MCMC Algorithms

Metropolis-Hastings algorithm

- 1 Initialise $x^{(0)}$
- **2** For t = 1, ..., n + N:
 - a Sample $y^{(t)} \sim q(y^{(t)}|x^{(t-1)})$
 - **b** Compute the acceptance probability $\alpha^{(t)} = \min \left\{ 1, \frac{\tilde{p}(y^{(t)})}{q(y^{(t)}|x^{(t-1)})} \middle/ \frac{\tilde{p}(x^{(t-1)})}{q(x^{(t-1)}|y^{(t)})} \right\}$
 - c Acceptance-rejection step: sample $u^{(t)} \sim \mathcal{U}_{[0;1]}$ $x^{(t)} = \begin{cases} y^{(t)} \text{ if } u^{(t)} \leq \alpha^{(t)} \\ x^{(t-1)} \text{ else} \end{cases}$

$$\alpha^{(t)} = \min \left\{ 1, \frac{\tilde{p}(y^{(t)})}{\tilde{p}(x^{(t-1)})} \frac{q(x^{(t-1)}|y^{(t)})}{q(y^{(t)}|x^{(t-1)})} \right\}$$

 \Rightarrow computable even if \tilde{p} is known only up to a constant ! (like the posterior)

Metropolis-Hastings: particular cases

Sometimes $\alpha^{(t)}$ computation simplifies:

- independent Metropolis-Hastings: $q(y^{(t)}|x^{(t-1)}) = q(y^{(t)})$
- random walk Metropolis-Hastings: $q(y^{(t)}|x^{(t-1)}) = g(y^{(t)} x^{(t-1)})$ If g is symetric (g(-x) = g(x)), then:

$$\frac{\tilde{p}(y^{(t)})}{\tilde{p}(x^{(t-1)})}\frac{q(y^{(t)}|x^{(t-1)})}{q(x^{(t-1)}|y^{(t)})} = \frac{\tilde{p}(y^{(t)})}{\tilde{p}(x^{(t-1)})}\frac{g(y^{(t)}-x^{(t-1)})}{g(x^{(t-1)}-y^{(t)})} = \frac{\tilde{p}(y^{(t)})}{\tilde{p}(x^{(t-1)})}$$

Pro and cons of Metropolis-Hastings

- e very simple & very general
- e allow sampling from uni- or multi-dimensional distributions
- e choice of the proposal is crucial, but hard
- ⇒ huge impact on algorithm performances
- e quickly becomes inefficient dimension is too high

NB: a high rejection rate often implies important computation timings





Simulated annealing

Change $\alpha^{(t)}$ computation during the algorithm:

- 1 $\alpha^{(t)}$ must first be large to explore all of the state space
- 2 then $\alpha^{(t)}$ must become smaller when the algorithm converges

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- 1 $\alpha^{(t)}$ must first be large to explore all of the state space
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 - 1 Initialise $x^{(0)}$
 - 2 For t = 1, ..., n + N:
 - a Sample $v^{(t)} \sim a(v^{(t)}|x^{(t-1)})$
 - Compute the acceptance probability

$$\alpha^{(t)} = \min \left\{ 1, \left(\frac{\tilde{p}(y^{(t)})}{\tilde{p}(x^{(t-1)})} \frac{q(x^{(t-1)}|y^{(t)})}{q(y^{(t)}|x^{(t-1)})} \right)^{\frac{1}{T(t)}} \right\}$$

c Acceptance-rejection step: sample $u^{(t)} \sim \mathcal{U}_{[0:1]}$

$$x^{(t)} := \begin{cases} y^{(t)} & \text{if } u^{(t)} \le \alpha^{(t)} \\ x^{(t-1)} & \text{else} \end{cases}$$

Simulated annealing

Change $\alpha^{(t)}$ computation during the algorithm:

- 1 $\alpha^{(t)}$ must first be large to explore all of the state space
- 2 then $\alpha^{(t)}$ must become smaller when the algorithm converges
 - 1 Initialise $x^{(0)}$
 - 2 For t = 1, ..., n + N:
 - a Sample $y^{(t)} \sim q(y^{(t)}|x^{(t-1)})$
 - **b** Compute the acceptance probability

$$\alpha^{(t)} = \min \left\{ 1, \left(\frac{\tilde{p}(y^{(t)})}{\tilde{p}(x^{(t-1)})} \frac{q(x^{(t-1)}|y^{(t)})}{q(y^{(t)}|x^{(t-1)})} \right)^{\frac{1}{T(t)}} \right\}$$

c Acceptance-rejection step: sample $u^{(t)} \sim \mathcal{U}_{[0;1]}$

$$x^{(t)} := \begin{cases} y^{(t)} & \text{if } u^{(t)} \le \alpha^{(t)} \\ x^{(t-1)} & \text{else} \end{cases}$$

Ex: $T(t) = T_0 \left(\frac{T_f}{T_0}\right)^{\frac{1}{n}} \Rightarrow$ particularly useful for avoiding local optima

Gibbs sampler

When the dimension $\nearrow \Rightarrow$ very hard to propose probable values

Gibbs samplers: re-actualisation coordinate by coordinate, while conditioning on the most recent values (no acceptance-rejection)

1 Initialise
$$x^{(0)} = (x_1^{(0)}, \dots, x_d^{(0)})$$

2 For
$$t = 1, ..., n + N$$
:

a Sample
$$x_1^{(t)} \sim p(x_1|x_2^{(t-1)},...,x_d^{(t-1)})$$

b Sample
$$x_2^{(t)} \sim p(x_2|x_1^{(t)}, x_3^{(t-1)}, \dots, x_d^{(t-1)})$$

d Sample
$$x_i^{(t)} \sim p(x_i|x_1^{(t)},...,x_{i-1}^{(t)},x_{i+1}^{(t-1)},...,x_d^{(t-1)})$$

f Sample
$$x_d^{(t)} \sim p(x_d | x_1^{(t)}, \dots, x_{d-1}^{(t)})$$

NB: if the conditional distribution is unknown for some coordinates, an acceptance-rejection step can be included for this coordinate only (Metropolis within gibbs)

Your turn!



Practical: exercise 4

