Probabilistic solvers for ODE's and Bayesian inference of parametrized models

Master Project - Master in CSE

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Outline of the presentation

1. Introduction on Bayesian inference and MCMC
2. Probabilistic solvers for ODE's
3. Bayesian inference inverse problems with differential equations

Consider Ω event space, $\mathcal{A}$ σ-algebra, P probability measure and $(\Omega, \mathcal{A}, P)$. Given A, B in Ω, Bayes' formula reads

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)} \propto P(B \mid A)P(A).$$

Normalization constant $P(B)$ can be replaced as

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{\int_\Omega P(B \mid A)P(A)},$$

as $P(A \mid B)$ is a probability distribution.

Problem. Consider two events A, B in Ω and the probability space $(\Omega, \mathcal{A}, P)$. We want to infer the probability distribution of A given B as

$$\underbrace{\pi(A \mid B)}_{\text{posterior}} \propto \overbrace{\mathcal{Q}(A)}^{\text{prior}} \underbrace{\mathcal{L}(B \mid A)}_{\text{likelihood}}$$

In models parametrized by a parameter θ, we deduce the distribution of θ through observations $\mathcal{Y}_n = \{y_1, y_2, \ldots, y_n\}$ as

$$\pi(\theta \mid \mathcal{Y}_n) \propto \mathcal{Q}(\theta)\mathcal{L}(\mathcal{Y}_n \mid \theta).$$

Goal. Approximate the expectation under the distribution $\pi(\theta \mid \mathcal{Y})$ of a functional of the parameter $\theta \in \mathbb{R}^{N_p}$ with a Monte Carlo sum, i.e.,

$$\mathbb{E}^{\pi}\left[g(\theta)\right] = \int_{\mathbb{R}^{N_p}} g(\theta)\pi(\mathrm{d}\theta \mid \mathcal{Y}) \approx \frac{1}{N}\sum_{k=1}^{N} g(\theta^{(k)}),$$

where $\theta^{(k)}$ are realizations of θ.

Problem. How do we generate samples $\theta^{(k)}$, with $k = 1, \ldots, N$ so that the approximation (5) holds?
$\rightsquigarrow$ MCMC [Gilks, 2005, e.g.]

Idea. Generate samples $\theta^{(k)}$, with from a Markov chain with kernel P until the chain reaches its stationary distribution. Different choices of the Markov kernel lead to different MCMC algorithms.

Metropolis-Hastings (MH). Choose a *proposal distribution* $q(x, y)$ such that

$$\int_{\mathbb{R}^{N_p}} q(x, y)\mathrm{d}y = 1,$$

Then, given current sample $\theta^{(i)}$, the transition kernel P_{MH} giving $\theta^{(i+1)}$ is defined as

$$P_{\mathrm{MH}}(\theta^{(i)}, \theta^{(i+1)}) := \alpha(\theta^{(i)}, \theta^{(i+1)})q(\theta^{(i)}, \theta^{(i+1)}) + \delta_{\theta^{(i)}}(\theta^{(i+1)})\rho(\theta^{(i)}),$$

where $\alpha(\theta^{(i)}, \vartheta)$ is the *acceptance probability* and is given by

$$\alpha(\theta^{(i)}, \vartheta) = \min\left\{ \frac{\pi(\vartheta)q(\vartheta, \theta^{(i)})}{\pi(\theta^{(i)})q(\theta^{(i)}, \vartheta)}, 1 \right\},$$

and ρ is defined as

$$\rho(\theta^{(i)}) := 1 - \int_{\mathbb{R}^{N_p}} \alpha(\theta^{(i)}, x)q(\theta^{(i)}, x)\mathrm{d}x.$$

Algorithm 1 Metropolis-Hastings.

Given $\theta^{(0)} \in \mathbb{R}^{N_p}$, $N \in \mathbb{N}_0$.
for $i = 0, \ldots, N$ **do**
  Draw ϑ from $q(\theta^{(i)}, \cdot)$;
  Compute the acceptance probability $\alpha(\theta^{(i)}, \vartheta)$ as

$$\alpha(\theta^{(i)}, \vartheta) = \min\left\{\frac{\pi(\vartheta)q(\vartheta, \theta^{(i)})}{\pi(\theta^{(i)})q(\theta^{(i)}, \vartheta)}, 1\right\};$$

  Draw u from $\mathcal{U}(0, 1)$;
  if $\alpha > u$ **then**
    Accept ϑ, set $\theta_{i+1} = \vartheta$;
  else
    set $\theta_{i+1} = \theta^{(i)}$
  end if
end for

Remark. If the proposal distribution is symmetric, i.e., $q(x, y) = q(y, x)$, then

$$\alpha(\theta^{(i)}, \vartheta) = \min\left\{\frac{\pi(\vartheta)}{\pi(\theta^{(i)})}, 1\right\}.$$

For example, Gaussian proposal [Kaipio and Somersalo, 2005]

$$q(x, y) \propto \exp\left(-\frac{1}{2}(x-y)^T\Sigma^{-1}(x-y)\right).$$

Problems. Two main problems

1. How to choose an efficient proposal distribution?
2. How to modify MH if it is not possible to evaluate the posterior distribution?

Problem. Bad proposal distribution $q(x, y) \implies$ inefficient algorithms. Measure efficiency with *acceptance ratio*.

Idea. Adapt $q(x, y)$ to obtain a chosen acceptance ratio α^*. Choose $q(x, y)$ Gaussian, the new guess ϑ is

$$\vartheta = \theta_k + S_n z_n, \quad Z_n \sim \mathcal{N}(0, I),$$

where $S_n \in \mathbb{R}^{N_p \times N_p}$ is lower triangular definite positive. Then,

$$S_{n+1} S_{n+1}^T = S_n \left(I + \eta_n \left(\alpha(\theta^{(n)}, \vartheta) - \alpha^* \right) \frac{z_n z_n^T}{z_n^T z_n} \right) S_n^T,$$

where $\eta_n \xrightarrow{n \to \infty} 0$.

Two-dimensional distribution π with density [Kaipio and Somersalo, 2005]

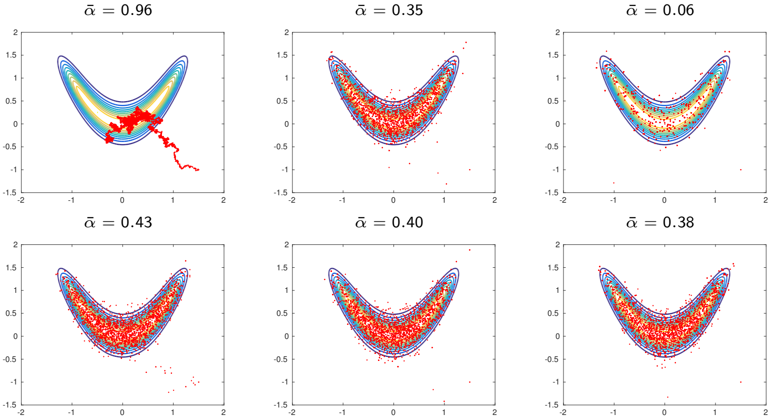
$$\pi(X) \propto \exp\left(-10(X_1^2 - X_2)^2 - (X_1 - 0.25)^4\right),$$

Setting of the experiment. Given $\sigma = \{0.01, 0.5, 2.0\}$, compare

- standard MH with Gaussian proposal with covariance σI,
- RAM with $S_0 = \sigma I$ and $\alpha^* = 0.4$.

Draw $N = 5000$ samples and compute final acceptance ratio $\bar{\alpha}$.

Robust adaptive Metropolis [Vihola, 2012], numerical experiment



Samples produced by MH and RAM for the distribution with standard MH (first row) and RAM (second row).

Problem. Impossible to evaluate $\pi(\theta)$ (no closed form available).

Idea. Find evaluable $\pi(\theta, \xi)$ that admits $\pi(\theta)$ as marginal distribution, then compute

$$\hat{\pi}_M(\theta) = \frac{1}{M} \sum_{i=1}^{M} \pi(\theta, \xi^{(i)}),$$

with $\xi^{(i)}$, $i = 1, \dots, M$ realizations of ξ. Use $\hat{\pi}_M$ for $\alpha(\theta^{(i)}, \vartheta)$.

Remark. The rest of MH is unchanged.

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Problem. Given $f \colon \mathbb{R}^d \to \mathbb{R}^d$ and the autonomous ODE

$$u'(t) = f(u), \quad u(0) = u_0,$$

build a probabilistic numerical solution. There exists flow map $\Phi_t(y)$ such that

$$u(t) = \Phi_t(u_0).$$

Idea. Given $h > 0$, the flow map of a Runge-Kutta method $\Psi_h(y)$ is

$$u_{k+1} = \Psi_h(u_k), \quad k = 0, 1, \dots,$$

consider $\xi_k(h)$ i.i.d. random variables in $\mathbb{R}^d$ and compute

$$U_{k+1} = \underbrace{\Psi_h(U_k)}_{\text{deterministic}} + \overbrace{\xi_k(h)}^{\text{random}}, \quad k = 0, 1, \dots,$$

Deterministic component $\rightsquigarrow$ Runge-Kutta methods.

Definition

Given $s \in \mathbb{N}^*$, $(b_i)_{i=1}^s$, $(a_{ij})_{i,j=1}^s$, $h > 0$, one step of an s-stage Runge-Kutta method is

$$
\begin{aligned}
K_i &= f\big(U_0 + h \textstyle\sum_{j=1}^s a_{ij} K_j\big), \quad i = 1, \dots, s, \\
U_1 &= U_0 + h \textstyle\sum_{i=1}^s b_i K_i.
\end{aligned}
$$

The method is of order q if $\exists C > 0$ independent of h such that

$$\|u(h) - U_1\| \leq C h^{q+1}.$$

Monte Carlo computations $\rightsquigarrow$ Explicit methods privileged.

Consider chaotic differential equation, e.g., Lorenz system

$$
\begin{aligned}
x' &= \sigma(y - x), & x(0) &= -10, \\
y' &= x(\rho - z) - y, & y(0) &= -1, \\
z' &= xy - \beta z, & z(0) &= 40.
\end{aligned}
$$

Small perturbation $\implies$ uncontrollable deviation of the solution.
Deterministic solvers not reliable for any time step $h > 0$.
$\rightsquigarrow$ Family of M probabilistic numerical solutions.

Relevant properties to be analyzed

- strong order of convergence,
- weak order of convergence,
- behavior Monte Carlo approximations,
- stability.

Recall. The probabilistic method is defined as

$$U_{k+1} = \Psi_h(U_k) + \xi_k(h), \quad k = 0, 1, \dots,$$

for suitable random variables $\xi_k(h)$.

It is possible to prove a result of strong convergence.

Definition (Strong convergence)

The probabilistic method has strong order r if $\exists C > 0$ independent of h such that for h small enough

$$\sup_{t_k = kh} \mathbb{E}|U_k - u(t_k)| \leq Ch^r.$$

Assumption (Variance of random variables)

The variables $\xi_k(t)$ *satisfy for* $p \geq 1$

$$\mathbb{E}|\xi_k(t)\xi_k(t)^T|_F^2 \leq Kt^{2p+1}.$$

Furthermore, there exists a matrix Q *independent of* h *such that*

$$\mathbb{E}[\xi_k(h)\xi_h(h)^T] = Qh^{2p+1},$$

Assumption (Order of the deterministic component)

The function f *and a sufficient number of its derivatives are bounded uniformly in* $\mathbb{R}^n$ *in order to ensure that* f *is globally Lipschitz and that the numerical flow map* Ψ_h *has uniform local truncation error of order* $q+1$*, i.e.,*

$$\sup_{u \in \mathbb{R}^n} |\Psi_t(u) - \Phi_t(u)| \leq Kt^{q+1}.$$

Theorem (Strong Convergence)

Under the assumptions above, there exists $K > 0$ *such that*

$$\sup_{0<kh<T} \mathbb{E}|u_k - U_K|^2 \leq Kh^{2\min\{p,q\}}.$$

Idea of the proof. Compute truncation error between exact and numerical solutions, divide deterministic and probabilistic contribution and derive a recurrence on the error. Apply then discrete Gronwall's lemma to bound the error.

Definition (Weak convergence)

The probabilistic method has weak order r if $\exists C > 0$ independent of h such that for any function φ sufficiently smooth

$$\sup_{t_k = kh} |\mathbb{E}[\varphi(U_k)] - \varphi(u(t_k))| \leq Ch^r,$$

for h small enough.

Idea. Introduce a modified SDE

$$\mathrm{d}\tilde{u} = f^h \tilde{u} \,\mathrm{d}t + \sqrt{h^{2p} Q} \,\mathrm{d}W \,, \tag{1}$$

and study the convergence of U_k and $\tilde{u}$ to u for $h \to 0$.

Theorem (Weak convergence)

For any function φ sufficiently smooth

$$|\varphi(u(T)) - \mathbb{E}[\varphi(U_k)]| \leq Kh^{\min\{2p,q\}}, \quad kh = T,$$

and

$$|\mathbb{E}[\varphi(\tilde{u}(T))] - \mathbb{E}[\varphi(U_k)]| \leq Kh^{2p+1}, \quad kh = T.$$

Idea of the proof. Use techniques of backwards error analysis, finding a modified ODE and SDE such that the numerical error is of higher order.

Problem. Study convergence of Monte Carlo approximations.

Numerical solution $\rightsquigarrow \mathcal{Q}_h$ (inaccessible),
M samples of numerical solution $\rightsquigarrow Q_h^M$ (accessible),
Exact solution $\rightsquigarrow \delta_u$.

Convergence scheme, we expect

$$\mathcal{Q}_h^M \xrightarrow{M \to \infty} \mathcal{Q}_h \xrightarrow{h \to 0} \delta_u .$$

Second convergence already treated, first unclear [Kersting and Hennig, 2016].

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