Structure-preserving model reduction of partially observed differential equations: molecular dynamics and beyond

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Model reduction is a major issue for control, optimization and simulation of large-scale systems. We present a formal procedure for model reduction of perturbed linear second-order differential equations. Second-order equations appear in a variety of physical contexts, e.g., in molecular dynamics or structural mechanics to mention just a few. Common spatial decomposition methods such as Proper Orthogonal Decomposition, Principal Component Analysis or the Karhunen-Loève expansion aim at identifying a subspace of "high-energy" modes onto which the dynamics is projected (Galerkin projection). These modes, however, may not be relevant for the dynamics. Moreover these methods tacitly assume that all degrees of freedom can actually be observed or measured. An alternative procedure is known by the name of Balanced Truncation which is a method of model reduction for stable input-output systems. Unlike the aforementioned approaches Balanced Truncation accounts for incomplete observability. It consists in finding a coordinate transformation such that modes which are least sensitive to the external perturbation (controllability) also give the least output (observability) and therefore can be neglected. Accordingly, a dimension-reduced model is obtained by restricting the dynamics to the subspace of the best controllable and observable modes. A great advantage of the method is that it gives computable *a priori* error bounds; a drawback is that it typically fails to preserve the problem's physical structure and suffers from lack of stability [1, 2].

Here we adopt the framework of port-Hamiltonian systems which covers the class of relevant problems and that allows for a generalization of Balanced Truncation to second-order problems, while preserving stability and the underlying Hamiltonian structure. The restriction to the controllable/observable subspace is done by imposing a holonomic constraint using techniques from singular perturbation theory for deterministic or stochastic differential equations.

Given a quadratic Hamiltonian $H : \mathbf{R}^n \times \mathbf{R}^n \to \mathbf{R}$, we consider the system

$$\begin{aligned} \dot{x}(t) &= (J - D)\, \nabla H(x(t)) + Bu(t) \\ y(t) &= C\nabla H(x(t))\,, \end{aligned} \tag{1}$$

where $J = -J^T$ is the invertible skew-symmetric structure matrix, $D = D^T \succeq 0$, and $y \in \mathbf{R}^l$ denotes a linear observable. The function $u(\cdot) \in \mathbf{R}^m$ may be either deterministic or random. As can be readily checked, the second-order equation

$$\begin{aligned} M\ddot{x}_1(t) + R\dot{x}_1(t) + Lx_1(t) &= B_2 u(t) \\ y(t) &= C_1 x_1(t) + C_2 \dot{x}_1(t) \end{aligned}$$

is an instance of the port-Hamiltonian system (1).

1. Deterministic systems

We shall make precise what it means that a state $x \in \mathbf{R}^n \times \mathbf{R}^n$ is controllable or observable. Let us assume that (1) is stable, i.e., all eigenvalues of $A = (J-D)\nabla^2 H$ are lying in the open left complex half-plane. Let us first confine ourselves to the case $u \in L^2(\mathbf{R})$ and consider the controllability function

$$L_c(x) = \min_{u \in L^2} \int_{-\infty}^{0} |u(t)|^2 \, dt \,, \quad x(-\infty) = 0, \, x(0) = x$$

that measures the minimum energy that is needed to steer the system from $x(-\infty) = 0$ to $x(0) = x$. In turn, the observability function

$$L_o(x) = \int_{0}^{\infty} |y(t)|^2 \, dt \,, \quad x(0) = x, \, u \equiv 0$$

measures the control-free energy of the output as the system evolves from $x(0) = x$ to $x(\infty) = 0$ (asymptotic stability). It is easy to see that

$$L_c(x) = x^T Q^{-1} x \,, \quad L_o(x) = x^T P x \,,$$

where the controllability Gramian Q and the observability P are the unique symmetric solutions of the Lyapunov equations

$$AQ + QA^T = -BB^T \,, \quad A^T P + PA = -W^T W$$

with the shorthands $A = (J - D)\nabla^2 H$ and $W = C\nabla^2 H$. Moore [3] has shown that if $Q, P \succ 0$ (complete controllability/observability) there exists a coordinate transformation $x \mapsto Tx$, such that the two Gramians become equal and diagonal,

$$T^{-1} Q T^{-T} = T^T P T = \operatorname{diag}(\sigma_1, \ldots, \sigma_{2n}) \,.$$

The σ_i are called the Hankel singular values of the system; they are positive and independent of the choice of coordinates. In the balanced representation all states that are least controllable also give the lowest output (small Hankel singular values), and it seems reasonable to truncate these states. The usual approach of projecting the system onto, say, the first $d < 2n$ column of T does not preserve the port-Hamiltonian structure as the balancing transformation mixes positions and generalized momenta. From a physical viewpoint it makes sense to consider the limit of vanishing small singular values, thereby forcing the system to the chosen subspace. To this end we scale the Hankel singular values according to

$$(2) \qquad (\sigma_1, \ldots, \sigma_d, \sigma_{d+1}, \ldots, \sigma_{2n}) \mapsto (\sigma_1, \ldots, \sigma_d, \delta\sigma_{d+1}, \ldots, \delta\sigma_{2n})$$

with $\delta > 0$ which implies that the balancing transformation $T = T_\delta$ becomes δ-dependent as well. Upon introducing balanced coordinates $\xi = T_\delta^{-1}x$, the port-Hamiltonian system (1) becomes the singularly perturbed system of equations

$$\begin{aligned} \dot{\xi}_1^\delta &= (\tilde{J}_{11} - \tilde{D}_{11})\frac{\partial \tilde{H}^\delta}{\partial \xi_1} + \frac{1}{\sqrt{\delta}}(\tilde{J}_{12} - \tilde{D}_{12})\frac{\partial \tilde{H}^\delta}{\partial \xi_2} + \tilde{B}_1 u \\ \dot{\xi}_2^\delta &= \frac{1}{\sqrt{\delta}}(\tilde{J}_{21} - \tilde{D}_{21})\frac{\partial \tilde{H}^\delta}{\partial \xi_1} + \frac{1}{\delta}(\tilde{J}_{22} - \tilde{D}_{22})\frac{\partial \tilde{H}^\delta}{\partial \xi_2} + \frac{1}{\sqrt{\delta}}\tilde{B}_2 u \\ y^\delta &= \tilde{C}_1\frac{\partial \tilde{H}^\delta}{\partial \xi_1} + \frac{1}{\sqrt{\delta}}\tilde{C}_2\frac{\partial \tilde{H}^\delta}{\partial \xi_2}\,, \end{aligned} \tag{3}$$

where $\tilde{J} - \tilde{D} = T_1^{-1}(J - D)T_1^{-T}$, $\tilde{B} = T_1^{-1}B$, $\tilde{C} = CT_1^{-T}$, and the partition of $\xi = (\xi_1, \xi_2) \in \mathbf{R}^d \times \mathbf{R}^{2n-d}$ is according to the separation of singular values. The balanced Hamiltonian is given by $\tilde{H}^\delta(\xi) = H(T_\delta\xi)$. We have proved in [4] borrowing arguments from geometric singular perturbation theory that the system collapses to the controllable/observable subspace as $\delta \to 0$. The limit system

$$\begin{aligned} \dot{\xi}_1(t) &= (\tilde{J}_{11} - \tilde{D}_{11})\nabla\bar{H}(\xi_1(t)) + \tilde{B}_1 u(t) \\ \bar{y}(t) &= \tilde{C}_1\nabla\bar{H}(\xi_1(t)) \end{aligned} \tag{4}$$

turns out to be a stable port-Hamiltonian system with the effective energy

$$\bar{H}(\xi_1) = \frac{1}{2}\xi_1^T\tilde{E}_1\xi_1\,, \quad \tilde{E}_1 = \tilde{E}_{11} - \tilde{E}_{12}\tilde{E}_{22}^{-1}\tilde{E}_{12}^T\,, \tag{5}$$

where $\tilde{E} = \nabla^2\tilde{H}^{\delta=1}$ in the last equation. As following from standard singular perturbation results [5] for linear control systems (4) satisfies the error bound

$$\sup_\omega \|G(i\omega) - \bar{G}(i\omega)\| < 4(\sigma_{d+1}, \ldots, \sigma_{2n})\,.$$

Here G and $\bar{G}$ are the matrix-valued transfer functions associated with (1) and (4) and $\|\cdot\|$ denotes spectral norm.

2. Partially observed Langevin equation

In equation (1), we replace the smooth control variable by Gaussian white noise, and consider the family of stable hypoelliptic Langevin equations

$$\begin{aligned} \dot{X}_t^\epsilon &= (J - D)\,\nabla H(X_t^\epsilon) + \sqrt{\epsilon}B\dot{W}_t \\ Y_t^\epsilon &= C\nabla H(X_t^\epsilon)\,, \end{aligned} \tag{6}$$

where W_t is standard Brownian motion in $\mathbf{R}^n$, and the parameter $\epsilon > 0$ controls the temperature in the system. If $2D = BB^T$ the system admits the ergodic invariant measure $d\mu^\epsilon \propto \exp(-H/\epsilon)$.

There is no control variable any longer, but we may ask to what extend a state can be excited by the noise. To this end we define the rate function

$$L_r(x) = \inf_{W \in H^1}\int_0^T |\dot{W}(t)|^2\,dt\,, \quad X_0^\epsilon = 0,\; X_T^\epsilon = x$$

and declare that $L_r(x) = \infty$ if no such realization $W \in H^1([0,T])$ exists. The typical white noise realizations are only Hölder continuous with exponent $\alpha = 1/2$, hence not absolutely continuous. At low temperature, however, Large Deviations Theory [6] asserts that the realizations of W concentrate around (measure-zero) paths that are smooth. As we have shown in [7] the rate function is given by

$$L_r(x) = x^T \Sigma_T^{-1} x\,, \quad \Sigma_T = \mathbf{E}(X_T^\epsilon \otimes X_T^\epsilon)\,.$$

For $T \to \infty$, the rate Gramian (i.e., the covariance matrix) can again be computed as the unique positive definite solution of the Lyapunov equation

$$A\Sigma + \Sigma A^T = -\epsilon BB\,.$$

Keeping the previous notion of observability (i.e., $L_o(x)$ for $\epsilon = 0$), we can balance the system such that states that are most sensitive to the noise also give the highest output. Scaling the Hankel singular values according to (2) yields again a singularly perturbed system of the form (3). Unlike in the deterministic case, sending δ to zero does not result in contraction to the most excitable/observable subspace but rather in fast random oscillations around this subspace. In the limit $\delta \to 0$ the fast modes become Gaussian random variables with mean $-\tilde{E}_{22}^{-1}\tilde{E}_{12}^T\xi_1$ and covariance $\epsilon\tilde{E}_{22}^{-1}$ and the Langevin process $Y_t^\epsilon = C\nabla H(X_t^\epsilon)$ converges in probability to the solutions of the low-dimensional Langevin equation (cf. [8])

$$\begin{aligned} \dot{Z}_t^\epsilon &= (\tilde{J}_{11} - \tilde{D}_{11})\nabla\bar{H}(Z_t^\epsilon) + \sqrt{\epsilon}\tilde{B}_1\dot{W}_t \\ \bar{Y}_t^\epsilon &= \tilde{C}_1\nabla\bar{H}(Z_t^\epsilon) \end{aligned} \tag{7}$$

with $2\tilde{D}_{11} = \tilde{B}_1\tilde{B}_1^T$ and $\bar{H}$ as given in (5). The reduced system admits an ergodic invariant measure $d\rho^\epsilon \propto \exp(-\bar{H}/\epsilon)$. Moreover $\bar{H}$ is independent of ϵ and has the meaning of the thermodynamical free energy

$$\bar{H}(z) = -\epsilon \ln \mathbf{P}_\epsilon(z)\,, \quad \mathbf{P}_\epsilon(z) = \int \delta(\xi_1 - z)d\mu^\epsilon\,.$$

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