BML: MCMC

http://github.com/rbardenet/bml-course

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Outline

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What comes to *your* mind when you hear "Monte Carlo"?

Expected utility requires computing integrals

Minimizing the posterior expected loss

If $\mathcal{A} = \{a_g\}$ and we partition $s = (s_{\text{obs}}, s_{\text{u}})$, then, given s_{obs}, we choose

$$g^\star(s_{\text{obs}}) = \arg\min_{g \in \mathcal{A}} \mathbb{E}_{s_{\text{u}}|s_{\text{obs}}} L(a, s).$$

The bottleneck is computing integrals w.r.t. the posterior

- E.g. for binary prediction with 0-1 loss

$$y^\star \in \arg\max_{y \in \{0,1\}} \int p(y|x, \theta) p(\theta | x_{1:n}, y_{1:n}) \mathrm{d}\theta$$

- or for estimation with squared loss

$$\theta^\star = \int \theta p(\theta | y_{1:n}) \mathrm{d}\theta.$$

Let π be a pdf w.r.t. $\mathrm{d}\theta$.

The problem of numerical integration

Find T nodes (θ_t) and weights (w_t) so that

$$\int f(\theta)\pi(\theta)\mathrm{d}\theta \quad \approx \quad \sum_{t=1}^{N} w_t f(\theta_t), \quad \forall f \in \mathcal{C},$$

where $\mathcal{C}$ is a large class of functions.

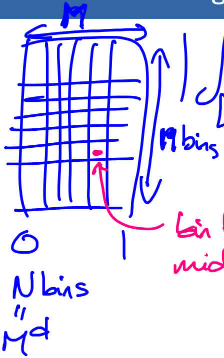
A constraint for Bayesians: π is only known up to a constant

E.g. in estimation,

$$\pi(\theta) = p(\theta|y_{1:n}) \propto p(y_{1:n}|\theta)p(\theta) =: \pi_u(\theta).$$

Or in classification/regression,

$$\pi(\theta) = p(\theta|x_{1:n}, y_{1:n}) \propto p(y_{1:n}|x_{1:n}, \theta)p(\theta) =: \pi_u(\theta).$$



bin B_i w/ middle x_i

$$\left|\int_{[0,1]^d} f(x)\,dx - \frac{1}{N}\sum_{i=1}^{N} f(x_i)\right|$$

$$= \left|\sum_{i=1}^{N} \int_{B_i} \big(f(x) - f(x_i)\big)\,dx\right|$$

$$\leq \sum_{i=1}^{N} \int_{B_i} \underbrace{|f(x) - f(x_i)|}_{\leq C_i \underbrace{\|x - x_i\|}_{\frac{1}{M}\sqrt{d}}}\,dx$$

$$\leq \sup C_i \, \frac{1}{M}\sqrt{d}$$

$$= \mathcal{O}\left(\frac{1}{N^{1/d}}\right).$$

- For modern developments, see quasi-Monte Carlo integration (Dick and Pilichshammer, 2010).

Outline

The Monte Carlo principle

Find a distribution on $\theta_1, \dots, \theta_T$ and weights w_t such that

$$\mathcal{E}_T(f) = \sum_{t=1}^{T} w_t f(\theta_t) - \int f(\theta)\pi(\theta)\mathrm{d}\theta$$

is small (with large probability, in quadratic mean, converges in law at some rate, etc.)

- If you knew how to sample from π, you could take $\theta_t \sim \pi$ i.i.d., $w_t = 1/T$, and prove e.g.

$$\mathbb{P}\left(\mathcal{E}_T(f) \geqslant \alpha \frac{\sigma(f)}{\sqrt{T}}\right) \leqslant \frac{1}{\alpha^2}, \quad \forall \alpha,$$

as soon as $\sigma(f)^2 := \mathbb{V}_\pi[f(\theta) - \int f(\theta)\pi(\theta)\mathrm{d}\theta] < +\infty$.

Self-normalized importance sampling

- Let $\pi_u(\theta) = Z\pi(\theta)$ be the unnormalized target pdf.
- Sample $\theta_{1:T}$ i.i.d. from q, and take

$$w_t = \frac{\pi_u(\theta_t)}{q(\theta_t)} \times \left(\sum_{t=1}^{T} \frac{\pi_u(\theta_t)}{q(\theta_t)} \right)^{-1}$$

  so that $\sum w_t = 1$.
- Then

- One can show that $\sqrt{T}\mathcal{E}_T(f) \to \mathcal{N}(0, \sigma^2_{\mathrm{NIS}}(f))$.
- Problem is that for reasonable choices of f, q, π, $\log \sigma_{\mathrm{NIS}}(f) \propto d$.

Outline

(Mostly) friendly faces

Figure: A few MCMC pioneers: N. Metropolis, S. Ulam, A. Rosenbluth, W. K. Hastings

Markov chain Monte Carlo (MCMC; (Robert and Casella, 2004))

- The idea is to take (θ_t) to be an ergodic Markov chain with limiting distribution π, so that for $f \in L^1(\pi)$,

- In MCMC research, when a new Markov kernel comes out, we typically first prove a law of large numbers, and then a central limit theorem, i.e., that under weak conditions on π and f,

and that $\sigma^2(f)$ can be estimated; see (Douc, Moulines, and Stoffer, 2014).

Let $(\theta_t)_{t\in\mathbb{N}}$ be a Markov chain on Θ, with Markov kernel P. If

- There exists π s.t.

$$\int \mathrm{d}\pi(\theta)P(\theta, B) = \pi(B).$$

- For any A with $\pi(A) > 0$, for any $\theta \in \Theta$,

$$\mathbb{P}_\theta\left(\sum_{t=0}^{\infty} 1_{\theta_t\in A} = +\infty\right) = 1,$$

then for any f such that $\int |f|\mathrm{d}\pi < \infty$, for any initial distribution μ_0 of θ_0, almost surely

$$\frac{1}{T}\sum_{t=1}^{T} f(\theta_t) \to \int f\mathrm{d}\pi.$$

See e.g. (Douc, Moulines, and Stoffer, 2014).

The Metropolis-Hastings algorithm

$\mathrm{MH}\big(\pi_u,\ q(\cdot|\cdot),\ \theta_0,\ T\big)$

for $t \leftarrow 1$ **to** T
  $\theta \leftarrow \theta_{t-1}$
  $\theta' \sim q(.|\theta),\ u \sim \mathcal{U}_{(0,1)},$
  $\alpha = 1 \wedge \frac{\pi(\theta')}{\pi(\theta)} \frac{q(\theta|\theta')}{q(\theta'|\theta)}.$
  if $u < \alpha,$
    $\theta_t \leftarrow \theta'$ $\triangleright$ *Accept*
  else $\theta_t \leftarrow \theta$ $\triangleright$ *Reject*
return $(\theta_t)_{t=1,\dots,N_{\mathrm{iter}}}$

... is given by

$$P_{\mathsf{MH}}(\theta, \theta') = \alpha(\theta, \theta') q(\theta' | \theta) + \delta_\theta(\theta') \left[1 - \int \alpha(\theta, \vartheta) q(\vartheta | \theta) \right] \mathrm{d}\vartheta,$$

where

$$\alpha(\theta, \theta') = 1 \wedge \frac{\pi(\theta')}{\pi(\theta)} \frac{q(\theta | \theta')}{q(\theta' | \theta)}.$$

MH leaves π invariant and satisfies the LLN

- We first show detailed balance, i.e., $\pi(\theta)P(\theta,\theta') = \pi(\theta')P(\theta',\theta)$.

- We deduce that P leaves π invariant.

Theorem (Robert and Casella, 2004)

If $\pi(A) > 0 \Rightarrow (\forall x) q(A|x) > 0$, then P_{MH} satisfies the LLN.

Some additional useful properties

- Note that if P_1 and P_2 leave π invariant, then so does

$$P_1 P_2(\theta,\theta') = \int P_1(\theta,\vartheta)P_2(\vartheta,\theta')\mathrm{d}\vartheta.$$

- The MH error scales polynomially with the dimension; see blog post.

Outline

The random scan Gibbs sampler

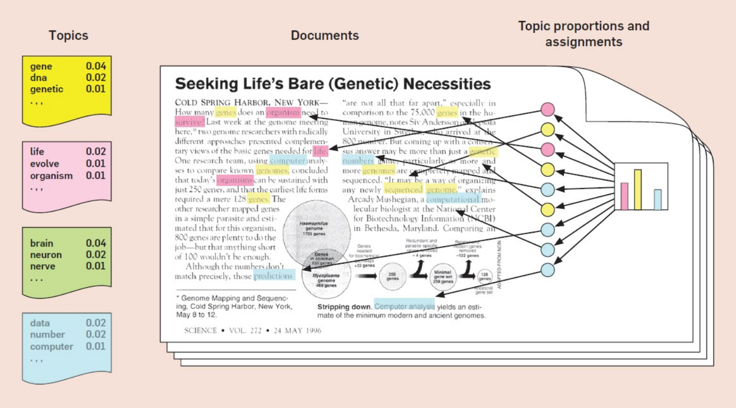
- Consider MH with

$$q(\theta'|\theta) = \frac{1}{d}\sum_{k=1}^{d} \pi(\theta'_k|\theta_{\setminus k}) 1_{\theta'_{\setminus k}=\theta_{\setminus k}}, \quad \theta_{\setminus k} := (\theta_1, \dots, \theta_{k-1}, \theta_{k+1}, \dots, \theta_d).$$

- Then the probability of acceptance $\alpha(\theta, \theta')$ is always 1.

- In practice, the systematic scan Gibbs sampler is more common, which consists in repeatedly: drawing $\theta_1|\theta_{\setminus 1}$, then $\theta_2|\theta_{\setminus 2}$, etc. always conditioning on the newest values available of each θ_k.
- You can also partition θ in arbitrary blocks.

An example: Latent Dirichlet allocation



A Gibbs sampler for LDA 1/2

Collapsed Gibbs sampling for LDA

An abstract variant of MH

- Let S be a linear involution of $\mathcal{X} \subset \mathbb{R}^{2d}$, such that $\eta \circ S = \eta$ for some (possibly unnormalized) PDF η.

- Let further $\Phi : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ be a C^1-diffeomorphism such that $S \circ \Phi = \Phi^{-1} \circ S$.
- Now let

$$\alpha(x) \triangleq 1 \wedge \frac{\eta(\Phi(x))}{\eta(x)} |\Phi'(x)|, \tag{1}$$

and consider the Markov kernel

$$P_{aHMC}(x, A) = \alpha(x) 1_{\Phi(x) \in A} + (1 - \alpha(x)) 1_{S(x) \in A}.$$

Proposition

P_{aHMC} leaves η invariant.

Hamilton's equations of motion

Consider a physical system described by Hamiltonian $H(q,p)$ in phase space $(q,p) \in \mathbb{R}^{2d}$. Then the trajectories are prescribed by

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{2}$$

- Given an initial point (q,p), solve (2) and denote the corresponding position in $\mathbb{R}^{2d}$ at time $t > 0$ by $\Phi_t(q,p)$.
- (2) implies that $t \mapsto H(\Phi_t(q,p))$ is constant.
- As an example, consider $H(q,p) = \frac{1}{2}q^2 + \frac{1}{2}p^2$.

Numerical approximations of the Hamiltonian flow

- One idea would be to put some monotone function of the target in the Hamiltonian, such as $H(q, p) = -\log \pi(q) + \frac{1}{2} p^T M p$.
- We know approximations of the Hamiltonian flow, such as the leapfrog (aka velocity Verlet) integrator. It is defined as $\psi_h^n = \psi_h \circ \ldots \psi_h$, where $(p', q') = \psi_h(p, q)$ is

$$\begin{aligned} p_{1/2} &= p + \frac{h}{2} \nabla \log \pi(q) \\ q' &= q + h M^{-1} p_{1/2} \\ p' &= p_{1/2} + \frac{h}{2} \nabla \log \pi(q'); \end{aligned}$$

Proposition

The leapfrog integrator satisfies $S \circ \psi_h^n = (\psi_h^n)^{-1} \circ S$ for $S(q, p) = (q, -p)$, and $|\det(\psi_h^n)'(q, p)| = 1$.

Hamiltonian Monte Carlo mimics a physical system

- Let $\log \widetilde{\pi}(q, p) = \log \pi(q) + \frac{1}{2} p^T M(q) p$.
- Consider the Markov kernel $P((q, p), (q', p'))$ given by the product of

$$p' \sim \mathcal{N}(0, M(q)^{-1})$$

and

$$P_{aHMC}(x, A) = \alpha(x) 1_{\psi_h^n(x) \in A} + (1 - \alpha(x)) 1_{S(x) \in A}, \text{ where } x = (p, q).$$

where

$$\alpha(x) \triangleq 1 \wedge \frac{\widetilde{\pi}(\psi_h^n(x))}{\widetilde{\pi}(x)} \cancel{|(\psi_h^n)'(x))|}, \tag{3}$$

Then P leaves π invariant.

What can go wrong?

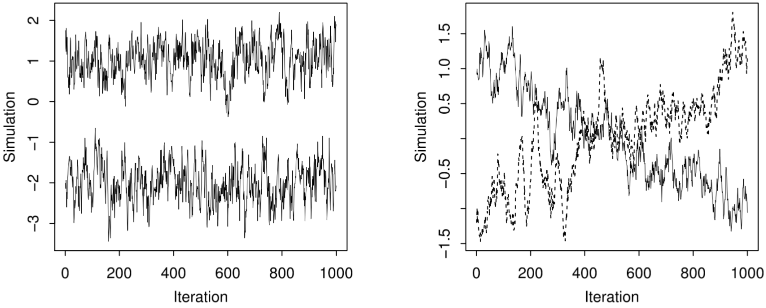


Figure: Taken from (Gelman et al., 2013)

We need to monitor both cross-chain and within-chain behavior.

Comparing P chains with overdispersed starting points

- The behaviour of the P traces should become similar.
- Always make visual sanity checks!
- Scalar estimates should converge to the same value.
- We can also compare the variance of a scalar estimate within- and across chains

The Gelman-Rubin diagnostic

- Choose an f of interest, e.g. $f(\theta) = \theta_1$.
- Compute $B := \frac{T}{P-1} \sum_{p=1}^{P} (\bar{f}_{\cdot p} - \bar{f}_{\cdot\cdot})^2$.
- Compute $W := \frac{1}{P} \sum_{p=1}^{P} \left[\frac{1}{T-1} \sum_{t=1}^{T} (\bar{f}_{tp} - \bar{f}_{\cdot p})^2 \right]$.
- Then check whether

$$\hat{R} = \sqrt{\frac{\frac{T-1}{T} W + \frac{1}{T} B}{W}} \in [1, 1.1].$$

- See (Vats and Knudson, 2021) for an insightful discussion.

More convergence diagnostics

Single-chain diagnostics

- The idea is to compare different chunks of a single chain.
- At stationarity, large chunks should be statistically indistinguishable.
- The Geweke diagnostic tests this similarity (Geweke, 1992)

Effective sample size

- Autocorrelation in each chain is what increases the variance of scalar estimands, compared to i.i.d. draws from π.
- We can estimate this autocorrelation, and build an estimator for PT times the ratio of the two variances $\widehat{ESS} \in [1, PT]$, called, the *effective sample size*; see Section 11.5 of (Gelman et al., 2013).
- Vats and Knudson, 2021 note that

$$\hat{R} \approx \sqrt{1 + P/\widehat{ESS}},$$

so $\hat{R} = 1.1$ only corresponds to $\widehat{ESS} = 5P$.

Take-home message

- MCMC approximates the integrals in the expected utility framework.
- Try to leverage the problem's structure to design your kernels.
- Otherwise, try standard kernels like HMC.
- Always monitor convergence.

- HMC with NUTS is the default choice in most probabilistic programming frameworks.
- MCMC is a rich research topic. Some keywords: Wang-Landau, Langevin, equi-energy, hit-and-run, bouncy particle sampler.
- Besides Markov chains, checkout sequential Monte Carlo samplers (Del Moral, Doucet, and Jasra, 2006).
- Deterministic methods are also investigated: quasi-Monte Carlo methods (Dick and Pilichshammer, 2010) have the best convergence rates as soon as the integrand is smooth.

Conclusion

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