

# CS340 Machine learning

## Gibbs sampling in Markov random fields

# Image denoising



$x$



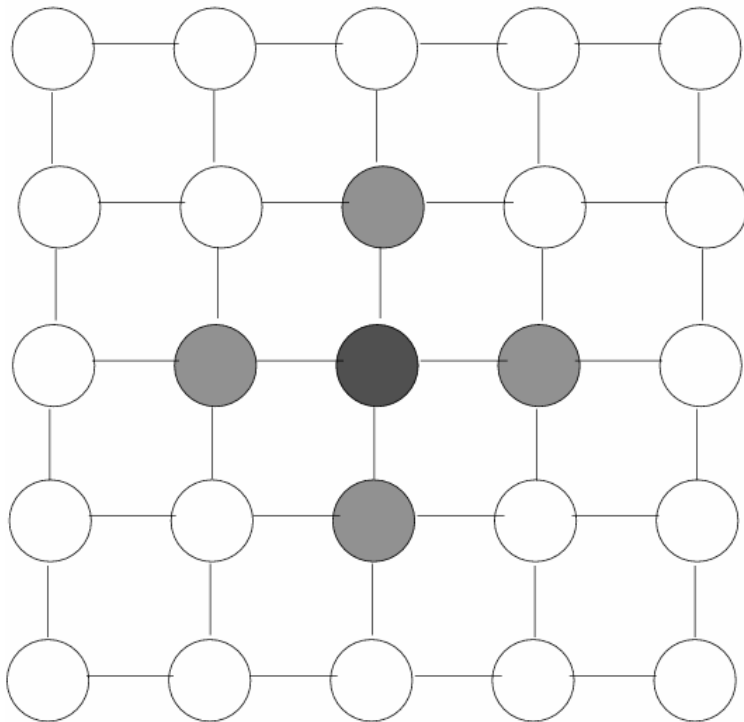
$y$



$$\hat{x} = E[x|y, \theta]$$

# Ising model

- 2D Grid on  $\{-1, +1\}$  variables
- Neighboring variables are correlated



$$p(\mathbf{x}|\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \prod_{\langle ij \rangle} \psi_{ij}(x_i, x_j)$$

# Ising model

$$\psi_{ij}(x_i, x_j) = \begin{pmatrix} e^W & e^{-W} \\ e^{-W} & e^W \end{pmatrix}$$

$W > 0$ : ferro magnet

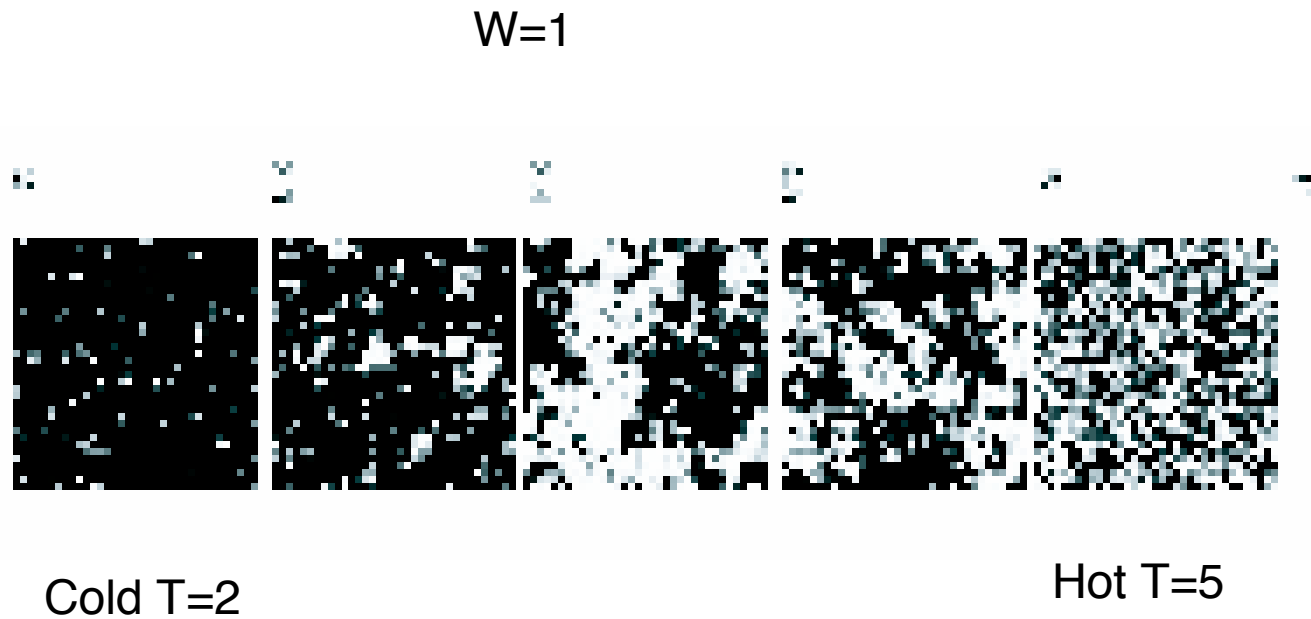
$W < 0$ : anti ferro magnet (frustrated system)

$$p(\mathbf{x}|\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \exp[-\beta H(\mathbf{x}|\boldsymbol{\theta})]$$

$$H(\mathbf{x}) = -\mathbf{x}^T \mathbf{W} \mathbf{x} = - \sum_{\langle ij \rangle} W_{ij} x_i x_j$$

$\beta = 1/T$  = inverse temperature

# Samples from an Ising model



# Boltzmann distribution

- Prob distribution in terms of clique potentials

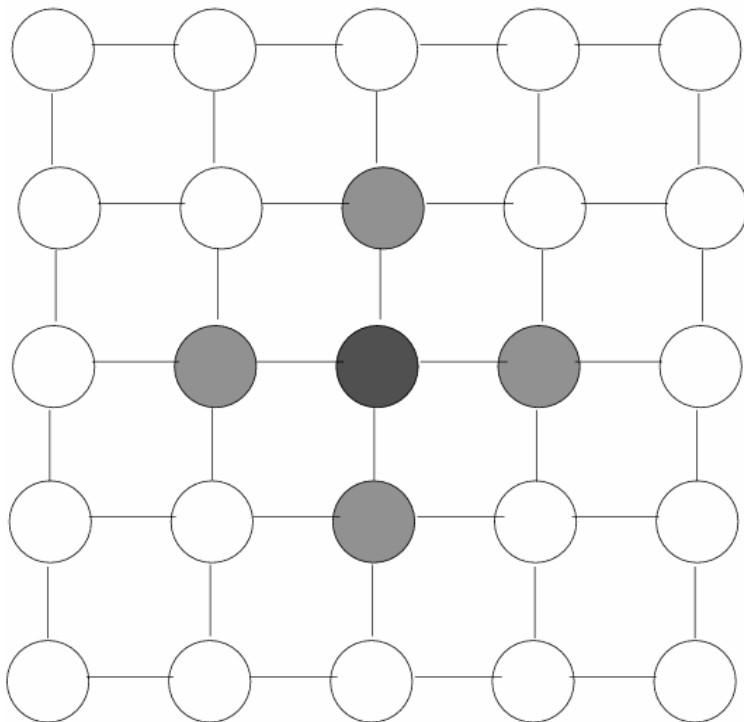
$$p(\mathbf{x}|\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \prod_{c \in \mathcal{C}} \psi_c(\mathbf{x}_c|\boldsymbol{\theta}_c)$$

- In terms of energy functions

$$\begin{aligned}\psi_c(\mathbf{x}_c) &= \exp[-H_c(\mathbf{x}_c)] \\ \log p(\mathbf{x}) &= -\left[\sum_{c \in \mathcal{C}} H_c(\mathbf{x}_c) + \log Z\right]\end{aligned}$$

# Ising model

- 2D Grid on  $\{-1,+1\}$  variables
- Neighboring variables are correlated



$$H_{ij} = \begin{pmatrix} W_{ij} & -W_{ij} \\ -W_{ij} & W_{ij} \end{pmatrix}$$

$W > 0$ : ferro magnet

$W < 0$ : anti ferro magnet (frustrated)

$$H(\mathbf{x}) = -\mathbf{x}^T \mathbf{W} \mathbf{x} = - \sum_{\langle ij \rangle} W_{ij} x_i x_j$$

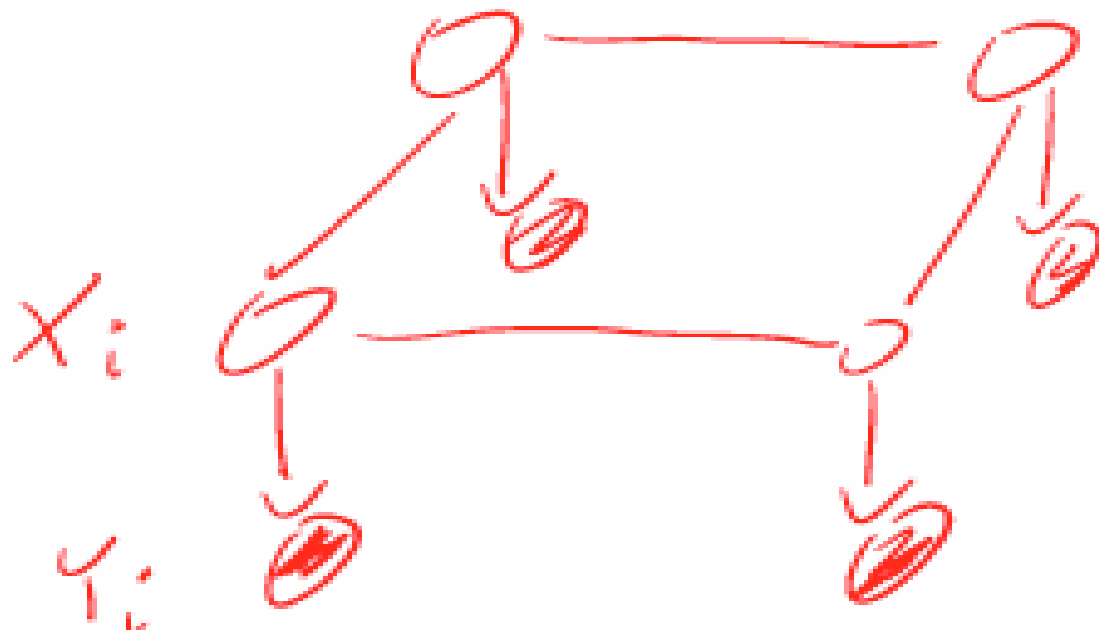
$$p(\mathbf{x}|\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \exp[-\beta H(\mathbf{x}|\boldsymbol{\theta})]$$

$\beta=1/T$  = inverse temperature

# Local evidence

$$p(x, y) = p(x)p(y|x) = \left[ \frac{1}{Z} \prod_{\langle ij \rangle} \psi_{ij}(x_i, x_j) \right] \left[ \prod_i p(y_i|x_i) \right]$$

$$p(y_i|x_i) = \mathcal{N}(y_i|x_i, \sigma^2)$$





# Gibbs sampling

- A way to draw samples from  $p(x_{1:D}|y, \theta)$  one variable at a time, ie.  $p(x_i|x_{-i})$

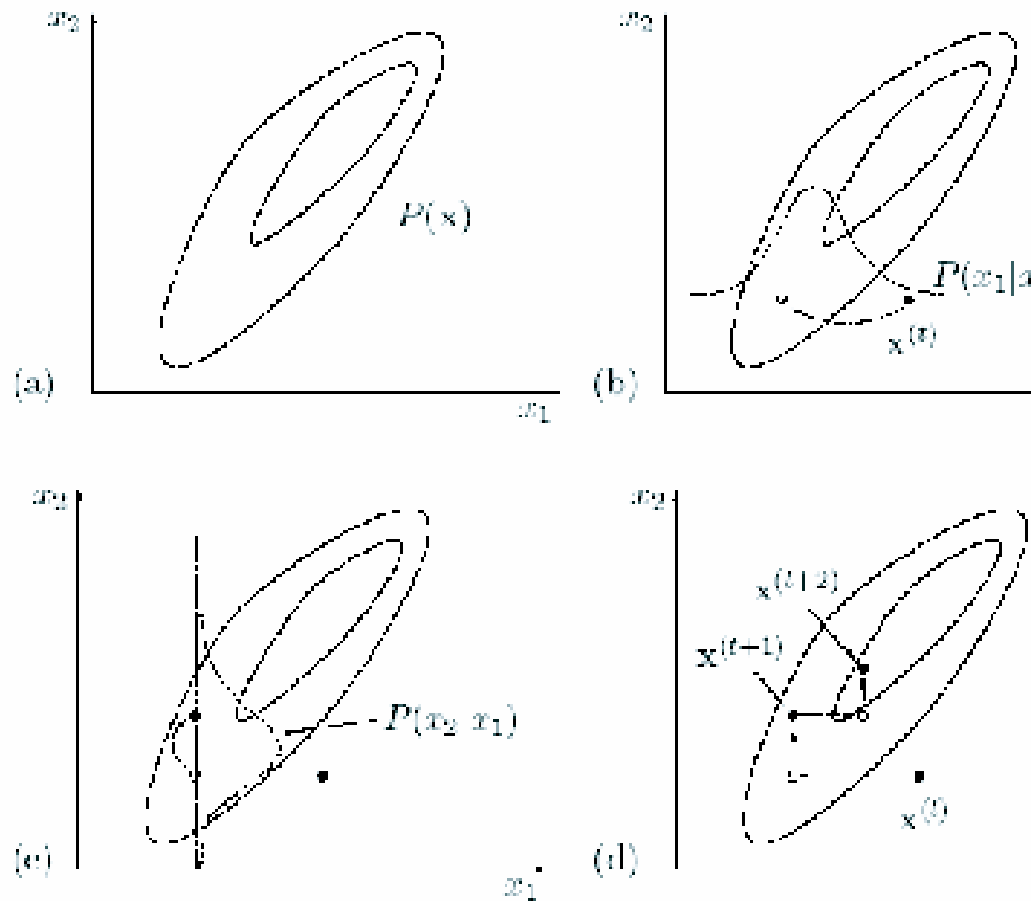
$$1. x_1^{s+1} \sim p(x_1|x_2^s, \dots, x_D^s)$$

$$2. x_2^{s+1} \sim p(x_2|x_1^{s+1}, x_3^s, \dots, x_D^s)$$

$$3. x_i^{s+1} \sim p(x_i|x_{1:i-1}^{s+1}, x_{i+1:D}^s)$$

$$4. x_D^{s+1} \sim p(x_D|x_1^{s+1}, \dots, x_{D-1}^{s+1})$$

# Gibbs sampling from a 2d Gaussian



# Gibbs sampling in an MRF

- Full conditional depends only on Markov blanket

$$\begin{aligned} p(X_i = \ell | x_{-i}) &= \frac{p(x_i = \ell, x_{-i})}{\sum_{\ell'} p(X_i = \ell', x_{-i})} \\ &= \frac{(1/Z) [\prod_{j \in N_i} \psi_{ij}(X_i = \ell, x_j)] [\prod_{\langle j,k \rangle: j,k \notin F_i} \psi_{jk}(x_j, x_k)]}{(1/Z) \sum_{\ell'} [\prod_{j \in N_i} \psi_{ij}(X_i = \ell', x_j)] [\prod_{\langle j,k \rangle: j,k \notin F_i} \psi_{jk}(x_j, x_k)]} \\ &= \frac{\prod_{j \in N_i} \psi_{ij}(X_i = \ell, x_j)}{\sum_{\ell'} \prod_{j \in N_i} \psi_{ij}(X_i = \ell', x_j)} \end{aligned}$$

# Gibbs sampling in an Ising model

- Let  $\psi(x_i, x_j) = \exp(W x_i x_j)$ ,  $x_i = +1, -1$ .

$$\begin{aligned} p(X_i = +1 | x_{-i}) &= \frac{\prod_{j \in N_i} \psi_{ij}(X_i = +1, x_j)}{\prod_{j \in N_i} \psi_{ij}(X_i = +1, x_j) + \prod_{j \in N_i} \psi_{ij}(X_i = -1, x_j)} \\ &= \frac{\exp[J \sum_{j \in N_i} x_j]}{\exp[J \sum_{j \in N_i} x_j] + \exp[-J \sum_{j \in N_i} x_j]} \\ &= \frac{\exp[Jw_i]}{\exp[Jw_i] + \exp[-Jw_i]} \\ &= \sigma(2Jw_i) \\ w_i &= \sum_{j \in N_i} x_j \end{aligned}$$

$$\sigma(u) = 1/(1 + e^{-u})$$

# Adding in local evidence

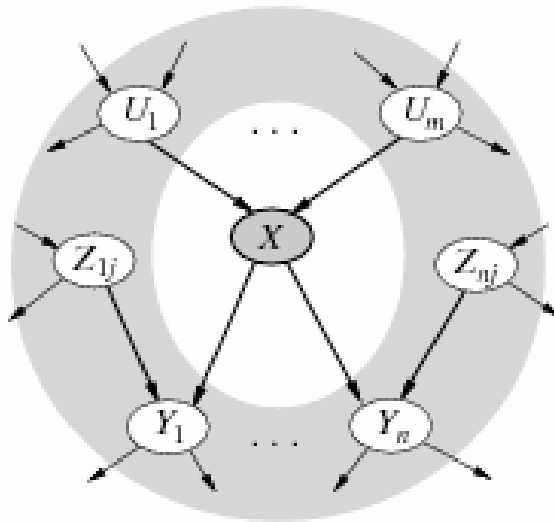
- Final form is

$$p(X_i = +1|x_{-i}, y) = \frac{\exp[Jw_i]\phi_i(+1, y_i)}{\exp[Jw_i]\phi_i(+1, y_i) + \exp[-Jw_i]\phi_i(-1, y_i)}$$

Run demo

# Gibbs sampling for DAGs

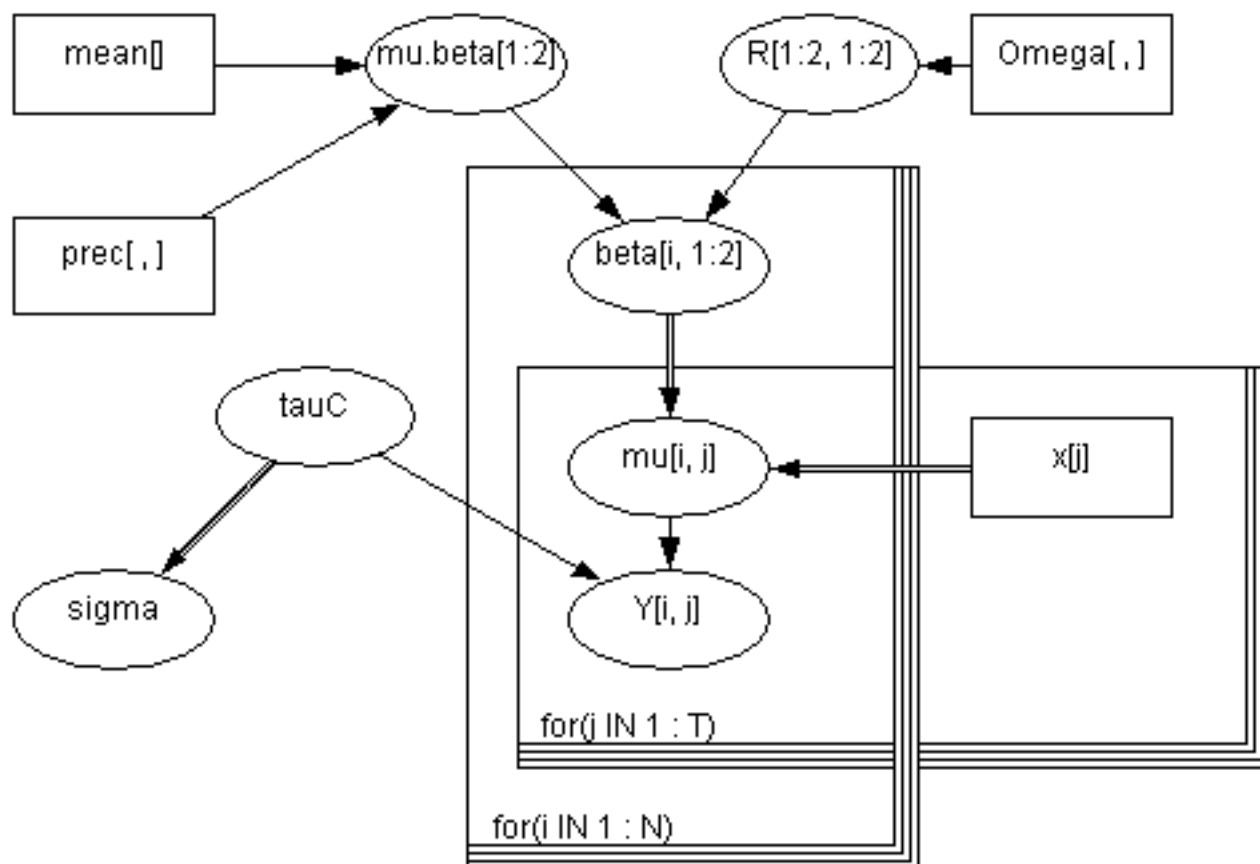
- The Markov blanket of a node is the set that renders it independent of the rest of the graph.
- This is the parents, children and co-parents.



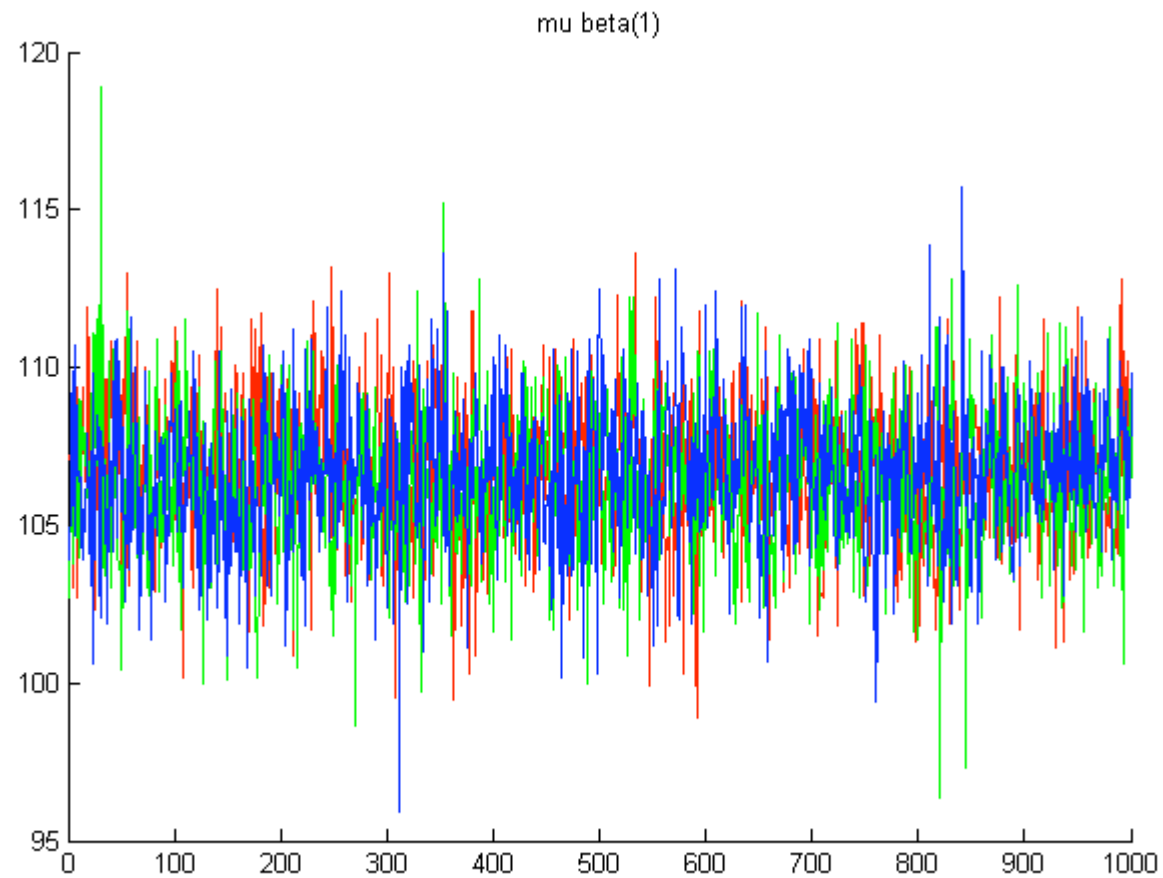
$$\begin{aligned}
 p(X_i | X_{-i}) &= \frac{p(X_i, X_{-i})}{\sum_x p(X_i, X_{-i})} \\
 &= \frac{p(X_i, U_{1:n}, Y_{1:m}, Z_{1:m}, R)}{\sum_x p(x, U_{1:n}, Y_{1:m}, Z_{1:m}, R)} \\
 &= \frac{p(X_i | U_{1:n}) [\prod_j p(Y_j | X_i, Z_j)] P(U_{1:n}, Z_{1:m}, R)}{\sum_x p(X_i = x | U_{1:n}) [\prod_j p(Y_j | X_i = x, Z_j)] P(U_{1:n}, Z_{1:m}, R)} \\
 &= \frac{p(X_i | U_{1:n}) [\prod_j p(Y_j | X_i, Z_j)]}{\sum_x p(X_i = x | U_{1:n}) [\prod_j p(Y_j | X_i = x, Z_j)]}
 \end{aligned}$$

$$p(X_i | X_{-i}) \propto p(X_i | Pa(X_i)) \prod_{Y_j \in ch(X_i)} p(Y_j | Pa(Y_j))$$

# Birats

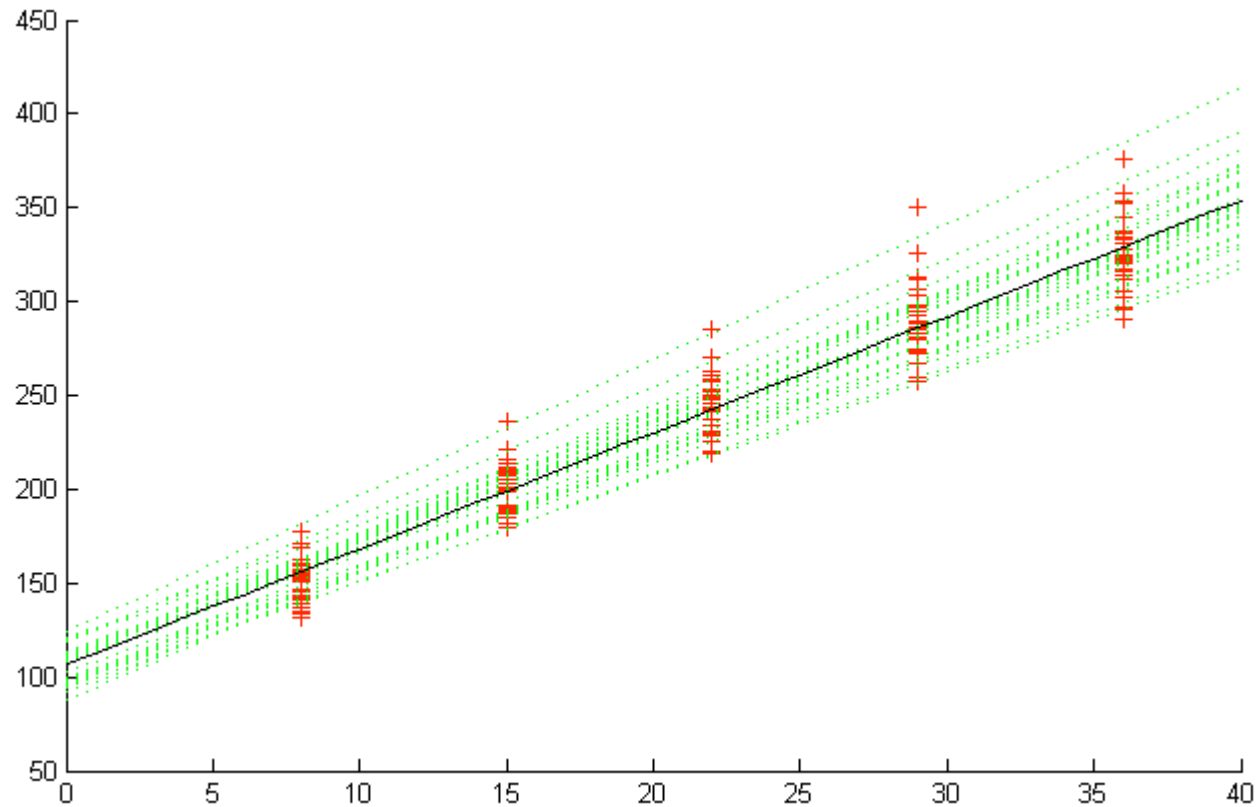


# Samples



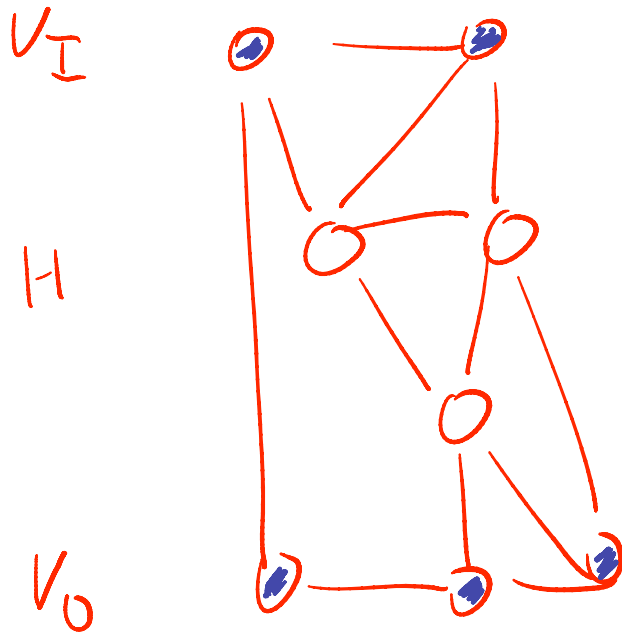


# Posterior predictive check

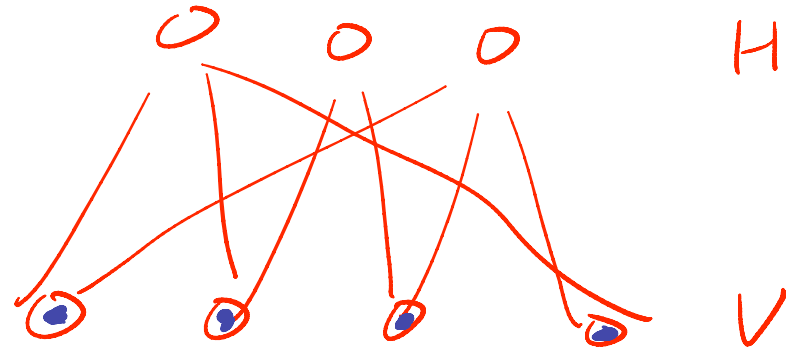


# Boltzmann machines

Ising model where the graph structure is arbitrary, and the weights  $W$  are learned by maximum likelihood



Restricted Boltzmann machine



# Hopfield network

Boltzmann machine with no hidden nodes (fully connected Ising model)

