Machine Learning 2 - Cheat Sheet

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1 Probability Theory

1.1 Independence

$$p(X,Y) = p(X)p(Y) \Leftrightarrow p(X|Y) = p(X) \Leftrightarrow p(Y|X) = p(Y)$$

1.2 Conditional Independence

 $X \perp \!\!\!\perp Y \mid Z \Longleftrightarrow p(X, Y|Z) = p(X|Z)p(Y|Z)$

1.3 Sum and Product Rules

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

1.4 Bayes' Theorem

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

2 Distributions

Binary Bernoulli Binomial Beta
Discrete Categorical Multinomial Dirichlet

2.1 Bernoulli Distribution

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

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(
$$\mu|a,b$$
) = $\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1}$, 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

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

2.6 Multinomial Distribution

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

2.7 Dirichlet Distribution

$$\operatorname{Dir}(\boldsymbol{\mu}|\boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1)\cdots\Gamma(\alpha_k)} \prod_{k=1}^K \mu_k^{\alpha_k - 1}, \qquad \alpha_0 = \sum_{k=1}^K \alpha_k$$

2.8 Gaussian Distribution

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

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

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

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

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

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

St(
$$x|\mu, \lambda, \nu$$
) = $\frac{\Gamma(\nu/2+1/2)}{\Gamma(\nu/2)} (\frac{\lambda^{1/2}}{(\pi\nu)^{D/2}}) [1 + \frac{\lambda(x-\mu)^2}{\nu}]^{-\nu/2-D/2},$
 $f_x(x) = \frac{\Gamma[(\nu+p)/2]}{\Gamma(\nu/2)\nu^{p/2}\pi^{p/2}|\Sigma|^{1/2}[1+1/\nu(x-\mu)^T\Sigma^{-1}(x-\mu)]^{(\nu+p)/2}}$
 $\mathbb{E}(\mathbf{x}) = \frac{\Gamma(D/2+\nu/2)}{\Gamma(\nu/2)} \frac{|\Lambda|^{1/2}}{(\pi\nu)^{D/2}} \int [1 + \frac{(x-\mu)^T\Lambda(x-\mu)}{\nu}]^{-D/2-\nu/2} x dx$

3 Graphical Models

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

3.1 Directed GMs a.k.a. Bayesian Networks

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

Directed Acyclic Graphs are BNs without directed loops.

3.1.1 Blocking Rules

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

3.1.2 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.

3.2 Markov Random Fields

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

3.2.1 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).

3.2.2 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.

3.2.3 Factorization

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

3.2.4 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.

3.3 Markov Blanket

 $p(x_i|x_{\mathrm{MB}_i}, x_{\mathrm{rest}}) = p(x_i|x_{\mathrm{MB}_i})$

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 .

3.4 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.

3.4.1 Inference on a chain

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

3.4.2 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.

3.4.3 Sum-product algorithm

Probability of the factor graph: $p(\vec{x}) = \frac{1}{Z} \prod_{\alpha} f_{\alpha}(\vec{x}_{\alpha})$ factor \rightarrow variable message $\mu_{\alpha \to i}(x_i) = \sum_{x_{\alpha \smallsetminus i}} f_{\alpha}(\vec{x}_{\alpha}) \prod_{j \in \alpha \smallsetminus i} \mu_{j \to \alpha}$ variable \rightarrow factor message $\mu_{j \to \alpha}(x_j) = \prod_{\beta \in \operatorname{ne}(j) \smallsetminus \alpha} \mu_{\beta \to j}(x_j)$

 $\begin{array}{lll} \text{leaf node messages} & x_l & \text{is a leaf node:} & \mu_{l \to \delta}(x_l) = 1 \\ \varepsilon & \text{is a leaf node:} & \mu_{\varepsilon \to k}(x_k) = f_\varepsilon(x_k) \end{array}$