# Machine Learning 2 - Cheat Sheet

Andrea Jemmett - April 19, 2016

# 1 Probability Theory

# 1.1 Independence

$$p(X,Y) = \overline{p(X)}p(Y) \Leftrightarrow p(X|Y) = p(X) \Leftrightarrow p(Y|X) = p(Y)$$

# 1.2 Conditional Independence

$$\begin{array}{l} X \perp \!\!\! \perp Y \mid Z \Longleftrightarrow p(X,Y|Z) = p(X|Z)p(Y|Z) \\ p(X,Y|Z) = p(X|Y,Z)p(Y|Z) = p(X|Z)p(Y|Z) \end{array}$$

#### 1.3 Sum and Product Rules

$$\begin{array}{ll} p(X,Y) = p(X)p(Y|X), & p(X,Y,Z) = p(X)p(Y|X)p(Z|X,Y) \\ p(X) = \sum_{Y} p(X,Y) & \end{array}$$

# 1.4 Bayes' Theorem

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}, \qquad p(Y|X,Z) = \frac{p(X|Y,Z)p(Y|Z)}{p(X|Z)}$$

# 1.5 Chain Rule

$$p(x_a, x_b, x_c) = p(x_c | x_a, x_b) p(x_b | x_a) p(x_a)$$
  $p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k | pa_k)$ 

# 1.6 Misc

$$p(a,b|c) = \frac{p(a,b,c)}{p(c)} \qquad p(a,b,c) = p(a|c)p(b|c)p(c)$$

# 2 Distributions

# 2.1 Bernoulli Distribution

$$\begin{array}{l} \mathrm{Ber}(x|n) = \mu^x (1-\mu)^{1-x}, \quad \mathbb{E}[x] = \mu, \quad \mathrm{Var}[x] = \mu - \mu^2, \\ P(D,\mu) = \prod_{n=1}^N \mu^{x_n} (1-\mu)^{1-x_n}, \quad \mu_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^N x_n \end{array}$$

# 2.2 Binomial Distribution

$$\begin{aligned} & \operatorname{Bin}(m|N,\mu) = \binom{N}{m} \mu^m (1-\mu)^{N-m}, & \frac{n!}{k!(n-k)!} = \binom{n}{k}, \\ & \mathbb{E}[m] = N\mu, & \operatorname{Var}[m] = N\mu (1-\mu), & \mu_{\operatorname{ML}} = \frac{m}{N} \end{aligned}$$

### 2.3 Categorical Distribution

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k} \mu_{k}^{x_{k}}, \quad \boldsymbol{\mu} \in \{0, 1\}^{K}, \quad \sum_{k} \mu_{k} = 1, \quad \boldsymbol{\mu}_{\mathrm{ML}} = \frac{\mathbf{m}}{N}, \\ m_{k} = \sum_{n} x_{nk}, \quad \mathrm{Mult}(m_{1} \dots, m_{k} | N, \boldsymbol{\mu}) = (\frac{N!}{m_{1}! \dots m_{k}} \prod_{k}) \mu_{k}^{mk}$$

# 2.4 Beta Distribution

Beta(
$$\mu|a,b$$
) =  $\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1}$ ,  $\mathbb{E}[\mu] = \frac{a}{a+b}$ ,  $Var[x] = \frac{ab}{(a+b)^2(a+b+1)}$ ,  $p(\mu|m,l,a,b) \propto \mu^{m+a-1}(1-\mu)^{l+b-1}$ 

# 2.5 Gamma Distribution

$$\begin{aligned} \operatorname{Gamma}(\tau|a,b) &= \frac{b^a}{\Gamma(a)} \tau^{a-1} e^{-b\tau}, & \mathbb{E}[\tau] &= \frac{a}{b}, & \operatorname{Var}[\tau] &= \frac{a}{b^2}, \\ \operatorname{mode}[\tau] &= \frac{a-1}{b} \text{ for } a \geq 1, & \mathbb{E}[\ln \tau] &= \psi(a) - \ln b, \\ H(\tau) &= \ln \Gamma(a) - (a-1) \psi(a) - \ln b + a \end{aligned}$$

#### 2.6 Multinomial Distribution

$$\begin{aligned} \mathbf{x} &= [0,0,0,0,1,0,0]^{\mathsf{T}}, & \sum_{k=1}^{K} x_k = 1, & p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_k^{x_k}, \\ \sum_{k=1}^{K} \mu_k = 1, & \mu_k^{\mathrm{ML}} = \frac{m_k}{N}, & m_k = \sum_{k=1}^{K} x_{nk} \end{aligned}$$

$$\begin{array}{ll} \textbf{2.7} & \textbf{Dirichlet Distribution} \\ \text{Dir}(\boldsymbol{\mu}|\boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1)\cdots\Gamma(\alpha_k)} \prod_{k=1}^K \mu_k^{\alpha_k-1}, \qquad \alpha_0 = \sum_{k=1}^K \alpha_k \end{array}$$

### 2.8 Gaussian Distribution

$$\mathcal{N}(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{1}{2\sigma^2}(x-\mu)^2),$$

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right\}$$

$$\Gamma(x) = \int_0^1 u^{x-1} e^{-u} = 1, \qquad \Gamma(x+1) = \Gamma(x)x, \qquad \Gamma(x+1) = x!$$

$$\frac{\Gamma(x)}{B(a,b)} = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$$

# 2.8.1 ML for the Gaussian

$$\begin{split} & \ln p(X|\boldsymbol{\mu},\boldsymbol{\Sigma}) = -\frac{ND}{2}\ln(2\pi) - \frac{N}{2}\ln|\boldsymbol{\Sigma}| - \frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n - \boldsymbol{\mu})^\mathsf{T}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n - \boldsymbol{\mu}), \\ & \boldsymbol{\mu}_{\mathrm{ML}} = 1/N\sum_{n=1}^{N}\mathbf{x}_n, \qquad \boldsymbol{\Sigma}_{\mathrm{ML}} = 1/N\sum_{n=1}^{N}(\mathbf{x}_n - \boldsymbol{\mu})^\mathsf{T}(\mathbf{x}_n - \boldsymbol{\mu}) \end{split}$$

# 2.8.2 Stochastic gradient descent Gaussian

$$\max P(x_1, \dots, x_n | \theta), \ \theta^N = \theta^{N-1} + \alpha_{N-1} \frac{\partial}{\partial \theta^{N-1}} \ln p(x_n | \theta^{N-1})$$

# 2.8.3 Marginal and Conditional Gaussians

Given 
$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1})$$
 and  $p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1})$ . We get  $p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\mathsf{T}})$  and  $p(\mathbf{x}|\mathbf{y}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\Sigma}[\mathbf{A}^{\mathsf{T}}\mathbf{L}(\mathbf{y} - \mathbf{b}) + \boldsymbol{\Lambda}\boldsymbol{\mu}], \boldsymbol{\Sigma})$  where  $\boldsymbol{\Sigma} = (\boldsymbol{\Lambda} + \mathbf{A}^{\mathsf{T}}\mathbf{L}\mathbf{A})^{-1}$ .

#### 2.9 Student's T distribution

The heavy tail of the student-t distribution makes it more robust against

$$St(x|\mu,\lambda,\nu) = \frac{\Gamma(\nu/2+1/2)}{\Gamma(\nu/2)} \left(\frac{\lambda^{1/2}}{(\pi\nu)^{D/2}}\right) \left[1 + \frac{\lambda(x-\mu)^2}{\nu}\right]^{-\nu/2-D/2},$$

$$f_x(x) = \frac{\Gamma[(\nu+p)/2]}{\Gamma(\nu/2)\nu^{p/2}\pi^{p/2}|\Sigma|^{1/2}[1+1/\nu(x-\mu)^T\Sigma^{-1}(x-\mu)]^{(\nu+p)/2}}$$

$$\mathbb{E}(\mathbf{x}) = \frac{\Gamma(D/2+\nu/2)}{\Gamma(\nu/2)} \frac{|\Lambda|^{1/2}}{(\pi\nu)^{D/2}} \int \left[1 + \frac{(x-\mu)^T\Lambda(x-\mu)}{\nu}\right]^{-D/2-\nu/2} x dx$$

# 3 Independent Component Analysis

We have a set of N observations:

$$D = \{\mathbf{x}^{(n)} \in \mathbb{R}^J\}_{n=1}^N$$

, with I independent sources. Thus:

 $\mathbf{x} = \mathbf{G}\mathbf{s}$ , where G is not known. We assume that the latent variables are independently distributed, with marginal distributions  $P(s_i|H) =$  $p_i(s_i)$ . The probability of the observables and the hidden nodes is:  $P(\{x^{(n)}, s^{(n)}\}_{n=1}^{N} | G, H) = \prod_{n=1}^{N} [P(x^{(n)} | s^{(n)}, G, H) P(s^{(n)} | H)]$  $=\prod_{n=1}^{N}[(\prod_{J}\delta(x_{j}^{(n)}-\sum_{i}G_{ji}s_{i}^{(n)}))(\prod_{i}p_{i}(s_{i}^{(n)}))].$  The factor x is generated without noise. For learning the G from the

data the likelihood is:  $P(D|G, H) = \prod_n P(x^{(n)}|G, H)$ 

, which is a product of factors if we marginalize over the latent variables. We can express each coefficient of G, as a summation over all coefficients multiplied by a delta function such that,  $G_{ii}s_i^{(n)} = \sum_i G_{ii}s_i^{(n)}$ . ( $\mathcal{H}$  denotes the model.)

$$p(\mathbf{x}^{(\mathbf{n})}|\mathbf{G}, \mathcal{H}) = \int p(\mathbf{x}^{(\mathbf{n})}|\mathbf{s}^{(n)}, \mathbf{G}, \mathcal{H})p(\mathbf{s}^{(n)}|\mathcal{H})d^{I}\mathbf{s}^{(n)}$$

$$= \int \prod_{j} \delta(x_{j}^{(n)} - G_{ji}s_{i}^{(n)}) \prod_{i} p_{i}(s_{i}^{(n)})d^{I}\mathbf{s}^{(n)}$$

$$= \frac{1}{|\det \mathbf{G}|} \prod_{i} p_{i}(G_{ji}^{-1}x_{j}) \Rightarrow$$

 $\ln p(\mathbf{x^{(n)}}|\mathbf{G}, H) = -\ln |\det \mathbf{G}| + \sum_{i} \ln p_i(G_{ii}^{-1}x_j)$ 

, which is the log-likelihood of the data D. Now, to find the gradient of the log-likelihood, we are introducing  $\mathbf{W} = \mathbf{G}^{-1}$ , now the log-likelihood can be written as:

$$\ln p(\mathbf{x}^{(\mathbf{n})}|\mathbf{G}, H) = -\ln |\det \mathbf{W}| + \sum_{i} \ln p_{i}(W_{ji}x_{j})$$

# The gradient of the log-likelihood equation will be: $\frac{\partial}{\partial W_{ij}} \ln p(\mathbf{x^{(n)}}|\mathbf{G},\mathcal{H}) = -\frac{\partial}{\partial W_{ij}} (\ln |\det \mathbf{W}|) + \frac{\partial}{\partial W_{ij}} (\sum_i \ln p_i(W_{ji}x_j))$ 4 Generative Models for Discrete Data

We can classify a feature vector **x** using the Bayes rule  $p(y = c | \mathbf{x}, \boldsymbol{\theta}) \propto p(\mathbf{x} | y = c, \boldsymbol{\theta}) p(y = c | \boldsymbol{\theta})$ 

We can use different models for the data when it's discrete, based on

what kind of distribution we expect the data to assume and a respective conjugate prior over the model parameters  $\boldsymbol{\theta}$ .

#### 4.1 Beta-Binomial Model

In this model we can observe a series of Bernoulli trials (e.g. coin tosses) or the number of heads (and the number of tails or total number of tosses), which is a Binomial, and it would result in the same likelihood:  $p(\mathcal{D}|\theta) = \theta^{N_1}(1-\theta)^{N_0}$ . A conjugate prior for this likelihood is given by Beta $(\theta|a,b) \propto \theta^{a-1}(1-\theta)^{b-1}$ . The **posterior** is then obtained by multiplying the prior with the likelihood,  $p(\theta|\mathcal{D}) \propto$  $p(\mathcal{D}|\theta)p(\theta) = \operatorname{Bin}(N_1|\theta, N_1 + N_0)\operatorname{Beta}(\theta|a, b) \propto \operatorname{Beta}(\theta|a + N_1, b + N_0).$ The evidence is obtained from  $p(\theta|\mathcal{D}) = \frac{1}{p(\mathcal{D})} p(\mathcal{D}|\theta) p(\theta)$  normalization of posterior is  $1/B(a+N_1,b+N_0)^2$ , of prior is 1/B(a,b), hence  $p(\mathcal{D}) = \binom{N}{N_1} B(a + N_1, b + N_0) / B(a, b).$ 

## 4.2 Dirichlet-Multinomial Model

For example N dice rolls or *multinomial* events (with K outcomes). The **likelihood** is  $p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{k=1}^K \theta_k^{N_k}$  where  $N_k$  counts times event k occurred (it's a suff. statistic). A conjugate prior is the Dirichlet distribution. The **posterior** is  $p(\theta|\mathcal{D}) \propto \text{Dir}(\theta|\alpha)p(\mathcal{D}|\theta) \propto \text{Dir}(\theta|\alpha_1 + \alpha_2)$  $N_1, \ldots, \alpha_k + N_k$ ). The **evidence** is (obtained as the previous model)  $p(\mathcal{D}) = B(\mathbf{N} + \boldsymbol{\alpha})/B(\boldsymbol{\alpha}).$ 

# 5 Graphical Models

Capture noise, for reasoning, enormous datasets, for causality, for designing models, CIR are encoded in the graph, for inference.

### 5.1 Discriminative

$$p(\mathbf{t}|w) = p(w) \prod_{n=1}^{N} p(t_n|w)$$

### 5.2 Generative

$$T^* = P(T^*|W, X^*, X_i, T_i, \sigma^2, a) =, [\prod_{i=1}^N P(X_i|W, \sigma^2)] P(W|a)P(T^*|X^*, W, \sigma^2)$$

# 5.3 Directed GMs a.k.a. Bayesian Networks

Nodes are connected by directed arrows. The full joint distribution is  $p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k | \text{pa}(x_k))$ 

Directed Acyclic Graphs are BNs without directed loops.

#### 5.3.1 Blocking Rules

$$\bigcirc \rightarrow \bigcirc \rightarrow \bigcirc \rightarrow \bigcirc \qquad \bigcirc \leftarrow \bigcirc \rightarrow \bigcirc \rightarrow \cdots \bigcirc \cdots \leftarrow \bigcirc$$

#### 5.3.2 D-separation

 $A \perp \!\!\!\perp B \mid C$  holds if each path that connects a node in A with a node in B is blocked, that is

- a) the arrows on the path meet either head-to-tail or tail-to-tail at the node and the node is in C, or
- b) the arrows meed head-to-head at the node and either the node nor any of its descendants is in C.

#### 5.4 Markov Random Fields

Graphical Models with undirected edges (a.k.a. Undirected Graphical

#### 5.4.1 Conditional Independence

 $A \perp \!\!\! \perp B \mid C$  holds if all paths connecting every node in A to every other node in B is 'blocked' by a node in C (blocked means passing through).

# 5.4.2 Cliques and Maximal Cliques

A *clique* is a subset of nodes in the graph such that there exists a link between all pairs of nodes in the subset (the set of nodes in a clique is fully connected). A *maximal clique* is a clique such that it is not possible to include any other nodes from the graph in without it ceasing to be a clique.

#### 5.4.3 Factorization

A MRF can be factorized using potential functions over its maximal cliques:  $p(\mathbf{x}) = \frac{1}{Z} \prod_C \psi_C(\mathbf{x}_C)$   $Z = \sum_T \prod_C \psi_C(\mathbf{x}_C)$ 

# 5.4.4 Relation to Directed Graphs

To transform a directed graph into an undirected one we have to perform a *moralization* process of "marrying the parents" of each node (by linking them) and removing all remaining arrows.

# 5.5 Markov Blanket

 $p(x_i|x_{MB_i}, x_{rest}) = p(x_i|x_{MB_i})$ 

**Directed case**: The MB of  $x_i$  consists of: the parents of  $x_i$ , the children of  $x_i$  and the co-parents of the children of  $x_i$ .

Undirected case: All neighboring nodes of  $x_i$ .

# 5.6 Naive Bayes

The problem of finding a label  $y^*$  for some previously unobserved vector of features  $\mathbf{x}^*$ , while having previously observed  $\{\mathbf{x}_n, y_n\}_{n=1,\dots,N}$ . We build a *generative* GM, linking the label  $y_n$  with each feature of the feature vector  $\mathbf{x}_n$ . This implies that all features are independent of each other given the label. For a single data case the joint probability is

$$p(y, x_1, \dots, x_D | \boldsymbol{\eta}, \boldsymbol{\theta}_i) = p(y | \boldsymbol{\eta}) \prod_{i=1}^D p(x_i | \boldsymbol{\theta}_i)$$

while the probability of the full dataset is  $\prod_{n=1}^{N} p(y_n | \boldsymbol{\eta}) \prod_{i=1}^{D} p(x_i | \boldsymbol{\theta}_i)$ Note that this generative form is chosen as the other option (features pointing towards the label) would imply a very highly parameterized model, as we would considering  $p(y|x_1,\ldots,x_D)$ .

Finding a label  $y^*$  implies finding

$$y^* = \operatorname{argmax}_y \left\{ \ln p(y|\boldsymbol{\eta}) + \sum_{i=1}^D \ln p(x_i^*|y, \boldsymbol{\theta}_i) \right\}$$

# 5.7 Maximum Likelihood Training in BNs

It is fast because the log-likelihood decomposes into a sum over all variables  $X_i$ . Learning all parameters reduces into a collection of independent tasks of learning  $p(x_i|pa_{x_i})$ .

$$p(x_i|\mathrm{pa}_{x_i}) = \frac{N(x_i,\mathrm{pa}_{x_i})}{N(\mathrm{pa}_{x_i})}$$

is the number of times  $x_i$  co-occurred with  $pa_{x_i}$  divided by the number of times  $pa_{x_i}$  occurred.

The probability of a set of variables  $\mathbf{x}$  in a Bayes Net is defined as  $p(x) = \prod_i p(x_i|x_{pa_i})$ . If we define a function  $\theta(x_i, x_{pa_i})$  and use it instead of  $p(x_i|x_{pa_i})$ , we have  $p(x) = \prod_i \theta(x_i, x_{pa_i})$ , if we constrain  $\theta$  such that  $\sum_{x_i} \theta(x_i, x_{pa_i}) = 1, \forall i$ . We now have that the probability of the full data set:  $p(\{\widetilde{x}_{in}\}) = \prod_n \prod_i \prod_{x_i n} \prod_{x_{pa_i}} \theta(x_i, x_{pa_i})^{\mathbb{I}[x_i = \widetilde{x}_{in} \land x_{pa_i} = \widetilde{x}_{pa_in}]}$ 

# 5.8 Inference in Graphical Models

In which some of the variables are observed and we wish to compute the posterior distribution of one or more subsets of other variables.

#### 5.8.1 Inference on a chain

$$\begin{split} p(\mathbf{x}) &= p(x_1, \dots, x_N) \\ &= \frac{1}{Z} \psi_{1,2}(x_1, x_2) \dots \psi_{N-1,N}(x_{N-1}, x_N) \\ &= \sum_{x_1} \sum_{x_2} \dots \sum_{x_{N-1}} \sum_{x_N} p(\mathbf{x}) \\ &= \sum_{x_1} \dots \sum_{x_{n-1}} \sum_{x_{n+1}} \dots \sum_{x_{N-1}} \sum_{x_N} p(\mathbf{x}) \\ &= \frac{1}{Z} \sum_{x_1} \dots \sum_{x_{n-1}} \psi_{x_1, x_2} \dots \psi_{x_{n-1}, x_n} \mu_{\beta}(x_n) \\ &\mu_{\beta}(x_n) &= \frac{1}{Z} \sum_{x_{n+1}} \psi_{x_n, x_{n+1}} \dots \sum_{x_N} \psi_{x_{N-1}, x_N} \\ &\mu_{\alpha}(x_n) &= \frac{1}{Z} \sum_{x_{n-1}} \psi_{x_{n-1}, x_n} \dots \sum_{x_1} \psi_{x_2, x_1} \\ &p(x_n) &= \frac{1}{z} \mu_{\alpha}(x_n) \mu_{\beta}(x_n) &O(NK^2) \end{split}$$

# 5.8.2 Factor Graphs

A tree is a graph with no loops. Both directed and undirected trees can be converted to a factor graph tree, but a directed tree could result in a non-tree structure when converted to an undirected representation. It is called a poly-tree (and not simply a tree) since its undirected representation (middle graph) includes a loop. The factor graph representation is again a tree. Factor graphs are the most general representation, and since any other tree representation can be easily converted to a factor tree, the sum-product algorithm is defined for factor trees.

# 5.8.3 Sum-Product Algorithm

It is used to find individual marginals.

Probability of the factor graph:  $p(\mathbf{x}) = \frac{1}{Z} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$ 

 $factor \rightarrow variable message:$ 

$$\mu_{f_{\alpha} \to x_{i}}(x_{i}) = \sum_{\mathbf{x}_{\alpha} \setminus x_{i}} f_{\alpha}(\mathbf{x}_{\alpha}) \prod_{m \in \text{ne}(f_{\alpha}) \setminus x_{i}} \mu_{x_{m} \to f_{\alpha}}(x_{m})$$

 $variable \rightarrow factor message:$ 

$$\mu_{x_m \to f_\alpha}(x_m) = \prod_{\beta \in ne(x_m) \setminus f_\alpha} \mu_{f_\beta \to x_m}(x_m)$$

 $\begin{array}{ll} \textbf{leaf nodes} & x_l & \text{is variable:} & \mu_{x_l \to f_\delta}(x_l) = 1 \\ & f_\varepsilon & \text{is factor:} & \mu_{f_\varepsilon \to x_k}(x_k) = f_\varepsilon(x_k) \\ \end{array}$ 

variable marginal:  $p(x) = \prod_{\alpha \in ne(x)} \mu_{f_{\alpha} \to x}(x)$ 

factor marginal: 
$$p(\mathbf{x}_{\alpha}) = f_{\alpha}(\mathbf{x}_{\alpha}) \prod_{i \in \text{ne}(f_{\alpha})} \mu_{x_i \to f_{\alpha}}(x_i)$$

By caching intermediate results and calculating two messages for each edge in a tree-structured factor graph, the Sum-Product algorithm efficiently computes all variable marginals in  $O(2EK^2)$  (where E is the number of edges and each variable is assumed to have K possible values).

### 5.8.4 Max-Sum Algorithm

It is used to find a setting of the variables that has the largest *joint* probability and the value of that probability.

$$\mathbf{x}^{\max} = \underset{\mathbf{x}}{\operatorname{argmax}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha}) \qquad p(\mathbf{x}^{\max}) = \underset{\mathbf{x}}{\max} \frac{1}{Z} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$$

 $\log p(\mathbf{x}^{\max}) = \max_{\mathbf{x}} \left\{ \log Z + \sum_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha}) \right\}$ factor  $\rightarrow$  variable message:

$$\mu_{f_{\alpha} \to x_{i}}(x_{i}) = \max_{\mathbf{x}_{\alpha} \setminus x_{i}} \left[ (\ln f_{\alpha}(\mathbf{x}_{\alpha})) + \sum_{m \in \text{ne}(f_{\alpha}) \setminus x_{i}} \mu_{x_{m} \to f_{\alpha}}(x_{m}) \right]$$

 $variable \rightarrow factor message:$ 

$$\mu_{x_m \to f_\alpha}(x_m) = \sum_{f_\beta \in \text{ne}(x_m) \setminus f_\alpha} \mu_{f_\beta \to x_m}(x_m)$$

$$\begin{array}{lll} \textbf{leaf nodes} & x_l & \text{is variable:} & \mu_{x_l \to f_\delta} = 0 \\ & f_\varepsilon & \text{is factor:} & \mu_{f_\varepsilon \to x_k} = \ln f_\varepsilon(x_k) \\ \textbf{at root} & p^{\max} = \max_x \left[ \sum_{f_\alpha \in \operatorname{ne}(x)} \mu_{f_\alpha \to x}(x) \right] \\ & x^{\max} = \operatorname{argmax}_x \left[ \sum_{f_\alpha \in \operatorname{ne}(x)} \mu_{f_\alpha \to x}(x) \right] \\ \textbf{max-marginals} & q(x_i) = -\ln Z + \sum_{f_\alpha \in \operatorname{ne}(x_i)} \mu_{f_\alpha \to x_i}(x_i) \\ \end{array}$$

Given max-marginals you have to perform a decoding step (the Viterbi algorithm) in order to find the global optimum. If  $q(x_i)$  has unique maximum, we can use  $x_i^* = \operatorname{argmax}_{x_i} q(x_i)$ .

#### 5.8.5 Variable Elimination

If we have some clusters  $C_i$  and  $C_j$ , then:

 $S_{ij} = C_i \cap C_j$  Define potential functions  $\Psi_i$  for each cluster  $C_i$ :  $\forall C_i : \Psi_i \coloneqq \prod_{\psi_j \in C_i} \psi_j \ m_i \to C_j = \sum_{C_i \smallsetminus S_{ij}} \Psi_i \prod_{k \in \text{ne}(i) \smallsetminus j} m_{k \to i}(C_i)$ 

Note that:  $C_i \setminus S_{ij} = C_i \setminus C_j$ 

Belief:  $\Psi_{\text{root}} \prod_{k \in \text{ne}(\text{root})} m_{k \to \text{root}}(C_{\text{root}}) \propto p(C_{\text{root}})$ 

Clusters replace factors, edges replace variables.

**Tree width** The width of a tree is one smaller than the biggest clique in the optimal ordering. Finding the optimal order is NP-hard.

Running Intersection Property A clique tree has the running intersection property if  $x \in C_i \land x \in C_j \Rightarrow x \in C_k$  on the clique path between  $C_i$  and  $C_j$ .

# 5.8.6 Loopy Belief Propagation

Is a way to approximate inference in graphs with loops. The idea is simply to apply the sum-product algorithm even though there is no guarantee that it will yield good results. This approach is possible because the message passing rules are purely local. However, because of the loops, information can flow many times around the graph; for some models it will converge, for others it will not. We will say that a node a has a **pending** message on its link to a node b if node a has received any message on any of its other links since the last time it sent a message to b. Thus, when a node receives a message on one of its links, this creates pending messages on all of its other links. Then we need to send only pending messages otherwise they will be duplicate. When there are no more pending messages, the product of the received messages at every node gives the (exact for tree) marginal. For loopy graphs however the algorithm may not converge and when we stop the marginals are approximate.

# 6 Mathematical Tricks

$$-\frac{1}{2}(x-\mu)^{\top}\Sigma^{-1}(x-\mu) = -\frac{1}{2}x^{\top}\Sigma^{-1}x + x^{\top}\Sigma^{-1}\mu + c$$

$$\frac{\partial a^{\top}Xb}{\partial X} = ab^{\top}, \quad \frac{\partial a^{\top}X^{\top}b}{\partial X} = ba^{\top}$$

$$\frac{\partial \det X}{\partial X} = \det(X)(X^{-1})^{\top}$$

$$M = M^{\top} \iff u^{\top}Mv = v^{\top}Mu$$

$$\mathbb{E}[(x-\mu)^{\top}\Sigma^{-1}(x-\mu)\mathcal{N}(x|\mu,\Sigma)] = \operatorname{Tr}(\Sigma^{-1}\Sigma) = D$$

$$\mathbb{E}[x] = \int_{-\infty}^{\infty} xf(x)dx$$
Product of Gaussians:  $\Sigma = (\Sigma_1^{-1} + \Sigma_2^{-1})^{-1}, \ \mu = \Sigma\Sigma_1^{-1}$ 

Product of Gaussians:  $\Sigma = (\Sigma_1^{-1} + \Sigma_2^{-1})^{-1}$ ,  $\mu = \Sigma \Sigma_1^{-1} \mu_1 + \Sigma \Sigma_2^{-1} \mu_2$  Other:  $(P^{-1} + B^{\top} R^{-1} B)^{-1} B^{\top} R^{-1} = P B^{\top} (B P B^{\top} + R)^{-1}$  Woodbury:  $(A + B D^{-1} C)^{-1} = A^{-1} - A^{-1} B (D + C A^{-1} B)^{-1} C A^{-1}$  Gradient in exp family wrt for  $\eta$ , for  $p(x|\eta) = h(x)g(\eta) \exp\{\eta^T u(x)\}$ , where  $g(\eta) \int h(x) \exp\{\eta^T u(x)\} dx = 1$ , we have the result: $-\nabla \ln g(\eta) = \mathbb{E}[u(x)]$