STA 414/2104:
Statistical Methods in Machine Learning II

Week 5: Markov Chain Monte Carlo (MCMC)

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Overview

We continue with sampling algorithms.

- Markov chains
- Markov chain Monte Carlo
  - Metropolis-Hastings
  - Gibbs sampling
  - Hamiltonian Monte-Carlo

Announcements:

- Assignment 2 to be released today.

Markov Chains

Sequential data

So far, we considered methods in which the generated samples are *i.i.d*:

- We generated T samples
$$x_{1:T} = \{x_1, ..., x_T\}.$$
- But each sample was independent from each other
$$x_t \sim p(x) \quad \text{i.i.d.}$$
- This lecture, we will generate samples that are dependent.

Sequential data

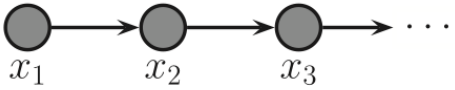
This also comes up when modelling the data. We generally assume data was i.i.d, however this may be a poor assumption:

- **Sequential data** are common:
  - time-series modelling (e.g. stock prices, speech, video analysis)
  - ordered data (e.g. textual data, gene sequences)
- Recall the general joint factorization via the chain rule

$$p(x_{1:T}) = \prod_{t=1}^{T} p(x_t|x_{t-1}, ..., x_1) \quad \text{where } p(x_1|x_0) = p(x_1).$$

- This quickly becomes intractable for high-dimensional data. Each factor requires exponentially many parameters to specify.

Markov chains



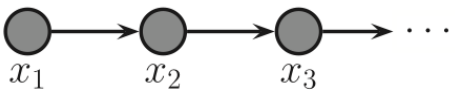
- We make the simplifying **first-order Markov chain** assumption:

$$p(x_t|x_{1:t-1}) = p(x_t|x_{t-1})$$

- This assumption greatly simplifies the factors in the joint distribution

$$p(x_{1:T}) = \prod_{t=1}^{T} p(x_t|x_{t-1})$$

Stationary Markov chains



Further assumptions may be useful:

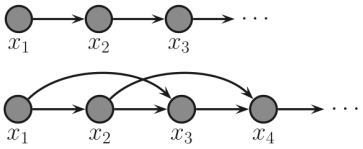
- **Stationary (homogeneous) Markov chain**: the distribution generating the data does not change through time

$$p(x_{t+1} = y | x_t = x) = p(x_{t+2} = y | x_{t+1} = x) \quad \text{for all } t.$$

- **Non-stationary Markov chain**: the transition probabilities $p(x_{t+1} = y | x_t = x)$ depend on the time t.

Here we only consider stationary Markov chains.

Higher-order Markov chains



In some cases, the first-order assumption may be restrictive (such as when modeling natural language, where long-term dependencies occur often). We can generalize to high-order dependence trivially

- Second order:

$$p(x_t|x_{1:t-1}) = p(x_t|x_{t-1}, x_{t-2})$$

- m-th-order

$$p(x_t|x_{1:t-1}) = p(x_t|x_{t-1:t-m})$$

Transition matrix

- When x_t is discrete (e.g. $x_t \in \{1, ..., K\}$), the conditional distribution $p(x_t|x_{t-1})$ can be written as a $K \times K$ matrix.
- We call this the **transition** (or stochastic) **matrix** A:

$$A_{ij} = p(x_t = j|x_{t-1} = i), \qquad A \in \mathbb{R}^{K \times K}.$$

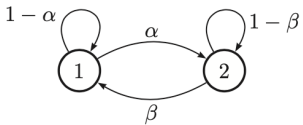
- Note that

$$\begin{aligned} p(x_t = j) &= \sum_i p(x_t = j|x_{t-1} = i)p(x_{t-1} = i), \\ &= \sum_i A_{ij} p(x_{t-1} = i). \end{aligned}$$

- Each row of the matrix sums to one, $\sum_j A_{ij} = 1$.

State transition diagram

- $A_{ij} = p(x_t = j | x_{t-1} = i)$ is the probability of going from state i to state j.



- We can visualize Markov chains via a directed graph, where nodes represent states and arrows represent legal transitions, i.e., non-zero elements of A.

- This is a **state transition diagram**.
- The weights associated with the arcs are the probabilities.
- The transition matrix for the 2-state chain shown above is given by

$$A = \begin{bmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{bmatrix}$$

Chapman-Kolmogorov equations

- The n-step transition matrix $A(n)$ is defined as

$$A_{ij}(n) = p(x_{t+n} = j | x_t = i)$$

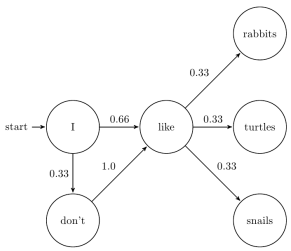
  which is the probability of getting from i to j in exactly n steps.
- Notice that $A(1) = A$.
- **Chapman-Kolmogorov** equations state that

$$A_{ij}(m+n) = \sum_{k=1}^{K} A_{ik}(m) A_{kj}(n) \quad \text{equivalently} \quad A(m+n) = A(m)A(n)$$

  the probability of getting from i to j in $m+n$ steps is just the probability of getting from i to k in m steps, and then from k to j in n steps, summed up over all k.
- So $A(n) = A \cdot A(n-1) = A \cdot A \cdot A(n-2) = \cdots = A^n$.

Application: Markov Language Models

- We use Markov chains as language models, which are distributions over sequences of words.
- State space is all words and x_t denotes the t-th word in a sentence.
- We may use a first-order Markov model.



- To estimate A and π, note that the probability of any particular sentence of length T is:

$$\begin{aligned} p(x_{1:T}|\theta) &= \pi(x_1)A(x_1, x_2)\cdots A(x_{T-1}, x_T) \\ &= \prod_{j=1}^{K} \pi_j^{1[x_1=j]} \prod_{t=2}^{T}\prod_{j=1}^{K}\prod_{k=1}^{K} A_{jk}^{1[x_t=k, x_{t-1}=j]} \end{aligned}$$

where $\pi(x_1)$ is the probability of the sentence starting with word x_1.

The estimating equations have a natural form $\rightarrow$ Tutorial

Stationary distribution of a (homogeneous) Markov chain

- We are often interested in the long term distribution over states, which is known as the **stationary distribution** of the chain.
- Let A be the transition matrix and let $\pi_t(j) = p(x_t = j)$ be the probability of being in state j at time t.
- The initial distribution is given by $\pi_0 \in \mathbb{R}^K$ and

$$\pi_1(j) = \sum_{i=1}^{K} p(x_1 = j | x_0 = i)\pi_0(i) = \sum_{i=1}^{K} A_{ij}\pi_0(i) = \sum_{i=1}^{K} (A^\top)_{ji}\pi_0(i).$$

- Using the vector notation $\pi_1 = A^\top \pi_0$ and more generally

$$\pi_t \;=\; A^\top \pi_{t-1} \;=\; A^\top A^\top \pi_{t-2} = \cdots = (A^\top)^t \pi_0.$$

- Do this infinitely many steps, the distribution of x_t may converge

$$\pi = A^\top \pi.$$

  Then we have reached the stationary distribution of the Markov chain.

Stationary distribution

A bit of linear algebra:

- Stationary distribution of a Markov chain can be found by solving the eigenvector equation

$$A^\top v = v \quad \text{and set} \quad \pi \propto v.$$

  v is the eigenvector of $A^\top$ with eigenvalue 1.

- Need to normalize!

- Since $A\mathbf{1} = \mathbf{1}$ (row sums are 1), 1 is an eigenvalue of A with eigenvector $\mathbf{1}$. A and $A^\top$ have the same eigenvalues (characteristic polynomials equal). It follows that 1 is also the eigenvalue of $A^\top$.

- The stationary distribution may not be unique.

Detailed balance equations

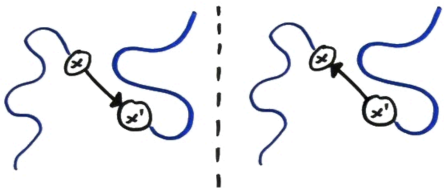
Markov Chain is called:

- **irreducible** if we can get from any state to any other state.
- **regular** if A^n has positive entries for some n.
- **time reversible** if there exists a distribution π such that

$$\pi_i A_{ij} = \pi_j A_{ji} \qquad \text{for all } i, j.$$

This is called the **detailed balance equations**.

Detailed balance means $\to x \to x'$ and $\to x' \to x$ are equally probable:



Detailed balance equations

Detailed balance equations (DB): $\pi_i A_{ij} = \pi_j A_{ji}$ for all i, j.

Theorem

If a Markov chain with transition matrix A satisfies detailed balance with respect to distribution π, then π is a stationary distribution.

Proof: Show that $A^\top \pi = \pi$ or, in other words, that

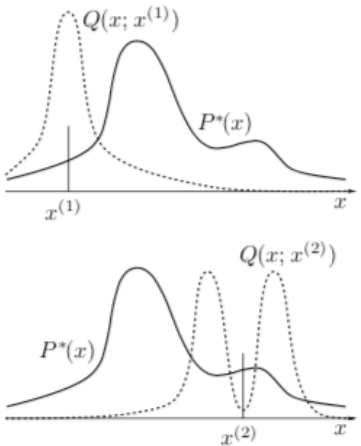
$$\sum_{i=1}^{K} \pi_i A_{ij} \;=\; \pi_j \qquad \text{for all } j.$$

Indeed, for every $j = 1, \ldots, K$, we have

$$\sum_{i=1}^{K} \pi_i A_{ij} \overset{\text{(DB)}}{=} \sum_{i=1}^{K} \pi_j A_{ji} \;=\; \pi_j \sum_{i=1}^{K} A_{ji} \;=\; \pi_j.$$

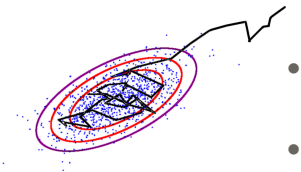
Metropolis-Hastings (first encounter with MCMC)

Importance and rejection sampling work only if the proposal density $q(x)$ is similar to $p(x)$. In high dimensions, it is hard to find one such q.



- The Metropolis-Hastings algorithm instead makes use of a proposal density q which depends on the current state $x^{(t)}$.
- The density $q(x|x^{(t)})$ might be a simple distribution such as a Gaussian centered on the current $x^{(t)}$, but can be any density from which we can draw samples.
- In contrast to importance and rejection sampling, it is not necessary that $q(x|x^{(t)})$ looks similar to $p(x)$.

Markov Chain Monte Carlo (MCMC)



- In contrast to rejection sampling, where the accepted points $\{x^{(t)}\}$ are independent, MCMC methods generate a dependent sequence.
- Each sample $x^{(t)}$ has a probability distribution that depends on the previous value, $x^{(t-1)}$.
- MCMC methods need to be run for a time in order to generate samples that are from the target distribution p.

We can still do Monte Carlo estimaton for large enough T to estimate the mean of a test function ϕ:

$$\mathbb{E}_{x\sim p}[f(x)] \approx \frac{1}{T}\sum_{t=1}^{T} f(x^{(t)}).$$

(good idea to discard a bunch of initial samples)

Metropolis-Hastings algorithm

As before, assume we can evaluate $\tilde{p}(x)$ for any x. Our procedure:

- A tentative new state x' is generated from the proposal density $q(x'|x^{(t)})$. We accept the new state with probability

$$A(x'|x^{(t)}) \quad = \quad \min\left\{1, \frac{\tilde{p}(x')q(x^{(t)}|x')}{\tilde{p}(x^{(t)})q(x'|x^{(t)})}\right\}$$

  - If accepted, set $x^{(t+1)} = x'$. Otherwise, set $x^{(t+1)} = x^{(t)}$.

- Metropolis: Simpler version when $q(x'|x) = q(x|x')$ for all x, x'.

- **Theorem:** This procedure defines a Markov chain with stationary distribution $\pi(x)$ equal to the target distribution $p(x)$.

Proof of the theorem

Recall $A(x'|x) = \min\left\{1, \frac{\tilde{p}(x')q(x|x')}{\tilde{p}(x)q(x'|x)}\right\} = \min\left\{1, \frac{p(x')q(x|x')}{p(x)q(x'|x)}\right\}$.

The resulting Markov chain has the following transition probabilities:

$$r(x'|x) = \begin{cases} q(x'|x)A(x'|x) & \text{if } x' \neq x \\ q(x|x) + \sum_{x' \neq x} q(x'|x)(1 - A(x'|x)) & \text{if } x' = x \end{cases}.$$

Show (DB) $r(x'|x)p(x) = r(x|x')p(x')$. If $x \neq x'$

$$r(x'|x)p(x) = p(x)q(x'|x)\min\left\{1, \frac{p(x')q(x|x')}{p(x)q(x'|x)}\right\} = \min\left\{p(x')q(x|x'), p(x)q(x'|x)\right\}$$

$$r(x|x')p(x') = p(x')q(x|x')\min\left\{1, \frac{p(x)q(x'|x)}{p(x')q(x|x')}\right\} = \min\left\{p(x')q(x|x'), p(x)q(x'|x)\right\}$$

Thus p is a stationary distribution of this Markov chain.

Overview for the remaining hour

- Gibbs sampling
- Hamiltonian Monte Carlo
- MCMC diagnostics

Gibbs Sampling Procedure

Suppose the vector x has been divided into d components

$$x = (x_1, ..., x_d).$$

Start with any $x^{(0)} = (x_1^{(0)}, \ldots, x_d^{(0)})$. In the t-th iteration:

- For $j = 1, \ldots, d$:
  - Sample $x_j^{(t)}$ from the conditional distribution given other components:

$$x_j^{(t)} \sim p(x_j | x_{-j}^{(t-1)})$$

Where $x_{-j}^{(t-1)}$ represents all the components of x except for x_j at their current values:

$$x_{-j}^{(t-1)} = (x_1^{(t)}, x_2^{(t)}, ..., x_{j-1}^{(t)}, x_{j+1}^{(t-1)}, ..., x_d^{(t-1)})$$

- No accept/reject, only accept.

Example: Bivariate Gaussian

Consider a (simple) problem of sampling from the bivariate Gaussian

$$X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \sim N_2(\mu, \Sigma), \qquad \mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \quad \Sigma = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}.$$

We have

$$X_1 | X_2 = x_2 \sim N(\mu_1 + \rho(x_2 - \mu_2), 1 - \rho^2)$$

$$X_2 | X_1 = x_1 \sim N(\mu_2 + \rho(x_1 - \mu_1), 1 - \rho^2)$$

Given $X^{(0)} = (0, 0)$ we proceed iteratively for $t \geq 1$:

$$X_1^{(t)} \sim N(\mu_1 + \rho(x_2^{(t-1)} - \mu_2), 1 - \rho^2)$$

$$X_2^{(t)} \sim N(\mu_2 + \rho(x_1^{(t)} - \mu_1), 1 - \rho^2)$$

Example: Bivariate Gaussian

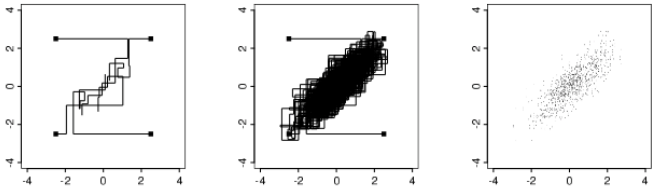


Figure 11.2 *Four independent sequences of the Gibbs sampler for a bivariate normal distribution with correlation $\rho = 0.8$, with overdispersed starting points indicated by solid squares. (a) First 10 iterations, showing the componentwise updating of the Gibbs iterations. (b) After 500 iterations, the sequences have reached approximate convergence. Figure (c) shows the points from the second halves of the sequences, representing a set of correlated draws from the target distribution.*

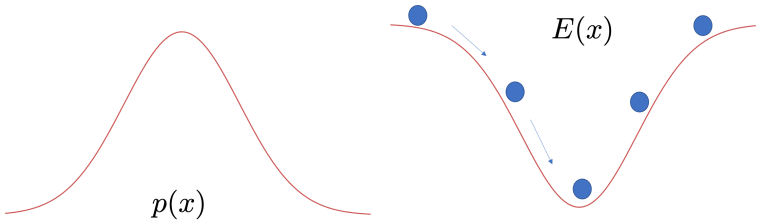
1

(The real power of Gibbs approach comes in situations when the distribution is hard but full-conditionals are simple, e.g. Ising)

[1] From "Bayesian Data Analysis Third edition" by Gelman, Carlin, Stern, Dunson, Vehtari, Rubin

Hamiltonian Monte Carlo

- This is essentially a Metropolis-Hastings algorithm with a specialized proposal mechanism.
- Algorithm uses a physical analogy to make proposals.
- Given the position x, the potential energy is $E(x)$



- Construct a distribution

$$p(x) \propto e^{-E(x)}, \quad \text{with} \quad E(x) = -\log(\tilde{p}(x))$$

where $\tilde{p}(x)$ is the unnormalized density we can evaluate.

Hamiltonian Monte Carlo

- Introduce **momentum** v carrying the kinetic energy

$$K(v) \;=\; \tfrac{1}{2}\|v\|^2 \;=\; \tfrac{1}{2}v^\top v.$$

- Total energy or **Hamiltonian**:

$$H(x, v) = E(x) + K(v).$$

- Energy is preserved:
  - Frictionless ball rolling $(x, v) \to (x', v')$
  - $H(x, v) = H(x', v')$.

- Ideal Hamiltonian dynamics are reversible: reverse v and the ball will return to its start point! $(x, v) \to (x', v')$ but also $(x', -v') \to (x, -v)$

Hamiltonian Monte Carlo

- The joint distribution:
  - $p(x, v) \propto e^{-E(x)} e^{-K(v)} = e^{-E(x)-K(v)} = e^{-H(x,v)}$
  - Momentum is Gaussian, and independent of the position ($K(v) = \frac{1}{2}\|v\|^2$).
- MCMC procedure
  - Sample the momentum from the standard Gaussian.
  - Simulate Hamiltonian dynamics. In the end flip sign of the momentum.
    - Hamiltonian dynamics is reversible.
    - Energy is constant $p(x, v) = p(x', v') = p(x', -v')$.
- How to simulate Hamiltonian dynamics? Take:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial H}{\partial v} = \frac{\partial K}{\partial v}$$
$$\frac{\mathrm{d}v}{\mathrm{d}t} = -\frac{\partial H}{\partial x} = -\frac{\partial E}{\partial x}$$

(Indeed: $\frac{\mathrm{d}H}{\mathrm{d}t} = \sum_i \frac{\partial E}{\partial x_i}\frac{\mathrm{d}x_i}{\mathrm{d}t} + \sum_i \frac{\partial K}{\partial v_i}\frac{\mathrm{d}v_i}{\mathrm{d}t}$ will be zero)

Leap-frog integrator

- A numerical approximation:

$$
\begin{aligned}
v(t+\tfrac{\epsilon}{2}) &= v(t) + \frac{\epsilon}{2}\frac{\mathrm{d}v}{\mathrm{d}t}(t) = v(t) - \frac{\epsilon}{2}\frac{\partial E}{\partial x}(x(t)) \\
x(t+\epsilon) &= x(t) + \epsilon\frac{\mathrm{d}x}{\mathrm{d}t}(t) = x(t) + \epsilon\frac{\partial K}{\partial v}(v(t+\tfrac{\epsilon}{2})) \\
v(t+\epsilon) &= v(t+\tfrac{\epsilon}{2}) - \frac{\epsilon}{2}\frac{\partial E}{\partial x}(x(t+\epsilon))
\end{aligned}
$$

  (Slightly more accurate than the standard Euler's method)

- We do a fixed number of leap-frog steps.
- Dynamics are still deterministic (and reversible)

HMC algorithm

The HMC algorithm (run until it mixes):

- Current position: $(x^{(t-1)}, v^{(t-1)}))$
- Sample momentum: $v^{(t)} \sim \mathcal{N}(0, I)$.
- Start at $(x, v) = (x^{(t-1)}, v^{(t)})$ and run Leapfrog integrator for L steps and reach (x', v')
- Accept new state $(x', -v')$ with probability:

$$\min\left\{1, \frac{\exp(H(x^{(t-1)}, v^{(t-1)}))}{\exp(H(x', v'))}\right\}$$

- Low energy points are favored.

MCMC Inference

- Sample from unnormalized posterior.
- Estimate statistics from simulated values of x:
  - mean
  - median
  - quantiles
- All of this however requires some care, as MCMC is not without problems.

MCMC diagnostics

- How do we know we have ran the algorithm long enough?
- What if we started very far from where our distribution is?
- Since there is correlation between each item of the chain (autocorrelation), what is the "effective" number of samples?

Good Ideas for MCMC

Some obvious things to consider:

- Parallel computation is cheap - we can run multiple chains in parallel starting at different points
- We should discard some initial samples - **burn-in phase**.
- We should examine how well the chain is "mixed".

(No need to memorize any of the formulas below)

R hat

- Start with m chains each of length n, $X = [x_{ij}] \in \mathbb{R}^{n \times m}$.
  - this will be already after a fixed burn-in phase.
- The **between sequence variance** B is:

$$B = \frac{n}{m-1} \sum_{j=1}^{m} (\bar{x}_{\cdot j} - \bar{x}_{\cdot\cdot})^2,$$

where:

$$\bar{x}_{\cdot j} = \frac{1}{n} \sum_{i=1}^{n} x_{ij} \quad \text{and} \quad \bar{x}_{\cdot\cdot} = \frac{1}{m} \sum_{j=1}^{m} \bar{x}_{\cdot j} = \frac{1}{mn} \sum_{i=1}^{n} \sum_{j=1}^{m} x_{ij}$$

(individual chain means, total mean)

R hat

- The **within sequence variance** W is:

$$W = \frac{1}{m} \sum_{j=1}^{m} s_j^2$$

where:

$$s_j^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_{ij} - \bar{x}_{.j})^2$$

(here s_j^2 estimates the variance in j-th sequence and W is the average variance)

- **Idea**: If one or more chain has not mixed well, the variance of all the chains combined together should be higher than that of individual chains.

R hat

- Next we compute the average variance:

$$\widehat{\text{var}}^{+}(x) = \frac{n-1}{n} W + \frac{1}{n} B$$

- Finally define **R-hat** coefficient:

$$\hat{R} = \sqrt{\frac{\widehat{\text{var}}^{+}(x)}{W}}$$

- If chains have not mixed well, R-hat is larger than 1.

- **Split-$\widehat{\mathbf{R}}$**: Split each chain into the first and second halves. This can detect non-stationarity within a single chain.

Effective Sample Size

- If $x_1, \ldots, x_n$ are i.i.d. with variance σ^2 then $\mathrm{var}(\bar{x}_n) = \frac{\sigma^2}{n}$.
- In general, without assuming independence

$$\mathrm{var}(\bar{x}) = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \mathrm{cov}(x_i, x_j) = \frac{\sigma^2}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \mathrm{corr}(x_i, x_j)$$

  so $\frac{n^2}{\sum_{i=1}^{n} \sum_{j=1}^{n} \mathrm{corr}(x_i, x_j)}$ measures "effective sample size".
- We define the **effective sample size** to be:

$$n_{\text{eff}} = \frac{mn}{1 + 2\sum_{t=1}^{\infty} \rho_t}$$

  where $\rho_t = \mathrm{corr}(x_0, x_t)$ are unknown, so we also estimate them.

Diagnostics Summary

- Once $\hat{R}$ is near 1, and $\hat{n}_{\text{eff}}$ is more than 10 per chain **for all scalar estimands** we collect the mn simulations, (excluding the burn-in).
- We can then draw inference based on our samples. However:
  - Even if the iterative simulations appear to have converged, passed all tests etc. It may still be far from convergence!
- When we declare "convergence" - we mean that all chains appear stationary and well mixed.
- Non of the checks we learned today are hypothesis test. There are no p-values, and no statistical significance.