Control of molecular dynamics and low-rank approximation of bilinear systems

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Outline

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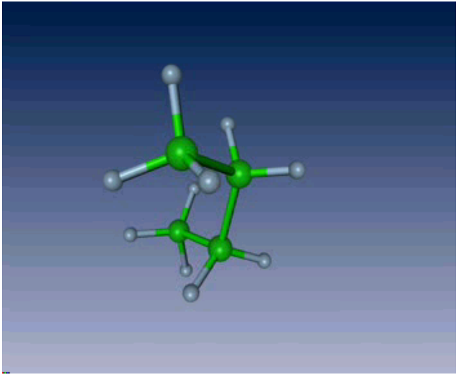
Bilinear control systems

Balanced model reduction

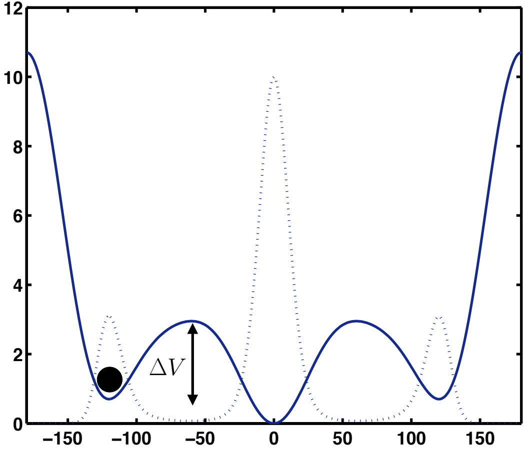
Numerical examples

Molecular conformations



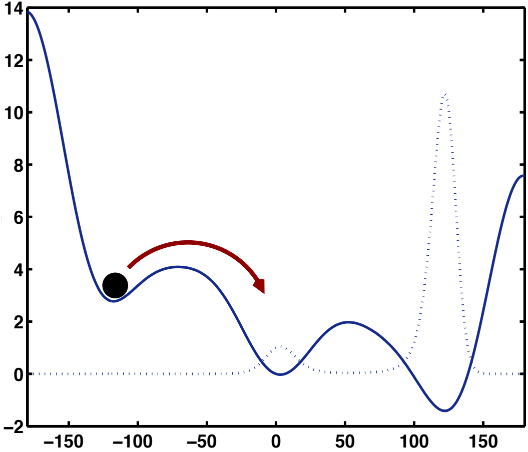
1.5ns simulation of butane at room temperature (vizualisation: Amira@ZIB).

The sampling problem



Metastable diffusion process at temperature $\theta \ll \Delta V$.

Biased molecular dynamics



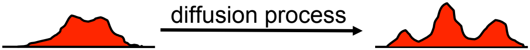
Biased molecular potential (e.g., using an optical tweezer).

Biased molecular dynamics (Fokker-Planck picture)

Swimming at low Reynolds numbers: **diffusion process**

$$dX_t = -\nabla V(X_t, u_t)dt + \sqrt{2\theta}\, dW_t\,, \quad X_0 = x_0\,,$$

in a **nonlinear energy landscape** $V\colon \mathbb{R}^d \times U \to \mathbb{R}$. (Here $\theta > 0$ and W is the standard d-dimensional Wiener process.)



The **probability distribution** $\rho(x,t)dx = \mathbb{P}\left[X_t \in [x, x+dx)\right]$ of X_t is governed by the **linear Fokker-Planck equation**

$$\frac{\partial \rho}{\partial t} = \theta\, \Delta\rho + \nabla \cdot (\rho \nabla V)\,, \quad \rho(x,0) = \rho_0(x)\,.$$

More on the sampling problem. . .

Metastability

Suppose $u = 0$. For V bounded below and satisfying appropriate growth conditions, there is a **unique stationary distribution**

$$\mu \propto \exp(-V/\theta)\,, \quad \int_{\mathbb{R}^n} d\mu = 1\,.$$

Theorem (Bakry & Emery, 1985)

The **rate of convergence** is determined by the spectral gap

$$\|\rho - \mu\|_{L^1} = C\exp(-\lambda_1 t)$$

with $\lambda_1 \asymp \exp(-\Delta V/\theta)$ and ΔV denoting the largest barrier.

Bakry & Emery, LNM 1123, 1985

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From the Fokker-Planck equation to bilinear systems

Now take your favourite spatial discretization scheme (FEM, finite-differences etc.) and **discretize the FP equation**:

$$\dot{\rho} = A\rho + (N\rho + B)u\,, \quad \rho(0) = \rho_0\,.$$

Here $-A \in \mathbb{R}^{n\times n}$ is an M-matrix with a simple eigenvalue 0, and $N \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^n$ are the **input coefficients**.

We augment our system by, say, k **output equations**, e.g., for observing the probability to be in certain state space regions:

$$\begin{aligned}\dot{\rho} &= A\rho + (N\rho + B)\,u\,, \quad \rho(0) = \rho_0\\ y &= C\rho\,.\end{aligned}$$

Model reduction problem

If the **space dimension** n **is very large**, then solving, e.g., an optimal control problem may be very tough or even infeasible.

Therefore we wish to find $\bar{A}, \bar{N} \in \mathbb{R}^{r\times r}$, $\bar{B} \in \mathbb{R}^r$ and $\bar{C} \in \mathbb{R}^{k\times r}$ with $r \ll n$ such that

$$\begin{aligned} \frac{d\zeta}{dt} &= \bar{A}\zeta + (\bar{N}\zeta + \bar{B})u\,, \quad \zeta(0) = \zeta_0 \\ y &= \bar{C}\zeta \end{aligned}$$

yields an **output** y **that is (in some sense) close to that of the original system** on any compact time interval $[0, T]$.

Model reduction strategy

Our approach is based on the **nonnegative controllability and observability Gramians** Q, P that are the solutions of

$$
\begin{aligned}
AQ + QA^* + NQN^* + BB^* &= 0 \\
A^*P + PA + N^*PN + C^*C &= 0
\end{aligned}
$$

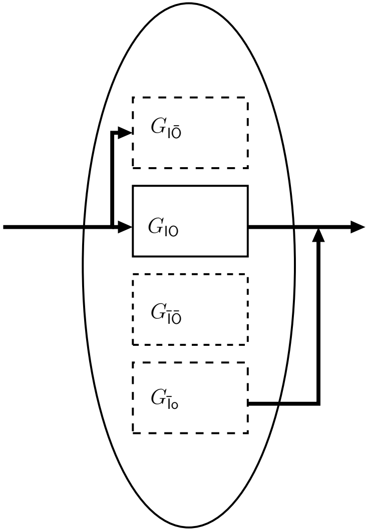
provided that they exist (e.g., we need that $\lambda(A) \subset \mathbb{C}^-$).

Realization theory of bilinear systems

1. States $\rho \in \mathbb{R}^n$ for which $Q\rho = 0$ are not accessible by any bounded measurable control.
2. States $\rho \in \mathbb{R}^n$ for which $P\rho = 0$ do not do not produce any output signal (for all bounded measurable controls).

Isidori, IEEE TAC, 1973; Al-Baiyat & Bettayeb, IEEE CDC, 1993; Benner & Damm, SICON, 2011

Model reduction paradigm: transfer function



Balancing controllability and observability

What if $Q, P > 0$? Then there exists a **balancing transformation** $\rho \mapsto T\rho$ by which the Gramians of the transformed system

$$\begin{aligned}
\dot{\rho} &= T^{-1}AT\rho + \left(T^{-1}NT\rho + T^{-1}B\right)u\,, \quad \rho(0) = \rho_0 \\
y &= CT\rho\,.
\end{aligned}$$

become equal and diagonal, i.e.,

$$T^{-1}Q(T^*)^{-1} = T^*PT = \mathrm{diag}(\sigma_1, \ldots, \sigma_n) > 0\,.$$

Balanced truncation: In the balanced form the least controllable states yield the lowest output, and can be neglected, i.e.,

$$\|Q\rho\| \approx 0 \quad \Leftrightarrow \quad \|P\rho\| \approx 0\,.$$

Moore, IEEE TAC, 1981; Glover, Int. J. Control, 1984

Model reduction strategy, cont'd

There are various ways to eliminate the least controllable and observable states. Projecting A, N, B, C onto the columns of T corresponding to the **dominant singular values** σ_i is just one.

Yet another way is to see where the **small singular values**, say, $\sigma_{r+1}, \ldots, \sigma_n$ enter the equations and then let

$$(\sigma_{r+1}, \ldots, \sigma_n) \to 0\,.$$

By being the square roots of the eigenvalues of QP, the σ_i are coordinate invariant and therefore sensible **small parameters**.

An averaging principle. . .

Elimination of irrelevant states

Suppose that $\sigma_{r+1} \ll \sigma_r$. To see how the $\sigma_{r+1}, \ldots, \sigma_n$ enter the equations we **scale them uniformly** according to

$$(\sigma_{r+1}, \ldots, \sigma_n) \mapsto \epsilon(\sigma_{r+1}, \ldots, \sigma_n)\,, \quad \epsilon > 0\,.$$

by which the balancing transformation becomes **ϵ-dependent**.

Balancing according to $A \mapsto T(\epsilon)^{-1} A T(\epsilon)$ etc. yields

$$\begin{aligned}
\frac{d\rho_1}{dt} &= (A_{11} + uN_{11})\,\rho_1 + \frac{1}{\sqrt{\epsilon}}\,(A_{12} + uN_{12})\,\rho_2 + B_1 u \\
\sqrt{\epsilon}\frac{d\rho_2}{dt} &= (A_{21} + uN_{21})\,\rho_1 + \frac{1}{\sqrt{\epsilon}}\,(A_{22} + uN_{22})\,\rho_2 + B_2 u \\
y &= C_1\rho_1 + \frac{1}{\sqrt{\epsilon}}C_2\rho_2
\end{aligned}$$

H. et al., *Multiscale Model. Simul., 2010; H., Math. Comput. Model. Dyn. Syst., 2011*

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An averaging principle

Theorem (H, 2010)

Technical details aside, denote by y_ϵ the output of the full bilinear system, and let y be the output of the reduced system

$$\begin{aligned} \dot{\rho}_1 &= \left(\bar{A} + u\bar{N}\right)\rho_1 + B_1 u\,, \quad \rho_1(0) = \rho_{0,1} \\ y &= \bar{C}\rho_1 \end{aligned}$$

where the coefficients $\bar{A}, \bar{N} \in \mathbb{R}^{r\times r}$ and $\bar{C} \in \mathbb{R}^{k\times r}$ are given by

$$\begin{aligned} \bar{A} &= A_{11} - A_{12}A_{22}^{-1}A_{21} \\ \bar{N} &= N_{11} - N_{12}A_{22}^{-1}A_{21} \\ \bar{C} &= C_1 - C_2A_{22}^{-1}A_{21}\,. \end{aligned}$$

Then $|y_\epsilon(t) - y(t)| \to 0$ uniformly on $[0, T]$ as $\epsilon \to 0$.

Hartmann et al., *submitted to SICON, 2010; cf. Watbled, J. Math. Anal. Appl., 2005*

A few remarks. . .

Properties of the averaged equations

As the small Hankel SVs go to zero, the dynamics collapse to the **invariant subspace of controllable and observable states**.

Recall that $\epsilon \sim \sigma_{r+1}/\sigma_r$ is our **smallness parameter**. If u belongs to the class of **relatively slow controls**, i.e., $u \in L^2(0,\infty)$ with $u = u(t/\epsilon^\gamma)$ and $0 < \gamma < 1$, then an error bound of the form

$$\sup_{t\in[0,T]} |y_\epsilon(t) - y(t)| \leq C\left(\epsilon^\gamma + \epsilon\|\rho_2(0) - m(\rho_1(0))\|^2\right)$$

can be proved where C grows exponentially with T.

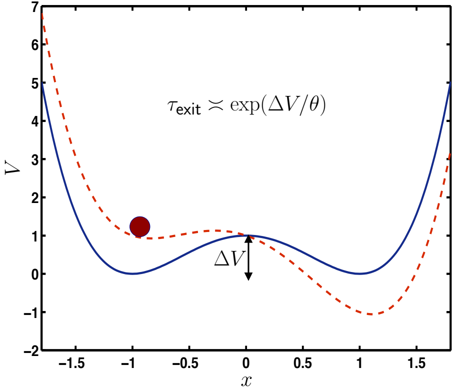
The transition from the full to the averaged system resembles the **Schur complement method** for PDEs.

Hartmann et al., *submitted to SICON, 2010; cf. Gaitsgory, SICON, 1992*

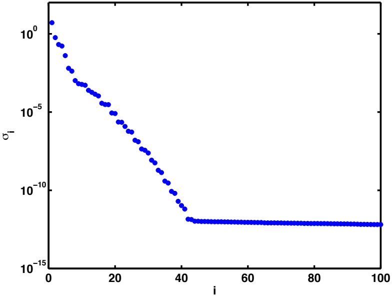
Biased molecular dynamics

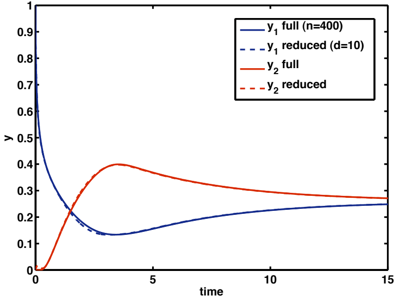
Dragged Brownian particle in a **tilted double-well potential**

$$dX_t = (u_t - \nabla V(X_t))\,dt + \sqrt{2\theta}\,dW_t\,,\quad X_0 \sim \mathcal{U}(\text{“left well”})\,.$$



Biased molecular dynamics





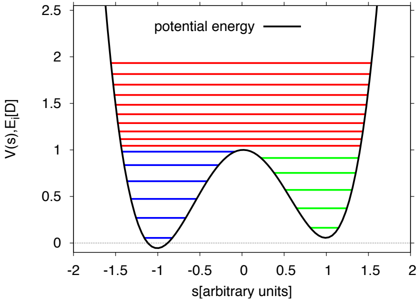
- **Finite-difference approximation** on $I = [-2, 2]$ with $n = 400$ gridpoints, control $u_t = \tanh(t - \pi) - 1$, and $y = (\pi_L, \pi_R)$.
- The **dominant eigenvalues** of the FP operator are well approximated (not true for projected system).

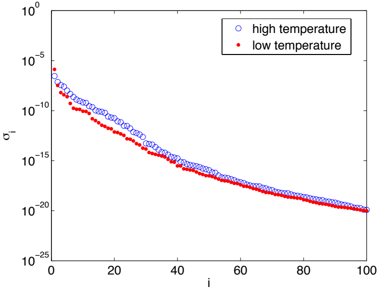
Hartmann et al., *submitted to SICON, 2010*

Control of open quantum systems

Dissipative Liouville-von-Neumann equation for density matrices

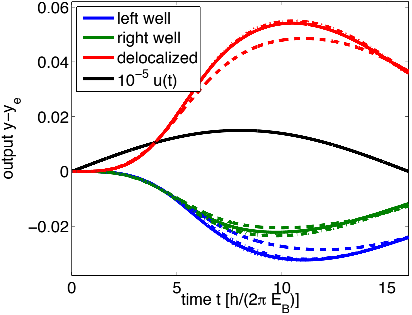
$$\frac{d\hat{\rho}}{dt} = [H + \mu u, \hat{\rho}] + D\hat{\rho}\,, \quad \hat{\rho} \in \mathbb{C}^{21\times 21}$$

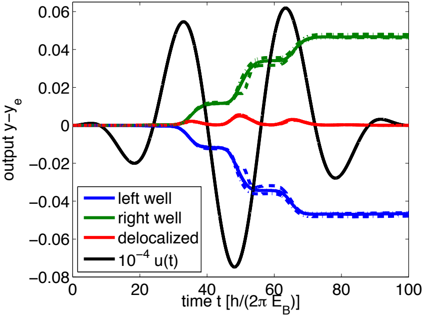




First 100 Hankel singular values (log plot).

Control of open quantum systems, cont'd





- The examples show the **response** of an open quantum system in equilibrium to a **long-wave laser pulse** (black curve).
- The low-θ approximation (right panel, $r = 15, 20, 25$) requires more states than the high-θ case (left panel $r = 5, 8, 11$).

Schäfer-Bung et al., *J. Chem. Phys., 2011*

Conclusions and open problems

- **Balanced truncation** can be powerful method for the optimal control of molecular systems.
- **It is fairly expensive, but it requires only an offline computation**. The Gramians can be sampled by Monte-Carlo.
- The small Hankel singular values are perfect parameters for the perturbation analysis. But **what if there is no gap?**
- The **dominant eigenvalues** of the Fokker-Planck operator are approximated extremely well. Why is this?
- **Quantum systems:** structure-preservation (density matrices) and control of the numerical effort are highly challenging.
- **Backward stability** for the optimal control is an open issue.

Thank you for your attention.

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