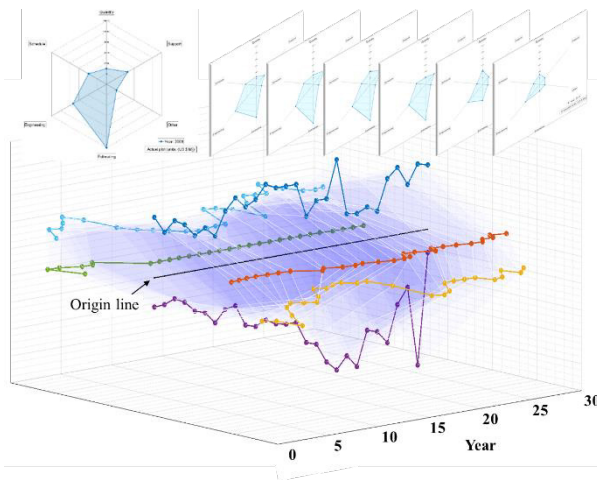


Fig. 1. Stacked plot example

Input time series data is formatted as row vectors where each column represents 1 time unit. This is split to train and test the network. As default, the network is trained on the first 70% and

tested on the last 30% to assess the network's accuracy with a comparable proportion of predicted and actual values for varying input dimensions. Training data is standardised to improve the training fit. When making predictions, the same mean and standard deviation parameters are used for the test data as for the training data. The training data is then shifted by 1 time step (responses) to enable the LSTM network to predict the next value and compare against the true value (predictors). The network architecture is illustrated in Fig. 2.

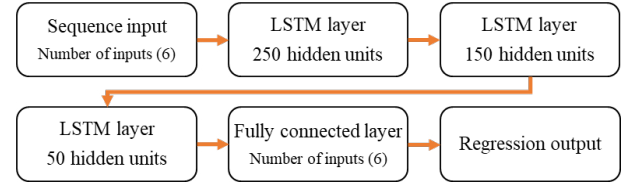


Fig. 2. LSTM network architecture

Network training options are given in Table 1 for the sample data. Training is initiated using the *trainNetwork* function. Network architecture and training options were devised from examples in literature and MATLAB tutorials [17–19].

Table 1. Network training options

Training options	Value
Solver	Adam
Max. Epochs	200
Gradient Threshold	1
Initial Learn Rate	0.001
Learn Rate Schedule	Piecewise
Learn Rate Drop Period	100
Learn Rate Drop Factor	0.2

Once trained, the *predictAndUpdateState* function is used to forecast multiple time steps ahead [28]. The network is updated after each predicted time step. The first predictions are made using the last time step of the training response. Where observed values exist between time step predictions, the network state can be updated to use those values in place of predicted values to further improve accuracy. Predictions are then unstandardised using the initial parameters. The time series data with forecasted values can then be plotted and root-mean-square error (RSME) calculated for each input via Eq. 5.

$$RSME = \sqrt{\frac{\sum_{i=1}^n (YPred - YTest)^2}{n}} \quad (5)$$

4. Results

The aggregated vectors for each input dimension are plotted in the polar chart in Fig. 3 below. It is clear from this and the 3D plot in Fig. 1 that the estimating factor prompts the greatest cost variance over the time period of the sample data. Further development of the model will show these in the 3D space.

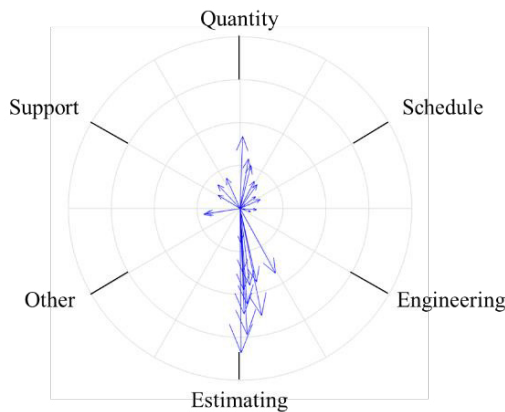


Fig. 3. Aggregated vectors for sample data over 28-year time period

For the size of the sample dataset used in this study and the development stage of the conceptual model, the LSTM network was not able to make predictions of cost variance using the end coordinate variables or symmetry in the state space that would enable confident and accurate forecasting. This could be due to the training parameters and architecture of the network or the inclusion of outliers in the dataset disrupting the training data.

To further test the model, the LSTM network was applied to the initial dataset before scaling. The forecasted values are shown in Fig. 4. The actual (observed) test data is plotted against the predicted data for each input dimension in Fig. 5.

The error between each data point (year) is plotted below, and the RMSE denoted in Table 2. It is important to note the scale and US \$Mil unit of the data here, $1.0e \times 10^4$ for the quality and estimating factors.

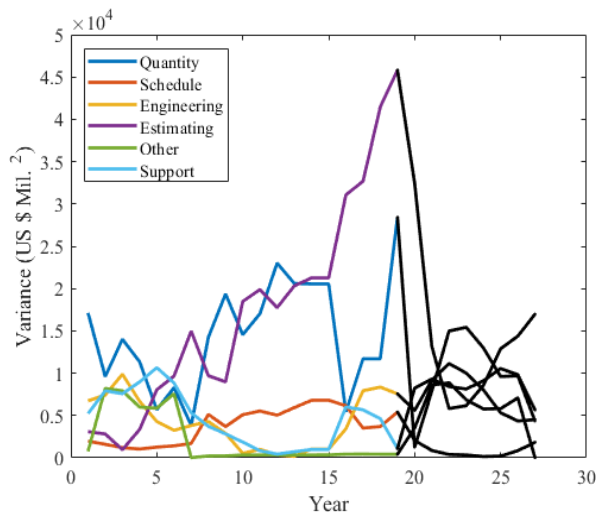


Fig. 4. Forecasted values for sample dataset using LSTM

While some parameters are mainly underestimated, others are overestimated. This is due to the training parameters of the LSTM being applied for all 6 input dimensions. The range of

each input used to train the network varies significantly. To increase the accuracy of predictions for each input dimension, different parameters should be applied for different ranges of data. This will be explored in further developments of the model. This may also explain the immediate predicted drop in the estimating and quantity factors in Fig. 4. The network architecture includes a regression layer to predict the future outputs. This typically relies on statistical data sufficient to fulfil the Central Limit Theorem, which the test data does not without artificial propagation through Monte Carlo simulation [24,29]. The regression outputs are therefore not able to provide accurate predictions on the given training data, as illustrated in Fig. 5. Alternative architectures of the LSTM network will be explored to enable the consideration of geometric symmetry under the point cloud topology presented by Schwabe et al. [23].

Table 2. RMSE of test data predicted values compared to actual

Input	RMSE (1.0×10^4 , US \$ Mil.)
Quantity	0.8294
Schedule	0.2916
Engineering	0.2938
Estimating	2.1965
Other	0.6170
Support	0.2367

5. Discussion and conclusions

The paper presented a conceptual framework to forecast and predict uncertainties in maintenance in-service where complete data is scarce. Incorporating deep learning LSTM networks with spatial geometry, the dynamic multistep prediction model analyses the geometric symmetry of given input variables through polar force-fields in vector space. The angle and magnitude of the aggregated vector illustrates the greatest source of uncertainty for each time unit. The 3D visualisation of each factor through time provides a clear and immersive view of which inputs result in the greatest uncertainty via the aggregated vector. These uncertainties require the most attention; be it mitigation, exploitation or simply increased awareness.

The LSTM network predictions are plotted as the difference in the actual and forecast uncertainty where actual data is available. Further optimisation of the training options may help to reduce this difference by considering the range of each input dimension over the relative time period, to which different training options will be applied to obtain the most accurate prediction for each input. The training function provides an element of self-validation to enable the user to determine if training options need adjusting.

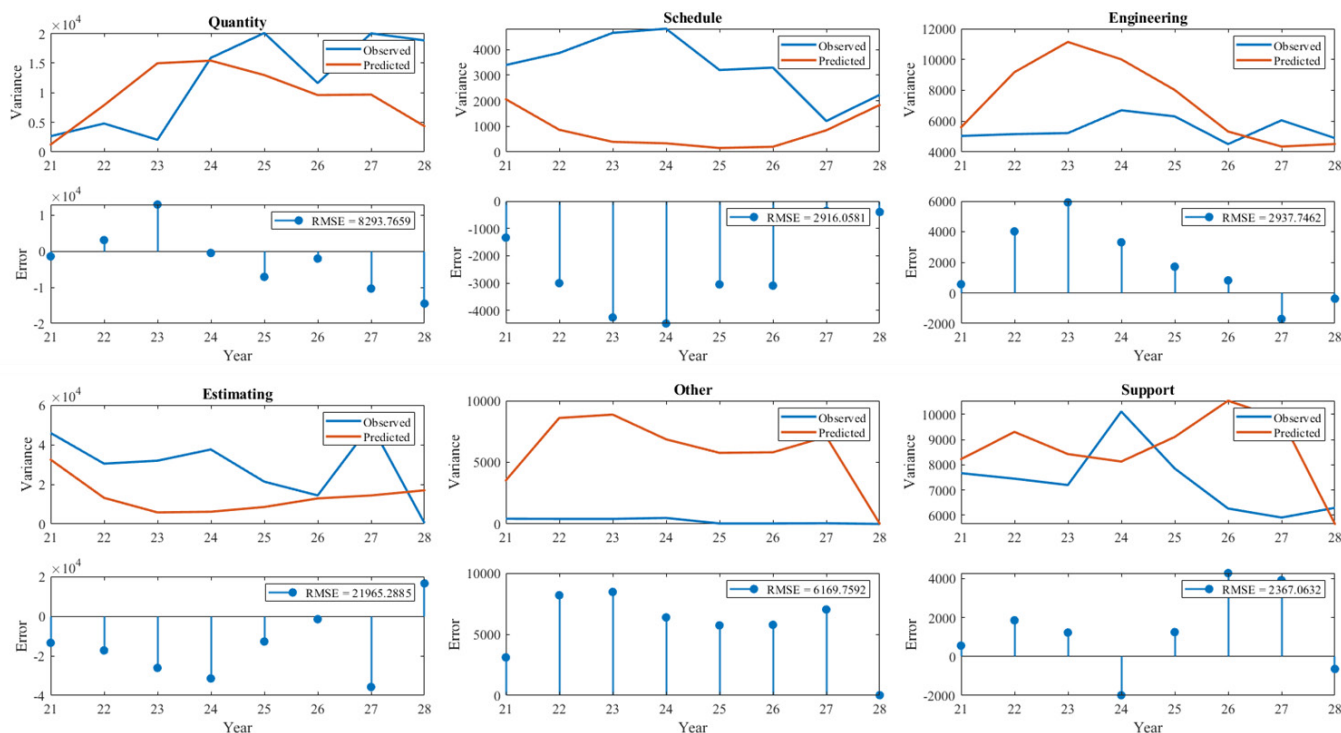


Fig. 5. Predicted vs. actual variance for sample dataset

The applicability of the conceptual framework was discussed with key personnel from the industrial sponsor in 4 hours of semi-structured interviews with positive feedback. Numerous data repositories and maintenance formats for different platforms present challenges that result in a large proportion of uncertainty, discussed in previous work by the author [22]. Modern proactive maintenance strategies utilise condition monitoring to obtain live equipment data to enable optimum predictive maintenance. The sensitive nature of such data often renders it confidential. Many systems are maintained on a corrective or time-based basis, where data is often sporadic. Continuous forecasting of these uncertainties is vital to facilitate dependable maintenance costing and ensure equipment availability.

The flexibility of the multistep prediction model to forecast uncertainties for a range of input dimensions and update future time steps when presented with new data reflects the theme of flexible mass customisation under life cycle engineering and design for manufacturing and maintenance. The ability to forecast uncertainties surrounding recorded data, experience and knowledge allows for comprehensive decisions to be made concerning equipment availability, turnaround time and unforeseen costs throughout the life cycle of the system, focused here on the in-service phase.

The evolving conceptual framework presented in this paper enables forecasting with limited data, but requires further development to optimise the projection and calculation of vector magnitude and corresponding coordinate points in future time steps. This will be achieved through further research into the network architecture and optimisation of the training options and plotting code in MATLAB. The ability to automatically adjust to accommodate fewer or additional input dimensions will also be added. Improved visualisation of

symmetry and vector magnitude in the 3D plot will boost usability of the model, making key points of information clear to the user. Additional future work will include the option to simulate and interpolate input data to enhance the accuracy of the LSTM by exploring suitable alternative to the regression layer and, further, suitable approaches to mitigate, tolerate or exploit uncertainty through deep learning.

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For access to the data underlying this paper, please see the Cranfield University repository, CORD, at DOI: 10.17862/cranfield.rd.12906716.

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