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Normalising Flows and Nonlinear Normal Modes

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Abstract: In the context of dynamic decoupling problems, engineering dynamics has long held *modal analysis* as an exemplar. The method allows the exact decomposition of linear multi-degree-of-freedom (MDOF) systems into single-degree-of-freedom (SDOF) oscillators, thus simplifying complex dynamic problems considerably. However, modal analysis is very much a linear theory; if applied to nonlinear systems, the decoupling property (among others) is lost. This unfortunate situation has led to numerous attempts to formulate workable nonlinear versions of the theory. The current paper extends previous work by the authors in using machine learning methods to *learn* nonlinear modal transformations on measured data, based on the premise that any latent modal variables should be statistically independent. Unlike previous work, the transformation here exploits the recent development of *normalising flows* in constructing the required transformations. The new approach is shown to overcome a number of the problems in the original approach when demonstrated on a simulated nonlinear system.

Keywords: Nonlinear modal analysis; nonlinear normal modes; machine learning, normalising flows.

1. INTRODUCTION

The field of structural dynamics has relied for decades on a particular decoupling technology. The method of *modal analysis* (Ewins [1984], Avitable [2018]), was developed in the 1960s and '70s as an experimental methodology with a mathematical basis which allowed a multi-degree-of-freedom (MDOF) system to be decomposed into a set of single-degree-of-freedom (SDOF) oscillators. The new variables in the transformed domain were termed *modal coordinates* and in machine learning terms were essentially *latent variables* which also offered the potential benefit of dimension reduction, in that the system could ofttimes be accurately described using fewer modal coordinates than the original physical ones. The theory was a fundamentally linear one, and provided – via the *principle of superposition* – a means of reconstructing the physical behaviour from the modal variables (Worden and Tomlinson [2001]). In fact, under certain circumstances, modal analysis proved to be exactly equivalent to the *Principle Orthogonal Decomposition* (POD) (Han and Feeny [2005]), which is in turn equivalent to the statistical technique of *Principal Component Analysis* (PCA) (Sharma [1995]).

Unfortunately, not all of the structures of interest to engineers prove to be linear, or allow a good approximation by linear dynamics. This issue has driven a long-standing programme of research with the aim of developing a fully-nonlinear variant of modal analysis. Sadly, it has not so far proved possible to create modal transformations for nonlinear systems which possess all of the desirable properties held in the linear theory. This situation has led to the development of different forms of nonlinear modal analysis, distinguished by the subset of properties which they preserve from the linear theory. The matter is discussed in more detail in Worden and Green [2017], where it is argued that the methods fall mainly into the *coherent motion* class, originating in the work of Rosenberg [1962], or the *decomposition* class exemplified by the invariant manifold approach of Shaw and Pierre [1993].

The main objective of the paper by Worden and Green [2017], was to propose a new definition of *nonlinear normal mode*, based on the geometrical ideas of Shaw and Pierre, but founded in ideas from machine learning. In fact, it proved possible to construct an (approximate) modal transformation using evolutionary optimisation in which the transformation was a multinomial expansion in the physical variables. Once the forward transformation was established, it then proved possible to learn the inverse transformation by supervised learning; the Gaussian process algorithm was used for the latter. The new method was demonstrated on a number of numerical case studies and one set of experimental data and proved to be very successful; however, it was not completely without problems.

The main idea of the new method in Worden and Green [2017] was to define the nonlinear modes in terms of their *statistical independence*; this is a natural idea, equivalent to the orthogonality concept in the original linear modal analysis. The problem was framed in terms of optimisation, whereby the free parameters in a multinomial map

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were tuned in order to maximise a measure of independence. At the time, the available measures of complete independence were too computationally expensive to form a feasible objective, so the problem was restricted to the minimisation of correlations up to third order; this was the first approximation. The second approximation enforced in the original paper was to truncate the multinomial forward transform at third order. Despite these approximations, the method worked very well on the benchmarks. However, the second approximation had a negative consequence; the multinomial forward transformation gave rise to a multi-valued inverse which gave problems in the 'superposition' of the nonlinear modes; i.e. the reconstruction of the original physical coordinates.

The objective of the current paper is to provide an alternative machine learning formulation of nonlinear modal analysis which overcomes the problems encountered in Worden and Green [2017]. The approach taken here is radically different and makes use of the concept of a *normalising flow* (NF) (Rezende and Mohamed [2015], Kobyzev et al. [2020]). The NF approach overcomes both of the main problems encountered in Worden and Green [2017]; in the first place, the forward transformation is constructed as a sequence of invertible mappings. The individual maps are learnt using neural networks which, unlike a truncated multinomial, are universal approximators; because each map is invertible, the inverse – the 'superposition' map – is single valued. Secondly, the objective of the NF is to map to variables with a prescribed probability density; the density in question here is a spherical (uncorrelated) Gaussian, and this is sufficient to enforce complete independence of the latent variables.

The layout of the paper is as follows: in the following section, a brief overview is given of the method proposed in Worden and Green [2017], and the problems with the approach are highlighted. In Section 3, the normalising flows are defined and in Section 4 they are demonstrated on a simulated benchmark two-DOF nonlinear system. The paper ends with a short section of conclusions.

2. NONLINEAR MODAL ANALYSIS

The basic principles of the approach in Worden and Green [2017], will be illustrated here via the two-DOF system presented there. The actual equation of motion will follow later as equation (19); for the moment, it suffices to say that there are two coupled physical variables of interest $(y_1, y_2) = \mathbf{y}$, which represent displacement responses from a highly-nonlinear system. The object of the analysis was to learn a transformation[1] $\mathbf{z} = f(\mathbf{y})$ into latent variables $(z_1, z_2) = \mathbf{z}$, which are *uncoupled* in some sense. The idea was that the transformation would be specified as a multinomial in the y_i with tunable coefficients a_{ij} and b_{ij} as follows,

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \end{pmatrix} \begin{pmatrix} y_1^3 \\ y_1^2 y_2 \\ y_1 y_2^2 \\ y_2^3 \end{pmatrix} \tag{1}$$

where, in the linear case, the first matrix A on the RHS would be the 'modal' matrix of linear theory (Worden and Green [2017]).

The coefficients a_{ij} and b_{ij} were then estimated in order to minimise an objective function which measured the degree of coupling of the new latent variables z_i. The measure of coupling was chosen to be a measure of statistical dependence between the variables. As discussed in Worden and Green [2017], measures of complete independence were desired, but proved too computationally costly; instead the chosen strategy was to minimise a sum of second and third-order correlations as follows,

$$\begin{aligned} J = & |\mathbf{a}_1.\mathbf{a}_2| \\ & + \mathrm{Cor}(z_1, z_2) + \mathrm{Cor}(z_1, z_2^2) + \mathrm{Cor}(z_1, z_2^3) \\ & + \mathrm{Cor}(z_1^2, z_2) + \mathrm{Cor}(z_1^3, z_2) + \mathrm{Cor}(z_1^2, z_2^2) \end{aligned} \tag{2}$$

The first term in the objective was added in order to make sure that the columns $\mathbf{a}_1$ and $\mathbf{a}_2$ of the matrix A would be orthogonal, as this would be required in the limit of linear modal analysis. The actual optimisation algorithm used was the self-adaptive differential evolution (SADE) algorithm; details of the implementation can be found in Worden and Green [2017].

Apart from the value of the objective function, the success of the algorithm was verified by considering the spectral densities of the z_i variables in the frequency domain. In linear structural dynamics, SDOF systems are characterised by having response spectra with a single peak, while MDOF system spectra have multiple peaks. As the objective here was to transform to decoupled SDOF systems, the transformed spectra should have single peaks. The results of the optimisation procedure on the 2DOF benchmark from Worden and Green [2017] are shown in Figure 1; one can see that the variables appear to have been decoupled as desired. (The level of excitation for the simulated data was chosen to be high enough that the y_i responses were significantly nonlinear; this is visible here in the shape and breadth of the second peak.)

There were a number of subtle issues with the analysis in Worden and Green [2017], but in the main, the transformation above was considered successful. At this point, the problem shifted to one of learning the inverse (superposition) transform. The important point there is that, as the variables $\mathbf{z}$ are now associated with the corresponding $\mathbf{y}$, the inverse map can be learnt using any appropriate supervised machine learning algorithm, and Gaussian Process regression models (GPs) were used in the paper. Following best practice with such algorithms, the data were divided into a training set and a test set. While the algorithm gave near-perfect reconstruction on the training set, the results on the testing set (Figure 2) showed a number of small 'glitches', some of which are highlighted in Figure 3.

[1] To avoid too much emphasis in the equations, transformations like f will not be emboldened, although they are vector valued.

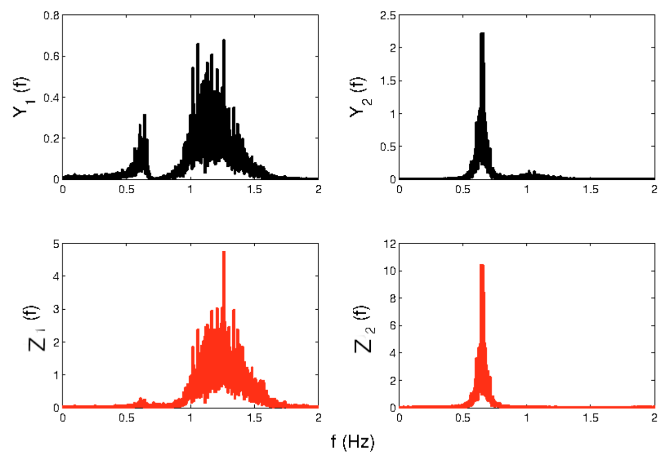

Fig. 1. Decomposition via the optimisation procedure in Worden and Green [2017]: Power spectral densities for the physical $\mathbf{y}$ and transformed $\mathbf{z}$ variables.

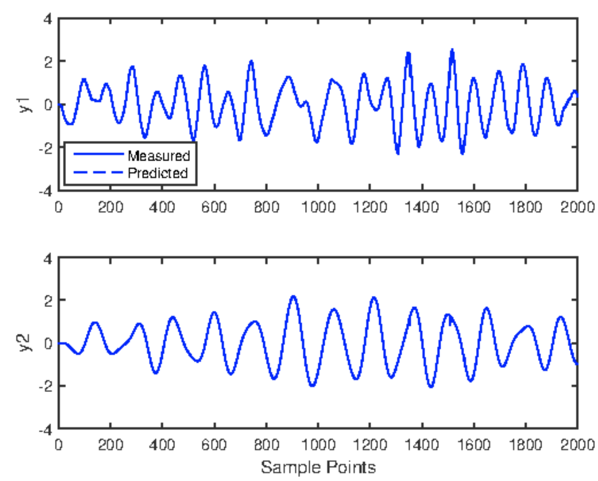

Fig. 2. Superposition of $\mathbf{z}$ variables using a Gaussian process (from Worden and Green [2017]).

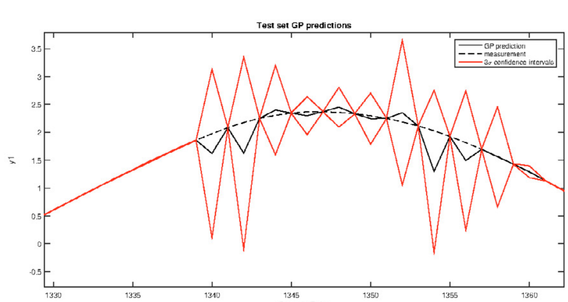

Fig. 3. Three-sigma confidence intervals (red) over the reconstructed physical variables (-) compared to the measurements (- -). Zoomed region of superposition of $\mathbf{z}$ variables using a Gaussian process (from Worden and Green [2017]).

The gliches are not the fault of the GP, they are symptomatic of a deeper problem. The issue is that the multinomial transformation (1) does not admit a single-valued inverse. Even if the results are perfect on the training set, small variations in the testing set can cause the inverse transformation to select the wrong root of the multivariate cubic equation represented by (1).

As discussed in the introduction, the solution to the problem as presented in this paper, is to propose an entirely different means of learning the forward transformation which is not only single-valued and invertible, but is also based on attaining true independence of the latent variables $\mathbf{z}$.

3. NORMALISING FLOWS

Normalising flows are capable of transforming simple *parametrised* probability distributions onto complex densities of unknown structure (Dinh et al. [2014]). This flexibility is useful, as the underlying density of practical data is often poorly described by any parametrised functions that are also easy to handle (the Gaussian distribution, for example). If a tractable probability density function (p.d.f) can be transformed via an invertible mapping, the density of complex data can be more easily modelled.

In more specific terms, Rezende and Mohamed [2015] define normalising flows as a transformation of a probability density through a *sequence* of invertible mappings. By repeatedly applying a change of variables rule, the initial density can *flow* through the sequence of invertible units, leading to a valid probability distribution at the end of the sequence (Rezende and Mohamed [2015]).

3.1 Change of Variables Formula

Let $\mathbf{Z} \in \mathbb{R}^d$ be a random variable with a known and tractable density function $p_{\mathbf{Z}}(\mathbf{z}_i)$ [2]. Then, considering an invertible (smooth) function $f : \mathbb{R}^{d'} \to \mathbb{R}^d$, such that,

$$\mathbf{Z} = f(\mathbf{Y}) \tag{3}$$

one can compute the p.d.f for the random variable $\mathbf{y}_i \in \mathbf{Y} \in \mathbb{R}^{d'}$, via the change of variable formula (Dinh et al. [2014], Kobyzev et al. [2020], Murphy [2012]),

$$\begin{aligned} p_{\mathbf{Y}}(\mathbf{y}_i) &= p_{\mathbf{Z}}(f(\mathbf{y}_i)) \left| \frac{\partial f(\mathbf{y}_i)}{\partial \mathbf{y}_i} \right| \\ &= p_{\mathbf{Z}}(\mathbf{z_i}) \left| \frac{\partial f(\mathbf{y}_i)}{\partial \mathbf{y}_i} \right| \end{aligned} \tag{4}$$

where $\left|\frac{\partial f(\mathbf{y}_i)}{\partial(\mathbf{y}_i)}\right|$ is the determinant of the Jacobian of the function f at $\mathbf{y}_i$. In conceptual terms, the determinant is effectively *scaling* the p.d.f by the factor in which the local area around $\mathbf{y}_i$ stretches/shrinks through the transformation f.

For normalising flows, f should be chosen such that the determinant of the Jacobian and the inverse f^{-1} are available. If these conditions are met, it becomes easy to sample the random variable $\mathbf{Y}$ via $\mathbf{Z}$,

$$\mathbf{z}_i \sim p_{\mathbf{Z}}(\mathbf{z}_i) \tag{5}$$
$$\mathbf{y}_i = f^{-1}(\mathbf{z}_i) \tag{6}$$

[2] Herein, subscripts index rows of matrices, while superscripts index columns of matrices

The inverse (f^{-1}) refers to the *generative* direction, while f is the *normalising* direction (Kobyzev et al. [2020]).

The construction of a complicated, nonlinear, and invertible function, with a defined Jacobian, is non-trivial. A popular approach considers that a composition (i.e. *chain*) of invertible functions is itself invertible, with a specific form for the Jacobian (Kobyzev et al. [2020]). That is, for a set of K invertible bijective functions,

$$f = f_1 \circ f_2 \circ \ldots \circ f_{K-1} \circ f_K \tag{7}$$

f is also bijective, with inverse,

$$f^{-1} = f_K^{-1} \circ f_{K-1}^{-1} \circ \ldots \circ f_2^{-1} \circ f_1^{-1} \tag{8}$$

and the determinant of the Jacobian is,

$$\left|\frac{\partial f(\mathbf{y}_i)}{\partial(\mathbf{y}_i)}\right| = \prod_{k=1}^{K}\left|\frac{\partial f_k(\mathbf{x}_i^{(k)})}{\partial(\mathbf{x}_i)}\right| \tag{9}$$

where $\mathbf{x}_i^{(k)}$ denotes the k^{th} intermediate flow, i.e. $\mathbf{x}_i^{(k)} = f_k^{-1} \circ \ldots \circ f_1^{-1}(\mathbf{z}_i) = f_{k+1} \circ \ldots \circ f_K(\mathbf{y}_i)$; thus, at the end of the sequence, $\mathbf{x}_i^{(K)} = \mathbf{y}_i$ (Kobyzev et al. [2020]). Consequently, K sets of nonlinear bijective functions can be composed to form successively more complicated functions.

3.2 Coupling layers

Dinh et al. [2014] showed that *coupling flows* can be used to define f, such that flexible and tractable transformations can be learnt. In general terms, coupling layers define units that are simple to invert, while depending on subsets of the input-features in a possibly complex way (Dinh et al. [2016]).

Briefly, consider a disjoint partition of the D-dimensional input into two subspaces, i.e. $\mathbf{x}_i^A, \mathbf{x}_i^B \in \mathbb{R}^d, \mathbb{R}^{D-d}$. Additionally, consider a bijection, referred to as the *coupling function* $h(\cdot, \theta)$ (Kobyzev et al. [2020]). The output of the coupling layer (in the generative direction, f_k^{-1}) can then be defined,

$$\mathbf{y}_i^B = \mathbf{x}_i^B \tag{10}$$

$$\mathbf{y}_i^A = h(\mathbf{x}_i^A; \mathbf{\Theta}(\mathbf{x}_i^B)) \tag{11}$$

i.e. the parameters θ are determined by some function $\mathbf{\Theta}$, which depends only on $\mathbf{x}_i^B$; the function $\mathbf{\Theta}$ is referred to as the *conditioner*.

The bijection and conditioner (h and $\mathbf{\Theta}$) combine to from a *coupling flow*, which is invertible iff h is invertible (Rezende and Mohamed [2015], Dinh et al. [2014]).

Importantly, the power of coupling flows lies in the fact that the conditioner $\mathbf{\Theta}$ can be arbitrarily complex, provided h is invertible, as established by Kobyzev et al. [2020],

$$\mathbf{x}_i^B = \mathbf{y}_i^B \tag{12}$$

$$\mathbf{x}_i^A = h^{-1}(\mathbf{y}_i^A; \mathbf{\Theta}(\mathbf{x}_i^B)) \tag{13}$$

Following Dinh et al. [2014], $\mathbf{\Theta}$ is defined by ReLU multilayer perceptrons in the experiments here, and h utilises the *affine* coupling function; in this case, (10) and (11) correspond to,

$$\mathbf{y}_i^B = \mathbf{x}_i^B \tag{14}$$

$$\mathbf{y}_i^A = \mathbf{x}_i^A \circ \exp(s(\mathbf{x}_i^B)) + t(\mathbf{x}_i^B) \tag{15}$$

where s and t are referred to as *scale* and *translation* neural networks, while $\circ$ is the Hadamard product, as defined in the RealNVP model (Dinh et al. [2016]) along with the inverse and the Jacobian.

3.3 Learning normalising flows onto an independent (spherical) Gaussian

The nonlinear transform f (onto the simple, parametrised base-distribution) is learnt via maximum likelihood. Considering the change of variables formulae, the log likelihood is (Dinh et al. [2014]),

$$\log(p_{\mathbf{Y}}(\mathbf{y}_i)) = \log(p_{\mathbf{Z}}(f(\mathbf{y}_i))) + \log\left|\frac{\partial f(\mathbf{y}_i)}{\partial \mathbf{y}_i}\right| \tag{16}$$

Because of the requirement of independence in this application, the base distribution is set to an isotropic Gaussian with independent dimensions, as suggested in Dinh et al. [2014, 2016], such that $\mathbf{z}_d \sim \mathcal{N}(0, 1)$. The likelihood can, therefore, be factorised, leading to a sum in the log-likelihood,

$$\log(p_{\mathbf{Y}}(\mathbf{y}_i)) = \sum_{d=1}^{D}\log(p_{\mathbf{Z}_d}(f_d(\mathbf{y}_i))) + \log\left|\frac{\partial f(\mathbf{y}_i)}{\partial \mathbf{y}_i}\right| \tag{17}$$

3.4 Combinations with the Principal Orthogonal Decomposition

To help enforce independence, a linear transform is applied at the each end of the normalising flow sequence. This projection is defined as in the Principal Orthogonal Decomposition (POD),

$$f(\mathbf{x}_i) = \mathbf{\Phi}\mathbf{x}_i \tag{18}$$

such that $\mathbf{\Phi}$ are the orthogonal eigenvectors of the covariance $\mathbf{\Sigma}_{\mathbf{x}} = \text{cov}(\mathbf{x}_i)$. These additional transforms are useful in the experiments, to further decouple the response of the nonlinear MDOF system ($\mathbf{y}_i$), as well as the features in the latent space ($\mathbf{z}_i$). While these transforms are not formally included in the normalising flow, they can be considered *linear* flows (Kobyzev et al. [2020]), since the inverse is trivial, i.e. $f^{-1} = \mathbf{\Phi}^\top \mathbf{z}_i$, and then the determinant of the Jacobian can be computed. In fact, orthogonal and linear projections are related to the *Householder flow* (Tomczak and Welling [2016]).

4. A CASE STUDY

As in the original work by Worden and Green [2017], a nonlinear two-DOF lumped mass system is simulated here for illustration. The equations of motion are,

$$\begin{bmatrix} m & 0 \\ 0 & m \end{bmatrix} \begin{bmatrix} \ddot{y_1}(t) \\ \ddot{y_2}(t) \end{bmatrix} + \begin{bmatrix} 2c & -c \\ -c & 2c \end{bmatrix} \begin{bmatrix} \dot{y_1}(t) \\ \dot{y_2}(t) \end{bmatrix} + \begin{bmatrix} 2k & -k \\ -k & 2k \end{bmatrix} \begin{bmatrix} y_1(t) \\ y_2(t) \end{bmatrix} + \begin{bmatrix} k_3 y_1(t)^3 \\ 0 \end{bmatrix} = \begin{bmatrix} u_1(t) \\ 0 \end{bmatrix} \tag{19}$$

The model parameters here are set to: $m = 1$, $c = 0.1$, $k = 10$, $k_3 = 1500$. The damping is proportional and the mass matrix is a multiple of the unit matrix (Han and Feeny [2005]); thus the underlying linear system truly uncouples via Principal Orthogonal Decomposition (POD) – with natural frequencies of 0.5hz and 0.87Hz. Data were simulated at a sampling frequency of 100Hz using a fourth-order Runge-Kutta method. The excitation $u_1(t)$ was a Gaussian white-noise sequence, applied to the first mass, with zero mean and standard deviation 5.5. The input $u_1(t)$ was filtered with a low-pass Butterworth filter, up to 50Hz. A total of 50000 points were simulated, with the first 10000 ignored, to remove the transient, such that $N = 40000$.

In the benchmark results below, the results of a standard *linear* modal analysis are shown via the POD; whereby the transformation $\mathbf{\Phi}$ is estimated using the standard eigenvalue approach (Worden and Green [2017]). The transformation from $\mathbf{Y} = \{\mathbf{y}_i\}_{i=1}^N$ to $\mathbf{Z} = \{\mathbf{z}_i\}_{i=1}^N$ can then be defined by,

$$\mathbf{Z} = \mathbf{\Phi}\mathbf{Y} \tag{20}$$

The result of the POD projection of the outputs is shown in Figure 4; this presents the power spectral densities $S(\cdot)$ for the physical variables $\mathbf{y}_i = \{y_i^{(1)}, y_i^{(2)}\}$ and the transformed variables $\mathbf{z}_i = \{z_i^{(1)}, z_i^{(2)}\}$. Clearly, the system is not uncoupled by linear modal analysis (in the visual sense defined earlier, whereby uncoupling results in single peaks in the spectra). Intuitively, as the system has been designed to produce a nonlinear response, the level of distortion is clearly visible – particularly in the spectrum of the first transformed variable $S(Z_1)$.

Normalising flows are now applied to learn the mapping from $\mathbf{Y} = \{\mathbf{y}_i\}_{i=1}^N$ to $\mathbf{Z} = \{\mathbf{z}_i\}_{i=1}^N$. To summarise, the mapping is defined as follows,

$$\mathbf{Z} = \mathbf{\Phi}_2 f(\mathbf{\Phi}_1 \boldsymbol{Y}) \tag{21}$$

i.e. there are two linear POD transforms $\mathbf{\Phi}_1$ and $\mathbf{\Phi}_2$ at the beginning and end of the normalising flow f. In the experiments here, the conditioner $\mathbf{\Theta}$ of the coupling layers is defined by two, two-layer perceptrons, with ReLu activation functions and four hidden units. The coupling functions h are constructed according to the *RealNVP* model, for details, see reference Dinh et al. [2016]. Six coupling layers are used in these experiments. The model is trained with a batch size of 1000, and a held-out validation set of 30% of the training data. The validation-set is used to monitor the negative-log-likelihood as validation-loss, to implement early stopping and help mitigate over-training. Because of the stochastic nature of training, a large number of models were learnt, the best result was then manually selected from the batch of models with the highest log-likelihood scores (on the validation set).

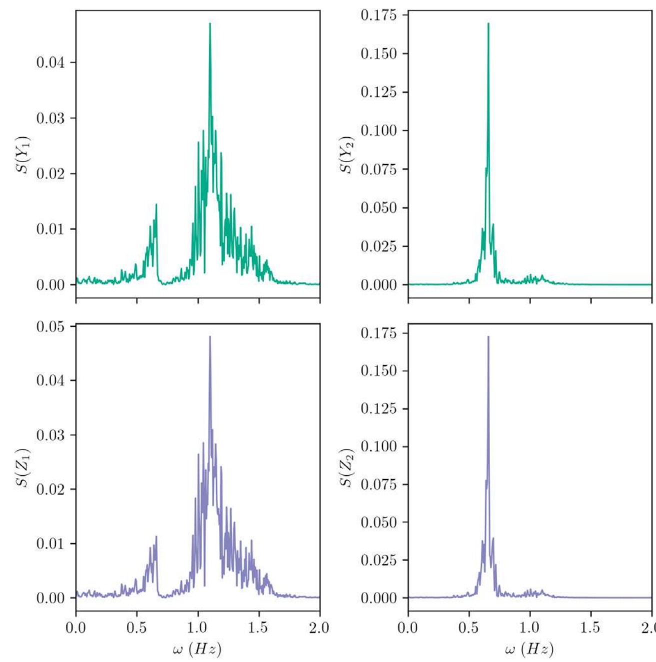

Fig. 4. Principal Orthogonal Decomposition: Power spectral densities for the physical $S(Y)$ and transformed $S(Z)$ variables.

The power spectral densities from the normalising flow projection are shown in Figure 5. The decomposed power spectra show a marked improvement over the linear modal analysis; i.e. there is uncoupling into what appears to be two individual '*modes*'. As in the original work of Worden and Green [2017], it is acknowledged here that this observation is based on the preconception that an isolated peak in the spectrum can be referred to as a *mode* – a possible artefact of linear thinking in a nonlinear context (Worden and Green [2017]).

To test the reconstruction, the inverse transform is used (generative direction) from the transformed variables, back to the physical variables,

$$\hat{\mathbf{Y}} = \mathbf{\Phi}_1^\top f^{-1}(\mathbf{\Phi}_2^\top \mathbf{Z}) \tag{22}$$

The time-series reconstruction $\hat{\mathbf{Y}}$ is compared to the original response in Figure 6. Visually, the inverse transform provides a near-perfect inverse modal transformation, verified by a mean-squared-error of 9.21×10^{-6}.

5. CONCLUSIONS

A new approach to nonlinear modal analysis, based on normalising flows (NFs) and the principal orthogonal decomposition (POD) is presented here and demonstrated on data from a simulated nonlinear system. As in previous work based on machine learning, the method is based on the idea that a 'modal' transformation into latent variables should induce pairwise statistical independence among those variables. However, the current approach is seen to overcome a number of shortcomings of the previous optimisation-based method; in particular, invertibility of the modal map – and thus a nonlinear principle of superposition – is ensured. Apart from invertibility, the method

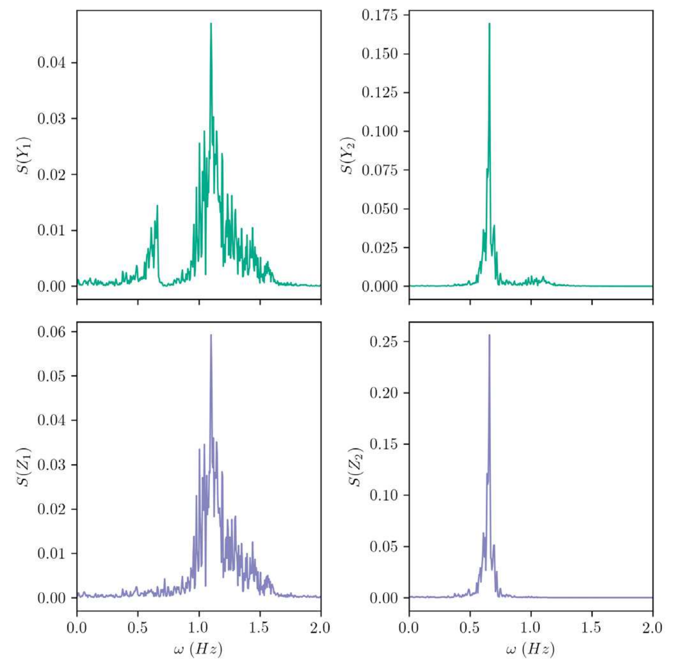

Fig. 5. Decomposition via normalising flows: Power spectral densities for the physical $S(Y)$ and transformed $S(Z)$ variables.

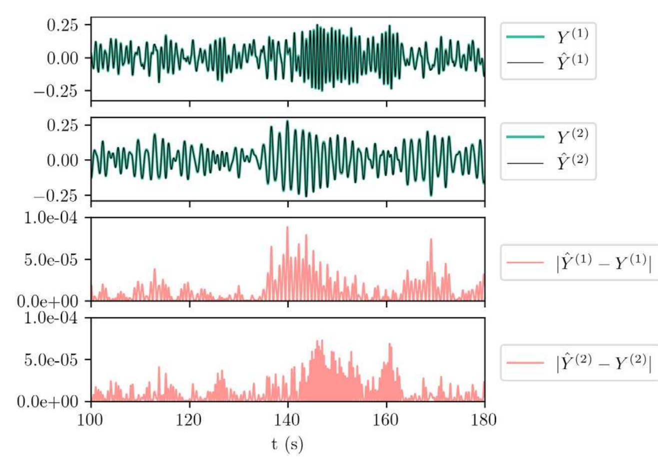

Fig. 6. Reconstruction (inverse modal transformations) of the time series via normalising flows (generative direction). Reconstructions $\hat{Y}$ are black lines and the true variables Y are the green lines. Mean-squared-error residuals shown by red lines.

also tries to ensure that the transformed variables are fully independent, rather than just uncorrelated to some order. In many ways, the new approach is more transparent and elegant than the optimisation-based method and also offers more direct ways forward in solving the outstanding problems. Furthermore, as will be shown in future work, the NFs offer the prospect of direct physical interpretation. Future work will also consider formally defining flow sequences that further prioritise independence in the transformed variables: Householder flows (Tomczak and Welling [2016]) present one approach to include orthogonal (POD-type) steps within the flow.

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