Balancing of dissipative Hamiltonian systems

C. Hartmann

Freie Universität Berlin, Germany

Corresponding author: C. Hartmann
Institut für Mathematik, Freie Universität Berlin
Arnimallee 6, 14195 Berlin, Germany
E-mail: `chartman@mi.fu-berlin.de`

Abstract. For stable linear input-output systems, the method of Balanced Truncation (B.C. Moore, IEEE Trans. Auto. Contr. AC-26, 17-32, 1981) is a rational model reduction strategy that allows for computable error bounds. A drawback is that projecting the original equations of motion onto the subspace of interest typically fails to preserve the problem's physical structure, e.g., if the original equations are of second-order form or Hamiltonian. For Hamiltonian systems, a natural way of restricting a system to a subspace is by means of constraints, and we show, employing singular perturbation arguments, that Balanced Truncation can be done in a structure-preserving fashion. The thus obtained reduced Hamiltonian system preserves stability and passivity and satisfies the usual Hankel norm error bound. Moreover the approach allows for a straightforward generalization to stochastic systems which has also useful implications for the numerical realization of Balanced Truncation.

1 Introduction

Model reduction is a major issue for control, optimization and simulation of large-scale systems [1]. We present a method for model reduction of perturbed linear Hamiltonian systems. The Hamiltonian approach involves also second-order equations that appear in a variety of physical contexts, e.g., in molecular dynamics or structural mechanics. 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. Unlike the aforementioned approaches *Balanced Truncation* accounts for incomplete observability [2]. It consists in finding a coordinate (or balancing) transformation such that modes which are least sensitive to the input variable (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 (truncation). A great advantage of the method is that it gives computable *a priori* error bounds [3]; a drawback is that it typically fails to preserve the problem's physical structure (e.g., being Hamiltonian) and that its second-order variants suffers from lack of stability [4, 5].

Here we adopt a Hamiltonian framework that allows for a generalization of Balanced Truncation to second-order problems [6, 7]. The control variable function may be either deterministic or random where systems of the latter class are known by the name of second-order (also: underdamped) Langevin equations [8]. Confining a Hamiltonian system to a given subspace is well understood in terms of (holonomic) constraints and, although the balancing transformation mixes positions and momenta, the truncation step can be formulated as a holonomic constraints. The negligible modes in the system are associated with certain small *Hankel singular values*, and by borrowing arguments from singular perturbation theory, we show that sending them to zero forces the dynamics to the best controllable and observable subspace. The resulting low-dimensional system is a again a stable and passive Hamiltonian system with collocated inputs and outputs.

It is interesting to note that the singular perturbation argument applies to both the deterministic and the noisy case, and it turns out that the coefficients of the reduced systems are exactly the same. The types of convergence are very different though; in particular the stochastic dynamics does not converge point-wise to the controllable and observable subspace as the small singular values go to zero but rather in the sense of expectations over all realizations of the driving noise process. The deterministic problem has been addressed in [7] and we shall focus mainly on the stochastic case here, discussing convergence and issues of structure-preservation. To see how the classical notions of controllability and observability carry over to stochastic systems, we employ a large deviations principle that allows for relating the sample paths of noise process to a smooth control variable [9]. This connection is not new indeed, and a variety of large deviations problems boil down to control arguments. What is new, however, is the systematic use of controllability arguments for the purpose of model reduction of stochastic differential equations. For the stochastic system, the balancing transformation can be computed from simulation data without solving Lyapunov equations, and the similarity between the deterministic and the stochastic case suggests to exploit this correspondence as well for the deterministic system if the dimension of state space is too high to solve the corresponding Lyapunov equations.

2 Set-up: balancing dissipative Hamiltonian systems

Given a quadratic Hamiltonian

$$H \colon \mathbf{R}^{2n} \supseteq \mathbf{X} \to \mathbf{R}, \quad H(x) = \frac{1}{2} x \cdot Ex$$

with $E = E^T \succ 0$ ("$\succ$" means positive definite), we consider systems of the form

$$\dot{x}(t) = (J - D) \nabla H(x(t)) + Bu(t)$$
$$y(t) = C \nabla H(x(t)), \tag{2.1}$$

where $J \in \mathbf{R}^{2n \times 2n}$ is an invertible skew-symmetric matrix, $D \in \mathbf{R}^{2n \times 2n}$ is symmetric positive semi-definite, $B \in \mathbf{R}^{2n \times m}$ and $C \in \mathbf{R}^{l \times 2n}$ (all constant). The vector $y(\cdot) \in \mathbf{R}^l$ denotes a linear observable, and the input variable $u(\cdot) \in \mathbf{R}^m$ may be either deterministic (typically L^2) or random (white noise). For $C = B^T$ and deterministic input $u \in L^2(\mathbf{R})$, systems of type (2.1) are called port-Hamiltonian (see [10]).

As can be readily checked, the second-order system

$$M\ddot{q}(t) + R\dot{q}(t) + Kq(t) = B_2 u(t)$$
$$y(t) = C_1 q(t) + C_2 \dot{q}(t) \tag{2.2}$$

with $M, R, K \in \mathbf{R}^{n \times n}$ being symmetric positive definite, $B_2 \in \mathbf{R}^{n \times m}$ and $C_1, C_2 \in \mathbf{R}^{l \times n}$ is an instance of (2.1) where $x = (q, Mv)$ with (q, v) are coordinates on the tangent space $T\mathbf{R}^n$, and the total energy is given by the Hamiltonian

$$H(q, p) = \frac{1}{2} p \cdot M^{-1} p + \frac{1}{2} q \cdot Kq, \quad p = Mv. \tag{2.3}$$

Furthermore

$$J = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}, \quad D = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & R \end{pmatrix} \tag{2.4}$$

in (2.1) and control and observable matrices in (2.1) and (2.2) are related by

$$B = \begin{pmatrix} \mathbf{0} \\ B_2 \end{pmatrix}, \quad C = \begin{pmatrix} C_1 K^{-1} & C_2 \end{pmatrix}. \tag{2.5}$$

2.1 Stochastic Langevin equation

A prevalent model for Newtonian dynamics in a heat bath is the stochastic Langevin equation (e.g., [11])

$$M\ddot{q}(t) + \gamma \dot{q}(t) + Kq(t) = \xi(t) \tag{2.6}$$

where $\xi(t) \in \mathbf{R}^n$ denotes a Gaussian white noise process with covariance matrix

$$\mathbf{E}\left[\xi(t)\xi(t)^T\right] \propto \sigma\sigma^T.$$

Here and in the following we shall use the symbol $\mathbf{E}[\cdot]$ to denote the expectation of a (measurable) stochastic process over all its possible realizations. For equilibrium phenomena the noise process is chosen so as to balance the energy dissipation due to the viscous friction. That is, setting $\xi(t) = \sigma \dot{W}(t)$ with $\sigma \in \mathbf{R}^{n \times n}$ and $\dot{W}$ denoting Gaussian white noise, friction and noise coefficients are related by the *fluctuation-dissipation relation*

$$2\gamma = \beta \sigma \sigma^T, \quad \beta > 0. \tag{2.7}$$

The parameter $\beta = (kT)^{-1}$ with k denoting Boltzmann's constant and $T > 0$ being the temperature of the system is called the inverse temperature and has the physical dimension of energy.

An important entity associated with (2.6) is its infinitesimal generator that generates the semigroup of solutions. Using the notation of (2.1) the generator can be written as a the following second-order differential operator,

$$\mathscr{L} = \frac{1}{2} BB^T : \nabla^2 + (J - D) \nabla H \cdot \nabla \tag{2.8}$$

where $A : B = \mathrm{tr}(A^T B)$ denotes the matrix inner product. If $\gamma = \gamma^T \succ 0$ in (2.6), i.e., the noise acts on all the momentum variables, the Langevin process is stable and the operator $\mathscr{L}$ is hypoelliptic, satisfying Hörmander's condition [13]. As a consequence, (2.6) has a smooth ergodic invariant measure, given by the Boltzmann measure

$$d\mu(x) = \frac{1}{Z} \exp(-\beta H(x)) \, dx, \quad Z = \int_{\mathbf{X}} \exp(-\beta H(x)) \, dx$$

with $\beta > 0$ as defined by (2.7). Ergodicity means that any infinitely long realization of the Langevin process samples μ, and we shall exploit this property later on to extract balancing transformations from simulation data. Using the shorthand $A = (J - D)E$ with $E = \nabla^2 H(x)$ for the drift matrix and given an initial value $x(0) = x$, the solution $X(t), t > 0$ of (2.1) with white noise input $u(t) = \dot{W}(t)$ can be expressed by the stochastic integral

$$X(t) = x + \int_0^t AX(s)\,ds + \int_0^t B\,dW(s)\,.$$

As is straightforward to verify employing Itô's formula [12], the solution can be recast as

$$X(t) = \exp(At)x + \int_0^t \exp(A(t-s))B\,dW(s) \tag{2.9}$$

which resembles the known variation-of-constants-formula in the deterministic case.[1]

2.2   Balancing transformations

We shall make precise what it means that (2.1), (2.2) or (2.6) are easily controllable and observable. To this end we confine our attention to the deterministic case first and suppose that $u \in L^2(\mathbf{R})$ which obviously does not entail u being white noise. We further assume that the first-order system (2.1) is stable in the sense that all eigenvalues of

$$A = (J - D)E\,, \quad E = \nabla^2 H(x)$$

are lying in the open left complex half-plane; for, e.g., the coefficient matrices M, R, K in (2.2) being symmetric and positive definite matrices this will be the case [7]. If (2.1) is stable, the controllability function

$$L_c(x) = \min_{u \in L^2} \int_{-\infty}^0 |u(t)|^2\,dt\,, \quad x(-\infty) = 0, x(0) = x \tag{2.10}$$

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

$$L_o(x) = \int_0^\infty |y(t)|^2\,dt\,, \quad x(0) = x, u \equiv 0 \tag{2.11}$$

measures the control-free energy of the output as the system evolves from $x(0) = x$ to $x(\infty) = 0$. Note that $x(\infty) = 0$ if $u = 0$ by asymptotic stability. It is easy to see that controllability and observability function are of the form

$$L_c(x) = x \cdot W_c^{-1}x\,, \quad L_o(x) = x \cdot W_o x$$

where the controllability Gramian W_c and the observability Gramian W_o are the unique and symmetric solutions of the Lyapunov equations

$$AW_c + W_c A^T = -BB^T\,, \quad A^T W_o + W_o A = -Q^T Q \quad (Q = C\nabla^2 H)\,.$$

Moore [2] has shown that if $W_c, W_o \succ 0$ (positive definiteness = complete controllability/observability), there exists a coordinate transformation $x \mapsto Tx$ such that the two Gramians become equal and diagonal, i.e.,

$$T^{-1}W_c T^{-T} = T^T W_o T = \mathrm{diag}(\sigma_1, \ldots, \sigma_{2n})$$

where the Hankel singular values (HSV) $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{2n} > 0$ are independent of the choice of coordinates. A convenient way to express the balancing transformation is the following: Noting that Σ^2 contains the positive eigenvalues of the product $W_c W_o$ we decompose the two Gramians according to

$$W_c = XX^T\,, \quad W_o = YY^T$$

and do a singular value decomposition (SVD) of the matrix $Y^T X$, i.e.,

$$Y^T X = U\Sigma V^T = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} \Sigma_1 & \mathbf{0} \\ \mathbf{0} & \Sigma_2 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix}\,. \tag{2.12}$$

The partitioning $\Sigma_1 = \mathrm{diag}(\sigma_1, \ldots, \sigma_d)$ and $\Sigma_2 = \mathrm{diag}(\sigma_{d+1}, \ldots, \sigma_{2n})$ indicates which singular values are important and which are negligible. The remaining matrices satisfy $U_1^T U_1 = V_1^T V_1 = \mathbf{1}_{d \times d}$ and $U_2^T U_2 = V_2^T V_2 = \mathbf{1}_{r \times r}$ with $r = 2n - d$. In terms of the SVD the balancing transformation T and its inverse $S = T^{-1}$ take the form

$$T = XV\Sigma^{-1/2}\,, \quad S = \Sigma^{-1/2}U^T Y^T\,. \tag{2.13}$$

---

[1] Strictly speaking, the notation $\dot{W}$ does not make sense as the paths of the Brownian motion W are nowhere differentiable. However we will sometimes use this notation for the sake of convenience and point out that the Langevin equation has to be understood in the sense of (2.9).

It can be readily seen that the balancing transformation leaves the structure of the equations of motion (2.1) unchanged and preserves both stability and passivity. In the balanced variables $z = Sx$ our Hamiltonian system reads

$$\dot{z}(t) = (\tilde{J} - \tilde{D})\nabla \tilde{H}(z(t)) + \tilde{B}u(t)$$
$$y(t) = \tilde{C}\nabla \tilde{H}(z(t)) \tag{2.14}$$

with the balanced Hamiltonian $\tilde{H}(z) = H(Tz)$, i.e.,

$$\tilde{H}(\xi) = \frac{1}{2}z \cdot \tilde{E}z, \quad \tilde{E} = T^T ET, \tag{2.15}$$

where $E = \nabla^2 H(x)$. The transformed coefficients are given by

$$\tilde{J} = SJS^T, \quad \tilde{R} = SRS^T, \quad \tilde{B} = SB, \quad \tilde{C} = CS^T. \tag{2.16}$$

3 Balanced Truncation revisited

Balancing amounts to changing coordinates such that those states that are least influenced by the input also have least influence on the output. Accordingly *Balanced Truncation* consists in first balancing the system, and then truncating the least observable and controllable states which have little effect on the input-output behaviour.

3.1 Strong confinement limit

There are many possible ways to a truncate a balanced system such as (2.14)–(2.16); standard projection methods or naive singular perturbation methods, however, fail to preserve the systems inherent Hamiltonian structure. For mechanical system, a natural way to restrict a system to a subspace is by means of constraints which, in a Hamiltonian framework, amounts to a restriction of structure matrix (or symplectic form) *and* the Hamiltonian.

As has been shown in [7], letting the small Hankel singular values go to zero gradually eliminates the least observable and controllable states, thereby constraining the system to the dominant subspace. To understand the idea of the *confinement limit*, we suppose that d is even and scale the HSV uniformly according to

$$(\sigma_1, \ldots, \sigma_d, \sigma_{d+1}, \ldots, \sigma_{2n}) \mapsto (\sigma_1, \ldots, \sigma_d, \varepsilon\sigma_{d+1}, \ldots, \varepsilon\sigma_{2n}), \tag{3.1}$$

i.e., in (2.12)–(2.13) we replace Σ_2 by $\varepsilon\Sigma_2$ and partition the thus obtained balancing matrices accordingly,

$$S(\varepsilon) = \begin{pmatrix} S_{11} & S_{12} \\ \varepsilon^{-1/2}S_{21} & \varepsilon^{-1/2}S_{22} \end{pmatrix}, \quad T(\varepsilon) = \begin{pmatrix} T_{11} & \varepsilon^{-1/2}T_{12} \\ T_{21} & \varepsilon^{-1/2}T_{22} \end{pmatrix}.$$

Splitting the state variables $z = (z_1, z_2)$ in the same fashion and omitting the free variable in what follows, the balanced equations of motion (2.14) take the form

$$\dot{z}_1^\varepsilon = (\tilde{J}_{11} - \tilde{D}_{11})\frac{\partial \tilde{H}^\varepsilon}{\partial z_1} + \frac{1}{\sqrt{\varepsilon}}(\tilde{J}_{12} - \tilde{D}_{12})\frac{\partial \tilde{H}^\varepsilon}{\partial z_2} + \tilde{B}_1 u$$
$$\dot{z}_2^\varepsilon = \frac{1}{\sqrt{\varepsilon}}(\tilde{J}_{21} - \tilde{D}_{21})\frac{\partial \tilde{H}^\varepsilon}{\partial z_1} + \frac{1}{\varepsilon}(\tilde{J}_{22} - \tilde{D}_{22})\frac{\partial \tilde{H}^\varepsilon}{\partial z_2} + \frac{1}{\sqrt{\varepsilon}}\tilde{B}_2 u \tag{3.2}$$
$$y^\varepsilon = \tilde{C}_1\frac{\partial \tilde{H}^\varepsilon}{\partial z_1} + \frac{1}{\sqrt{\varepsilon}}\tilde{C}_2\frac{\partial \tilde{H}^\varepsilon}{\partial z_2}$$

where $\tilde{H}^\varepsilon$ denotes the scaled Hamiltonian

$$\tilde{H}^\varepsilon(z) = \frac{1}{2}z \cdot \tilde{E}^\varepsilon z, \quad \tilde{E}^\varepsilon = \begin{pmatrix} \tilde{E}_{11} & \varepsilon^{-1/2}\tilde{E}_{12} \\ \varepsilon^{-1/2}\tilde{E}_{21} & \varepsilon^{-1}\tilde{E}_{22} \end{pmatrix}.$$

Boundedness of the total energy implies that $z_2 = \mathcal{O}(\sqrt{\varepsilon})$ as $\varepsilon \to 0$. This suggests that we introduce new variables $(\zeta_1, \zeta_2) = (z_1, \varepsilon^{-1/2}z_2)$ in terms of which the scaled equations (3.2) become

$$\dot{\zeta}_1^\varepsilon = (\tilde{J}_{11} - \tilde{D}_{11})\frac{\partial \tilde{H}}{\partial \zeta_1} + \frac{1}{\varepsilon}(\tilde{J}_{12} - \tilde{D}_{12})\frac{\partial \tilde{H}}{\partial \zeta_2} + \tilde{B}_1 u$$
$$\dot{\zeta}_2^\varepsilon = \frac{1}{\varepsilon}(\tilde{J}_{21} - \tilde{D}_{21})\frac{\partial \tilde{H}}{\partial \zeta_1} + \frac{1}{\varepsilon^2}(\tilde{J}_{22} - \tilde{D}_{22})\frac{\partial \tilde{H}}{\partial \zeta_2} + \frac{1}{\varepsilon}\tilde{B}_2 u \tag{3.3}$$
$$y^\varepsilon = \tilde{C}_1\frac{\partial \tilde{H}}{\partial \zeta_1} + \frac{1}{\varepsilon}\tilde{C}_2\frac{\partial \tilde{H}}{\partial \zeta_2}$$

with $\tilde{H}(\zeta) = \tilde{H}^\varepsilon(\zeta_1, \sqrt{\varepsilon}\zeta_2)$ being now independent of ε. We have the following statement.

Theorem 3.1 (Hartmann 2008). *Let $(\zeta_1^\varepsilon(t), \zeta_2^\varepsilon(t)) \subset \mathbf{R}^d \times \mathbf{R}^{2n-d}$ be a solution of (3.3) with initial conditions $(\zeta_1^\varepsilon(0), \zeta_2^\varepsilon(0)) = (\zeta_1, \zeta_2)$ independent of ε. Then*

$$\zeta_2^\varepsilon(t) \to -\tilde{E}_{22}^{-1}\tilde{E}_{21}\zeta_1(t)$$

as $\varepsilon \to 0$ where $\zeta_1(t)$ is the solution of the stable system

$$\dot{\xi}(t) = (\tilde{J}_{11} - \tilde{D}_{11})\nabla\bar{H}(\xi(t)) + \tilde{B}_1 u(t)$$
$$y(t) = \tilde{C}_1 \nabla\bar{H}(\xi(t)).$$

(3.4)

with the effective Hamiltonian

$$\bar{H}(\xi) = \frac{1}{2}\xi \cdot \bar{E}_1 \xi, \quad \bar{E}_1 = \tilde{E}_{11} - \tilde{E}_{12}\tilde{E}_{22}^{-1}\tilde{E}_{21}.$$

(3.5)

Sketch of derivation   For a rigorous derivation of (3.4)–(3.5) using multiscale analysis of the perturbed equations (3.3) the reader is referred to [7], but we shall give some brief motivation using an energy argument. Equation (3.3) is an instance of a slow/fast system, and we seek an effective equation for the slow variable $z_1 = \zeta_1$. Now let $(\zeta_1(t), \zeta_2(t)) \subset \mathbf{R}^d \times \mathbf{R}^{2n-d}$ be a solution of (3.3). By definition, it obeys the energy balance

$$\frac{d\tilde{H}}{dt} = -\frac{\partial\tilde{H}}{\partial\zeta_1} \cdot \tilde{D}_{11}\frac{\partial\tilde{H}}{\partial\zeta_1} - \frac{2}{\varepsilon}\frac{\partial\tilde{H}}{\partial\zeta_1} \cdot \tilde{D}_{12}\frac{\partial\tilde{H}}{\partial\zeta_2} - \frac{1}{\varepsilon^2}\frac{\partial\tilde{H}}{\partial\zeta_2} \cdot \tilde{D}_{22}\frac{\partial\tilde{H}}{\partial\zeta_2} + \frac{\partial\tilde{H}}{\partial\zeta_1} \cdot \tilde{B}_1 u + \frac{1}{\varepsilon}\frac{\partial\tilde{H}}{\partial\zeta_2} \cdot \tilde{B}_2 u$$

as follows immediately upon differentiating H and inserting the equations of motion. Assuming that $\tilde{H}$ remains bounded as ε goes to zero and using the asymptotic stability of the overall dynamics, we conclude that

$$\frac{\partial\tilde{H}}{\partial\zeta_2} \to 0 \quad \text{as} \quad \varepsilon \to 0.$$

Latter implies that the dynamics admit an invariant manifold that is defined by

$$\zeta_2 = -\tilde{E}_{22}^{-1}\tilde{E}_{21}\zeta_1.$$

It furthermore follows from the stability results in [7] that the invariant manifold is uniformly hyperbolic, i.e., all trajectories with finite initial energy are exponentially attracted to the invariant manifold as $\varepsilon \to 0$. Inserting the last identity into (3.3), we obtain a closed equation for $z_1 = \zeta_1$, viz.,

$$\dot{z}_1 = (\tilde{J}_{11} - \tilde{D}_{11})(\tilde{E}_{11} - \tilde{E}_{12}\tilde{E}_{22}^{-1}\tilde{E}_{21})z_1 + \tilde{B}_1 u$$
$$y = \tilde{C}_1(\tilde{E}_{11} - \tilde{E}_{12}\tilde{E}_{22}^{-1}\tilde{E}_{21})z_1.$$

Equation (3.4) is Hamiltonian with the energy

$$\bar{H}(z_1) = \frac{1}{2}z_1 \cdot \bar{E}_1 z_1, \quad \bar{E}_1 = \tilde{E}_{11} - \tilde{E}_{12}\tilde{E}_{22}^{-1}\tilde{E}_{21}$$

and hence the assertion follows. Notice that $\tilde{J}_{11} = -\tilde{J}_{11}^T$ and $\tilde{D}_{11} = \tilde{D}_{11}^T \succcurlyeq 0$ are simply the original structure and friction matrices restricted to the subspace of the most controllable and observable states. That is, in the limit of vanishing small HSV the dynamics are confined to the controllable and observable subspace. Moreover $E = E^T \succ 0$ implies $\bar{E}_1 = \bar{E}_1^T \succ 0$ for the Schur complement, and it is easy to see that the reduced system is passive if the original system was. As for the stability of the limiting system and the invariant manifold we refer to [7].

Transfer function   Theorem 3.1 is an assertion regarding convergence of the (possibly unobserved) state variables. By the linear dependence of the observable y on the state variable x this clearly entails clearly convergence of the observable. Another (and perhaps more common way) to prove convergence of the output variable refers directly to the transfer function that can be regarded as a mapping $G: L^2([0, \infty[, \mathbf{R}^m) \to L^2([0, \infty[, \mathbf{R}^l)$ in the Laplace domain that maps the system's input to the output. In case of (3.3), the transfer function reads (see [15])

$$G^\varepsilon(s) = \tilde{C}^\varepsilon \tilde{E}(s - (\tilde{J}^\varepsilon - \tilde{D}^\varepsilon)\tilde{E})^{-1}\tilde{B}^\varepsilon$$

(3.6)

where $\tilde{E} = \nabla^2\tilde{H}$ is independent of ε, and the scaled coefficient matrices are given by

$$\tilde{J}^\varepsilon - \tilde{D}^\varepsilon = \begin{pmatrix} \tilde{J}_{11} - \tilde{D}_{11} & \varepsilon^{-1}(\tilde{J}_{12} - \tilde{D}_{12}) \\ \varepsilon^{-1}(\tilde{J}_{21} - \tilde{D}_{21}) & \varepsilon^{-2}(\tilde{J}_{22} - \tilde{D}_{22}) \end{pmatrix}$$

and

$$\tilde{B}^\varepsilon = \begin{pmatrix} \tilde{B}_1 \\ \varepsilon^{-1}\tilde{B}_2 \end{pmatrix}, \quad \tilde{C}^\varepsilon = \begin{pmatrix} \tilde{C}_1 & \varepsilon^{-1}\tilde{C}_2 \end{pmatrix}.$$

Provided that the system is stable, the transfer function is analytic in the open right half-plane, and the H^∞ norm of G can be defined as the supremum of the largest singular value of the transfer function on the imaginary axis [1],

$$\|G\|_\infty = \sup_{\omega \in \mathbf{R}} \left\{ \sigma_{\max} \left(G(i\omega) \right) \right\}.$$

It has been shown in [7] that the transfer function G^ε converges in H^∞ to the limiting transfer function

$$\bar{G}(s) = \tilde{C}_1 \bar{E}_1 (s - (\tilde{J}_{11} - \tilde{D}_{11}) \bar{E}_1)^{-1} \tilde{B}_1 \tag{3.7}$$

as $\varepsilon \to 0$. That is, we have

$$\|G^\varepsilon - \bar{G}\|_\infty \to 0 \quad \text{as} \quad \varepsilon \to 0.$$

The following can be easily shown by adapting the results in [14]:

Theorem 3.2 (Liu 1989). *Let (3.7) be the transfer function of the limit system (3.4)–(3.5). Then*

$$\|G - \bar{G}\|_\infty < 2(\sigma_{d+1} + \ldots + \sigma_{2n})$$

where $G = G^{\varepsilon=1}$ is the transfer function associated with (2.1).

4 The stochastic Langevin equation

In equation (2.1), we replace the smooth control variable by Gaussian white noise and consider the family of stable hypoelliptic Langevin equations (i.e., degenerate diffusion equations)

$$\begin{aligned} dX(t) &= (J - D)\nabla H(X(t))dt + B dW(t), \quad X(0) = x \\ Y(t) &= C\nabla H(X(t)). \end{aligned} \tag{4.1}$$

The Itô equation (4.1) is the differential version of (2.9) with W denoting standard Brownian motion in $\mathbf{R}^n$ so that $B \in \mathbf{R}^{2n \times n}$. If moreover the fluctuation-dissipation relation (2.7) is in force, i.e., if $2D = \beta BB^T$, the system admits the ergodic invariant probability measure (so-called Boltzmann measure)

$$d\mu(x) = \frac{1}{Z} \exp(-\beta H(x)) dx, \quad Z = \int_{\mathbf{X}} \exp(-\beta H(x)) dx. \tag{4.2}$$

There is no control variable any longer, yet we may ask to what extend a state can be excited by the noise. Roughly speaking and in analogy with the controllability function (2.10), we would like define a function of the form

$$\tilde{L}_c(x) = \inf_{W \in H^1} \int_0^T |\dot{W}(t)|^2 dt, \quad X(0) = 0, X(T) = x$$

where we declare that $\tilde{L}_c(x) = \infty$ if no such realization $W \in H^1([0,T])$ exists. However the typical realizations of W are Hölder continuous with exponent $\alpha \le 1/2$, hence not absolutely continuous. Even worse, the admissible H^1 realizations form a set of measure zero which renders the naive definition of the function $\tilde{L}_c(x)$ useless.

4.1 A large deviations principle

We should bear in mind that the Langevin dynamics admit the invariant measure (4.2) with smooth density $\rho(x) \propto \exp(-\beta H(x))$. Since ρ has full topological support and is positive everywhere, this suggests that all states $x \in \mathbf{X}$ are reachable in the sense of control theory. To come up with a meaningful notion of controllability of the Langevin equation, we exploit the correspondence between stochastic differential equations and control systems that is established by the famous *Support Theorem* of Stroock and Varadhan [9].

For this purpose we replace $dW(t)$ in (4.1) by the control force $u(t)dt$ with $u(\cdot) \in \mathbf{R}^n$ in which case the Langevin equation boils down to the deterministic system (2.1). Now let $V = C([0,T])$ be the space of continuous functions φ taking values on $\mathbf{X} \subseteq \mathbf{R}^{2n}$, and define $V_x = \{\varphi \in V : \varphi(0) = x\}$. Let further $X_x(t)$ be the (unique) solution of the Langevin equation (4.1) with initial value $X_x(0) = x$. Obviously, $X_x \in V_x$ and we may define the support of the diffusion process X as the smallest closed subset $U_x \subset V_x$ for which

$$\mathbf{P}[X \in U_x] = 1$$

with $\mathbf{P}[\cdot]$ being the probability measure on the path space V_x that is induced by the Brownian motion W.

Theorem 4.1 (Stroock & Varadhan 1972). *Let $F_x(t; u)$ denote the solution of the deterministic equation (2.1) with control u. Then the support of the (degenerate) diffusion process X_x is given by*

$$U_x = \overline{\{F_x(t; u) : u \in L(\mathbf{R})\}}$$

where $L(\mathbf{R})$ is the space of piecewise constant functions with values in $\mathbf{R}^n$.

Rate function It is a straight consequence of the last theorem that the reachable subspace of the Langevin equation is given by the set of states that can be reached using piecewise constant control input. In particular the space of integrable step functions is dense in L^2, so we can approximate any L^2 control by a series of step functions. This implies that we can carry over the balancing procedure to the Langevin equation by introducing the *rate function*

$$L_r(x) = \inf_{u \in L^2} \int_0^T |u(t)| ds, \quad F_0(T;u) = x \tag{4.3}$$

where $F_x(\cdot;u) \colon [0,T] \to \mathbf{X}$ is given by the map

$$F_x(t;u) = \exp(At)x + \int_0^t \exp(A(t-s))Bu(s)\, ds.$$

The term *rate function* for L_r is owed to its use in Large Deviations Theory [16]. For our purposes it suffices to say that the rate function measures the minimum noise that is needed for the process to reach $x \in \mathbf{X}$ after time $t = T$, when it was started at $x = 0$ at time $t = 0$. Now we can state:

Lemma 4.2. *The rate function of the Langevin equation (4.1) is given by*

$$L_r(x) = x \cdot \Sigma(T)^{-1}x, \tag{4.4}$$

where

$$\Sigma(t) = \mathbf{E}\left[X(t)X(t)^T\right]$$

is the $2n \times 2n$ covariance matrix of the Langevin process (2.9) started at $X(0) = 0$.

Proof. We start by revisiting the well-known property of linear control systems to have a quadratic controllability function, and then show that it can be expressed in terms of the covariance matrix. Regarding the first, let $u \in L^2$ be such that $F_0(T;u) = x$ and consider the linear mapping $S \colon L^2([0,T]) \to \mathbf{X}$ defined by

$$Su = \int_0^T \exp(A(T-s))Bu(s)\, ds.$$

By construction, we have $x = Su$. The adjoint map $S^* \colon \mathbf{X} \to L^2([0,T])$ is defined by means of the inner products

$$\langle S^*x, u\rangle_{L^2} = x \cdot Su.$$

Hence

$$(S^*x)(t) = B^T \exp(A^T(T-t))x$$

is an admissible control, i.e., the process with control $u = S^*x$ reaches x at time T. Since the Langevin process $X(t)$ is hypoelliptic (i.e., its generator $\mathscr{L}$ satisfies Hörmander's condition), the associated control system (2.1) is completely controllable. Consequently the map S is onto which implies that $SS^* \colon \mathbf{X} \to \mathbf{X}$ is invertible. Now consider *any* $u \in L^2$ with the property that $x = Su$. The optimal such u is given by minimizing $\|u\|_{L^2}^2$ subject to the linear constraint $x = Su$. The solution to this problem is known and given by the projection theorem, viz.,

$$u_* = S^* (SS^*)^{-1}x.$$

Obviously $u_* \in L^2$ and, by the definition of the rate function, we obtain

$$L_r(x) = x \cdot (SS^*)^{-1}x$$

which completes the first part of the proof. As for the identity $SS^* = \Sigma(t)$ recall equation (2.9) and consider the solution of the Langevin equation (4.1) for the initial value $X(0) = 0$:

$$X(t) = \int_0^t \exp(A(t-s))B\, dW(s).$$

The covariance matrix of $X(t)$ is defined as

$$\text{cov}(X(t)) = \mathbf{E}\left[(X(t) - \mathbf{E}X(t))(X(t) - \mathbf{E}X(t))^T\right].$$

Since $\mathbf{E}X(t) = 0$ by the first Itô isometry [12], the covariance matrix at time $t = T$ turns out to be

$$
\begin{aligned}
\mathbf{E}\left[X(T)X(T)^T\right] &= \mathbf{E}\left[\int_0^T \exp(A(T-s))B\,dW(s)\int_0^T dW(s)^T B^T \exp(A^T(T-s))\right]\\
&= \int_0^T \exp(A(T-s))BB^T \exp(A^T(T-s))\,ds\\
&= \int_0^T \exp(As)BB^T \exp(A^T s)\,ds
\end{aligned}
$$

where we have used the second Itô isometry in the second line. The assertion follows upon noting that the last integral equals SS^* from above, evaluated at time $t = T$. $\qquad\square$

4.2 Balanced Averaging of the Langevin equation (main result)

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

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

Keeping the previous notion of observability (i.e., $L_o(x)$ measures the noise-free output), 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 (3.1) yields again a singularly perturbed system of the form (see Section 3.1 for details)

$$
\begin{aligned}
d\zeta_1^\varepsilon &= (\tilde{J}_{11} - \tilde{D}_{11})\frac{\partial \tilde{H}}{\partial \zeta_1}dt + \frac{1}{\varepsilon}(\tilde{J}_{12} - \tilde{D}_{12})\frac{\partial \tilde{H}}{\partial \zeta_2}dt + \tilde{B}_1 dW\\
d\zeta_2^\varepsilon &= \frac{1}{\varepsilon}(\tilde{J}_{21} - \tilde{D}_{21})\frac{\partial \tilde{H}}{\partial \zeta_1}dt + \frac{1}{\varepsilon^2}(\tilde{J}_{22} - \tilde{D}_{22})\frac{\partial \tilde{H}}{\partial \zeta_2}dt + \frac{1}{\varepsilon}\tilde{B}_2 dW \qquad\qquad (4.5)\\
y^\varepsilon &= \tilde{C}_1\frac{\partial \tilde{H}}{\partial \zeta_1} + \frac{1}{\varepsilon}\tilde{C}_2\frac{\partial \tilde{H}}{\partial \zeta_2}
\end{aligned}
$$

with $\tilde{H}(\zeta) = \tilde{H}^\varepsilon(\zeta_1, \sqrt{\varepsilon}\zeta_2)$ being independent of ε.

Unlike in the deterministic case, sending ε to zero does not result in contraction to the most excitable (i.e. controllable) and observable subspace as the white noise process is not of bounded variation. Hence the unbounded noise will eventually push the dynamics arbitrarily far away from the essential subspace, no matter how small ε is. Still the process is stable in the sense that its stationary distribution is Gaussian with finite covariance matrix. This can be rephrased by saying that the limit $\varepsilon \to 0$ leads to fast random oscillations of the fast modes around the essential subspace with the fast variables becoming *stationary* Gaussian random variables with mean $-\tilde{E}_{22}^{-1}\tilde{E}_{21}\zeta_1$ and covariance $\beta^{-1}\tilde{E}_{22}^{-1}$ whereas the slow variables remain nonstationary on time scales of order one.

Since the distribution of the fast variables follows the slow variables instantaneously we might well replace them by their stationary distribution (i.e., their stationary averages), thereby eliminating the fast variables from the equation. The following *Averaging Principle* is our main result.

Theorem 4.3. *Let $Y^\varepsilon(t) = C\nabla H(\zeta^\varepsilon(t))$ be the observed solution of the Langevin equation (4.5) with initial conditions independent of ε. Then, as ε goes to zero, $Y^\varepsilon(t)$ converges in probability to $Y(t)$, i.e.,*

$$
\lim_{\varepsilon \to 0}\mathbf{P}\left[\sup_{t\in[0,T]}|Y^\varepsilon(t) - Y(t)| > \delta\right] \to 0 \quad \forall \delta > 0, T > 0\,.
$$

where $Y(t)$ is a Markov process that is governed by the reduced Langevin equation

$$
\begin{aligned}
d\xi(t) &= (\tilde{J}_{11} - \tilde{D}_{11})\nabla \bar{H}(\xi(t))dt + \tilde{B}_1 dW(t)\\
y(t) &= \tilde{C}_1\nabla \bar{H}(\xi(t))
\end{aligned} \qquad\qquad (4.6)
$$

with all coefficients and the effective Hamiltonian as in Theorem 3.1. If the original friction and noise coefficients satisfy the fluctuation-dissipation relation (2.7) for some $\beta > 0$, then also $2\tilde{D}_{11} = \beta\tilde{B}_1\tilde{B}_1^T$ and the reduced system admits an ergodic invariant measure that is given by the marginal Boltzman measure

$$
d\bar{\mu}(x) = \frac{1}{\bar{Z}}\exp(-\beta\bar{H}(\xi))d\xi, \quad \bar{Z} = \int_{\mathbf{R}^d}\exp(-\beta\bar{H}(\xi))d\xi\,.
$$

Moreover $\bar{H}$ can be expressed as the thermodynamical free energy

$$
\bar{H}(\xi) = -\beta^{-1}\ln\mathbf{P}_\mu(\xi), \quad \mathbf{P}_\mu(\xi) = \int_{\mathbf{X}}\delta(\zeta_1 - \xi)d\mu
$$

which is independent of β.

Proof. For the sake of brevity, we give only a formal justification of the limit equations and refer to [17] regarding convergence issues. For the observables y are linear transformations of the state variables, it suffices to restrict one's attention to them. We aim at a perturbative expansion of the solutions to (4.5). To this end we observe that the associated generator $\mathscr{L}^\varepsilon$ that generates the semigroup of solutions can be split acccording to

$$\mathscr{L}^\varepsilon = \mathscr{L}_0 + \frac{1}{\varepsilon}\mathscr{L}_1 + \frac{1}{\varepsilon^2}\mathscr{L}_2$$

with

$$\mathscr{L}_0 = \frac{1}{2}\tilde{B}_1\tilde{B}_1^T : \frac{\partial}{\partial\zeta_1} \otimes \frac{\partial}{\partial\zeta_1} + f_{11}(\zeta_1,\zeta_2)\cdot\frac{\partial}{\partial\zeta_1}$$

$$\mathscr{L}_1 = f_{12}(\zeta_1,\zeta_2)\cdot\frac{\partial}{\partial\zeta_1} + f_{21}(\zeta_1,\zeta_2)\cdot\frac{\partial}{\partial\zeta_2}$$

$$\mathscr{L}_2 = \frac{1}{2}\tilde{B}_2\tilde{B}_2^T : \frac{\partial}{\partial\zeta_2} \otimes \frac{\partial}{\partial\zeta_2} + f_{22}(\zeta_1,\zeta_2)\cdot\frac{\partial}{\partial\zeta_2}$$

and the shorthand

$$f_{ij} = (\tilde{J}_{ij} - \tilde{D}_{ij})\frac{\partial\tilde{H}}{\partial\zeta_j}.$$

Suppose $\mathscr{L}^\varepsilon$ is equipped with appropriate boundary conditions, and consider the following Cauchy problem

$$\partial_t v^\varepsilon(\zeta,t) = \mathscr{L}^\varepsilon v^\varepsilon(\zeta,t), \quad v^\varepsilon(\zeta,0) = f(\zeta) \tag{4.7}$$

that is fully equivalent to the Langevin equation (4.5) and for which we seek a perturbative expansion of the form

$$v^\varepsilon = v_0 + \varepsilon v_1 + \varepsilon^2 v_2 + \dots.$$

Plugging the ansatz in the backward equation (4.7) and equating equal powers of ε yields a hierarchy of equations the first three of which are

$$\mathscr{L}_2 v_0 = 0 \tag{4.8}$$
$$\mathscr{L}_2 v_1 = -\mathscr{L}_1 v_0 \tag{4.9}$$
$$\mathscr{L}_2 v_2 = -\mathscr{L}_0 v_0 - \mathscr{L}_1 v_1 + \partial_t v_0. \tag{4.10}$$

We proceed step by step: First of all, note that $\mathscr{L}_2$ is a differential operator in ζ_2 only and that the nullspace of $\tilde{J}_{22} - \tilde{D}_{22}$ is empty (cf. [7]). It is then easy to show that the operator satisfies a Hörmander condition, and, employing the maximum principle, we conclude that the only functions that solve (4.8) are constant in ζ_2, i.e., $v_0 = v_0(\zeta_1,t)$. By the Fredholm alternative [18], equation (4.9) has a solution if and only if the right hand side is orthogonal to the kernel of $\mathscr{L}_2^*$ where orthogonality is meant in the L^2 sense. Since the fast subsystem

$$d\zeta_2(t) = (\tilde{J}_{22} - \tilde{D}_{22})(\tilde{E}_{21}\xi + \tilde{E}_{22}\zeta_2(t))dt + \tilde{B}_2 dW(t), \quad \zeta_2(0) = \zeta_2, \tag{4.11}$$

i.e., the diffusion process generated by $\mathscr{L}_2$, is exponentially mixing for each $\zeta_1 = \xi$ fixed, the dynamics relax exponentially fast towards their invariant probability distribution. Solvability of (4.9) therefore requires that the right hand is zero when we integrate it against any function that is in the nullspace of $\mathscr{L}_2^*$, i.e., an invariant measure of the fast dynamics. By the exponential mixing results in [17] the invariant measure is unique and is given by

$$d\mu_\xi(\zeta_2) = \rho(\zeta_2;\xi)d\zeta_2, \quad \rho(\cdot;\xi) = \mathscr{N}\left(-\tilde{E}_{22}^{-1}\tilde{E}_{21}\xi, \beta^{-1}\tilde{E}_{22}^{-1}\right).$$

As v_0 is independent of ζ_2 we find that

$$\int_{\mathbf{R}^{2n-d}} \mathscr{L}_1 v_0 \, d\mu_\xi = 0,$$

i.e., the solvability condition $\mathscr{L}_1 v_0 \perp \ker\mathscr{L}_2^*$ is met. To solve equation (4.9) for the unknown v_1 we follow the route taken in [19] and observe that v_1 must be of the form

$$v_1(\zeta_1,\zeta_2,t) = \phi(\zeta_1,\zeta_2)^T \nabla v_0(\zeta_1,t) + \psi(\zeta_1,t)$$

where $\psi \in \ker \mathscr{L}_2$ plays no role in what follows so we set it to zero. Equation (4.9) can now be recast as an equation for $\phi : \mathbf{X} \to \mathbf{R}^d$, the so-called cell problem

$$\mathscr{L}_2 \phi = -f_{12}^T. \tag{4.12}$$

In (4.7), the initial condition is independent of ε, therefore $v_1(\zeta, 0) = 0$ which leaves the only possible choices $v_0 = c$ or $\phi = 0$. If we exclude the trivial stationary solution v_0 being constant, consistency of (4.12) requires that $f_{12} = 0$, i.e., the initial conditions for ζ_2 are drawn from the equilibrium distribution μ_ξ. (In the language of the deterministic system this means that the admissible initial condition are restricted to the invariant subspace.) To conclude, the Fredholm alternative for equation (4.10) entails the solvability condition

$$\int_{\mathbf{R}^{2n-d}} \left(\partial_t v_0 - \mathscr{L}_0 v_0 - \mathscr{L}_1 \phi \nabla v_0 \right) d\mu_\xi = 0$$

which, for $\phi = 0$, can be recast as an equation for ζ_1, namely,

$$\partial_t v_0(\zeta_1, t) = \left(\frac{1}{2} \tilde{B}_1 \tilde{B}_1^T : \nabla^2 + \bar{f} \cdot \nabla \right) v_0(\zeta_1, t) \tag{4.13}$$

where we have introduced the abbreviation

$$\bar{f} \quad = \quad (\tilde{J}_{11} - \tilde{D}_{11})(\tilde{E}_{11} - \tilde{E}_{12}\tilde{E}_{22}^{-1}\tilde{E}_{21})\zeta_1 .$$

As can be readily checked, (4.6) is the stochastic Langevin equation associated with (4.13). The free energy property of the Hamiltonian follows upon completing the square in the expression for the marginal distribution

$$\begin{aligned} \bar{H}(\xi) \quad &= \quad -\beta^{-1} \ln \int_{\mathbf{X}} \delta(\zeta_1 - \xi) d\mu \\ &= \quad -\beta^{-1} \ln \frac{1}{Z} \int_{\mathbf{R}^{2n-d}} \exp(-\beta \tilde{H}(\xi, \eta)) \sqrt{\det T} d\eta \\ &= \quad \frac{1}{2} \xi \cdot (\tilde{E}_{11} - \tilde{E}_{12}\tilde{E}_{22}^{-1}\tilde{E}_{21})\xi + \text{const.} \end{aligned}$$

with T in the second equation denoting the balancing transformation (2.13). Ergodicity of the limit dynamics with respect to $\bar{\rho} \propto \exp(-\beta \bar{H})$ follows once more from Hörmander's condition and reference [17]. $\qquad \square$

5 Numerical issues and examples

The argument from Section 4 establishes a relation between controllability and the covariance matrix of a stable linear stochastic differential equation, and we may exploit this correspondence so as to compute controllability and obervability Gramians without solving Lyapunov equations.

Given any discrete realization $\{X_0, X_1, \ldots\}$ of (4.1) with arbitrary initial value $X_0 = x$, we define the empirical covariance matrix by

$$\Sigma_N = \frac{1}{N} \sum_{i=0}^{N-1} (X_i - \bar{X}_N)(X_i - \bar{X}_N)^T ,$$

where

$$\bar{X}_N = \frac{1}{N} \sum_{i=0}^{N-1} X_i .$$

By stability of the Langevin process and the law of large numbers (i.e., ergodicity) we have $\Sigma_N \to \Sigma$ as $N \to \infty$ with probability one for almost all initial conditions $X_0 = x$. But as the covariance matrix for $N \to \infty$ equals the controllability Gramian W_c — the reader should compare the respective Lyapunov equations —, we have just computed the controllability Gramian for (2.1). Conversely, we may compute the observability Gramian W_o from a sufficiently long realization of the adjoint stochastic system (complete observability assumed), which is numerically feasible, even if the system's dimension is too high to solve the corresponding Lyapunov equations.

The situation is even easier if the fluctuation-dissipation relation (2.7) is in force. In this case any (sufficiently long) discrete trajectory $\{X_0, X_1, \ldots\}$ is distributed according to the equilibrium distribution $\rho \propto \exp(-\beta H)$. In other words, the distribution of sample points $X_0, X_1, \ldots$ is Gaussian with mean zero and covariance given by $\beta^{-1}E^{-1}$ where $E = \nabla^2 H$ is the constant Hessian of H. Consequently the rate or observability Gramian for an equilibrium system, i.e., with coefficients satisfying (2.7), is simply given by the inverse Hessian of the Hamiltonian.
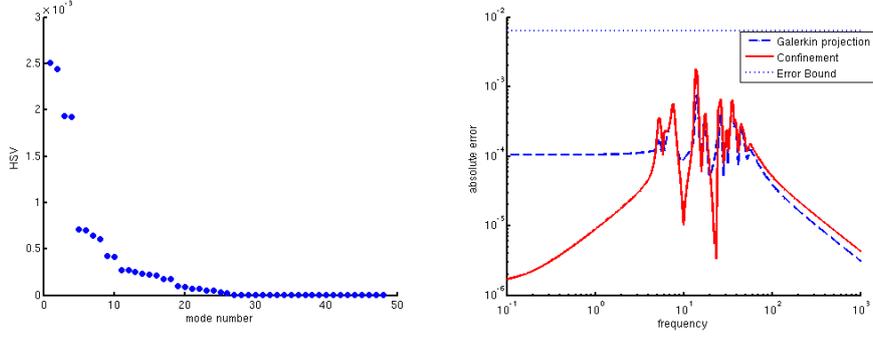
Figure 1: Hankel singular values of the building model (left panel) and a comparison between Balanced Truncation (a.k.a. Galerkin projection) and strong confinement (right panel) for an approximant of order $d = 8$.

Remark The empirical covariance matrix is the chief ingredient for computing low rank approximants of a given data set. For $\{X_0, X_1, \ldots, X_{N-1}\}$, the optimal rank-$d$ approximation

$$\min_P \sum_{i=0}^{N-1} \|X_i - PX_i\|^2 \quad \text{s.t.} \quad P^2 = P, \text{ rank } P = d$$

is obtained by choosing P to be the orthogonal projection onto the first d eigenvectors of Σ_N. Upon replacing the Euclidean inner product in the last equation by the Gramian-weighted one $\|x\|_o = \sqrt{\langle W_o x, x \rangle}$ and letting $N \to \infty$, the projection method recovers Balanced Truncation as has been pointed out in [20].

5.1 Deterministic systems: an example from structural mechanics

For a deterministic second-order system of the form (2.2), we compare two different model reduction methods: standard Balanced Truncation and reduction by strong confinement as explained in Section 3.1. As a test example we choose a stable building model with single input and output that is described in [21]. The comparison is made by computing the spectral norms of $\delta \bar{G}_d = G - \bar{G}_d$ in the frequency domain, where $\bar{G}_d : L^2([0, \infty[, \mathbf{R}) \to L^2([0, \infty[, \mathbf{R})$ stands for the respective d-th order transfer functions. For the constrained system the transfer function is given by (3.7) whereas Balanced Truncation yields a transfer function of the form

$$\bar{G}_k(s) = \tilde{Q}_1 (s - \tilde{A}_{11})^{-1} \tilde{B}_1 \,.$$

Here $\tilde{Q}_1 \in \mathbf{R}^{1 \times d}$ consists of the first d columns of $Q = C \nabla^2 H$ after balancing, $\tilde{A}_{11} \in \mathbf{R}^{d \times d}$ denotes the upper left $d \times d$ block of $A = (J - D) \nabla^2 H$ after balancing, and $\tilde{B}_1 \in \mathbf{R}^{d \times 1}$ is simply the balanced and truncated input matrix B; the transfer function G of the original system is given by (3.6) with $\varepsilon = 1$.

Figure 1 shows the results for an 8-dimensional approximation of the 48-dimensional building model. We see that both methods are well within the usual upper H^∞ bound

$$\|G - \bar{G}_k\|_\infty \leq 2(\sigma_{k+1} + \ldots + \sigma_{2n})$$

that is due to Glover [3] and that hold similarly for Balanced Truncation and singular perturbation approaches.

5.2 Stochastic systems: high friction limit of the Langevin equation

The second example is concerned with stochastic dynamics and is purely pedagogical. As we have seen Balanced Averaging preserves the structure of the Langevin equation, including its statistical equilibrium properties. However there may be situations in which the structure-preservation turns out be very subtle. An interesting scenario in this respect is the overdamped limit of the Langevin equation that also known by the name of diffusion limit or Smoluchowski equation. The following remarkable result is due to Nelson [22].

Theorem 5.1. *Let* $(Q_t^\varepsilon, P_t^\varepsilon) \subset \mathbf{R}^n \times \mathbf{R}^n$ *denote the solutions of*

$$\dot{q}(t) = \frac{\partial H^\varepsilon}{\partial p}, \quad dp(t) = -\left(\frac{\partial H^\varepsilon}{\partial q} + \gamma \frac{\partial H^\varepsilon}{\partial p}\right) dt + \sigma dW(t)$$

where friction and noise coefficients satisfy $2\gamma = \sigma \sigma^T$, *and* H^ε *is a family of Hamiltonians given by*

$$H^\varepsilon(q, p) = \frac{1}{2\varepsilon} p \cdot M^{-1} p + \frac{1}{2} q \cdot Lq \,.$$

Then, as $\varepsilon \to 0$, *the process* Q_t^ε *converges with probability one to a diffusion process* Q_t^0 *that is the solution of*

$$\gamma dq(t) = -Lq(t)dt + \sigma dW(t) \,.$$

The above limit is an example of a model reduction procedure, in which the reduced equations have a genuinely different structure (second-order vs. first-order). Nonetheless we can interpret the above result nicely in terms of our method as we shall illustrate with a simple example (cf. [8]). For $x \in \mathbf{R}^2$, consider the equation

$$
\begin{aligned}
\dot{x}_1(t) &= x_2(t) \\
dx_2(t) &= -(\varepsilon x_1(t) + x_2(t))dt + \sqrt{2\varepsilon}dW(t)
\end{aligned}
$$
(5.1)

that is a rescaled version of the above system describing damped oscillations of a stochastic particle of mass ε. By standard perturbation arguments, we might guess that, as $\varepsilon \to 0$, the dynamics degenerates to the system

$$
\begin{aligned}
\dot{x}_1 &= x_2 \\
\dot{x}_2 &= -x_2
\end{aligned}
$$

which implies $x_2(t) \approx \exp(-t)x_2(0)$ and $x_1(t) \approx -x_2(t)$ for $\varepsilon \ll 1$. However we have to be careful in neglecting terms involving ε, for the white noise is unbounded and, hence, both εx_1 and $\sqrt{2\varepsilon}\dot{W}$ can be become arbitrarily large. Now suppose we observe only the first component $y = x_1$ of the system (5.1). The two Gramians are

$$
\Sigma = \left(\begin{array}{cc} 1 & 0 \\ 0 & \varepsilon \end{array} \right), \quad W_o = \frac{1}{2\varepsilon} \left(\begin{array}{cc} 1+\varepsilon & 1 \\ 1 & 1 \end{array} \right)
$$

with corresponding Hankel singular values $\sigma_1 \sim 1/\sqrt{\varepsilon}$ and $\sigma_2 \sim \sqrt{\varepsilon}$ for $\varepsilon \to 0$. After balancing and averaging over the low energy mode we obtain the correct diffusion equation for the balanced variable $\xi = x_1$, viz.,

$$
d\xi(t) = -\varepsilon\xi(t)dt + \sqrt{2\varepsilon}dW(t).
$$

6   References

[1] A.C. Antoulas. Approximation of Large-Scaled Dynamical Systems. SIAM, 2005.

[2] B.C. Moore. Principal component analysis in linear systems: controllability, observability, and model reduction. *IEEE Trans. Auto. Contr.* **AC-26**, pp. 17–32, 1981.

[3] K. Glover. All optimal Hankel-norm approximations of linear multivariable systems and their L^∞-error bounds. *Int. J. Control* **39**, pp. 1115–1193, 1984.

[4] Y. Chahlaoui, D. Lemonnier, A. Vandendorpe and P. Van Dooren. Second-order balanced truncation. *Linear Algebra and its Applications* **415**, pp. 373–384, 2006.

[5] T. Reis and T. Stykel. Balanced truncation model reduction of second-order systems. *To appear in Math. Comput. Model. Dyn. Syst.*, 2008.

[6] R. Lopezlena, J.M.A. Scherpen, and K. Fujimoto. Energy-Storage Balanced Reduction of Port-Hamiltonian Systems. *Proc. IFAC workshop of Lagrangian and Hamiltonian Methods for Nonlinear Control, Sevilla, Spain*, pp. 79–84, 2003.

[7] C. Hartmann, V.-M. Vulcanov, and Ch. Schütte. Balanced truncation of linear second-order systems: a Hamiltonian approach. *Submitted to Mult. Mod. Sim.*, 2008.

[8] C. Hartmann and Ch. Schütte. Balancing of partially-observed stochastic differential equations. *To appear in 47th IEEE Conf. Decisions and Control*, 2008.

[9] D.W. Stroock and S.R.S. Varadhan. On the support of diffusion processes with applications to the strong maximum principle. *Proc. Sixth Berkeley Symp. Math. Statist. Prob.* **3**, pp. 333–359, 1972.

[10] A. van der Schaft. L_2-*Gain and Passivity Techniques in Nonlinear Control.* Springer, 1996.

[11] T. Schlick. *Molecular Modeling and Simulation: An Interdisciplinary Guide.* Springer, 2002.

[12] B. Øksendal. *Stochastic differential equations : an introduction with applications.* Springer, 2003.

[13] K. Ichihara and H. Kunita. A classification of second order degenerate elliptic operators and its probabilistic characterization. *Z. Wahrscheinlichkeitstheorie verw. Gebiete* **30**, pp. 235–254, 1974.

[14] Y. Liu and B.D.O. Anderson. Singular perturbation approximation of balanced systems. *Int. J. Control* **50**, pp. 1379–1405, 1989.

[15] K. Zhou, J.C. Doyle and K. Glover. *Robust and Optimal Control.* Prentice Hall, New Jersey, 1998.

[16] A. Dembo and O. Zeitouni. *Large Deviations Techniques and Applications.* Springer, 1998.

[17] A. Yu Veretennikov. On rate of mixing and the averaging principle for hypoelliptic stochastic differential equations. *Math. USSR Izv.* **33**, pp. 221–231, 1989.

[18] E. Zeidler. *Applied Functional Analysis.* Springer, 1995.

[19] G.A. Pavliotis and A.M. Stuart. *Multiscale Methods: Averaging and Homogenization.* Springer, 2008.

[20] C.W. Rowley. Model Reduction for Fluids, Using Balanced Proper Orthogonal Decomposition. *Int. J. on Bifurcation and Chaos* **15**(3):997–1013, 2005.

[21] Y. Chahlaoui and P. Van Dooren. Benchmark examples for model reduction of linear time invariant dynamical systems. In: P. Benner, D.C. Sorensen and V. Mehrmann, (eds). *Dimension Reduction of Large-Scale Systems. LNCSE 45*, pp. 379-392, Springer, 2005.

[22] E. Nelson. *Dynamical Theories of Brownian Motion.* Princeton University Press, 1967.