Computational Statistics - MCMC

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Group 2

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Introduction

What is MC & MC?

Markov Chain:

- Transition kernel K:

$$K(A|x) = \mathbb{P}(X_t \in A|X_{t-1} = x).$$

- This kernal then has transition density p:

$$K(A|x) = \int_A p(y|x)\mathrm{d}y$$

- The chain then has an invariant distribution Π with density $\pi(x)$:

$$\Pi(A) = \int K(A|x)\pi(x)\mathrm{d}x$$

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Monte Carlo (Integration):

- Mathematically:

$$\theta = \mathbb{E}\left[\phi(X)\right] = \int \phi(x)\pi(x)\mathrm{d}x$$

- Allows us to take a sample average:

$$\hat{\theta} = \frac{1}{n}\sum_{i=1}^{n}\phi(x_i)$$

What is MCMC?

Joining the two MCs together:

- We know a distribution, $\pi(x)$, up to some constant of proportionality.
- Construct a Markov Chain whose stationary distribution is $\pi(x)$.
- Simulate N samples, $x_1, \ldots, x_N$. Remove the burn-in period.
- Using Monte Carlo we can estimate posterior expectations and probabilities.

This is the base idea of MCMC.

Metropolis-Hastings

For some proposal density, q, we have an acceptance probability that we 'move' states of,

$$\alpha(x|y) = \min\left\{1, \frac{\pi(x)q(y|x)}{\pi(y)q(x|y)}\right\},$$

where π is the stationary distribution of our Markov chain.

Metropolis-Hastings

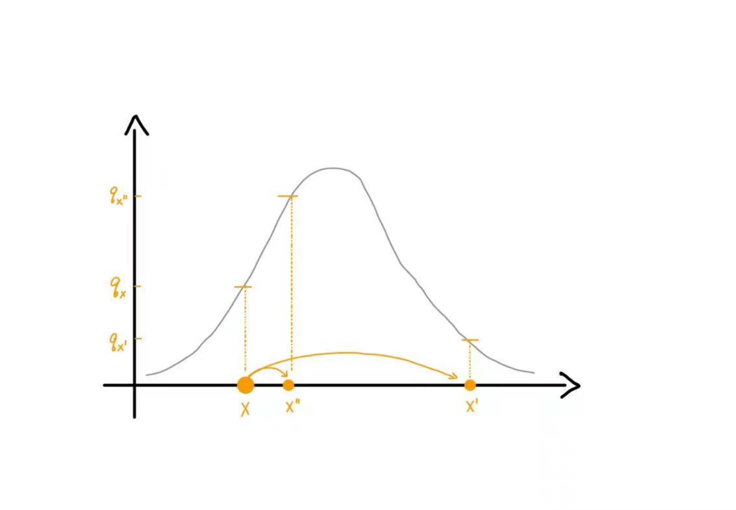

Figure 1: Proposal Distribution Illustrated

MCMC Algorithms

MCMC Algorithms

There exist a number of algorithms that can give us a proposal density for our Markov chain's dynamics.

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By using the Metropolis-Hastings algorithm we can obtain an acceptance probability for each proposed change of state within the Markov Chain.

Random Walk

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If in the current state x, the proposed next state x' is obtained using the random variable X':

$$X' = x + \epsilon$$

Where ϵ is a zero mean random variable.

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Where ϵ is a zero mean random variable.

This transition is accepted with probability $\alpha(x' \mid x)$, obtained using the Metropolis-Hastings algorithm.

Random Walk

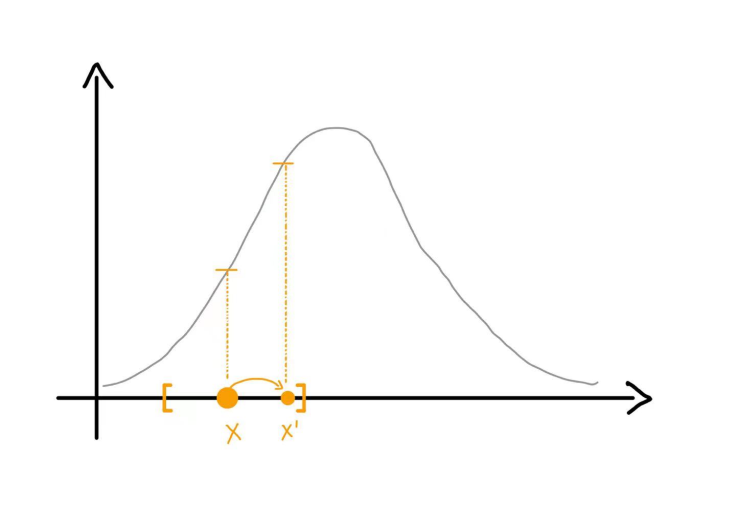

Figure 2: Visualisation of RWM

Random Walk

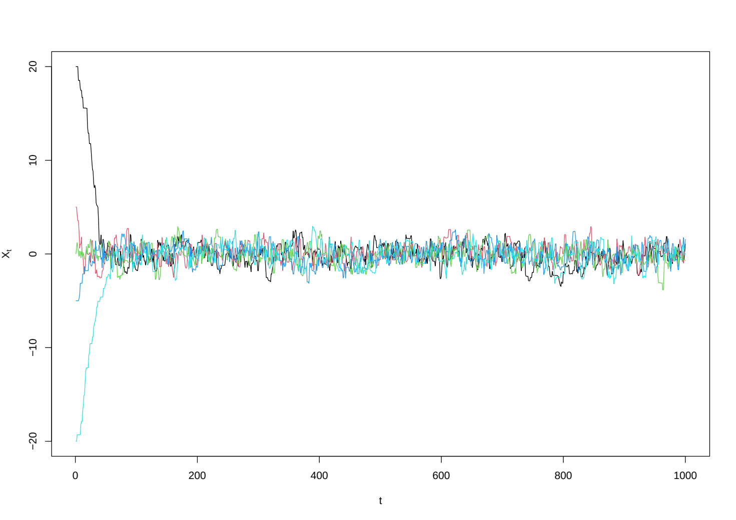

Figure 3: Trace plot of RW for N(0,1) with starting values: 20,5,0,-5,-20

Random Walk

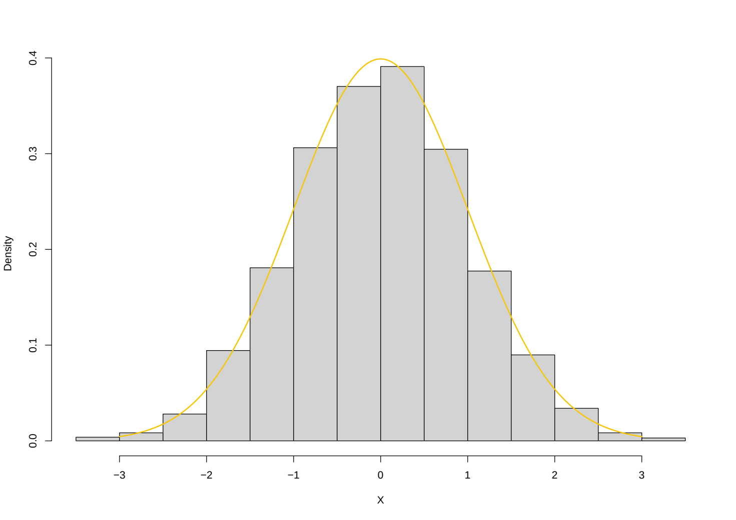

Figure 4: Histogram of RW for N(0,1)

Metropolis-adjusted Langevin algorithm

Even with appropriately tuned parameters, RWM proposes a new state x' at random.

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If we instead, try to model our Markov chain as a discretised Langevin diffusion, we can use Langevin dynamics to propose a new state based upon a random walk displaced by some factor of the gradient of the proposed density.

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If we instead, try to model our Markov chain as a discretised Langevin diffusion, we can use Langevin dynamics to propose a new state based upon a random walk displaced by some factor of the gradient of the proposed density.

$$x' = x + \frac{h}{2}\nabla log(\pi(x)) + \sqrt{h}\epsilon_t$$

Where $\epsilon_t \sim \mathcal{N}(0, 1)$.

Metropolis-adjusted Langevin algorithm

If at every timepoint we were to select the proposed x' then we would be carrying out the Unadjusted Langevin Algorithm (ULA).

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If at every timepoint we were to select the proposed x' then we would be carrying out the Unadjusted Langevin Algorithm (ULA).

Whilst not producing samples exactly from the proposed density $\pi(x)$ it is particularly useful in Big Data settings.

If were instead to accept the proposed x' with probability α (obtained from using the MH algorithm) we would be using the Metropolis-adjusted Langevin algorithm which does sample from the proposed density $\pi(x)$.

$$q\left(x' \mid x\right) = N\left(x'; x + \frac{h}{2}\nabla \log \pi(x), h\right)$$

Metropolis-adjusted Langevin algorithm

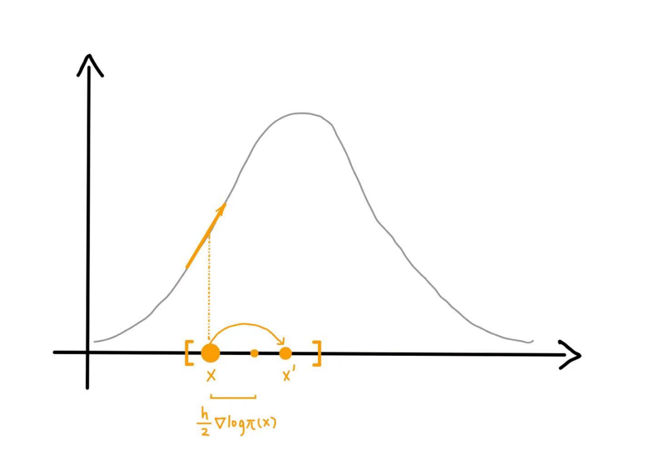

Figure 5: MALA Visualisation

Metropolis-adjusted Langevin algorithm

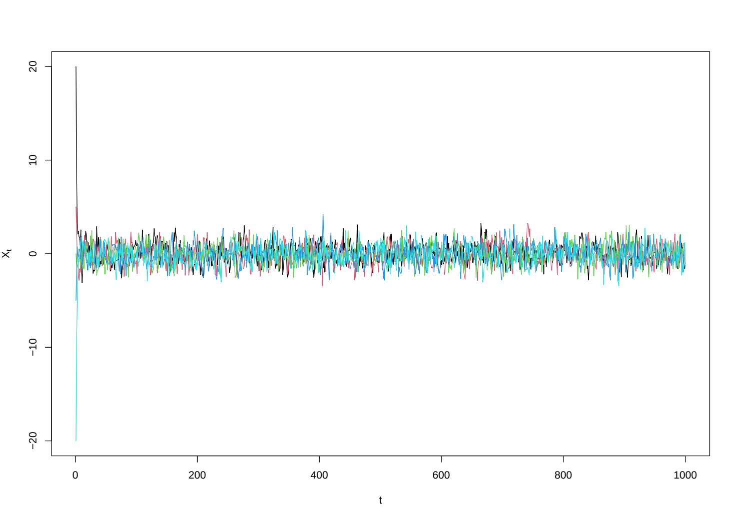

Figure 6: Trace plot of MALA for N(0,1) with starting values: 20,5,0,-5,-20

Metropolis-adjusted Langevin algorithm

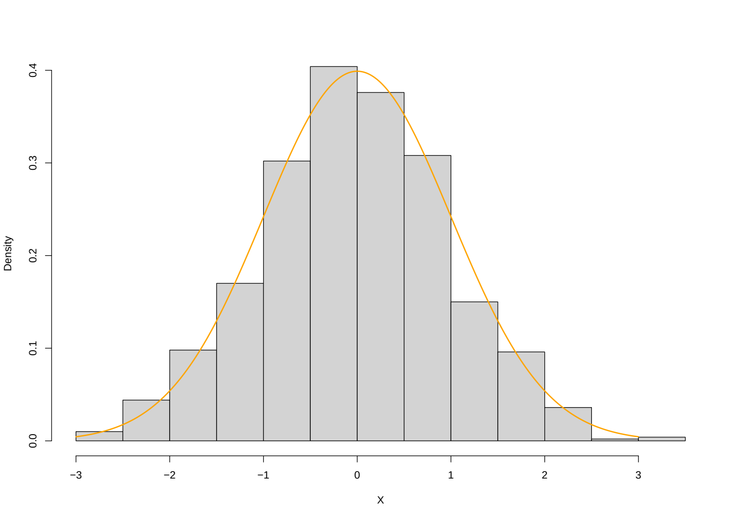

Figure 7: Histogram of MALA for N(0,1)

Gibbs Sampling

For $x = (x_1, x_2, ..., x_d)$ the joint distribution of x may be complicated. But if some conditional distributions are known this can be taken advantage of.

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We make a proposal of

$$q(x' \mid x) = \pi(x_i \mid x_{-i})$$

.

Gibbs Sampling

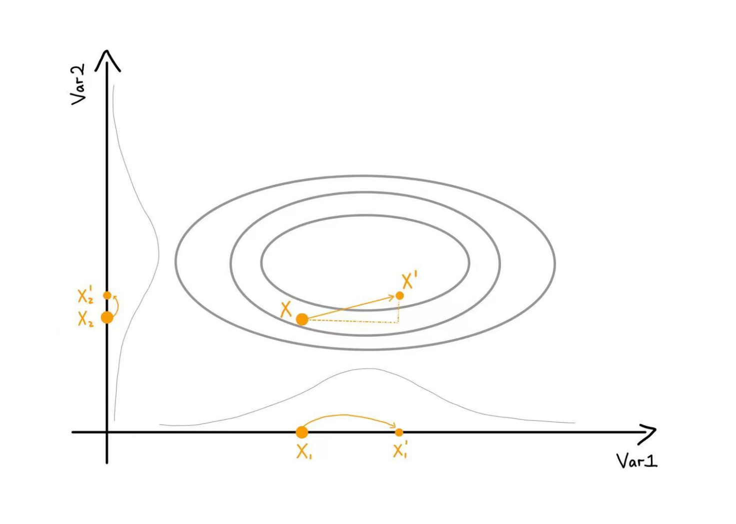


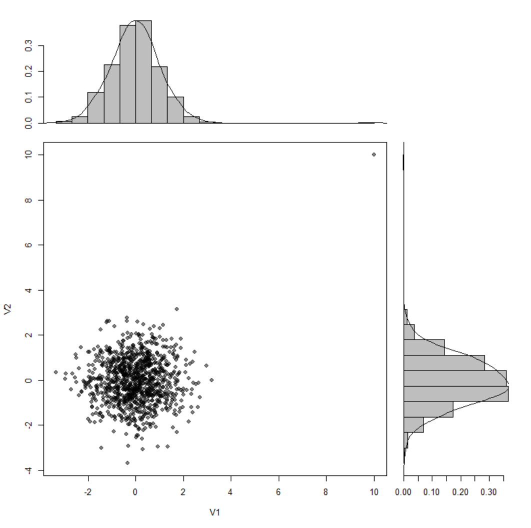
Figure 8: Gibbs Visualisation

Gibbs Sampling

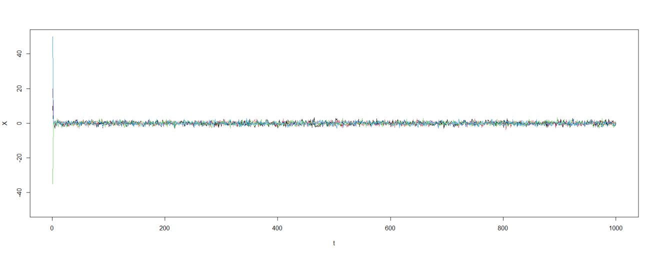
In the context of Metropolis-Hastings the acceptance probability is always 1.

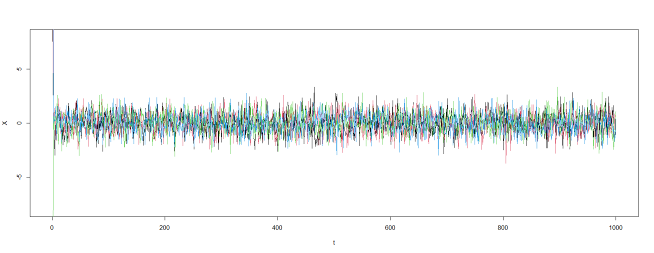
$$
\begin{aligned}
\alpha(x' \mid x) &= \min\left\{1, \frac{\pi(x')q(x \mid x')}{\pi(x)q(x' \mid x)}\right\} \\
\alpha(x_i \mid x_{-i}) &= \min\left\{1, \frac{\pi(x_i)\pi(x_{-i} \mid x_i)}{\pi(x_{-i})\pi(x_i \mid x_{-i})}\right\} \\
&= \min\left\{1, \frac{\pi(x_i) \times \frac{\pi(x_{-i}, x_i)}{\pi(x_i)}}{\pi(x_{-i}) \times \frac{\pi(x_i, x_{-i})}{\pi(x_-i)}}\right\} \\
&= \min\left\{1, \frac{\pi(x)}{\pi(x)}\right\} \\
&= 1
\end{aligned}
$$

Gibbs Sampling-Implementation

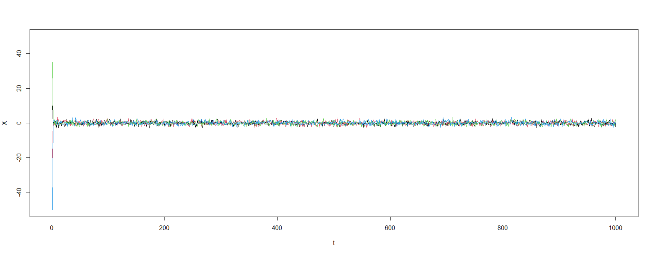


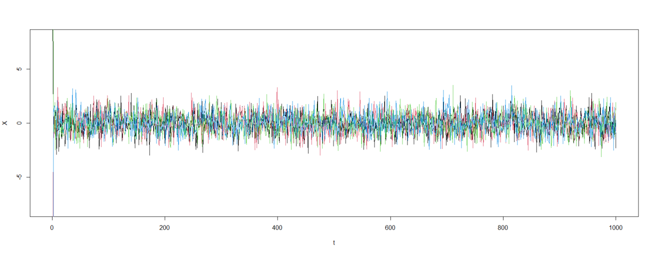
Gibbs Sampling-Implementation X_1





Gibbs Sampling-Implementation X_2

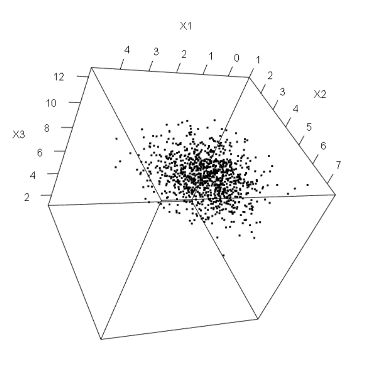




Gibbs Sampling - 3D case

$$\mu = \begin{pmatrix} 2 \\ 5 \\ 10 \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} 1 & 0.5 & 0.2 \\ 0.5 & 1 & 0.4 \\ 0.2 & 0.4 & 1 \end{pmatrix}$$



Comparisons

Target Distribution

In order to test the limitations of each of the algorithms, we trial them using a number of different target distributions:

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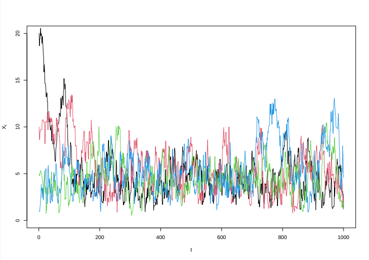
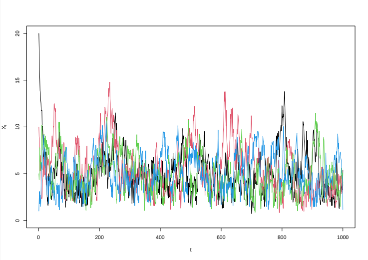
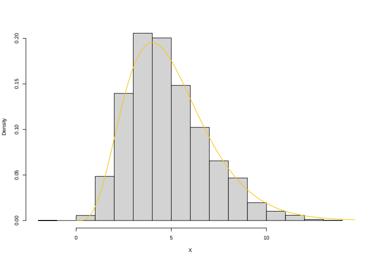
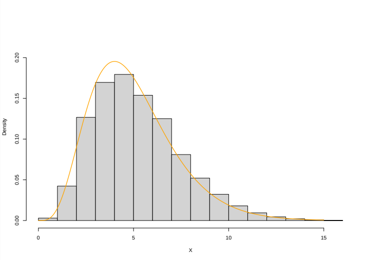
- Skewed distribution
- Heavy tailed distribution
- Multi-mode distribution

Target Distribution: Gamma(5,1)

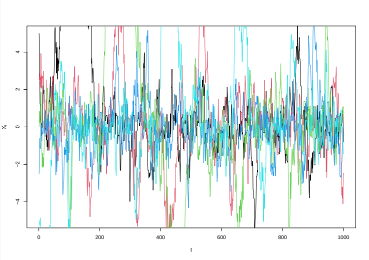


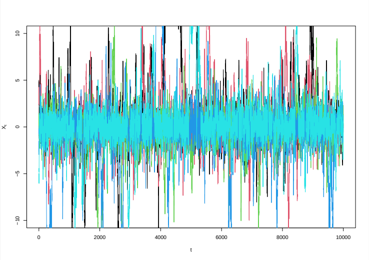


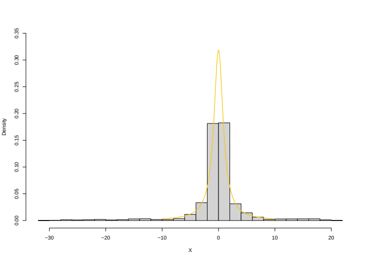


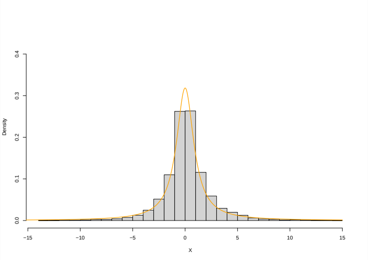


Target Distribution: Student t(1)

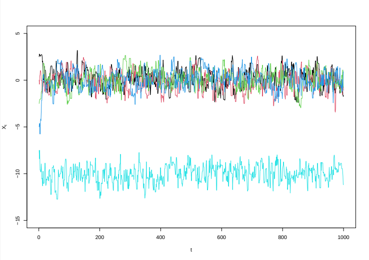


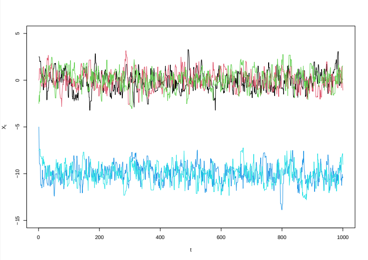


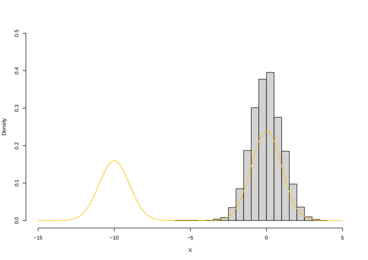


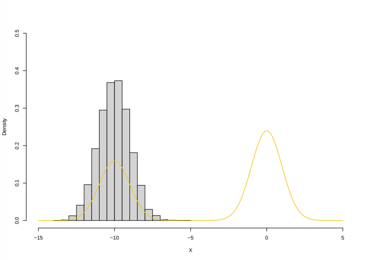


Target Distribution: Bimodal(-10,0) - RW

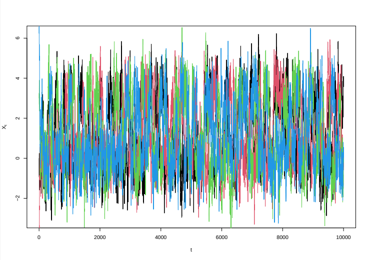


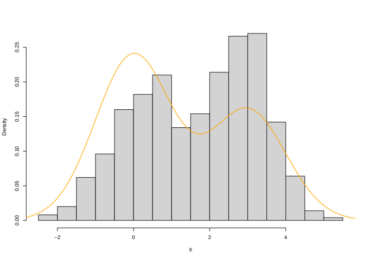


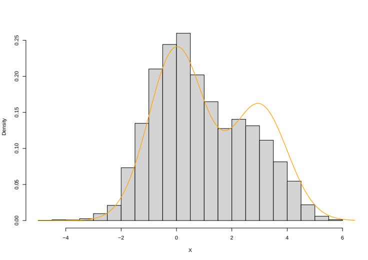


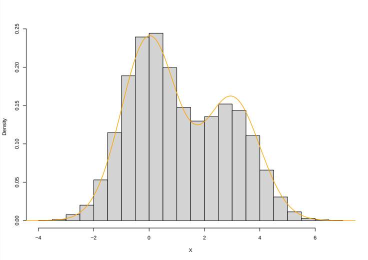


Target Distribution: Bimodal(0,3) - MALA

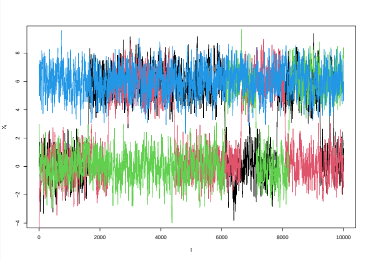


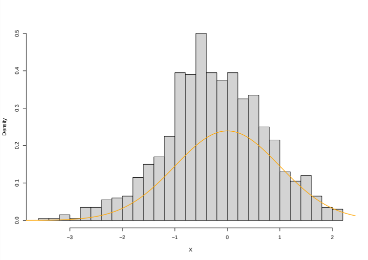


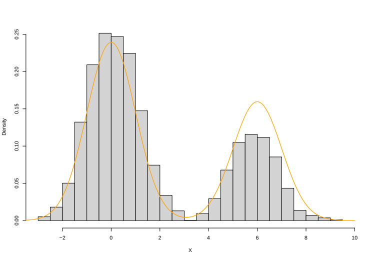


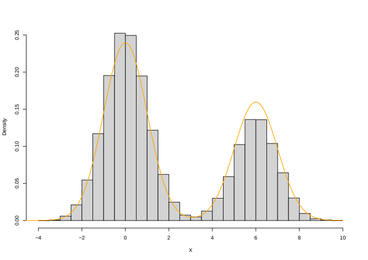


Target Distribution: Bimodal(0,6) - MALA

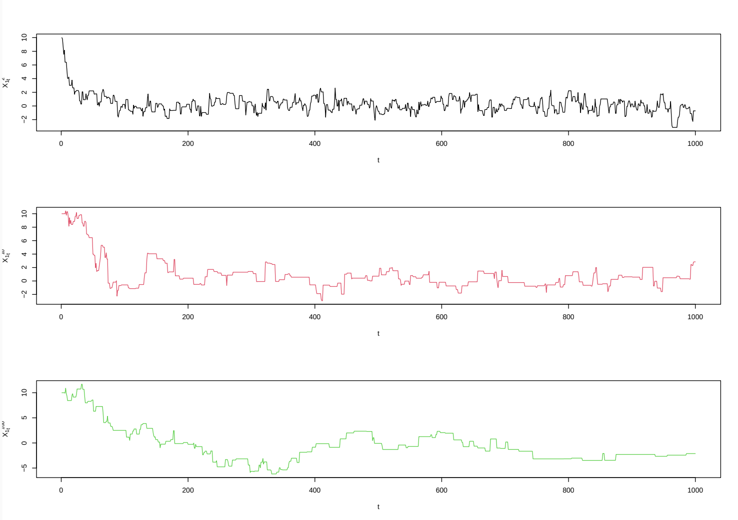




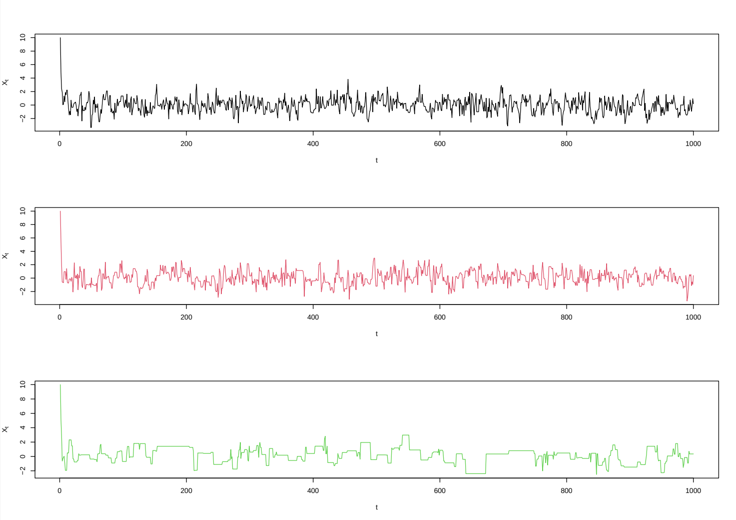




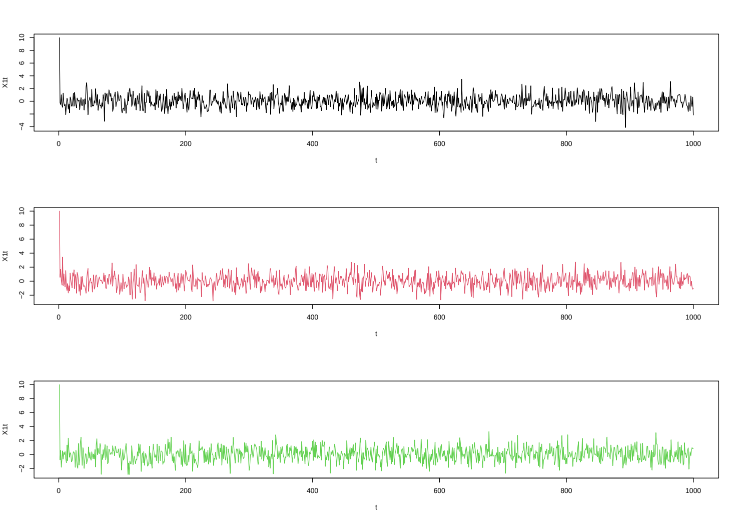
Dimensions: RW d=2,10,100



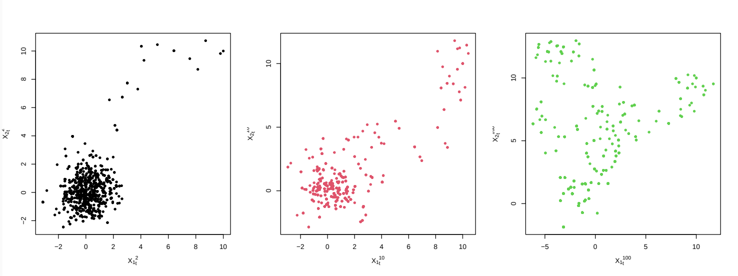
Dimensions: MALA d=2,10,100



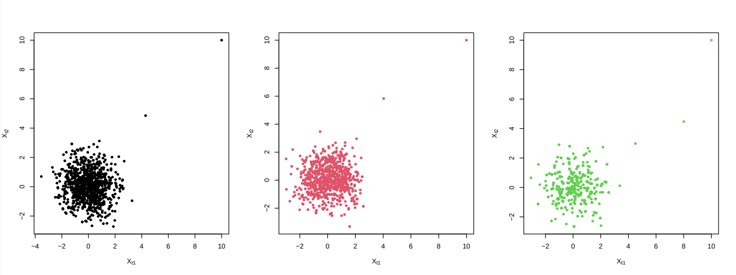
Dimensions: Gibbs d=2,10,100



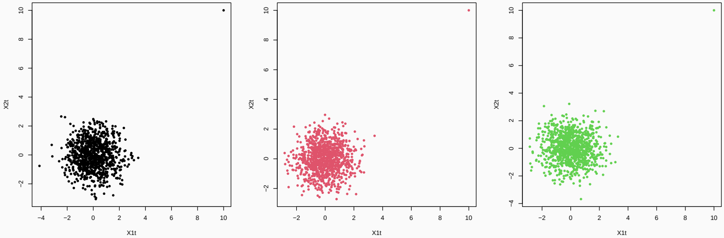
Dimensions: RW d=2,10,100



Dimensions: MALA d=2,10,100



Dimensions: Gibbs d=2,10,100



Convergence Diagnostics

Asymptotic Distribution

CLT for Markov Chain:

$$\sqrt{n}\left(\frac{1}{n}\sum_{i=1}^{n} g\left(X_i\right) - \mathrm{E}(g(X))\right) \xrightarrow{d} N\left(0, \sigma^2\right) \quad (n \to \infty)$$

$$\begin{aligned}\sigma^2 &= \operatorname{Var}\left(g\left(X_0\right)\right) + 2\sum_{k=1}^{\infty} \operatorname{cov}\left(g\left(X_0\right), g\left(X_k\right)\right) \\ &= \operatorname{Var}(g(X_0)[1 + 2\sum_{k=1}^{\infty} \operatorname{corr}(g(X_0), g(X_k))]\end{aligned}$$

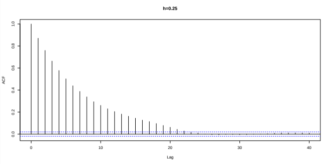
Effective Sample Size

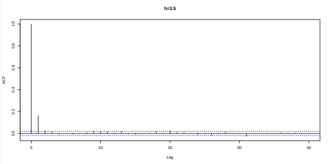
Size k of an iid sample $Y_1, \ldots Y_k \sim f$ whose average $\frac{1}{k}\sum_{i=1}^{k} g(Y_i)$ has the same variance as $\frac{1}{n-b}\sum_{i=1}^{k} g(X_i)$

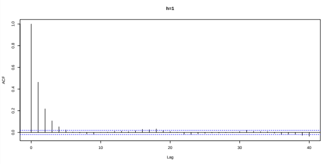
$$k = \frac{n-b}{1 + 2\sum_{k=1}^{\infty} \operatorname{corr}\left(g\left(X_0\right), g\left(X_k\right)\right)}$$

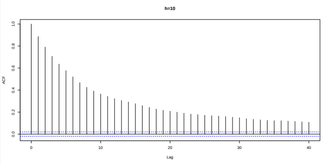
Step Size Tuning: MALA

```
h: 0.25 ESS: 686.5147 Accept Rate: 0.9916
h: 1 ESS: 3433.997 Accept Rate: 0.9266
h: 3.5 ESS: 7196.557 Accept Rate: 0.5604
h: 10 ESS: 325.0788 Accept Rate: 0.1602
```

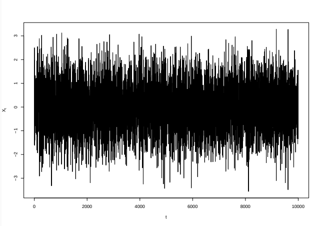


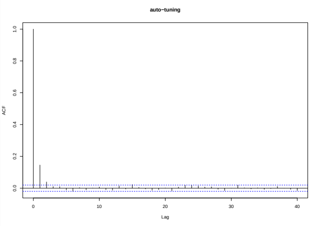






Step Size Tuning: MALA





$$h_{k+1} = h_k + \frac{h_k}{k}(R_k - \hat{\alpha})$$

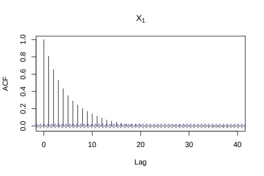
$$\hat{\alpha} \approx 0.576$$

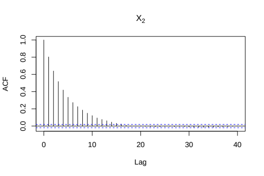
$$\hat{h} \approx 3.3401$$

Figure 9: Starting h = 10, Effective sample size = 7187

Correlation

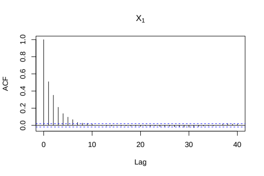
RW

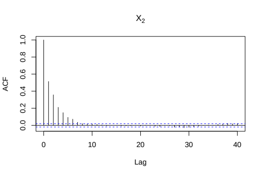




ESS: X1=1054; X2=1077;

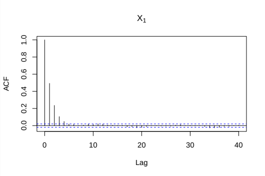
MALA

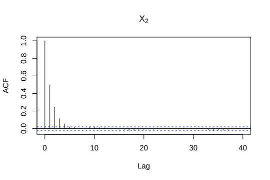




ESS: X1=2530; X2=2481;

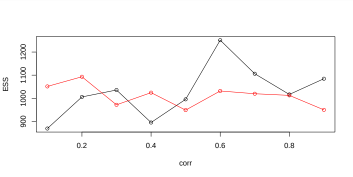
Gibbs

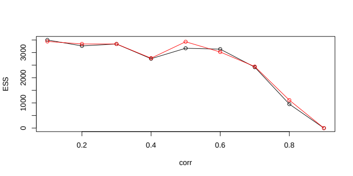


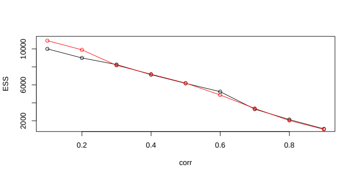


ESS: X1=3396; X2=3344;

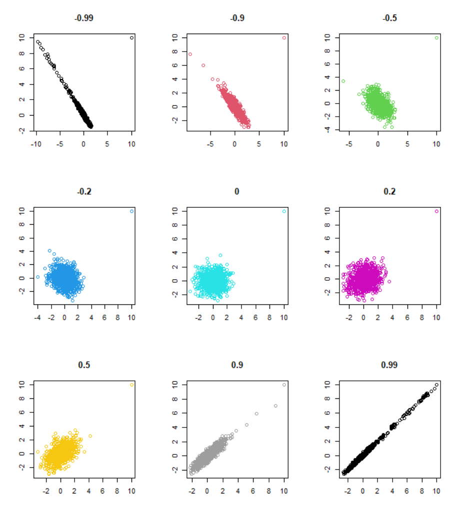
Correlation







Gibbs Sampling with High Correlation



X_1	X_2
24.09	19.48
125.55	113.87
692.36	610.60
1000.00	907.24
1119.07	1000.00
858.51	1000.00
539.68	620.75
109.73	84.94
9.26	9.29

Conclusion

Summary

- Implementation of RWM, MALA, Gibbs Sampler.
- Experimentation with dimensionality, correlation of variables, target distributions, hyper-parameter tuning.
- Further research directions.
    - Hamiltonian Dynamics - HMC, NUTS

Thank you for listening. Questions?