Adiabatic Approximation of Coarse Grained Second
Order Response

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Abstract

We propose estimators for dynamic second order response theory in coarse
grained variables for driven out-of-equilibrium subsystems. The error is con-
trolled through the the notion of subsystem spectral gap for the convergence of
course grained observables.

1 Introduction and main result

This note addresses the problem of forecasting the dynamic behaviour of driven out-
of-equilibrium subsystems, using only equilibrium subsystem measurements. As a
prototype consider a tracer interacting with an else unknown and unobserved particle
system which is driven out of equilibrium by an additional force acting only on the
tracer, e.g. [15, 10]. How can one make a sensible prediction on the dynamics of the
forced tracer from probing it in the unforced regime when the whole system is still
unknown but can be assumed in equilibrium?

We treat this as a nonparametric statistical problem for a \( \mathbb{R}^d \)-valued solution \( x_\varepsilon \)
to an overdamped Langevin SDE

\[
\begin{aligned}
dx_\varepsilon^t &= -\nabla U(x_\varepsilon^t)dt - \varepsilon f(x_\varepsilon^t)dt + \sqrt{2}dW_t \\
x_\varepsilon^0 &\sim \mu = \frac{1}{Z}e^{-U}dx,
\end{aligned}
\]

where only \( f : \mathbb{R}^d \to \mathbb{R}^d \) is known and only partial observations \( \pi(x) \in \mathbb{R}^m, m \leq d, \)
of the states \( x \) are possible under a fixed measurable (‘coarse graining’) map

\( \pi : \mathbb{R}^d \to \mathbb{R}^m, \quad m \leq d, \)

describing the passage to the observable subsystem. Assuming that \( f(x) = f(\pi(x)) \)
is also coarse grained, given \( \kappa : \mathbb{R}^m \to \mathbb{R} \) we want to estimate

\[
\mathbb{E}_\mu(\kappa(\pi(x_\varepsilon^t))),
\]

in terms of quantities of the form

\[
\mathbb{E}_\mu(\Phi(\pi(x_0^s)_{s\in[0,t]})),
\]

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where $\Phi \in (\mathbb{R}^m)^{0,t}$ are suitably chosen path functionals. In practice such expectations of $\Phi(\pi(x)_{s \in [0,t]})$ at equilibrium can be obtained from corresponding time-averaged subsystem observations, using the ergodicity of $x$.

This inference problem from unperturbed $\pi(x^0)$ to perturbed $\pi(x^\varepsilon)$ is non-trivial due to the interaction with the hidden degrees of freedom. Standard response theory (c.f. e.g. [1, 14]) does not give an answer since it relies on full system measurements at equilibrium which might not be available or too costly in practice. The aim of this note is to suggest a simple and practical work around for such a situation.

Using a suitable semigroup expansion and a variant of adiabatic approximation, in case when $f = \nabla V$ with $V(x) = v(\pi(x))$ we propose the approximation

$$E_{\mu}(k(\pi(x^\varepsilon_T))) \approx \langle k \rangle + \varepsilon \left[ \langle V k \rangle - \langle V P_T k \rangle \right]$$

which can be estimated empirically up to arbitrary precision from equilibrium $\pi(x)$-observations. Hence only some structural information about the full systems and the precise form of the perturbation needs to be known, and no effective model for the dynamics of the tracer e.g. by stochastic delay differential equations or via averaging as in e.g. [7, 13, 4] is used. The estimator above extends the standard first order expansion from [1, 14, 17] and is complimentary to a previous approach via linearization of higher order correlations in [2, 16]. Its accuracy depends critically on the mixing of the (generally non-Markovian) subsystem $\pi(x)$, and which we quantify through the notion of subsystem spectral gap, see definition 3.1 and proposition 3.5 below. In particular, the subsystem and not the environment needs to be fast for reasonable accuracy, contrary to the standard assumptions in e.g. averaging.

The method is illustrated by numerical simulations towards the end.

2 Dyson formula and semigroup expansion

We will treat the given statistical inference problem in the framework of perturbations of overdamped Langevin dynamics and their associated Markov semigroups, where for simplicity we assume full regularity of the coefficients throughout. To this aim, for $\varepsilon \geq 0$ we consider the unique strong solutions to the SDE in $\mathbb{R}^d$

$$\begin{align*}
dx_t^\varepsilon f &= -\nabla U(x_t^\varepsilon f)dt - \varepsilon f_t(x_t^\varepsilon f)dt + \sqrt{2}dW_t \\
nx_0^\varepsilon f &= \xi
\end{align*}$$

where $U : \mathbb{R}^d \rightarrow \mathbb{R}$ and $f : \mathbb{R}^d \times \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}^d$ satisfy appropriate growth and regularity assumptions, $W$ is a $d$-dimensional Brownian motion, $\xi$ is independent of $W$. We shall assume also that the solutions have infinite life time and induce the family of time-inhomogeneous Feller semigroups $(P_{s,t}^{\varepsilon f})_{0 \leq s \leq t}$ on the Banach space $C_0(\mathbb{R}^d)$ via

$$P_{s,t}^{\varepsilon f} g(x) = \mathbb{E} \left[ g(x_T^\varepsilon f) | x_s^\varepsilon = x \right],$$

2
and write $P_{s,t}^0 = P_{t-s}$. The corresponding family of generators $(L^\varepsilon f)_t \geq 0$ read
\[ L^\varepsilon f g(x) = L^0 g(x) - \varepsilon f_t(x) \cdot \nabla g(x), \]
where
\[ L^0 g(x) = -\nabla U(x) \cdot \nabla g(x) + \Delta g(x). \]

In this situation one verifies the following implicit relation between $(P_{s,t}^\varepsilon)_{0 \leq s \leq t}$ and $(P_{s,t}^0)_{0 \leq s \leq t}$.

**Proposition 2.1 (‘Dyson Formula’).** For regular $U$ and $f$ it holds that
\[ P_{s,t}^\varepsilon g = P_{t-s}^0 g - \varepsilon \int_s^t P_{s_1-s}^0 (f_{s_1} \cdot \nabla P_{s_1,t}^\varepsilon) ds_1 \] (2)

Nested iteration of (2) produces explicit expressions for the power series expansion of $P_{s,t}^\varepsilon$ in $\varepsilon$. Here we record the first and second order terms, given that $\xi$ is distributed according to the equilibrium invariant measure $\mu$. We denote by $\langle \cdot \rangle$ the expectation w.r.t. $\mu$.

**Proposition 2.2.** Let $(x^\varepsilon f_{t\in[0,T]})_{\varepsilon,f}$, $(P_{s,t}^\varepsilon)_{0 \leq s \leq t}$ and $L^\varepsilon f_t$ as above with $f_t = -h_t \nabla V$ and $\xi \sim \mu$ with $\mu(dx) = e^{-U(x)}Z d x$. Then,
\[ \frac{d}{d\varepsilon} \bigg|_{\varepsilon=0} \mathbb{E}_\mu[k(x^\varepsilon f_T)] = -\int_0^T h_t \langle V L^0 P^0_{T-t} k \rangle dt \]
and
\[ \frac{d^2}{d\varepsilon^2} \bigg|_{\varepsilon=0} \mathbb{E}_\mu[k(x^\varepsilon f_T)] = -2 \int_0^T \int_0^{t_1} h_{t_1} h_{t_2} \langle \langle L^0 V \rangle P_{t_1-t_2} \langle \nabla V \cdot \nabla P_{T-t_1} k \rangle \rangle dt_2 dt_1 \]

**Proof.** As for the first order term, differentiation of (2) w.r.t. $\varepsilon$ yields
\[ \frac{d}{d\varepsilon} \bigg|_{\varepsilon=0} \mathbb{E}_\mu[k(x^\varepsilon f_T)] = \int_0^T h_t \langle P^0_t (\nabla V \cdot \nabla P^0_{T-t} k) \rangle dt \]
\[ = \int_0^T h_t \langle \nabla V \cdot \nabla P^0_{T-t} k \rangle dt \]
\[ = -\int_0^T h_t \langle V, L^0 P^0_{T-t} k \rangle dt, \]
where used the $P^0_t$-invariance of $\mu$ and integration by parts in the second resp. third line. As for the second order term, we expand the time integral on the r.h.s. of (2) by another application of Dyson’s formula and differentiate twice w.r.t. $\varepsilon$. This yields
\[ \frac{d^2}{d\varepsilon^2} \bigg|_{\varepsilon=0} \mathbb{E}_\mu[k(x^\varepsilon f_T)] = 2 \int_0^T \int_0^{t_1} h_{t_1} h_{t_2} \langle \nabla V \cdot \nabla P_{t_1-t_2} \langle \nabla V \cdot \nabla P_{T-t_1} k \rangle \rangle dt_2 dt_1 \]
and hence the claim via another integration by parts. \(\square\)
In case of a conservative and time-homogeneous perturbation \( f(t, x) = -\nabla V(x) \) the expressions above simplify further.

**Lemma 2.3.** In a setting as in proposition 2.2 but for \( h_t = 1 \) for all \( t \geq 0 \), the response simplifies to

\[
\frac{d}{d\varepsilon} \bigg|_{\varepsilon=0} \mathbb{E}_\mu \left[ k(x_\varepsilon^T) \right] = \langle V k \rangle - \langle VP_0^0 k \rangle
\]

and

\[
\frac{d^2}{d\varepsilon^2} \bigg|_{\varepsilon=0} \mathbb{E}_\mu \left[ k(x_\varepsilon^T) \right] = \langle V^2 k \rangle - \langle VP_0^0 (V k) \rangle + \int_0^T \langle VP_0^0 (L^0 V P_{-t}^0) \rangle \, dt .
\]

**Proof.** Starting from proposition 2.2 in case of \( h = 1 \)

\[
\frac{d}{d\varepsilon} \bigg|_{\varepsilon=0} \mathbb{E}_\mu \left[ k(x_\varepsilon^T) \right] = - \int_0^T \langle V L^0 P_{-t}^0 k \rangle dt
\]

\[
= \int_0^T \frac{d}{dt} \langle VP_0^0 P_{-t}^0 k \rangle dt
\]

\[
= \langle V k \rangle - \langle VP k \rangle.
\]

Likewise, for the second order term

\[
\frac{d^2}{d\varepsilon^2} \bigg|_{\varepsilon=0} \mathbb{E}_\mu \left[ k(x_\varepsilon^T) \right] = -2 \int_0^T \int_{t_1}^{t_1+T} \langle (L^0 V) P_{t_1-t_2}^0 (\nabla V \cdot \nabla P_{-t_1}^0) \rangle \, dt_2 dt_1
\]

\[
= 2 \int_0^T \langle V \nabla V \cdot \nabla P_{-t}^0 \rangle \, dt - 2 \int_0^T \langle VP_{t_1}^0 (\nabla V \cdot \nabla P_{-t_1}^0) \rangle \, dt_1
\]

\[
= - \int_0^T \langle V^2 L^0 P_{-t}^0 \rangle \, dt - \int_0^T \frac{d}{dt_1} \langle VP_{t_1}^0 (VP_{-t_1}^0) \rangle \, dt
\]

\[
+ \int_0^T \langle VP_{t_1}^0 (L^0 V P_{-t}^0) \rangle \, dt
\]

\[
= \langle V^2 k \rangle - \langle VP_0^0 (V k) \rangle + \int_0^T \langle VP_{t_1}^0 (L^0 V P_{-t}^0) \rangle \, dt_1 .
\]

Here, we have used that \( 2V \nabla V = \nabla V^2 \) and \( \frac{d}{dt} \langle VP_{t}^0 (VP_{-t}^0) \rangle = \langle VP_0^0 (L^0 V P_{-t}^0) \rangle + 2 \langle VP_{t_1}^0 (\nabla V \cdot \nabla (P_{-t}^0)) \rangle . \)

\[
\square
\]

3 **Subsystem spectral gap and coarse graining**

The above mentioned inference problem corresponds to the situation when both the observable \( k \) and the potential \( V \) are coarse grained, i.e. when

\[
k(x) = \kappa(\pi(x)) \text{ and } V(x) = v(\pi(x))
\]
for some measurable map $\pi : \mathbb{R}^d \rightarrow \mathbb{R}^m$, $m \leq d$, and where $\kappa, v : \mathbb{R}^m \rightarrow \mathbb{R}$ are known functions. A natural idea is to use power series expansion in $\varepsilon$ and use lemma 2.3. However, the time integral in the the second order coefficient (3) involves $L^0V$ which in general is not coarse grained, i.e. not a subsystem observable and hence cannot be estimated from time-averaged equilibrium $\pi(x^0)$-measurements. To overcome this problem, we shall propose an approximation by certain subsystem observables below.

To estimate the induced error, we introduce a new quantity which controls the rate of convergence of subsystem observables.

Here and in the sequel we shall assume for simplicity that the generator $L$ of the equilibrium process has discrete spectrum.

**Definition 3.1.** Let $L$ be the generator of an $\mathbb{R}^d$-valued $\mu$-reversible Markov process $x$ and let $\pi : \mathbb{R}^d \rightarrow \mathbb{R}^m$, $m \leq d$ measurable. Let

$$S = L^2_\mu(\mathbb{R}^d, \sigma(\pi)) \subset L^2_\mu(\mathbb{R}^d),$$

where $\sigma(\pi)$ denotes the sigma algebra generated on $\mathbb{R}^d$ by $\pi$, be the closed subspace of square integrable subsystem observables and denote by $\text{Sp}(-L)$ the spectrum of $-L$, then the quantity

$$\lambda_{\pi} = \inf \left\{ \lambda \in \text{Sp}(-L) \setminus \{0\} | \perp (\text{Eig}(\lambda) \perp L^2(\mathbb{R}^d, \sigma(\pi), \mu)) \right\}$$

is called **subsystem spectral gap** of $\pi(x^0)$.

The coarse grained process $(\pi(x^0_t))_{t \geq 0}$ is not assumed to be Markovian in the definition above. The following statement is a simple consequence and yields a criterion when the passage to the subsystem improves the spectral gap.

**Corollary 3.2.** In the situation as above let $\lambda_*$ be the spectral gap of the full system $x^0$, then

$$\lambda \geq \lambda_*$$

with strict inequality if and only if

$$\mathbb{E}_\mu(g|\sigma(\pi)) = 0 \quad \forall g \in \text{Eig}(\lambda_*) .$$

**Example 3.3.** Consider the time-continuous Markov chain $(x_t)_{t \geq 0}$ on the state space $E = \{1, 2, 3, 4\}$ with generator

$$Q = \begin{pmatrix}
-\frac{9}{10} & \frac{8}{10} & 0 & \frac{1}{10} \\
\frac{8}{10} & -\frac{9}{10} & \frac{1}{10} & 0 \\
0 & \frac{1}{10} & -1 & \frac{9}{10} \\
\frac{1}{10} & 0 & \frac{9}{10} & -1
\end{pmatrix}$$

$Q$ is symmetric w.r.t. the invariant distribution $\mu = \frac{1}{4}(1, 1, 1, 1)$ with spectral gap $\lambda_* = \frac{1}{\delta}$. Dividing the system into two subsystems $E_1 = \{1, 4\}, E_2 = \{2, 3\}$
{2, 3} yields a new (non Markovian) stochastic process \( \pi(x_t) = 1_{\{x_t \in E_1\}} - 1_{\{x_t \in E_2\}} \) on the state space \( E' = \{1, -1\} \), which has a subsystem spectral gap of \( \lambda_\pi = \frac{18}{10} - \sqrt{2} \).

In fact, the other eigenvectors other than \( \mu \) for \( Q \) are \( v_2^T = (-1, -1, 1, 1), v_3^T = (1 + \sqrt{2}, -1 - \sqrt{2}, -1, 1), v_4 = (1 - \sqrt{2}, 1 + \sqrt{2}, -1, 1) \) with eigenvalues \( -\lambda_2 = -\frac{1}{5}, -\lambda_3 = -\frac{18+\sqrt{2}}{10}, -\lambda_4 = -\frac{18-\sqrt{2}}{10} \) and \( v_2 \perp L_\mu^2(E, \sigma(\pi)) = \{(u, v, u)^T \in \mathbb{R}^4 | u, v \in \mathbb{R}\} \).

The quantity \( \lambda_\pi \) controls the exponential decay to equilibrium for subsystem observables in \( L^2 \)-sense.

**Proposition 3.4.** For \( f \in L_\mu^2(\mathbb{R}^d, \sigma(\pi)) \) with \( \langle f \rangle = 0 \), it holds that

\[
\langle (P_t f)^2 \rangle \leq c_{L, \pi} e^{-2\lambda_\pi t} \langle f^2 \rangle
\]

(4)

**Proof.** Denote by \( \lambda_0 = 0 < \lambda_1 = \lambda_\pi < \lambda_2 < \cdots \) the set of eigenvalues of \( -L \) and \( (\varphi_n)_{n\in\mathbb{N}} \subset L_\mu^2(\mu) \) a set of orthonormal eigenfunctions. Then, for any \( f \in L_\mu^2(\mathbb{R}^d, \sigma(\pi)) \) with \( \langle f \rangle = 0 \), by the spectral theorem

\[
P_t f = \sum_{n=1}^{\infty} \langle \varphi_n, f \rangle e^{-\lambda_n t} \varphi_n
\]

\[
= \sum_{n \geq 1} \langle \varphi_n, f \rangle e^{-\lambda_n t} \varphi_n, \quad \varphi_n \in L_\mu^2(\mathbb{R}^d, \sigma(\pi))
\]

hence

\[
\langle (P_t f)^2 \rangle = \sum_{n \geq 1} \langle \varphi_n, f \rangle^2 e^{-2\lambda_n t} \sum_{n \geq 1} \langle \varphi_n, f \rangle^2 e^{-2\lambda_n t} \leq e^{-2\lambda_\pi t} \sum_{n \geq 1} \langle \varphi_n, f \rangle^2 e^{-2\lambda_n t} \langle f^2 \rangle.
\]

We can now introduce our estimator for the dynamic second order response in terms of subsystem observables as follows.

**Proposition 3.5.** Let \( (x_t^\pi)_{t \geq 0} \) be the solution to (1) with \( f_t(x) = -\nabla V \) with \( V(x) = v(\pi(x)) \) and let \( (P_t) \) denote the semigroup associated to \( x_0^\pi \). Then, for all \( T > 0 \) and \( k(x) = \kappa(\pi(x)) \)

\[
\frac{d^2}{dx^2} \mathbb{E}_{\mu} [k(x_T^\pi)] = \langle V^2 k \rangle - \langle VP_TVk \rangle + \langle V \rangle \left( \langle P_{T/2} k, V \rangle - \langle k V \rangle \right)
\]

\[
+ \langle k \rangle \left( \langle P_{T/2} V, V \rangle - \langle V^2 \rangle \right) + f_k(T) + f_V(T)
\]
where

\[ |f_V(T) + f_k(T)| \]
\[ \leq (\|k\|_{L^\infty} \|V\|_{L^2} + \|V\|_{L^\infty} \|k\|_{L^2}) \|LV\|_{L^2} \frac{1}{\lambda_\pi} (e^{-\lambda_\pi T/2} - e^{-\lambda_\pi T}) \]

and \( \lambda_\pi \) denotes the subsystem spectral gap associated to \( \pi(x^0) \).

**Proof.** We need to approximate the remaining integral

\[
\int_0^T \langle VP_t ((LV)P_{T-t}k) \rangle \, dt
\]
\[
= \int_0^T \langle VP_{T-t} ((LV)P_t k) \rangle \, dt
\]
\[
= \int_0^T \langle (P_{T-t}V)(P_t k) \rangle \, dt
\]
\[
= \int_0^{T/2} \langle V \rangle \langle (P_t k) \rangle \, dt + \int_0^{T/2} \langle (P_{T-t}V - \langle V \rangle)(P_t k) \rangle \, dt
\]
\[
+ \int_{T/2}^T \langle k \rangle \langle (P_{T-t}V) \rangle \, dt + \int_{T/2}^T \langle (P_t k - \langle k \rangle)(P_{T-t}V) \rangle \, dt
\]
\[
= \langle V \rangle (\langle P_{T/2}k, V \rangle - \langle k V \rangle) + f_V(T)
\]
\[
+ \langle k \rangle (\langle P_{T/2}V, V \rangle - \langle V^2 \rangle) + f_k(T)
\]

with

\[ f_V(T) = \int_0^{T/2} \langle (P_{T-t}V - \langle V \rangle)(P_t k) \rangle \, dt \]

and

\[ |f_V(T)| \leq \int_0^{T/2} \|P_{T-t}V - \langle V \rangle\|_{L^2} \|P_t k\|_{L^\infty} \|LV\|_{L^2} \, dt \]
\[
\leq \|LV\|_{L^2} \|k\|_{L^\infty} \int_0^{T/2} e^{-\lambda_\pi (T-t)} \|V\|_{L^2} \, dt
\]
\[
= \|LV\|_{L^2} \|k\|_{L^\infty} \frac{1}{\lambda_\pi} (e^{-\lambda_\pi T/2} - e^{-\lambda_\pi T}) \|V\|_{L^2}
\]

where we have used Cauchy-Schwarz and the contractivity of the semigroup \((P_t)_t\).

Similarly,

\[ f_k(T) = \int_{T/2}^T \langle (P_t k - \langle k \rangle)(P_{T-t}V) \rangle \, dt, \]
hence

$$|f_k(T)| \leq \|LV\|_{L^2} \|V\|_{L^\infty} \|k\|_{L^2} \frac{1}{\lambda_\pi} \left( e^{-\lambda_\pi T/2} - e^{-\lambda_\pi T} \right).$$

Summing all terms yields the claim. \qed

**Remark 3.6.** In the event that the potential is unbounded, we can still make an estimate, namely

$$|f_k(T)| \leq \int_T^{T/2} \|(P_{T-t}V)(LV)\|_{L^2} \|P_t k - \langle k \rangle_{\mu_0}\|_{L^2}$$

$$\leq \int_T^{T/2} \|(P_{T-t}V)\|_{L^{2p}} \|LV\|_{L^{2q}} \|P_t k - \langle k \rangle_{\mu_0}\|_{L^2}$$

$$\leq \|V\|_{L^{2p}} \|LV\|_{L^{2q}} \|k\|_{L^2} \frac{1}{\lambda_\pi} \left( e^{-\lambda_\pi T/2} - e^{-\lambda_\pi T} \right)$$

where we again applied Hölder inequality again and used the fact that the $L^\infty$ contractivity of the semigroup implies contractivity $L^p$ for any $1 \leq p \leq \infty$, c.f. [5].

## 4 Numerical experiments

As a consequence of lemma 2.3 and proposition 3.5 we arrive at the following estimator for $E_\mu(k(\pi(x^\varepsilon_t)))$

$$e_\mu(k(\pi(x^\varepsilon_t))) = \langle k \rangle + \varepsilon \left[ \langle V k \rangle - \langle VP_t k \rangle \right]$$

$$+ \frac{\varepsilon^2}{2} \left[ \langle V^2 k \rangle - \langle VP_t V k \rangle + \langle V \rangle \left( \langle P_{T/2} k, V \rangle - \langle k V \rangle \right) \right] + \frac{\varepsilon^3}{3} \left( \langle \left( P_{T/2} V, V \right) - \langle V^2 \rangle \rangle \right),$$

which is composed entirely of equilibrium subsystem observables. Hence $e_\mu(k(\pi(x^\varepsilon_t)))$ can be estimated from ergodic averages of corresponding subsystem measurements at equilibrium. The statistical error in this ergodic approximation is also controlled by the subsystem spectral gap, which however may be difficult to estimate in practice.

We present two examples of the performance of this approach, using a straightforward Euler-Maruyama scheme for the numerical simulation of the full system trajectories $x^0$ and $x^\varepsilon$.

### 4.1 A system with two time scales

Let $x^\varepsilon_t \in \mathbb{R}^2$ be the solution to the Ito SDE

$$d x^\varepsilon_t = - \left( ax^\varepsilon_t + V'(\pi^1 x^\varepsilon_t) \right) dt + dW_t$$

$$x^\varepsilon_0 = \xi \quad \xi \sim e^{-U(x)} dx$$

5
given a 2 dimensional BM \((W_t)_t\) and

\[
a = \begin{pmatrix} 2 & -r \\ -r & 2r \end{pmatrix}
\]  

(6)

Hence, the (strong) solution to the equilibrium equation is an Ornstein-Uhlenbeck process

\[
x^0_t = e^{-at}\xi + \sqrt{2}\int_0^t e^{-a(t-s)}dW_s.
\]  

(7)

We consider the projection \(\pi(x) = e_1 \cdot x\).

\[
P^0_t\pi(x) = e_1^T \cdot e^{-at}x \quad \forall \ x \in \mathbb{R}^2.
\]  

(8)

It is useful to know that the eigenvalues of \(a\) are \(\lambda_{1/2} = \mp \sqrt{2r^2 - 2r + 1 + r + 1}\). Note that \(\lambda_1(r = 0) = 0\) so that the spectral gap vanishes when \(r = 0\).

\[
a^{-1} = \frac{1}{4r - r^2} \begin{pmatrix} 2r & r \\ r & 2 \end{pmatrix}
\]

The error of observing the position of the projected observable \(k(x) = \pi(x)\) can be estimated by proposition 3.5 by

\[
|f_V(T) + f_k(T)| \leq (\|k\|_{L^2}^p \|V\|_{L^2}^p \|LV\|_{L^2}^q + \|V\|_{L^\infty} \|k\|_{L^2}) \|LV\|_{L^2} \frac{1}{\lambda} \left( e^{-\lambda T/2} - e^{-\lambda T} \right)
\]

where we estimate the constant by

\[
(\|k\|_{L^2}^p \|V\|_{L^2}^p \|LV\|_{L^2}^q + \|V\|_{L^\infty} \|k\|_{L^2}) \|LV\|_{L^2}
\]

\[
\leq \left( 3 \left( \frac{2r}{4r - r^2} \right) \right)^2 \left( \left( (2x_1 - rx_2) \sin(x_1 - \frac{\pi}{4}) - \cos(x_1 - \frac{\pi}{4}) \right)^4 \right)^{1/4} + \frac{2}{\sqrt{4 - r}} \left( \left( (2x_1 - rx_2) \sin(x_1 - \frac{\pi}{4}) - \cos(x_1 - \frac{\pi}{4}) \right)^2 \right)^{1/2}
\]

\[
\leq \left( 3 \left( \frac{2r}{4r - r^2} \right) \right)^2 \left( \left( \frac{3}{(4r - r^2)^2} \right)^4 (64r^2 + 32r^3 + 20r^4 - 8r^5) \right)^{1/4} + \frac{2}{\sqrt{4 - r}} \left( \frac{2r + 4}{4 - r} \right)^{1/2}
\]

\[\approx 2.564\]

for the choice of \(r = 0.1\) with \(p = q = 2\). The spectral gap in this case is \(\lambda = \lambda_1 \approx 0.194\). Note that nevertheless, the approximation of the second order response yields an improved estimate of the nonequilibrium trajectory as seen from figure 1.
For SDEs we construct a potential landscape mimicking the behaviour of the Markov chain in example 3.3:

\[ U = U_{\Gamma_1} + U_{\Gamma_2} + \sum_{i=1}^{4} U_i + U_C \]

\[ U_{\Gamma_1}(x,y) = -\frac{\sqrt{2\pi}}{\sigma} e^{-(y-1)^2/2} \quad U_{\Gamma_2}(x,y) = -\frac{\sqrt{2\pi}}{\sigma_m} e^{-(y+1)^2/2} \]

\[ U_1(x,y) = -\frac{1}{2\sigma_1} e^{-(x-1)^2-(y-1)^2} \quad U_2(x,y) = -\frac{1}{2\sigma_1} e^{-(x+1)^2-(y-1)^2} \]

\[ U_3(x,y) = -\frac{1}{2\sigma_2} e^{-(x+1)^2-(y+1)^2} \quad U_4(x,y) = -\frac{1}{2\sigma_2} e^{-(x-1)^2-(y+1)^2} \]

\[ U_C(x,y) = \frac{x^2 + y^2}{10}. \]

As a coarse-grained variable, consider the projection onto the x axis \( \pi(x,y) = x \). Figure 2 shows the mean value of \( k(x,y) = \pi(x,y) = x \) under the perturbing potential, which increases the probability to remain in one of the right hand side minima:

\[ V(x,y) = v(x) = \exp \left( -(x-1)^2/4 \right) \]
(a) The potential $U$ of the unperturbed dynamics with $\sigma = \frac{1}{2}$, $\sigma_m = \frac{1}{4}$ and $\sigma_1 = \sigma_2 = \frac{1}{10}$.

(b) The linear and second order response of the $x$ coordinate in a system evolving in the potential landscape on the left hand side to the potential $v(x) = \exp \left( -(x - 1)^2/4 \right)$ (blue).

Figure 2: Evolution in a multiwell potential

By Kramer’s rule the relaxation along the $x$-axis is much faster than the one along the $y$-axis. Therefore, projecting onto the $x$ axis should yield a better approximation of the second order response than projecting onto the $y$ axis. Furthermore, figure 2 (b) is consistent with the error bound of 3.5: the approximation up to second order is very good for small times, and large times but cannot fully capture the dynamics on intermediate time scales.

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