# BML. 3. Intro to MCMC From Gibbs to Hamilton

DataLab CSIC

# Brief description

1. presented key methods in Bayesian inference and basic models and faced ‘severe’ computational problems quite rapidly (beta-binomial, logistic regression)

2. overviewed Bayesian computational strategies

3. Will focus on MCMC (Markov chain Monte Carlo): Gibbs, Metropolis, Hybrid, Hamiltonian.

Other stuff, including SG-MCMC later on

# Computational problems in Bayesian analysis

Computing the posterior

$$f(\theta|x) = \frac{f(x|\theta)\, f(\theta)}{f(x)} = \frac{f(x|\theta)\, f(\theta)}{\int f(x|\theta)\, f(\theta)\, d\theta} \propto f(x|\theta)\, f(\theta)$$

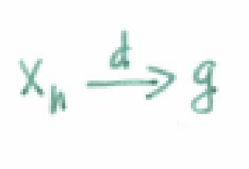
Computing posterior expectations

$$\int h(\theta)\, f(\theta|x)\, d\theta$$

$$\frac{1}{N} \sum_{i=1}^{n} h(\theta_i) \qquad \theta_i \sim f(\theta|x)$$

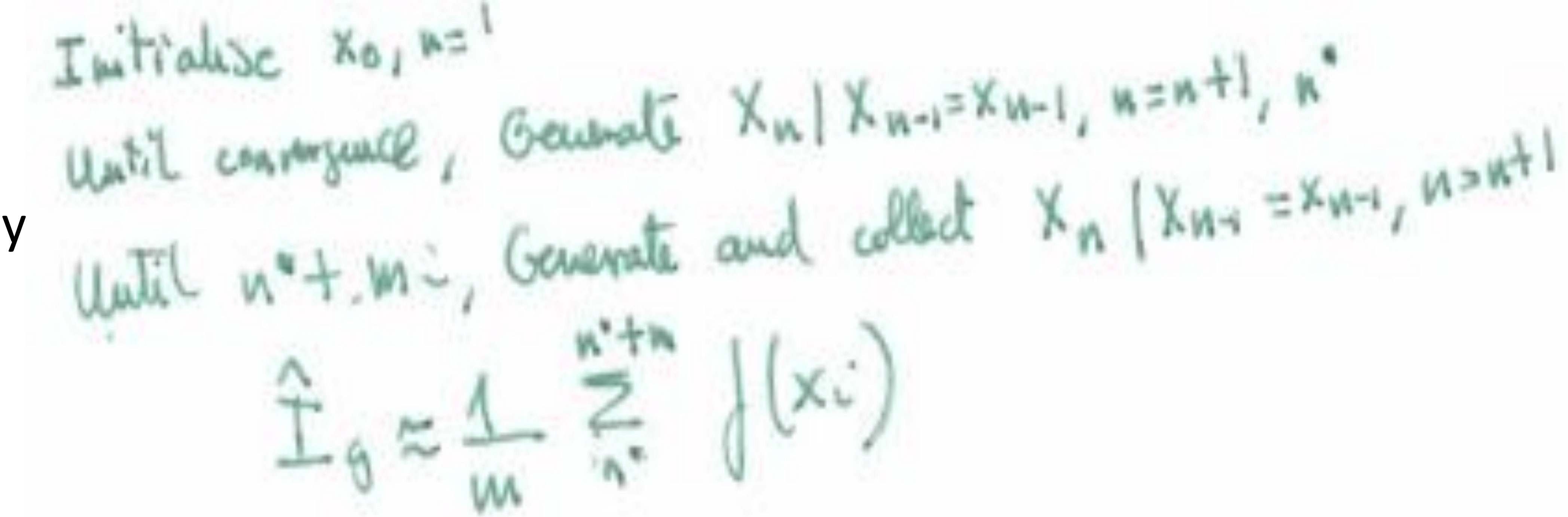
# General idea MCMC

Markov chain $X_n$ with same state space as target and convergent to target distribution g



$$x_n \xrightarrow{d} g$$

Strategy



```
Initialise $x_0$, $n=1$
Until convergence, Generate $X_n | X_{n-1}=x_{n-1}$, $n=n+1$, $n^*$
Until $n^*+m$, Generate and collect $X_n | X_{n-1}=x_{n-1}$, $n=n+1$
```

$$\hat{I}_g \approx \frac{1}{m}\sum_{n^*}^{n^*+m} f(x_i)$$

# a. Gibbs sampling

# Sources

French and DRI  (2000) Ch 7

DRI et al (2010) Ch4

BDA3 (2015) Ch11, 12

Hoff (2009) Ch 6,7

# Labs

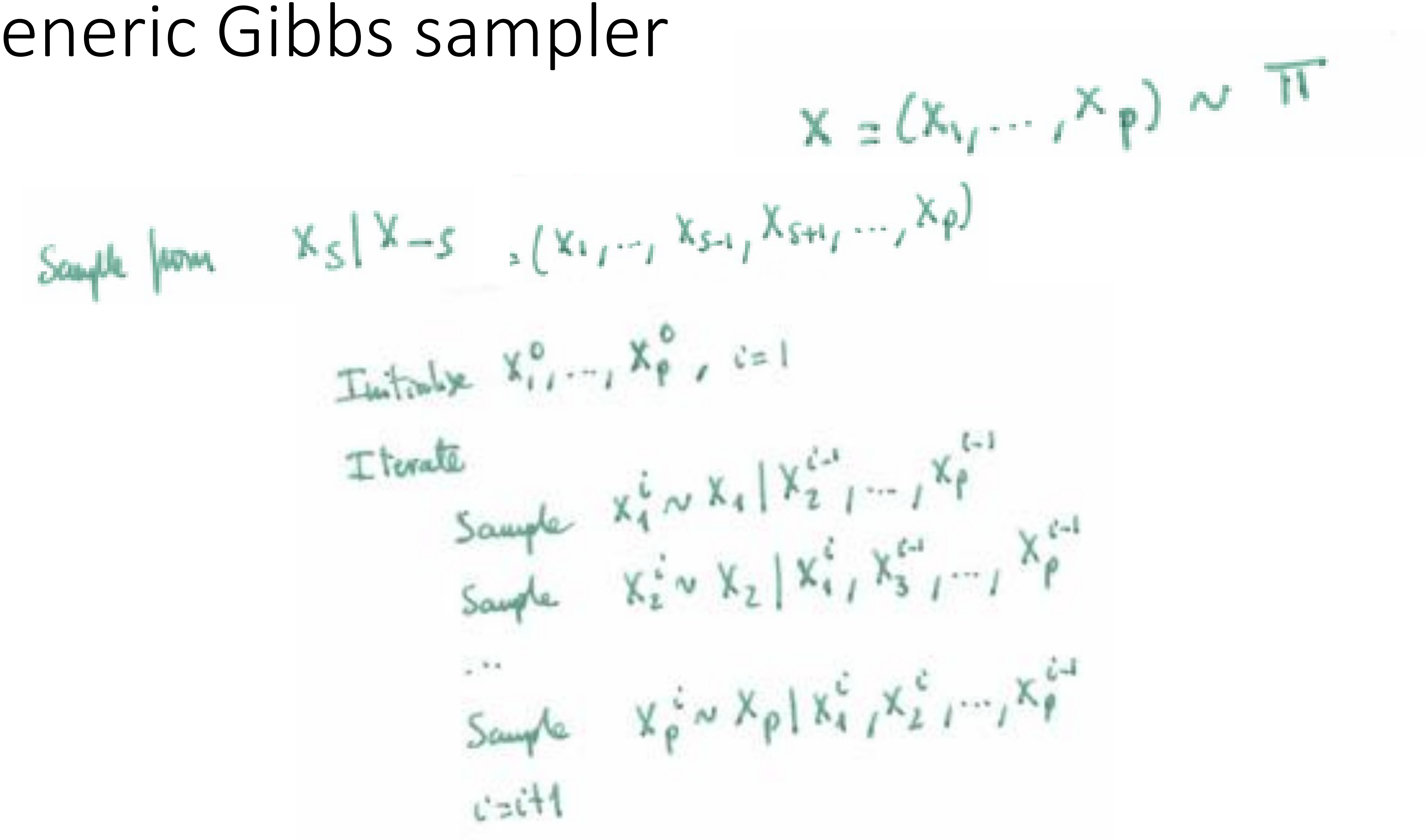
3.1 Gibbs

Basic, Re-usable,Paralel chains

Multivariate normal

Normal-gamma inverse

# Generic Gibbs sampler



$X = (X_1, \dots, X_p) \sim \pi$

Sample from $X_s | X_{-s} = (X_1, \dots, X_{s-1}, X_{s+1}, \dots, X_p)$

```
Initialize $X_1^0, \dots, X_p^0$, $i = 1$
Iterate
    Sample $X_1^i \sim X_1 | X_2^{i-1}, \dots, X_p^{i-1}$
    Sample $X_2^i \sim X_2 | X_1^i, X_3^{i-1}, \dots, X_p^{i-1}$
    ...
    Sample $X_p^i \sim X_p | X_1^i, X_2^i, \dots, X_p^{i-1}$
    $i = i + 1$
```

# Important Gibbs sampling examples

# Purpose

Through several important examples reinforce Gibb sampling concept

Motivation

Model and prior

Posterior conditionals

Gibbs sampler

Use

(Many implemented in labs)

# Sampling the bi-variate normal

Simple example to recall approach

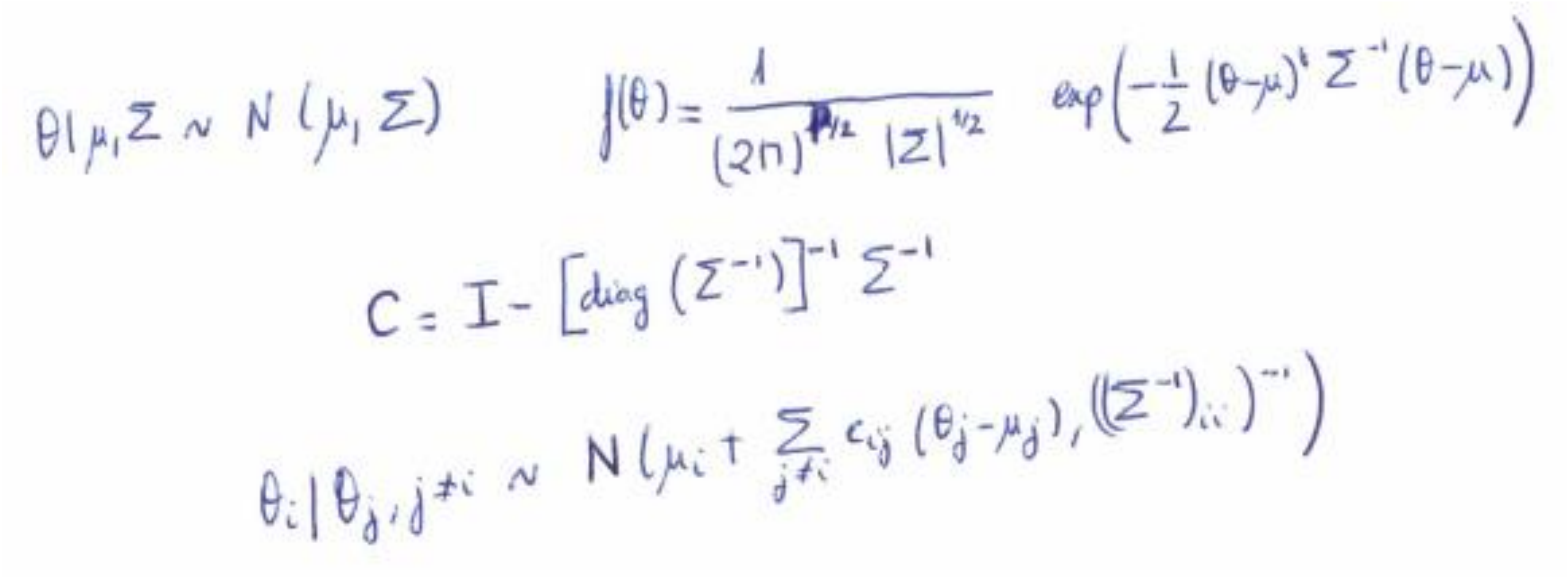
**Model**. Bivariate normal with unknown means. Variances 1. Known correlation $\varrho$

1 observation

Prior. Uniform

**Use**. Expected value and variance of parameters, Expected cross product, Probability that parameter belongs to a set

# Auxiliary result (eg Handbook of the Normal Distribution)



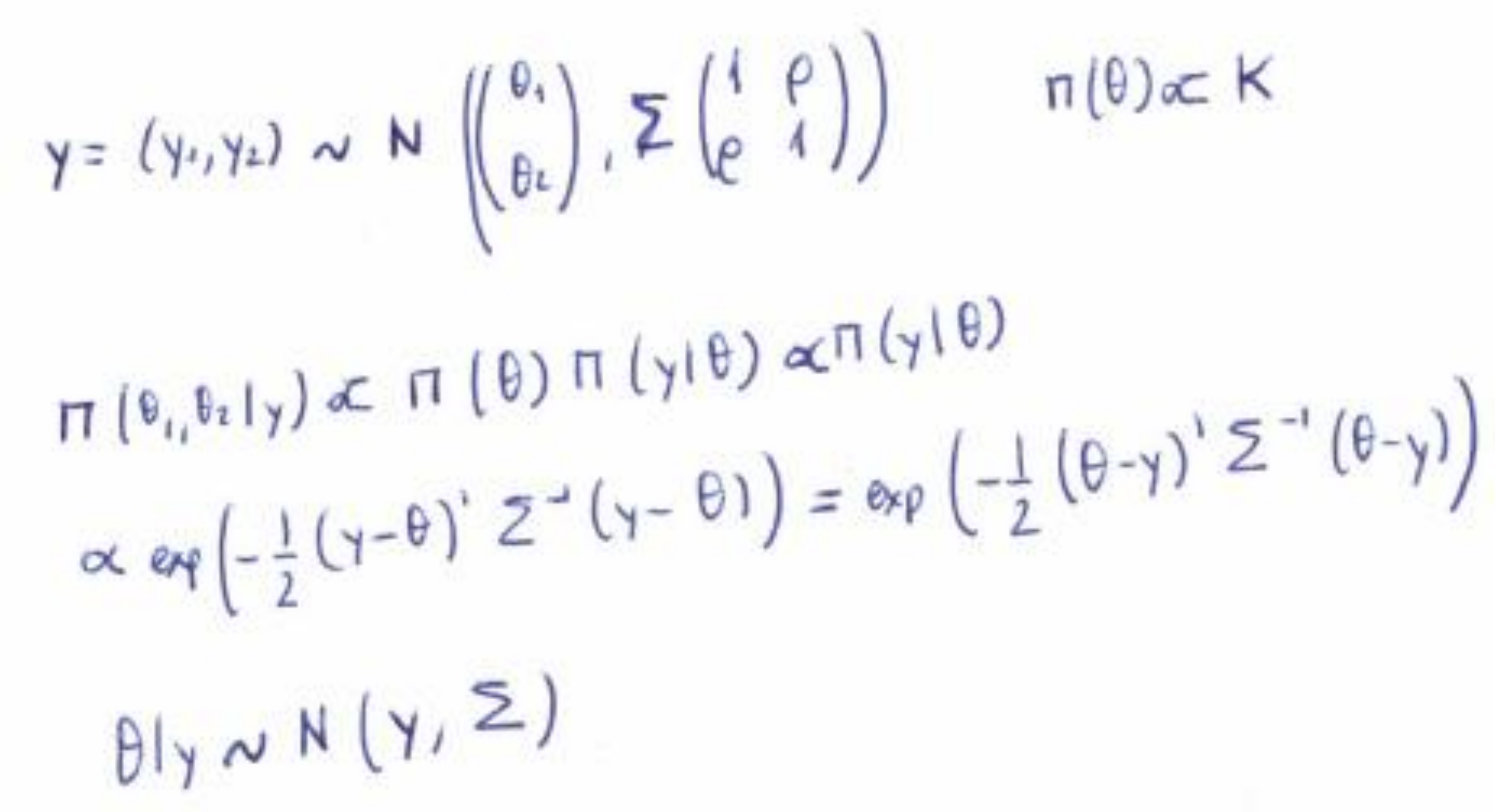
$\theta | \mu, \Sigma \sim N(\mu, \Sigma)$

$$f(\theta) = \frac{1}{(2\pi)^{p/2} \, |\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\theta-\mu)' \Sigma^{-1} (\theta-\mu)\right)$$

$$C = I - \left[\mathrm{diag}(\Sigma^{-1})\right]^{-1} \Sigma^{-1}$$

$$\theta_i | \theta_j, j \neq i \sim N\left(\mu_i + \sum_{j \neq i} c_{ij} (\theta_j - \mu_j), ((\Sigma^{-1})_{ii})^{-1}\right)$$

# Sampling the bi-variate normal. Model and posterior



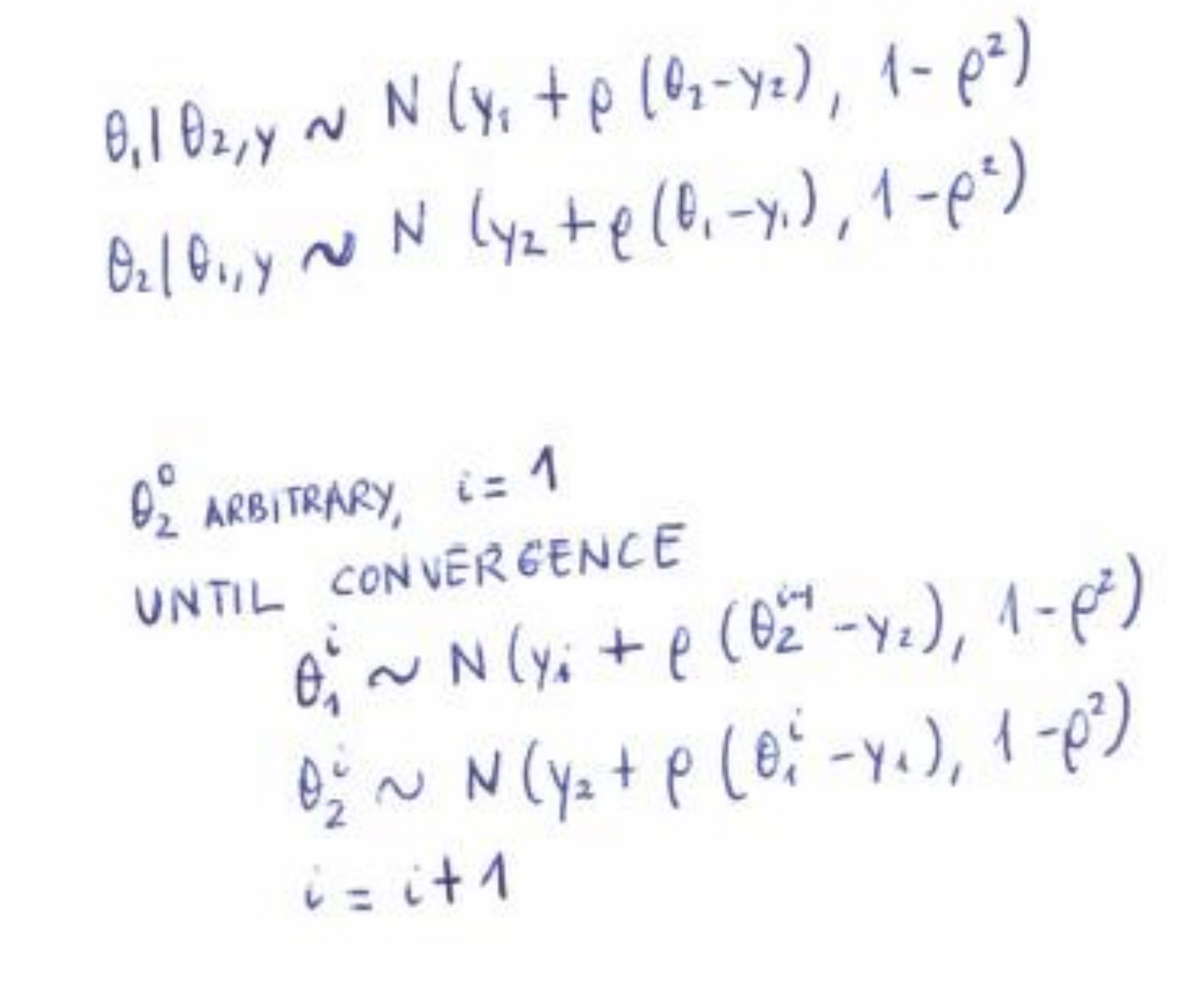
$$y = (y_1, y_2) \sim N\left(\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix}, \Sigma\begin{pmatrix}1 & \rho\\ \rho & 1\end{pmatrix}\right) \qquad \pi(\theta) \propto K$$

$$\pi(\theta_1, \theta_2 | y) \propto \pi(\theta)\,\pi(y|\theta) \propto \pi(y|\theta)$$

$$\propto \exp\left(-\frac{1}{2}(y-\theta)'\,\Sigma^{-1}(y-\theta)\right) = \exp\left(-\frac{1}{2}(\theta-y)'\,\Sigma^{-1}(\theta-y)\right)$$

$$\theta | y \sim N(y, \Sigma)$$

# Sampling the bi-variate normal. Gibbs sampler

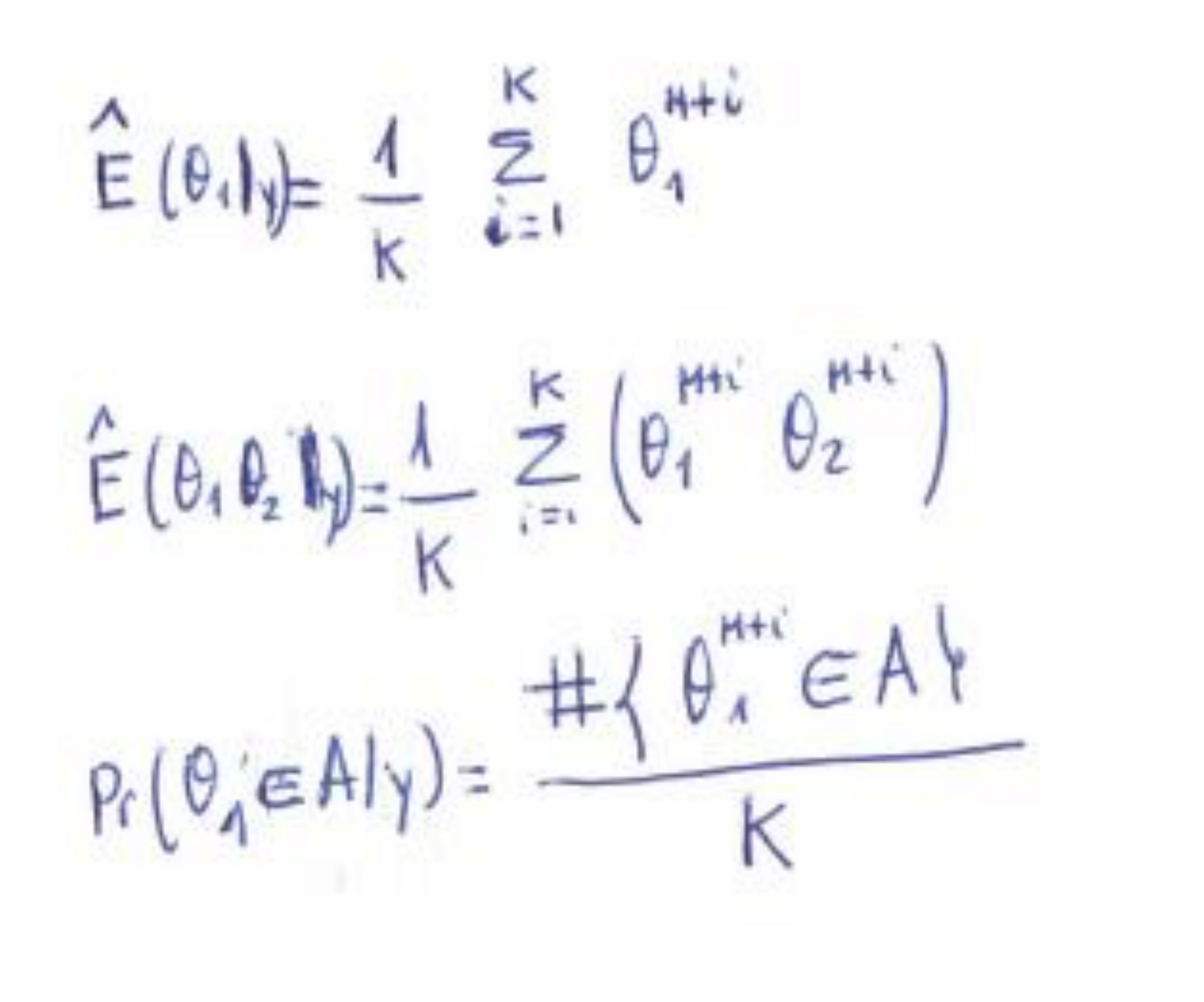


$$\theta_1 \mid \theta_2, y \sim N\left(y_1 + \rho\,(\theta_2 - y_2),\ 1 - \rho^2\right)$$

$$\theta_2 \mid \theta_1, y \sim N\left(y_2 + \rho\,(\theta_1 - y_1),\ 1 - \rho^2\right)$$

```
$\theta_2^0$ ARBITRARY, $i = 1$
UNTIL CONVERGENCE
    $\theta_1^i \sim N(y_1 + \rho\,(\theta_2^{i-1} - y_2),\ 1 - \rho^2)$
    $\theta_2^i \sim N(y_2 + \rho\,(\theta_1^i - y_1),\ 1 - \rho^2)$
    $i = i + 1$
```

# Sampling the bi-variate normal. Answers



$$\hat{E}(\theta_1|y) = \frac{1}{K}\sum_{i=1}^{K} \theta_1^{M+i}$$

$$\hat{E}(\theta_1\theta_2|y) = \frac{1}{K}\sum_{i=1}^{K}\left(\theta_1^{M+i}\;\theta_2^{M+i}\right)$$

$$Pr(\theta_1^{i} \in A|y) = \frac{\#\{\theta_1^{M+i} \in A\}}{K}$$

# Inference for normal-gamma

A very important example. Analytic solution available. Serves as benchmark

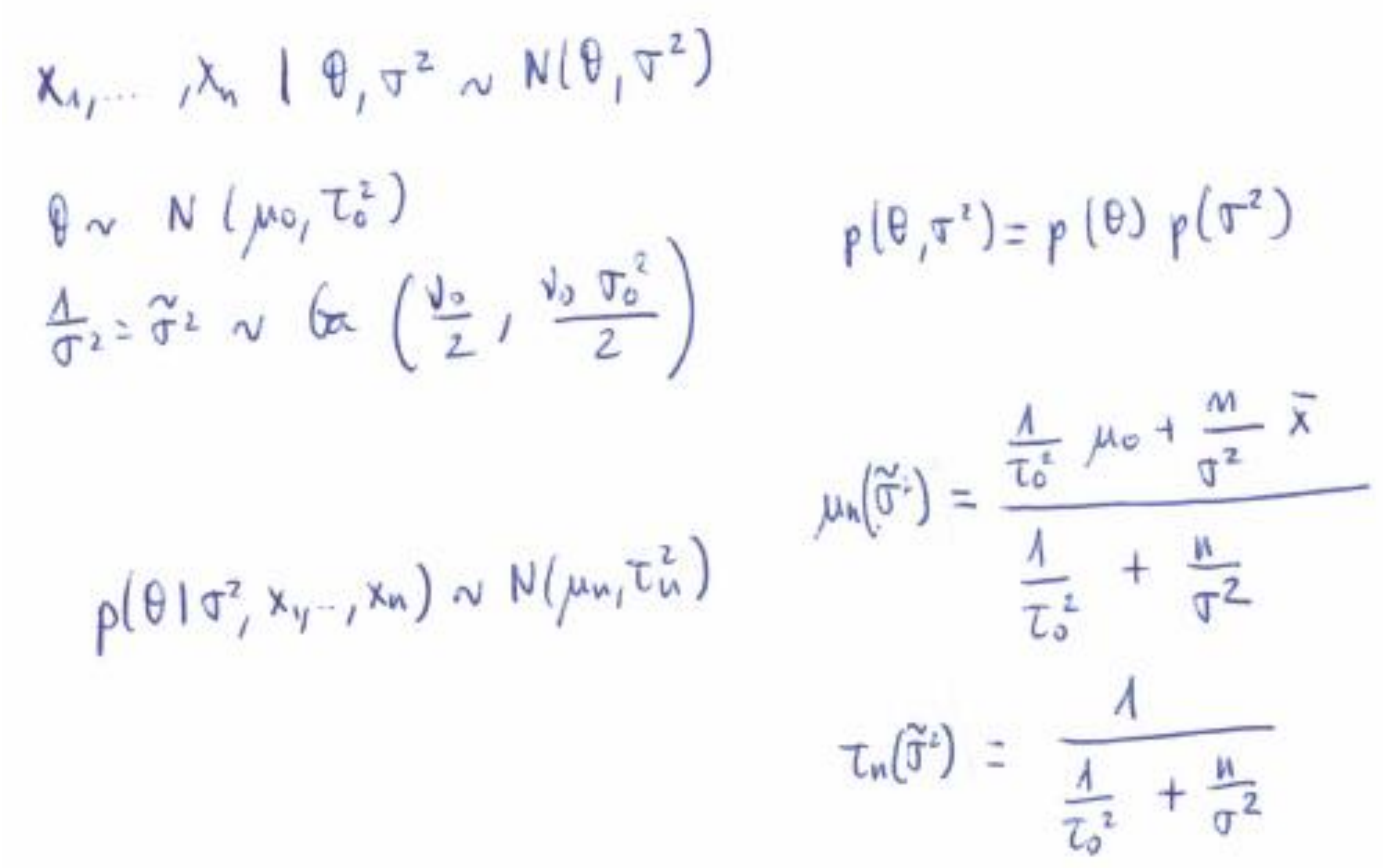
**Model**. Normal with unknown mean and variance.  Prior normal-gamma.

**Use.** Quartiles of mean, Interval of probability 0.7, Test null that mean is bigger than 0

https://en.wikipedia.org/wiki/Inverse-gamma_distribution

https://en.wikipedia.org/wiki/Normal-inverse-gamma_distribution

# Inference for normal-gamma. Model



$$X_1, \dots, X_n \mid \theta, \sigma^2 \sim N(\theta, \sigma^2)$$

$$\theta \sim N(\mu_0, \tau_0^2)$$

$$\frac{1}{\sigma^2} = \tilde{\sigma}^2 \sim Ga\left(\frac{\nu_0}{2}, \frac{\nu_0 \sigma_0^2}{2}\right)$$

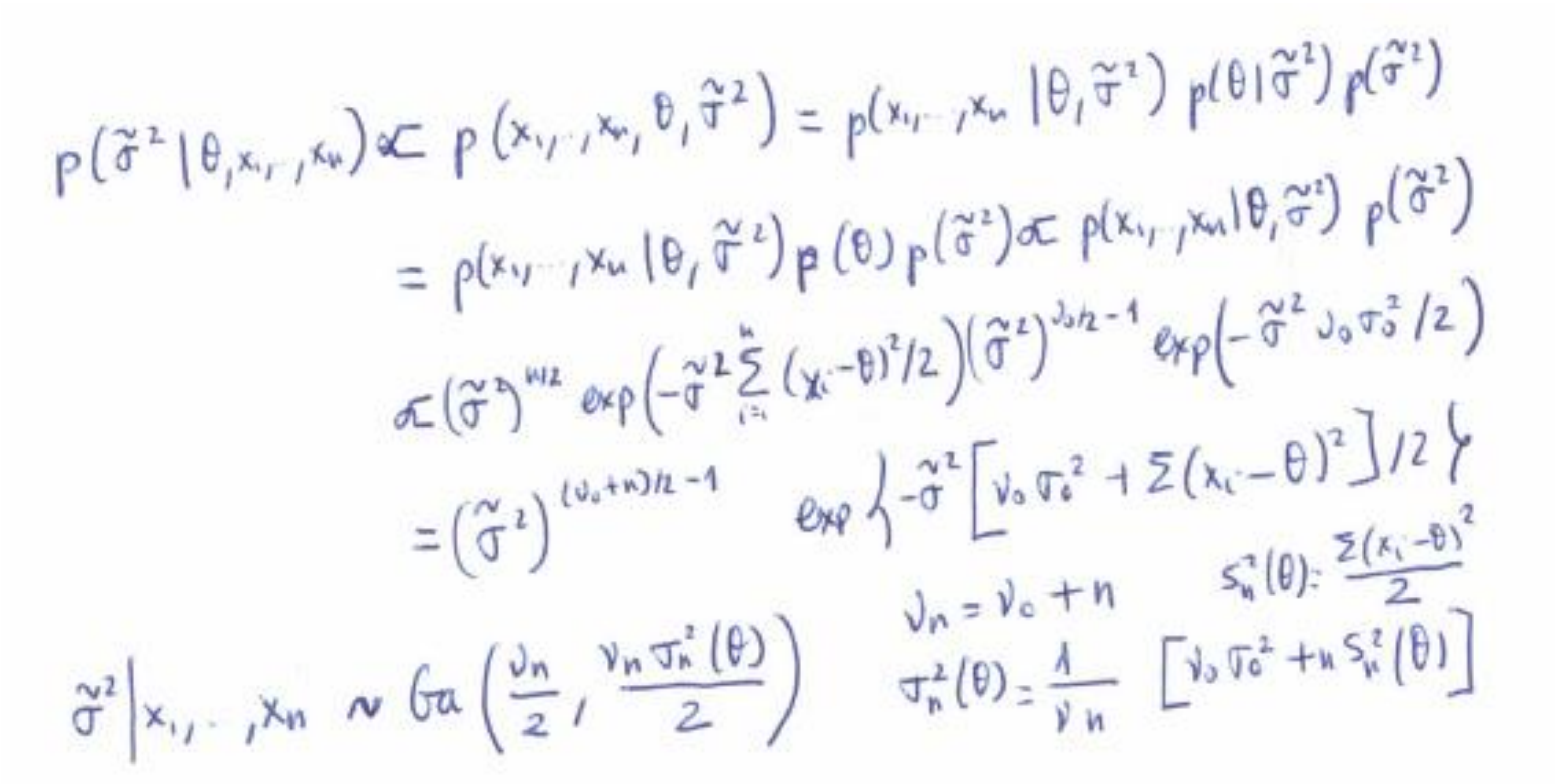
$$p(\theta, \sigma^2) = p(\theta)\, p(\sigma^2)$$

$$\mu_n(\tilde{\sigma}^2) = \frac{\frac{1}{\tau_0^2} \mu_0 + \frac{n}{\sigma^2} \bar{x}}{\frac{1}{\tau_0^2} + \frac{n}{\sigma^2}}$$

$$p(\theta \mid \sigma^2, x_1, \dots, x_n) \sim N(\mu_n, \tau_n^2)$$

$$\tau_n(\tilde{\sigma}^2) = \frac{1}{\frac{1}{\tau_0^2} + \frac{n}{\sigma^2}}$$

# Inference for normal-gamma. Conditional



$$p(\tilde\sigma^2|\theta,x_1,\dots,x_n) \propto p(x_1,\dots,x_n,\theta,\tilde\sigma^2) = p(x_1,\dots,x_n|\theta,\tilde\sigma^2)\,p(\theta|\tilde\sigma^2)\,p(\tilde\sigma^2)$$

$$= p(x_1,\dots,x_n|\theta,\tilde\sigma^2)\,p(\theta)\,p(\tilde\sigma^2) \propto p(x_1,\dots,x_n|\theta,\tilde\sigma^2)\,p(\tilde\sigma^2)$$

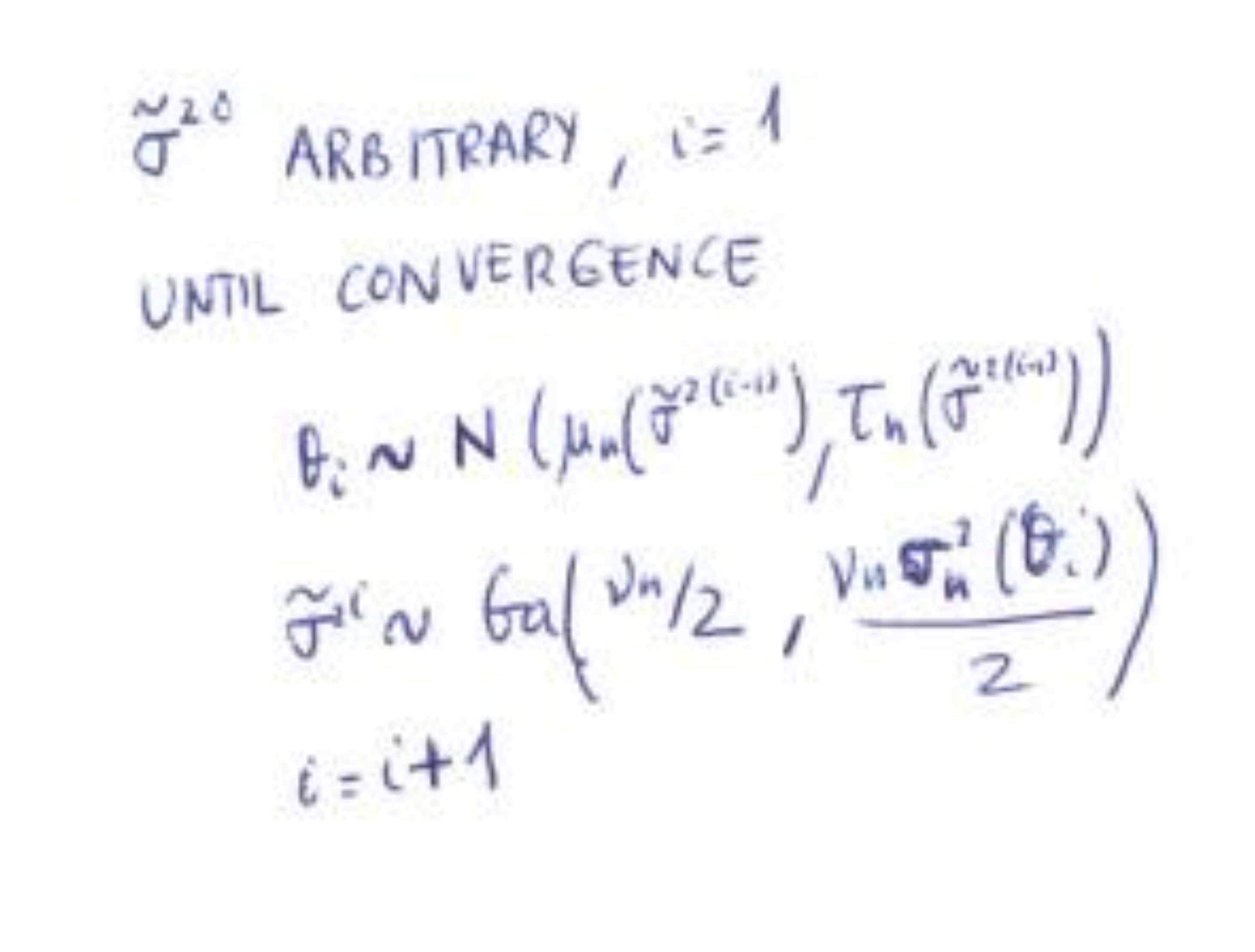
$$\propto (\tilde\sigma^2)^{n/2}\exp\left(-\tilde\sigma^2\sum_{i=1}^{n}(x_i-\theta)^2/2\right)(\tilde\sigma^2)^{\nu_0/2-1}\exp\left(-\tilde\sigma^2\nu_0\sigma_0^2/2\right)$$

$$=(\tilde\sigma^2)^{(\nu_0+n)/2-1}\exp\left\{-\tilde\sigma^2\left[\nu_0\sigma_0^2+\sum(x_i-\theta)^2\right]/2\right\}$$

$$\nu_n=\nu_0+n \qquad s_n^2(\theta)=\frac{\sum(x_i-\theta)^2}{2}$$

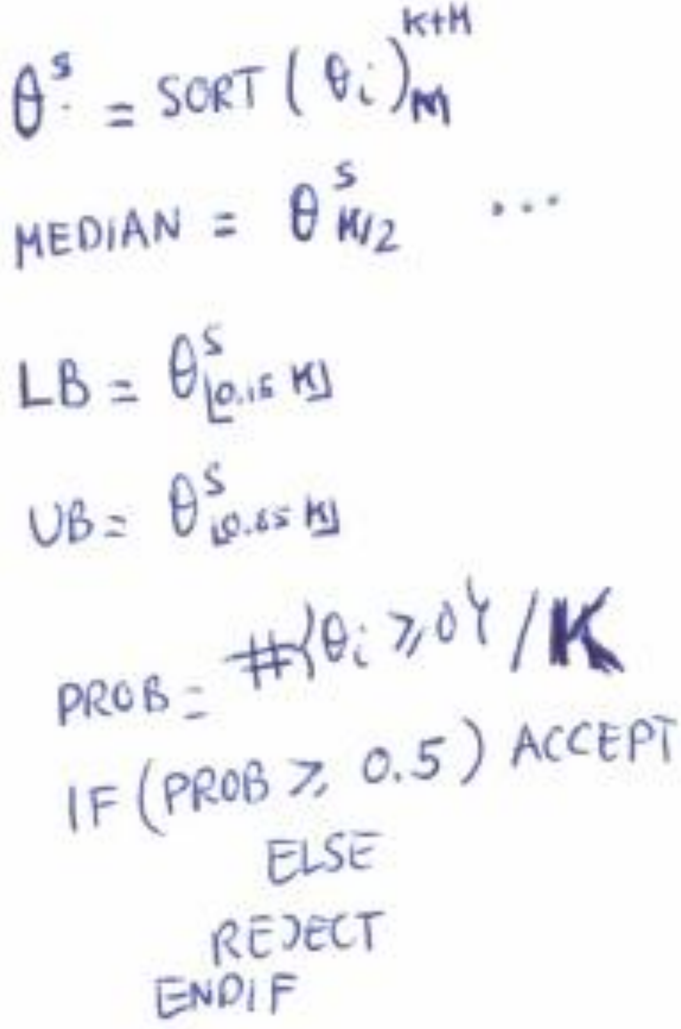
$$\tilde\sigma^2|x_1,\dots,x_n \sim Ga\left(\frac{\nu_n}{2},\frac{\nu_n\sigma_n^2(\theta)}{2}\right) \qquad \sigma_n^2(\theta)=\frac{1}{\nu_n}\left[\nu_0\sigma_0^2+n s_n^2(\theta)\right]$$

# Inference for normal-gamma. Sampler



```
$\tilde{\sigma}^{2\,0}$ ARBITRARY, $i=1$
UNTIL CONVERGENCE
    $\theta_i \sim N\left(\mu_n(\tilde{\sigma}^{2(i-1)}), \tau_n(\tilde{\sigma}^{2(i-1)})\right)$
    $\tilde{\sigma}^{i} \sim Ga\left(\nu_n/2, \frac{\nu_n \sigma_n^2(\theta_i)}{2}\right)$
    $i = i+1$
```

# Inference for normal-gamma. Answers



```
$\theta^{s}_{\cdot} = \mathrm{SORT}(\theta_i)_{M}^{K+M}$
MEDIAN = $\theta^{s}_{K/2}$ ...
LB = $\theta^{s}_{\lfloor 0.15 K \rfloor}$
UB = $\theta^{s}_{\lfloor 0.85 K \rfloor}$
PROB = $\#\{\theta_i \geq 0\} / K$
IF (PROB $\geq$ 0.5) ACCEPT
    ELSE
    REJECT
ENDIF
```

# Inference for a mixture of exponentials

An example with mixtures. Very important in modern statistics and machine learning, e.g. Latent Dirichlet allocation. Used in clustering, density estimation,… Also introduces latent variables.

**Model**. Mixture of k exponentials, gamma priors. Dirichlet-multinomial on labels.

**Use**. Predictive distribution, group for first observation

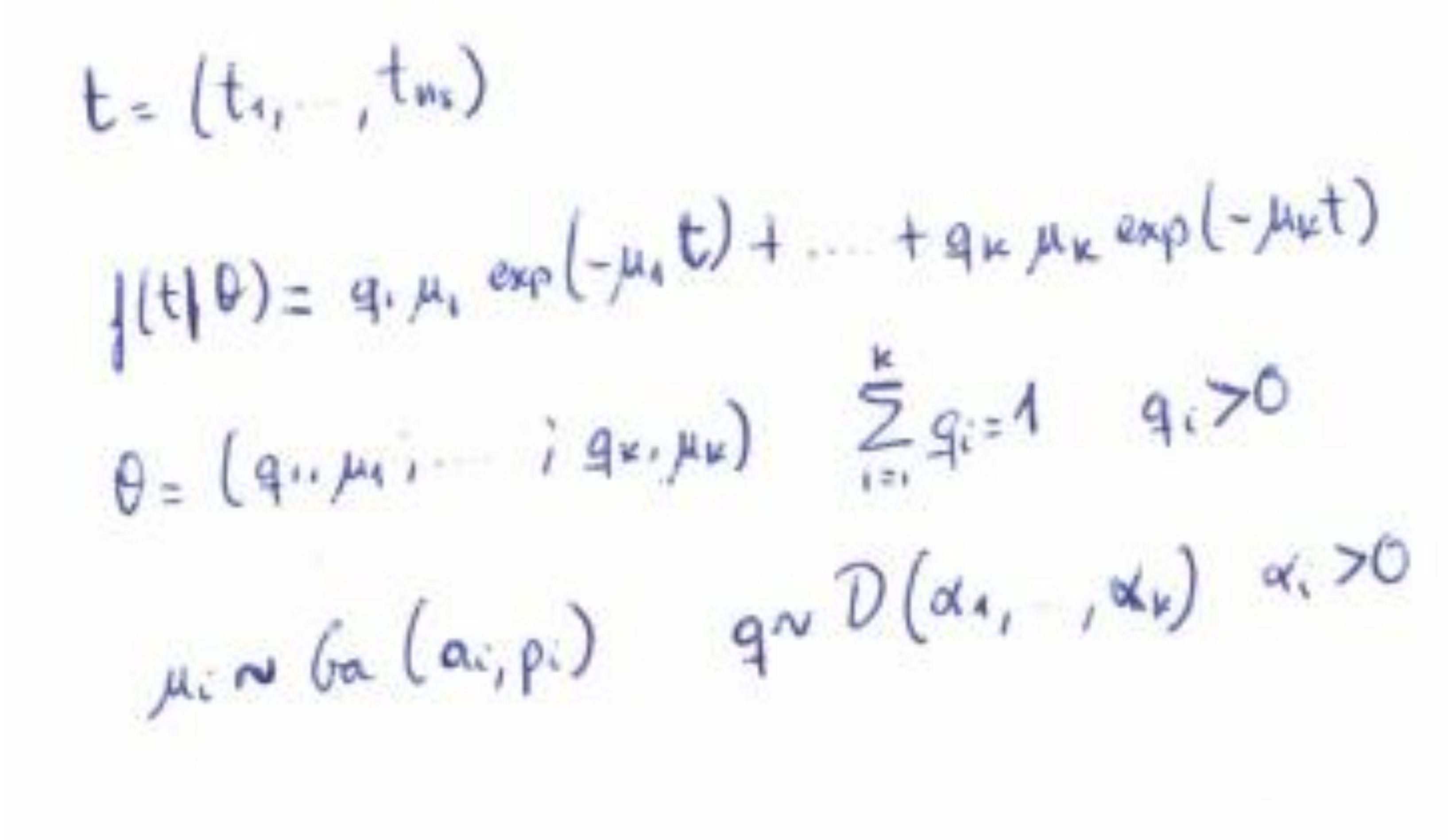
https://en.wikipedia.org/wiki/Multinomial_distribution

https://en.wikipedia.org/wiki/Dirichlet_distribution

https://en.wikipedia.org/wiki/Latent_Dirichlet_allocation

# Inference for a mixture of exponentials

Model



$t = (t_1, \dots, t_{n_s})$

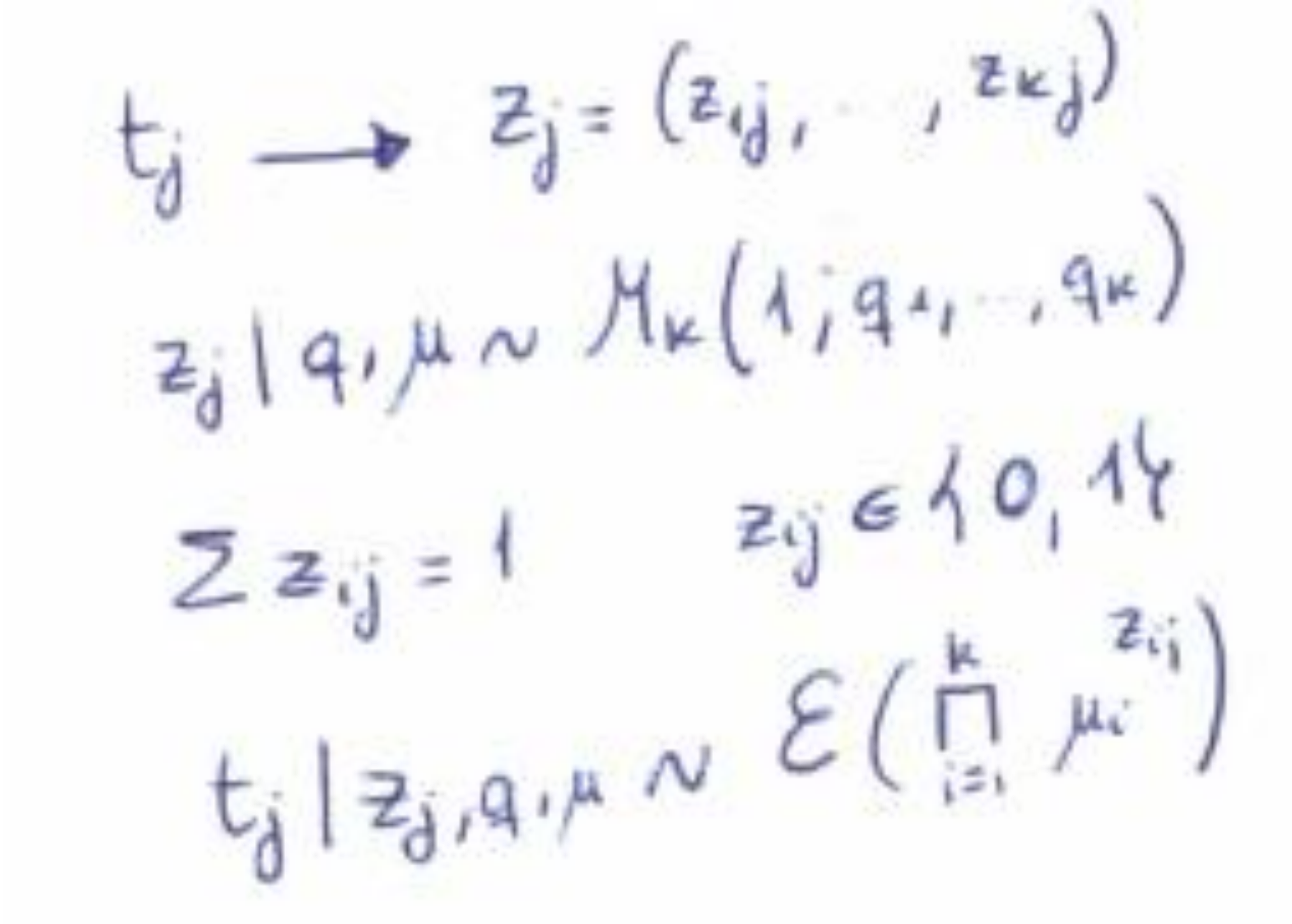
$f(t|\theta) = q_1 \mu_1 \exp(-\mu_1 t) + \dots + q_K \mu_K \exp(-\mu_K t)$

$\theta = (q_1, \mu_1; \dots; q_K, \mu_K)$ $\sum_{i=1}^{K} q_i = 1$ $q_i > 0$

$\mu_i \sim Ga(a_i; p_i)$ $q \sim D(\alpha_1, \dots, \alpha_K)$ $\alpha_i > 0$

# Inference for a mixture of exponentials

Latent variables



$$t_j \longrightarrow z_j = (z_{1j}, \dots, z_{kj})$$

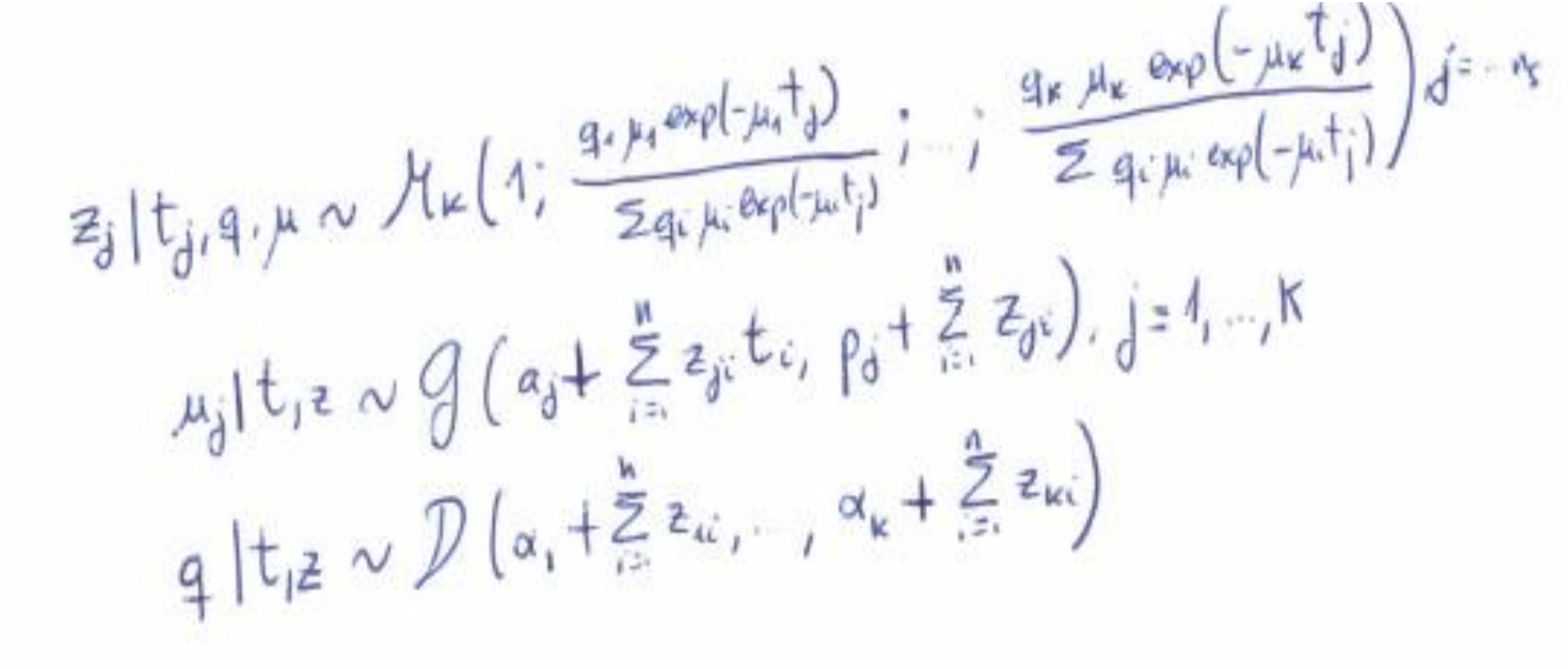
$$z_j \mid q, \mu \sim \mathcal{M}_k(1; q_1, \dots, q_k)$$

$$\sum z_{ij} = 1 \qquad z_{ij} \in \{0, 1\}$$

$$t_j \mid z_j, q, \mu \sim \mathcal{E}\left(\prod_{i=1}^{k} \mu_i^{z_{ij}}\right)$$

# Inference for a mixture of exponentials

Posterior conditionals



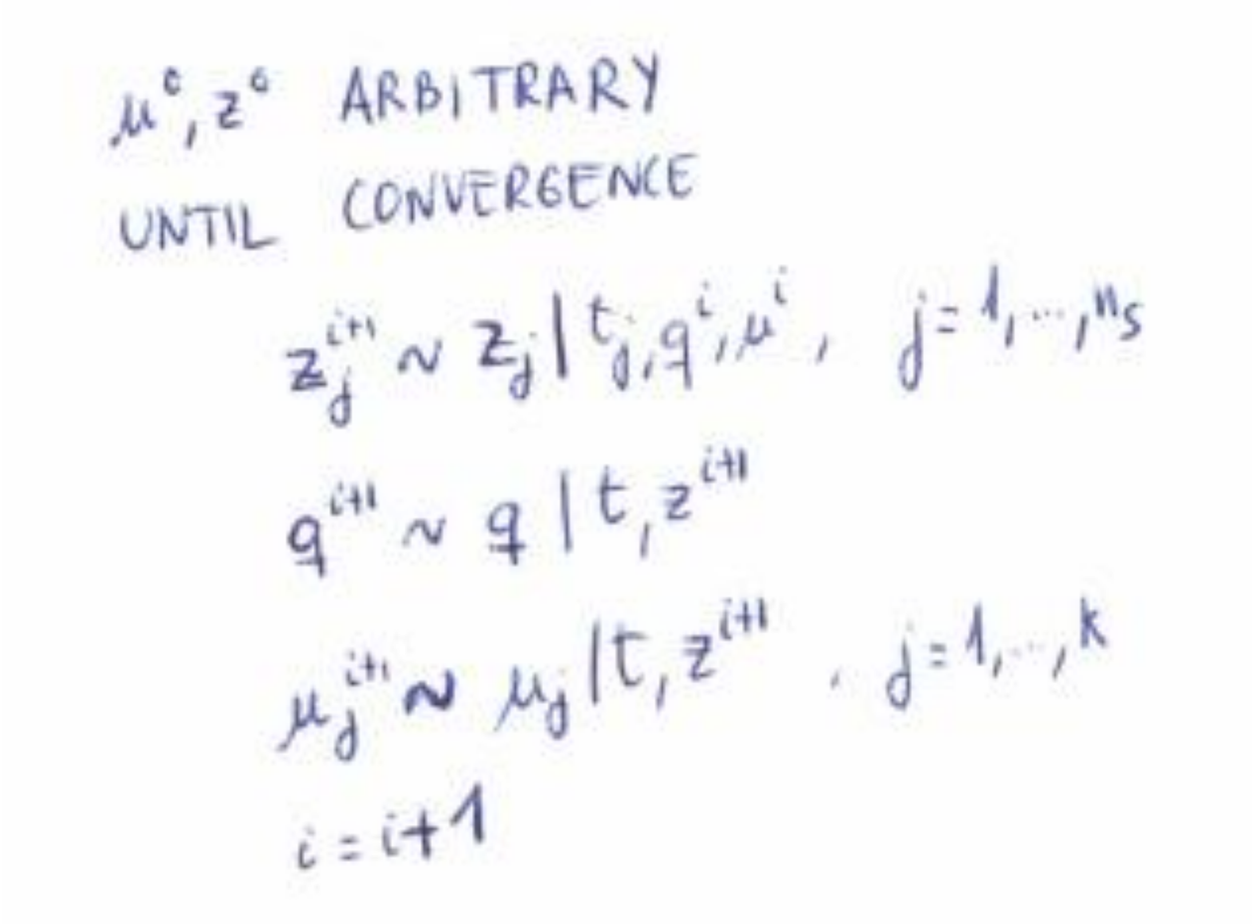
$$z_j \mid t_j, q, \mu \sim \mathcal{M}_K\left(1; \frac{q_1 \mu_1 \exp(-\mu_1 t_j)}{\Sigma q_i \mu_i \exp(-\mu_i t_j)}; \dots; \frac{q_K \mu_K \exp(-\mu_K t_j)}{\Sigma q_i \mu_i \exp(-\mu_i t_j)}\right) j = \dots n$$

$$\mu_j \mid t, z \sim \mathcal{G}\left(a_j + \sum_{i=1}^{n} z_{ji} t_i, \beta_j + \sum_{i=1}^{n} z_{ji}\right), j = 1, \dots, K$$

$$q \mid t, z \sim \mathcal{D}\left(\alpha_1 + \sum_{i=1}^{n} z_{1i}, \dots, \alpha_K + \sum_{i=1}^{n} z_{Ki}\right)$$

# Inference for a mixture of exponentials

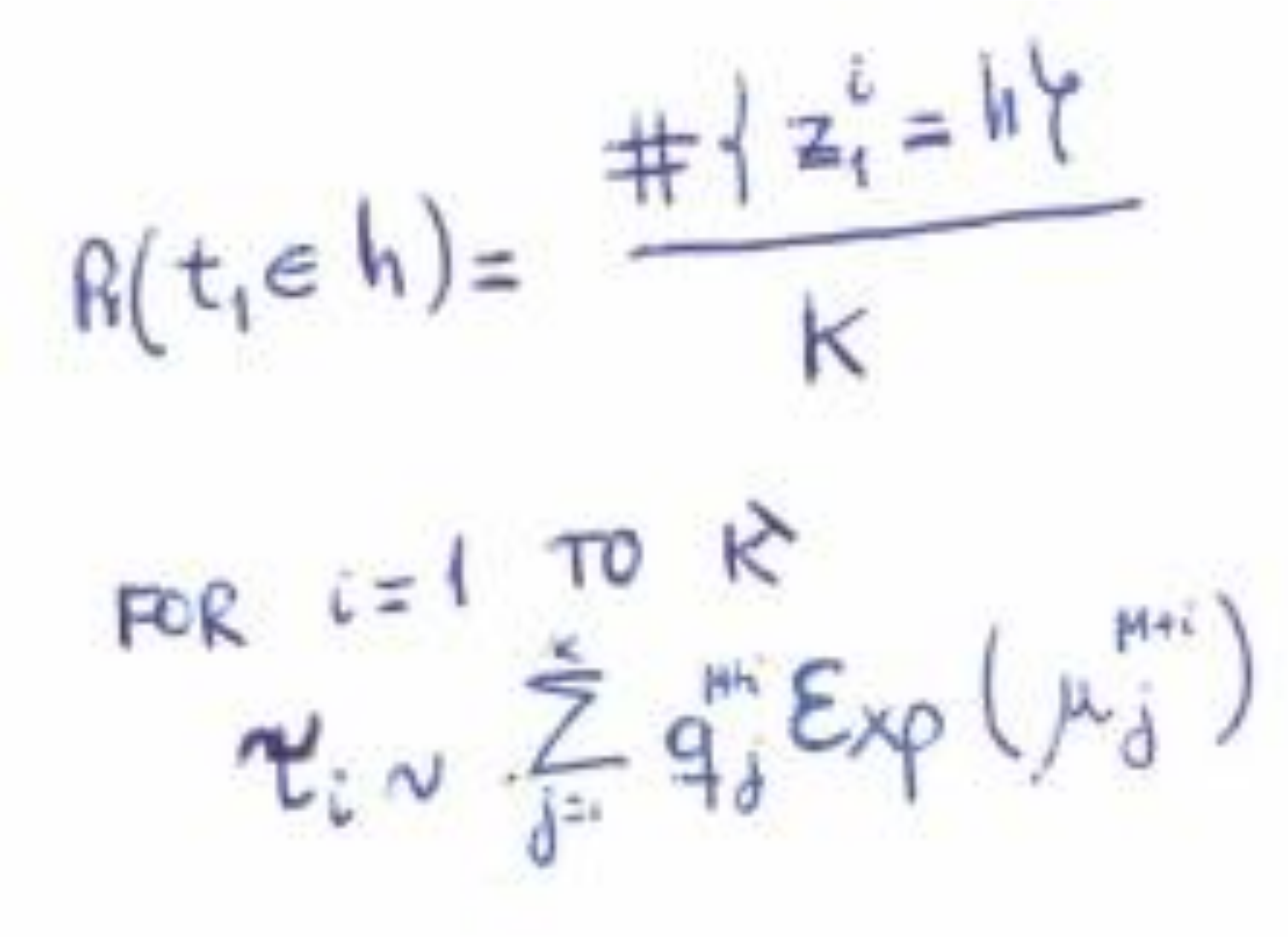
Gibbs sampler



```
$\mu^0, z^0$ ARBITRARY
UNTIL CONVERGENCE
    $z_j^{i+1} \sim z_j \mid t_j, q^i, \mu^i$ ,  $j = 1, \dots, n_s$
    $q^{i+1} \sim q \mid t, z^{i+1}$
    $\mu_j^{i+1} \sim \mu_j \mid t, z^{i+1}$ ,  $j = 1, \dots, k$
    $i = i+1$
```

# Inference for a mixture of exponentials

Answers



$$P(t_1 \in h) = \frac{\#\{z_1^i = h\}}{K}$$

FOR $i = 1$ TO $K$

$$\tau_i \sim \sum_{j=1}^{K} q_j^{M+i} \mathcal{E}xp(\mu_j^{M+i})$$

# Inference for normal multivariate

Again ultra-important. Bread and butter of multivariate analysis

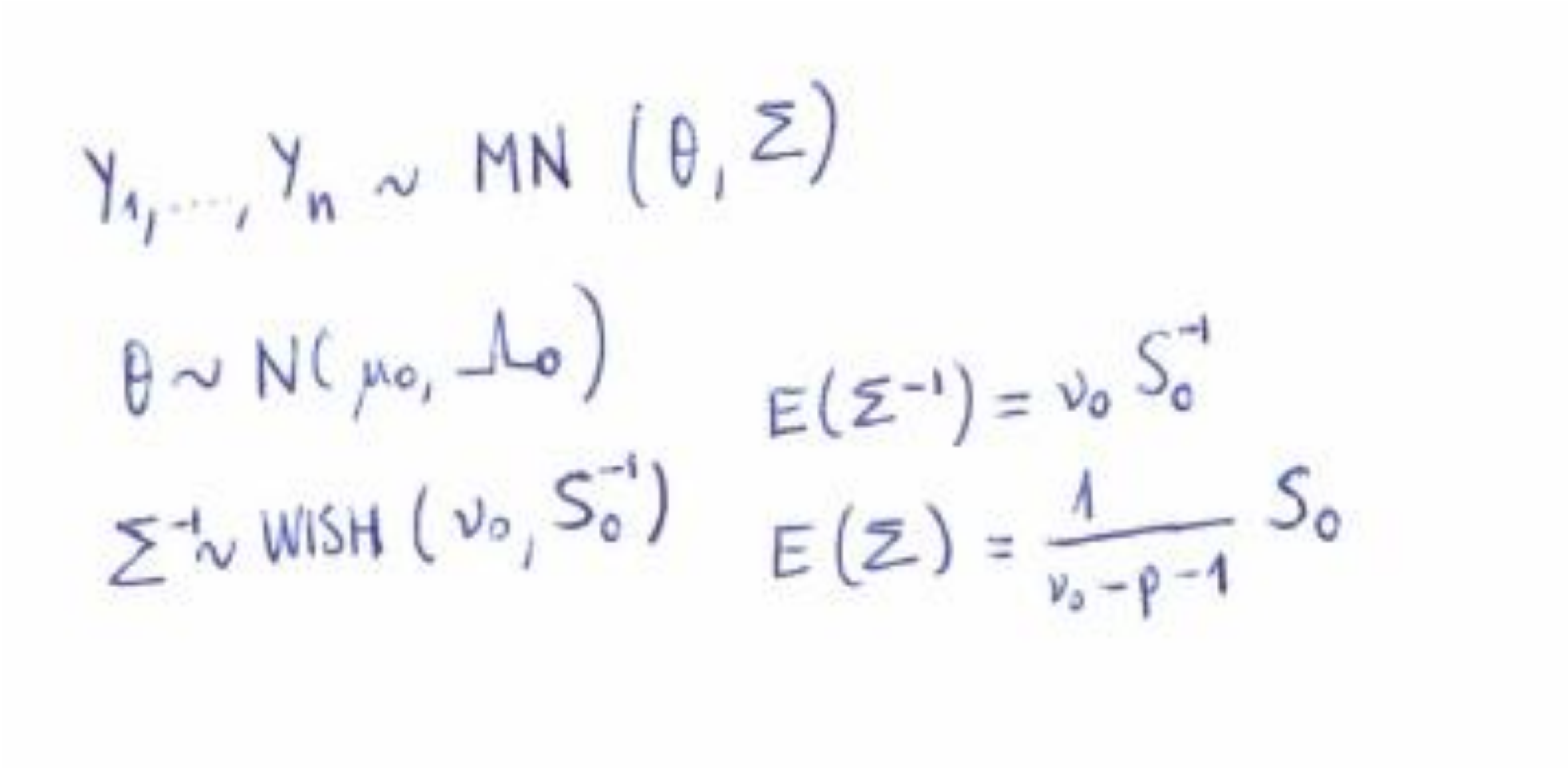
**Model.** Multivariate normal (means and covariance matrix). Normal-Wishart prior

**Use**. Expected value of maximum, Probability that product of means is bigger than 4

https://en.wikipedia.org/wiki/Wishart_distribution

# Inference for normal multivariate

Model



$$Y_1, \dots, Y_n \sim MN(\theta, \Sigma)$$

$$\theta \sim N(\mu_0, \Lambda_0)$$

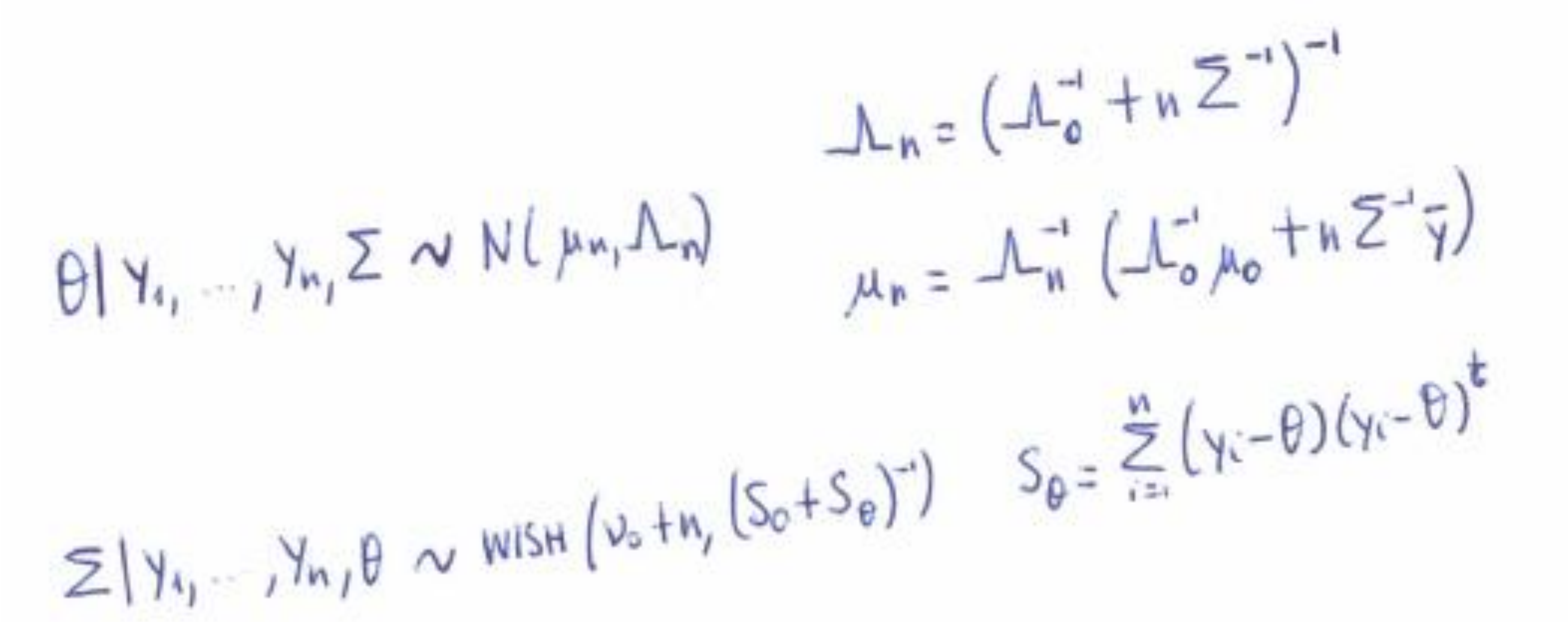
$$\Sigma^{-1} \sim WISH(\nu_0, S_0^{-1})$$

$$E(\Sigma^{-1}) = \nu_0 S_0^{-1}$$

$$E(\Sigma) = \frac{1}{\nu_0 - p - 1} S_0$$

# Inference for normal multivariate

## Posterior conditionals



$$\Lambda_n = \left(\Lambda_0^{-1} + n\Sigma^{-1}\right)^{-1}$$

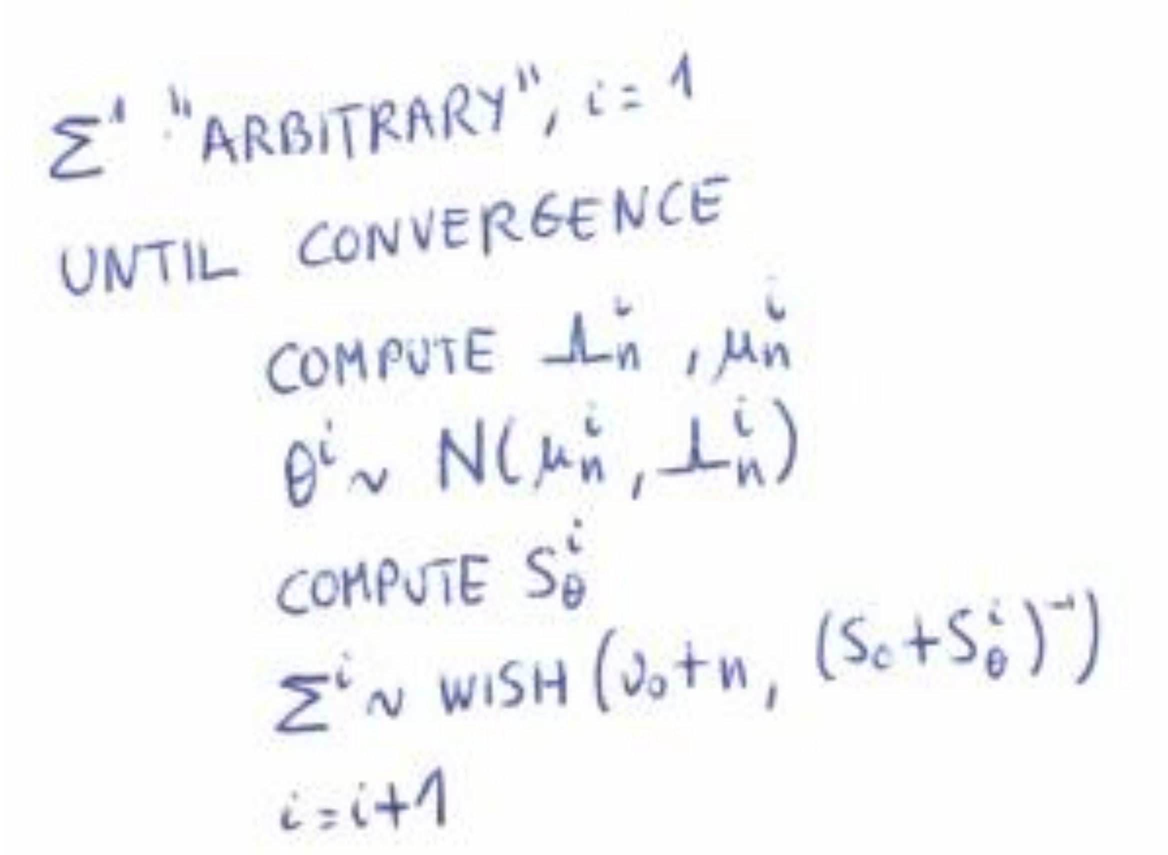
$$\theta | y_1, \dots, y_n, \Sigma \sim N(\mu_n, \Lambda_n) \qquad \mu_n = \Lambda_n^{-1}\left(\Lambda_0^{-1}\mu_0 + n\Sigma^{-1}\bar{y}\right)$$

$$S_\theta = \sum_{i=1}^{n}(y_i-\theta)(y_i-\theta)^t$$

$$\Sigma | y_1, \dots, y_n, \theta \sim \text{WISH}\left(\nu_0 + n, (S_0+S_\theta)^{-1}\right)$$

# Inference for normal multivariate

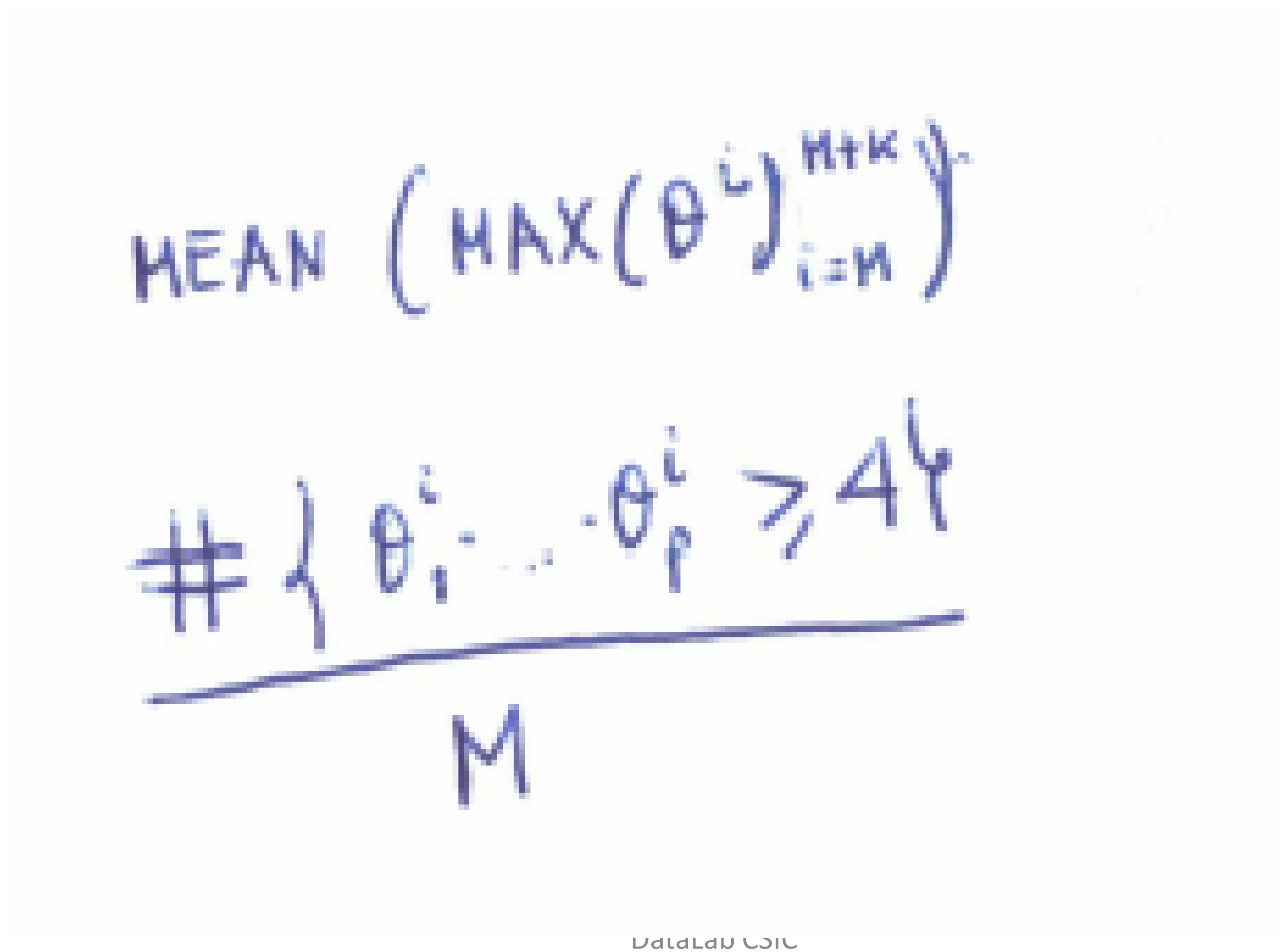
## Gibbs sampler



```
$\Sigma^1$ "ARBITRARY", $i=1$
UNTIL CONVERGENCE
        COMPUTE $\Lambda_n^i$ , $\mu_n^i$
        $\theta^i \sim N(\mu_n^i, \Lambda_n^i)$
        COMPUTE $S_\theta^i$
        $\Sigma^i \sim$ WISH$(\nu_0+n, (S_0+S_\theta^i)^{-1})$
        $i=i+1$
```

# Inference for normal multivariate

Answers

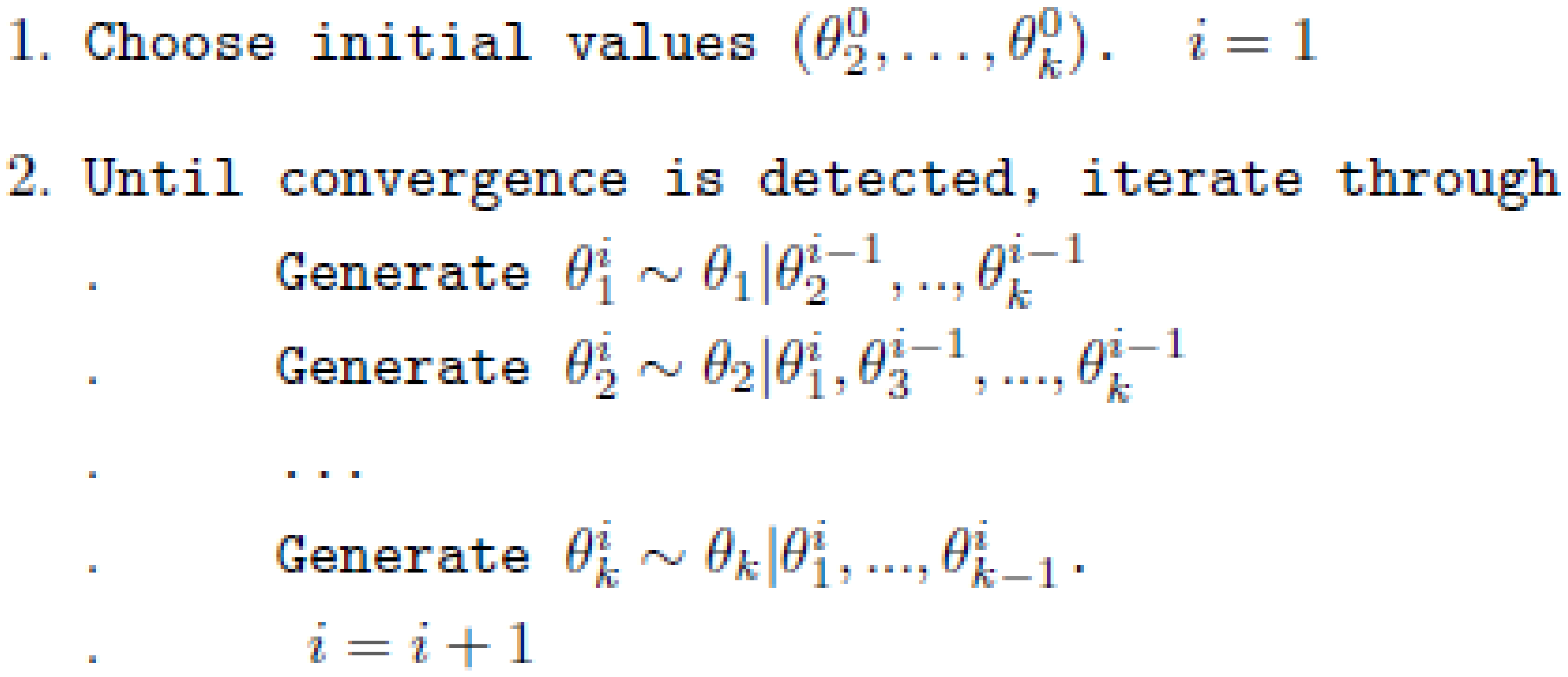


$$\text{MEAN}\left(\text{MAX}(\theta^{i})_{i=M}^{M+K}\right)$$

$$\frac{\#\{\theta_1^{i} \cdots \theta_p^{i} \geq 4\}}{M}$$

# Gibbs sampling theory

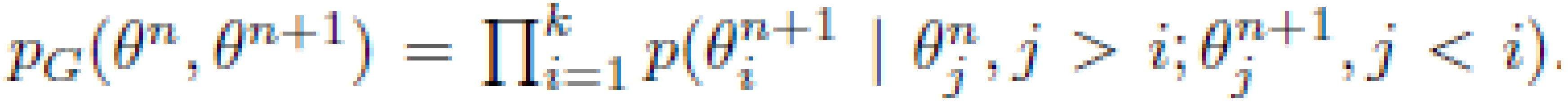
# Recall



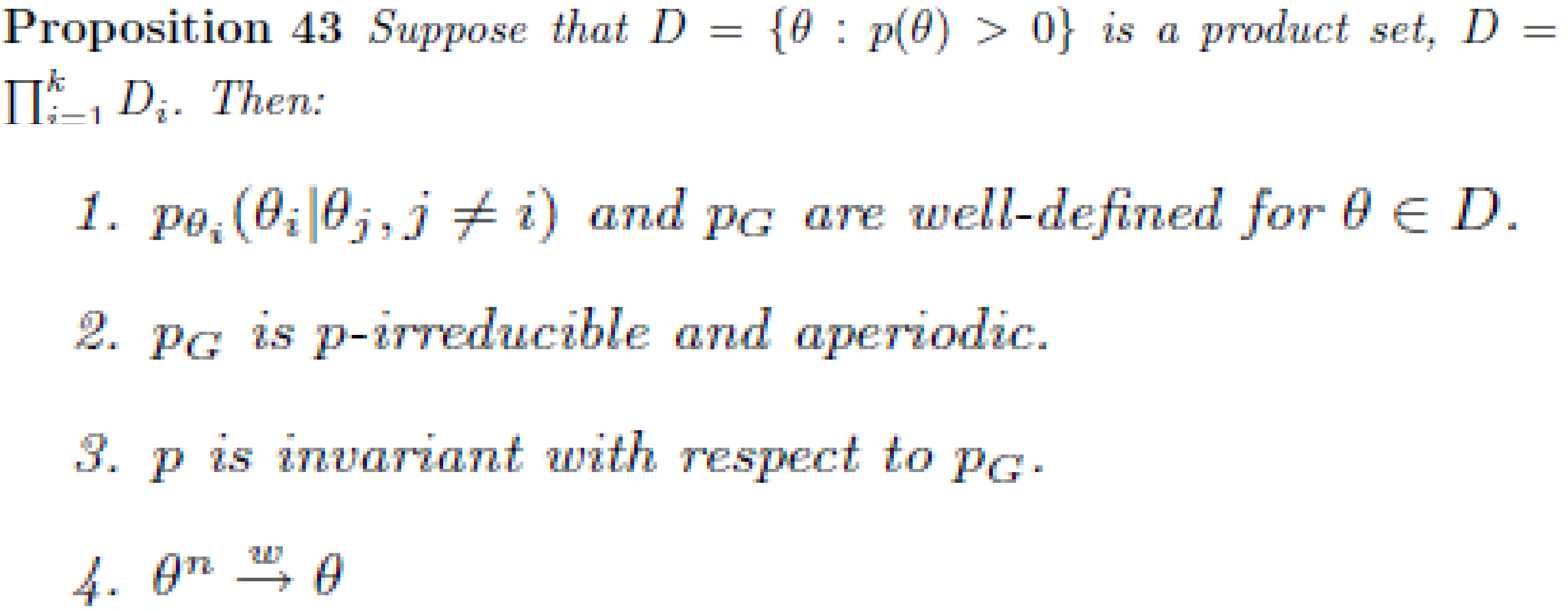
```
1. Choose initial values $(\theta_2^0, \ldots, \theta_k^0)$.   $i = 1$
2. Until convergence is detected, iterate through
   .      Generate $\theta_1^i \sim \theta_1|\theta_2^{i-1}, .., \theta_k^{i-1}$
   .      Generate $\theta_2^i \sim \theta_2|\theta_1^i, \theta_3^{i-1}, ..., \theta_k^{i-1}$
   .      ...
   .      Generate $\theta_k^i \sim \theta_k|\theta_1^i, ..., \theta_{k-1}^i$.
   .       $i = i + 1$
```

# Convergence

Kernel



$$p_G(\theta^n, \theta^{n+1}) = \prod_{i=1}^k p(\theta_i^{n+1} \mid \theta_j^n, j > i; \theta_j^{n+1}, j < i).$$



**Proposition 43** *Suppose that $D = \{\theta : p(\theta) > 0\}$ is a product set, $D = \prod_{i=1}^k D_i$. Then:*

1. *$p_{\theta_i}(\theta_i | \theta_j, j \neq i)$ and $p_G$ are well-defined for $\theta \in D$.*

2. *$p_G$ is p-irreducible and aperiodic.*

3. *$p$ is invariant with respect to $p_G$.*

4. *$\theta^n \xrightarrow{w} \theta$*

# b. Metropolis Hastings algos

# Brief description

The intro presented key methods in Bayesian inference and basic models and faced ‘severe’ computational problems quite rapidly (beta-binomial, logistic regression)

We have introduced MCMC and Gibbs sampling

We focus here on Metropolis-Hastings and hybrid samplers

More to be followed

# Sources

French and DRI (2000) Ch 7

DRI et al (2010) Ch4

BDA3 (2015) Ch11, 12

Hoff (2009) Ch 6,7

# Labs

3.2 Metropolis

Basic, Standard, MH

Multivariate normal

Linear regression (ecology)

Poisson regression (ecology)

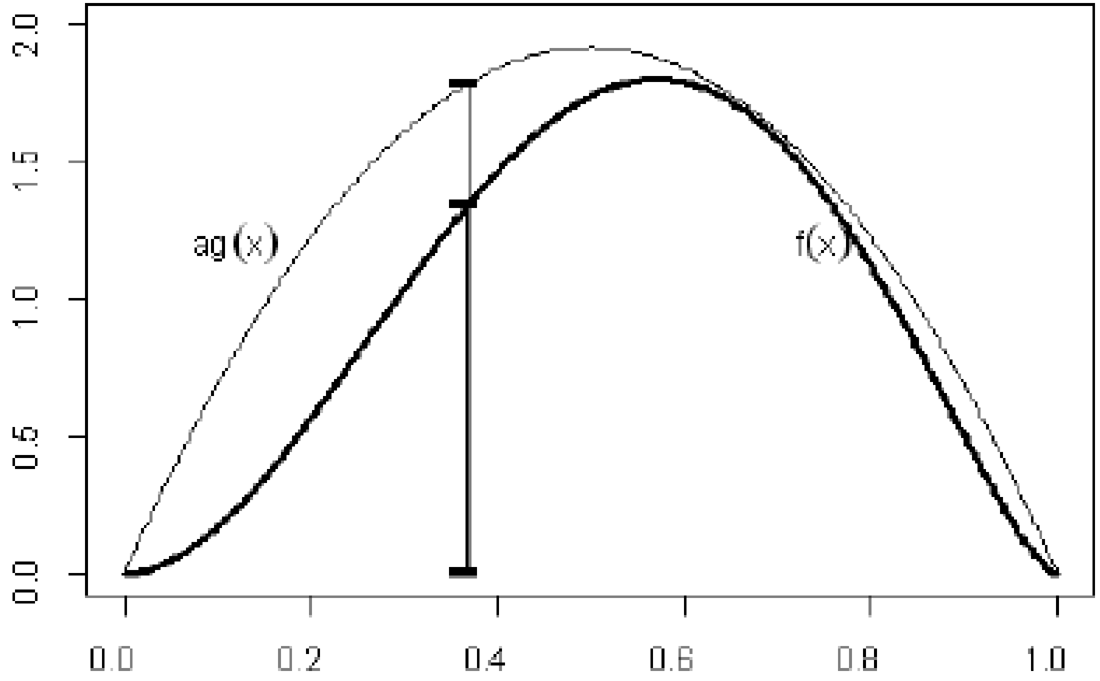
# Understanding the Metropolis-Hastings algorithm

# Recall: Acceptance-rejection sampling

TARGET DENSITY $\pi(x) = f(x)/K$, K POSSIBLY UNKNOWN

SAMPLING DENSITY $g(x)$ : $f(x) \leq a g(x)$ , $\forall x$

```
WHILE $U > f(x) / (a g(x))$
    GENERATE $X \sim g$, $U \sim \mathcal{U}[0,1]$
OUTPUT $X$
```



$P(X \leq x \mid X \text{ ACCEPTED}) = F(x)$ ($F$ cdf of $X$)

# Metropolis-Hastings rationale I

Transition kernel of Markov chain $P(x,A)$

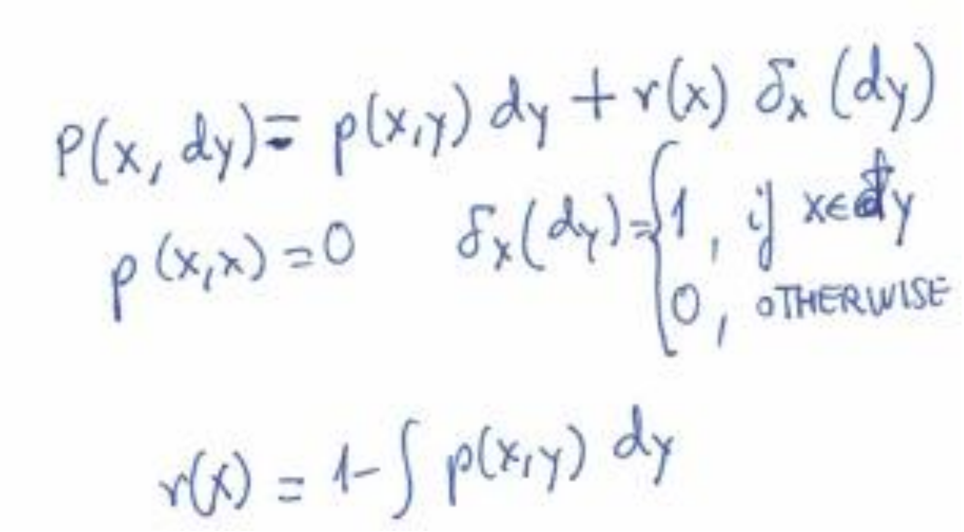
Invariant distribution $\pi^*(dy) = \int P(x,dy)\,\pi(x)\,dx$

n-th iterate

$$P^{(n)}(x,A) = \int P^{(n-1)}(x,dy)\;P(y,A)$$

# Metropolis-Hastings rationale II

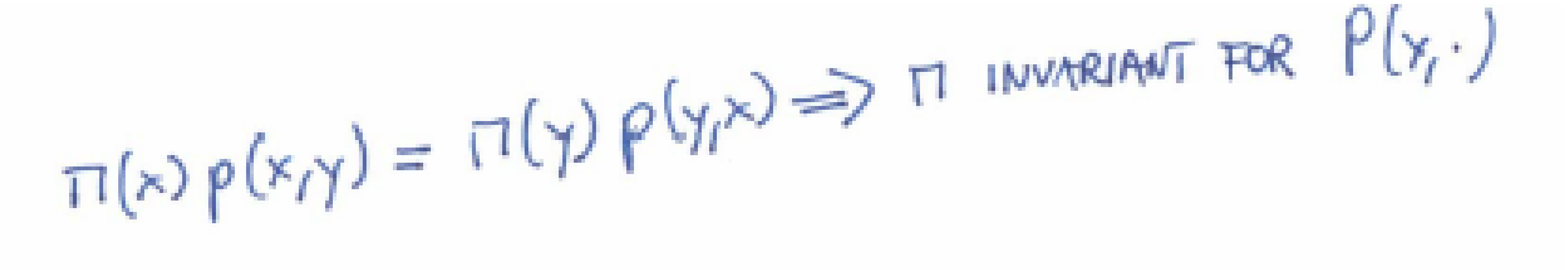
Invariant distribution and reversibility. Suppose that for p kernel (x,y)



$$P(x, dy) = p(x,y)\,dy + r(x)\,\delta_x(dy)$$

$$p(x,x) = 0 \qquad \delta_x(dy) = \begin{cases} 1, & \text{if } x \in dy \\ 0, & \text{OTHERWISE} \end{cases}$$

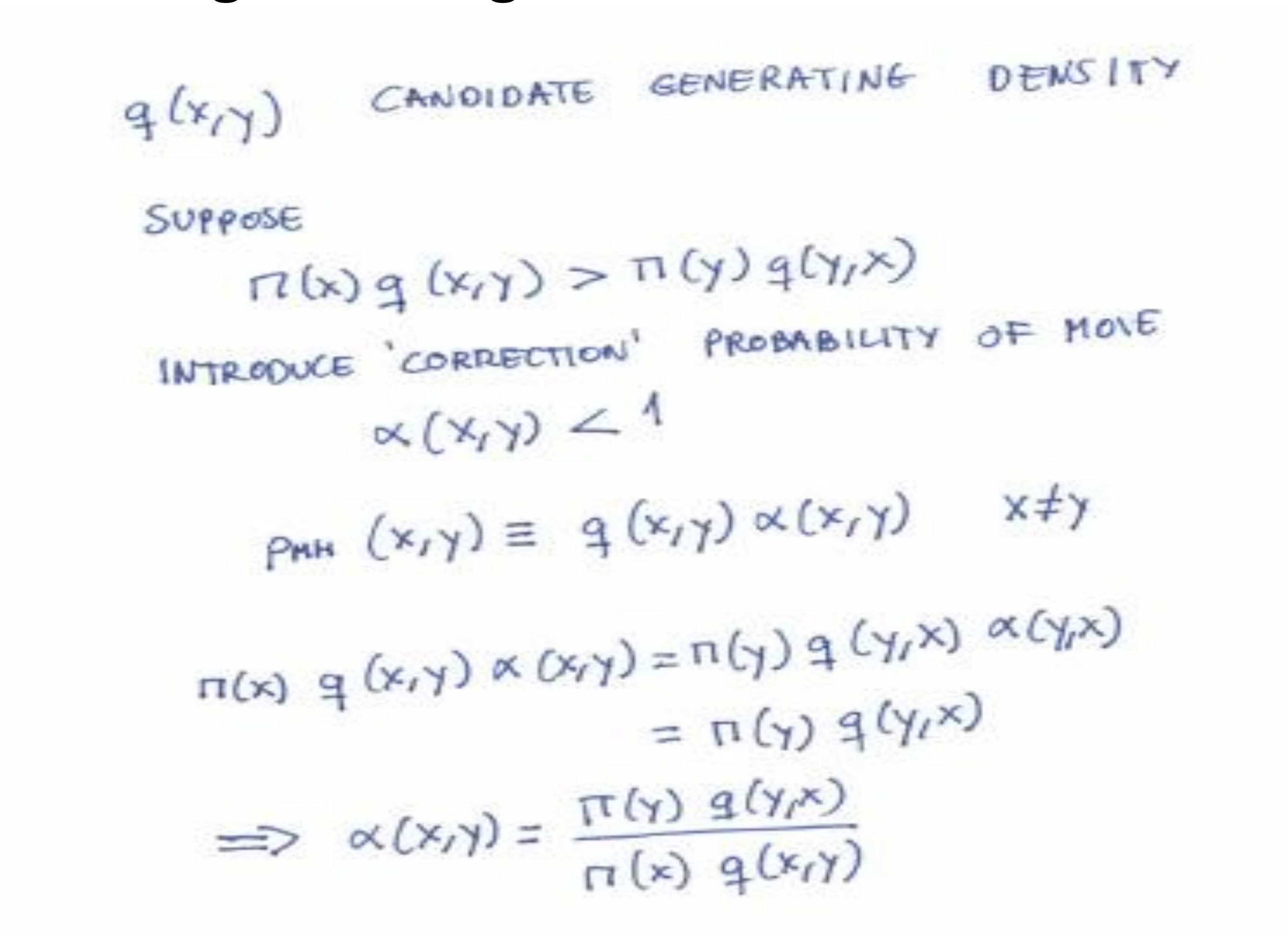
$$r(x) = 1 - \int p(x,y)\,dy$$



$$\pi(x)\,p(x,y) = \pi(y)\,p(y,x) \Longrightarrow \pi \text{ INVARIANT FOR } P(y,\cdot)$$

# Metropolis-Hastings rationale III

Adjusting a candidate generating distribution



$q(x,y)$ CANDIDATE GENERATING DENSITY

SUPPOSE

$$\pi(x)\, q(x,y) > \pi(y)\, q(y,x)$$

INTRODUCE 'CORRECTION' PROBABILITY OF MOVE

$$\alpha(x,y) < 1$$

$$p_{MH}(x,y) \equiv q(x,y)\,\alpha(x,y) \qquad x \neq y$$

$$\begin{aligned}\pi(x)\, q(x,y)\,\alpha(x,y) &= \pi(y)\, q(y,x)\,\alpha(y,x) \\ &= \pi(y)\, q(y,x)\end{aligned}$$

$$\Longrightarrow \alpha(x,y) = \frac{\pi(y)\, q(y,x)}{\pi(x)\, q(x,y)}$$

# Metropolis-Hastings rationale IV

Balance condition

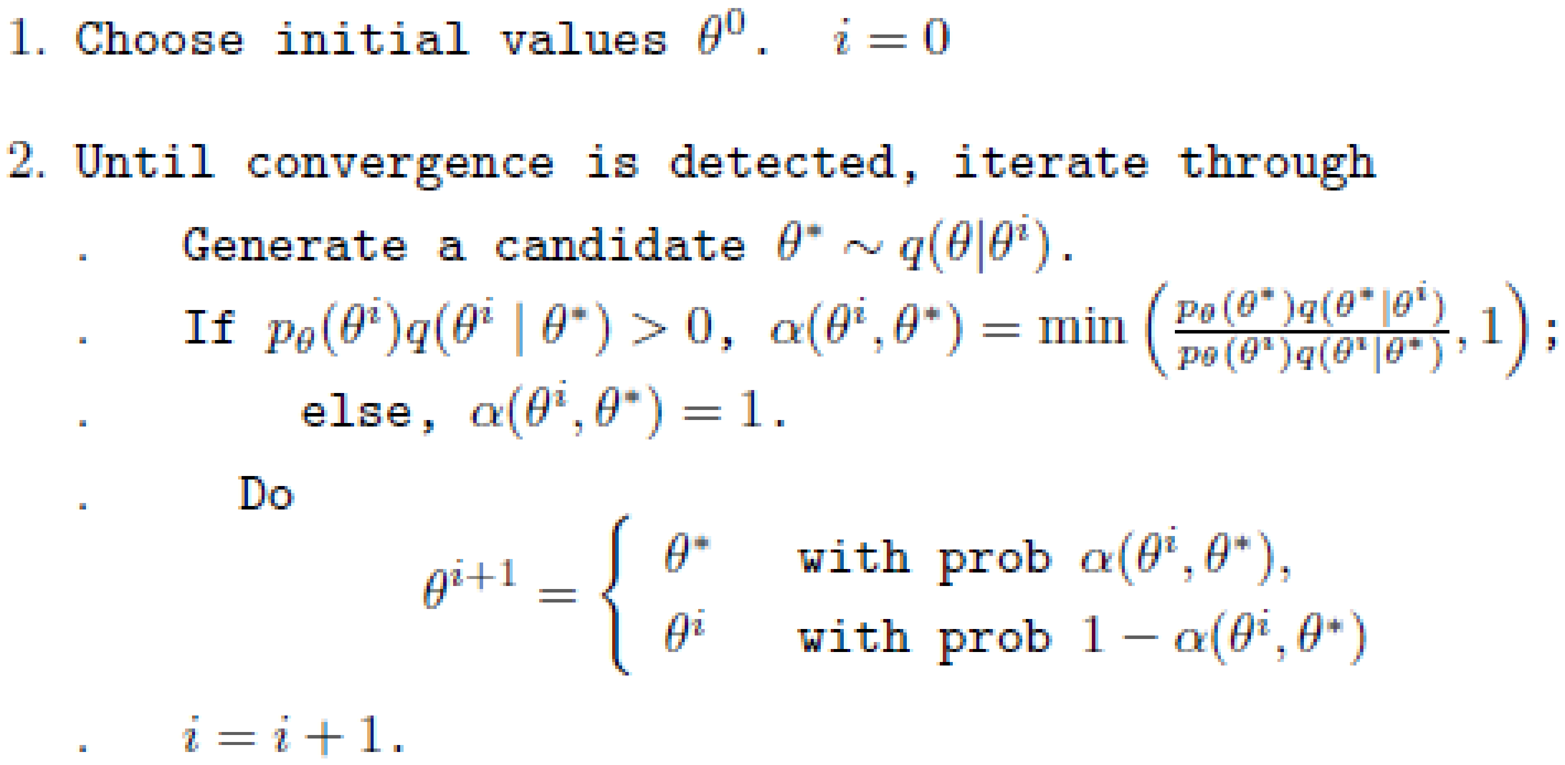
$$\alpha(x,y) = \begin{cases} \min\left(\frac{\pi(y)\,q(y,x)}{\pi(x)\,q(x,y)}, 1\right), & \text{IF } \pi(x)\,q(x,y)>0 \\ 1, & \text{OTHERWISE} \end{cases}$$

Observations

- Normalising constant not required
- If q symmetric, Metropolis

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

# Metropolis-Hastings algo



```
1. Choose initial values $\theta^0$.   $i = 0$

2. Until convergence is detected, iterate through
   .   Generate a candidate $\theta^* \sim q(\theta|\theta^i)$.
   .   If $p_\theta(\theta^i)q(\theta^i \mid \theta^*) > 0$, $\alpha(\theta^i, \theta^*) = \min\left(\frac{p_\theta(\theta^*)q(\theta^*|\theta^i)}{p_\theta(\theta^i)q(\theta^i|\theta^*)}, 1\right)$;
   .       else, $\alpha(\theta^i, \theta^*) = 1$.
   .     Do
           $\theta^{i+1} = \begin{cases} \theta^* & \text{with prob } \alpha(\theta^i, \theta^*), \\ \theta^i & \text{with prob } 1 - \alpha(\theta^i, \theta^*) \end{cases}$
   .   $i = i + 1$.
```

# Metropolis-Hastings variants I

Random walk chain

$$q(x,y) = q_1(x-y)$$

$$y = x+z, \quad z \sim q_1$$

→ NORMAL

→ t

Metropolis algorithm

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

Independence chain

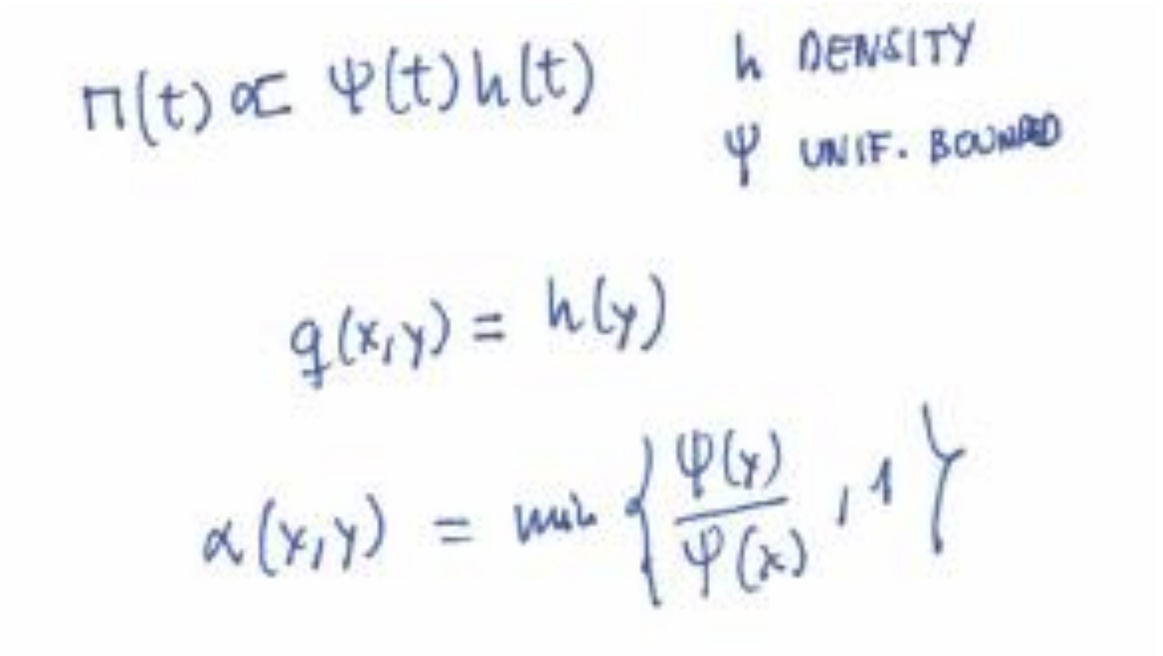
$$q(x,y) = q_2(y)$$

→ NORMAL

→ t

# Metropolis-Hastings variants II

Exploiting form of target



$$\pi(t) \propto \psi(t)\, h(t)$$

$h$ DENSITY

$\psi$ UNIF. BOUND

$$q(x,y) = h(y)$$

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

Acceptance rate not too high, not too low (23%). Tuning parameters

# Examples

# Sampling the bi-variate normal

Simple example to recall approach

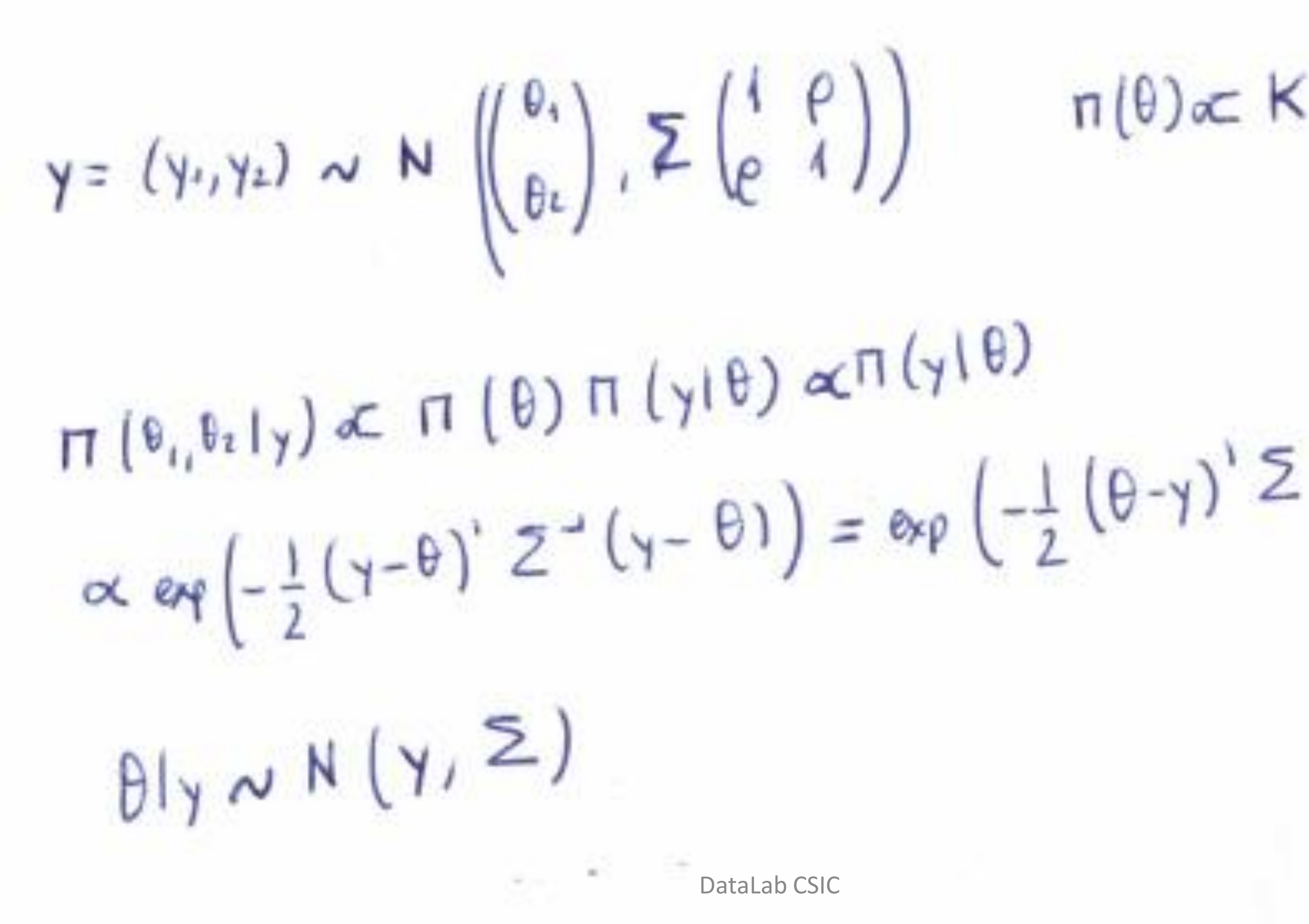
**Model**. Bivariate normal with unknown means. Variances 1. Known correlation $\varrho$

1 observation

Prior. Uniform

**Use**. Expected value and variance of parameters, Expected cross product, Probability that parameter belongs to a set

# Sampling the bi-variate normal. Model and posterior



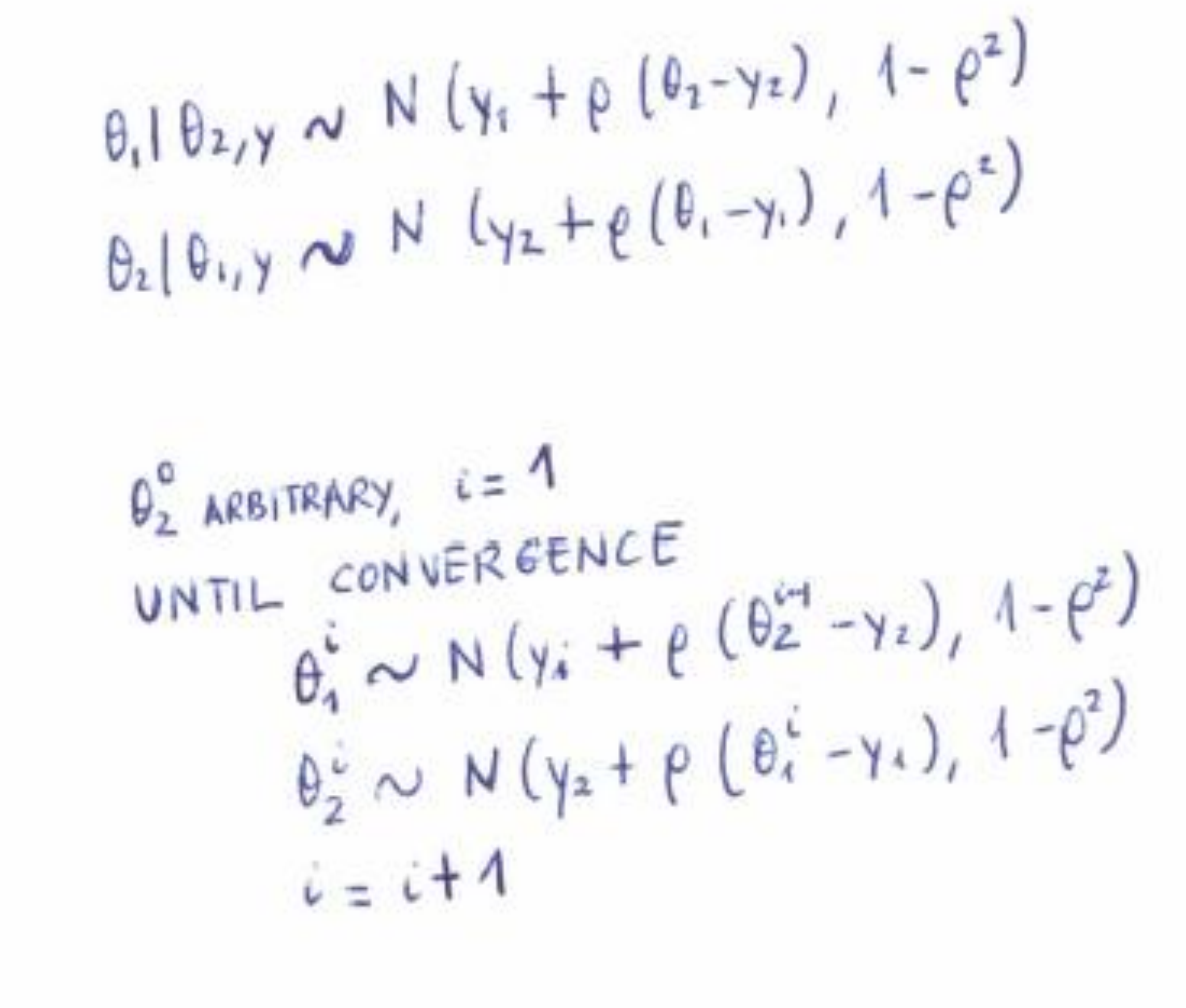
$$y = (y_1, y_2) \sim N\left(\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix}, \Sigma\begin{pmatrix}1 & \rho\\ \rho & 1\end{pmatrix}\right) \qquad \pi(\theta) \propto K$$

$$\pi(\theta_1, \theta_2 | y) \propto \pi(\theta)\, \pi(y|\theta) \propto \pi(y|\theta)$$

$$\propto \exp\left(-\frac{1}{2}(y-\theta)' \Sigma^{-1} (y-\theta)\right) = \exp\left(-\frac{1}{2}(\theta-y)' \Sigma^{-1} (\theta-y)\right)$$

$$\theta|y \sim N(y, \Sigma)$$

# Sampling the bi-variate normal. Gibbs sampler

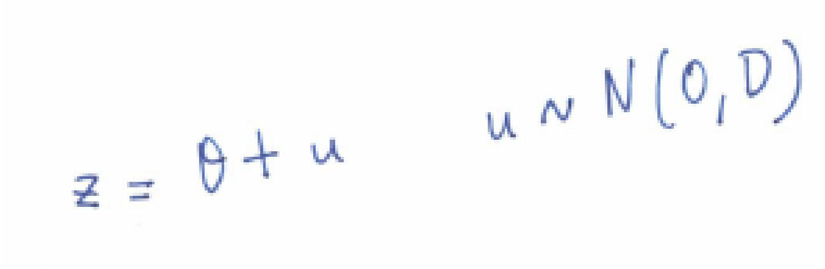


$$\theta_1 | \theta_2, y \sim N(y_1 + \rho(\theta_2 - y_2), 1-\rho^2)$$

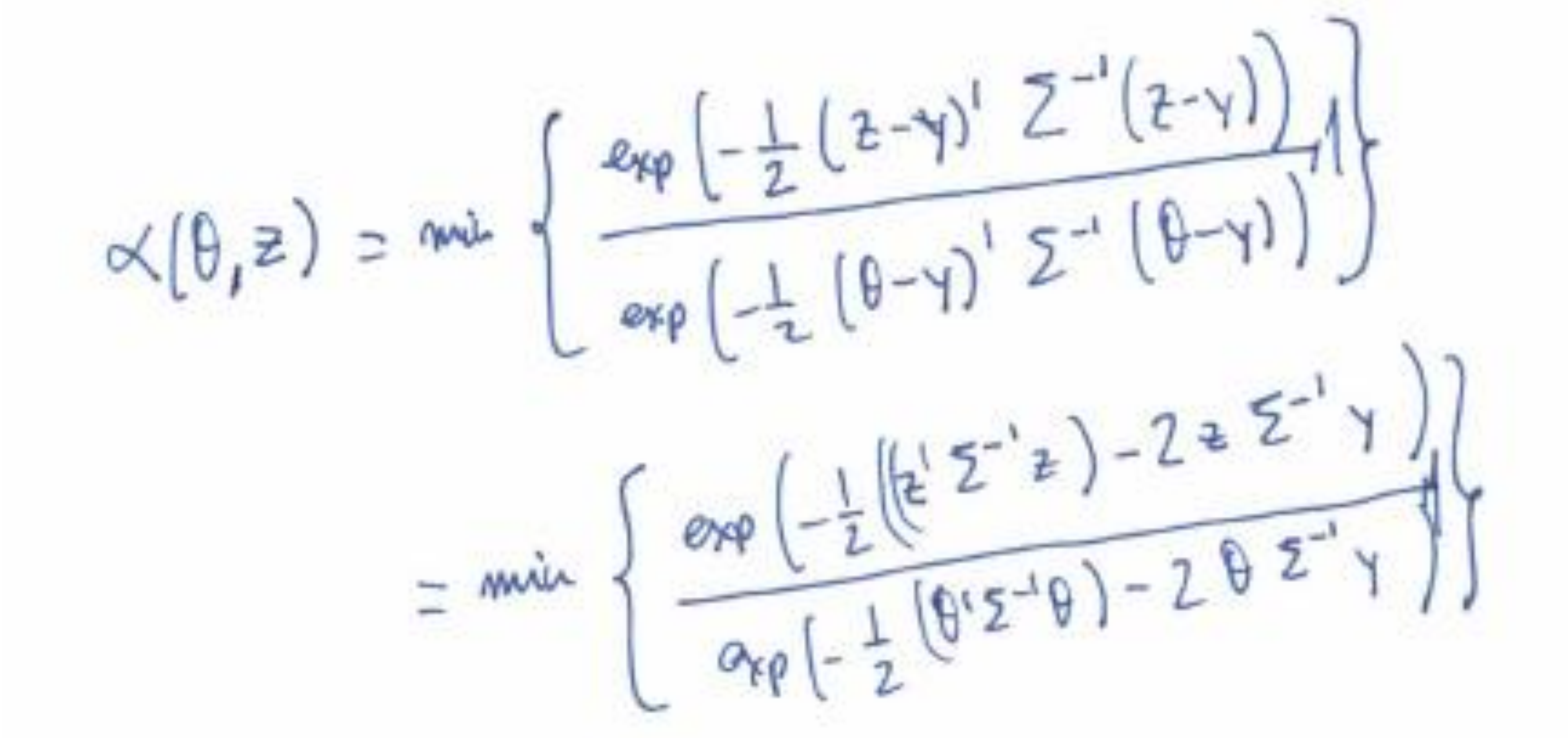
$$\theta_2 | \theta_1, y \sim N(y_2 + \rho(\theta_1 - y_1), 1-\rho^2)$$

```
$\theta_2^0$ ARBITRARY, $i = 1$
UNTIL CONVERGENCE
    $\theta_1^i \sim N(y_1 + \rho(\theta_2^{i-1} - y_2), 1-\rho^2)$
    $\theta_2^i \sim N(y_2 + \rho(\theta_1^i - y_1), 1-\rho^2)$
    $i = i+1$
```

# Sampling the bi-variate normal. Metropolis Hastings



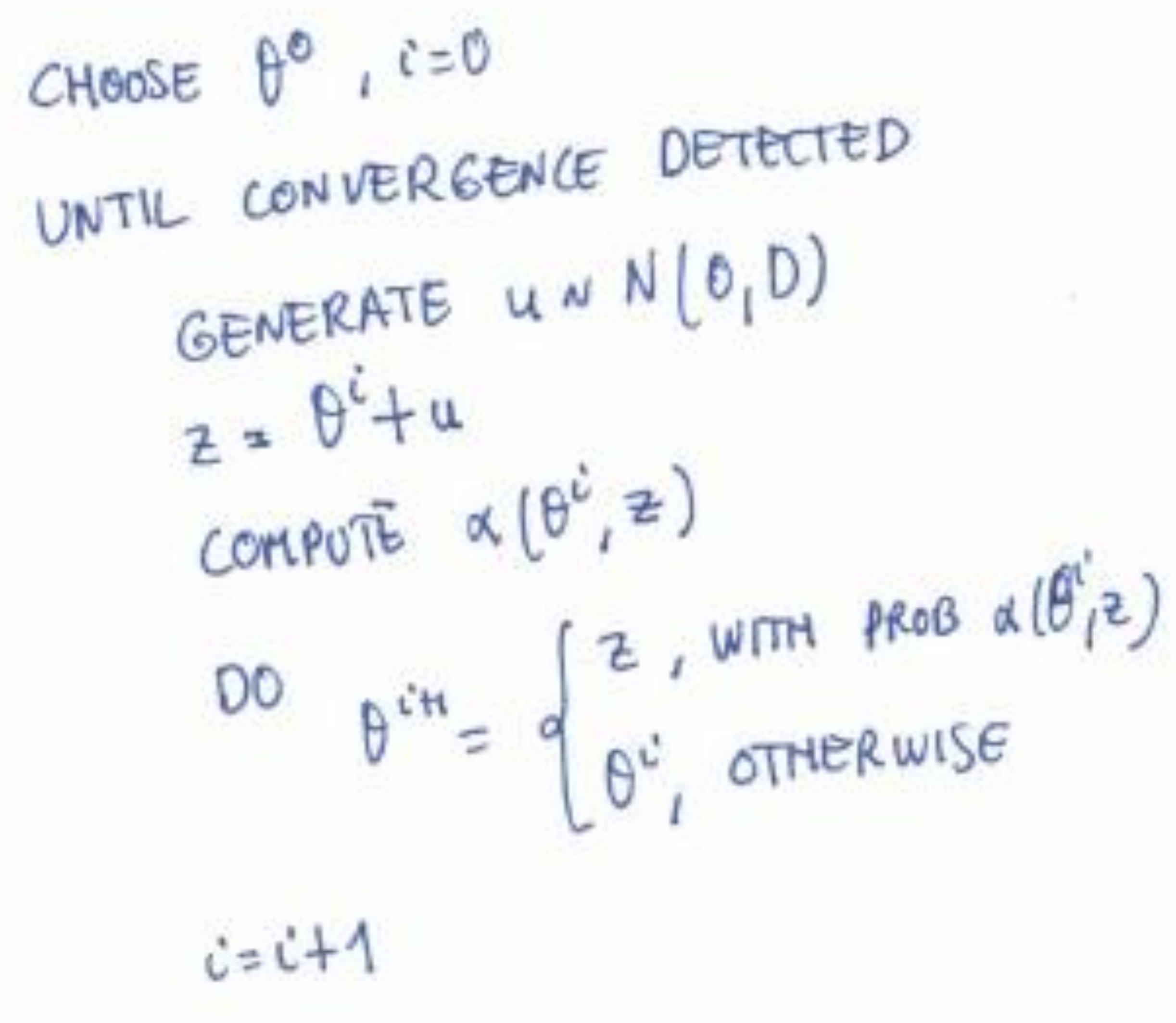
$$z = \theta + u \qquad u \sim N(0, D)$$



$$\alpha(\theta, z) = \min\left\{ \frac{\exp\left(-\frac{1}{2}(z-y)'\,\Sigma^{-1}(z-y)\right)}{\exp\left(-\frac{1}{2}(\theta-y)'\,\Sigma^{-1}(\theta-y)\right)}, 1 \right\}$$

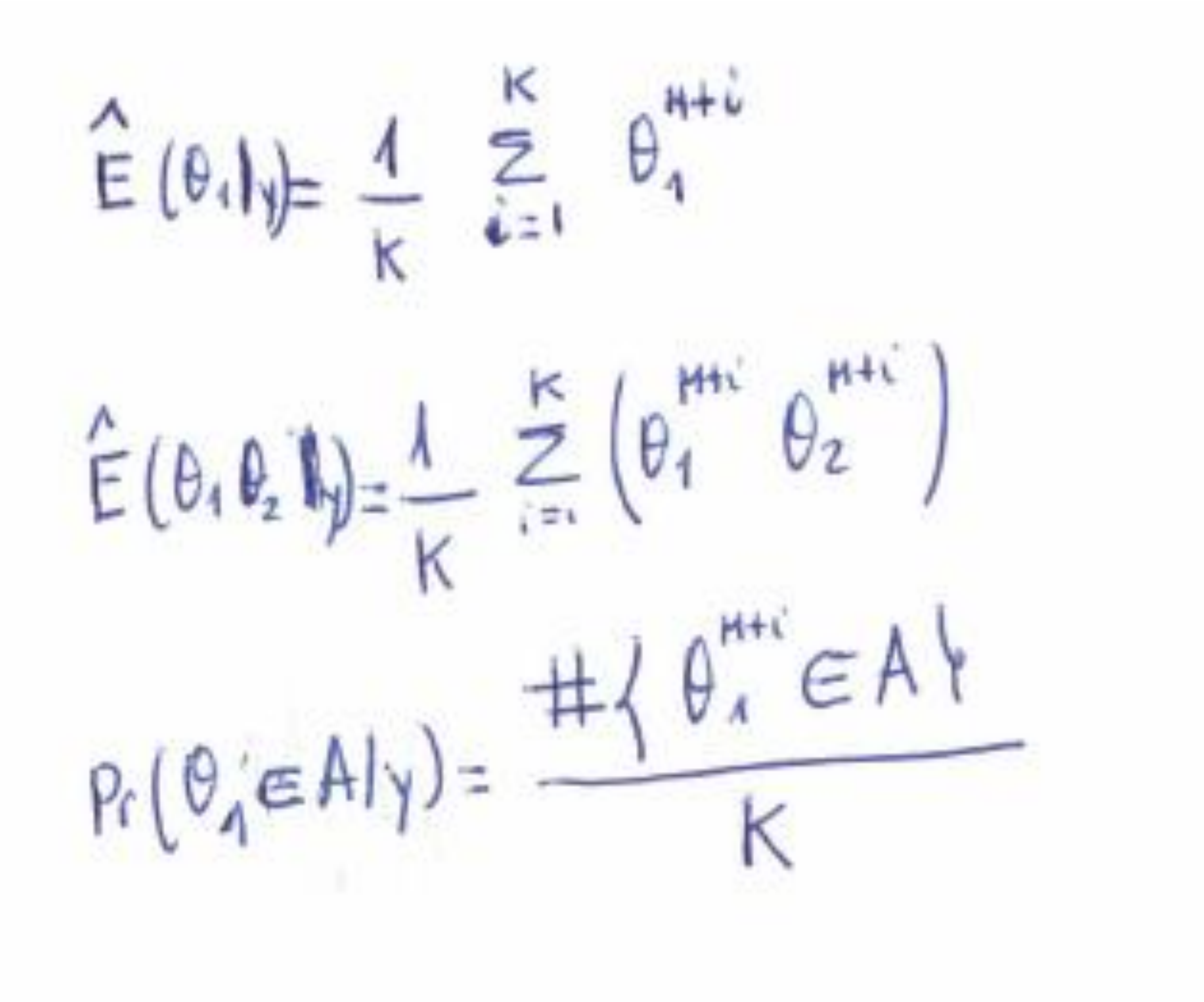
$$= \min\left\{ \frac{\exp\left(-\frac{1}{2}\left((z'\Sigma^{-1}z) - 2z\Sigma^{-1}y\right)\right)}{\exp\left(-\frac{1}{2}(\theta'\Sigma^{-1}\theta) - 2\theta\Sigma^{-1}y\right)}, 1 \right\}$$

# Sampling the bi-variate normal. Metropolis Hastings



```
CHOOSE $\theta^0$, $i=0$
UNTIL CONVERGENCE DETECTED
    GENERATE $u \sim N(0,D)$
    $z = \theta^i + u$
    COMPUTE $\alpha(\theta^i, z)$
    DO $\theta^{i+1} = \begin{cases} z, & \text{WITH PROB } \alpha(\theta^i, z) \\ \theta^i, & \text{OTHERWISE} \end{cases}$

    $i = i+1$
```

# Sampling the bi-variate normal. Answers….

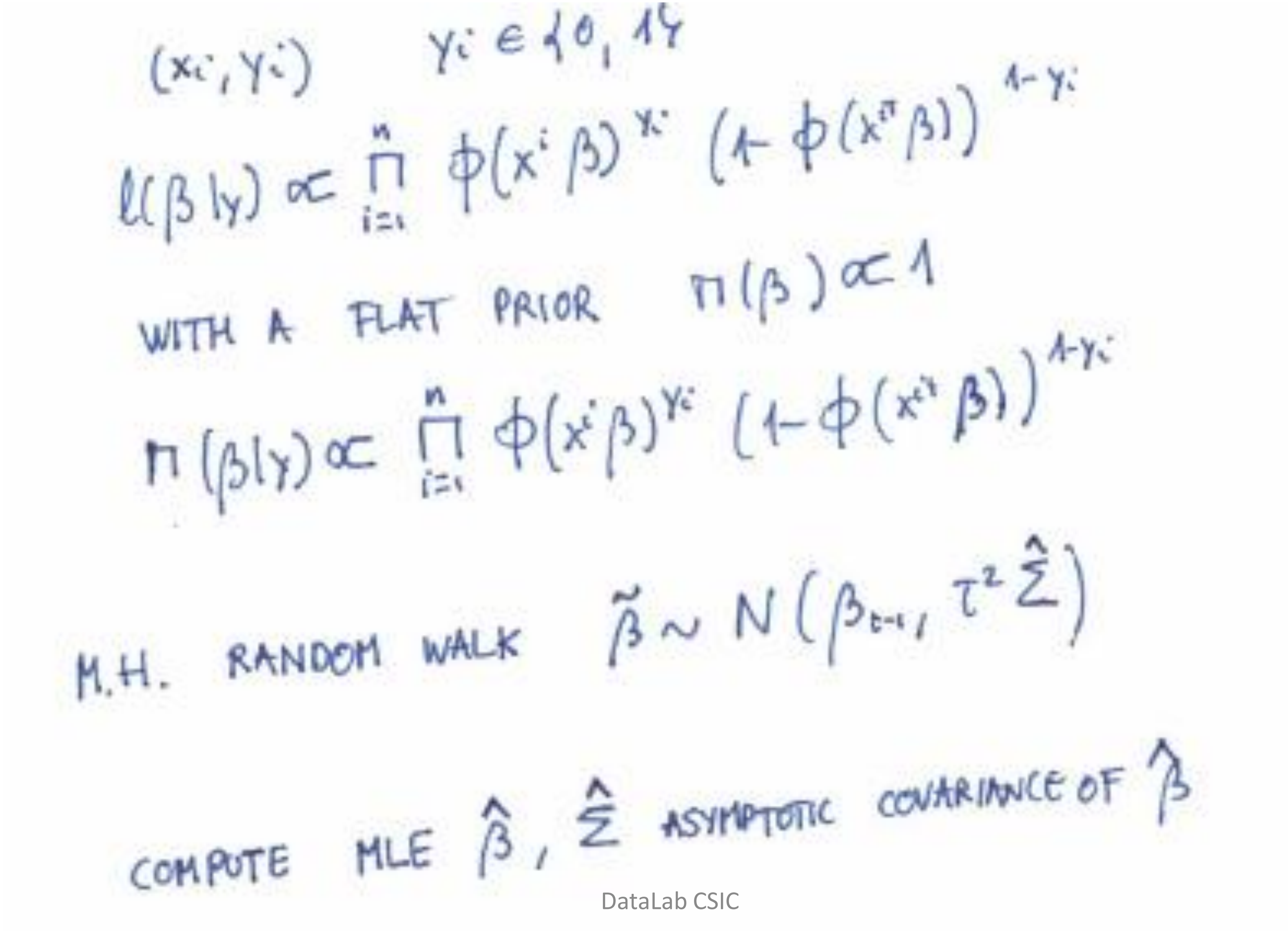


$$\hat{E}(\theta_1|y) = \frac{1}{K}\sum_{i=1}^{K} \theta_1^{M+i}$$

$$\hat{E}(\theta_1\theta_2|y) = \frac{1}{K}\sum_{i=1}^{K}\left(\theta_1^{M+i}\ \theta_2^{M+i}\right)$$

$$Pr(\theta_1' \in A|y) = \frac{\#\{\theta_1^{M+i} \in A\}}{K}$$

# Bayesian Probit Regression



$(x_i, y_i)$ $\quad y_i \in \{0, 1\}$

$$\ell(\beta|y) \propto \prod_{i=1}^{n} \phi(x^i \beta)^{y_i} \left(1 - \phi(x^{iT} \beta)\right)^{1-y_i}$$

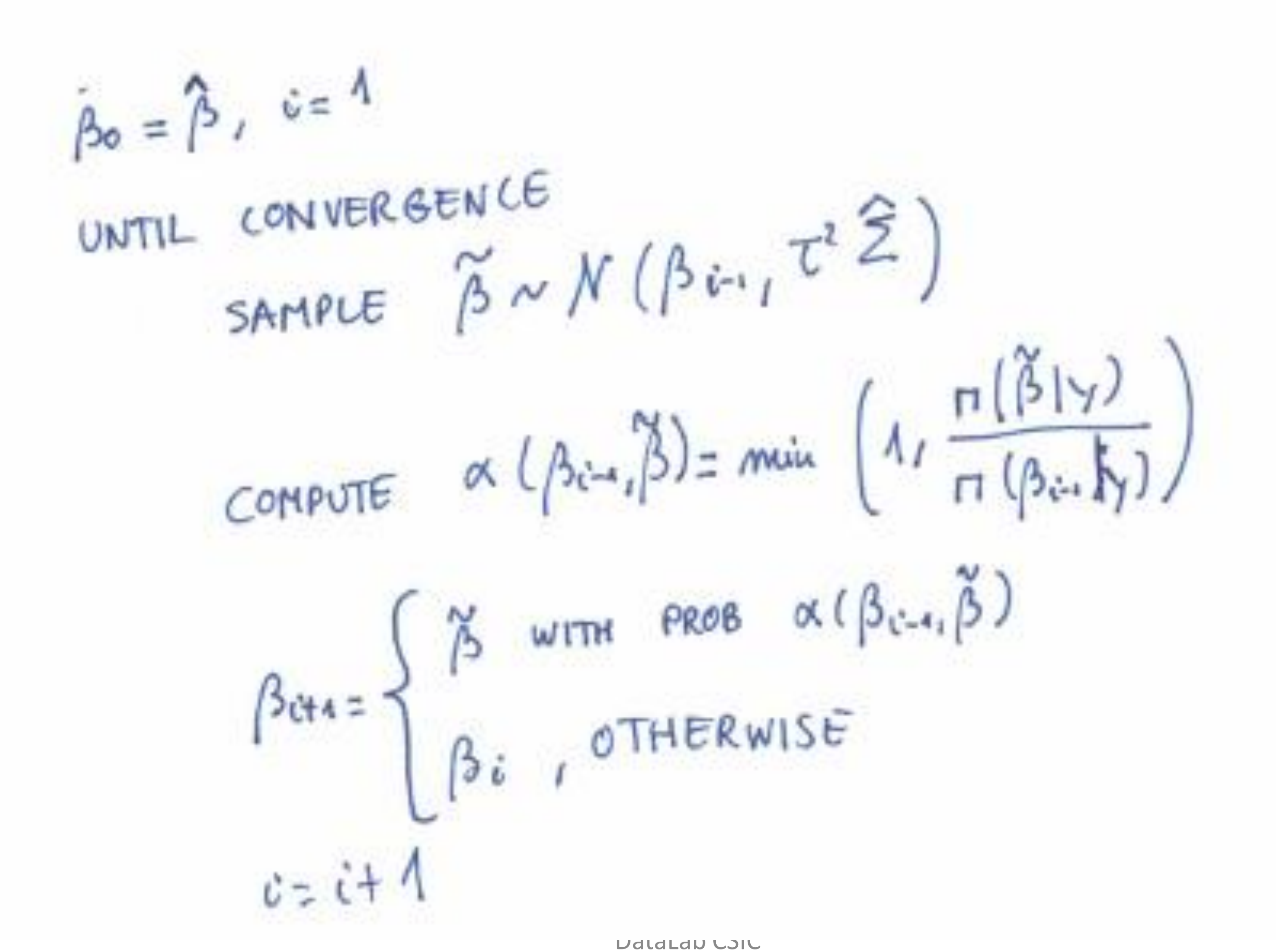
WITH A FLAT PRIOR $\pi(\beta) \propto 1$

$$\pi(\beta|y) \propto \prod_{i=1}^{n} \phi(x^i \beta)^{y_i} \left(1 - \phi(x^{iT} \beta)\right)^{1-y_i}$$

M.H. RANDOM WALK $\tilde{\beta} \sim N(\beta_{t-1}, \tau^2 \hat{\Sigma})$

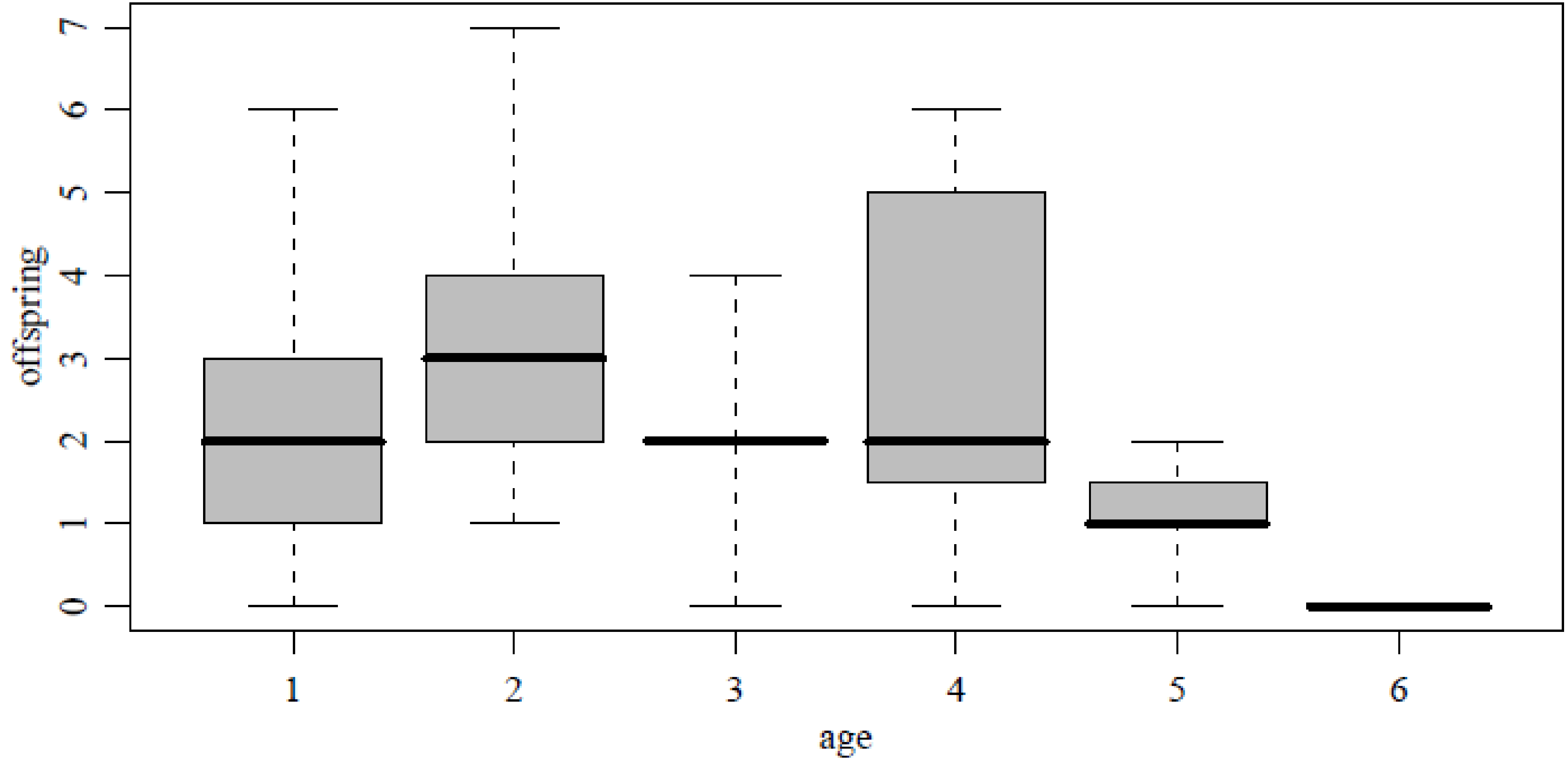
COMPUTE MLE $\hat{\beta}$, $\hat{\Sigma}$ ASYMPTOTIC COVARIANCE OF $\hat{\beta}$

# Bayesian Probit Regression  MH



```
$\beta_0 = \hat{\beta}$, $i = 1$
UNTIL CONVERGENCE
    SAMPLE $\tilde{\beta} \sim N(\beta_{i-1}, \tau^2 \hat{\Sigma})$
    COMPUTE $\alpha(\beta_{i-1}, \tilde{\beta}) = \min\left(1, \frac{\pi(\tilde{\beta}|y)}{\pi(\beta_{i-1}|y)}\right)$
    $\beta_{i+1} = \begin{cases} \tilde{\beta} & \text{WITH PROB } \alpha(\beta_{i-1}, \tilde{\beta}) \\ \beta_i, & \text{OTHERWISE} \end{cases}$
    $i = i + 1$
```

# Bayesian Poisson Regression. Offspring of birds given age



# Bayesian Poisson Regression

Offspring Y given age?? Per age?? Linear??

$$Y|x \sim \text{POISSON}(\theta_x)$$

$$\theta_x = \beta_1 + \beta_2 x + \beta_3 x^2 ??$$

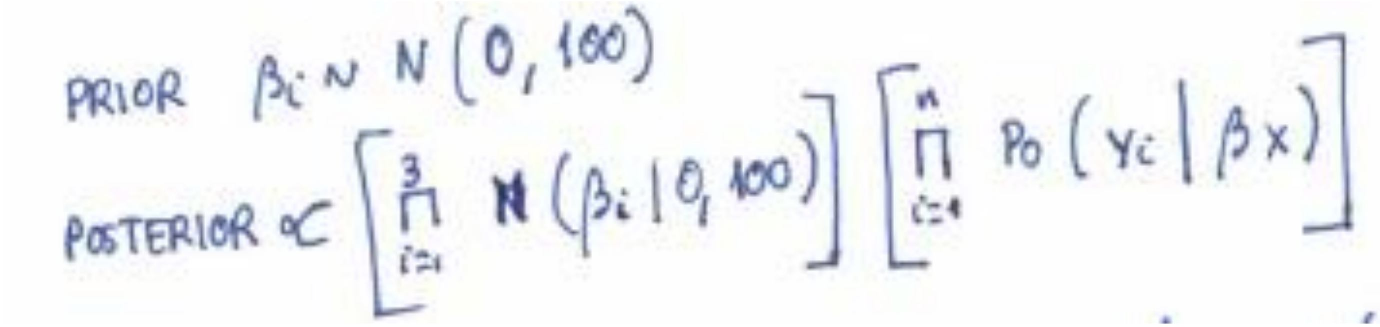
$$\log \theta_x = \beta_1 + \beta_2 x + \beta_3 x^2$$

$$E(Y|x) = \exp(\beta_1 + \beta_2 x + \beta_3 x^2)$$

$$Y|x \sim \text{POISSON}(\exp(\beta^T x))$$

# Bayesian Poisson Regression

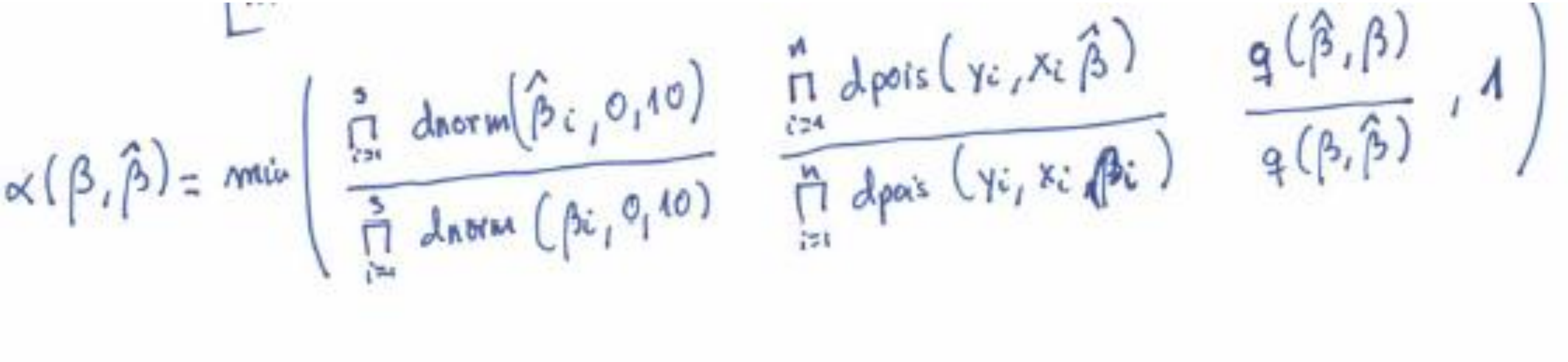
## Prior and posterior



PRIOR $\beta_i \sim N(0, 100)$

POSTERIOR $\propto \left[\prod_{i=1}^{3} N(\beta_i \mid 0, 100)\right] \left[\prod_{i=1}^{n} Po(y_i \mid \beta x)\right]$

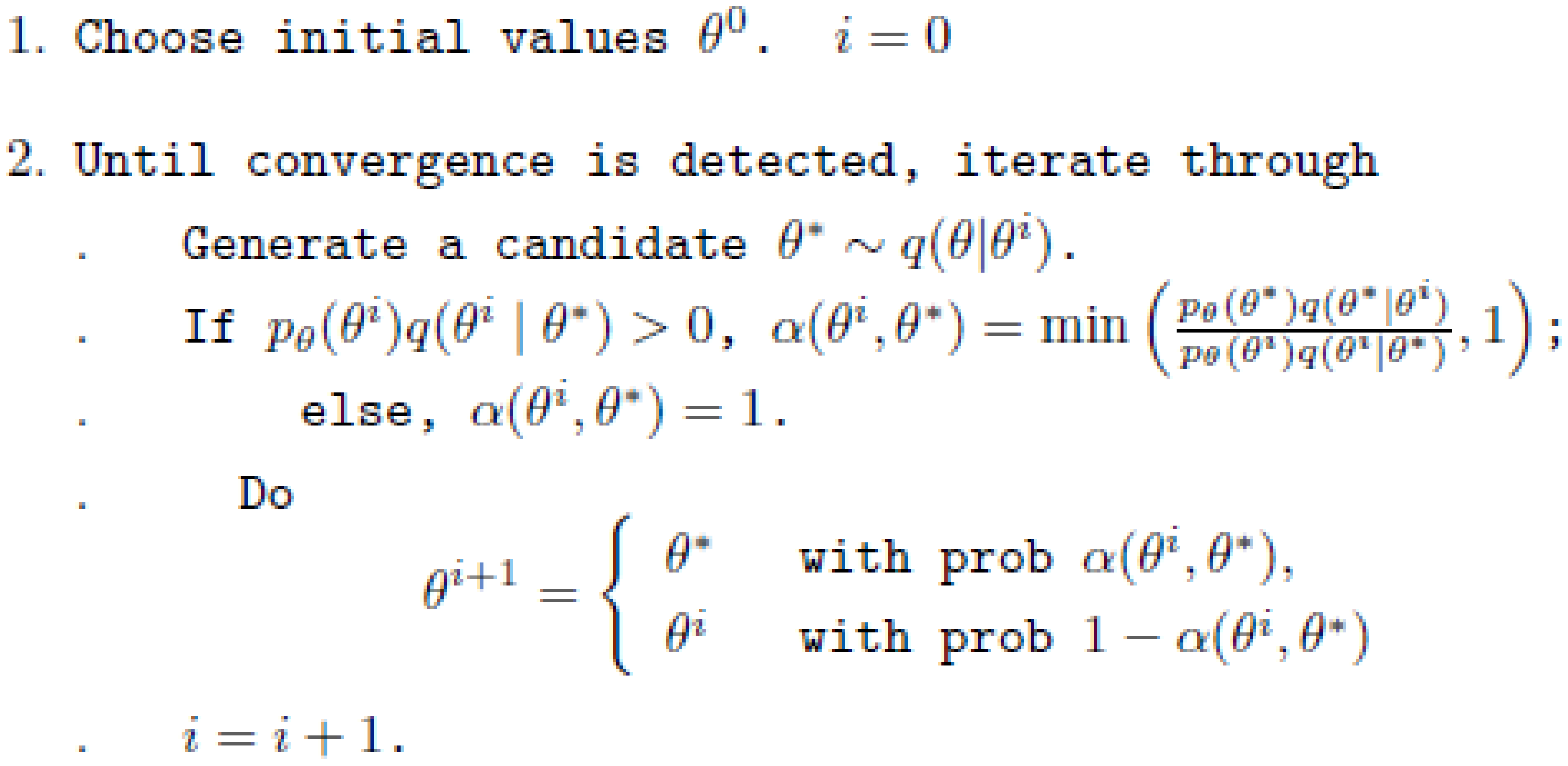
## Acceptance probability in MH



$$\alpha(\beta, \hat{\beta}) = \min \left( \frac{\prod_{i=1}^{3} dnorm(\hat{\beta}_i, 0, 10)}{\prod_{i=1}^{3} dnorm(\beta_i, 0, 10)} \; \frac{\prod_{i=1}^{n} dpois(y_i, x_i \hat{\beta})}{\prod_{i=1}^{n} dpois(y_i, x_i \beta_i)} \; \frac{q(\hat{\beta}, \beta)}{q(\beta, \hat{\beta})}, 1 \right)$$

# MH  theory

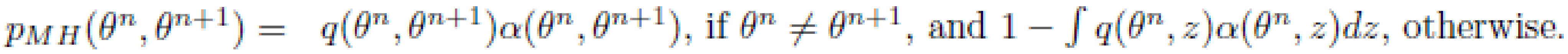
# Recall



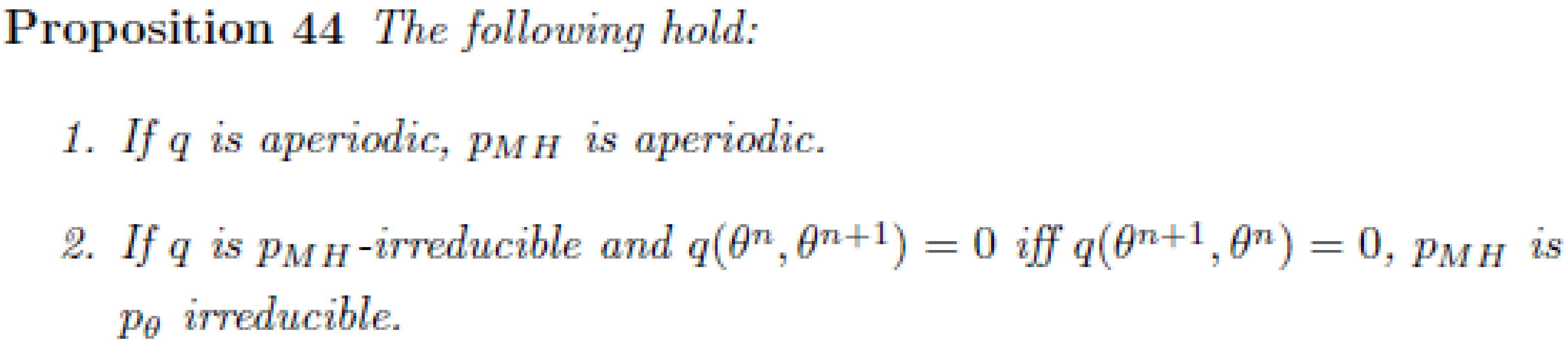
```
1. Choose initial values $\theta^0$.   $i = 0$

2. Until convergence is detected, iterate through
   .   Generate a candidate $\theta^* \sim q(\theta|\theta^i)$.
   .   If $p_\theta(\theta^i)q(\theta^i \mid \theta^*) > 0$, $\alpha(\theta^i,\theta^*) = \min\left(\frac{p_\theta(\theta^*)q(\theta^*|\theta^i)}{p_\theta(\theta^i)q(\theta^i|\theta^*)}, 1\right)$;
   .       else, $\alpha(\theta^i,\theta^*) = 1$.
   .     Do
             $\theta^{i+1} = \begin{cases} \theta^* & \text{with prob } \alpha(\theta^i,\theta^*), \\ \theta^i & \text{with prob } 1-\alpha(\theta^i,\theta^*) \end{cases}$
   .   $i = i + 1$.
```

# Convergence

Kernel



$p_{MH}(\theta^n, \theta^{n+1}) = \; q(\theta^n, \theta^{n+1})\alpha(\theta^n, \theta^{n+1})$, if $\theta^n \neq \theta^{n+1}$, and $1 - \int q(\theta^n, z)\alpha(\theta^n, z)dz$, otherwise.



**Proposition 44** *The following hold:*

1. *If $q$ is aperiodic, $p_{MH}$ is aperiodic.*
2. *If $q$ is $p_{MH}$-irreducible and $q(\theta^n, \theta^{n+1}) = 0$ iff $q(\theta^{n+1}, \theta^n) = 0$, $p_{MH}$ is $p_\theta$ irreducible.*

# Hybrid algos

# Typical situation

Frequently

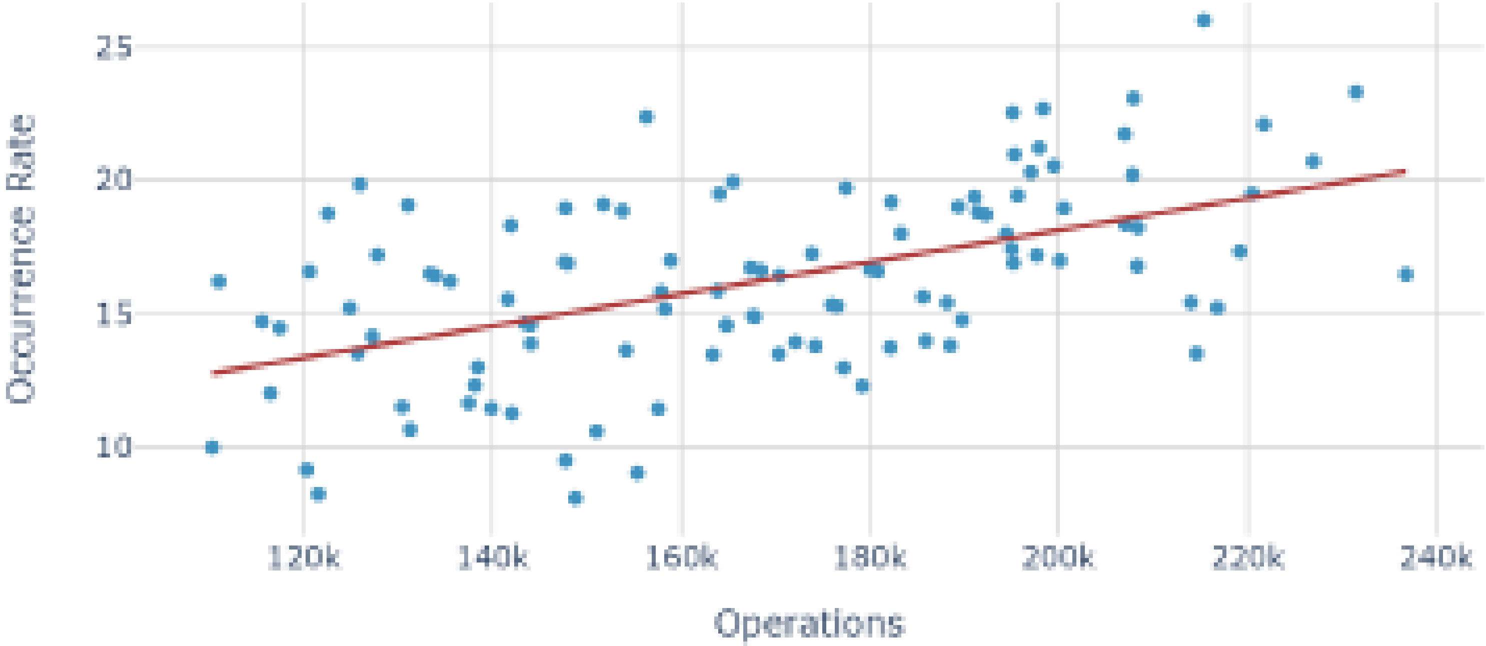
1. Some posterior conditionals available for efficient sampling
2. For others, just known up to a constant

Hybrid samplers

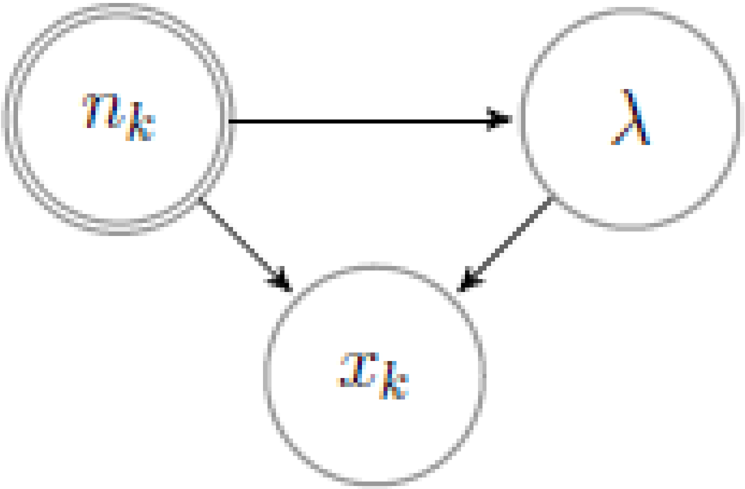
- Gibbs steps for type 1 conditionals
- MH steps for type 2 conditionals

# Case study: Aviation safety

## Development of National Aviation Safety Plan. TCAS warnings



# Aviation safety. Stress effect



$$x_k|\lambda, n_k \sim Po(\lambda n_k),$$

$$\lambda = a n_k + b + \epsilon_k, \quad \epsilon_k \sim N(0, \sigma^2),$$

$$a \sim N(\mu_a, \sigma_a^2), \quad b \sim N(\mu_b, \sigma_b^2), \quad \sigma^2 \sim Inv\text{-}Gamma(\alpha, \beta)$$

# Aviation safety. Stress effect

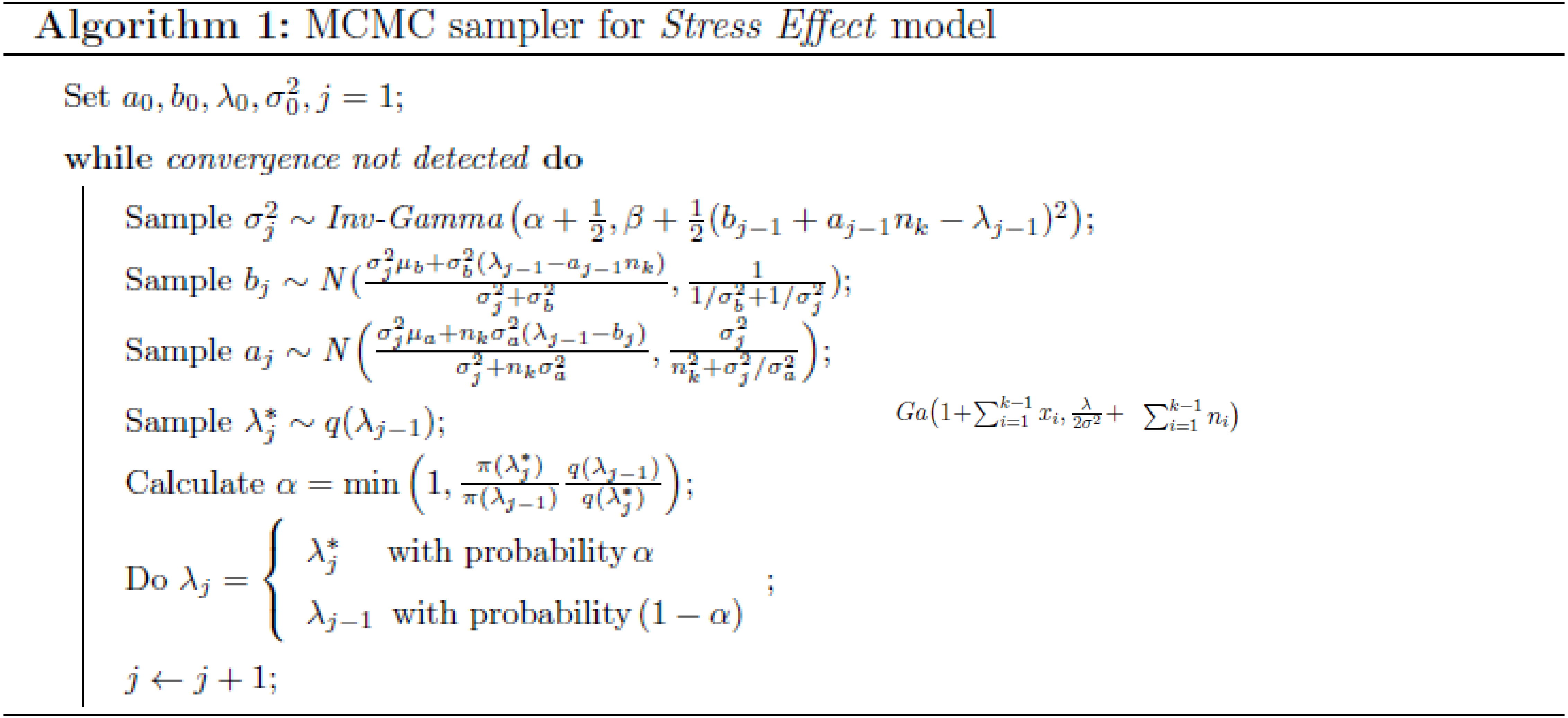
Posterior proportional to

$$\lambda^{\sum_{i=1}^{k-1} x_i} \sigma^{-3-2\alpha} \exp\left( -\lambda \sum_{i=1}^{k-1} n_i - \frac{(\lambda - a n_k - b)^2}{2\sigma^2} - \frac{(a-\mu_a)^2}{2\sigma_a^2} - \frac{(b-\mu_b)^2}{2\sigma_b^2} - \frac{\beta}{\sigma^2} \right)$$

Posterior conditionals

$$\begin{aligned}
p(a|\lambda, b, \sigma^2, D_k) &\sim N\left( a \,\middle|\, \frac{\sigma^2\mu_a + n_k\sigma_a^2(\lambda - b)}{\sigma^2 + n_k\sigma_a^2}, \frac{\sigma^2}{n_k^2 + \sigma^2/\sigma_a^2} \right), \\
p(b|\lambda, a, \sigma^2, D_k) &\sim N\left( b \,\middle|\, \frac{\sigma^2\mu_b + \sigma_b^2(\lambda - a n_k)}{\sigma^2 + \sigma_b^2}, \frac{1}{1/\sigma_b^2 + 1/\sigma^2} \right), \\
p(\sigma^2|\lambda, a, b, D_k) &\sim \mathit{Inv\text{-}Gamma}\left( \sigma^2 \,\middle|\, \alpha + \frac{1}{2}, \beta + \frac{1}{2}(b + a n_k - \lambda)^2 \right), \\
p(\lambda|a, b, \sigma^2, D_k) &\propto \lambda^{\sum x_i} \exp\left( -\frac{1}{2\sigma^2} \left( \lambda^2 - 2\lambda \left( a n_k + b - \sigma^2 \sum n_i \right) \right) \right).
\end{aligned}$$

# Aviation safety. Stress effect  algo



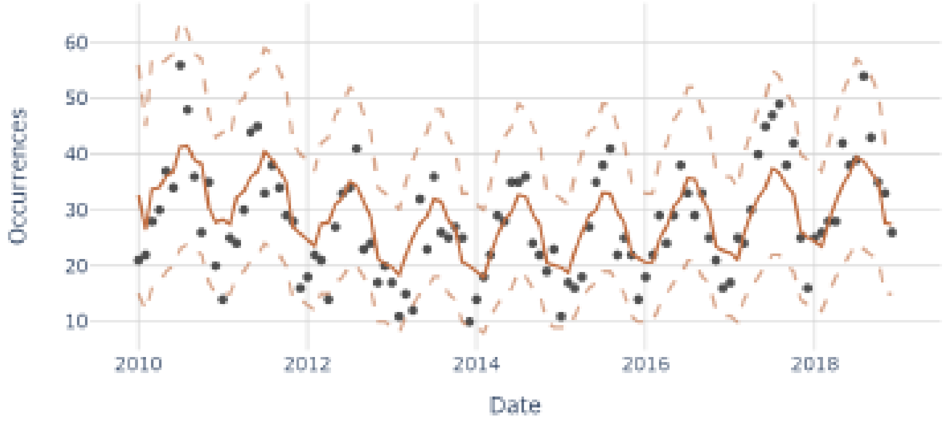
**Algorithm 1:** MCMC sampler for *Stress Effect* model

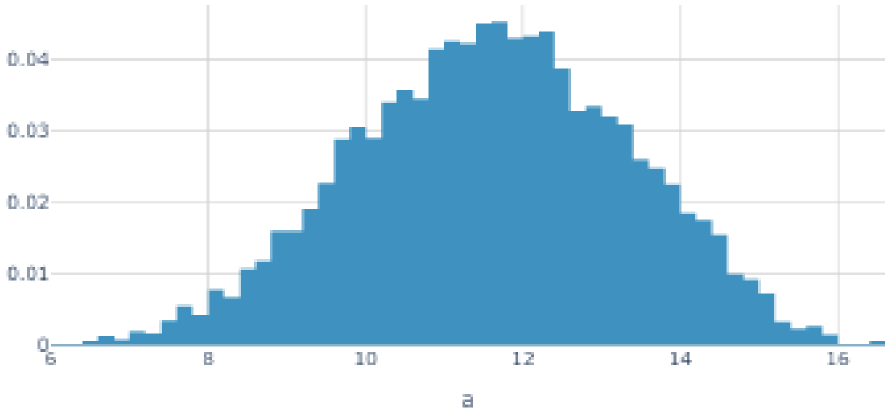
```
Set $a_0, b_0, \lambda_0, \sigma_0^2, j = 1$;
while convergence not detected do
    Sample $\sigma_j^2 \sim \mathit{Inv\text{-}Gamma}\left(\alpha + \frac{1}{2}, \beta + \frac{1}{2}(b_{j-1} + a_{j-1}n_k - \lambda_{j-1})^2\right)$;
    Sample $b_j \sim N(\frac{\sigma_j^2\mu_b + \sigma_b^2(\lambda_{j-1} - a_{j-1}n_k)}{\sigma_j^2 + \sigma_b^2}, \frac{1}{1/\sigma_b^2 + 1/\sigma_j^2})$;
    Sample $a_j \sim N\left(\frac{\sigma_j^2\mu_a + n_k\sigma_a^2(\lambda_{j-1} - b_j)}{\sigma_j^2 + n_k\sigma_a^2}, \frac{\sigma_j^2}{n_k^2 + \sigma_j^2/\sigma_a^2}\right)$;
    Sample $\lambda_j^* \sim q(\lambda_{j-1})$;
    Calculate $\alpha = \min\left(1, \frac{\pi(\lambda_j^*)}{\pi(\lambda_{j-1})}\frac{q(\lambda_{j-1})}{q(\lambda_j^*)}\right)$;
    Do $\lambda_j = \begin{cases} \lambda_j^* & \text{with probability}\,\alpha \\ \lambda_{j-1} & \text{with probability}\,(1-\alpha) \end{cases}$;
    $j \leftarrow j + 1$;
```

$Ga\left(1+\sum_{i=1}^{k-1} x_i, \frac{\lambda}{2\sigma^2}+ \ \sum_{i=1}^{k-1} n_i\right)$

# Aviation safety. Uses

$$Pr(x_k = z|D_k) = \iiiint Pr(x_k = z|\lambda, n_k)\, p(\lambda|a, b, \sigma^2, D_k)\, p(a, b, \sigma^2|D_k)\, d\lambda\, da\, db\, d\sigma^2$$
$$\approx \frac{1}{N}\sum_{j=1}^{N} Pr(x_k = z|\lambda_j, n_k) = \frac{n_k^z}{N z!}\sum_{j=1}^{N} \exp(-\lambda_j n_k)\, (\lambda_j)^z\,,$$





# Comments

Gibbs requires more analysis. Not always feasible

Metropolis requires less analysis. Not so fast. More automatic

Recall potentially severe autocorrelation problems, slow mixing, convergence,…

# c. Hamiltonian Monte Carlo

# Brief description

We have introduced MCMC, Gibbs sampling and Metropolis-Hastings

We focus here on Hamiltonian Monte Carlo HMC

# Sources

Sources:

BDA3 (2015) 12.4 and 12.5

Thomas and Tu. Learning HMC in R

Betancourt. A conceptual intro to HMC

Neal. MCMC using Hamiltonian dynamics

# Labs

3.3 Hamiltonian MC

Multivariate normal

Hmclearn: Linear regression, Logistic regression (ecology)

Stan afterwards!!

# Hamiltonian MC. Basics

# HMC. Pros and cons

- Improved computational efficiency over MH et al (specially in high dimensional complex problems)

- Difficulties in implementation…. But Stan is available now: automates tuning of HMC parameters (and can be called from R and Python)
- But Stan a bit of a black box, hmclearn+this session before going through it

- Still insufficient for Bayesian analysis of deep learning models… soon

# The drawback of MH

Balance condition in MH and M algos. Current x, proposed y

$$\alpha(x,y) = \begin{cases} \min\left(\frac{\pi(y)\, q(y,x)}{\pi(x)\, q(x,y)}, 1\right), & \text{IF } \pi(x)\, q(x,y) > 0 \\ 1, & \text{OTHERWISE} \end{cases}$$

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

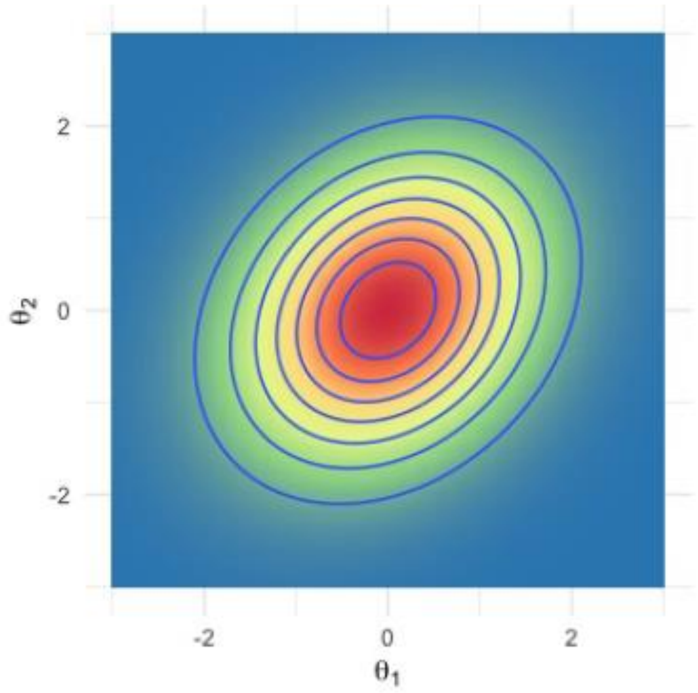
Frequents regions of higher posterior density.  Sample from the right region

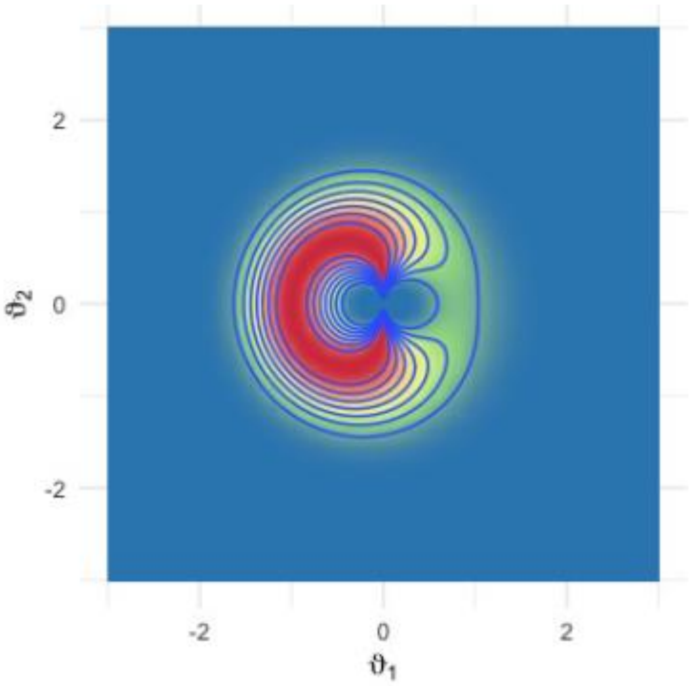
Ocasionally visits low density regions. Fully explore the sample space

As proposals are random, may take quite some time to get in HPD regions

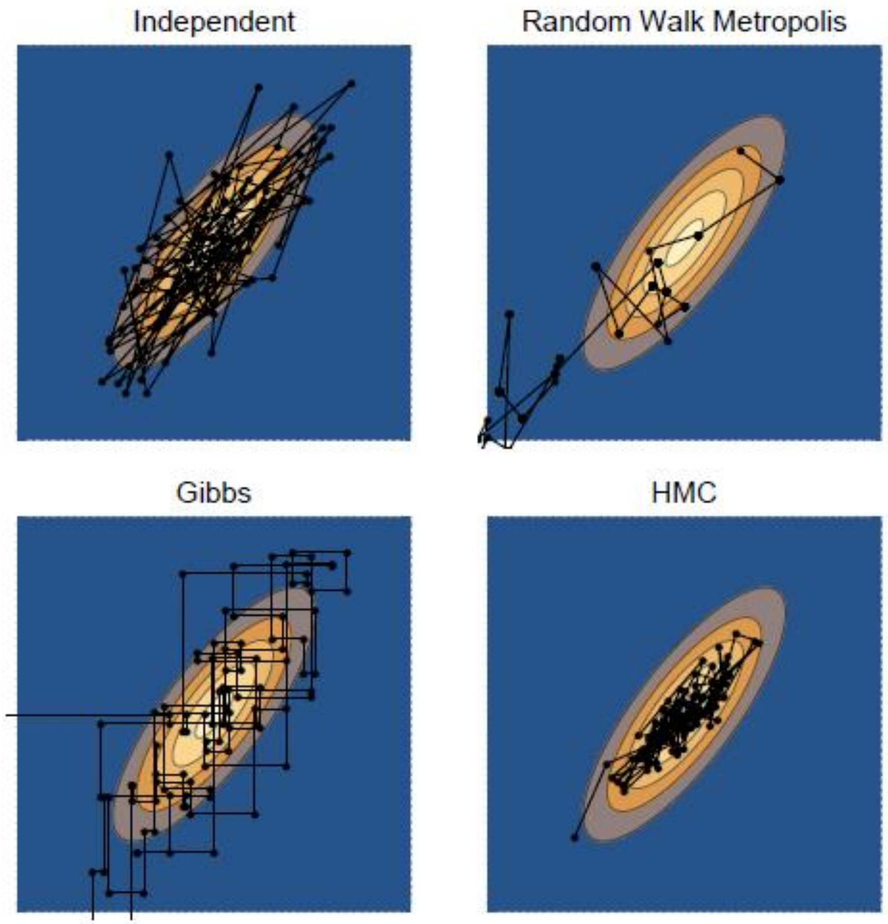
May get stuck

# The drawback of MH





# Comparing four MCMC algos



# HMC. Qualitative description

- A guided proposal generation scheme

- Uses the gradient of log posterior to direct MC towards HPD regions:

A well-tuned HMC accepts proposals at much higher rate than MH

- But still samples the tails properly

# HMC. Idea

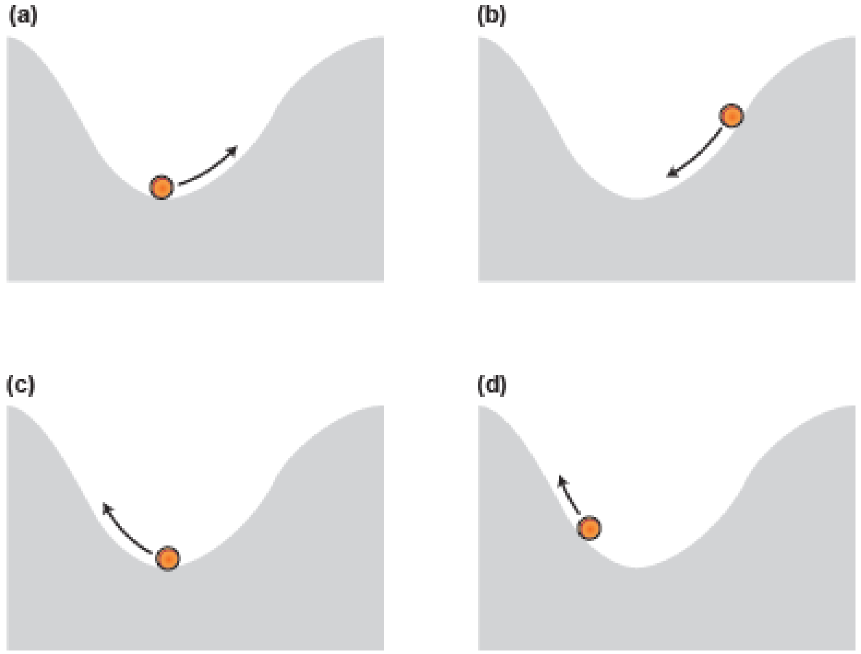
f is the posterior

-log (f) inverse bell-shaped

lower values reached guided by its gradient

In classical mechanics, exchanges between kinetic and potential energy dictate location through hamiltonian equations

( $\theta, p$) horizontal and vertical positions. p is a momentum (auxiliary variable to actually simulate from $\theta$) mass x velocity



# Hamiltonian equations and MCMC

Target is posterior. Auxiliary momentum (same dimension)

$$\theta \sim f(\theta) \qquad \dim(\theta) = \dim(p)$$

Hamiltonian as potential + kinetic

$$H(\theta, p) = U(\theta) + K(p)$$

$$U(\theta) = -\log f(\theta) \qquad p \sim N(0, M)$$

$$H(\theta, p) = -\log f(\theta) + \frac{1}{2} p^T M^{-1} p$$

Hamiltonian equations

$$\left.\begin{aligned} \frac{dp}{dt} &= -\frac{\partial H(\theta, p)}{\partial \theta} = \nabla_\theta \log(f(\theta)) \\ \frac{d\theta}{dt} &= \frac{\partial H(\theta, p)}{\partial p} = M^{-1} p \end{aligned}\right] (\theta, p)$$

# Hamiltonian equations through leapfrog

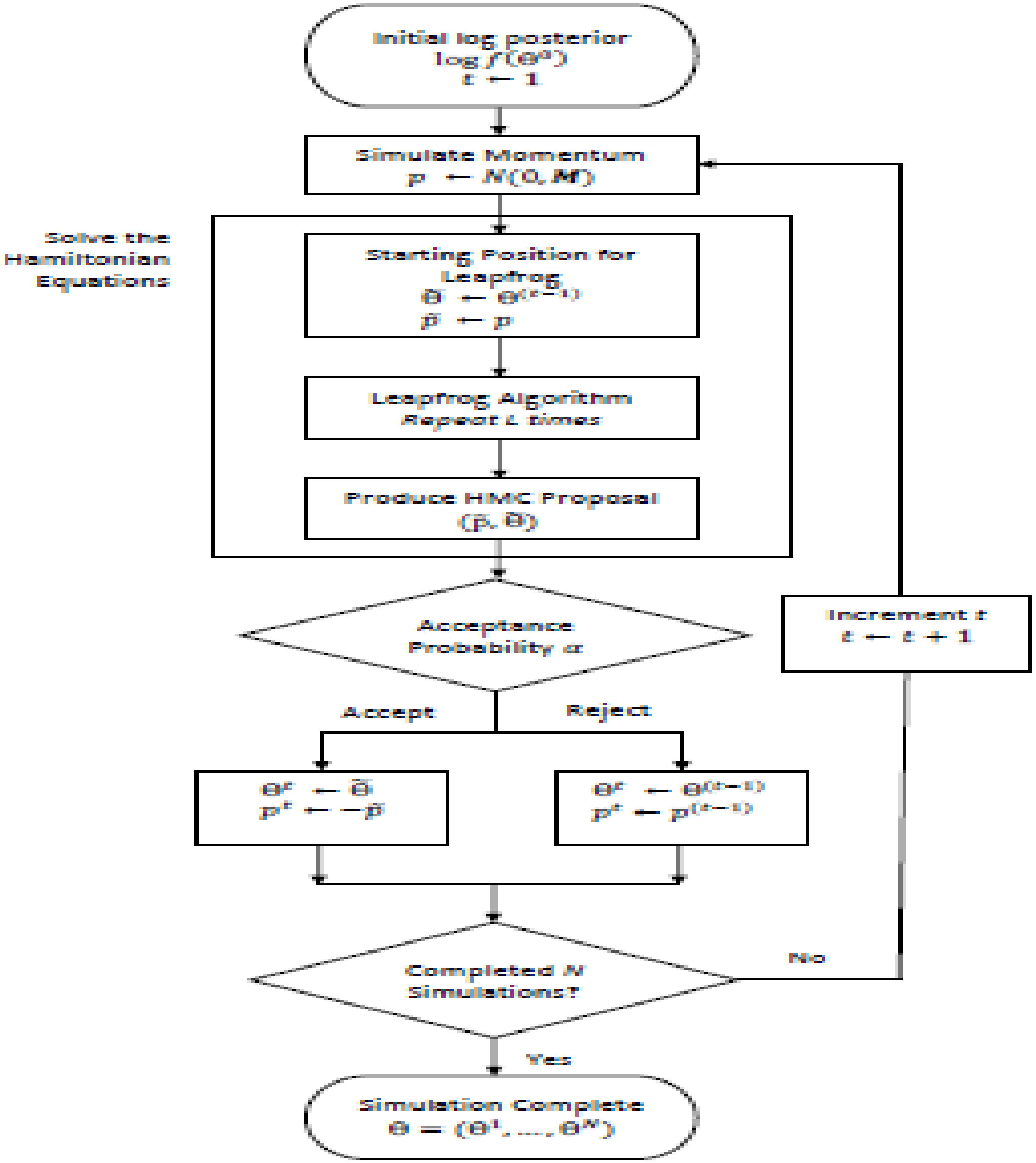
$$\left.\begin{aligned} \frac{dp}{dt} &= -\frac{\partial H(\theta,p)}{\partial \theta} = \nabla_\theta \log(f(\theta)) \\ \frac{d\theta}{dt} &= \frac{\partial H(\theta,p)}{\partial p} = M^{-1} p \end{aligned}\right] (\theta,p)$$

$$\mathbf{p}(t+\epsilon/2) = \mathbf{p}(t) + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\boldsymbol{\theta}(t)),$$

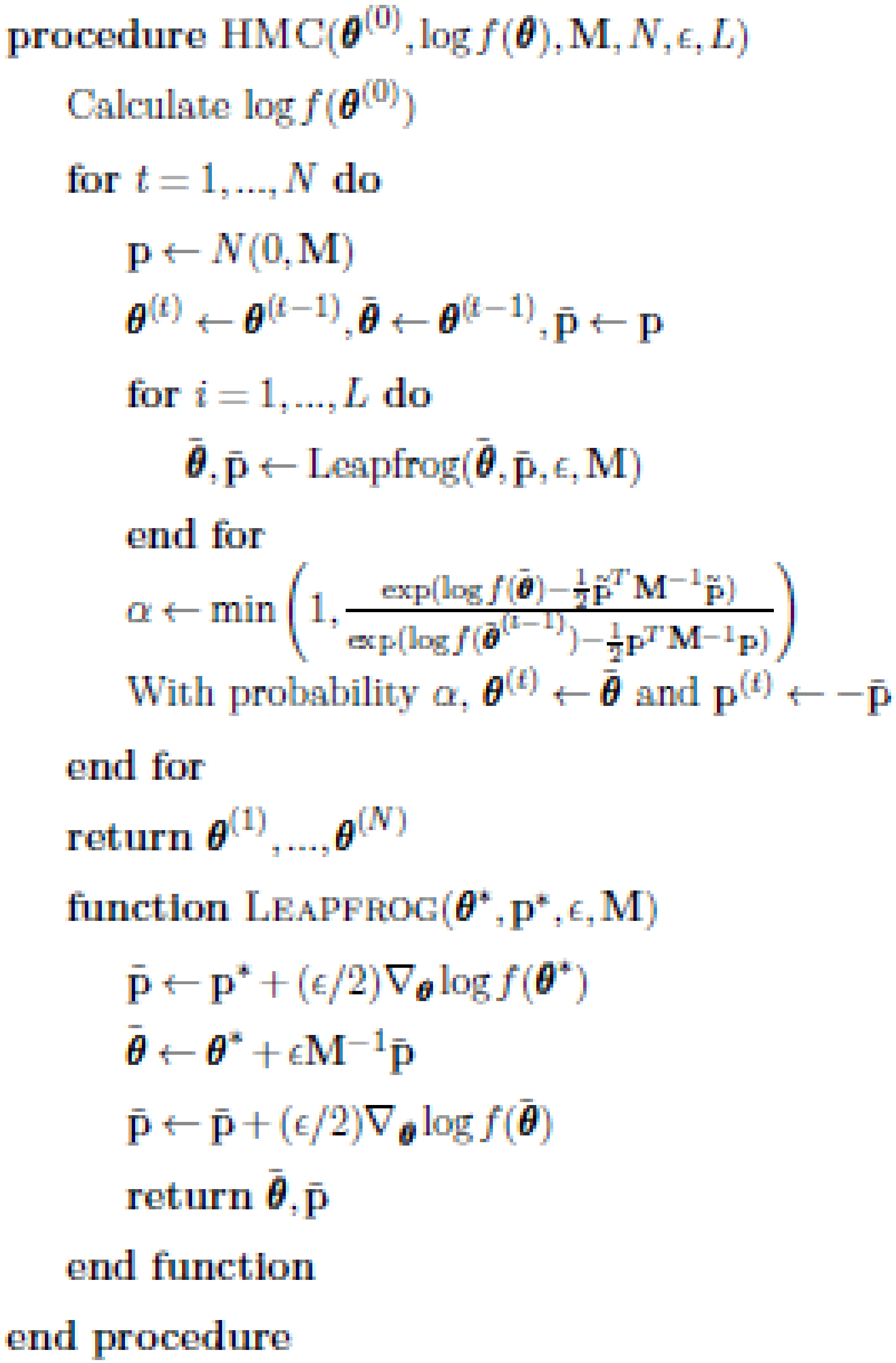
$$\boldsymbol{\theta}(t+\epsilon) = \boldsymbol{\theta}(t) + \epsilon \mathbf{M}^{-1}\mathbf{p}(t+\epsilon/2),$$

$$\mathbf{p}(t+\epsilon) = \mathbf{p}(t+\epsilon/2) + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\boldsymbol{\theta}(t+\epsilon)).$$

# HMC. Algo I


Initial log posterior
$\log f(\theta^0)$
$t \leftarrow 1$
Simulate Momentum
$p \leftarrow N(0, M)$
Solve the Hamiltonian Equations
Starting Position for Leapfrog
$\tilde{\theta} \leftarrow \theta^{(t-1)}$
$\tilde{p} \leftarrow p$
Leapfrog Algorithm
*Repeat L times*
Produce HMC Proposal
$(\tilde{p}, \tilde{\theta})$
Acceptance Probability $\alpha$
Accept
Reject
$\theta^t \leftarrow \tilde{\theta}$
$p^t \leftarrow -\tilde{p}$
$\theta^t \leftarrow \theta^{(t-1)}$
$p^t \leftarrow p^{(t-1)}$
Completed $N$ Simulations?
No
Yes
Increment $t$
$t \leftarrow t + 1$
Simulation Complete
$\theta = (\theta^1, \ldots, \theta^N)$

# HMC. Algo II



```
procedure HMC($\boldsymbol{\theta}^{(0)}, \log f(\boldsymbol{\theta}), \mathrm{M}, N, \epsilon, L$)
    Calculate $\log f(\boldsymbol{\theta}^{(0)})$
    for $t = 1, ..., N$ do
        $\mathrm{p} \leftarrow N(0, \mathrm{M})$
        $\boldsymbol{\theta}^{(t)} \leftarrow \boldsymbol{\theta}^{(t-1)}, \bar{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta}^{(t-1)}, \bar{\mathrm{p}} \leftarrow \mathrm{p}$
        for $i = 1, ..., L$ do
            $\bar{\boldsymbol{\theta}}, \bar{\mathrm{p}} \leftarrow \mathrm{Leapfrog}(\bar{\boldsymbol{\theta}}, \bar{\mathrm{p}}, \epsilon, \mathrm{M})$
        end for
        $\alpha \leftarrow \min\left(1, \frac{\exp(\log f(\bar{\boldsymbol{\theta}}) - \frac{1}{2}\bar{\mathrm{p}}^T \mathbf{M}^{-1} \bar{\mathrm{p}})}{\exp(\log f(\bar{\boldsymbol{\theta}}^{(t-1)}) - \frac{1}{2}\mathrm{p}^T \mathbf{M}^{-1} \mathrm{p})}\right)$
        With probability $\alpha$, $\boldsymbol{\theta}^{(t)} \leftarrow \bar{\boldsymbol{\theta}}$ and $\mathrm{p}^{(t)} \leftarrow -\bar{\mathrm{p}}$
    end for
    return $\boldsymbol{\theta}^{(1)}, ..., \boldsymbol{\theta}^{(N)}$
    function LEAPFROG($\boldsymbol{\theta}^*, \mathrm{p}^*, \epsilon, \mathrm{M}$)
        $\bar{\mathrm{p}} \leftarrow \mathrm{p}^* + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\boldsymbol{\theta}^*)$
        $\bar{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta}^* + \epsilon \mathrm{M}^{-1} \bar{\mathrm{p}}$
        $\bar{\mathrm{p}} \leftarrow \bar{\mathrm{p}} + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\bar{\boldsymbol{\theta}})$
        return $\bar{\boldsymbol{\theta}}, \bar{\mathrm{p}}$
    end function
end procedure
```

# HMC Tuning

epsilon.  Small relative to parameter of interest

x Number of leapfrog steps. L small, random walk nature

L large, wasted computation

Jointly acceptance rate of 65%

Examine for correlations

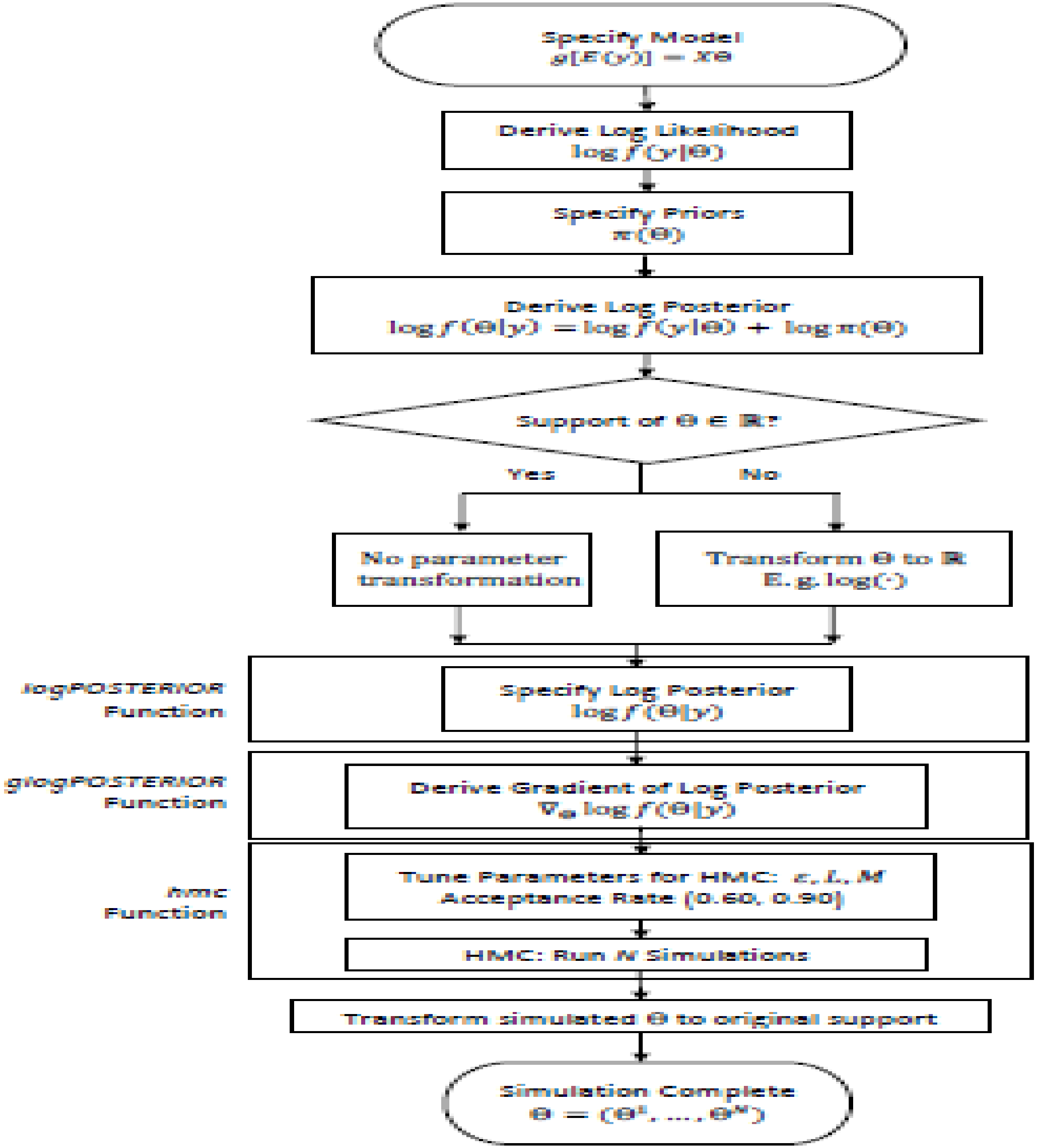
Adaptively select L as in No U-turn Sampler (NUTS) .  Hoffman and Gelman

Implemented in Stan. Also adaptively chooses epsilon

Covariance matrix M

# Hamiltonian MC. Examples

# Typical setup



Specify Model
$g[E(y)] = X\Theta$

Derive Log Likelihood
$\log f(y|\Theta)$

Specify Priors
$\pi(\Theta)$

Derive Log Posterior
$\log f(\Theta|y) = \log f(y|\Theta) + \log \pi(\Theta)$

Support of $\Theta \in \mathbb{R}$?

Yes

No

No parameter transformation

Transform $\Theta$ to $\mathbb{R}$
E.g. $\log(\cdot)$

*logPOSTERIOR*
Function

Specify Log Posterior
$\log f(\Theta|y)$

*glogPOSTERIOR*
Function

Derive Gradient of Log Posterior
$\nabla_\Theta \log f(\Theta|y)$

*hmc*
Function

Tune Parameters for HMC: $\varepsilon, L, M$
Acceptance Rate (0.60, 0.90)

HMC: Run $N$ Simulations

Transform simulated $\Theta$ to original support

Simulation Complete
$\Theta = (\Theta^1, \ldots, \Theta^N)$

# Sampling the bi-variate normal

Simple example to recall approach

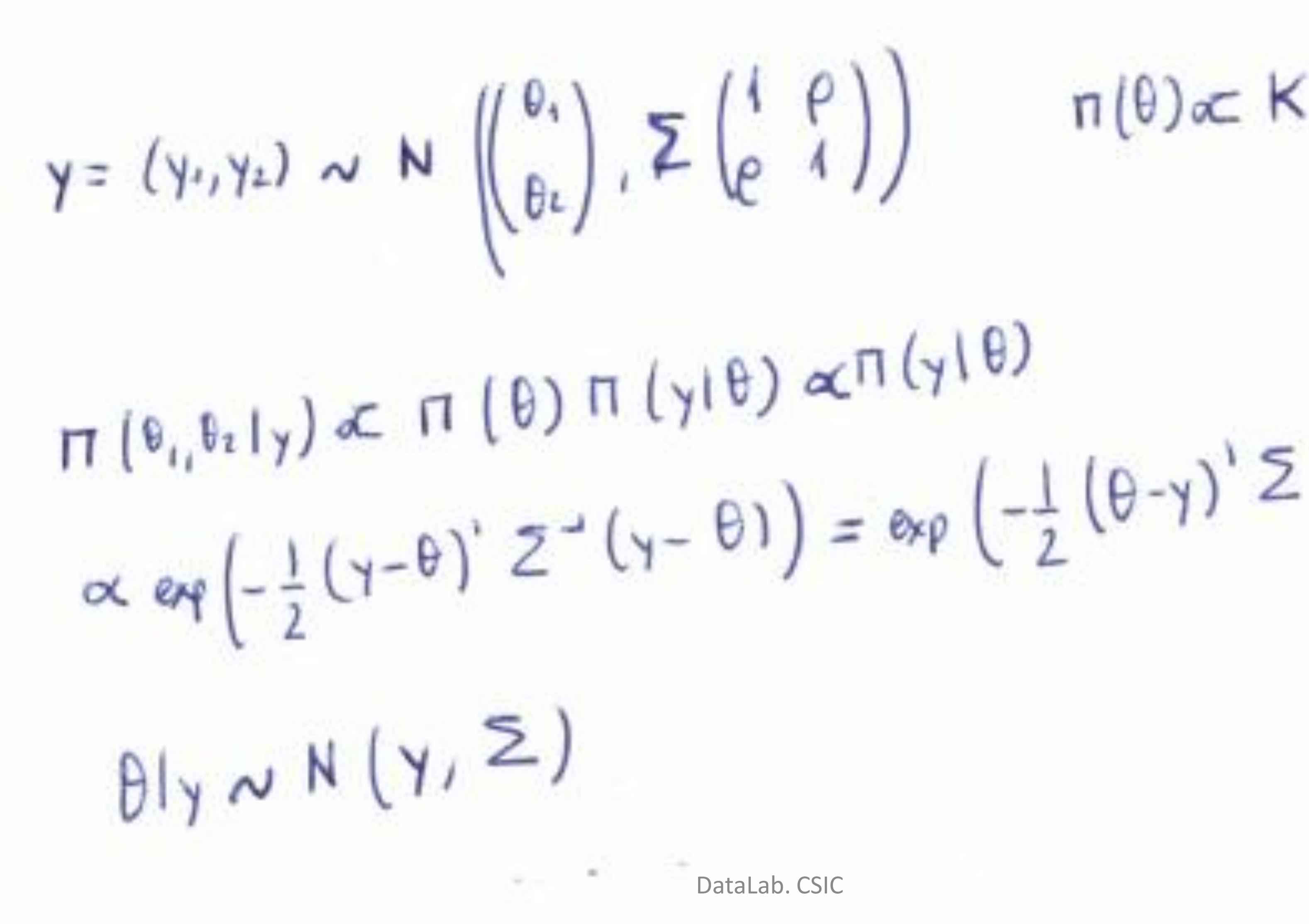
**Model**. Bivariate normal with unknown means. Variances 1. Known correlation $\varrho$

1 observation

Prior. Uniform

**Use**. Expected value and variance of parameters, Expected cross product, Probability that parameter belongs to a set

# Sampling the bi-variate normal. Model and posterior



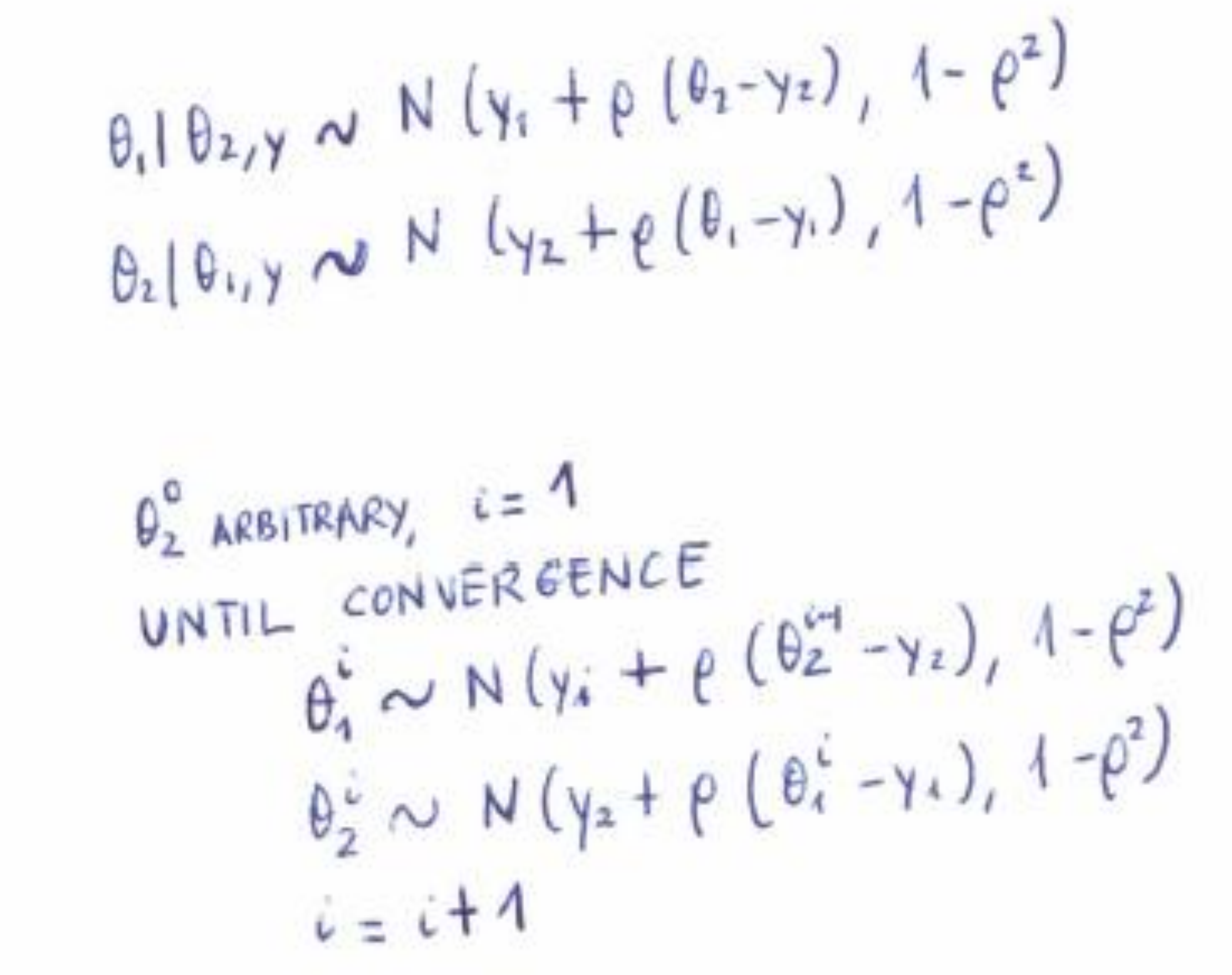
$$y = (y_1, y_2) \sim N\left(\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix}, \Sigma\begin{pmatrix}1 & \rho\\ \rho & 1\end{pmatrix}\right) \qquad \pi(\theta) \propto K$$

$$\pi(\theta_1, \theta_2 | y) \propto \pi(\theta)\, \pi(y|\theta) \propto \pi(y|\theta)$$

$$\propto \exp\left(-\frac{1}{2}(y-\theta)' \Sigma^{-1}(y-\theta)\right) = \exp\left(-\frac{1}{2}(\theta-y)' \Sigma^{-1}(\theta-y)\right)$$

$$\theta|y \sim N(y, \Sigma)$$

# Sampling the bi-variate normal. Gibbs sampler

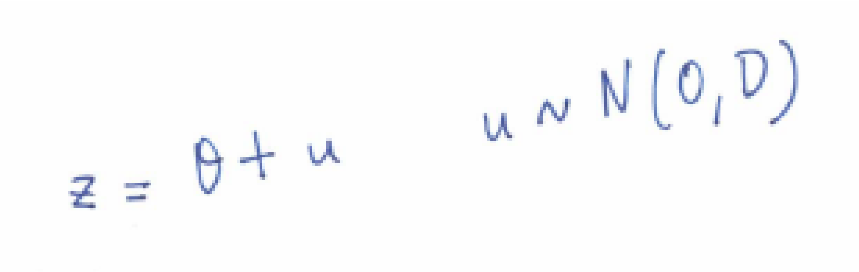


$$\theta_1 \mid \theta_2, y \sim N\left(y_1 + \rho\,(\theta_2 - y_2),\ 1 - \rho^2\right)$$

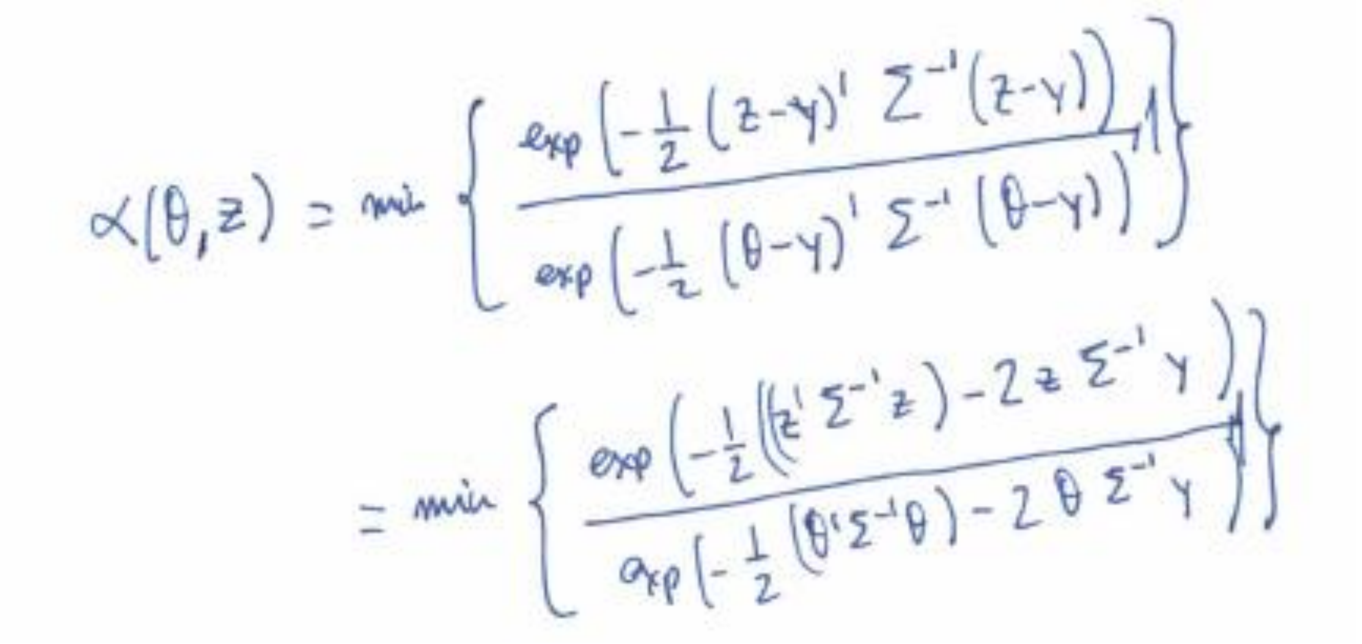
$$\theta_2 \mid \theta_1, y \sim N\left(y_2 + \rho\,(\theta_1 - y_1),\ 1 - \rho^2\right)$$

```
$\theta_2^0$ ARBITRARY, $i = 1$
UNTIL CONVERGENCE
    $\theta_1^i \sim N(y_1 + \rho\,(\theta_2^{i-1} - y_2),\ 1 - \rho^2)$
    $\theta_2^i \sim N(y_2 + \rho\,(\theta_1^i - y_1),\ 1 - \rho^2)$
    $i = i + 1$
```

# Sampling the bi-variate normal. Metropolis Hastings



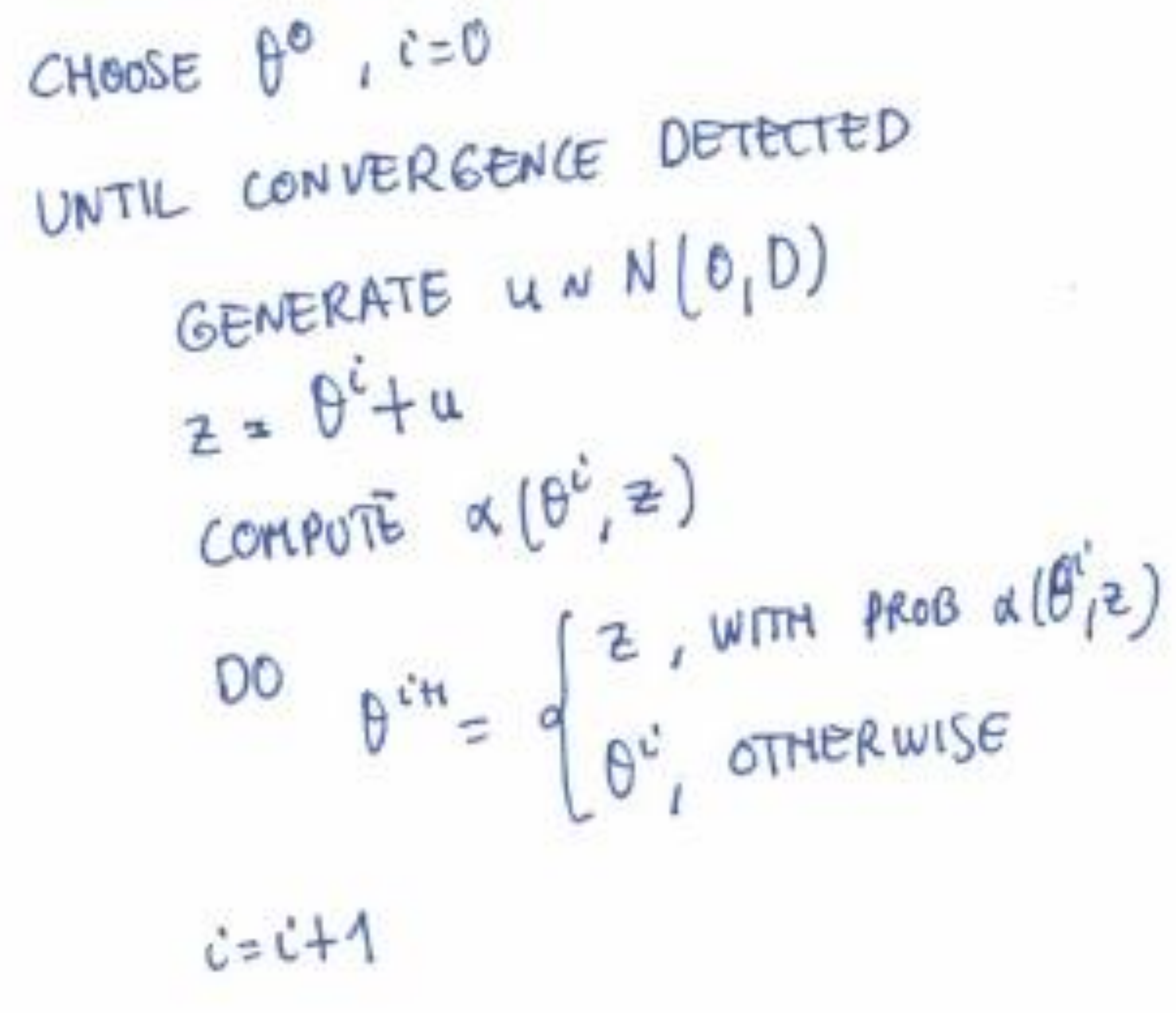
$$z = \theta + u \qquad u \sim N(0, D)$$



$$\alpha(\theta, z) = \min\left\{ \frac{\exp\left(-\frac{1}{2}(z-y)'\Sigma^{-1}(z-y)\right)}{\exp\left(-\frac{1}{2}(\theta-y)'\Sigma^{-1}(\theta-y)\right)}, 1 \right\}$$

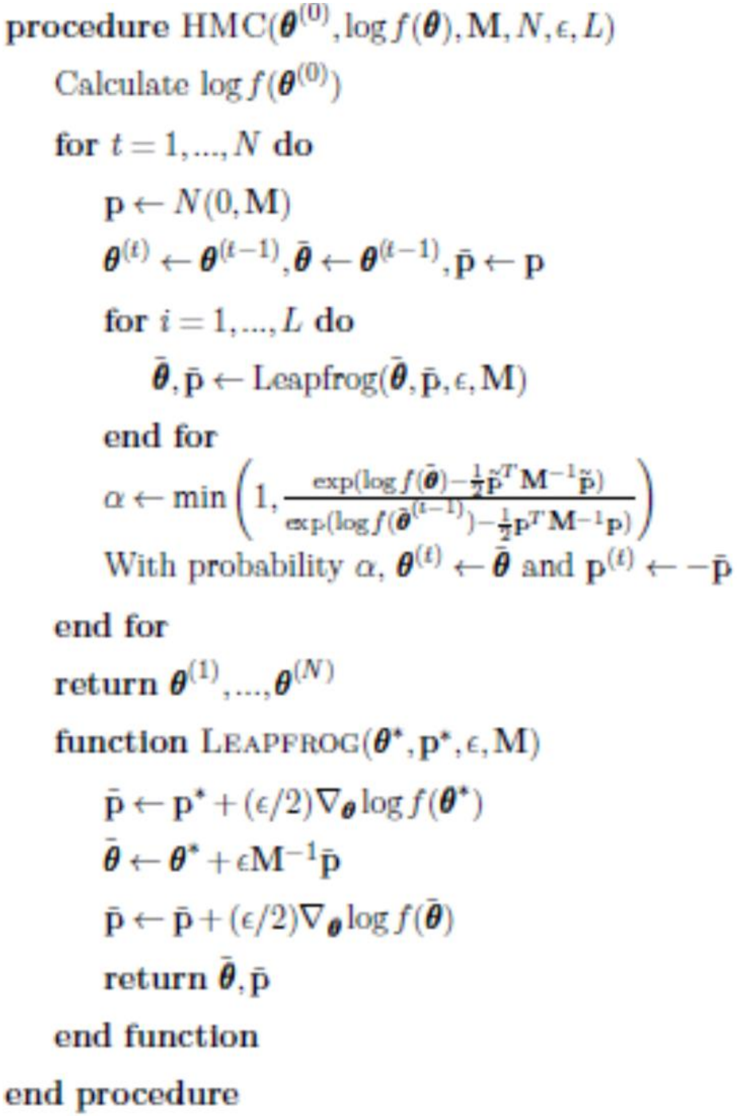
$$= \min\left\{ \frac{\exp\left(-\frac{1}{2}\left((z'\Sigma^{-1}z) - 2z\Sigma^{-1}y\right)\right)}{\exp\left(-\frac{1}{2}(\theta'\Sigma^{-1}\theta) - 2\theta\Sigma^{-1}y\right)}, 1 \right\}$$

# Sampling the bi-variate normal. Metropolis Hastings

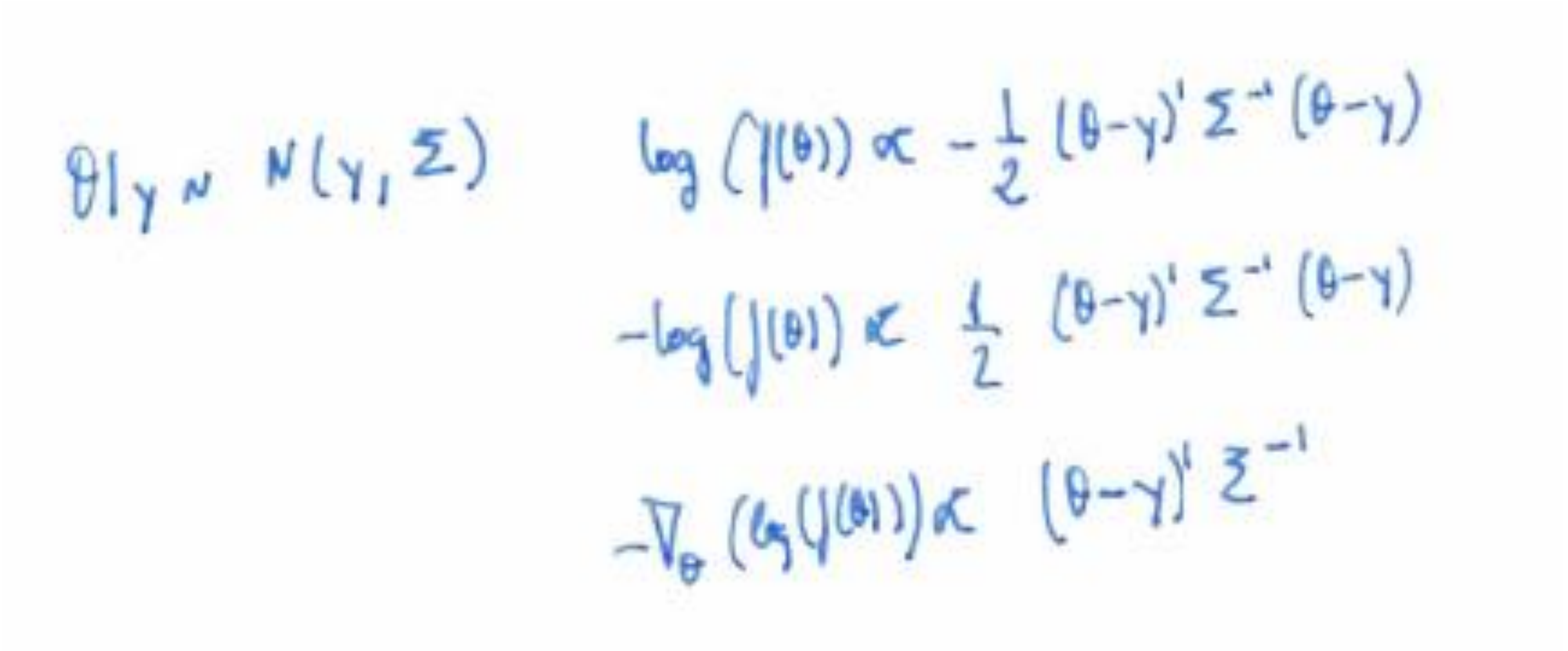


```
CHOOSE $\theta^0$ , $i=0$
UNTIL CONVERGENCE DETECTED
    GENERATE $u \sim N(0,D)$
    $z = \theta^i + u$
    COMPUTE $\alpha(\theta^i, z)$
    DO $\theta^{i+1} = \begin{cases} z, & \text{WITH PROB } \alpha(\theta^i, z) \\ \theta^i, & \text{OTHERWISE} \end{cases}$
    $i = i+1$
```

# Sampling the bi-variate normal. Hamiltonian MC



```
procedure HMC($\boldsymbol{\theta}^{(0)}, \log f(\boldsymbol{\theta}), \mathbf{M}, N, \epsilon, L$)
    Calculate $\log f(\boldsymbol{\theta}^{(0)})$
    for $t = 1, ..., N$ do
        $\mathbf{p} \leftarrow N(0, \mathbf{M})$
        $\boldsymbol{\theta}^{(t)} \leftarrow \boldsymbol{\theta}^{(t-1)}, \bar{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta}^{(t-1)}, \bar{\mathbf{p}} \leftarrow \mathbf{p}$
        for $i = 1, ..., L$ do
            $\bar{\boldsymbol{\theta}}, \bar{\mathbf{p}} \leftarrow$ Leapfrog($\bar{\boldsymbol{\theta}}, \bar{\mathbf{p}}, \epsilon, \mathbf{M}$)
        end for
        $\alpha \leftarrow \min\left(1, \frac{\exp(\log f(\bar{\boldsymbol{\theta}}) - \frac{1}{2}\bar{\mathbf{p}}^T \mathbf{M}^{-1} \bar{\mathbf{p}})}{\exp(\log f(\bar{\boldsymbol{\theta}}^{(t-1)}) - \frac{1}{2}\mathbf{p}^T \mathbf{M}^{-1} \mathbf{p})}\right)$
        With probability $\alpha$, $\boldsymbol{\theta}^{(t)} \leftarrow \bar{\boldsymbol{\theta}}$ and $\mathbf{p}^{(t)} \leftarrow -\bar{\mathbf{p}}$
    end for
    return $\boldsymbol{\theta}^{(1)}, ..., \boldsymbol{\theta}^{(N)}$
    function LEAPFROG($\boldsymbol{\theta}^*, \mathbf{p}^*, \epsilon, \mathbf{M}$)
        $\bar{\mathbf{p}} \leftarrow \mathbf{p}^* + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\boldsymbol{\theta}^*)$
        $\bar{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta}^* + \epsilon \mathbf{M}^{-1} \bar{\mathbf{p}}$
        $\bar{\mathbf{p}} \leftarrow \bar{\mathbf{p}} + (\epsilon/2)\nabla_{\boldsymbol{\theta}} \log f(\bar{\boldsymbol{\theta}})$
        return $\bar{\boldsymbol{\theta}}, \bar{\mathbf{p}}$
    end function
end procedure
```



$\theta | y \sim N(y, \Sigma)$

$\log(f(\theta)) \propto -\frac{1}{2}(\theta - y)' \Sigma^{-1} (\theta - y)$

$-\log(f(\theta)) \propto \frac{1}{2}(\theta - y)' \Sigma^{-1} (\theta - y)$

$-\nabla_\theta (\log(f(\theta))) \propto (\theta - y)' \Sigma^{-1}$

# Sampling the bi-variate normal. Hamiltonian MC. Bonus

$$H(\theta,p) = \frac{1}{2}(\theta-y)^t \Sigma^{-1}(\theta-y) + \frac{1}{2} p^t M^{-1} p$$

$$\frac{dp}{dt} = -\frac{\partial H(\theta,p)}{\partial \theta} = (\theta-y)'\Sigma^{-1}$$

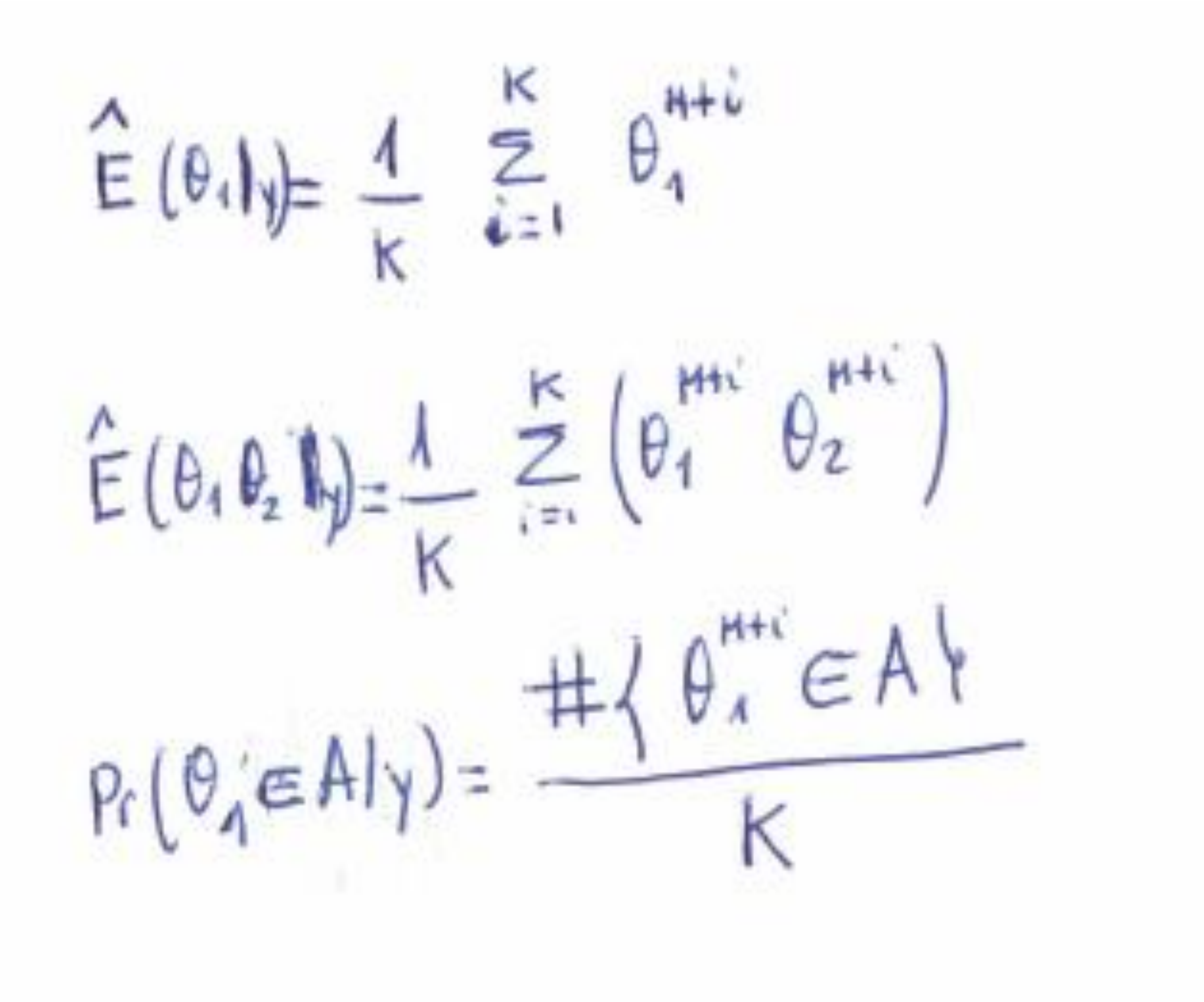
$$\frac{d\theta}{dt} = \frac{\partial H(\theta,p)}{\partial p} = M^{-1} p$$

$$p(t+\tfrac{\varepsilon}{2}) = p(t) + \frac{\varepsilon}{2}(y-\theta(t))' \Sigma^{-1}$$

$$\theta(t+\varepsilon) = \theta(t) + \varepsilon M^{-1} p(t+\varepsilon/2)$$

$$p(t+\varepsilon) = p(t+\tfrac{\varepsilon}{2}) + \frac{\varepsilon}{2}(y-\theta(t+\tfrac{\varepsilon}{2}))'\Sigma^{-1}$$

# Sampling the bi-variate normal. Answers (Whatever the method used)



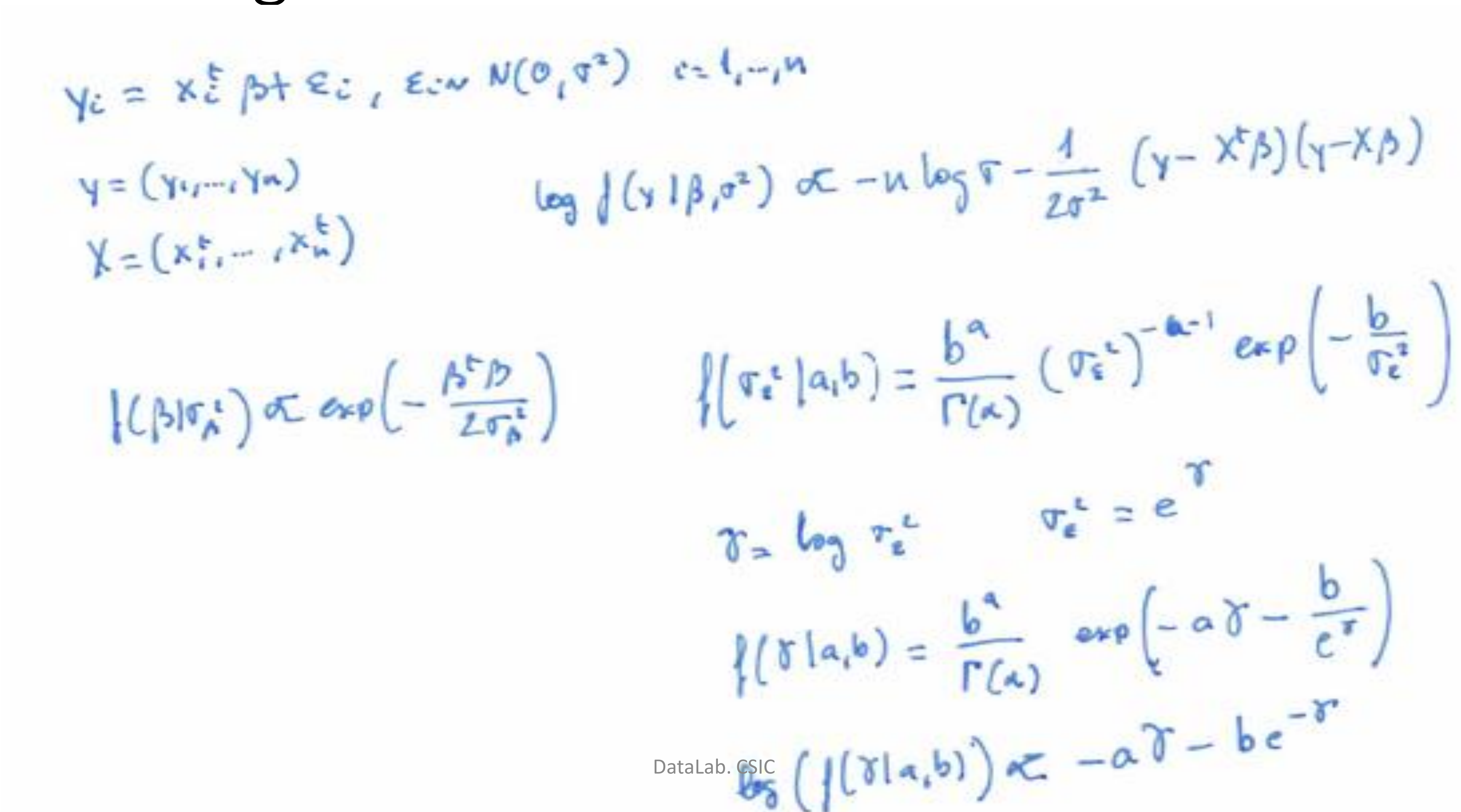
$$\hat{E}(\theta_1|y) = \frac{1}{K}\sum_{i=1}^{K}\theta_1^{M+i}$$

$$\hat{E}(\theta_1\theta_2|y) = \frac{1}{K}\sum_{i=1}^{K}\left(\theta_1^{M+i}\,\theta_2^{M+i}\right)$$

$$Pr(\theta_1\in A|y) = \frac{\#\{\theta_1^{M+i}\in A\}}{K}$$

# Linear regression model

Normal Prior for weights



$$y_i = x_i^t \beta + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2) \quad i = 1, \dots, n$$

$$y = (y_1, \dots, y_n)$$

$$X = (x_1^t, \dots, x_n^t)$$

$$\log f(y \mid \beta, \sigma^2) \propto -n \log \sigma - \frac{1}{2\sigma^2} (y - X^t \beta)(y - X\beta)$$

$$f(\beta \mid \sigma_\beta^2) \propto \exp\left(-\frac{\beta^t \beta}{2\sigma_\beta^2}\right)$$

$$f(\sigma_\varepsilon^2 \mid a, b) = \frac{b^a}{\Gamma(a)} (\sigma_\varepsilon^2)^{-a-1} \exp\left(-\frac{b}{\sigma_\varepsilon^2}\right)$$

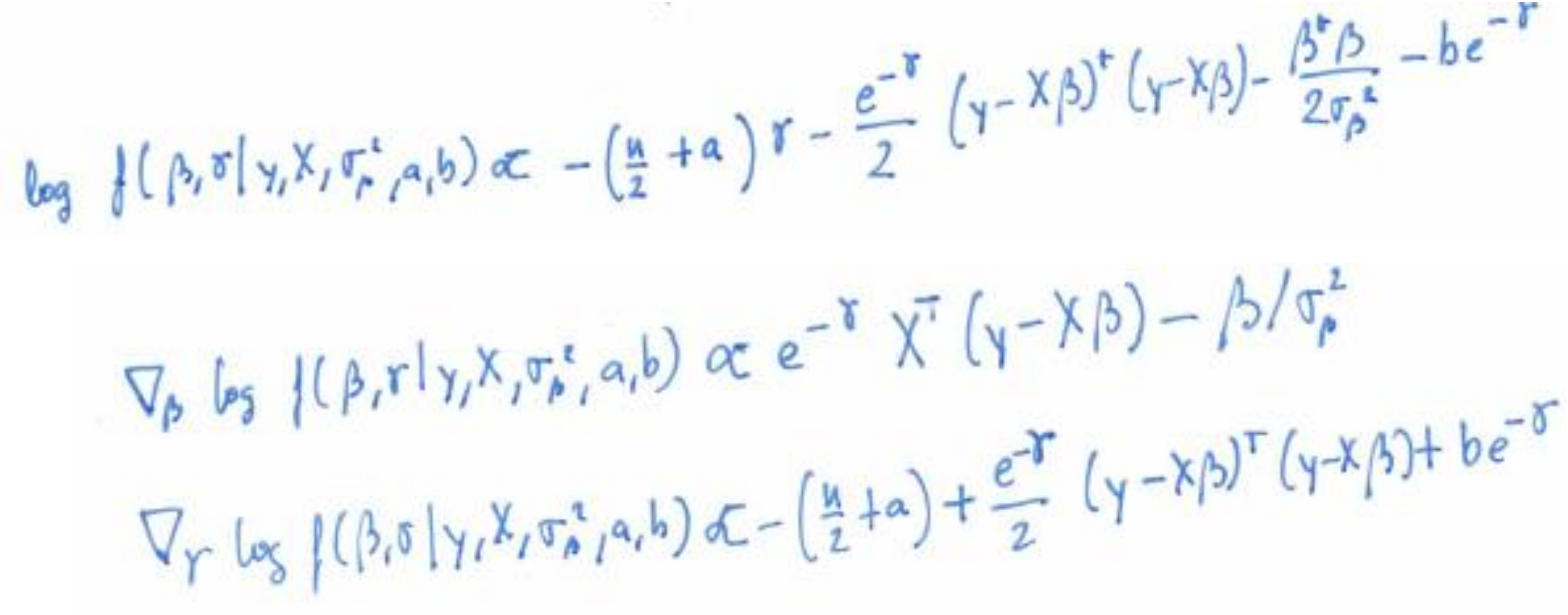
$$\gamma = \log \sigma_\varepsilon^2 \qquad \sigma_\varepsilon^2 = e^\gamma$$

$$f(\gamma \mid a, b) = \frac{b^a}{\Gamma(a)} \exp\left(-a\gamma - \frac{b}{e^\gamma}\right)$$

$$\log\left(f(\gamma \mid a, b)\right) \propto -a\gamma - b e^{-\gamma}$$

Inv-gamma prior for variance

# Linear regression model

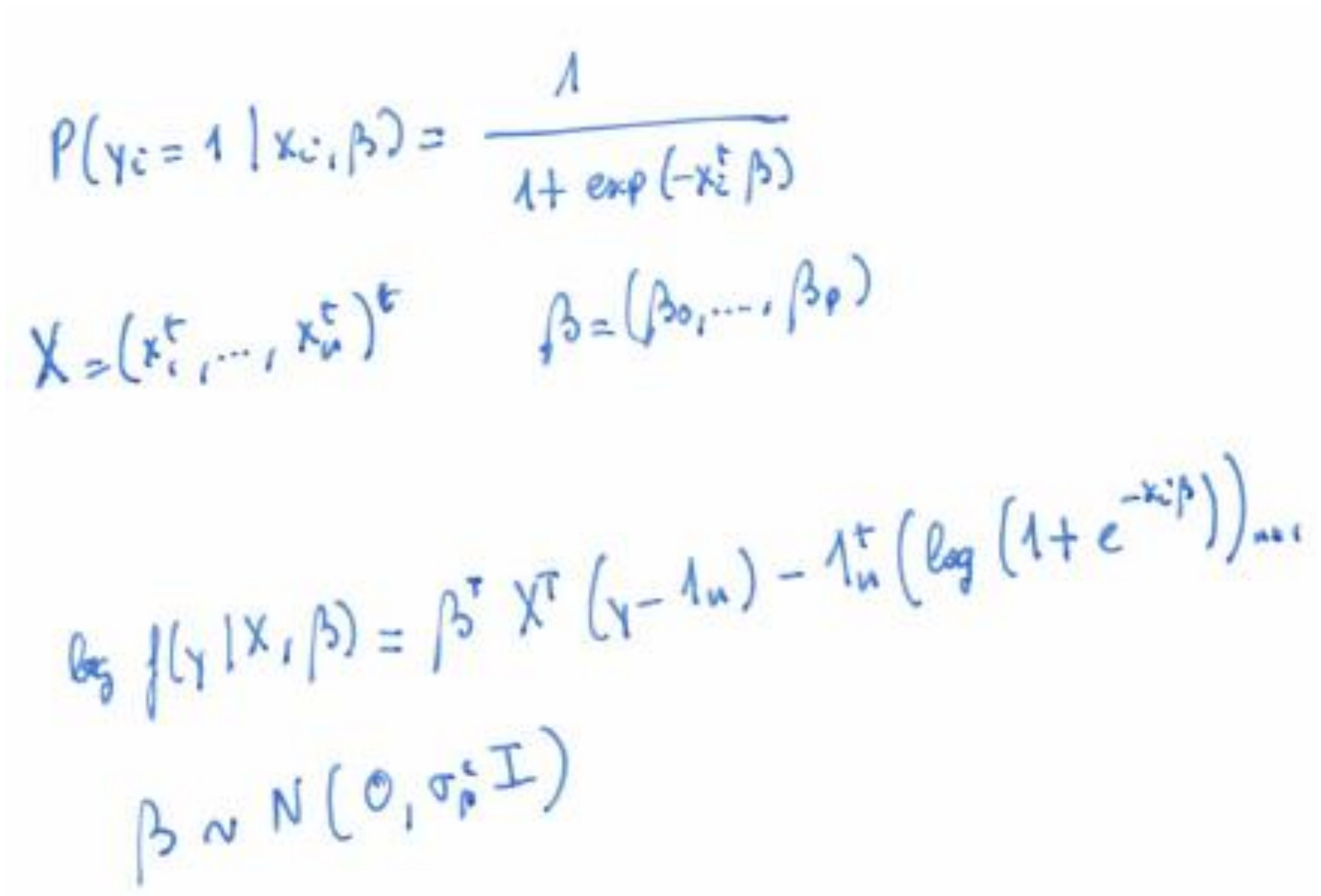


$$\log f(\beta, \gamma \mid y, X, \sigma_\beta^2, a, b) \propto -\left(\frac{n}{2} + a\right)\gamma - \frac{e^{-\gamma}}{2}(y - X\beta)^T (y - X\beta) - \frac{\beta^T\beta}{2\sigma_\beta^2} - b e^{-\gamma}$$

$$\nabla_\beta \log f(\beta, \gamma \mid y, X, \sigma_\beta^2, a, b) \propto e^{-\gamma} X^T (y - X\beta) - \beta / \sigma_\beta^2$$

$$\nabla_\gamma \log f(\beta, \gamma \mid y, X, \sigma_\beta^2, a, b) \propto -\left(\frac{n}{2} + a\right) + \frac{e^{-\gamma}}{2}(y - X\beta)^T (y - X\beta) + b e^{-\gamma}$$

# Logistic regression model



$$P(y_i = 1 \mid x_i, \beta) = \frac{1}{1+\exp(-x_i^t \beta)}$$

$$X = (x_1^t, \dots, x_n^t)^t \qquad \beta = (\beta_0, \dots, \beta_p)$$

$$\log f(y \mid X, \beta) = \beta^T X^T (y - 1_n) - 1_n^t \left(\log\left(1+e^{-x_i^t \beta}\right)\right)_{n \times 1}$$

$$\beta \sim N(0, \sigma_\beta^2 I)$$

# Logistic regression model

$$\log f(\beta \mid y, X, \sigma_\beta^2) \propto \beta^T X^T (y - 1_n) - 1_n^t \left(\log\left(1 + e^{-x_i^t \beta}\right)\right)_{n \times 1} - \frac{\beta^T \beta}{2\sigma_\beta^2}$$

$$\nabla_\beta \log f(\beta \mid y, X, \sigma_\beta^2) \propto X^T \left( y - 1_n + \left[ \frac{e^{-x_i^t \beta}}{1 + e^{-x_i^t \beta}} \right]_{n \times 1} \right) - \beta / \sigma_\beta^2$$

# Almost final comments

Gibbs. Lots of hard prior work. Not always implementable. If so may work well.

Metropolis Hastings. Less prior work. Quite general. May work slowly.

Hamiltonian. Even less work (although gradient needs to be computed) Quite general. Works more efficiently if well tuned) …. Yet suffers in large scale problems

We turn now into Stan

More when introducing SG-MCMC and Variational inference

# HMC. Stan

- PPL
- Syntaxis inherited from BUGS
- Stan files defining models
- Automatic transformations!!!
- Automatic differentiation!!!
- Automatic tuning of parameters!!!
- Monitoring convergence, etc

Stan 1. Learning mean, normal model + variants

Stan 2. Learning proportion + variants

Stan 3. Learning linear model + ANOVA

# d. Complements

# Further variants

# Further variants

There’s many other variants

Slice sampling, simulated tempering, parallel tempering,…

We sketch here two: reversible jump sampling and particle filtering

Later we mention SG-MCMC variants

# Reversible jump

In many complex problems  we need to do trans-dimensional Markov chain simulation

- Mixtures with unknown number of components
- Shallow neural nets with unknown number of hidden nodes
- Model averaging
- Bartmachine

Parameters=(indicator of model, parameters of such model)

Within the model, a ‘standard’ Markov chain (Gibbs, MH, HMC, etc…)

Between models, Metropolis Hastings with reversible moves (jumps, collapsing and splitting models…)

See classic paper by Peter Green

# Particle filtering

For nonlinear sequential problems, MCMC gets complex

Generate initial sample at time t=0

Let them evolve (and learn) according to nonlinear sequential model

Introduce rules to avoid collapse of particles

# Inference and assessing convergence

# Inference

Once convergence detected, collect samples from posterior and perform inference (point estimates, intervals, hypothesis tests, predictions and expected utility computations) via Monte Carlo (recall uncertainty associated, they are stochastic algos!!!)

# Difficulties

If iterations have not proceeded long enough, target is not approximated well, samples are unrepresentative of target!!!

Early iterations may bias results

Autocorrelation impacts precision of estimates and the effective number of samples may be smaller than the one actually drawn (as if we’d be using a smaller number of samples)

# Solutions

Runs to allow for effective monitoring of convergence (based on multiple chains, recall labs)

Monitor convergence by comparing variation within and between simulated sequences (until within and between variation are similar)

Modifying the algorithm by reparameterising or learning good parameterisations, if efficiency is very low (algo too slow)

Discarding initial values

Thinning

Take into account AC when estimating precisions

# Discarding early iterations

Rule of thumb: Discard first half of iterations (warm-up, burn-in) and use the second half of iterations for inference and prediction

Warm-up fraction may vary

Warm-up fraction may adapt

Example. Run 200. Discard first 100. If second 200, do not suggest convergence, run 200 more and discard first 200.

# Thinning iterations

Mitigate autocorrelation: keep every k-th simulation draw and discard the rest (to avoid storage problems also!!!)

Rule of thumb: Choose k to save up to 1000 draws

# Assessing convergence

Comparing different simulated sequences from multiple chains with overdispersed starting points

- Compare variance within each sequence with variance between sequences
- Monitoring various scalar estimands (and other quantities of interest like the logposterior) separately
- Checking mixing and stationarity
  - Split each series in two parts
    - after discarding burn-in

    - Check R

- coda
- monitor

$$\psi \longrightarrow \psi_{ij} \quad \left( \begin{array}{ll} i = 1, \dots, n & \text{\# length of each chain} \\ j = 1, \dots, m & \text{\# of chains} \end{array} \right)$$

$$B = \frac{n}{m-1} \sum_{i=1}^{m} \left( \overline{\psi}_{.j} - \overline{\psi}_{..} \right)^2 \qquad \overline{\psi}_{.j} = \frac{1}{n} \sum_{i}^{n} \psi_{ij} \qquad \overline{\psi}_{..} = \frac{1}{m} \sum_{i=1}^{m} \overline{\psi}_{.j}$$

$$s_j^2 = \frac{1}{n-1} \sum_{i=1}^{n} \left( \psi_{ij} - \overline{\psi}_{.j} \right)^2$$

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

$$\widehat{\mathrm{var}}(\psi | y) = \frac{n-1}{n} W + \frac{1}{n} B$$

$$\hat{R} = \sqrt{\frac{\widehat{\mathrm{var}}(\psi | y)}{W}} \downarrow 1$$

# Effective number of simulation draws

Once simulated sequences judged to have mixed, estimate effective number of simulation draws for any estimand of interest

If draws within each sequence truly independent, B would be an unbiased estimator of the posterior variance and we’d have mn independent observations

But typically will be autocorrelated and E(B) will be larger than the posterior variance

# Effective number of simulation draws

We have

$$\overline{\psi}_{..} = \frac{1}{m}\sum_{j=1}^{m}\overline{\psi}_{.j} \qquad \lim_{n\to\infty} mn\,\mathrm{var}(\overline{\psi}_{..}) = \left(1+2\sum_{t=1}^{\infty}\rho_t\right)\mathrm{var}(\psi|y)$$

And define the effective simple size as

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

We estimate it through

$$\widehat{\mathrm{var}}^{+}(\psi|y) = \frac{n-1}{n}W + \frac{1}{n}B \qquad V_t = \frac{1}{m(n-t)}\sum_{j=1}^{m}\sum_{i=t+1}^{n}(\psi_{i,j}-\psi_{i-t,j})^2$$

$$E(\psi_i-\psi_{i-t})^2 = 2(1-\rho_t)\,\mathrm{var}(\psi) \longrightarrow \hat{\rho}_t = 1-\frac{V_t}{2\,\widehat{\mathrm{var}}^{+}}$$

$$\hat{n}_{eff} = \frac{mn}{1+2\sum_{t=1}^{T}\hat{\rho}_t} \qquad T \overset{\text{first}}{:=} \hat{\rho}_{T+1}+\hat{\rho}_{T+2}<0$$