Monte Carlo Methods and Uncertainty Quantification

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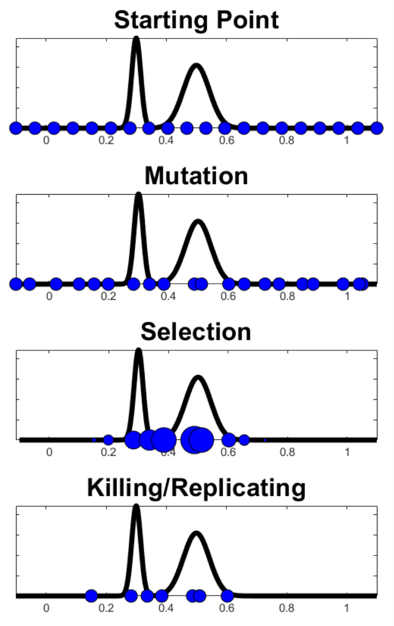
Monte Carlo Methods

- **Aim 1:** sample from a probability distribution π on $\mathbb{R}^d$ and approximate expectations w.r.t. $\pi(x) = \eta(x)/\mathcal{Z}$ whose normalising constant might be unknown

$$\int f(x)\pi(x)\mathrm{d}x \approx \sum_{i=1}^{N} W_i f(X_i)$$

- **Motivation:** compute posterior expectations in Bayesian inference
- **Aim 2:** estimate the unknown normalising constant $\mathcal{Z}$
- **Motivation:** model selection/parameter inference

Sequential Monte Carlo (SMC)



Example I: Optimisation

Consider the following data-generating process

$$x \sim p_\theta(\cdot)$$
$$y \sim p_\theta(\cdot|x)$$

for some parameter $\theta \in \mathbb{R}^{d_\theta}$, where $x \in \mathbb{R}^{d_x}$ is a latent variable which cannot be observed.

Given a data point y we want to find $\theta^\star$ maximising the marginal log-likelihood

$$\log p_\theta(y) = \log \int_{\mathbb{R}^{d_x}} p_\theta(x, y)\mathrm{d}x,$$

where $p_\theta(x, y) = p_\theta(x)p_\theta(y|x)$.

Example I: Optimisation

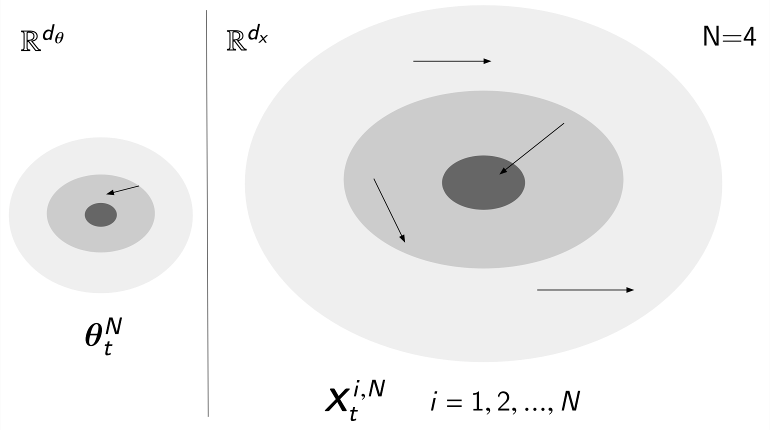
Maximising $\log p_\theta(y)$ amounts to finding the maximum likelihood estimator for the latent variable model above. Can be achieved by defining

$$\pi^N(\theta, x_1, x_2, ..., x_N) \propto \prod_{i=1}^{N} p_\theta(x_i, y);$$

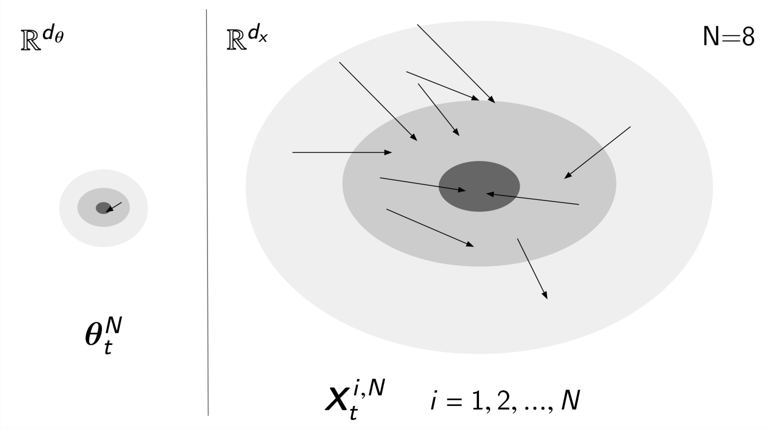
since the **theta-marginal** π_Θ^N is given as

$$\begin{aligned}\pi_\Theta^N(\theta) &\propto \int_{\mathbb{R}^{d_x}} ... \int_{\mathbb{R}^{d_x}} \prod_{i=1}^{N} p_\theta(x_i, y)\mathrm{d}x_1\mathrm{d}x_2 \ldots \mathrm{d}x_N \\ &= \left(\int_{\mathbb{R}^{d_x}} p_\theta(x, y)\mathrm{d}x \right)^N.\end{aligned}$$

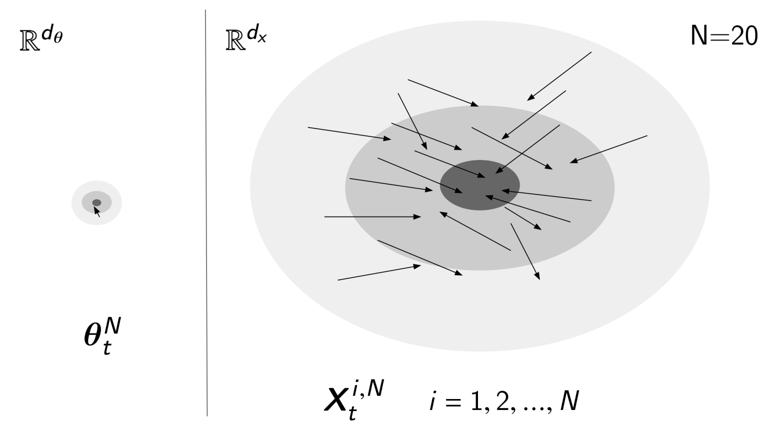
Optimisation with Monte Carlo



Optimisation with Monte Carlo



Optimisation with Monte Carlo

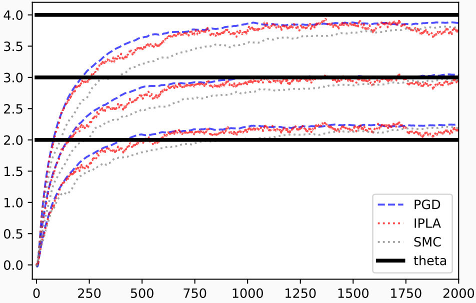


Optimisation: Bayesian Logistic Regression

We consider the Bayesian logistic regression LVM where for $\theta \in \mathbb{R}^{d_\theta}$

$$p_\theta(x) = \mathcal{N}(x; \theta, \sigma^2 \mathrm{Id}_{d_x}), \qquad p_\theta(y|x) = \prod_{j=1}^{d_y} s(v_j^T x)^{y_j} (1 - s(v_j^T x))^{1-y_j},$$

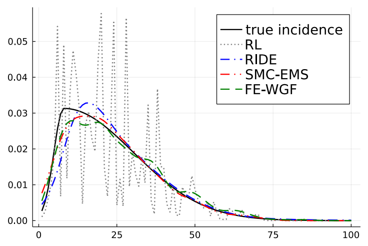
with $s(u) := e^u/(1+e^u)$ the logistic function and $\{v_j\}_{j=1}^{d_y} \in \mathbb{R}^{d_x}$ a set of covariates with corresponding binary responses $\{y_j\}_{j=1}^{d_y} \in \{0, 1\}$.

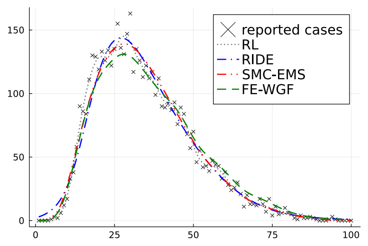


Example III: Integral equations

$$\mu(y) = \int_{\mathbb{R}^d} k(x, y)\pi(x)\mathrm{d}x := \pi[k(\cdot, y)], \qquad y \in \mathbb{R}^p$$

- μ = distribution of hospitalisations over time
- k = delay between infection and hospitalisation
- π = distribution of infections over time





Conclusions

Monte Carlo methods are a powerful alternative to numerical integration to approximate $\int f(x)\pi(x)\mathrm{d}x$. They can be used in several "applications"

- posterior computation in Bayesian inference
- optimisation
- general numerical integration
- inverse problems