# BALANCED MODEL REDUCTION OF BILINEAR SYSTEMS WITH APPLICATIONS TO POSITIVE SYSTEMS 

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#### Abstract

We study balanced model reduction for stable bilinear systems in the limit of partly vanishing Hankel singular values. We show that the dynamics admit a splitting into fast and slow subspaces and prove an averaging principle for the slow dynamics. We illustrate our method with an example from stochastic control (density evolution of a dragged Brownian particle) and discuss issues of structure preservation and positivity.


## 1. Introduction

Modelling of chemical, physical or biological phenomena often leads to highdimensional systems of differential equations, resulting from semi-discretized partial differential equations. Examples involve stochastic control problems [1], dissipative quantum dynamics [2], or metabolic networks [3].

For linear systems, balanced model reduction going back to [4] provides a rational basis for various approximation techniques that include easily computable error bounds [5]; see also [6, 7] and the references given there. The general idea of balanced model reduction is to restrict the system onto the subspace of easily controllable and observable states which can be determined by the Hankel singular values associated with the system. For bilinear systems, however, neither a comprehensive theory nor the corresponding numerical algorithms for efficiently solving the corresponding generalized Lyapunov equations are available, at least not to same extend as in the linear case (cf., e.g., $[8,9,10,11,12]$ ). This article is supposed to contribute to the theoretical aspects, where only little attention is given to the numerics; regarding numerical issues we refer to, e.g, [13, 14].

For a certain class of bilinear systems, namely, stable ones, we derive balanced reduced-order models by studying the limit of vanishing Hankel singular values. To the best of our knowledge a systematic multiscale analysis of the equations of motion in the limit of vanishing Hankel singular values is new; see, e.g., [15] for a similar approach or $[16,17,18]$ for approaches in which low-rank perturbative approximations of transfer functions of linear systems are sought. Our approach resembles the well-known averaging method (see, e.g., [19] and the references therein) where the Hankel singular values serve to identify suitable small parameters. By sending the small parameters in the bilinear system to zero, we obtain an averaged lower-dimensional equation that inherits many properties of the original one.

The structure of the article is as follows: In Section 2 we briefly review controllability and observability for bilinear systems. Section 3 states the averaging problem and contains the main result, Theorem 3.2. Two numericals examples of positive systems and the problem of structure-preservation are discussed in Section 4. In Appendix A we propose an alternative approach to compute the solutions of generalized Lyapunov equations as the covariance matrix of a Markov process.

[^0]
## 2. Bilinear control systems

We consider bilinear control systems of the form

$$
\begin{align*}
& \dot{x}=A x+\sum_{k=1}^{m} N_{k} x u_{k}+B u, \quad x(0)=x_{0}  \tag{2.1}\\
& y=C x
\end{align*}
$$

where $x \in \mathbb{R}^{n}$ is the state vector, $u \in L^{2}\left(\mathbb{R}, \mathbb{R}^{m}\right)$ is the control and $y \in \mathbb{R}^{l}$ denotes vector of outputs. The matrices $A, B, C$ and $N_{k} \in \mathbb{R}^{n \times n}, k=1, \ldots, m$ are of appropriate dimensions. We suppose that the matrix $A$ is Hurwitz, i.e., all eigenvalues of $A$ have strictly negative real part.
2.1. Controllability and observability. We follow the work of Scherpen [20] on balancing of nonlinear systems and define controllability and observability of a state $x \in \mathbb{R}^{n}$ in the terms of energy norms:

Definition 2.1. The controllability and observability functions associated with the bilinear system (2.1) are defined as

$$
\begin{equation*}
E_{c}\left(x_{0}\right)=\inf _{u \in L^{2}}\left\{\int_{-\infty}^{0}|u(t)|^{2} d t: x(0)=x_{0}, x(-\infty)=0\right\} \tag{2.2}
\end{equation*}
$$

and

$$
\begin{equation*}
E_{o}\left(x_{0}\right)=\left\{\int_{0}^{\infty}|y(t)|^{2} d t: x(0)=x_{0}, u=0\right\} \tag{2.3}
\end{equation*}
$$

The function $E_{c}$ measures the minimum control effort needed to steer the system from the zero state at $t=-\infty$ to a prescribed state $x_{0} \in \mathbb{R}^{n}$ at $t=0$; note that $E_{c}$ may be infinite if a state is uncontrollable. Conversely $E_{o}$ measures the control-free output generated by a particular initial state $x_{0} \in \mathbb{R}^{n}$. It can be readily seen that

$$
\begin{equation*}
E_{o}(x)=\left\langle x, W_{o} x\right\rangle \tag{2.4}
\end{equation*}
$$

with $\langle x, z\rangle=x^{*} z$ denoting the inner product between vectors and the observability Gramian $W_{o}$ being the unique and symmetric solution of the Lyapunov equation

$$
\begin{equation*}
A^{*} W_{o}+W_{o} A+C^{*} C=0 \tag{2.5}
\end{equation*}
$$

In principle, the controllability function $E_{c}$ can be computed as the solution to some Hamilton-Jacobi PDE (see, e.g., [20]) which is not very handy for high-dimensional problems though. To avoid this problem we introduce the controllability Gramian as the solution to the generalized Lyapunov equation

$$
\begin{equation*}
A W_{c}+W_{c} A^{*}+\sum_{k=1}^{m} N_{k} W_{c} N_{k}^{*}+B B^{*}=0 \tag{2.6}
\end{equation*}
$$

that has the property

$$
\begin{equation*}
E_{c}(x)>\left\langle x, W_{c}^{-1} x\right\rangle, \quad x \neq 0 \tag{2.7}
\end{equation*}
$$

Inequality (2.7) holds true in a sufficiently small open neighbourhood of $x=0$ in which $E_{c}$ is analytic [9]. In our case it serves as a worst-case-scenario to identify hardly controllable states, for it bounds the controllability function from below.

Remark 2.2. The choice of controllability and observability function is not unique, nor is their approximation by quadratic forms as in (2.7). Ideally the choice of what well controllable and observable means should depend upon the underlying problem; cf, e.g., $[9,21,22]$. We see this flexibility as a strength of our approach, for what is going to follow does not depend on how this choice is made.

## 3. Balanced model Reduction

Let us come back to our system (2.1). Consider a coordinate transformation $x \mapsto T^{-1} x$ under which the Gramians transform according to

$$
T^{-1} W_{\mathrm{c}} T^{-*}, \quad T^{*} W_{\mathrm{o}} T
$$

Suppose that the symmetric Gramians $W_{c}, W_{o}$ are both positive definite. Then $T$ can be chosen in such a way that

$$
T^{-1} W_{\mathrm{c}} T^{-*}=\left(\begin{array}{cc}
\Sigma_{1} & 0 \\
0 & \Sigma_{2}
\end{array}\right)=T^{*} W_{\mathrm{o}} T
$$

As in the linear case the Hankel singular values (HSV) $\sigma_{i}$, i.e., the diagonal entries of $\Sigma=\left(\Sigma_{1}, \Sigma_{2}\right)$, are the square roots of the eigenvalues of the product $W_{c} W_{o}$. Hence they are independent of the choice of coordinates.

The rationale behind the balancing approach is that all states $x \in \mathbb{R}^{n}$ for which $E_{c}(x)$ is large and $E_{o}(x)$ is small do not contribute much to the system's overall input-output behaviour. Therefore, in the balanced representation $[4,5]$

$$
\left(A, B, N_{k}, C\right) \mapsto\left(T^{-1} A T, T^{-1} B, T^{-1} N_{k} T, C T\right), \quad k=1, \ldots, m
$$

we may expect that we can safely neglect all those variables corresponding to the invariant subspace of the smallest singular values $\Sigma_{2} \ll \Sigma_{1}$.

Small parameters. We shall now explain, starting from a balanced representation, how to derive a dimension-reduced version of our bilinear system (2.1). By positive definiteness we may decompose the two Gramians according to

$$
W_{c}=X X^{*}, \quad W_{o}=Y Y^{*}
$$

and do a singular value decomposition of the full-rank matrix $Y^{*} X$, i.e.,

$$
Y^{*} X=U \Sigma V^{*}=\left(\begin{array}{cc}
U_{1} & U_{2}
\end{array}\right)\left(\begin{array}{cc}
\Sigma_{1} & \mathbf{0}  \tag{3.1}\\
\mathbf{0} & \Sigma_{2}
\end{array}\right)\binom{V_{1}^{*}}{V_{2}^{*}}
$$

The partitioning $\Sigma_{1}=\operatorname{diag}\left(\sigma_{1}, \ldots, \sigma_{d}\right)$ and $\Sigma_{2}=\operatorname{diag}\left(\sigma_{d+1}, \ldots, \sigma_{n}\right)$ indicates which singular values are important and which are negligible. The remaining matrices satisfy $U_{1}^{*} U_{1}=V_{1}^{*} V_{1}=I_{d \times d}$ and $U_{2}^{*} U_{2}=V_{2}^{*} V_{2}=I_{r \times r}$ with $r=n-d$. In terms of the SVD the balancing transformation $T$ and its inverse $S=T^{-1}$ read

$$
\begin{equation*}
T=X V \Sigma^{-1 / 2}, \quad S=\Sigma^{-1 / 2} U^{*} Y^{*} \tag{3.2}
\end{equation*}
$$

as can be readily verified.
Now suppose $\sigma_{d+1} \ll \sigma_{d}$. As HSV are coordinate invariants, the $\sigma_{d+1}, \ldots, \sigma_{n}>0$ may serve a dimensionless small parameters. Upon replacing $\Sigma_{2}$ by $\epsilon \Sigma_{2}$ in equation (3.2) and changing coordinates $x \mapsto S x$ tells us where the small parameters $\Sigma_{2}$ enter the equations. Partitioning the thus obtained balancing matrices accordingly then yields

$$
S(\epsilon)=\left(\begin{array}{cc}
S_{11} & S_{12} \\
\epsilon^{-1 / 2} S_{21} & \epsilon^{-1 / 2} S_{22}
\end{array}\right), \quad T(\epsilon)=\left(\begin{array}{cc}
T_{11} & \epsilon^{-1 / 2} T_{12} \\
T_{21} & \epsilon^{-1 / 2} T_{22}
\end{array}\right)
$$

In terms of the balanced variables $z=S(\epsilon) x$ with $z=\left(z_{1}, z_{2}\right)$ our bilinear system (2.1) turns into the following singularly perturbed system of equations

$$
\begin{align*}
\dot{z}_{1} & =A_{11} z_{1}+\frac{1}{\sqrt{\epsilon}} A_{12} z_{2}+\left(N_{11} z_{1}+\frac{1}{\sqrt{\epsilon}} N_{12} z_{2}+B_{1}\right) u \\
\sqrt{\epsilon} \dot{z}_{2} & =A_{21} z_{1}+\frac{1}{\sqrt{\epsilon}} A_{22} z_{2}+\left(N_{21} z_{1}+\frac{1}{\sqrt{\epsilon}} N_{22} z_{2}+B_{2}\right) u  \tag{3.3}\\
y & =C_{1} z_{1}+\frac{1}{\sqrt{\epsilon}} C_{2} z_{2}
\end{align*}
$$

where without loss of generality we have set $m=1$, thereby omitting the summation over the bilinear terms. (The partitioning of the balanced matrices $A, B, N, C$ is evidently in accordance with the splitting into large and small HSV.)

Remark 3.1. In general we cannot be sure that the system is minimal, in which case the Gramians are only semidefinite and the balancing transformation becomes

$$
T^{-1} W_{\mathrm{c}} T^{-*}=\left(\begin{array}{cccc}
\Sigma_{1} & 0 & 0 & 0 \\
0 & \Sigma_{2} & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}\right), \quad T^{*} W_{\mathrm{o}} T=\left(\begin{array}{cccc}
\Sigma_{1} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & \Sigma_{3} & 0 \\
0 & 0 & 0 & 0
\end{array}\right)
$$

with $\Sigma_{1}, \Sigma_{2}, \Sigma_{3}$ invertible and positive definite [7]. To save the previous scaling argument we may resort to some kind of regularization approach and replace the zero HSV by entries of order $\epsilon^{s}$ with $s>1$. This will introduce an additional scale in equation (3.3) that must be taken into account. For the sake of clarity of the presentation, however, we refrain from treating the problem is such generality and assume throughout that our system (2.1) is minimal.
3.1. An averaging principle: adiabatic approximation. We now want to study the limit $\epsilon \rightarrow 0$ of vanishing small HSV. Assuming that the solutions stay bounded for all $u \in L^{2}\left(\mathbb{R}, \mathbb{R}^{m}\right)$ and for all $\epsilon>0$ we may expect that $z_{2} \rightarrow 0$ as $\epsilon \rightarrow 0$ while $z_{2} / \sqrt{\epsilon}=\mathcal{O}(1)$. It is therefore convenient to introduce the scaled variables $z_{2} \mapsto \sqrt{\epsilon} z_{2}$ by which (3.3) becomes

$$
\begin{align*}
\dot{z}_{1} & =A_{11} z_{1}+A_{12} z_{2}+\left(N_{11} z_{1}+N_{12} z_{2}+B_{1}\right) u \\
\epsilon \dot{z}_{2} & =A_{21} z_{1}+A_{22} z_{2}+\left(N_{21} z_{1}+N_{22} z_{2}+B_{2}\right) u  \tag{3.4}\\
y & =C_{1} z_{1}+C_{2} z_{2}
\end{align*}
$$

Equation (3.4) is an instance of a slow-fast system with $z_{1}$ being the slow variable and $z_{2}$ being fast. Hence, for non-pathological controls $u$, the averaging principle applies [24]. The associated (fast) system for frozen slow variable $z_{1}=\zeta$ reads $^{1}$

$$
\begin{equation*}
\dot{z}_{2}=A_{21} \zeta+A_{22} z_{2}+\left(N_{21} \zeta+N_{22} z_{2}+B_{2}\right) u \tag{3.5}
\end{equation*}
$$

The idea of the averaging principle now is to view the state space of the associated system as a fibre over the state space of the slow one. As we speed up the fast motion, i.e., as we let $\epsilon \rightarrow 0$ the influence of the fast motion on the slow one is effectively given by its stationary state (provided that it exists).

More precisely, if we denote by $\varphi_{\zeta}^{t}\left(z_{2}\right):=\varphi_{\zeta}^{t, t_{0}}\left(z_{2}\right)$ for fixed $t_{0}=0$ the solution of (3.5) for frozen slow variable $z_{1}=\zeta$, then the averaging principle asserts that in (3.4) we may replace $z_{2}$ by its asymptotic value given by

$$
m(\zeta)=\lim _{t \rightarrow \infty} \varphi_{\zeta}^{t}\left(z_{2}\right)
$$

Note that in general $m(\zeta)$ may depend on both the control $u$ and the initial value $z_{2}=\varphi_{\zeta}^{0}\left(z_{2}\right)$. But since $u$ is square integrable it follows that $u \rightarrow 0$ asymptotically which, by stability of $A$, entails $m(\zeta)=-A_{22}^{-1} A_{21} \zeta$; for details regarding the convergence of $z_{2}$ to the invariant subspace we refer to in the appendix.

The adiabatic approximation of (3.4) then consists in substituting $m\left(z_{1}\right)$ for $z_{2}$ which yields a closed equation for $z_{1}$ and the output variable $y$. We have:

Theorem 3.2. Let $y_{\epsilon}(t)$ be the observed solution of the system (3.4). Further let $\bar{y}(t)=y_{0}(t)$ be the output of the averaged or reduced system

$$
\begin{align*}
& \dot{\zeta}=\bar{A} \zeta(t)+\left(\bar{N} \zeta+B_{1}\right) u, \quad \zeta(0)=\zeta_{0} \\
& \bar{y}=\bar{C} \zeta \tag{3.6}
\end{align*}
$$

[^1]with the coefficients
$$
\bar{A}=A_{11}-A_{12} A_{22}^{-1} A_{21}, \bar{N}=N_{11}-N_{12} A_{22}^{-1} A_{21}, \bar{C}=C_{1}-C_{2} A_{22}^{-1} A_{21}
$$

Then

$$
\lim _{\epsilon \rightarrow 0}\left|y_{\epsilon}(t)-\bar{y}(t)\right|=0
$$

uniformly for $t \in[0, T]$ and for all initial conditions $\left(z_{1}(0), z_{2}(0)\right)$ with $z_{1}(0)=\zeta_{0}$.
Comparison with balanced truncation. The reader may wonder how the adiabatic approximation relates to the usual method of balanced truncation. Roughly speaking balanced truncation amounts to setting $z_{2}=0$ in the balanced equations (3.4), whereas singular perturbation methods seek a closure of the equations by arguing that $\dot{z}_{2} \approx 0$ (see, e.g., [16]). Clearly, our approach belongs to the second category as we use that $\dot{z}_{2} \rightarrow 0$ in the limit of vanishing small HSV (cf. [24]). In case of linear systems, both truncation and singular perturbation approximation can be shown to yield reduced systems that preserve stability and that obey the usual $H^{\infty}$ error bound [5]. Although we strongly believe that a similar result may hold for bilinear systems, it is clear that proving such a result would require completely different mathematical techniques which is beyond the scope of this article.

Remark 3.3. It is interesting to note that the limiting equations (3.6) resemble the result of the Schur complement method that is employed for solving partial differential equations on complicated domains (see, e.g., [25]). In the language of our approach this is to say that we decompose our system's state space (i.e., the computational domain) into controllable/observable and hardly controllable/observable subspaces and restrict the solution to the first one where the latter enters the problem in form of stationary boundary terms.
3.2. Proof of the averaging principle. For the proof of Theorem 3.2 is suffices to prove convergence for the state space variables $z_{1}, z_{2}$, ignoring the output $y$. Let us assume that the system (3.4) is completely controllable, i.e., its controllability function (2.2) is finite. For the sake of convenience, we write the first two equations in (3.4) as the abstract system of equations

$$
\begin{align*}
\dot{z}_{1} & =f\left(z_{1}, z_{2}, u\right) \\
\epsilon \dot{z}_{2} & =g\left(z_{1}, z_{2}, u\right) \tag{3.7}
\end{align*}
$$

with $\left(z_{1}, z_{2}\right) \in \mathbb{R}^{d} \times \mathbb{R}^{n-d}$ and $0<\epsilon \ll 1$ and $\left(z_{1}, z_{2}\right)=(0,0)$ being a globally asymptotically stable fixed-point.

We prove that in the limit $\epsilon \rightarrow 0$ and for $u$ being square-integrable on the real line, the slow component $z_{1}$ converges uniformly to $\zeta$ that is governed by

$$
\dot{\zeta}=f(\zeta, m(\zeta), u)
$$

where $z_{2}=m(\zeta)$ is the graph representation of the limiting invariant subspace

$$
M=\left\{\left(\zeta, z_{2}\right) \in \mathbb{R}^{d} \times \mathbb{R}^{n-d}: g\left(\zeta, z_{2}, 0\right)=0\right\} \subset \mathbb{R}^{n}
$$

that the fast dynamics approach as $\epsilon \rightarrow 0$.
Contractivity and admissible controls. Suppose that $z_{1}=\zeta$ is fixed. By asymptotic stability of the global fixed-point $(0,0) \in \mathbb{R}^{d} \times \mathbb{R}^{n-d}$ the fast subsystem has a stable fixed-point too if $u$ decays as $t \rightarrow \infty$ (recall that $u$ is assumed to be in $\left.L^{2}\right)$. That is, for all $\zeta \in \mathbb{R}^{d}$ fixed, the solution $\varphi_{\zeta}^{t}\left(z_{2}\right):=\varphi_{\zeta}^{t, t_{0}}\left(z_{2}\right)$ of the associated system (here and in the following we set $t_{0}=0$ )

$$
\dot{z}_{2}=g\left(\zeta, z_{2}, u\right)
$$

has a unique exponentially attracting fixed point, i.e.,

$$
\lim _{t \rightarrow \infty} \varphi_{\zeta}^{t}\left(z_{2}\right)=m(\zeta)
$$

uniformly in $\zeta$ and $\epsilon>0$ and independently of the initial condition $\varphi_{\zeta}^{0}\left(z_{2}\right)=z_{2}$. For this purpose, we note that $g(\zeta, m(\zeta), 0)=0$ where $g$ meets the following contractivity condition: for any $\zeta \in \mathbb{R}^{d}$ and $z_{2}, \tilde{z}_{2} \in \mathbb{R}^{n-d}$ there exist $\alpha, \delta>0$ such that

$$
\begin{equation*}
\left\langle g\left(\zeta, z_{2}, u\right)-g\left(\zeta, \tilde{z}_{2}, u\right), z_{2}-\tilde{z}_{2}\right\rangle \leq-\alpha\left|z_{2}-\tilde{z}_{2}\right|^{2} \tag{3.8}
\end{equation*}
$$

for all admissible controls $u$ with $|u| \leq \delta$.
The convergence of the fast dynamics to their fixed-point on finite time intervals (with respect to the time scale of the slow variables) requires to impose further restrictions on the control. Recall that the balancing method assumes that $u$ is in $L^{2}$, hence $u \rightarrow 0$ as $t \rightarrow \infty$. Furthermore, in the argument above, we have assumed that the controls are still active on the time scale of the fast variables. Specifically, we restrict $u$ to the class of relatively slow controls that has been introduced by Gaitsgory [26]; see also [27]. Roughly speaking we assume that as $\epsilon \rightarrow 0$ the control law has the asymptotic form $u\left(t / \epsilon^{\gamma}\right)$ with $0<\gamma<1$, so that the controls act on an intermediate time scale between the slow and the fast variables.

Convergence to the invariant subspace. We implement the following standing assumptions that are justified by the non-explosiveness of the solutions to (3.7) on any finite time interval $[0, T]$ : we suppose that there exists a uniform Lipschitz constant $L>0$ and an open set $U \times V \subset \mathbb{R}^{d} \times \mathbb{R}^{n-d}$ such that

$$
\begin{aligned}
\left|f\left(z_{1}, z_{2}, u\right)\right| \leq L & \forall\left(z_{1}, z_{2}\right) \in U \times V \\
\left|\nabla f\left(z_{1}, z_{2}, u\right)\right| \leq L & \forall\left(z_{1}, z_{2}\right) \in U \times V \\
\left|\nabla m\left(z_{1}\right)\right| \leq L & \forall z_{1} \in U
\end{aligned}
$$

for a suitable class of admissible controls, e.g., $u \in L^{2}\left(\mathbb{R}, \mathbb{R}^{m}\right) \cap L^{\infty}\left(\mathbb{R}, \mathbb{R}^{m}\right)$ with $|u|<\delta$. We further assume that

$$
\left|g\left(z_{1}, m\left(z_{1}\right), u\right)\right| \leq L u \quad \forall\left(z_{1}, z_{2}\right) \in U \times V
$$

and define the deviations of the fast variable from the invariant manifold by

$$
\eta=z_{2}-m(\zeta)
$$

As a first step we estimate the rate at which $\eta$ goes to zero as $\epsilon \rightarrow 0$. Since

$$
\dot{\eta}=\dot{z}_{2}-\nabla m(\zeta) \dot{\zeta}
$$

the augmented set of variables $\left(\zeta, \eta, z_{2}\right)$ is governed by the joint system of equations

$$
\begin{aligned}
\dot{\zeta} & =f(\zeta, m(\zeta)+\eta, u) \\
\dot{\eta} & =\frac{1}{\epsilon} g(\zeta, m(\zeta)+\eta, u)-\nabla m(\zeta) f(\zeta, m(\zeta), u) \\
\dot{z}_{2} & =\frac{1}{\epsilon} g(\zeta, m(\zeta)+\eta, u)
\end{aligned}
$$

that is equivalent to (3.7). By adding zero, the second equation can be recast as

$$
\dot{\eta}=\frac{1}{\epsilon}(g(\zeta, m(\zeta)+\eta, u)-g(\zeta, m(\zeta), u)+g(\zeta, m(\zeta), u))-\nabla m(\zeta) f(\zeta, m(\zeta), u)
$$

Lipschitz continuity of $f, g$ and $m$ and the Cauchy-Schwarz inequality entail

$$
g(\zeta, m(\zeta), u) \leq L u, \quad\langle\nabla m(\zeta) f(\zeta, m(\zeta), u), \eta\rangle \leq L^{2}|\eta|
$$

Using further equation (3.8), i.e.,

$$
\langle g(\zeta, m(\zeta)+\eta, u)-g(\zeta, m(\zeta), u), \eta\rangle \leq-\alpha|\eta|^{2}
$$

we obtain the following differential inequality for $\eta$ :

$$
\begin{aligned}
\frac{1}{2} \frac{d}{d t}|\eta|^{2} & =\langle\eta, \dot{\eta}\rangle \\
& =\frac{1}{\epsilon}\langle g(\zeta, m(\zeta)+\eta, u), \eta\rangle-\langle\nabla m(X) \bar{f}(X), \eta\rangle \\
& \leq-\frac{\alpha}{\epsilon}|\eta|^{2}+M|\eta|
\end{aligned}
$$

with $M=L^{2}+L u / \epsilon$. Completing the square yields

$$
\frac{1}{2}\left(\delta M-\frac{|\eta|}{\delta}\right)^{2}>0 \Rightarrow \frac{1}{2}\left(\delta^{2} M^{2}+\frac{|\eta|^{2}}{\delta^{2}}\right)>L|\eta|
$$

for any $\delta \in \mathbb{R}$. Setting $\delta=\sqrt{\epsilon / \alpha}$, we therefore find

$$
\begin{aligned}
\frac{1}{2} \frac{d}{d t}|\eta|^{2} & \leq-\frac{\alpha}{\epsilon}|\eta|^{2}+\frac{1}{2}\left(\delta^{2} M^{2}+\frac{|\eta|^{2}}{\delta^{2}}\right) \\
& \leq-\frac{\alpha}{2 \epsilon}|\eta|^{2}+\frac{\epsilon}{2 \alpha} M^{2}
\end{aligned}
$$

Thus Gronwall's Lemma gives the bound

$$
|\eta|^{2} \leq \exp \left(-\frac{\alpha}{2 \epsilon} t\right)\left(|\eta(0)|^{2}+\frac{\epsilon}{2 \alpha} \int_{0}^{t} \exp \left(\frac{\alpha}{2 \epsilon} s\right) M_{s}^{2} d s\right)
$$

where the subscript $M_{s}$ indicates the time dependence of $M$ through $u$. If we set $\hat{u}=\max \left\{u\left(t / \epsilon^{\gamma}\right): t \in[0, T]\right\}$ the integral can be bounded from above by

$$
\begin{equation*}
|\eta|^{2} \leq \exp \left(-\frac{\alpha}{2 \epsilon} t\right)|\eta(0)|^{2}+\frac{\epsilon^{2} \hat{M}^{2}}{\alpha^{2}}\left(1-\exp \left(-\frac{\alpha}{2 \epsilon} t\right)\right) \tag{3.9}
\end{equation*}
$$

with $\epsilon^{2} \hat{M}^{2}=\epsilon^{2} L^{4}+2 \epsilon L^{3} u+L^{2} \hat{u}^{2}$. Since $u \sim u\left(t / \epsilon^{\gamma}\right)$ as $\epsilon \rightarrow 0$ and therefore $\hat{u} \rightarrow 0$ we conclude that

$$
\lim _{\epsilon \rightarrow 0}|\eta(t)|^{2}=0
$$

for all $t \in[0, T]$ which implies $\eta \rightarrow 0$. This completes the first part of the proof.
Convergence of solutions. In order to show that convergence of the fast dynamics to the invariant subspace implies uniform convergence $z_{1} \rightarrow \zeta$, we note that

$$
\dot{z}_{1}=f(\zeta, m(\zeta)+\eta, u)
$$

by definition of $\eta$, and

$$
\dot{\zeta}=f(\zeta, m(\zeta), u)
$$

Using Cauchy-Schwarz and Lipschitz continuity of $f$, it readily follows that

$$
\begin{aligned}
\frac{1}{2} \frac{d}{d t}\left|z_{1}-\zeta\right|^{2} & =\left\langle z_{1}-\zeta, f(\zeta, m(\zeta)+\eta, u)-f(\zeta, m(\zeta), u)\right\rangle \\
& \leq\left|z_{1}-\zeta\right||f(\zeta, m(\zeta)+\eta, u)-f(\zeta, m(\zeta), u)| \\
& \leq L\left|z_{1}-\zeta\right||\eta|
\end{aligned}
$$

By completing the square we obtain the inhomogeneous differential inequality

$$
\frac{d}{d t}\left|z_{1}-\zeta\right|^{2} \leq L^{2}\left|z_{1}-\zeta\right|^{2}+|\eta|^{2}
$$

with $|\eta|^{2}$ as given by (3.9) above. For $z_{1}(0)=\zeta(0)$, Gronwall's Lemma yields

$$
\left|z_{1}-\zeta\right|^{2} \leq \int_{0}^{t} \exp (L(t-s))|\eta(s)|^{2} d s
$$

The assertion that $z_{1} \rightarrow \zeta$ uniformly on $[0, T]$ follows upon inserting (3.9) in the last inequality and integrating, viz.,

$$
\begin{equation*}
\left|z_{1}-\zeta\right|^{2} \leq C e^{L t}\left(\epsilon|\eta(0)|^{2}+\epsilon^{\gamma}\right) \tag{3.10}
\end{equation*}
$$



Figure 1. The optical tweezer acting with force $u$ tilts the original double well $W$ potential (solid line) to $V=W-u x$ (dashed line).

In equation (3.4), $y$ is a linear transformation of the state variables $z_{1}$ and $z_{2}=$ $\eta+m\left(z_{1}\right)$. Hence (3.10) implies convergence $y \rightarrow \bar{y}$ which proves Theorem 3.2.

Remark 3.4. We should mention a similar result that is due to Watbled [28]. Therein the author proves uniform convergence of the slow process on the interval $[0, T]$ for all $T>0$ to the solutions of a differential inclusion. The proof relies on the construction of a suitable Lyapunov functional by which convergence of the fast dynamics to an invariant manifold can be shown. Although the result is far more involved than ours, it does not give convergence rates for $\epsilon \rightarrow 0$.

Upon inspecting (3.10) we see that our error bound consist of two parts the first of which depends on the deviation of the initial condition $z_{2}(0)$ from the invariant subspace $m\left(z_{1}(0)\right)$. That is, the first term is due to the initial relaxation of the fast dynamics to the steady state, whereas the second term describes the actual approximation error that arises from replacing $f\left(z_{1}, z_{2}, u\right)$ by $f\left(z_{1}, m\left(z_{1}\right), u\right)$. Further notice that the upper bound for the error grows exponentially like $\exp (L t)$, i.e., for $t=\mathcal{O}(-\ln \epsilon)$ the upper bound becomes essentially of order 1.

## 4. Applications and numerical illustration

We shall now illustrate the balanced model reduction approach with an example from stochastic control: a semi-discretized Fokker-Planck equation with external forcing.

As the Fokker-Planck equation describes the evolution of probability distributions associated with stochastic differential equations, the state variables are nonnegative. Moreover, the system comes with a simple eigenvalue zero that corresponds to the stationary distribution of the system, i.e., the system is not asymptotically stable.
4.1. Dragged Brownian particle. Consider a stochastic particle on the real line assuming states $x \in \mathbb{R}$ that is confined by a double-well potential

$$
W(x)=\left(x^{2}-1\right)^{2}
$$

Suppose, initially, the particle is in the left well and we want to drag it to the right well; even without external forcing the particle will eventually hop to the right well, but on a time scale that is of the order $\exp (\Delta W / \sigma)$ where $\Delta W=W(0)$ denotes the energy barrier that the particle has to overcome and $\sigma>0$ is the temperature of the system [29]; in typical application scenarios $\sigma$ is small, so by dragging the particle over the barrier the transition rate can be considerably augmented.

Situations of this kind arise, e.g., in atomic force microscopy [30, 31] or singlemolecule pulling experiments $[32,33]$ in which the system is typically manipulated by an optical tweezer. To lowest order, a reasonably good model for the interaction with the particle with an optical tweezer is

$$
\phi(x ; u)=-u x
$$

where $u$ denotes the force exerted on the particle (see Figure 1). The motion of the particle is then governed by the stochastic differential equation

$$
\begin{equation*}
d X_{t}=-\nabla V\left(X_{t}, t\right) d t+\sqrt{2 \sigma} d W_{t}, \quad X_{0} \text { in the left well, e.g., } X_{0}=-1 \tag{4.1}
\end{equation*}
$$

with $0<\sigma<1 / 2$ and $V(x, t)=W(x)+\phi\left(x, u_{t}\right)$. Equivalently, the dynamics of the particle can be described in terms of its probability distribution function

$$
\rho(x, t) d x=\mathbf{P}\left[X_{t} \in[x, x+d x)\right]
$$

that is governed by the Fokker-Planck equation

$$
\begin{equation*}
\frac{\partial \rho}{\partial t}=\sigma \Delta \rho+\nabla \cdot(\rho \nabla V), \quad \rho(x, 0)=\rho_{0}(x) . \tag{4.2}
\end{equation*}
$$

Here $\rho_{0}$ denotes a smooth probability distribution that concentrates in the left potential well. For $u=0$ and for smooth potentials $W$ that grow at least quadratically (as in our case) all solutions converge exponentially fast to the Boltzmann distribution $\rho_{\infty} \propto \exp (-W / \sigma)$ that is the unique solution of the elliptic equation

$$
\sigma \Delta \rho+\nabla \cdot(\rho \nabla V)=0
$$

Discrete Fokker-Planck equation. Now let us discretize the parabolic problem on a finite spatial domain $I \subset \mathbb{R}$, say, $I=[a, b]$. Conservation of probability then requires that the (outwards) probability flux

$$
J(\rho)=\sigma \nabla \rho+\rho \nabla V
$$

vanishes at the boundaries $a$ and $b$, so that (4.2) assumes the form

$$
\begin{align*}
\frac{\partial \rho}{\partial t}=\sigma \Delta \rho+\nabla \cdot(\rho \nabla V) & (x, t) \in(a, b) \times(0, T] \\
0=\sigma \nabla \rho+\rho \nabla V & (x, t) \in\{a, b\} \times[0, T]  \tag{4.3}\\
\rho_{0}=\rho & (x, t) \in(a, b) \times\{0\}
\end{align*}
$$

As we are not interested in particularly sophisticated spatial discretization schemes we choose the simplest finite difference scheme to illustrate the basic idea: given a $\operatorname{grid}\left\{x_{1}=a, x_{2}=a+h, x_{3}=a+2 h, \ldots, x_{n}=b\right\}$ and defining $\rho_{i}(t)=\rho\left(x_{i}, t\right)$ the finite difference discretization of the initial boundary value problem (4.3) reads

$$
\dot{\rho}_{i}=\frac{\sigma}{h^{2}}\left(\rho_{i+1}-2 \rho_{i}+\rho_{i-1}\right)+\frac{W^{\prime}\left(x_{i}\right)-u}{2 h}\left(\rho_{i+1}-\rho_{i-1}\right)+W^{\prime \prime}\left(x_{i}\right) \rho_{i}
$$

for $i=2, \ldots, n-1$. At the boundaries $x_{1}=a$ and $x_{n}=b$ we have

$$
\dot{\rho}_{1}=\frac{2 \sigma}{h^{2}}\left(\rho_{2}-\rho_{1}\right)+\left(\frac{2 W^{\prime}(a)}{h}-\frac{\left(W^{\prime}(a)\right)^{2}}{\sigma}+W^{\prime \prime}(a)+\frac{u W^{\prime}(a)}{\sigma}\right) \rho_{1}
$$

and

$$
\dot{\rho}_{n}=\frac{2 \sigma}{h^{2}}\left(\rho_{n-1}-\rho_{n}\right)+\left(-\frac{2 W^{\prime}(b)}{h}-\frac{\left(W^{\prime}(b)\right)^{2}}{\sigma}+W^{\prime \prime}(b)+\frac{u W^{\prime}(b)}{\sigma}\right) \rho_{n}
$$

The initial value is given by the vector with the non-negative entries $\rho_{i}(0)=\rho_{0}\left(x_{i}\right)$. In matrix-vector notation, the last equations can be compactly written as

$$
\begin{equation*}
\dot{\rho}=A \rho+N \rho u, \quad \rho(0)=\rho_{0} \tag{4.4}
\end{equation*}
$$

where $-A \in \mathbb{R}^{n \times n}$ is an $M$-matrix with a simple eigenvalue 0 that corresponds to the discretized stationary distribution $\exp (-W / \sigma)$ on $I \subset \mathbb{R}$. Since the diffusion


Figure 2. Controlled Fokker-Planck equation: the first 15 HSV (left panel) and the approximant of degree $d=10$ (right panel). The blue curve shows the probability in the left well whereas the red curve shows how the right well is populated.
process (4.1) is reversible, i.e., satisfies detailed balance, it follows moreover that $A$ has only real eigenvalues (provided that the discretization is sufficiently fine).

We augment (4.4) by an output equation. To this end, we introduce the observable $y=\left(y_{1}, y_{2}\right)$ with $y_{i} \geq 0$ denoting the probabilities to be in the left well or the right well which yields the homogeneous system

$$
\begin{align*}
\dot{\rho} & =A \rho+N \rho u \\
y & =C \rho \tag{4.5}
\end{align*}
$$

The observation matrix $C \in \mathbb{R}^{2 \times n}$ is given by $C=\left(P_{L}, P_{R}\right)$ where $P_{L}, P_{R} \in \mathbb{R}^{n}$ denote the discrete characteristic functions of left and right potential well.

We suppose that the discrete Fokker-Planck equation (4.5) is already in balanced form, i.e., we assume that Gramians, HSV and balancing transforms have been computed (see Section 4.3 below for the details). In partitioned form (4.5) reads

$$
\begin{align*}
\dot{\rho}_{1} & =A_{11} \rho_{1}+A_{12} \rho_{2}+\left(N_{11} \rho_{1}+N_{12} \rho_{2}\right) u \\
\epsilon \dot{\rho}_{2} & =A_{21} \rho_{1}+A_{22} \rho_{2}+\left(N_{21} \rho_{1}+N_{22} \rho_{2}\right) u  \tag{4.6}\\
y & =C_{1} \rho_{1}+C_{2} \rho_{2}
\end{align*}
$$

where we have inserted the scaling parameter $\epsilon>0$ for the sake of clearness.
Since the stationary distribution, i.e., the kernel of $A$ is easily controllable and observable, we may assume the system the weakly controllable and observable modes lie in the complementary subspace. Hence we may assume that $A_{22}$ is Hurwitz (which can be easily checked numerically) so that the dominant subspace is asymptotically stable as we have assumed in the proof of Theorem 3.2. Then, as $\epsilon \rightarrow 0$, the dynamics converge to the solutions of the averaged system

$$
\begin{align*}
\dot{\rho}_{1} & =\left(A_{11}-A_{12} A_{22}^{-1} A_{21}\right) \rho_{1}+\left(N_{11}-N_{12} A_{22}^{-1} A_{21}\right) \rho_{1} u \\
y & =\left(C_{1}-C_{2} A_{22}^{-1} A_{21}\right) \rho_{1} . \tag{4.7}
\end{align*}
$$

Averaged dynamics. Notice that $\epsilon$ in equation (4.6) is a fake parameter, i.e., it does not appear in the actual equations of motion. Nonetheless it marks where the negligible HSV enter the equations which is why we can expect (4.7) to yield a reasonable approximation whenever the negligible HSV are small compared to the dominant ones.

By the $M$-matrix property of $A$ that is preserved by the balancing transformation and by the Schur complement, $\bar{A}=A_{11}-A_{12} A_{22}^{-1} A_{21}$ is a singular $M$-matrix with a simple eigenvalue zero (see [34] and the references therein). As a consequence the reduced system is positivity-preserving provided that the initial value remains positive upon balancing (which need not be the case). By the approximation result,


Figure 3. Contractivity of the invariant subspace: the left panel shows the largest 10 eigenvalues of the matrix $A_{22}$ that are responsible for the fast relaxation of the dynamics to the invariant subspace as the right plot shows (here $d=10$ ).
however, we know that when the singular values decay sufficiently fast, the output variable $y=\left(y_{1}, y_{2}\right)$ will remain non-negative. If the balanced variables stay positive the vector $\bar{v}$ solving $\bar{A} \bar{v}=0$ can moreover be interpreted as the marginal equilibrium distribution of the dominant variables (again a simple computation that exploits the fact that $\bar{A}$ is the Schur complement of the $A_{22}$ block of $A$ ).

For comparing (4.5) and (4.7) we consider the following scenario: we discretize the Fokker-Planck equation (4.2) on the domain $I=[-2,2]$ using $n=400$ grid points. As initial value we choose $\rho_{0}(x) \propto \chi_{L}(x)$ where $\chi_{L}$ is the characteristic function of the set $L \subset \mathbb{R}$ and $L=[-1.2,-0.8]$ is symmetric around the left potential minimum at $x=-1$. The forcing $u$ is given by the mollified step function

$$
u(t)=\frac{1}{2}(\tanh (t-\pi)-1),
$$

that goes to zero as $t$ grows large. For the time-discretization we use a simple forward Euler scheme with constant step size $\Delta t=5 \cdot 10^{-5}$. The temperature was set to $\sigma=1 / 2$. The dominant Hankel SV and the 400-dimensional reference trajectory together with its approximant of dimension $d=10$ are shown in Figure 2. ${ }^{2}$ The blue curve is the probability in the left well whereas the red curve depicts how the right well is populated; observe that the population maximum is reached about $t \approx \pi$ slightly before the control is turned down. Once the control is switched off, the populations of left and right well start approaching their equilibrium values.

Note that the initial values in the right panel of Figure 2 have not been projected to the invariant subspace; in point of fact starting from the invariant subspace would require that $u(0)=0$. But if the initial values do not lie in the invariant subspace of the fast dynamics then the dynamics have to relax to the invariant subspace before the averaged dynamics yields a good approximation (see also the discussion below). The relaxation to the invariant subspace is demonstrated in the right panel of Figure 3. It can be seen that for sufficiently small HSV (i.e., small $\epsilon$ ) the relaxation occurs quickly; notice that the fast dynamics relaxes even though the control force is still of order 1. The latter is due to the fact that the invariant subspace is contractive whenever $u$ is not too large (compare Section 3.2). The contraction condition is further justified by noting all the eigenvalues of $A_{22}$ in equation (3.4) are strictly negative (see left panel).
4.2. Non-decaying control force and positivity. The second example is to illustrate some of the subtleties and pitfalls of the method. To this end we consider

[^2]

Figure 4. Skew potential $W_{\mathrm{s}}$ : Hankel singular values (the first 15 are shown) and the time evolution of the population of the right well for various approximants $(d=11,12,20)$.
a skew double well potential defined by

$$
W_{\mathrm{s}}(x)=\left(x^{2}-1\right)^{2}+x .
$$

In comparison with the symmetric potential, the left potential well is lowered and therefore carries the overall statistical weight if the system is in equilibrium.

Suppose that initially at $t=0$ the system is in the stationary state $\rho_{0}$ given by the eigenvector $\rho_{0}$ of $A$ to the simple eigenvalue zero. Apart from the modified potential, the discretization is essentially the same as before with $I=[-2,2], n=400, \sigma=1 / 2$ and zero-flux boundary conditions. In contrast to the previous example and in violation of the theoretical assumptions that underly the averaging result we choose an external force that is non-decaying. More precisely we set

$$
u(t)=2(1-\exp (-2 t))
$$

which is clearly not square integrable over the real line. As a consequence, the effective potential $V(x, u)=W_{\mathrm{s}}(x)-u x$ converges to $W_{\mathrm{s}}^{-}=\left(x^{2}-1\right)^{2}-x$ as $t \rightarrow \infty$ which is exactly the reverse of $W_{\mathrm{s}}$ with the right well lowered.

As observable we choose the population of the right potential well, i.e., $C=P_{R}$ with $P_{R}$ denoting again the discrete characteristic function of the right well. The initial populations in the left and right wells are $\rho_{0, L}=0.9685$ and $\rho_{0, R}=0.0315$. We integrate the system up to the final time $T=10$ at which $W(x, u) \approx W_{\mathrm{s}}^{-}(x)$ and the population are $\rho_{L}=0.0404$ and $\rho_{R}=0.9596$.

Balancing and averaging is performed after a change of variables $\rho \rightarrow \rho-\rho_{0}$ and shifting $A \rightarrow A-\alpha I$ with $\alpha=10^{-3}$ or, likewise, after splitting off the stationary state; the results are found not to depend on this choice. In order to obtain a converged controllability Gramian $W_{c}, N$ and $B$ are scaled by $\mu=1 / 2$ (for details see Section 4.3 below). Singular values and the time evolution of the observable $y=P_{R} \rho$ for various orders of approximation, $d$, are shown in Figure 4. Apparently the dynamics are well reproduced for $d \geq 12$ (see right panel of the figure).

But as usual the devil is in the details: Closer inspection reveals that the state variables other than the observables do not remain positive when $d$ is too small. Figure 5 shows an instance for $d=12$; it can be seen that the both initial and final state $\rho(0)$ and $\rho(T)$ assume negative values in regions of low density (here: in the left well). The negative outliers disappear for $d \geq 20$. This behaviour is well in accordance with the limit result: Firstly, the $M$-matrix property of $A$ or $\bar{A}$, respectively, preserves positivity of the solution provided that the initial values are positive. This however does not need to be the case, because the balanced and truncated initial value is not necessarily positive. Secondly, the limit result essentially asserts that the approximation error is of the order of the negligible


Figure 5. Negative densities: the left panel shows the spatial density distribution for $t=0$ and $t=10$ (final state) for an approximant of order $d=12$ (cf. left panel of Figure 4). The complete spatio-temporal density evolution for is depicted in the right panel.

HSV, so it does not come as a surprise that the negative values appear in regions of low density; as $d$ is increased the outliers vanish which is in agreement with the numerical findings. Thirdly, the projection to the invariant subspace may produce initial values that are no longer non-negative; the same is true for the observables although the balancing transformation itself leaves the output variable invariant.

Remark 4.1. For the sake of completeness we computed also the truncated version of (4.5), i.e., the reduced system that is obtained from (4.6) by setting $\rho_{2}=0$ and compared the solutions to the averaged ones (cf. [12]). In terms of the output variables $y$ both methods yielded almost equally accurate approximants. However, other than the Schur complement, truncation does not preserve the $M$-matrix property with the simple eigenvalue zero. As a consequence, the truncated system may not admit a stationary distribution.
4.3. Numerical issues. Consider the generalized Lyapunov equation

$$
A W_{c}+W_{c} A^{*}+\sum_{k=1}^{m} N_{k} W_{c} N_{k}^{*}+B B^{*}=0
$$

and recall that if $A$ is Hurwitz there are constants $\lambda, \mu>0$, such that $\|\exp (A t)\| \leq$ $\lambda \exp (-\mu t)$ where $\|\cdot\|$ is any suitable matrix norm. If moreover

$$
\begin{equation*}
\frac{\lambda^{2}}{2 \mu} \sum_{k=1}^{m}\left\|N_{k}\right\|^{2}<1 \tag{4.8}
\end{equation*}
$$

the controllability Gramian $W_{c}$ exist [9]. If the pair $(A, B)$ is completely controllable, i.e., if $\operatorname{rank}\left(B A B A^{2} B \ldots A^{n-1} B\right)=n$, then $W_{c}$ is positive definite [36].

Since direct methods for solving generalized Lyapunov equations have a numerical complexity $\mathcal{O}\left(n^{6}\right)$ computing Gramians is challenging even for medium-sized systems. For $A$ Hurwitz, the obvious iterative scheme is (see, e.g., [37])

$$
\begin{equation*}
A X_{j+1}+X_{j+1} A^{*}=-\sum_{k=1}^{m} N_{k} X_{j} N_{k}^{*}-B B^{*}, \quad X_{0}=0 \tag{4.9}
\end{equation*}
$$

which requires the solution of a standard Lyapunov equation in each step. Convergence $X_{j} \rightarrow W_{c}$ is guarenteed by the following result that is to Damm [14].

Lemma 4.2. Let the linear operator $\mathcal{L}_{A}: \mathbb{R}^{n \times n} \rightarrow \mathbb{R}^{n \times n}$ be defined by $\mathcal{L}_{A}(X)=$ $A X+X A^{*}$ and let $\Pi: \mathbb{R}^{n \times n} \rightarrow \mathbb{R}^{n \times n}$ be nonnegative in the sense that $\Pi(X) \geqslant 0$ for $X \geqslant 0$. Further assume that the spectrum of $\mathcal{L}_{A}$ is contained in the closed left half-plane (including the imaginary axis) and for a given $Y \geqslant 0$ there exists a
nonnegative definite matrix $\hat{X} \geqslant 0$ such that $\left(\mathcal{L}_{A}+\Pi\right) \hat{X} \leqslant-Y$. Then there exists a minimal nonnegative definite solution $X_{-}$with satisfying
(1) $X_{-} \geqslant 0$ and $\left(\mathcal{L}_{A}+\Pi\right) X_{-}=-Y$
(2) If $\hat{X} \geqslant 0$ such that $\left(\mathcal{L}_{A}+\Pi\right) \hat{X} \leqslant-Y$, then $\hat{X} \geqslant X_{-}$.
(3) $X_{j} \rightarrow X_{-}$, where $X_{j}$ for $j=0,1,2, \ldots$ is defined via

$$
X_{j+1}=-\mathcal{L}_{A-\alpha I}^{-1}\left(\Pi\left(X_{j}\right)+2 \alpha X_{j}+Y\right), \quad X_{0}=0, \quad \alpha>0
$$

Setting $\Pi(X)=\sum_{k=1}^{m} N_{k} X N_{k}^{*}$ and $\alpha=0$ Lemma 4.2 implies that (4.9) converges to $W_{c}$ if the solvability condition (4.8) is met (cf. [12]).

Unstable systems I. In both of the previous numerical examples the matrix $A$ has a simple eigenvalue zero and $B=0$. However we may exploit the fact that $A$ has a nontrivial kernel and transform the homogeneous equation

$$
\dot{\rho}=A \rho+\sum_{k=1}^{m} N_{k} \rho u_{k}, \quad \rho(0)=\rho_{0}
$$

by doing a change of variables $\rho \mapsto \rho+v$ with $A v=0$. This yields

$$
\dot{\rho}=A \rho+\sum_{k=1}^{m} N_{k} \rho u_{k}+B u, \quad \rho(0)=\rho_{0}+v
$$

with $B=-\left(N_{1} v, \ldots, N_{m} v\right)$. The difference between the homogeneous and the inhomogeneous system is that the latter has $\rho=v$ as stationary state whereas the other one has the stationary state $\rho=0$.

Clearly the Gramians do not exists if $A$ is not Hurwitz. In accordance with Lemma 4.2 we may enforce stability by shifting the matrix $A$ according to $A \mapsto$ $A-\alpha I$ for a suitable $\alpha>0$; cf. also [35]. Physically, shifting amounts to a constant killing rate $\alpha$ in the Fokker-Planck equation and makes the zero state $\rho=0$ the unique asymptotically stable fixed point. Alternatively one may split off the stationary state $x=v$ and balance only the orthogonal complement in which the dynamics are asymptotically stable. This approach has the advantage that it preserves the stationary state and that the computed Gramians are the Gramians associated with the true dynamics. In both of our examples neither method turned out to be better than the other one in terms of the approximation quality of the reduced systems.

Unstable systems II. Now suppose that (4.8) does not hold while $A$ is Hurwitz. In this case we may replace the control by the scaled control $u \mapsto u / \mu$ for $0<\mu<1$. Invariance of (2.1) or (4.5) then requires that the coefficients scale according to $B \mapsto \mu B$ and $N_{k} \mapsto \mu N_{k}$ whereupon the system is altered according to

$$
\begin{aligned}
& \dot{\rho}=A \rho+\sum_{k=1}^{m}\left(\mu N_{k}\right) \rho \frac{u_{k}}{\mu}+(\mu B) \frac{u}{\mu}, \quad \rho(0)=\rho_{0} \\
& y=C \rho
\end{aligned}
$$

and the generalized Lyapunov equation has to be replaced by

$$
A W_{c}+W_{c} A^{*}+\mu^{2} \sum_{k=1}^{m} N_{k} W_{c} N_{k}^{*}+\mu^{2} B B^{*}=0
$$

The scaling as such clearly changes the Gramian $W_{c}$. Roughly speaking, we may expect that the HSV decay faster as $\mu$ becomes small (for $\mu \rightarrow 0$ the system becomes completely uncontrollable). But since the nullspace of $W_{c}$ is not affected by the scaling we may still expect that, to lowest order, the ordering of the HSV is not changed as long as $\mu$ is not too small.

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## Appendix A. Sampling the controllability Gramian

Instead of solving the generalized Lyapunov equation (2.6) directly, we may compute $W_{c}$ as the covariance matrix of a continuous-time Markov process that is governed by the following stochastic differential equation

$$
\begin{equation*}
d X_{t}=A X_{t} d t+\sum_{k=1}^{m} N_{k} X_{t} d W_{k, t}+B d W_{t}, \quad X_{0}=0 \tag{A.1}
\end{equation*}
$$

that is the stochastic analog of the deterministic control system

$$
\begin{equation*}
\dot{x}=A x+\sum_{k=1}^{m} N_{k} x u_{k}+B u, \quad x(0)=0 \tag{A.2}
\end{equation*}
$$

Here $W_{t}$ denotes standard Brownian motion in $\mathbb{R}^{m}$. To see this, it is helpful to note that $\mathbf{E} X_{t}=0$ as following from the first Itô isometry [23]. By Itô's formula,

$$
d\left(X_{t} X_{t}^{*}\right)=X_{t} d X_{t}^{*}+d X_{t} X_{t}^{*}+\sum_{k=1}^{m}\left(N_{k} X_{t}+b_{k}\right)\left(N_{k} X_{t}+b_{k}\right)^{*}
$$

with the $b_{k} \in \mathbb{R}^{n}$ denoting the columns of the matrix $B$, i.e., $B=\left(b_{1}, \ldots, b_{m}\right)$. Now set $S_{t}=\mathbf{E} X_{t} X_{t}^{*}$. Inserting the differential equation for $d X_{t}$, taking the expectation, and interchanging expectation and differentiation, it follows that

$$
\begin{equation*}
\dot{S}_{t}=A S_{t}+S_{t} A^{*}+\sum_{k=1}^{m} N_{k} S_{t} N_{k}^{*}+B B^{*} \tag{A.3}
\end{equation*}
$$

Recall that the existence of the Gramian $W_{c}$ in (2.6) follows from (4.8). Equivalently the solvability condition (4.8) guarantees that the solutions of (A.1) are mean-square stable, i.e., for $B=0$, we have $\mathbf{E}\left|X_{t}\right|^{2} \rightarrow 0$ as $t \rightarrow \infty$ (see, e.g., [38] and the references therein). For $B \neq 0$ it therefore follows that $\dot{S}_{t} \rightarrow 0$ which entails

$$
W_{c}=\lim _{t \rightarrow \infty} S_{t}
$$

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[^1]:    ${ }^{1}$ The associated system can be constructed from the coupled system (3.4) by rescaling time according to $t \mapsto t / \epsilon$ and then sending $\epsilon$ to zero.

[^2]:    ${ }^{2}$ The balancing transformation was computed doing first a state transformation to the zero state and then stabilizing $A$ by shifting $A \mapsto A-\alpha I$ with $\alpha=10^{-3}$; see Section 4.3 below.

