

# A quadratic decoder approach to nonintrusive reduced-order modeling of nonlinear dynamical systems

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Linear projection schemes like Proper Orthogonal Decomposition can efficiently reduce the dimensions of dynamical systems but are naturally limited, e.g., for convection-dominated problems. Nonlinear approaches have shown to outperform linear methods in terms of dimension reduction versus accuracy but, typically, come with a large computational overhead. In this work, we consider a quadratic reduction scheme which induces nonlinear structures that are well accessible to tensorized linear algebra routines. We discuss that nonintrusive approaches can be used to simultaneously reduce the complexity in the equations and propose an operator inference formulation that respects dynamics on nonlinear manifolds.

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## 1 Introduction

Both the idea and the promise of model order reduction are the identification and employment of coordinate systems that can best encode states and behaviors with the least amount of degrees of freedom. Linear projection schemes like the proper orthogonal decomposition (POD) have proven their universality and efficiency but come with limits in terms of low-dimensionality that is related to the notion of the *Kolmogorov n-width*; cp. [10].

In the very low-dimensional regime, techniques that use nonlinear relations between the actual and the reduced coordinates seem to outperform POD; see, e.g., [5, 6, 9]. While nonlinearities may lead to fewer dimensional coordinates, their inclusion in simulation schemes comes with extra computational efforts.

A potential general approach to soften the computational disadvantages over linear methods lies in consideration of tensor-structured nonlinearities. These can well encode or approximate general types of nonlinear relations and are structured to be efficiently treated by numerical linear algebra tools. As an example and as the basic approach in this paper, we consider the quadratic relation that decodes some  $r$ -dimensional coordinates  $q$  to approximate some  $n$ -dimensional coordinates  $x$  as

$$x(t) \approx \tilde{x}(t) = \Gamma(q(t)) := Vq(t) + \frac{1}{2}\Omega(q(t) \otimes q(t)), \quad (1)$$

with the matricized tensor  $\Omega \in \mathbb{R}^{n \times k^2}$  and where  $\otimes$  stands for the *Kronecker product*.

In this work, we focus on data-driven reduced order modeling of quadratic model systems of the form

$$\dot{x}(t) = Ax(t) + H(x(t) \otimes x(t)) + B, \quad x(0) = x_0, \quad (2)$$

with the (full order) state  $x(t) \in \mathbb{R}^n$ . As a benchmark and to introduce the basic concepts, we briefly discuss the method of *Proper Orthogonal Decomposition* (POD): Given a matrix  $X \in \mathbb{R}^{n \times k}$  of  $k$  solution snapshots

$$X = [x(t_1), x(t_2), \dots, x(t_k)], \quad (3)$$

then POD identifies a matrix  $V \in \mathbb{R}^{n \times r}$  with  $r \leq k$ , with  $V^\top V = I_r$ , so that, measured in the *Frobenius norm*  $\|\cdot\|_F$ , the projection error  $\|X - VV^\top X\|_F$ , is minimal over all possible matrices  $V \in \mathbb{R}^{n \times r}$ . This choice means that the coordinates

$$q(t) = V^\top x(t) \quad (4)$$

encode the state  $x$  in an  $r$ -dimensional space optimally on average with respect to the linear decoding

$$\tilde{x}(t) = Vq(t)$$

and with respect to the data collected in  $X$ . If, in (2), the state  $x$  is replaced by the parametrization  $\tilde{x} = Vq$  and the equations are projected onto the span of  $V^\top$ , then the POD reduced order model is obtained as

$$\dot{q}(t) = V^\top AVq(t) + V^\top H(Vq(t) \otimes Vq(t)) + V^\top B, \quad q(0) = V^\top x_0.$$

The motivations for this work are:

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- to follow the POD approach to identify low-dimensional coordinates from data
- with a quadratic decoding
- to be used for *nonintrusive model reduction* by means of *operator inference*
- with a nonlinear projection of the state equations.

The idea of using quadratic decoding has been proposed in [7] for mechanical systems, where the reduced-order coordinates can be derived from first principles. In [1], a data-driven approach for finding the coordinates has been investigated and applied in an *intrusive* way as an enhancement of POD. As we will illustrate here, this *intrusive* use of nonlinear decodings induces higher-order nonlinearities. Thus, as we will argue, the combination with *operator inference* (see, e.g., [11]), seems to make the best use of nonlinear decoding and reduced-order modelling. This idea has been followed in [4] though in a *one-sided* fashion, meaning that the nonlinear embedding is used for decoding the coordinates but not respected in the projection of the equations. Thus, one can also interpret the methodology in [4] as obtaining a classical operator inference [11] with a quadratic nonlinearity and, additionally, a quadratic correction term for decoding the original coordinates from POD coordinates.

The paper is structured as follows. In Section 2, we lay out how an intrusive model reduction based on nonlinear decodings would look like. The *nonintrusive* approach of inferring the operators for a system approximation of a lower degree is explained in Section 3 with implementation details provided in Section 4. In Section 5, we present the setup and numerical results for an example application of two-dimensional incompressible flows before concluding the paper with a summarizing discussion in Section 6.

## 2 Intrusive Model Reduction with Nonlinear Decoding

We will refer to a (*quadratic*) *manifold* of dimension  $r$ , when talking about a domain  $\mathcal{Q} \subset \mathbb{R}^r$  that is embedded into  $\mathbb{R}^n$  by a (quadratic) map  $\Gamma: \mathcal{Q} \mapsto \mathbb{R}^n$  that is differentiable and onto with a differentiable left inverse.

Assume that a low-dimensional manifold  $\mathcal{Q} \in \mathbb{R}^r$  is given that well encodes the state of (2) with the embedding  $\Gamma: \mathbb{R}^r \rightarrow \mathbb{R}^n$ . Then, replacing  $x(t)$  by  $\tilde{x}(t) = \Gamma(q(t))$  in (2) and respecting the chain rule of differentiation, we obtain the dynamical system in the reduced coordinates as

$$\partial\Gamma(q(t))\dot{q}(t) = A\Gamma(q(t)) + H(\Gamma(q(t)) \otimes \Gamma(q(t))) + B. \quad (5)$$

Since  $\Gamma$  is onto, it holds that its Jacobian  $\partial\Gamma(q(t)) =: \partial\Gamma_q$  has full column rank, so that a premultiplication by  $\partial\Gamma(q(t))^\top$  turns (5) into a regular ODE:

$$\partial\Gamma_q^\top \partial\Gamma_q \dot{q}(t) = \partial\Gamma_q^\top A\Gamma(q(t)) + \partial\Gamma_q^\top H(\Gamma(q(t)) \otimes \Gamma(q(t))) + \partial\Gamma_q^\top B \quad (6)$$

**Remark 2.1** As for the choice of the projection, we would like to make the following relevant remarks:

- Notice that the projected system (6) possesses a matrix  $\partial\Gamma_q^\top \partial\Gamma_q$  which is full rank. Hence, the system (6) is a regular ODE. This justifies the use of a  $q(t)$  dependent projection. It is worth noticing that if the reduced model was obtained by enforcing Petrov-Galerkin with the constant matrix  $W \in \mathbb{R}^{n \times r}$ , the projected mass matrix would have the form  $W^\top \partial\Gamma(q(t))$  and might not be necessarily invertible for all  $t$ .
- Doing so, as in the standard POD projection approach, we also make sure that  $\dot{q}(t)$  is the minimizer to

$$\min_{\zeta \in \mathbb{R}^r} \|\partial\Gamma(q(t))\zeta - A\Gamma(q(t)) - H(\Gamma(q(t)) \otimes \Gamma(q(t))) - B\|_F.$$

- The choice of  $\partial\Gamma(q(t))^\top$  as a projection matrix can also be motivated by  $\partial\Gamma(q(t))$  describing a basis for the tangent space to the manifold  $\Gamma(\mathcal{Q})$  at  $\Gamma(q(t))$ .

If the map  $\Gamma$  is quadratic in form of (1), its Jacobian at point  $q(t)$  is given as the linear map

$$\tilde{q} \mapsto V\tilde{q} + \frac{1}{2}(\Omega(q(t) \otimes \tilde{q}) + \Omega(\tilde{q} \otimes q(t))) \quad (7)$$

that can be realized as a matrix as in the formulas provided in [2, Sec. 7.2].

From (7), it can be seen that  $\partial\Gamma(q(t))$  itself is linear in  $q(t)$ , so that premultiplication by  $\partial\Gamma_q^\top$  will increase the degrees of the polynomials in the states  $q(t)$ , e.g., the projected constant term will be realized as

$$\partial\Gamma_q^\top B = \tilde{B}_1 + \tilde{B}_2 q(t).$$

Overall, the nonlinearly reduced model using the quadratic manifold projection that approximates (2) will have the form

$$M_{q(t)}\dot{q}(t) = \tilde{A}_1 q(t) + \tilde{A}_2 \otimes^2 q(t) + \tilde{A}_3 \otimes^3 q(t) + \tilde{A}_4 \otimes^4 q(t) + \tilde{A}_5 \otimes^5 q(t) + \tilde{B}_1, \quad (8)$$

where  $\otimes^m q(t) := \bigotimes_{i=1}^m q(t)$ , with the  $q(t)$  dependent mass matrix  $M_{q(t)} := \partial \Gamma_q^\top \partial \Gamma_q$ , and with coefficients that, in an intrusive MOR scheme, have to be derived from the original coefficients  $A$ ,  $H$ , and  $B$  and their products with  $\partial \Gamma(q(t))^\top$ .

We will use, however, the approach of *operator inference* to extract lower-order coefficients that best approximate (8) with respect to given trajectory data.

Apart from being purely data-driven, i.e., no knowledge of the original coefficients is required, the use of *operator inference* for a model with a lower polynomial degree comes with the conceptual advantage that higher orders are possibly compensated by them. Thus, only coefficients of moderate size can be inferred, stored, and later evaluated, and possible numerical instabilities that come with large exponents are avoided. For this reason, in this work, we will limit ourselves to surrogate models of the form

$$M_{q(t)}\dot{q}(t) = \tilde{A}_1 q(t) + \tilde{A}_2 \otimes^2 q(t) + \tilde{B}_1. \quad (9)$$

### 3 Operator Inference for Low-order Approximation

In this section, we propose a non-intrusive method enabling to infer surrogate models for (2) using a quadratic encoding as in (1). Our main goal is to infer reduced-order models of the form (9). To this aim, we will require two steps. The first step is to construct the quadratic encoding using snapshots of the state. Then, based on this quadratic encoding, we will infer this reduced system operators by means of a tailored operator inference approach.

We assume that we are given a matrix  $X \in \mathbb{R}^{n \times k}$  of  $k$  solution snapshots of a dynamical system with state  $x(t) \in \mathbb{R}^n$  on a grid  $t_1 < t_2 < \dots < t_k$  as in (3) and a POD based encoding and decoding

$$q(t) = V^\top x(t) \quad \text{and} \quad \tilde{x}(t) = V q(t)$$

as in (4) with  $V \in \mathbb{R}^{n \times r}$ .

As in [1] and [4], we define the quadratic decoding as a correction of the POD decoding, which can be formulated as  $\Omega \in \mathbb{R}^{n \times k^2}$  being a minimizer for

$$\min_{\Omega \in \mathbb{R}^{n \times r^2}} \|X - VQ - \frac{1}{2}\Omega(Q \otimes_c Q)\|_F^2, \quad (10)$$

with the matrix

$$V^\top X =: Q := [q_1, q_2, \dots, q_r] \in \mathbb{R}^{r \times k}$$

and where we define

$$Q \otimes_c Q = [q_1 \otimes q_1, q_2 \otimes q_2, \dots, q_k \otimes q_k] \in \mathbb{R}^{r^2 \times k}.$$

With  $\Omega$  at hand, we realize the gradient  $\partial \Gamma q_j$  as in (7) at all snapshots  $j = 1, \dots, k$ , and, having approximated the time derivatives  $\dot{q}_j$  of the snapshots  $q_j$ , we can set up the matrix

$$\dot{Q}_M := [M_{q_1} \dot{q}_1, M_{q_2} \dot{q}_2, \dots, M_{q_r} \dot{q}_r],$$

with  $M_{q_k} = \partial \Gamma_{q_k} \partial \Gamma_{q_k}$ , and state the operator inference problem as

$$\min_{\hat{A}_1 \in \mathbb{R}^{r \times r}, \hat{A}_2 \in \mathbb{R}^{r \times r^2}, \hat{B}_1 \in \mathbb{R}^{r \times 1}} \|\dot{Q}_M - \hat{A}_1 Q - \hat{A}_2 (Q \otimes_c Q) - \hat{B}_1\|_F^2. \quad (11)$$

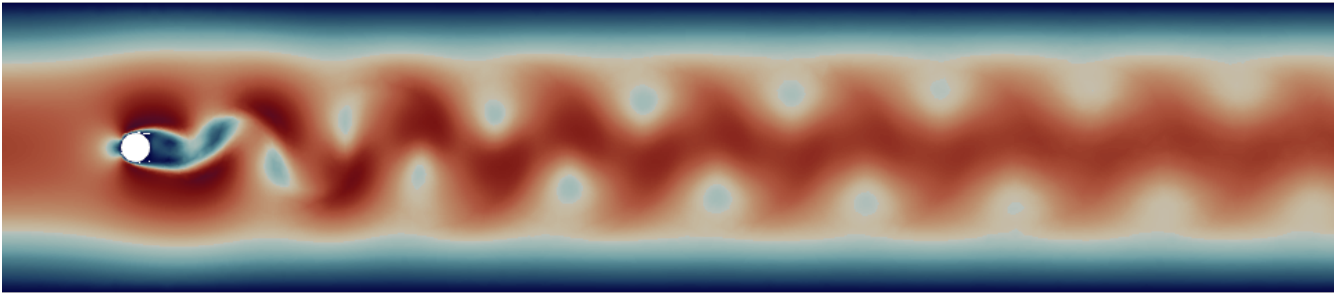
Given (approximately) minimizing solutions  $\hat{A}_1$ ,  $\hat{A}_2$ , and  $\hat{B}_1$  to (11), a lower-order approximation to (8), and via  $x(t) \approx \tilde{x}(t) = V q(t) + \frac{1}{2}\Omega q(t) \otimes q(t)$ , a reduced-order model of the dynamics of (2), is defined through

$$M_{q(t)}\dot{q}(t) = \hat{A}_1 q(t) + \hat{A}_2 (q(t) \otimes q(t)) + \hat{B}_1, \quad q(0) = V^\top x(0).$$

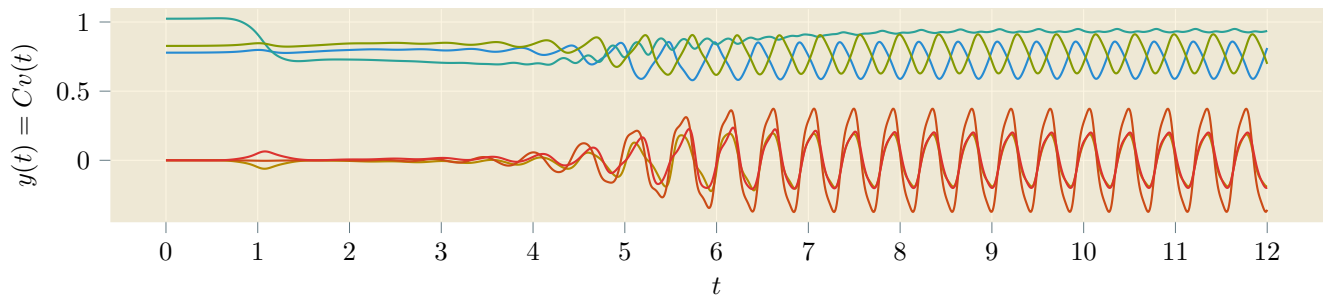
### 4 Implementation Details

Regarding the numerical implementation of the *operator inference* approach of Section 3, we address two issues.

Firstly, for a vector  $q \in \mathbb{R}^r$ , the Kronecker product  $q \otimes q \in \mathbb{R}^{r^2}$  has only  $\frac{(r+1)r}{2}$  different entries. Accordingly, the function  $\Omega(q \otimes q)$ , with  $\Omega \in \mathbb{R}^{r \times r^2}$ , can be equivalently realized by a matrix  $\tilde{\Omega} \in \mathbb{R}^{r \times \frac{(r+1)r}{2}}$  and a corresponding removal of the



**Fig. 1:** Snapshot of the velocity magnitude of the considered setup in the fully developed transient regime of  $Re = 30$ .



**Fig. 2:** Output of the full order simulation.

redundant entries of  $q \otimes q$ . We make use of this compression by directly inferring the reduced realizations of  $\Omega$  and  $A_2$  in (10) and (11).

Secondly, it has been commonly observed that an overfitting of the coefficients in (10) and (11) has adversary effects. The best results are obtained by trading in some accuracy for a smaller norm of the solutions to the optimization problems. When using the SVD to compute the coefficients, this tradeoff can be achieved by truncating the SVD at suitably chosen threshold values; see [3] for a heuristic strategy for choosing these parameters based on *L-curves*. We further note that this truncation has a similar effect as a regularization of the optimization problem as done in [4].

## 5 Numerical Example

We consider the flow past a cylinder in 2D at Reynolds number  $Re = 30$  in the startup phase from the associated steady-state *Stokes* solution and in the fully developed transient regime. The geometrical setup and a snapshot of the developed flow is presented in Figure 1; for a detailed description see [6, Sec. 5].

In the spatial domain, we use a *Finite Element* discretization that approximates the flow velocity with 41,682 degrees of freedom. We consider a time frame from  $t = 0$  to  $t = 12$  and take 2000 snapshots of the velocity solution  $v$  at equispaced time instances that cover the whole time range.

The approximation will target the actual system states  $v(t)$ , and we will report the numerical realization of the approximation error

$$\|v(t) - \tilde{v}(t)\|_{L^2(\mathcal{D}; \mathbb{R}^2)},$$

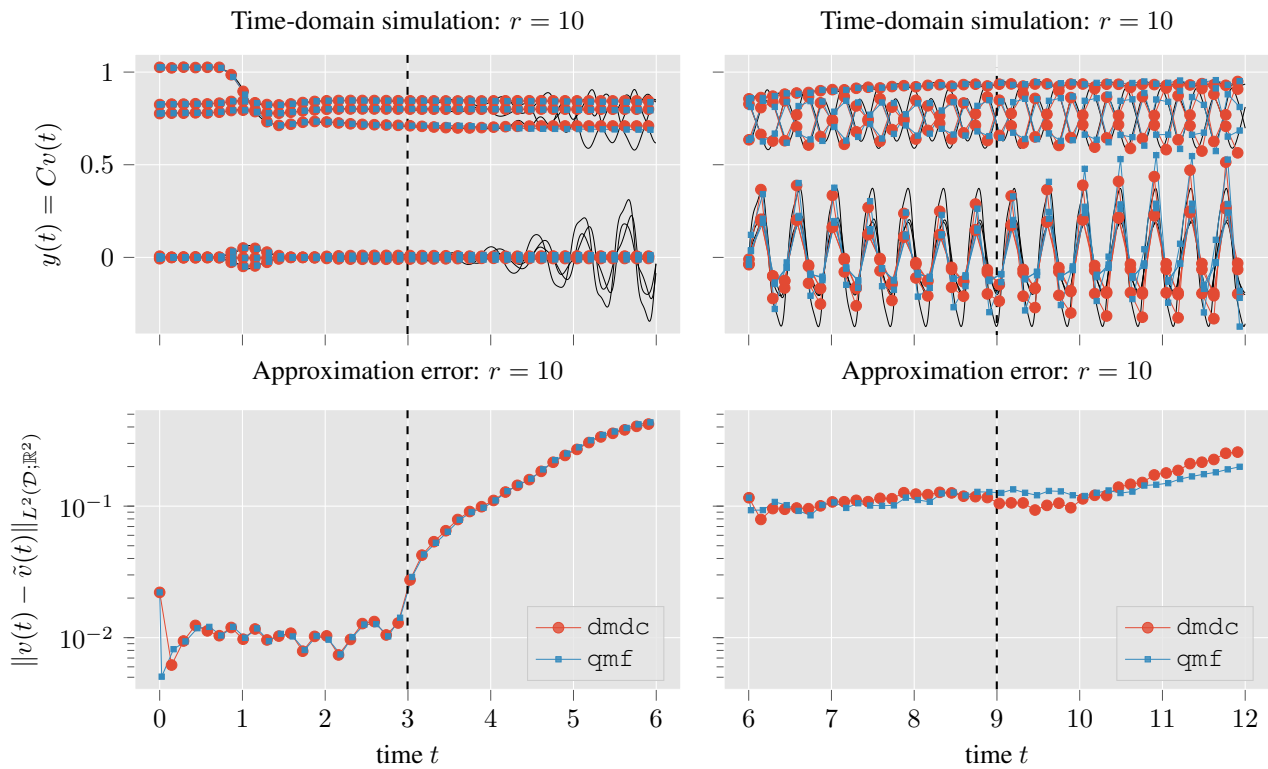
where  $(t_0, t_e)$  defines the time interval,  $v(t)$  is described by the snapshots,  $\tilde{v}(t)$  is the reconstruction from the reduced order model, and  $\mathcal{D} \subset \mathbb{R}^2$  denotes the computational domain. For illustration purposes, we report an output  $y(t) = Cv(t) \in \mathbb{R}^6$  that is obtained by measuring the locally spatially averaged values of the two components of the velocity at three *sensor locations* in the cylinder wake. The output of the full order simulation is depicted in Figure 2, showing the development of the flow from the initial state to the characteristic periodic vortex-shedding regime.

We check the performance of the following two methods:

`qm f` – the quadratic manifold approach as developed in Section 3 and

`dmdc` – the *Dynamic Mode Decomposition* with a bias term; see, e.g., [12].

Both methods are completely data-driven, and `dmdc` has shown to be a suitable benchmark because of its good performance independent of hyperparameters other than the dimension  $r$  of the reduced order model; see [3, Sec. 7.2]



**Fig. 3:** Outputs and approximation errors for the  $qmf$  and  $dmddc$  model of reduced order  $r = 10$  in the initial phase (left) and the periodic regime (right). The thin black lines in the upper plots denote the output of the full order model; cp. Figure 2. The dashed vertical lines in the lower plots separate the regions of the training data (left of the dashed line) and the region that is extrapolated by the model.

As none of the methods could encode the full transition of the rather nonphysical *Stokes* steady state towards the fully developed periodic regime, we checked the performance for the initial phase for  $t \in (0, 6)$  and the final phase for  $t \in (6, 12)$  separately with separate models. In both cases, the first 500 of the 1000 snapshots that fell into the corresponding subinterval were used to infer the models and the remaining snapshots served as an estimation for the prediction capabilities of the approaches.

The approximation results for  $r = 10$  and truncations of the SVDs that solve (10) and (11) to keep only the first 7 and 10 largest singular values, respectively, are plotted in Figure 3.

In the initial phase, both methods perform similarly. While an initial transient response is well captured, the developing transition to the periodic regime is not reflected in the outputs, and the approximation error suddenly grows once the subinterval that was covered by the training data is left. In the transient phase, both approaches show good extrapolation capabilities. Overall, on this example, the  $qmf$  approach well competes with established methods. Additional potentials and good adaptivity to other problem classes are to be provided, e.g., by a systematic optimization of the hyperparameters.

The code and the raw data of the presented numerical results are available as noted in Figure 4.

## 6 Conclusion and Discussion

The presented approach to constructing reduced-order models is purely data-driven. Future theoretical research could address system analytical investigations of low-dimensional manifolds that encode system states, e.g., as in [8] or rigorous reasoning, as in [7], that for the system under consideration, a quadratic manifold suggests itself for efficiently encoding the state.

The presented numerical results show the potential but no clear advantage over the very robust  $dmddc$  method. Future work would seek algorithmic improvements like the choice of different norms for the involved optimization problems or reliable strategies to choose hyperparameters. In a finite-element context, e.g., the corresponding discrete Sobolev norms will provide targeted measures for the optimizations that are consistent with the underlying PDE model and useful for estimating truncation errors independent of other model parameters.

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**Fig. 4:** Code and Data Availability.

The raw data and the source code of the implementations used to compute the presented results is available from  
`doi:10.5281/zenodo.7126187`  
 under the MIT license and is authored by Jan Heiland.

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