Bayesian inference of multiscale diffusion processes

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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

Multiscale SDE - first order Langevin

$$\mathrm{d} x^{\varepsilon}(t) = -\underbrace{\alpha \nabla V_0(x^{\varepsilon}(t))}_{\text{large-scale potential}} - \underbrace{\frac{1}{\varepsilon} \nabla V_1(\frac{x^{\varepsilon}(t)}{\varepsilon})}_{\text{fluctuating potential}} \, \mathrm{d} t + \underbrace{\sqrt{2\sigma} \, \mathrm{d} W(t)}_{\text{diffusion}}.$$

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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 $C^{0}((0, T), \mathbb{R}^{d})$ for $\varepsilon \to 0$.

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

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Inverse problem 2 – MS / HOM

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

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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

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 ⇒ marginalization

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

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

Inverse problem 1 - MS / MS

Find
$$\theta^{\varepsilon} = (\alpha, \sigma)^{\top}$$
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Likelihood: Needs more work ⇒ marginalization

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

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

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 ⇒ marginalization

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

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: $p^{\varepsilon}(x_k \mid x_{k-1}, \theta^{\varepsilon}) \Rightarrow \text{only "ingredient" depending on } \varepsilon$.

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

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

with

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

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

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Proposition

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

Thank you for your attention!

References

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