

CMPE 58N - Lecture 4

Monte Carlo methods

The Gibbs Sampler, Applications



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Outline

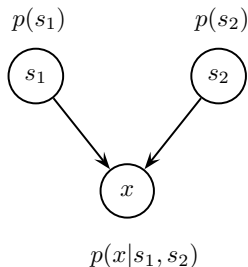
- ▶ Motivating Example
- ▶ The Gibbs sampler
- ▶ Gibbs Application: Change point model
- ▶ MH Application: Sensor fusion

The Gibbs sampler

Algorithm 1 Gibbs sampler

```
1: Initialize:  $x^{(0)} \sim q(x)$ 
2: for  $i = 1, 2, \dots$  do
3:    $x_1^{(i)} \sim p(x_1 | X_2 = x_2^{(i-1)}, X_3 = x_3^{(i-1)}, \dots, X_N = x_N^{(i-1)})$ 
4:    $x_2^{(i)} \sim p(x_2 | x_1 = x_1^{(i)}, X_3 = x_3^{(i-1)}, \dots, X_N = x_N^{(i-1)})$ 
5:    $\vdots$ 
6:    $x_N^{(i)} \sim p(x_N | x_1 = x_1^{(i)}, X_2 = x_2^{(i)}, \dots, X_{N-1} = x_{N-1}^{(i)})$ 
7: end for
```

Motivating Example : Gibbs Sampler



This graph encodes the joint: $p(x, s_1, s_2) = p(x|s_1, s_2)p(s_1)p(s_2)$

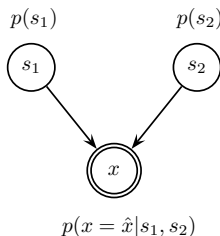
$$s_1 \sim p(s_1) = \mathcal{N}(s_1; \mu_1, P_1)$$

$$s_2 \sim p(s_2) = \mathcal{N}(s_2; \mu_2, P_2)$$

$$x|s_1, s_2 \sim p(x|s_1, s_2) = \mathcal{N}(x; s_1 + s_2, R)$$

Toy example

Suppose, we observe $x = \hat{x}$.



- By Bayes' theorem, the posterior is given by:

$$\mathcal{P} \equiv p(s_1, s_2 | x = \hat{x}) = \frac{1}{Z_{\hat{x}}} p(x = \hat{x} | s_1, s_2) p(s_1) p(s_2) \equiv \frac{1}{Z_{\hat{x}}} \phi(s_1, s_2)$$

- The function $\phi(s_1, s_2)$ is proportional to the exact posterior.
($Z_{\hat{x}} \equiv p(x = \hat{x})$)

Toy example, cont.

$$\log p(s_1) = \mu_1^T P_1^{-1} s_1 - \frac{1}{2} s_1^T P_1^{-1} s_1 + \text{const}$$

$$\log p(s_2) = \mu_2^T P_2^{-1} s_2 - \frac{1}{2} s_2^T P_2^{-1} s_2 + \text{const}$$

$$\log p(x|s_1, s_2) = \hat{x}^T R^{-1} (s_1 + s_2) - \frac{1}{2} (s_1 + s_2)^T R^{-1} (s_1 + s_2) + \text{const}$$

Toy example, cont.

$$\begin{aligned}\log \phi(s_1, s_2) &= \log p(x = \hat{x} | s_1, s_2) + \log p(s_1) + \log p(s_2) \\&= + \left(\mu_1^T P_1^{-1} + \hat{x}^T R^{-1} \right) s_1 + \left(\mu_2^T P_2^{-1} + \hat{x}^T R^{-1} \right) s_2 \\&\quad - \frac{1}{2} \mathbf{Tr} \left(P_1^{-1} + R^{-1} \right) s_1 s_1^T - \underbrace{s_1^T R^{-1} s_2}_{(*)} \\&\quad - \frac{1}{2} \mathbf{Tr} \left(P_2^{-1} + R^{-1} \right) s_2 s_2^T\end{aligned}$$

- The (*) term is the cross correlation term that makes s_1 and s_2 a-posteriori dependent.

Toy example, cont.

Completing the square

$$\begin{aligned}\log \phi(s_1, s_2) = & + \begin{pmatrix} P_1^{-1}\mu_1 + R^{-1}\hat{x} \\ P_2^{-1}\mu_2 + R^{-1}\hat{x} \end{pmatrix}^\top \begin{pmatrix} s_1 \\ s_2 \end{pmatrix} \\ & - \frac{1}{2} \begin{pmatrix} s_1 \\ s_2 \end{pmatrix}^\top \begin{pmatrix} P_1^{-1} + R^{-1} & R^{-1} \\ R^{-1} & P_2^{-1} + R^{-1} \end{pmatrix} \begin{pmatrix} s_1 \\ s_2 \end{pmatrix}\end{aligned}$$

Remember: $\log \mathcal{N}(s; m, \Sigma) = + (\Sigma^{-1}m)^\top s - \frac{1}{2}s^\top \Sigma^{-1}s$

$$\Sigma = \begin{pmatrix} P_1^{-1} + R^{-1} & R^{-1} \\ R^{-1} & P_2^{-1} + R^{-1} \end{pmatrix}^{-1} \quad m = \Sigma \begin{pmatrix} P_1^{-1}\mu_1 + R^{-1}\hat{x} \\ P_2^{-1}\mu_2 + R^{-1}\hat{x} \end{pmatrix}$$

Gibbs sampler

- ▶ We define the following iterative schema to generate a Markov Chain

$$\begin{aligned}s_1^{(t+1)} &\sim p(s_1 | s_2^{(t)}, x = \hat{x}) && \propto \phi(s_1, s_2^{(t)}) \\ s_2^{(t+1)} &\sim p(s_2 | s_1^{(t+1)}, x = \hat{x}) && \propto \phi(s_1^{(t+1)}, s_2)\end{aligned}$$

- ▶ The desired posterior $\mathcal{P}$ is the stationary distribution of T

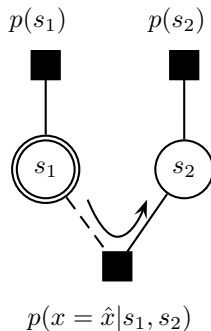
Gibbs sampler

- ▶ A remarkable fact is that we can estimate any desired expectation by ergodic averages

$$\langle f(\mathbf{s}) \rangle_{\mathcal{P}} \approx \frac{1}{t - t_0} \sum_{n=t_0}^t f(\mathbf{s}^{(n)})$$

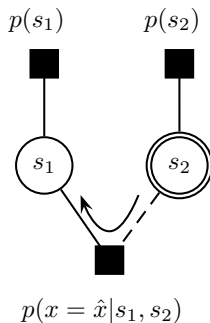
- ▶ Consecutive samples $\mathbf{s}^{(t)}$ are dependent but we can “pretend” as if they are independent!

Gibbs Sampler



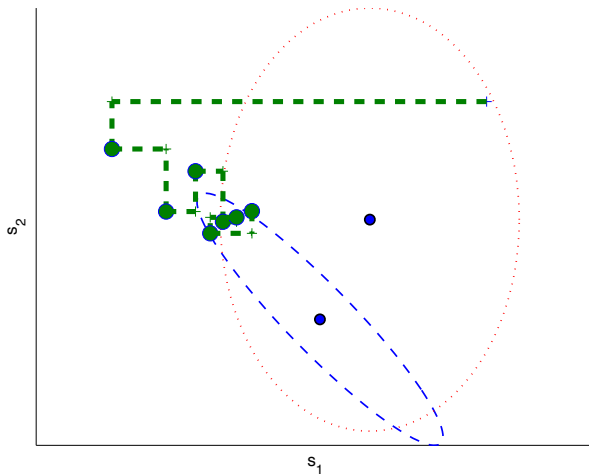
$$\textcolor{red}{s}_2^{(t+1)} \sim \mathcal{N}(s_2; m_2(s_1^{(t+1)}), S_2)$$

Gibbs Sampler

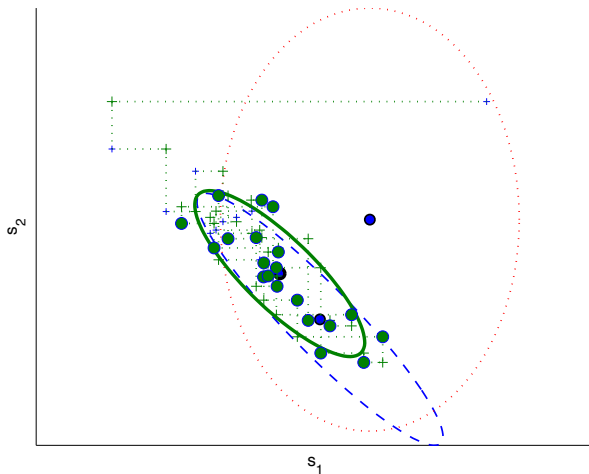


$$\textcolor{red}{s}_1^{(t+1)} \sim \mathcal{N}(s_1; m_1(s_2^{(t)}), S_1)$$

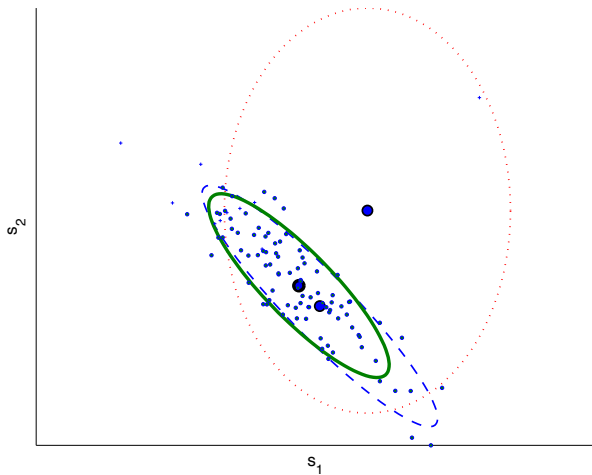
Gibbs Sampler



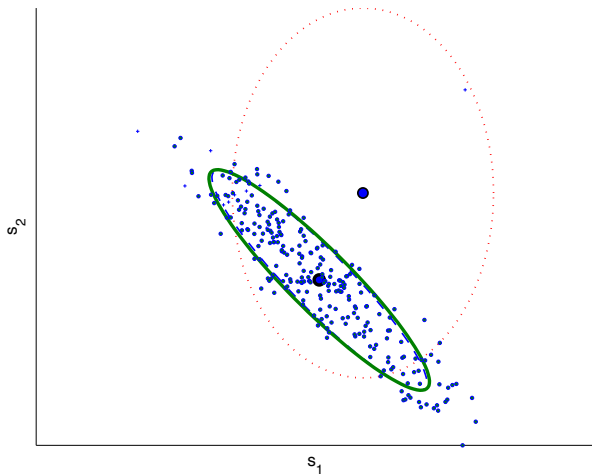
Gibbs Sampler, $t = 20$



Gibbs Sampler, $t = 100$



Gibbs Sampler, $t = 250$



Technicalities: Finding the full conditionals

$$\mathbf{s}_1^{(t+1)} \sim p(\mathbf{s}_1 | \mathbf{s}_2^{(t)}, x = \hat{x}) \propto \phi(\mathbf{s}_1, \mathbf{s}_2^{(t)}) \equiv \phi_1$$

Eliminate terms that don't depend on $\mathbf{s}_1$

$$\begin{aligned} \log \phi_1 &= \log p(x = \hat{x} | \mathbf{s}_1, \mathbf{s}_2^{(t)}) + \log p(\mathbf{s}_1) + \log p(\mathbf{s}_2^{(t)}) \\ &= + \underbrace{\mu_1^\top P_1^{-1} \mathbf{s}_1 - \frac{1}{2} \mathbf{s}_1^\top P_1^{-1} \mathbf{s}_1}_{\log p(\mathbf{s}_1)} \\ &\quad + \underbrace{\hat{x}^\top R^{-1} (\mathbf{s}_1 + \mathbf{s}_2^{(t)}) - \frac{1}{2} (\mathbf{s}_1 + \mathbf{s}_2^{(t)})^\top R^{-1} (\mathbf{s}_1 + \mathbf{s}_2^{(t)})}_{p(x = \hat{x} | \mathbf{s}_1, \mathbf{s}_2^{(t)})} \end{aligned}$$

Technicalities: Finding the full conditionals (cont.)

$$\begin{aligned}\log \phi_1 = &^+ \left(\mu_1^\top P_1^{-1} + (\hat{x} - s_2^{(t)})^\top R^{-1} \right) \mathbf{s}_1 \\ & - \frac{1}{2} \mathbf{Tr} \left(P_1^{-1} + R^{-1} \right) \mathbf{s}_1 \mathbf{s}_1^\top\end{aligned}$$

$$p(\mathbf{s}_1 | s_2^{(t)}, x = \hat{x}) = \mathcal{N}(s_1; m_1, S_1)$$

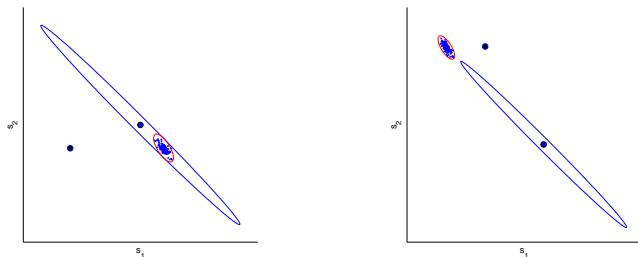
$$\begin{aligned}S_1 &= \left(P_1^{-1} + R^{-1} \right)^{-1} \\ m_1(s_2^{(t)}) &= S_1 \left(P_1^{-1} \mu_1 + R^{-1} (\hat{x} - s_2^{(t)}) \right)\end{aligned}$$

The transition kernel

$$\begin{aligned}T(s_{1:2}^{(t+1)} | s_{1:2}^{(t)}, s_2^{(t)}) &= T(s_2^{(t+1)} | s_1^{(t+1)}, s_1^{(t)}, s_2^{(t)}) T(s_1^{(t+1)} | s_1^{(t)}, s_2^{(t)}) \\&= T(s_2^{(t+1)} | s_1^{(t+1)}) T(s_1^{(t+1)} | s_2^{(t)}) \\&= \mathcal{N}(s_2^{(t+1)}; m_2(s_1^{(t+1)}), S_2) \mathcal{N}(s_1^{(t+1)}; m_1(s_2^{(t)}), S_1)\end{aligned}$$

Therefore, the transition kernel is also Gaussian.

The transition kernel



- ▶ But why does the chain converge to the target distribution?
- ▶ The Gibbs sampler is a special MH algorithm

Metropolis-Hastings

Algorithm 2 Metropolis-Hastings

- 1: Initialize: $x^{(0)} \sim q(x_0)$
- 2: **for** $i = 1, 2 \dots$ **do**
- 3: Propose: $\xi^{(i)} \sim q(x|x^{(i-1)})$
- 4: Acceptance Probability:

$$\alpha(\xi^{(i)}|x^{(i-1)}) = \min\left\{1, \frac{q(x^{(i-1)}|\xi^{(i)})\pi(\xi^{(i)})}{q(\xi^{(i)}|x^{(i-1)})\pi(x^{(i-1)})}\right\}$$

- 5: Uniform: $u \sim \mathcal{U}(u; 0, 1)$
- 6: **if** $u < \alpha$ **then**
- 7: Accept: $x^{(i)} \leftarrow \xi^{(i)}$
- 8: **else**
- 9: Reject: $x^{(i)} \leftarrow x^{(i-1)}$
- 10: **end if**
- 11: **end for**

The acceptance probability for Gibbs

$$\begin{aligned}\xi &\sim p(x_n | x_{-n} = x_{-n}^{(i-1)}) \\ \alpha &\equiv \alpha(\xi, x_{-n}^{(i-1)} | x_n^{(i-1)}, x_{-n}^{(i-1)})\end{aligned}$$

$$\begin{aligned}\alpha &= \min \left\{ 1, \frac{q(x_n^{(i-1)}, x_{-n}^{(i-1)} | \xi, x_{-n}^{(i-1)}) p(\xi, x_{-n}^{(i-1)})}{q(\xi, x_{-n}^{(i-1)} | x_n^{(i-1)}, x_{-n}^{(i-1)}) p(x_n^{(i-1)}, x_{-n}^{(i-1)})} \right\} \\ &= \min \left\{ 1, \frac{p(x_n^{(i-1)} | x_{-n}^{(i-1)}) p(\xi, x_{-n}^{(i-1)})}{p(\xi | x_{-n}^{(i-1)}) p(x_n^{(i-1)}, x_{-n}^{(i-1)})} \right\} \\ &= \min \left\{ 1, \frac{p(x_n^{(i-1)} | x_{-n}^{(i-1)}) p(\xi | x_{-n}^{(i-1)}) p(x_{-n}^{(i-1)})}{p(\xi | x_{-n}^{(i-1)}) p(x_n^{(i-1)} | x_{-n}^{(i-1)}) p(x_{-n}^{(i-1)})} \right\} = 1\end{aligned}$$

Example: A change-point model

- ▶ We have a sequence of counts x_j .
- ▶ The average of the counts is jumping to a new value after an unknown index

Generative model

- ▶ We can model the counts with Poisson random variables $x_j, j = 1 \dots M$

$$\begin{aligned}\mathcal{PO}(x; \lambda) &= e^{-\lambda} \frac{\lambda^x}{x!} \\ &= \exp(+x \log \lambda - \lambda - \log(x!))\end{aligned}$$

- ▶ The unknown intensity can be modelled by a Gamma random variable

$$\begin{aligned}\mathcal{G}(\lambda; a, b) &\equiv \frac{1}{\Gamma(a)} b^a \lambda^{a-1} \exp(-b\lambda) \\ &= \exp((a-1) \log \lambda - b\lambda - \log \Gamma(a) + a \log b)\end{aligned}$$

- ▶ The unknown intensity λ_1 is jumping to a new unknown value λ_2 after an unknown index m

Generative model

$$m \sim \mathcal{U}\{1 \dots M\}$$

$$\lambda_i \sim \mathcal{G}(\lambda_i; a, b)$$

$$x_j \sim \begin{cases} \mathcal{PO}(x_j; \lambda_1) & 1 \leq j \leq m \\ \mathcal{PO}(x_j; \lambda_2) & m < j \leq M \end{cases}$$

Goal: Compute $p(\lambda_1, \lambda_2, m | x_{1:M})$

Generate data

```
% Fix the seeds for reproducibility
randn('seed', 1); rand('seed', 1);

% Hyperparameters
data.M = 50;
data.a = 2; data.b = 1;

% Changepoint
data.m = ceil(data.M*rand);

% Intensities, % !! Beware of the Gamma parametrisation !!
data.lambda = gamrnd(data.a, 1/data.b, [1 2]);

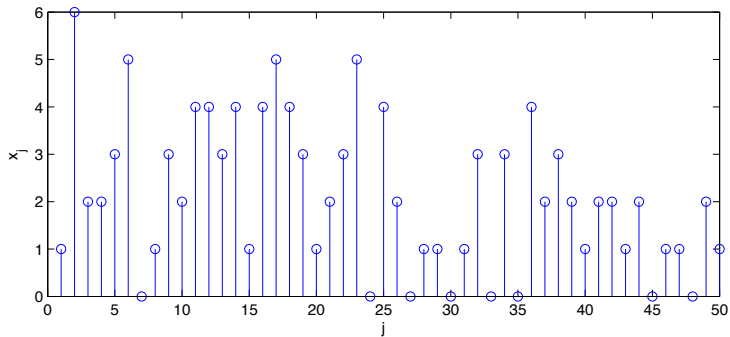
Lambda = zeros(1, M);
Lambda(1:data.m) = data.lambda(1);
Lambda((data.m+1):data.M) = data.lambda(2);

% Counts
data.x = poissrnd(Lambda);
```

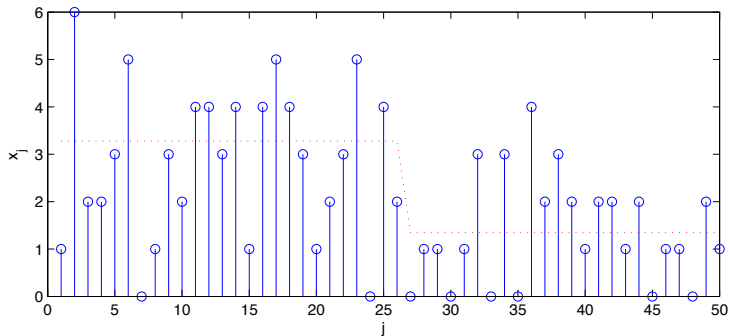
Generate data (cont.)

```
%% Visualise  
stem(data.x); xlabel('j'); ylabel('x_j')
```

A Change-point model



A Change-point model



Full Joint Density

$$\begin{aligned} p(x_{1:M}, \lambda_1, \lambda_2, m) &= p(x_{1:M} | \lambda_1, \lambda_2, m) p(\lambda_1) p(\lambda_2) p(m) \\ &= \left(\prod_{j=1}^m p(x_j | \lambda_1) \right) \left(\prod_{j=m+1}^M p(x_j | \lambda_2) \right) p(\lambda_1) p(\lambda_2) p(m) \end{aligned}$$

Full Conditional Distributions

$$\begin{aligned}\mathcal{L} &= \log p(x_{1:M} | \lambda_1, \lambda_2, m) + \log p(\lambda_1) + \log p(\lambda_2) + \log p(m) \\ &= \sum_{j=1}^m (+x_j \log \lambda_1 - \lambda_1 - \log(x_j!)) \\ &\quad + \sum_{j=m+1}^M (+x_j \log \lambda_2 - \lambda_2 - \log(x_j!)) \\ &\quad + (a-1) \log \lambda_1 - b \lambda_1 - \log \Gamma(a) + a \log b \\ &\quad + (a-1) \log \lambda_2 - b \lambda_2 - \log \Gamma(a) + a \log b - \log M\end{aligned}$$

Full Conditional Distributions

$$\begin{aligned}\log p(\lambda_1 | m, \lambda_2, x_{1:M}) &=^+ \sum_{j=1}^m (+x_j \log \lambda_1 - \lambda_1) \\ &\quad + (a - 1) \log \lambda_1 - b \lambda_1 \\ &= \left(a + \sum_{j=1}^m x_j - 1 \right) \log \lambda_1 - (m + b) \lambda_1 \\ &=^+ \log \mathcal{G}(a + \sum_{j=1}^m x_j, m + b)\end{aligned}$$

Full Conditional Distributions

$$\begin{aligned}\log p(\lambda_2 | m, \lambda_1, x_{1:M}) &=^+ \sum_{j=m+1}^M (+x_j \log \lambda_2 - \lambda_2) \\ &\quad + (a-1) \log \lambda_2 - b \lambda_2 \\ &=^+ \log \mathcal{G}(a + \sum_{j=m+1}^M x_j, M - m + b)\end{aligned}$$

Full Conditional Distributions

$$\begin{aligned}\log p(m|\lambda_1, \lambda_2, x_{1:M}) &= \sum_{j=1}^m (+x_j \log \lambda_1 - \lambda_1 - \log(x_j!)) \\ &\quad + \sum_{j=m+1}^M (+x_j \log \lambda_2 - \lambda_2 - \log(x_j!)) \\ &= + \left(\sum_{j=1}^m x_j \right) \log \lambda_1 - m\lambda_1 \\ &\quad + \left(\sum_{j=m+1}^M x_j \right) \log \lambda_2 - (M-m)\lambda_2\end{aligned}$$

The Gibbs sampler

```
% Gibbs sampler
EP = 5200; % Number of epochs
BURN_IN = 200;

% Initial state of the Markov chain
m = 10; lam = zeros(2,1);
% Storage
chain.m = zeros(1, EP-BURN_IN);
chain.lambda = zeros(2, EP-BURN_IN);
```

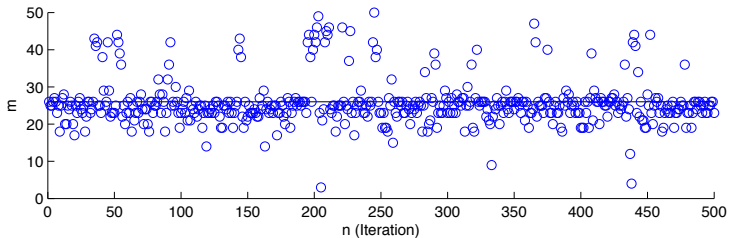
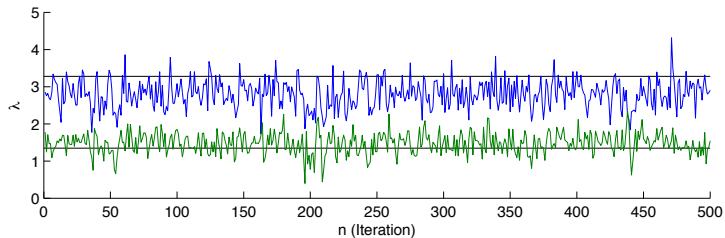
The Gibbs sampler (cont.)

```
for e=1:EP,
    % lambda ~ p(lambda | x, m)
    lam(1) = gamrnd(data.a + sum(data.x(1:m)), 1/(m+data.b) );
    lam(2) = gamrnd(data.a + sum(data.x(m+1:end)), 1/(data.M-m+d));

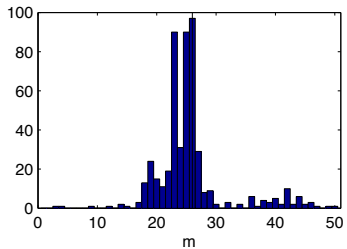
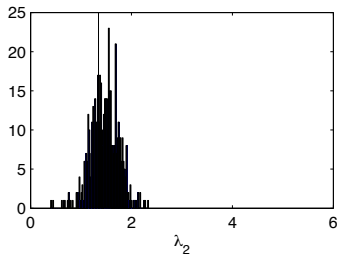
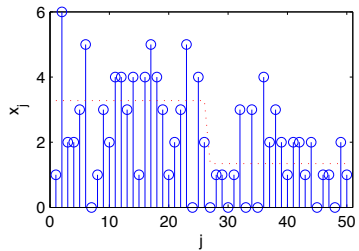
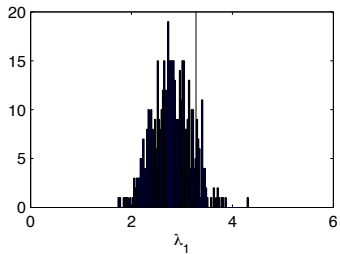
    % m ~ p(m | x, lambda)
    lp = zeros(1, data.M);
    for i=1:data.M,
        lp(i) = sum(data.x(1:i)).*log(lam(1)) - i*lam(1) +...
        sum(data.x((i+1):data.M)).*log(lam(2)) - (data.M-i)*lam(2) ;
    end;
    m = randgen(exp(lp-max(lp)));

    if e>BURN_IN,
        chain.lambda(:, e-BURN_IN) = lam;
        chain.m(1, e-BURN_IN) = m;
    end;
end;
```

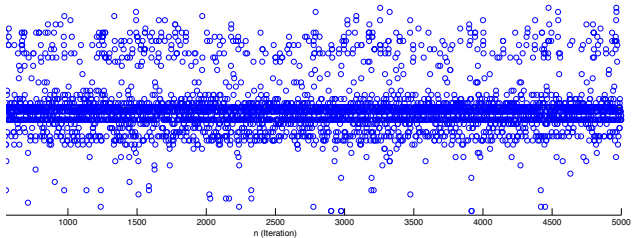
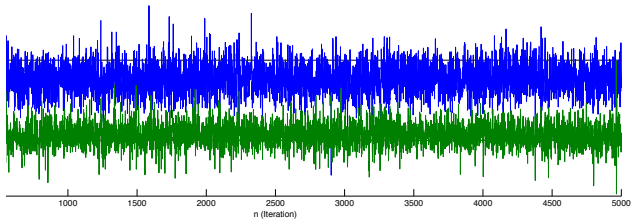
Results



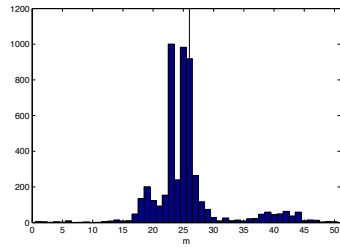
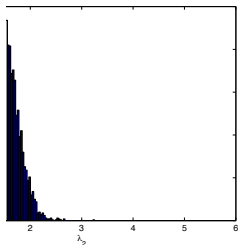
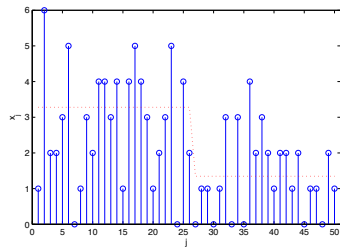
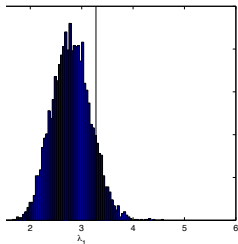
Results



Results, Longer chain



Results, Longer chain



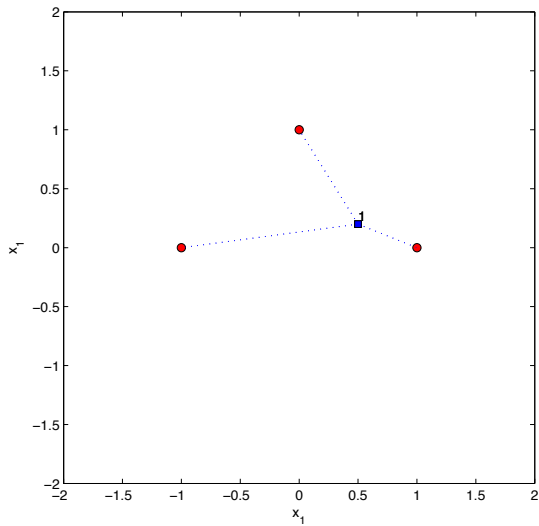
Metropolis Hastings Example

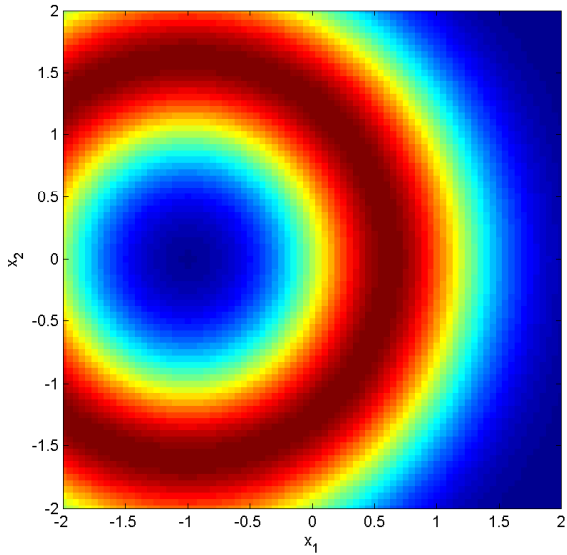
- ▶ Problem : Object position estimation from range measurements
- ▶ We have L sensors at known positions $s_j, j = 1 \dots L$, each measuring the distance of a point object with noise

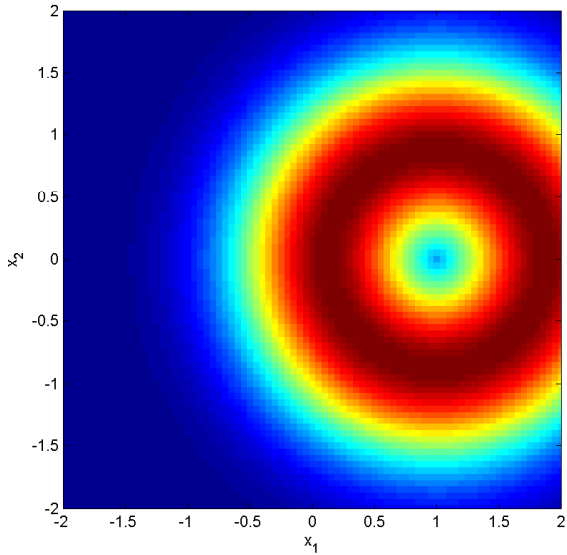
Range measurements

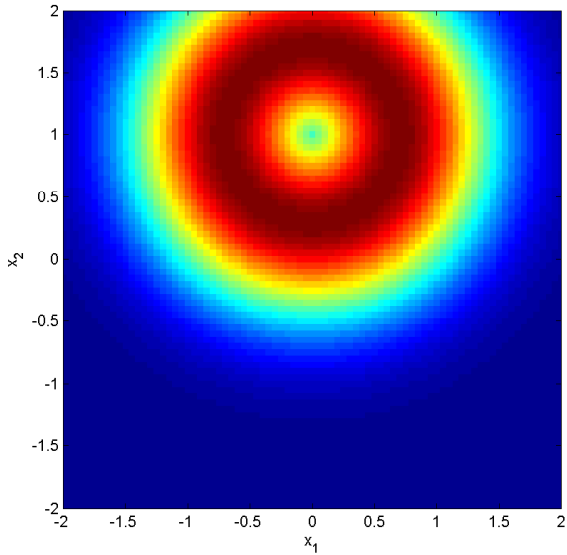
$$\begin{aligned}x &\sim p(x) \propto 1 \\ y_j|x, s_j &\sim \mathcal{N}(y_j; \|x - s_j\|, R)\end{aligned}$$

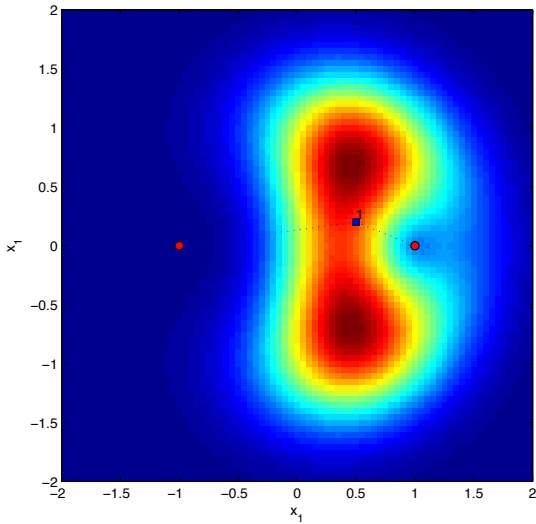
$$\|x\| \equiv \left(\sum_k x_k^2 \right)^{1/2}$$

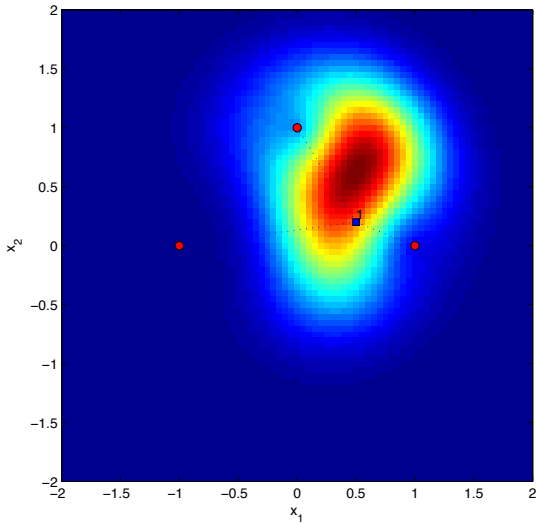












Generative Model

```
% Fix the seeds for reproducibility
randn('seed', 11); rand('seed', 1);

% Sensor positions
s = [-1 0; 1 0; 0 1]';
L = size(s, 2); % Number of sensors

M = 1; % Number of targets
x = [0.5;0.2]; % True Target position
R_r = 0.3; %% Range sensor noise variance

m_r = zeros(M, L);
for i=1:M, % For each target
    % Find the true distance from the sensor
    d = repmat(x(:,i), [1 L] ) - s;
    m_r(i, :) = sqrt(d(1,:).^2 + d(2,:).^2);
end;

y_r = sqrt(R_r)*randn(size(m_r)) + m_r;
```

Finding numerically the true posterior

```
% Prepare a uniform grid
xx = -2:0.05:2;
[X1 X2] = meshgrid(xx);

llk = zeros([size(X1) L]);

i = 1; %% Target idx, assume M = 1;
for j=1:L,
    d = sqrt((X1-s(1,j)).^2 + (X2 - s(2, j)).^2);
    llk(:, :, j) = -0.5*(d-y_r(i, j)).^2/R_r -0.5*log(2*pi*R_r);
end;
lk = sum(llk, 3);

imagesc(xx, xx, exp(lk-max(lk(:))))
```

Metropolis

```
% Metropolis
EP = 50200; % Number of epochs
BURN_IN = 200;
R_q = 0.4; % proposal variance
i = 1; % Which target ?
% Storage
chain.x = zeros(2, EP-BURN_IN);
chain.lk = zeros(1, EP-BURN_IN);
```

Metropolis (cont.)

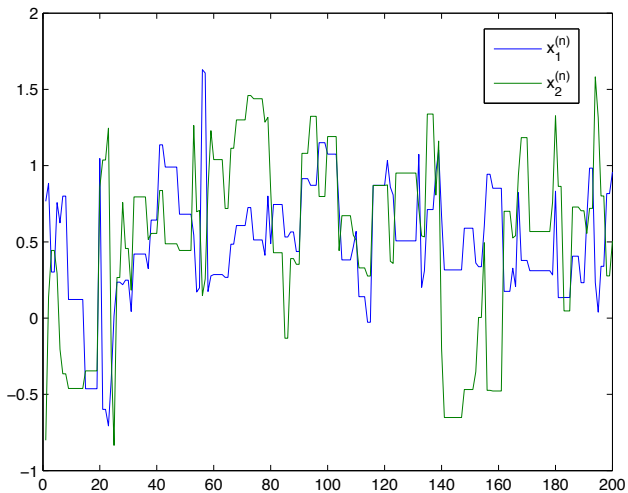
```
x_c = [0; 0]; lk = -Inf;
for e=1:EP,
    % propose a new position
    x_new = x_c + sqrt(R_q)*randn(size(x_c));
    % Evaluate the unnormalised joint posterior
    d = sqrt((x_new(1)-s(1,:)).^2 + (x_new(2) - s(2, :)).^2);
    lk_new = sum(-0.5*(d-y_r(i, :)).^2/R_r -0.5*log(2*pi*R_r));
    % Compute the log-acceptance probability
    log_a = min(0, lk_new - lk);

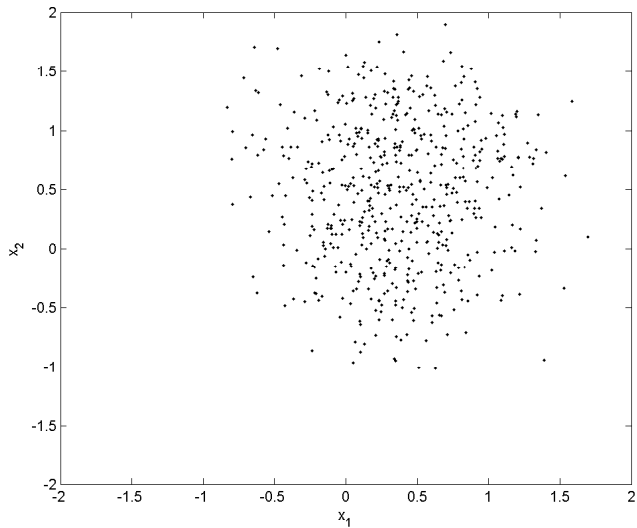
    if log(rand)<log_a, % Accept,
        x_c = x_new; lk = lk_new;
    end;    % else reject

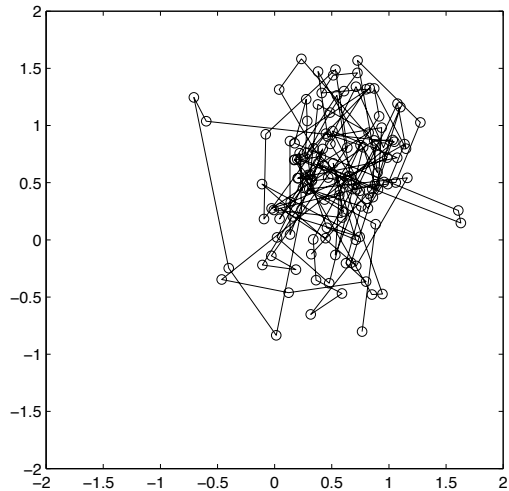
    if e>BURN_IN,
        chain.x(:, e-BURN_IN) = x_c;
        chain.lk(1, e-BURN_IN) = lk;
    end;
end;
```

Metropolis (cont.)

```
[z] = hist3(chain.x', 'ctrs', {xx',xx' });  
imagesc(xx, xx, z'); set(gca, 'ydir', 'n')  
xlabel('x_1');  
ylabel('x_2');
```







A 2-D histogram from a longer chain

