

# Model Reduction via Projection onto Nonlinear Manifolds, with Applications to Analog Circuits and Biochemical Systems

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**Abstract**—Previous model order reduction methods fit into the framework of identifying the low-order linear subspace and using the linear projection to project the full state space into the low-order subspace. Despite its simplicity, the macromodel might automatically include redundancies.

In this paper, we present a model order reduction approach, named *maniMOR*, which extends the linear projection framework to a general nonlinear projection framework. The two key ideas of *maniMOR* are (1) it explicitly separates the construction of the low-order subspace and projection operation; (2) it constructs a nonlinear manifold which captures important system responses and defines the corresponding nonlinear projection operator.

The low-order manifold subspace in *maniMOR* is identified by stitching together the low-order linear subspaces around a set of sample points on the manifold. After the manifold is determined, it is embedded into a global nonlinear coordinate system. The projection function is defined in a piece-wise linear manner, and the model evaluation is conducted directly in the manifold subspace using cheap matrix-vector product computations. As a result, a compact model is generated by pre-computing all the functions and Jacobians and storing them in a look-up table.

We apply *maniMOR* on two analog circuits and a bio-chemical system to validate its correctness. Extensive comparisons with the results of the full model and other macromodels are provided. Experimental results show that *maniMOR* manages to obtain a huge reduction – e.g., from 52 to 5 for the I/O buffer circuit and from 304 to 30 for yeast pheromone pathway system. This is less than half of the size of the TPWL model with the same accuracy. With great promise to capture important system responses, *maniMOR* presents a novel and powerful paradigm for nonlinear model reduction, and casts inspirations for further researches.

## I. INTRODUCTION

Model order reduction (MOR) has been an active research topic in CAD area for a long time. The goal of model order reduction is to automatically extract a smaller macromodel for a subcircuit/subsystem, thus enabling fast simulations/verifications of large complex systems. MOR for bio-chemical systems is also of great importance and has received much more concern than ever. Those systems have the feature that even a very small system has hundreds of reactants reacting with each other. Therefore the size of the corresponding differential equations describing the chemical reaction kinetics [1] is extremely large. In this context, macromodels enable the simulation of large higher-level chemical systems.

So far, MOR techniques for linear time invariant systems have been well-developed and widely used, such as Krylov subspace methods [2], [3], TBR methods [4], [5], and the combination of the two [6], [7]. On the other hand, nonlinear systems present a lot of challenges for MOR, and much less robust, efficient, and generally-applicable methods are available. Some of the most influential works include the TVP method [8] for time varying systems, projection-based methods based on linearization or bilinearization [9] for weakly nonlinear time-varying systems, and trajectory-based methods [10]–[13]. Almost all existing methods are based on the idea of projecting the full state space on a linear subspace, where the system dynamics evolve. However, macromodels generated under this framework seem not to achieve the most reduction in size.

In this paper, we present an approach, named *maniMOR*, to nonlinear model order reduction, based on nonlinear manifold projection. Employing *nonlinear* projection of the full state space into a low-order *nonlinear* manifold/subspace, instead of *linear* projection into

*linear* subspace in previous works, *maniMOR* is able to extract a smaller macromodel of a nonlinear system. *maniMOR* first constructs the nonlinear manifold in a way such that it captures the main behavior of the original system. (e.g., asymptotic DC response, small signal AC response, frequency conversion and distortion effects, etc.) In the course of the manifold construction, a coordinate system in the manifold subspace is built up. Accordingly, the nonlinear projection/mapping between the original space and the manifold subspace is defined – since the projection operator becomes nonlinear, it is defined and stored in a piece-wise linear fashion, rather than a single projection matrix in the linear case. Finally, in order to achieve computation reduction of the model, compact computation of the macromodel directly in the manifold coordinate is ensured by simplifying the function computation to cheap matrix-vector product operations.

The first main contribution of this paper is to extend the *linear* projection framework of previous methods to a general *nonlinear* projection framework, and to demonstrate that through nonlinear projection into a nonlinear manifold, more reduction can be obtained than its linear counterpart. In this view point, methods based on linear projection can be regarded as a special case in the nonlinear projection framework.

The second main contribution of this paper is that we propose to explicitly split the MOR procedure into two sub-problems, i.e., (1) the construction/parameterization of the nonlinear manifold where system dynamics evolve; (2) projection between the original state space and the manifold subspace. To the best of our knowledge, previous literatures have not brought into attention the concept of separating the construction of subspace and projection into the subspace, although this is implicitly done in linear-projection-based methods (where the projector defines the low-order subspace). This separation gives a better understanding of MOR methods.

The third main contribution of this paper is that we present a procedure to identify the nonlinear manifold, define the manifold coordinate system, and generate a compact model for fast simulation. The procedure identifies the nonlinear manifold and the coordinate system in a correct-by-construction manner – i.e., we ensure that the major system responses do lie on the nonlinear manifold we construct. Since the manifold is nonlinear, it is approximated by stitching together the local tangent subspaces around a set of sample points on the manifold, and the coordinate system is built along *nonlinear axes*. Accordingly, the nonlinear projection/mapping function is also defined by a piece-wise linear approximation around several nearest sample points. The generated compact model enables us to convert function and Jacobian computations into efficient matrix-vector products, by employing a piece-wise linear approximation. This is similar but distinguishable to the technique used in previous trajectory-based approaches.

The rest of the paper is organized as follows. In Section II, we briefly review the projection framework of existing MOR methods, and the trajectory-based methods. In Section III, we discuss in detail the procedure of *maniMOR*, together with some implementation details. Three examples of application of *maniMOR* are presented in Section IV. Finally, Section V concludes the paper, and proposes future research directions.





TABLE I

Methods	SEPARATION OF SUBSPACE CONSTRUCTION AND PROJECTION	
	Subspace construction guideline	Projection
Krylov-subspace	matches first few derivatives of the transfer function	$x = Vz$
TBR	matches largest few Hankel singular values	$x = Vz$
Trajectory-based	the union of subspaces at all sampled points	$x = Vz$

- Precompute the functions, Jacobians, local projection matrices at all samples, and store the model, which is essentially a look-up table.

### C. Construction of the Nonlinear Manifold and Its Coordinate System: From Linear Subspace to Nonlinear Manifold

Intuitively motivated in Section II-C and Fig. 1(b), we see that a nonlinear manifold contains more information than linear subspaces, and therefore has the potential ability to exploit more reduction of the model. Here we present the detailed procedure to construct such a nonlinear manifold.

1) *The first dimension*: The first intuition to construct our nonlinear manifold is motivated by the inverter example we mentioned in Section II-C, *i.e.*, a 1-D (size 1) model should be enough to capture the DC response of the system. In the linear case, the DC operating points constitutes a straight line going through the origin in the state space, which is defined by  $Gx + Bu = 0$ . For a nonlinear system, the DC operating points are  $x$ 's that satisfy  $f(x) + Bu = 0$ , which represent a curve in the state space. This curve can be easily computed by performing a DC sweep simulation.

Now that we have obtained a "DC curve", we regard it as a nonlinear axis. Suppose the state variable in the reduced space is  $z = [z_1, z_2, \dots, z_q]^T$ , we designate the coordinates of  $z_1$  along this "DC curve". Doing so, we ensure the DC response of the full system be exactly matched in the reduced-order model. This simple coordinate designation scheme is a natural generalization of the linear case to the nonlinear case. In linear-projection methods,  $z_1$  is along the direction of  $v_1$ , the first column of the projection matrix  $V$ . Specifically, in Krylov-subspace methods,  $v_1 = G^{-1}B$ , which exactly matches the equation for DC operating points  $Gx + Bu = 0$ .

One important question is that what should the value  $z_1$  be at different points on the "DC curve". We formulate the procedure as follows: (1) arbitrarily choose a DC operating point, and let  $z_1$  for this point to be 0; (2) choose the point  $x_j$  that is closest to points that have been designated a coordinate, among which the closest point to  $x_j$  is  $x_i$ , choose its  $z_1$  value  $z_{1j}$  such that (6) is satisfied, where the sign is determined by their relative position along the "DC curve".

$$\|z_{1j} - z_{1i}\|_2 = \|x_j - x_i\|_2 \quad (6)$$

Since locally a curve can be approximated by a straight line, the distance between two nearby points *along the curve* could reasonably be approximated by the distance between the two points. We claim this procedure is valid because it preserves the distance information between nearby points – in other words, it preserves the *geodesic* distance information between pairs of points.

2) *Beyond the first dimension*: The second thing to be captured in the nonlinear manifold is the small signal response at each DC operating point. Since locally around each DC operating point, the low-order subspace is linear, and this linear subspace can be efficiently calculated, (*e.g.*, Krylov-subspace methods), we approximate the nonlinear manifold by stitching the low-order linear subspace around each DC operating point together. Thus, all the small signal responses are captured exactly in the model.

In this case, all the axes except for the first one are linear, and the coordinates are trivially chosen, just as the linear case.

This idea could be examined in view of model order reduction for time-varying systems. Suppose the input of a time varying system is decomposed into a large signal  $u_L(t)$  and a small signal  $u_S(t)$ , *i.e.*,  $u(t) = u_L(t) + u_S(t)$ . Each value of  $u_L$  corresponds to an equilibrium

point and a local low-order linear subspace. Suppose  $q$  is size of the reduced model, and Krylov-subspace methods are used for each linearized system. The first  $q$  moments of the transfer function are matched. In trajectory-based methods, all the  $q$ -D linear subspaces at different equilibrium points are aggregated together. Therefore they render a more redundant model than *maniMOR*.

The last thing to be included in the manifold is the large signal response. It can naturally be extrapolated from the previous two ideas that we need to make the rest  $q - 1$  axes *nonlinear*. Obviously, this is a hard problem since there is no easy simulation such as the DC sweep simulation that could give us the manifold.

Based on the fact that at each point on the nonlinear manifold, the tangent linear subspace is a good approximation to the local manifold, we could say that *a point on this tangent linear subspace and close to the expansion point is also on the manifold*. Therefore, starting at any DC operating point  $x_0$ , we first calculate its Krylov subspace, and the corresponding projection matrix  $V_0 = [v_1, v_2, \dots, v_q]$ . Then, we can go an Euler step along any of the  $q - 1$  directions from  $x_0$ , and claim that the new point is also on the manifold.

For example, the simplest way is the forward Euler method in (7), where  $x_{j-1}$  is the known point on the manifold,  $x_i$  is the new point,  $v_j$  is the  $j$ -th Krylov basis,  $h$  is the step size.

$$x_i = x_{i-1} + hv_j \quad (7)$$

Accordingly, the  $z$  coordinate is chosen by increasing the corresponding  $z$  element by  $h$ . For example, if a size  $h$  step is performed along  $v_j$  direction,  $z_j$  is increased by  $h$ . When the Euler step is small enough, our assumption that the new point does lie on the nonlinear manifold is correct.<sup>4</sup>

### D. Projection Between the Nonlinear Manifold and the Full State Space

Similar to the linear-projection-based methods [10], there are two projection operations: projection of the state space  $x = f_V(z)$  and the projection of the differential equations  $W^T(z)$ . After the projection, the differential equations in the reduced-order subspace is (8).

$$W^T(z) \frac{d}{dt} q(f_V(z)) + f(f_V(z)) + Bu(t) = 0 \quad (8)$$

1) *Nonlinear projection of the state space*: We express the nonlinear projection between  $x \in \mathbb{R}^n$  and  $z \in \mathbb{R}^q$  by a nonlinear equation  $x = f_V(z)$ . However, since there is no particular form (*e.g.*, polynomial) for this nonlinear equation, we use a piece-wise linear function as an approximation.

At any sample point  $z_i$ , we write the first-order Taylor expansion of  $f_V(\cdot)$  in (9). In (9),  $f_V(z_i)$  is exactly  $x_i$ , and the term  $\frac{\partial f_V}{\partial z}$  is essentially the projection matrix  $V_i$  of the linearized system at  $x_i$ , which can be efficiently computed (*e.g.*, by Krylov subspace methods). So (9) can be simplified to (10).

$$x = f_V(z) \approx f_V(z_i) + \frac{\partial f_V}{\partial z}(z - z_i) \quad (9)$$

$$x \approx x_i + V_i(z - z_i) \quad (10)$$

<sup>4</sup>The problems are also obvious in this heuristic: (1) the number of points needed to be visited on the manifold could increase exponentially; (2) there is no theoretical proof that such a nonlinear manifold could capture large signal responses. We have been trying some other heuristics combined with this one, and some of them do give good experimental results. Though, we seek more theoretically sound manifolds to be used here.







