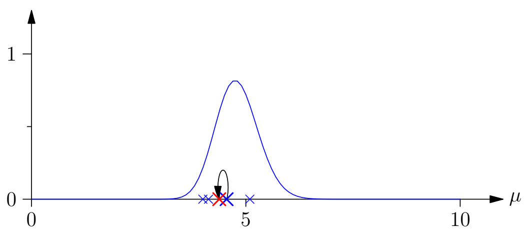
Advanced Machine Learning

MCMC

$$\mathcal{D} = \{4, 4, 6, 4, 2, 2, 5, 9, 5, 4, 3, 2, 5, 4, 4, 11, 6, 2, 3, 11\}$$

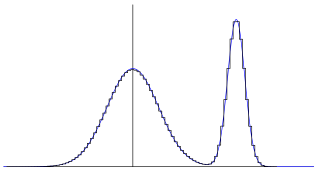


Monte Carlo methods, MCMC, Variational Methods

Outline

1. **Sampling**
2. Random Number Generation
3. MCMC

$T = 10000000$, acceptence rate $=0.897$



Bayesian Inference Gets Hard

- We saw that in some cases if we had a simple likelihood (normal, binomial, Poisson, multinomial) you can choose a conjugate prior (gamma-normal/Wishart, beta, gamma, Dirchlet) so that the posterior has the same form as the prior
- Very often we are working with more complex models where no conjugate prior exists
- The posterior is not described by a known distribution
- We have to work a lot harder—particularly with multivariate distributions

Bayesian Inference

- Recall our problem is that we are given some data $\mathcal{D}$
- Our posterior is given by

$$\mathbb{P}(\boldsymbol{\theta}|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|\boldsymbol{\theta})\,\mathbb{P}(\boldsymbol{\theta})}{\mathbb{P}(\mathcal{D})} \qquad \text{or} \qquad f(\boldsymbol{\theta}|\mathcal{D}) = \frac{f(\mathcal{D}|\boldsymbol{\theta})\,f(\boldsymbol{\theta})}{f(\mathcal{D})}$$

- Where $\boldsymbol{\theta}$ are the parameters we are trying to infer
- But our likelihood (and/or prior) might be quite complicated
- Typically we don't have a closed form representation for our posterior distibution

Histograms, Samples and Means

- We could represent our posterior as a histogram, although for multivariate distributions (i.e. when we are modelling more than one variable) a histogram can be unwieldy
- A sample from the posterior distribution is often sufficient e.g. in our topic models (LDA) a typical set of topics is what we are after
- However, when samples vary a lot, often the most useful quantities are expectation, e.g.

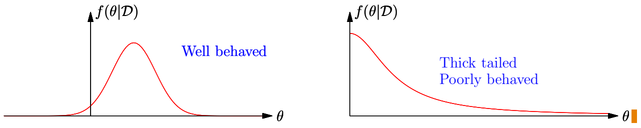
$$\begin{array}{ll} \mathbb{E}[\boldsymbol{\Theta}] & \mathbb{E}\left[\Theta_i^2\right] - \mathbb{E}[\Theta_i]^2 \\ \mathbb{E}[\Theta_i \Theta_j] - \mathbb{E}[\Theta_i]\,\mathbb{E}[\Theta_j] & \mathbb{E}\left[\boldsymbol{\Theta}\boldsymbol{\Theta}^{\mathsf{T}}\right] - \mathbb{E}[\boldsymbol{\Theta}]\,\mathbb{E}[\boldsymbol{\Theta}]^{\mathsf{T}} \end{array}$$

Sample Estimation

- If we can draw independent **deviates** (aka **variates**), $\boldsymbol{\Theta}_i$, from our posterior distribution then we can obtain an estimate of our expectation

$$\mathbb{E}[g(\boldsymbol{\Theta})] \approx \frac{1}{n}\sum_{i=1}^{n} g(\boldsymbol{\Theta}_i)$$

- Provided our posterior distribution is well behaved the relative error in our estimate will drop off as $1/\sqrt{n}$



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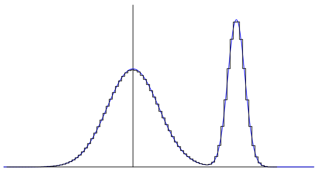
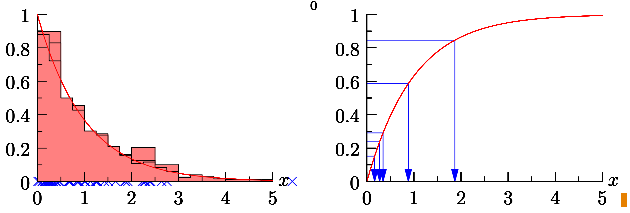


Drawing Random Samples

- Drawing (pseudo) random variables from a distribution is known as **Monte Carlo**
- For some very simple distributions we can use the **transformation methods** to transform a uniform distribution

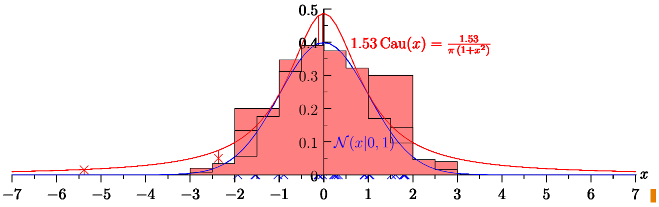
$$\mathrm{Exp}(x|1) = \mathrm{e}^{-x} \qquad F(x|1) = \int_0^x \mathrm{Exp}(y|1)\,\mathrm{d}y = 1 - \mathrm{e}^{-x}$$



Rejection Method

- The transformation method only works when we can easily compute the inverse *cumulative distribution function* (CDF)
- A more general technique is the **rejection method** where we generate deviates from $g_Y(y)$ such that $c g_Y(x) \geq f_X(x)$
- To draw deviates from $f_X(x)$ we draw a deviate $Y \sim g_Y$ and then accept the deviate with probability $f_X(Y)/(c g_Y(Y))$
- The expected rejection rate is $c - 1$
- Need to choose a good distribution $g_Y(y)$

Drawing Normal Deviates



Problems with Rejection

- The rejection method is very general and often the method of choice (although for normal deviates there is a clever transformation method which is faster)
- However, for complicated probability distributions it can be difficult to find a good proposal distribution $g_Y(y)$
- This is particular true for multivariate distributions
- If the proposal distribution is poor c might be very high and the number of rejections is stupidly high

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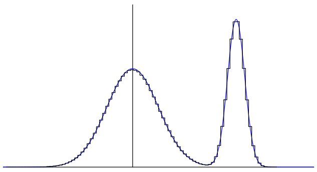


Detailed Balance

- Suppose we have a set of states $\mathcal{S}$ and want to draw sample from a probability distribution $\boldsymbol{\pi} = (\pi_i | i \in \mathcal{S})$
- We invent a dynamical system with a transition probability M_{ij} from state j to state i such that

$$M_{ij}\pi_j = M_{ji}\pi_i$$

- This is known as **detailed balance**
- Summing both sides over j

$$\sum_j M_{ij}\pi_j = \sum_j M_{ji}\pi_i = \pi_i \qquad \mathbf{M}\boldsymbol{\pi} = \boldsymbol{\pi}$$

Convergence of MCMC

- Suppose we start from a state $\boldsymbol{x}(0) = \sum_i c_i \boldsymbol{v}^{(i)}$ where the $\boldsymbol{v}^{(i)}$'s are an eigenvectors of the transition matrix $\mathbf{M}$ with eigenvalues λ_i
- It I apply $\mathbf{M}$ many times then

$$\boldsymbol{x}(t) = \mathbf{M}^t \boldsymbol{x}(0) = \mathbf{M}^t \sum_i c_i \boldsymbol{v}^{(i)} = \sum_i \lambda_i^t c_i \boldsymbol{v}^{(i)}$$

- And $\lim_{t\to\infty} \boldsymbol{x}(t) = \boldsymbol{v}^*$ where $\boldsymbol{v}^*$ is the eigenvector with the maximum eigenvalue
- Now $\|\mathbf{M}\boldsymbol{v}\|_1 \leq \|\mathbf{M}\|_1 \|\boldsymbol{v}\|_1 = \|\boldsymbol{v}\|_1$ so the maximum eigenvalue is 1 with eigenvector $\boldsymbol{\pi}$ ($\mathbf{M}$ is known as a **stochastic matrix**)

Metropolis Algorithm

- A very easy way to achieve detailed balance is starting from state j choose a "neighbouring" state, i with equal probability
- We accept the move if either
  - ⋆ $\pi_i > \pi_j$ or
  - ⋆ we make the move with a probability π_i/π_j
- If $\pi_i > \pi_j$ then $M_{ij} = 1$ and $M_{ji} = \pi_j/\pi_i$. Thus

$$M_{ij}\pi_j = \pi_j \qquad M_{ji}\pi_i = \frac{\pi_j}{\pi_i}\pi_i = \pi_j$$

- Note that we require the state i to have the same number of neighbours as state j so that detailed balance is satisfied

Continuous Variables

- If we are working with continuous variables $\boldsymbol{\theta}$ then the equation for detailed balance for the transition probability $W(\boldsymbol{\theta} \to \boldsymbol{\theta}')$ is

$$W(\boldsymbol{\theta} \to \boldsymbol{\theta}')\pi(\boldsymbol{\theta}) = W(\boldsymbol{\theta}' \to \boldsymbol{\theta})\pi(\boldsymbol{\theta}')$$

- where $\pi(\boldsymbol{\theta})$ is the probability distribution we wish to sample from
- The update rule is to choose a nearby value $\boldsymbol{\theta}'$, compute $r = \pi(\boldsymbol{\theta}')/\pi(\boldsymbol{\theta})$ and accept the update with probability $\min(1,r)$
- We require that the probability of choosing $\boldsymbol{\theta}$ from $\boldsymbol{\theta}'$ is the same as the reverse

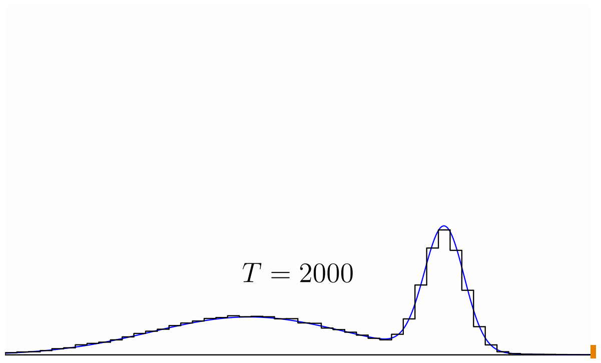
What Makes MCMC Nice

- Because we are free to choose where we move (and choose close by neighbours) $\pi(\boldsymbol{\theta}') \approx \pi(\boldsymbol{\theta})$ so that moves are not too infrequent
- Also very importantly the updates depend only on the ratio $\pi(\boldsymbol{\theta}')/\pi(\boldsymbol{\theta})$
- We only need to know our probabilities up to a multiplicative scaling factor
- For sampling from the posterior we only need to know the likelihood and prior $\mathbb{P}(\mathcal{D}|\boldsymbol{\theta})\,\mathbb{P}(\boldsymbol{\theta})$ (or $f(\mathcal{D}|\boldsymbol{\theta})\,f(\boldsymbol{\theta})$)
- We don't need to know $\mathbb{P}(\mathcal{D})$ which we generally don't know

What Makes MCMC Nasty

- It can take a long time until our states occur with the probability $\boldsymbol{\pi}$ (i.e. we have forgotten our initial state)
- We don't even know how long we have to wait
- Even when we have reached this *equilibration time* each sample is correlated with the previous sample
- To get a good approximation to the posterior expectation requires running for many times the equilibration time
- Note, if we are just finding sample averages then we can use all samples after equilibrating even if they are not independent

Burn-In



Proposals and Metropolis-Hastings

- We have some freedom in choosing a new proposal $\boldsymbol{\theta}'$ from our current position $\boldsymbol{\theta}$—a good choice can increase the acceptance rate making the MCMC more efficient
- We define the proposal distribution $p(\boldsymbol{\theta}'|\boldsymbol{\theta})$
- For the standard Metropolis algorithm to work we require $p(\boldsymbol{\theta}'|\boldsymbol{\theta}) = p(\boldsymbol{\theta}|\boldsymbol{\theta}')$
- In some cases (e.g when $\theta_i \geq 0$) this can be hard to achieve
- We can modify our update rule to accept a move with probability

$$\min\left(1, \frac{p(\boldsymbol{\theta}|\boldsymbol{\theta}')\,f(\mathcal{D}|\boldsymbol{\theta}')\,f(\boldsymbol{\theta}')}{p(\boldsymbol{\theta}'|\boldsymbol{\theta})\,f(\mathcal{D}|\boldsymbol{\theta})\,f(\boldsymbol{\theta})}\right)$$

Traffic Rate

- Consider monitoring the flow of traffic where we have data

$$\mathcal{D} = (N_1, N_2, \ldots, N_n)$$

where N_i is the number of car that past on day i

- We assume $N_i \sim \text{Poi}(\mu)$ and want to infer μ
- The Poisson distribution has a beta conjugate prior
- We don't have any prior knowledge on μ so we use a non-informative prior $\text{Gam}(\mu|0,0) = 1/\mu$
- Note that we can solve this problem exactly—however, lets compare with MCMC

Proposal Distribution

- If we can choose our proposal distribution $p(\mu'|\mu)$ to be close to the posterior distribution then our acceptance rate would be close to 1
- We choose $p(\mu'|\mu) = \text{Gam}(\mu'|\mu,\mu^2)$ which has $\mathbb{E}[\mu'] = \mu$ and variance 1
- We update with probability $\min(1,r)$ where

$$\begin{aligned} r &= \frac{\text{Gam}(\mu|\mu'^2,\mu')\frac{1}{\mu'}\prod_{i=1}^{n}\text{Poi}(N_i|\mu')}{\text{Gam}(\mu'|\mu^2,\mu)\frac{1}{\mu}\prod_{i=1}^{n}\text{Poi}(N_i|\mu)} \\ &= \frac{\mu\,\text{Gam}(\mu|\mu'^2,\mu')}{\mu'\,\text{Gam}(\mu'|\mu^2,\mu)}\mathrm{e}^{-n(\mu'-\mu)+\sum_{i=1}^{n} N_i \log\left(\frac{\mu'}{\mu}\right)} \end{aligned}$$

MCMC in Practice

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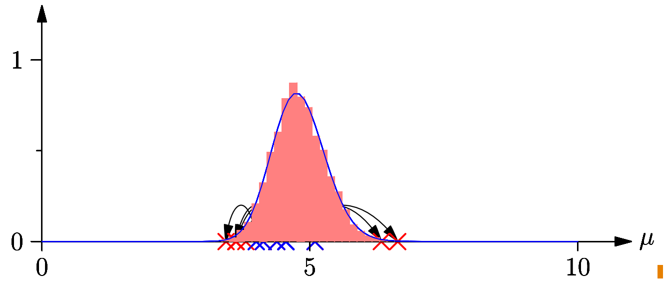

MCMC Details

- To compute correct histograms you need to count samples where no move is made multiple times
- On modern computers its quite quick to compute millions of samples
- The code is not very difficult to write (although care is need to get everything correct)
- This can be used on complicated problems such as topic models (LDA) with thousands of parameters
- The accuracy of MCMC is slow if it takes a long time to sample the posterior distribution

The MCMC Industry

- MCMC provides a means to accurately sample from very complex models▮
- There have been many advanced techniques developed to improve MCMC performance▮
- E.g. hybrid MCMC simulates a dynamics to find good proposals with similar probability far from the starting point▮
- Often it seems that MCMC is complicated because there are so many optimisations, but often simple implementations are sufficient▮

Conclusions

- As soon as we use complex models we are no longer able to compute the posterior in closed form▮
- Monte Carlo techniques and particularly MCMC are a very general method for computing samples from the posterior▮
- These techniques have been highly developed, but very frequently even simple implementations are sufficient to do good inference▮
- Variational methods provide an approximate closed form solution to problems with complex likelihoods▮
- Variational methods are mathematically challenging, but are potentially far faster to compute than MCMC▮