STA 414/2104:
Statistical Methods of Machine Learning II

Week 5 - 2/2: Sampling II

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Overview

- Gibbs sampling

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- Hamiltonian Monte Carlo

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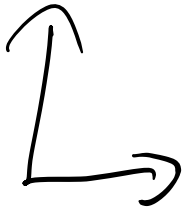
- Hamiltonian Monte Carlo
- MCMC diagnostics

Gibbs Sampling



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- At each iteration, the **Gibbs Sampler**, cycles through the components of θ, drawing each subset conditional on the value of all others.
- This means we perform d steps at each sampling iteration t to obtain $\theta^{(t+1)}$

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- For $j = 1$ to $j = d$:
  - Sample θ_j^t from the conditional distribution given all the other components:

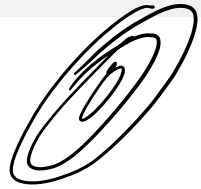
$$p(\theta_j | \theta_{-j}^{t-1}, y)$$

Where θ_{-j}^{t-1} represents all the components of θ except for θ_j at their current values:

$$\theta_{-j}^{t-1} = (\theta_1^t, \theta_2^t, ..., \theta_{j-1}^t, \theta_{j+1}^{t-1}, ..., \theta_d^{t-1})$$

$$\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{pmatrix} \qquad \theta_{-2}^{t-1} = \begin{pmatrix} \theta_1^t \\ \\ \theta_3^{t-1} \end{pmatrix}$$

Gibbs Sampling Example



Consider a single observation (y_1, y_2) from a bivariate normal, with unknown mean $\mu = (\mu_1, \mu_2)$ and known covariance matrix: $\Sigma = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$ with a uniform prior distibution on μ

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Although it is simple to draw from this posterior we can alternatively use the Gibbs sampler. To do that we must first deterimine the conditional posterior distributions for μ_1 and μ_2

Gibbs Sampling Example

Using the properties of the multivariate normal distribution we have:

$$\mu_1|\mu_2, y \sim N(y_1 + \rho(\mu_2 - y_2), 1 - \rho^2)$$
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Then given some previous (possibly initial) value of μ, the sampling would be:

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Gibbs Sampling Example

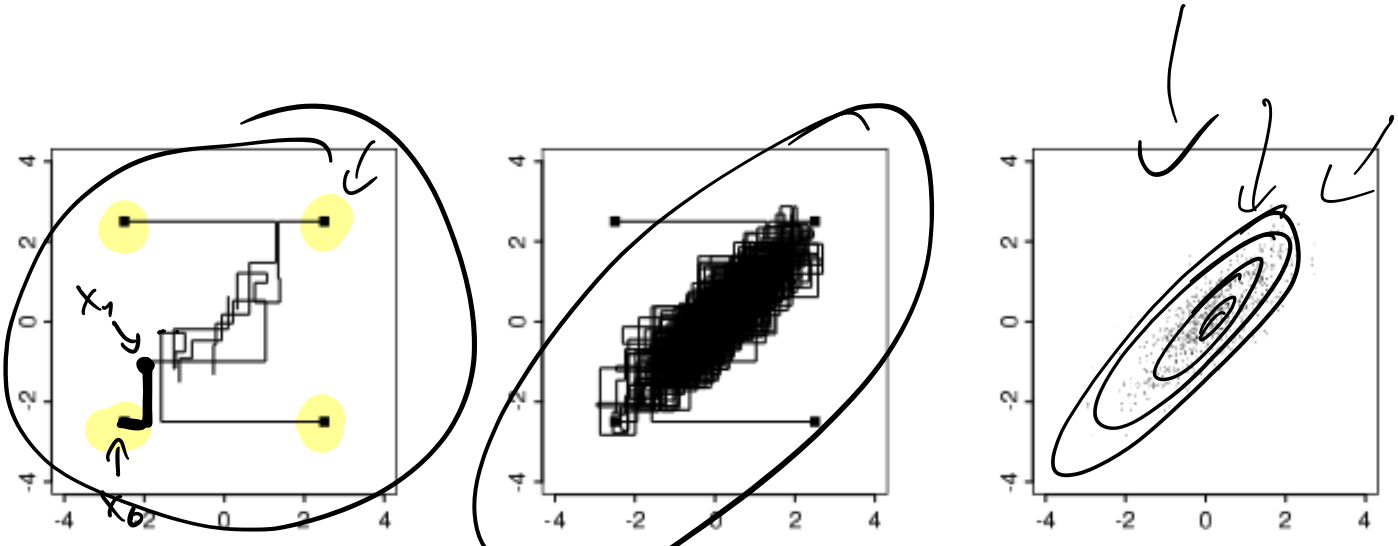


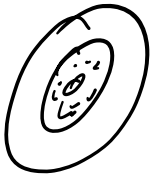
Figure 11.2 *Four independent sequences of the Gibbs sampler for a bivariate normal distribution with correlation $\rho = 0.8$, with overdispersed starting points indicated by solid squares. (a) First 10 iterations, showing the componentwise updating of the Gibbs iterations. (b) After 500 iterations, 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

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

Volumes in High dimensional Spaces and Typical sets

- In high dimensional spaces, a very large proportion of the density will be far away from the modes



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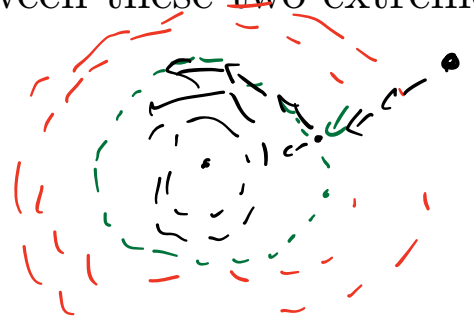
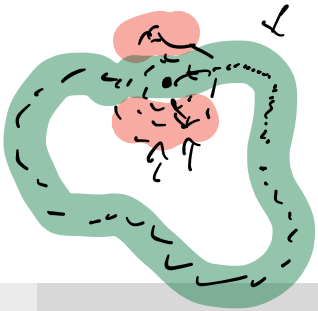
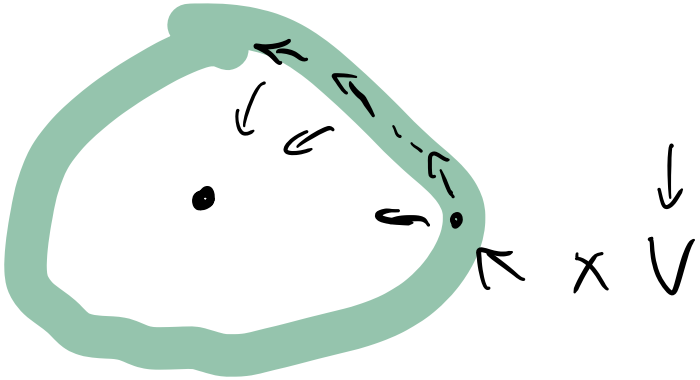
- The neighbourhood around the mode(s) features large densities but a very small volume
- The space far away from the mode(s) might have very large volumes, but very low densities
- The only significant contributions to expecations will be a balance between these two extremes known as the **typical set**





Typical Set - Satelite analogy



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- Ideal Hamiltonian dynamics are reversible: reverse v and the ball will return to its start point!

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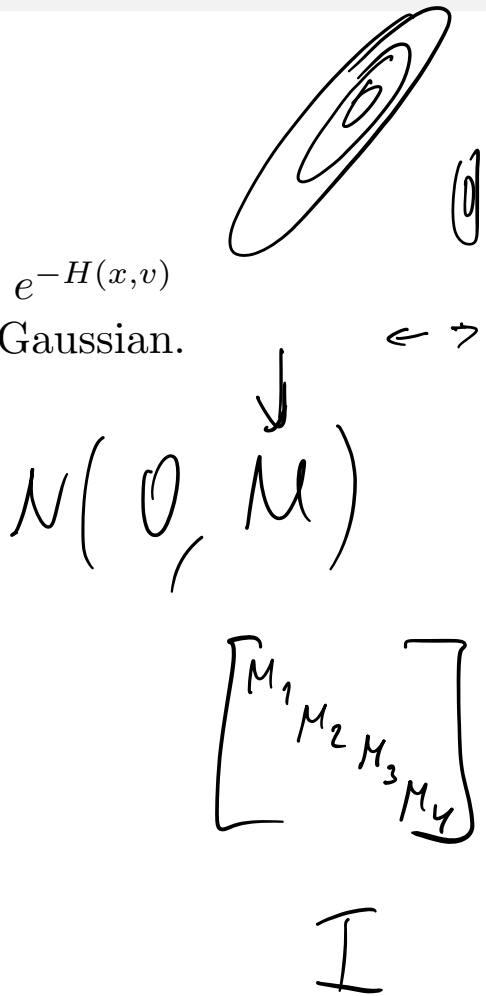

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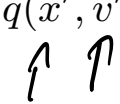

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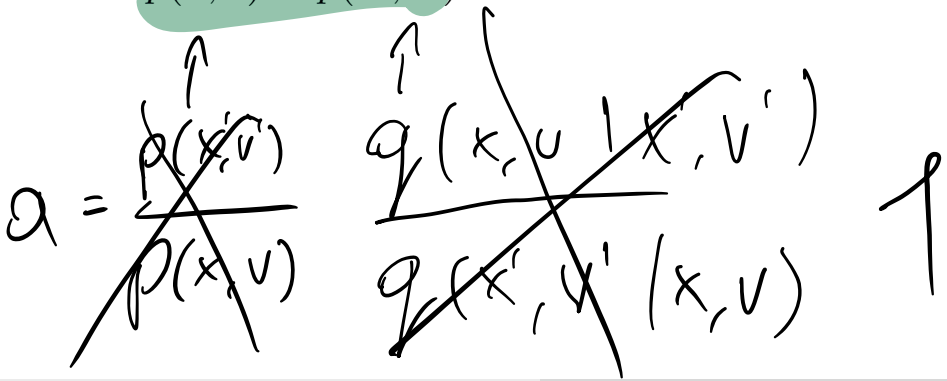

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    - Metropolis acceptance probability is 1.
- How to simulate Hamiltonian dynamics?

Leap-frog integrator

- A numerical approximation:

$$
\begin{cases}
v_i(t+\frac{\epsilon}{2}) &= v_i(t) - \frac{\epsilon}{2}\frac{\partial E(x(t))}{\partial x_i} \\
x_i(t+\epsilon) &= x_i(t) + \epsilon\, v_i(t+\frac{\epsilon}{2}) \\
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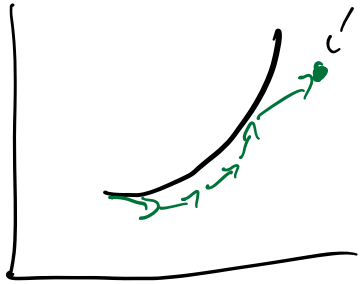

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- Dynamics are still deterministic (and reversible)

Leap-frog integrator

- A numerical approximation:

$$\text{Single step} \begin{cases} v_i(t+\frac{\epsilon}{2}) &= v_i(t) - \frac{\epsilon}{2}\frac{\partial E(x(t))}{\partial x_i} \\ x_i(t+\epsilon) &= x_i(t) + \epsilon\, v_i(t+\frac{\epsilon}{2}) \\ v_i(t+\epsilon) &= v_i(t+\frac{\epsilon}{2}) - \frac{\epsilon}{2}\frac{\partial E(x(t+\epsilon))}{\partial x_i} \end{cases}$$

- H is not conserved.
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- Acceptance probability :

$$\min\{1, \exp(H(x,v) - H(x',v'))\}$$

HMC algorithm

The HMC algorithm (run until it mixes):

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The HMC algorithm (run until it mixes):

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- Run Leapfrog integrator for L steps
- Accept new position x' with probability:

$$\min\{1, \exp(H(x, v) - H(x', v'))\}$$

MCMC Inference

- Compute the unnormalized posterior

$$\frac{p(\theta) L(\theta)}{\to Z}$$

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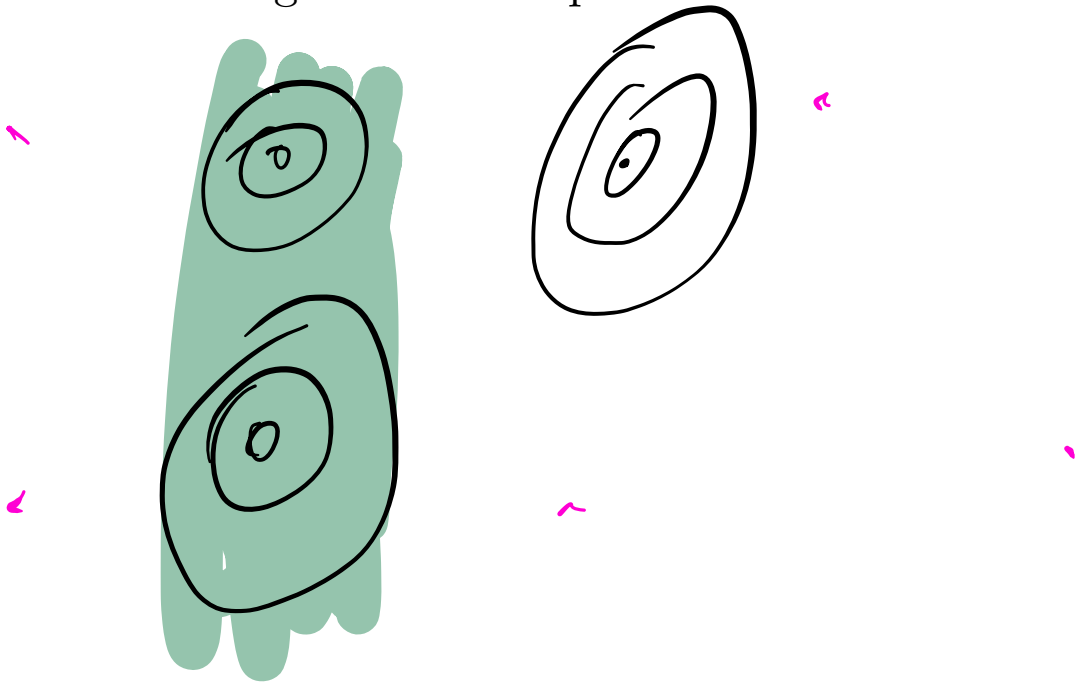
- **Posterior predictive** simulations of unobserved outcomes $\tilde{y}$ can be obtained by further simulation conditional on drawn values of θ
- All of this however requires some care, as MCMC is not without problems

MCMC demo

Good Ideas for MCMC

- Parallel computation is cheap - we can run multiple chains in parallel starting at different points



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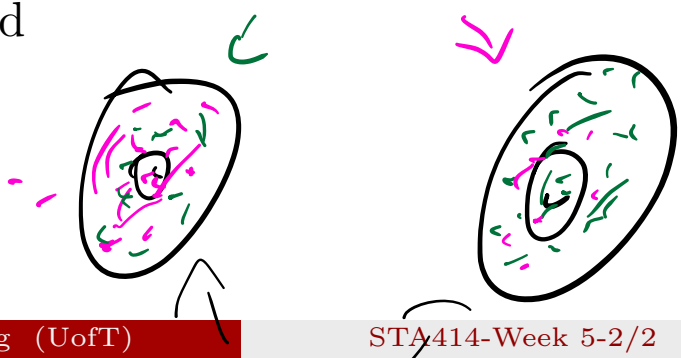
- We should examine how well the chains have "mixed" together - i.e. how much overlap is there in the parameter space each of them explored



MCMC diagnostics

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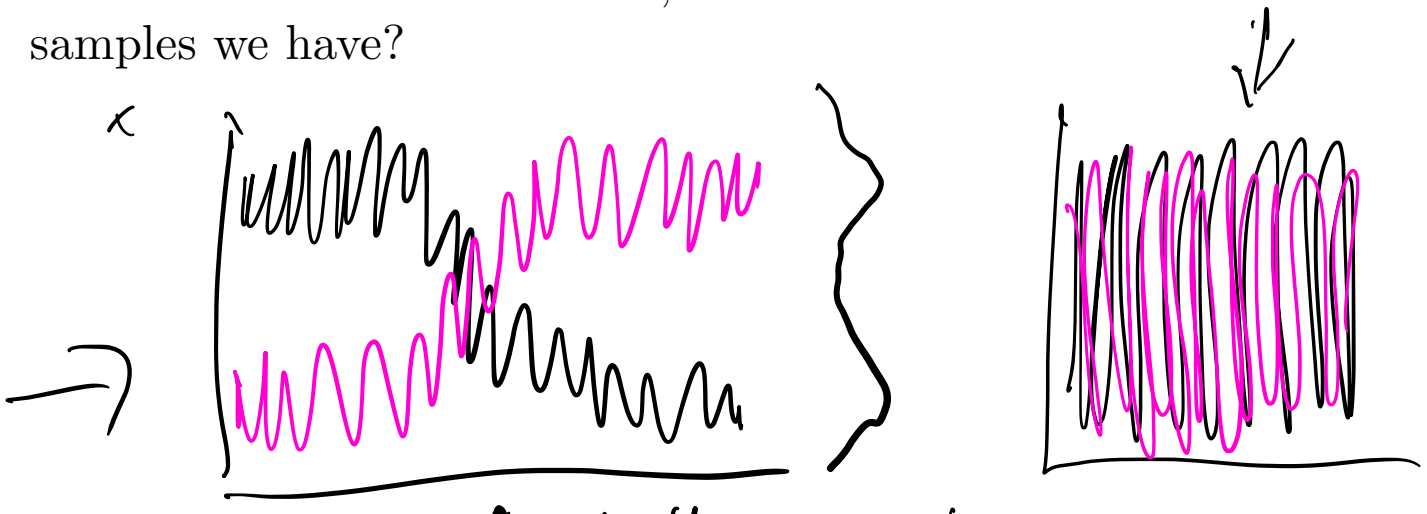
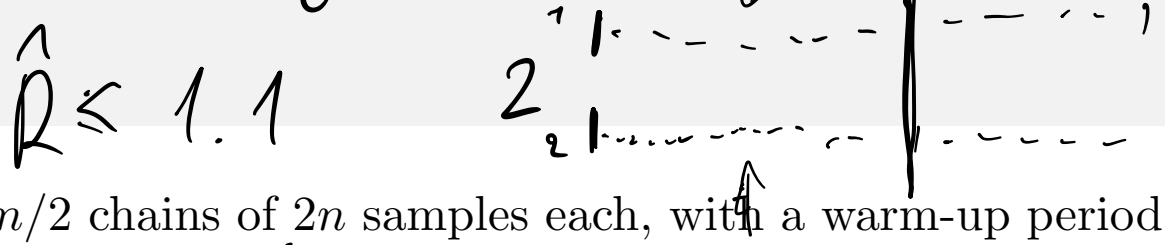
- What if we started very far from where our distribution is?
- Since there is autocorrelation, what is the "effective" number of samples we have?



R hat



Start with $m/2$ chains of $2n$ samples each, with a warm-up period of n. Split them in half so that we have m chains total (half of which are burn-in) of length n each. Label each scalar estimand with $\psi_{i,j}$ with $(i = 1, ..., n; j = 1, ..., m)$ The **between sequence variance** B is:

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and:

$$\bar{\psi}_{..} = \frac{1}{m} \sum_{j=1}^{m} \bar{\psi}_{.j}$$

R hat

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

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

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- In the limit the expectation of W approaches $var(\psi|y)$

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- We estimate the factor by which the scale of the current distribution for ψ might be reduced if we were continue to infinity by:

$$\hat{R} = \sqrt{\frac{\widehat{var}^{+}(\psi|y)}{W}}$$

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- in the presence of correlation we define the **effective sample size** to be:

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

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- For large values of t this becomes very noisy so we usually cut off the sum over $\hat{\rho}_t$ when two consecutive summands were negative

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- All of the checks we learned today are not hypothesis test. There are no p-values, and no statistical significance.