

Bayesian inference of multiscale diffusion processes

Assyr Abdulle ¹ Giacomo Garegnani ¹ Grigoris Pavliotis ²

MATHICSE Retreat

Champéry – 11/13 June 2019

¹Institute of Mathematics, EPFL

²Department of Mathematics, Imperial College London

Motivation

Bayesian inference

- Fit model to data
- Full UQ approach

Diffusion processes

- Intrinsically stochastic phenomena
- Analysis for BM noise

Multiscale

- Numerous real-world applications
- Theory of homogenization applies

Problem statement

Multiscale SDE – first order Langevin

$$dx^\varepsilon(t) = - \underbrace{\alpha \nabla V_0(x^\varepsilon(t))}_{\text{large-scale potential}} dt - \underbrace{\frac{1}{\varepsilon} \nabla V_1\left(\frac{x^\varepsilon(t)}{\varepsilon}\right)}_{\text{fluctuating potential}} dt + \underbrace{\sqrt{2\sigma} dW(t)}_{\text{diffusion}}.$$

Problem statement

Multiscale SDE – first order Langevin

$$dx^\varepsilon(t) = - \underbrace{\alpha \nabla V_0(x^\varepsilon(t))}_{\text{large-scale potential}} dt - \underbrace{\frac{1}{\varepsilon} \nabla V_1\left(\frac{x^\varepsilon(t)}{\varepsilon}\right)}_{\text{fluctuating potential}} dt + \underbrace{\sqrt{2\sigma} dW(t)}_{\text{diffusion}}.$$

Homogenized SDE

$$dx^0(t) = -A \nabla V_0(x^0(t)) dt + \sqrt{2\Sigma} dW(t), \quad A = K\alpha, \Sigma = K\sigma.$$

Homogenization result: $x^\varepsilon \Rightarrow x^0$ in $\mathcal{C}^0((0, T), \mathbb{R}^d)$ for $\varepsilon \rightarrow 0$.

Problem statement

Multiscale SDE – first order Langevin

$$dx^\varepsilon(t) = \underbrace{-\alpha \nabla V_0(x^\varepsilon(t)) dt}_{\text{large-scale potential}} - \underbrace{\frac{1}{\varepsilon} \nabla V_1\left(\frac{x^\varepsilon(t)}{\varepsilon}\right) dt}_{\text{fluctuating potential}} + \underbrace{\sqrt{2\sigma} dW(t)}_{\text{diffusion}}.$$

Homogenized SDE

$$dx^0(t) = -A \nabla V_0(x^0(t)) dt + \sqrt{2\Sigma} dW(t), \quad A = K\alpha, \Sigma = K\sigma.$$

Homogenization result: $x^\varepsilon \Rightarrow x^0$ in $\mathcal{C}^0((0, T), \mathbb{R}^d)$ for $\varepsilon \rightarrow 0$.

Inverse problem 1 – MS / MS

Find $\theta^\varepsilon = (\alpha, \sigma)$ given $\mathbf{y} = \mathbf{x}^\varepsilon(\theta^\varepsilon) + \boldsymbol{\eta}$, $\boldsymbol{\eta} \sim \rho_\eta$.

Notation: $\mathbb{R}^{Nd} \ni \mathbf{x}^\varepsilon = (x_1^\varepsilon, x_2^\varepsilon, \dots, x_N^\varepsilon)$, $x_k^\varepsilon = x^\varepsilon(t_k)$.

Problem statement

Multiscale SDE – first order Langevin

$$dx^\varepsilon(t) = \underbrace{-\alpha \nabla V_0(x^\varepsilon(t)) dt}_{\text{large-scale potential}} - \underbrace{\frac{1}{\varepsilon} \nabla V_1\left(\frac{x^\varepsilon(t)}{\varepsilon}\right) dt}_{\text{fluctuating potential}} + \underbrace{\sqrt{2\sigma} dW(t)}_{\text{diffusion}}.$$

Homogenized SDE

$$dx^0(t) = -A \nabla V_0(x^0(t)) dt + \sqrt{2\Sigma} dW(t), \quad A = K\alpha, \Sigma = K\sigma.$$

Homogenization result: $x^\varepsilon \Rightarrow x^0$ in $\mathcal{C}^0((0, T), \mathbb{R}^d)$ for $\varepsilon \rightarrow 0$.

Inverse problem 2 – MS / HOM

Find $\theta^0 = (A, \Sigma)$ given $\mathbf{y} = \mathbf{x}^\varepsilon(\theta^\varepsilon) + \boldsymbol{\eta}$, $\boldsymbol{\eta} \sim \rho_\eta$.

Notation: $\mathbb{R}^{Nd} \ni \mathbf{x}^\varepsilon = (x_1^\varepsilon, x_2^\varepsilon, \dots, x_N^\varepsilon)$, $x_k^\varepsilon = x^\varepsilon(t_k)$.

Bayesian framework

Inverse problem 1 – MS / MS

Find $\theta^\varepsilon = (\alpha, \sigma)^\top$ given $\mathbf{y} = \mathbf{x}^\varepsilon(\theta^\varepsilon) + \boldsymbol{\eta}$, $\boldsymbol{\eta} \sim \rho_\eta$.

Posterior distribution $\mu^\varepsilon(\theta^\varepsilon \mid \mathbf{y})$ with density

$$p^\varepsilon(\theta^\varepsilon \mid \mathbf{y}) = \frac{1}{Z^\varepsilon} \underbrace{p(\theta^\varepsilon)}_{\text{prior}} \underbrace{p^\varepsilon(\mathbf{y} \mid \theta^\varepsilon)}_{\text{likelihood}}, \quad Z^\varepsilon \text{ s.t. } \int p^\varepsilon(\theta \mid \mathbf{y}) d\theta = 1.$$

Prior: Easy to evaluate (e.g. Gaussian), independent of ε

Likelihood: Needs more work

Bayesian framework

Inverse problem 1 – MS / MS

Find $\theta^\varepsilon = (\alpha, \sigma)^\top$ given $\mathbf{y} = \mathbf{x}^\varepsilon(\theta^\varepsilon) + \boldsymbol{\eta}$, $\boldsymbol{\eta} \sim \rho_\eta$.

Likelihood: Needs more work \Rightarrow marginalization

$$p^\varepsilon(\mathbf{y} \mid \theta^\varepsilon) = \int_{\mathbb{R}^{Nd}} p^\varepsilon(\mathbf{y} \mid \mathbf{x}, \theta^\varepsilon) p^\varepsilon(\mathbf{x} \mid \theta^\varepsilon) d\mathbf{x}.$$

where (observation independence)

$$p^\varepsilon(\mathbf{y} \mid \mathbf{x}, \theta^\varepsilon) = \prod_{k=1}^N p^\varepsilon(y_k \mid x_k, \theta^\varepsilon).$$

Observation density: $p(y_k \mid x_k, \theta^\varepsilon) = \rho_\eta^{(k)}(y_k - x_k)$

Bayesian framework

Inverse problem 1 – MS / MS

Find $\theta^\varepsilon = (\alpha, \sigma)^\top$ given $\mathbf{y} = \mathbf{x}^\varepsilon(\theta^\varepsilon) + \boldsymbol{\eta}$, $\boldsymbol{\eta} \sim \rho_\eta$.

Likelihood: Needs more work \Rightarrow marginalization

$$p^\varepsilon(\mathbf{y} \mid \theta^\varepsilon) = \int_{\mathbb{R}^{Nd}} p(\mathbf{y} \mid \mathbf{x}, \theta^\varepsilon) p^\varepsilon(\mathbf{x} \mid \theta^\varepsilon) d\mathbf{x}.$$

where (observation independence)

$$p(\mathbf{y} \mid \mathbf{x}, \theta^\varepsilon) = \prod_{k=1}^N p(y_k \mid x_k, \theta^\varepsilon).$$

Observation density: $p(y_k \mid x_k, \theta^\varepsilon) = \rho_\eta^{(k)}(y_k - x_k) \Rightarrow$ independent of ε .

Bayesian framework

Inverse problem 1 – MS / MS

Find $\theta^\varepsilon = (\alpha, \sigma)^\top$ given $\mathbf{y} = \mathbf{x}^\varepsilon(\theta^\varepsilon) + \boldsymbol{\eta}$, $\boldsymbol{\eta} \sim \rho_\eta$.

Likelihood: Needs more work \Rightarrow marginalization

$$p^\varepsilon(\mathbf{y} \mid \theta^\varepsilon) = \int_{\mathbb{R}^{Nd}} p(\mathbf{y} \mid \mathbf{x}, \theta^\varepsilon) p^\varepsilon(\mathbf{x} \mid \theta^\varepsilon) d\mathbf{x}.$$

where (Markov property)

$$p^\varepsilon(\mathbf{x} \mid \theta^\varepsilon) = p(x_0) \prod_{k=1}^N p^\varepsilon(x_k \mid x_{k-1}, \theta^\varepsilon).$$

Transition density: $p^\varepsilon(x_k \mid x_{k-1}, \theta^\varepsilon) \Rightarrow$ only “ingredient” depending on ε .

Bayesian framework

Inverse problem 1 – MS / MS

Find $\theta^\varepsilon = (\alpha, \sigma)^\top$ given $\mathbf{y} = \mathbf{x}^\varepsilon(\theta^\varepsilon) + \boldsymbol{\eta}$, $\boldsymbol{\eta} \sim \rho_\eta$.

Idea: Replace $p^0(\mathbf{x} \mid \theta^\varepsilon) \approx p^\varepsilon(\mathbf{x} \mid \theta^\varepsilon) \Rightarrow$ cheaper!

Result: Homogenized posterior $\mu^0(\theta \mid \mathbf{y})$ with density

$$p^0(\theta^\varepsilon \mid \mathbf{y}) = \frac{1}{Z^0} p(\theta^\varepsilon) p^0(\mathbf{y} \mid \theta^\varepsilon), \quad Z^0 \text{ s.t. } \int p^0(\theta \mid \mathbf{y}) d\theta = 1,$$

with

$$p^0(\mathbf{y} \mid \theta^\varepsilon) = \int_{\mathbb{R}^{Nd}} p(\mathbf{y} \mid \mathbf{x}, \theta^\varepsilon) p^0(\mathbf{x} \mid \theta^\varepsilon) d\mathbf{x}.$$

High-dimensional integral \Rightarrow Compute unbiased estimator $\hat{p}^0(\mathbf{y} \mid \theta^\varepsilon)$.

Bayesian framework

Inverse problem 1 – MS / MS

Find $\theta^\varepsilon = (\alpha, \sigma)^\top$ given $\mathbf{y} = \mathbf{x}^\varepsilon(\theta^\varepsilon) + \boldsymbol{\eta}$, $\boldsymbol{\eta} \sim \rho_\eta$.

Idea: Replace $p^0(\mathbf{x} \mid \theta^\varepsilon) \approx p^\varepsilon(\mathbf{x} \mid \theta^\varepsilon) \Rightarrow$ cheaper!

Result: Homogenized posterior $\mu^0(\theta \mid \mathbf{y})$ with density

$$p^0(\theta^\varepsilon \mid \mathbf{y}) = \frac{1}{Z^0} p(\theta^\varepsilon) p^0(\mathbf{y} \mid \theta^\varepsilon), \quad Z^0 \text{ s.t. } \int p^0(\theta \mid \mathbf{y}) d\theta = 1,$$

Proposition

Hellinger distance $d_{\text{Hell}}(\mu^\varepsilon(\cdot \mid \mathbf{y}), \mu^0(\cdot \mid \mathbf{y})) \rightarrow 0$ for $\varepsilon \rightarrow 0$.

Thank you for your attention!

References