Nonparametric Drift Estimation for Stochastic Differential Equations

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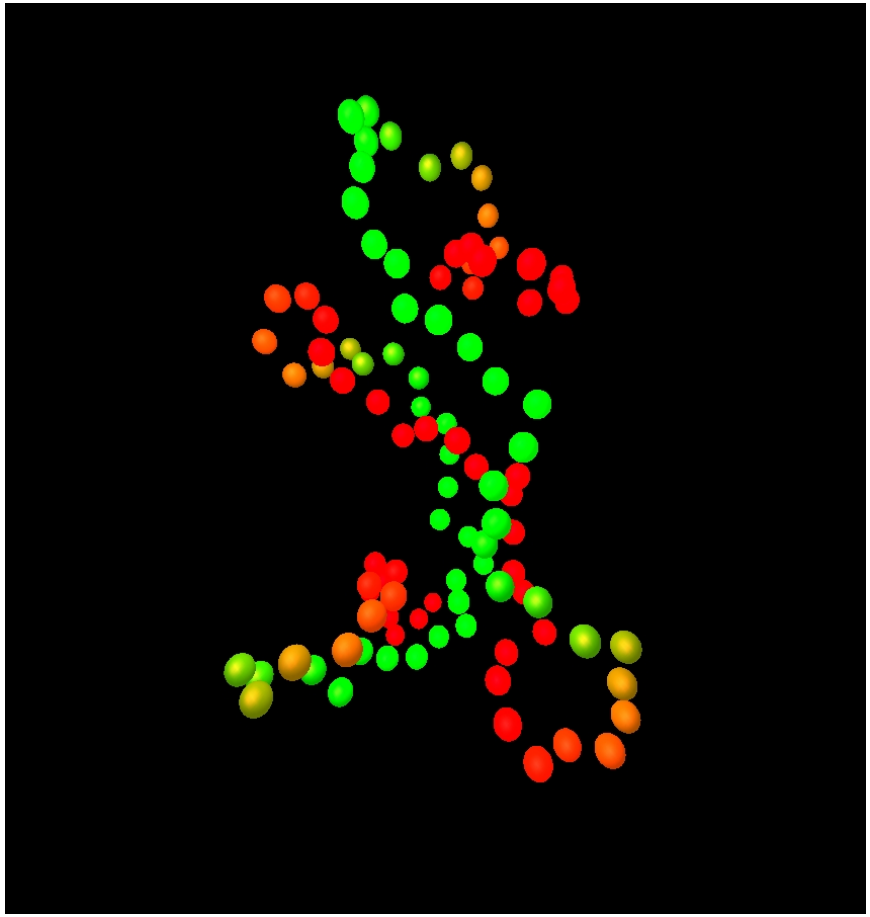
EPSRC Symposium on MCMC and Related Methods
Joint work with O. Papaspiliopoulos, G. Roberts and A. Stuart

Outline

Fitting SDEs to Molecular Dynamics

MD data



$$X(n\Delta t) \in \mathbb{R}^N$$

- Multiple Timescales
- High frequency data
- High dimension, only few dimensions of chemical interest
- Diffusion good description at some timescales only.

Programme

Start from SDE

$$dx = b(x)dt + dB, \quad x(0) = x_0$$

and high-frequency discrete time observations x_i.

- Write down likelihood for $b(\cdot)$ on function space H.
- Modify likelihood to make the local time L an (almost) sufficient statistic.
- Specify prior on function space H, compute posterior. Make Bayesian framework rigorous.
- Application: Toy example from Molecular Dynamics

SDE properties - Girsanov

$$dx = b(x)dt + dB$$

- Generates measure $\mathbb{P}$ on path space $\mathcal{C}([0, T], [0, 2\pi))$.
- $\mathbb{P}$ is absolutely continuous w.r.t. $\mathbb{Q}$ generated by Brownian Motion.
- The Radon-Nikodym derivative is

$$\frac{d\mathbb{P}}{d\mathbb{Q}} = \exp(I[b])$$

$I[b]$ viewed as functional of the drift:

$$I[b] = -\frac{1}{2}\int_0^T \left(b^2(x)dt - 2b(x)dx\right)$$

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Local Time

Local time is the empirical occupation density:

$$\frac{1}{T}\int_0^T f(x_t)dt = \int_{\mathbb{R}} f(a)\frac{L(a)}{T}da$$

- L is continuous but not differentiable.
- In the limit $T \to \infty$ it becomes smooth:

$$\lim_{T\to\infty}\frac{1}{T}L = \varrho^{\infty}$$

The Likelihood Functional

$$l[b] = \log \frac{d\mathbb{P}}{d\mathbb{Q}} = -\frac{1}{2}\int_0^T \left(b^2(x)dt - 2b(x)dx\right)$$

- Start from the Girsanov change of measure.
- Apply the Ito formula for $V(x)$ to rewrite the stochastic integral as boundary terms plus correction.
- Replace Integrals along the trajectory by integral against local time $L(a)da$.

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If local time was smooth

$$
\begin{aligned}
l[b] =& \text{Boundary} - \frac{1}{2}\int \left(b^2 + 2b'\right) L da \\
=& \text{Boundary} - \frac{1}{2}\int b^2 L - 2bL' da \\
\leq& \text{Boundary} - \|L\|_\infty \|b\|_{L^2}^2 - \|b\|_{L^2}^2 - \|L'\|_{L^2}^2
\end{aligned}
$$

- the log-likelihood $l[b]$ is bounded above on $b \in L^2(0, 2\pi)$.
- Taking the functional derivative yields the MLE

$$\widehat{b} = \frac{L'}{2L}$$

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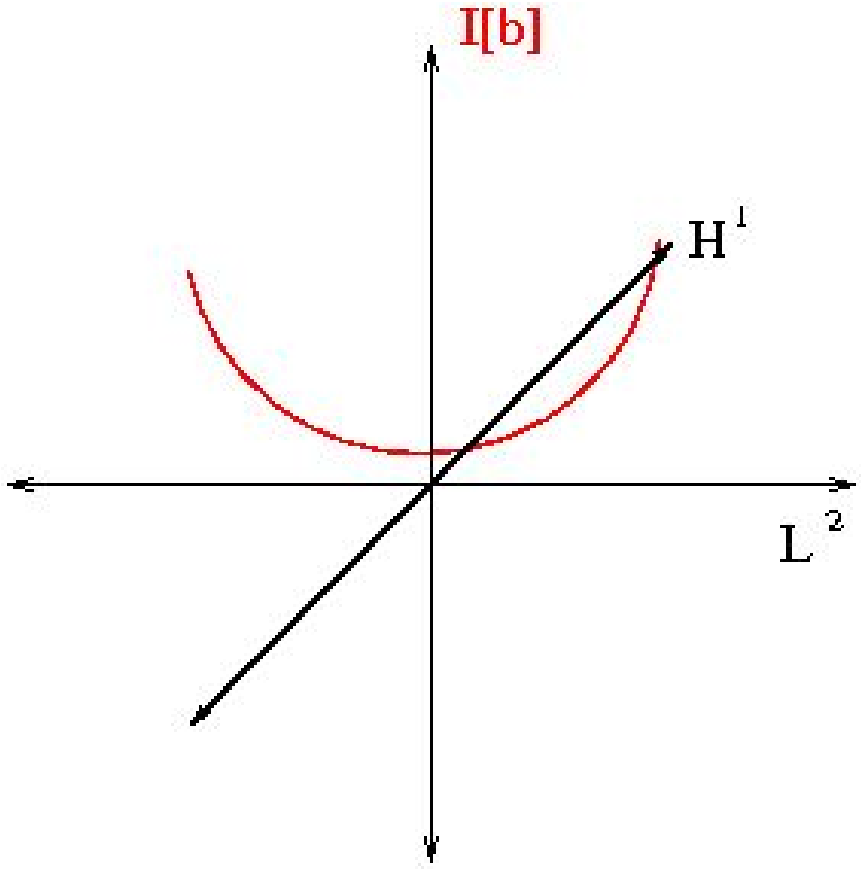
Infinite Dimensional Trouble

$$-I[b] = \int_0^{2\pi} |b(a)|^2 L(a) + b'(a) L(a) da$$

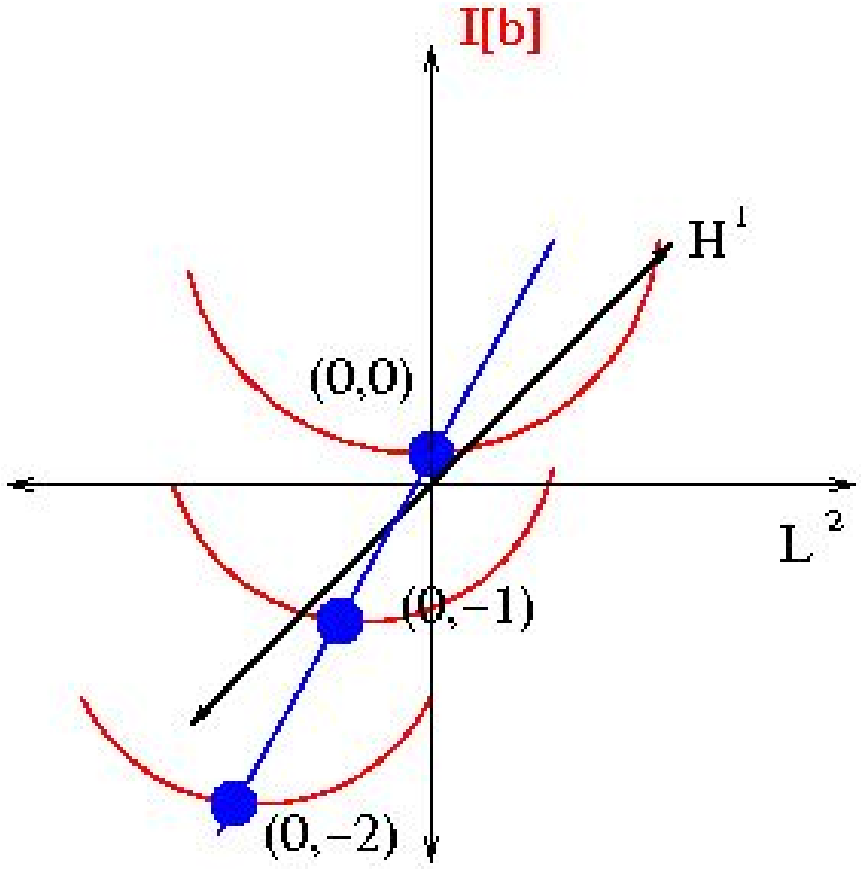
- For smooth L the functional is positive definit.
- Quadratic positive definit functionals are bounded below.
- **BUT** L is not differentiable!



Infinite Dimensional Trouble

$$-I[b] = \int_0^{2\pi} \underbrace{|b(a)|^2 L(a)}_{\text{Term A}} + \underbrace{b'(a)L(a)}_{\text{Term B}} \, da$$

- Quadratic in the L^2-direction (Term A)
- Linear in the Derivative-direction (Term B)
- Hence cylindrical paraboloid - not bounded below!



Three Options

$$\text{Boundary} - \frac{1}{2}\int_0^{2\pi} \left(|b(a)|^2 + b'(a)\right) L(a)da.$$

1. Assume a parametric form $b(x, \theta)$
2. Introduce a regularised version of $L(a)da$.
3. Introduce a prior measure on drift functions $b(\cdot)$ and perform Bayesian estimation.

Gaussian Prior on drift functions

Specify a prior Gaussian measure for zero-mean drift functions by

- Its Mean:

$$b_0 \in H^2_{\text{per}}([0, 2\pi])$$

- Its Precision (operator): $\mathcal{C}_0 = \Delta^2$ on $[0, 2\pi]$ periodic, mean-zero.

Formally:

$$db \propto \exp\left(-\int_0^{2\pi} |\Delta b(a) - \Delta b_0(a)|^2 \, da\right) d\lambda$$

Finding the Posterior - formally

Multiply prior "density" by likelihood:

$$\mu \propto \exp\left(-\int_0^{2\pi} |\Delta b(a)|^2 \, da\right) \cdot \exp\left(\int_0^{2\pi} |b(a)|^2 L(a) + b'(a) L(a) da\right)$$

Complete the square to find that the posterior is Gaussian with

- Mean

$$\left(\Delta^2 + L\right) \widehat{b} = \frac{1}{2} L' + \tilde{\chi} x_0, x_T + W$$

- Posterior Covariance

$$\left(\Delta^2 + L\right)^{-1}$$

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Posterior Mean is the solution of a PDE

Theorem

Let $L \in \mathcal{C}([0, 2\pi])$ be continuous and periodic and not identically zero. Then the PDE for the posterior mean

$$\Delta^2 u + Lu = \frac{1}{2}L' + W + \tilde{\chi}_{x_0, x_T} \tag{1}$$

has a unique weak solution $u \in H^2_{\mathrm{per}}([0, 2\pi])$.

Robustness of the Posterior Mean

Theorem

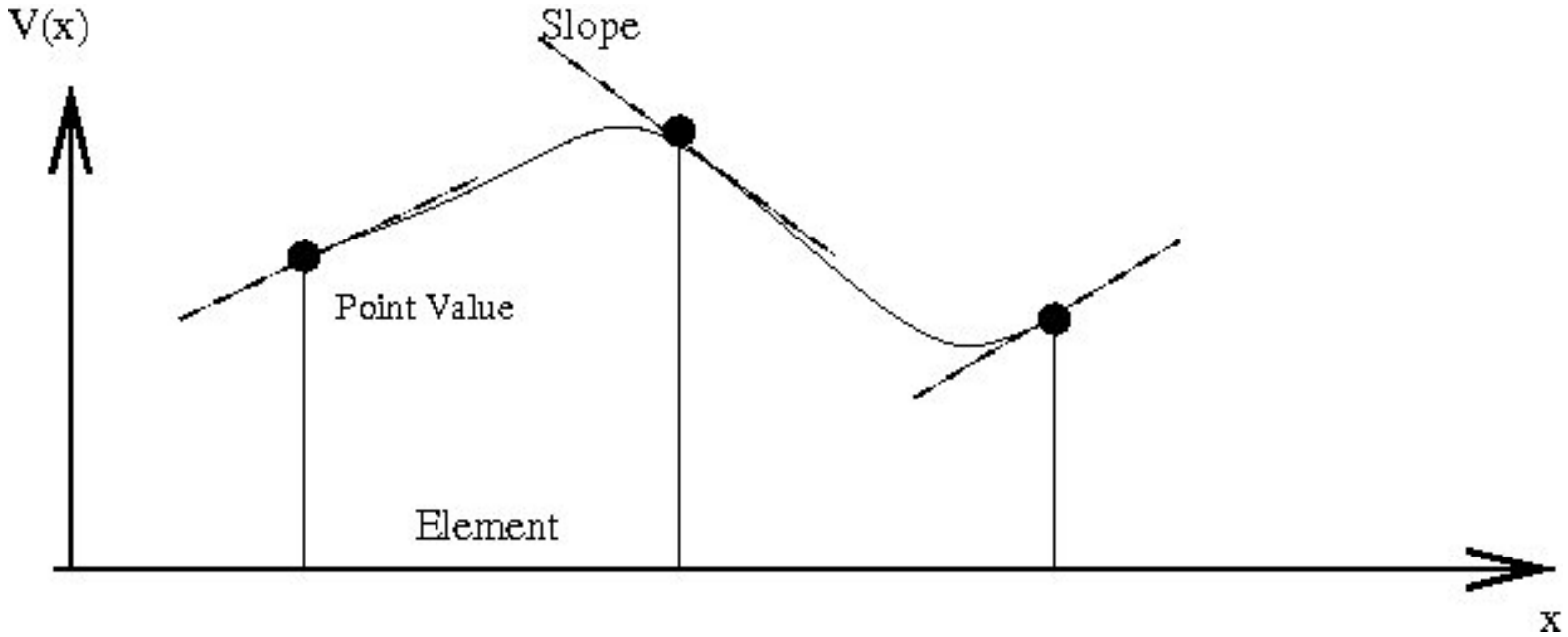
There exists a constant $C(W, \|L\|_\infty) > 0$ such that for all admissible perturbed local times $\tilde{L}$ the deviation of the perturbed posterior mean $\tilde{u}$ from the unpterturbed posterior mean u is bounded in the H^2-norm:

$$\|\tilde{u} - u\|_{H^2} \leq C(W, \|L\|_\infty)\|\tilde{L} - L\|_{L^2} \tag{2}$$

Cleanup

- Observe absolute continuity of posterior and prior measure, Δ^2 and $\Delta^2 + L$ differ only in lower order differential parts.
- Compute the Radon-Nikodym derivative and identify with the likelihood.
- Simple estimate of local time from pointwise estimations combined with Hölder continuity of local time, so that $\|\hat{L} - L\|_{L^2}$ is small.

Numerical Treatment

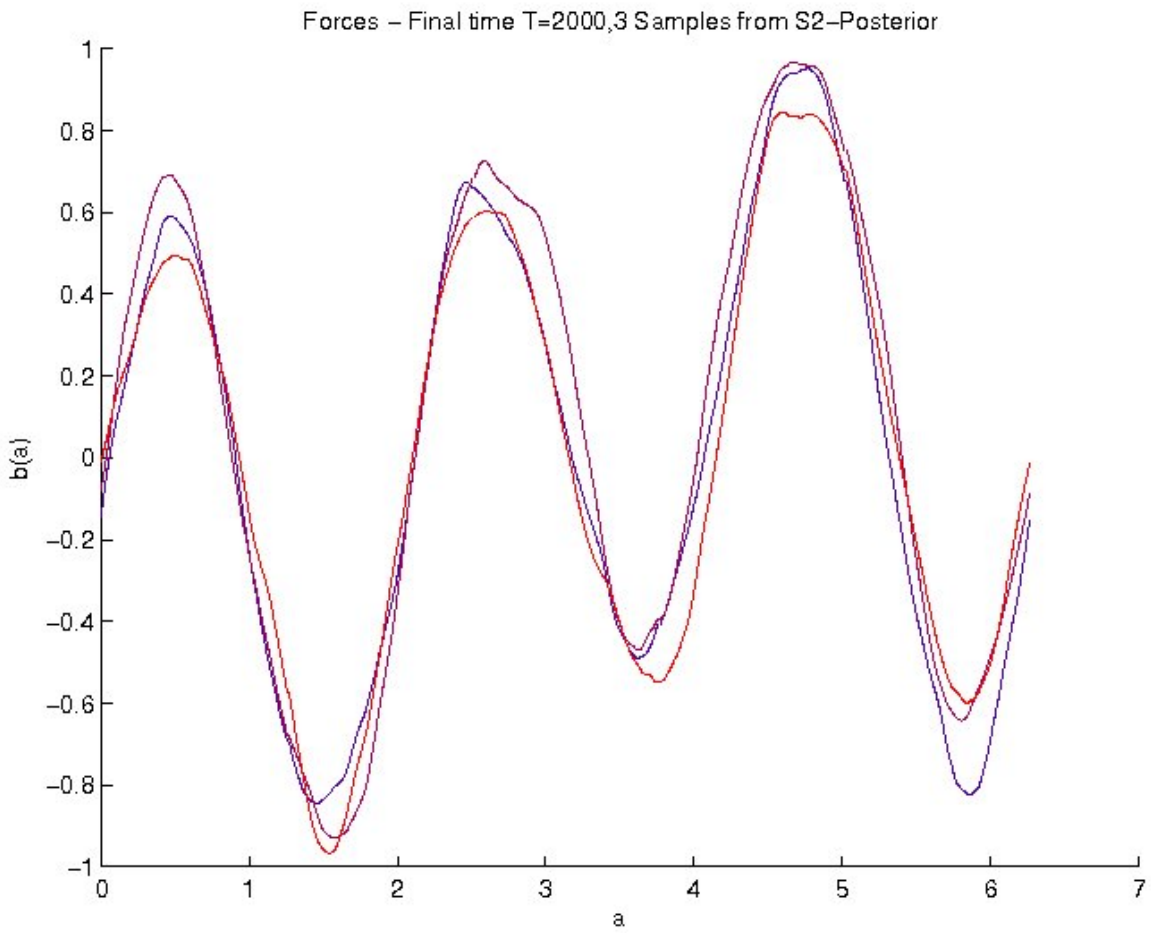


- Fourth order elliptic PDE with non-regular right hand side.
- Use piecewise cubic polynomial base functions on each finite element.

$$b(a) = \sum_{e=1}^{K} \sum_{f=1}^{4} B_{e,f} \phi_{e,f}(a)$$

Numerics: Samples from Posterior

$$dx = -sin(x) + 3cos^2(x)sin(x)dt + dB$$



Second order prior covariance: $\mathcal{A} = \Delta^{-2}$

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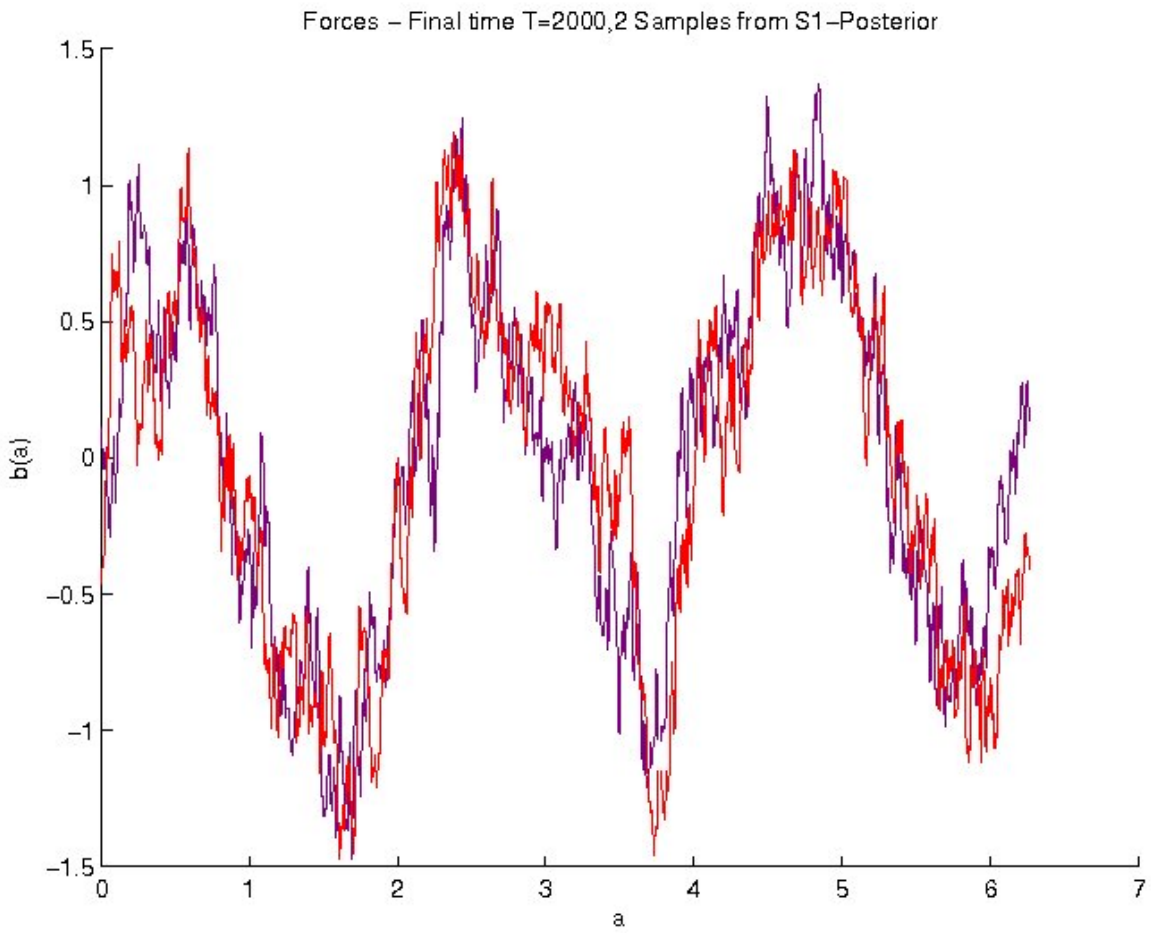
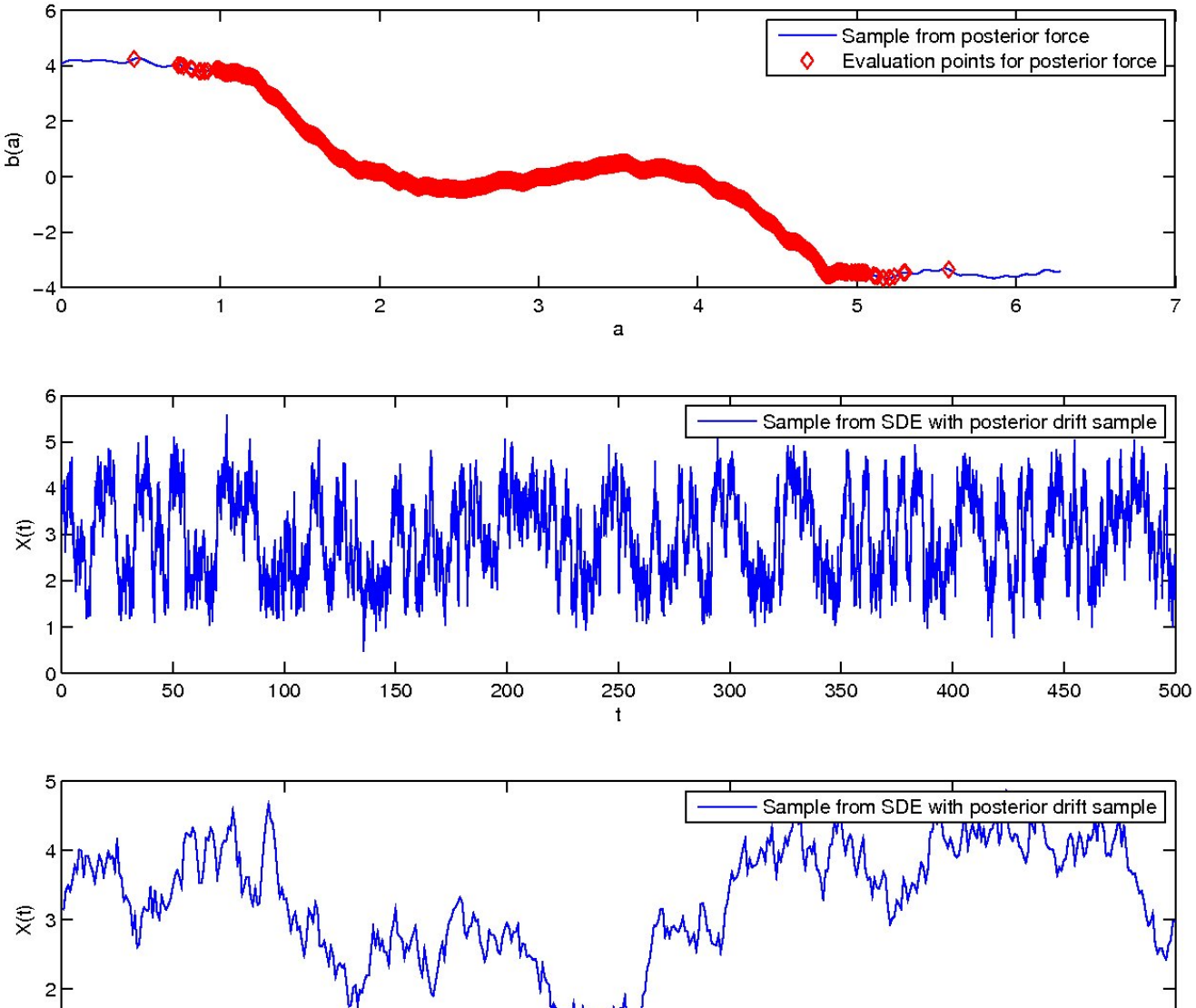


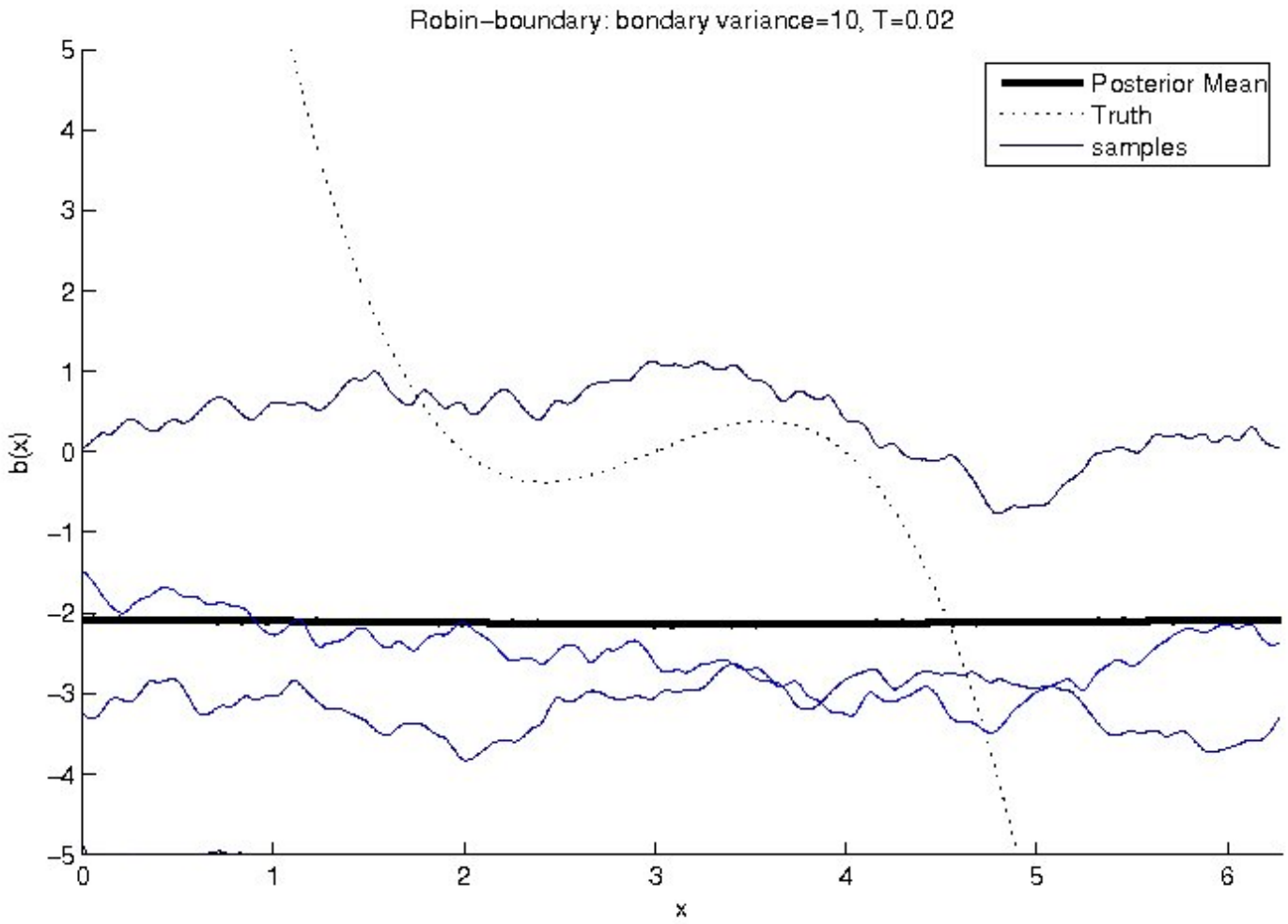
First order prior covariance: $\mathcal{A} = \Delta^{-1}$

Samples from the Posterior are usable



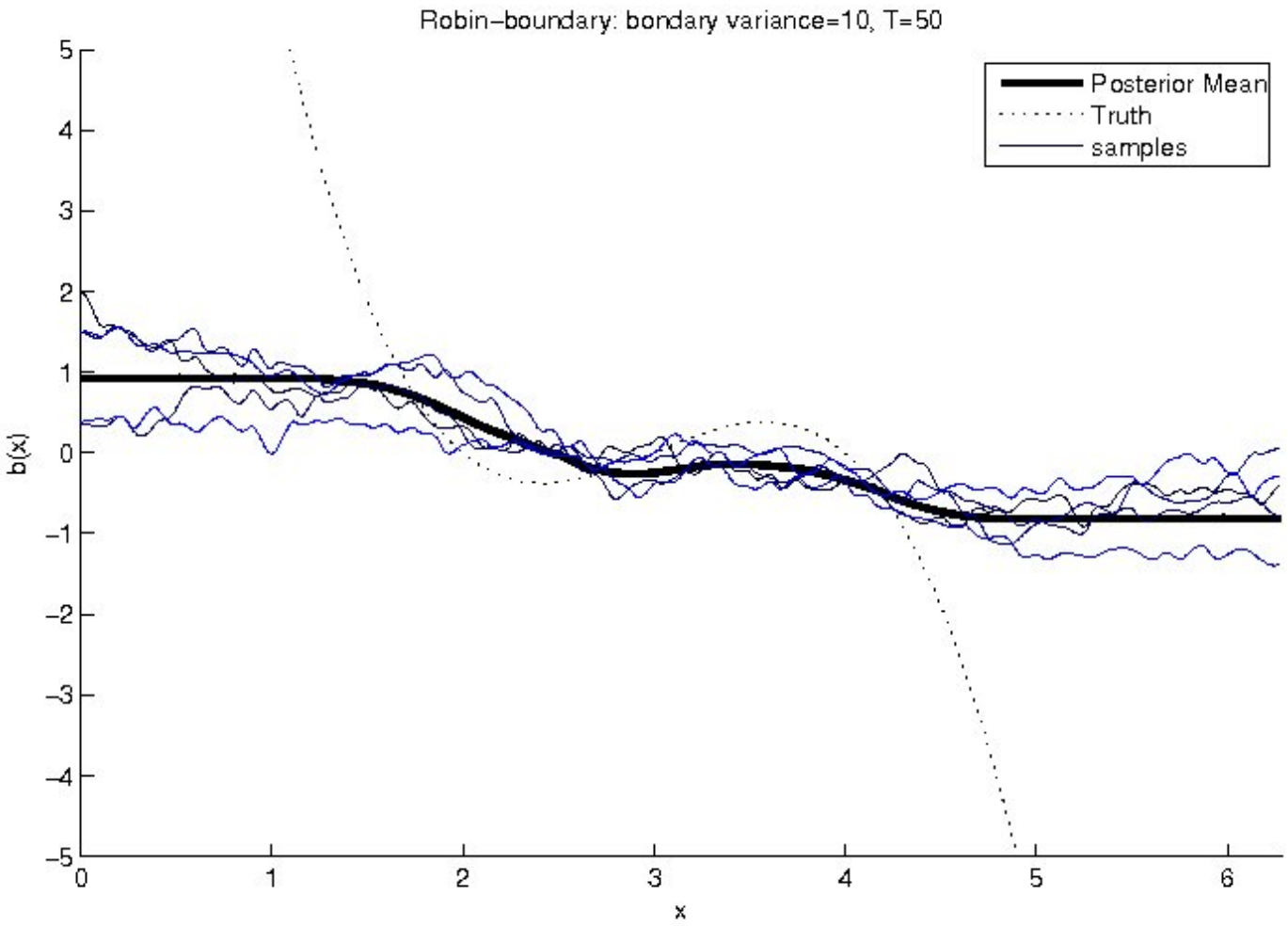
Convergence as $T \to \infty$

Gaussian boundary conditions with second order covariance operator. $T = 0.02$



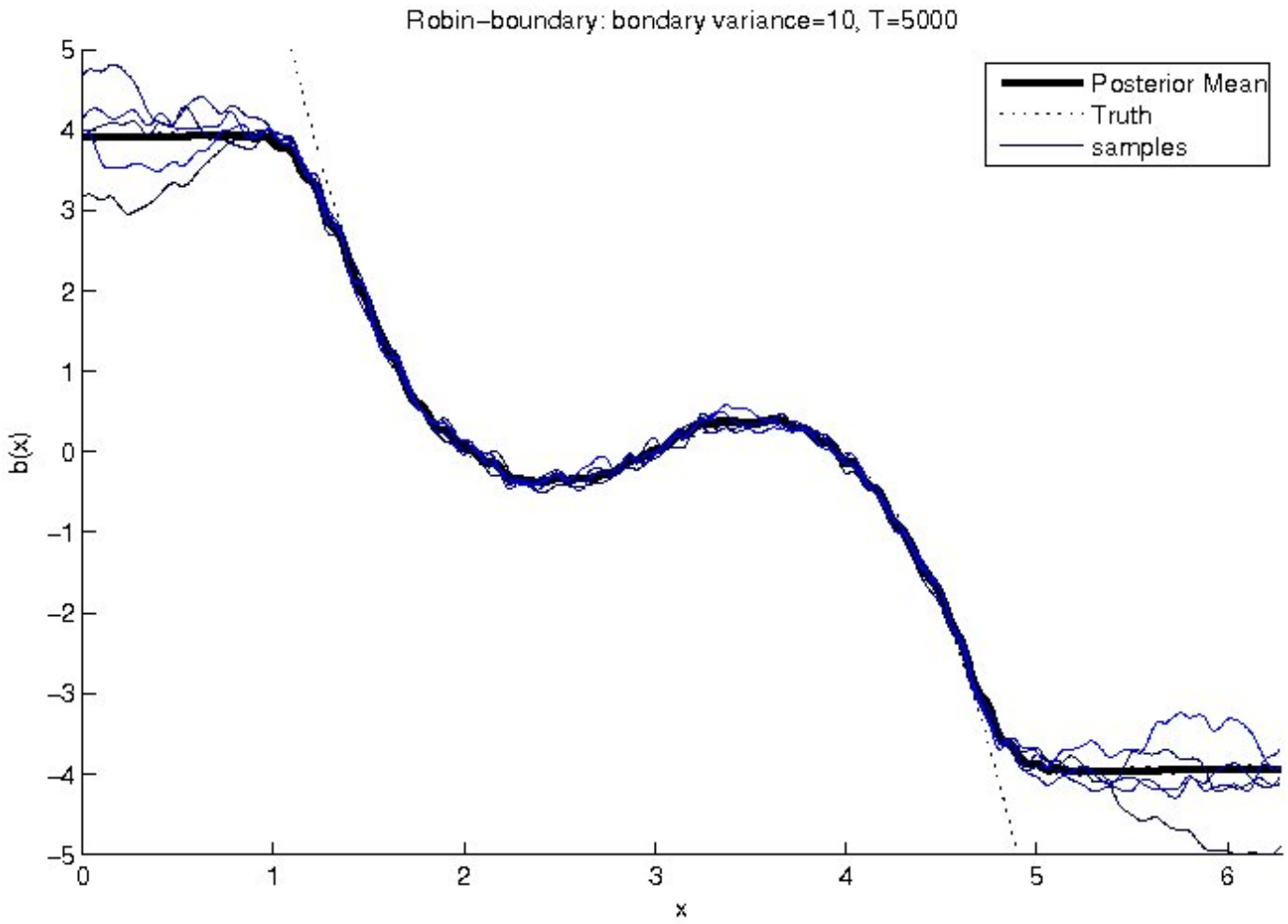
Convergence as $T \to \infty$

Gaussian boundary conditions with second order covariance operator. $T = 50$



Convergence as $T \to \infty$

Gaussian boundary conditions with second order covariance operator. $T = 5000$



Rates of posterior contraction

For $Z_1 = \hat{b}(0.38\pi) - b(0.38\pi)$ and $Z_2 = \int_0^{2\pi} \hat{b}(a)\sin(a)da$.
Questions:

- Do we have a law of large numbers $Z_i \to 0$ as $T \to \infty$?
- Do we get CLT-like convergence? $\mathrm{Var}(Z_i) = \mathcal{O}\left(\frac{1}{T}\right)$

(Numerical) Answers:

- Numerically, $\lim_{T\to\infty} Z_i = 0$ is observed.
- Decay of Variance: Answer depends on i!
  High frequency components of L' can dominate the convergence.

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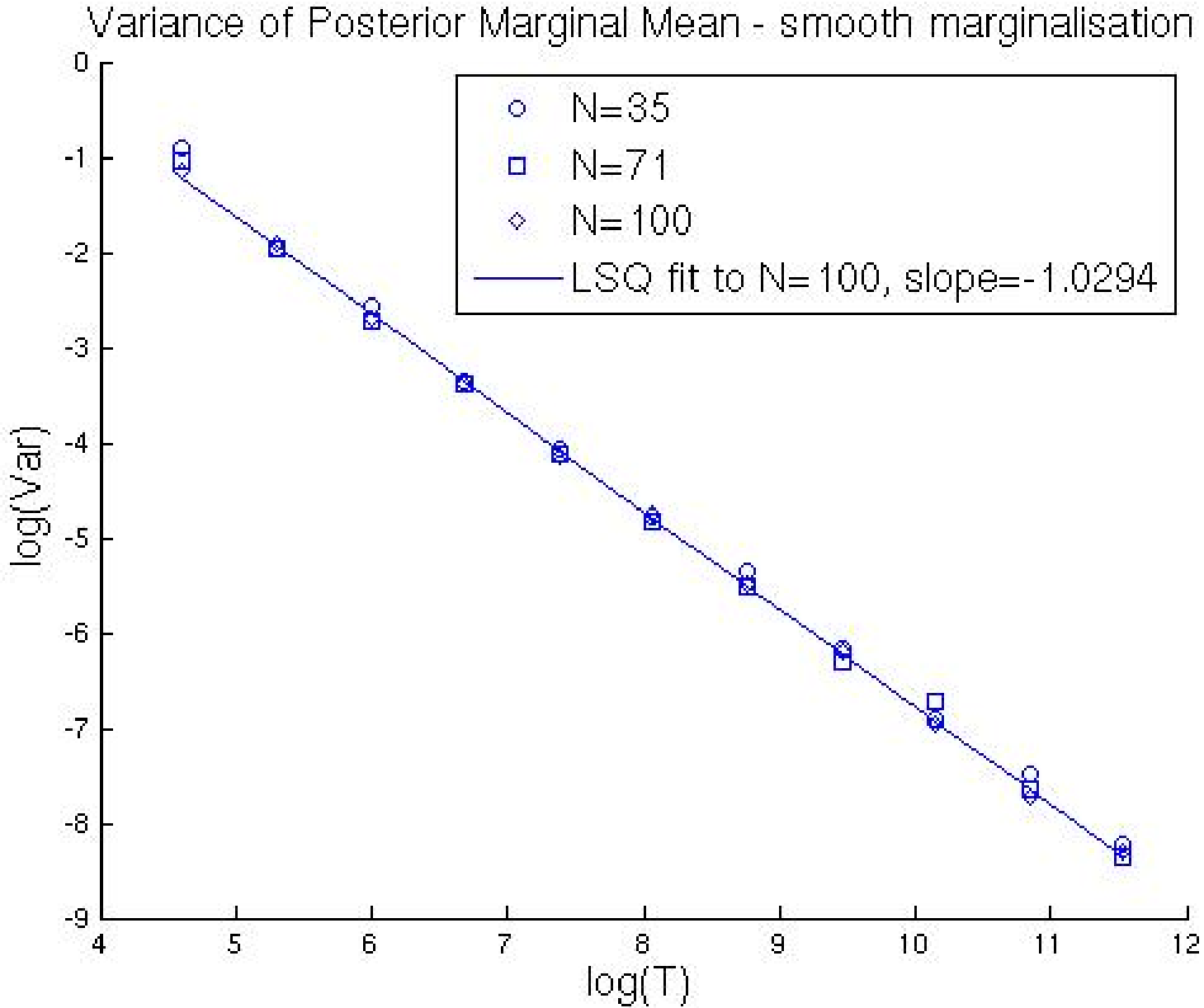
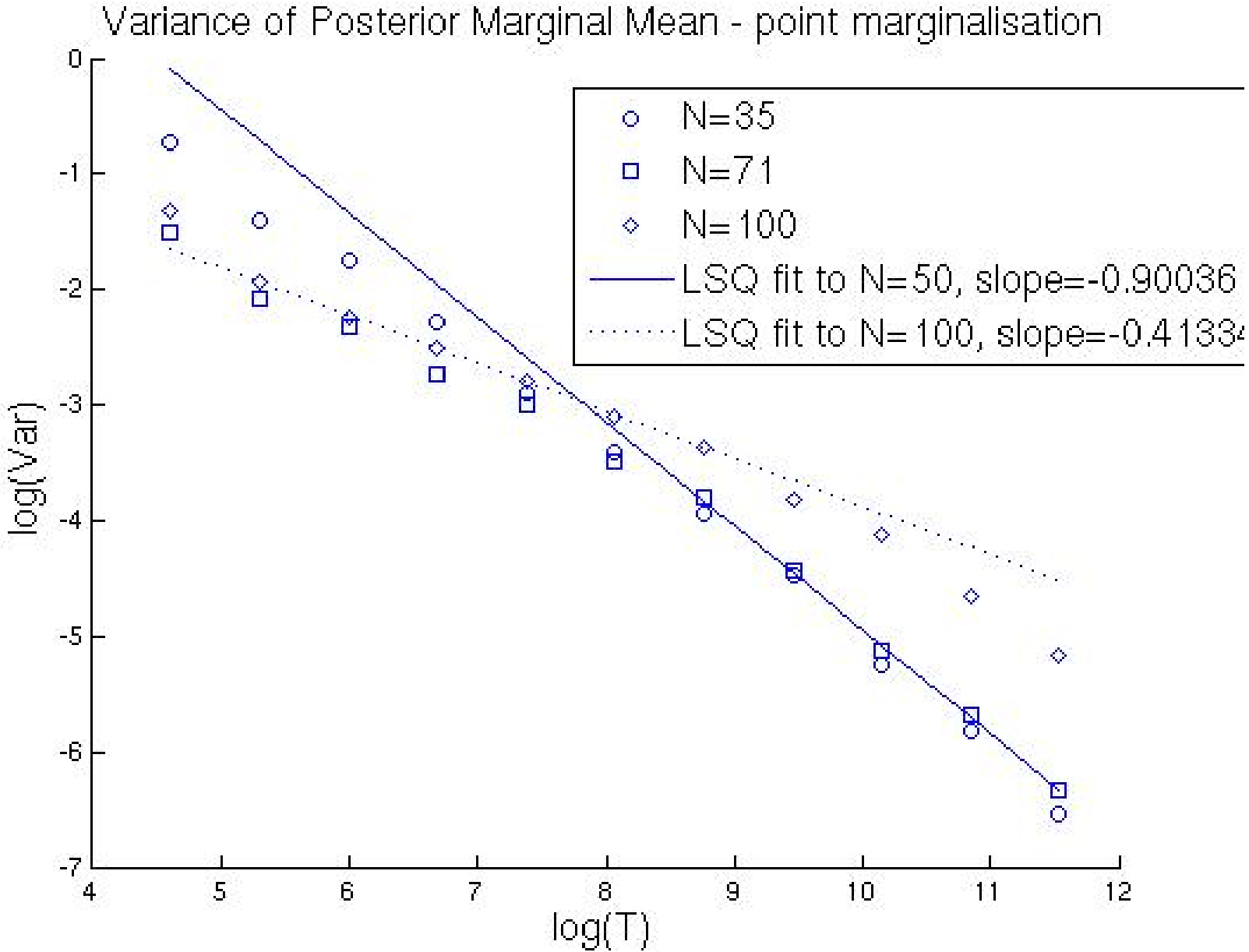
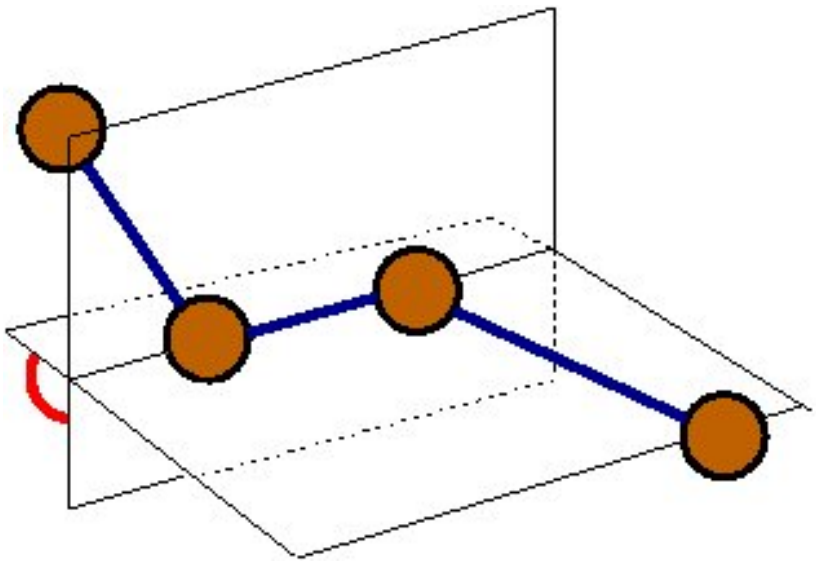
Rate of Posterior Contraction – Smooth Functional

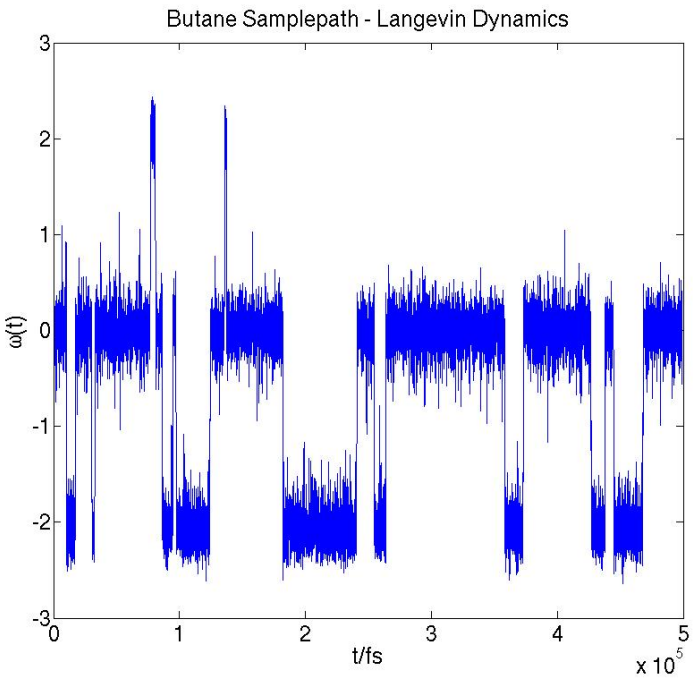


Rate of Posterior Contraction – Point Evaluation



Molecular Dynamics

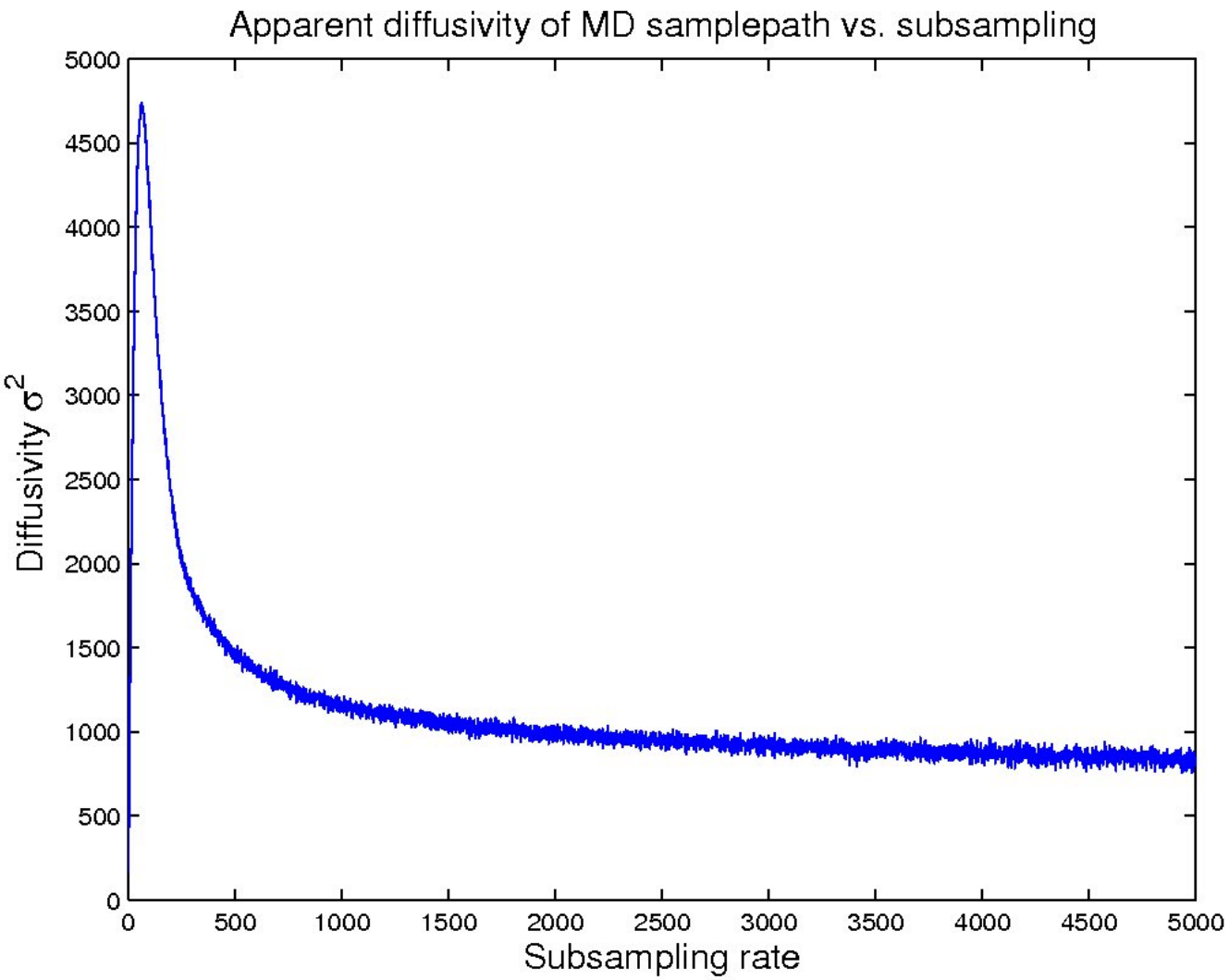




$$
\begin{aligned}
M\ddot{X}(t) &= -\nabla V(X(t)) - \gamma M\dot{X}(t) + \sqrt{2\gamma k_B T M}\dot{B} \\
X &\mapsto \omega(X)
\end{aligned}
$$

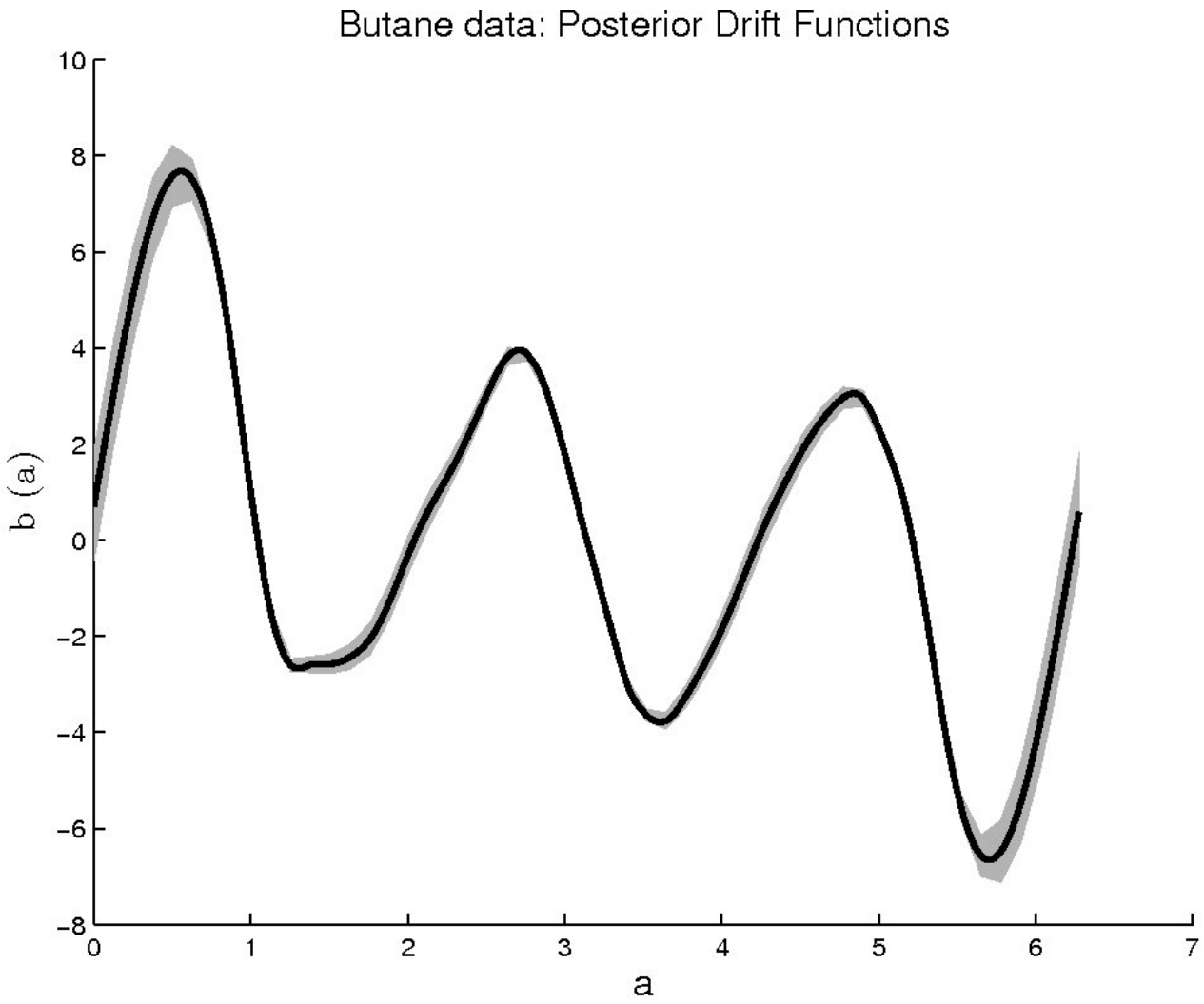
Fitting Result

Whether data looks like a diffusion depends on *timescale*.



Fitting Result

Posterior mean and standard deviation band for $k = 1000$:



Extensions

Numerically, the method also works for

- second order covariance operators
- Gaussian boundary conditions
- the whole real line

Future work:

- Extension to higher dimensions (2,3)
- Low-frequency data by sampling from missing local time.
- Convergence properties for various test functionals (singular limit problem in PDE theory)

Summary

- Nonparametric drift estimation for diffusions on the circle can be performed rigorously for Gaussian prior (conjugate prior).
- Finite element implementation enables error control from discrete time high frequency samples all the way to numerically obtained posterior means.
- Applications are in molecular dynamics and other areas where data with multiple timescales pose problems.