# Formula

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## Abstract

Mathematical formulas with special emphasis on statistical distributions. The formulas are sketchy and not necessarily complete or correct. Corrections can be sent to fn@imm.dtu.dk.

Thanks to Berkan Dulek

# Contents

# Chapter 1

# Distributions

## 1.1 Normal distributions

The "stationary colored noise" matrix normal $\mathbf{X}(N \times P) \sim N_{N\times P}(\mathbf{M}, \mathbf{\Sigma} \otimes \mathbf{\Omega})$ (Triantafyllopoulos, 2002, p. 234)

$$p(\mathbf{X}|\mathbf{M},\mathbf{\Omega},\mathbf{\Sigma}) = (2\pi)^{-NP/2}|\mathbf{\Omega}|^{-P/2}|\mathbf{\Sigma}|^{-N/2}\exp\left\{-\frac{1}{2}\mathrm{tr}\left[\mathbf{\Omega}^{-1}(\mathbf{X}-\mathbf{M})\mathbf{\Sigma}^{-1}(\mathbf{X}-\mathbf{M})^{\mathsf{T}}\right]\right\} \tag{1.1}$$

The probability density function for $\mathbf{X}(N \times P)$ for "white noise" matrix normal, i.e., $N$ independent $P$-dimensional $\mathbf{x}_n$ with $\boldsymbol{\mu}^{\mathsf{T}}\mathbf{1} = \mathbf{M}$ and $\mathbf{\Omega} = \mathbf{I}_N$ (Mardia et al., 1979, section 2.5.5)

$$p(\mathbf{X}|\boldsymbol{\mu},\mathbf{\Sigma}) = |2\pi\mathbf{\Sigma}|^{-N/2}\exp\left[-\frac{1}{2}\sum_n^N(\mathbf{x}_n-\boldsymbol{\mu})^{\mathsf{T}}\mathbf{\Sigma}^{-1}(\mathbf{x}_n-\boldsymbol{\mu})\right] \tag{1.2}$$

$$= |2\pi\mathbf{\Sigma}|^{-N/2}\exp\left[-\frac{1}{2}\mathrm{tr}\left\{\mathbf{\Sigma}^{-1}(\mathbf{X}-\mathbf{1}\boldsymbol{\mu}^{\mathsf{T}})^{\mathsf{T}}(\mathbf{X}-\mathbf{1}\boldsymbol{\mu}^{\mathsf{T}})\right\}\right] \tag{1.3}$$

with sufficient statistics $\bar{\mathbf{x}}$ and $\mathbf{S}$ (Mardia et al., 1979, equation 4.1.20)

$$= |2\pi\mathbf{\Sigma}|^{-N/2}\exp\left[-\frac{N}{2}(\bar{\mathbf{x}}-\boldsymbol{\mu})^{\mathsf{T}}\mathbf{\Sigma}^{-1}(\bar{\mathbf{x}}-\boldsymbol{\mu}) - \frac{N}{2}\mathrm{tr}(\mathbf{\Sigma}^{-1}\mathbf{S})\right] \tag{1.4}$$

The multinormal distribution (the Gaussian distribution) of a $P$-dimensional $\mathbf{x} \sim N_P(\boldsymbol{\mu},\mathbf{\Sigma})$ for a single case $N = 1$ (Mardia et al., 1979, equation 2.5.1)

$$p(\mathbf{x}|\boldsymbol{\mu},\mathbf{\Sigma}) = |2\pi\mathbf{\Sigma}|^{-1/2}\exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}}\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right] \tag{1.5}$$

With an isotropic (co-)variance

$$p(\mathbf{x}|\boldsymbol{\mu},\sigma^2) = (2\pi\sigma^2)^{-P/2}\exp\left[-\frac{(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}}(\mathbf{x}-\boldsymbol{\mu})}{2\sigma^2}\right] \tag{1.6}$$

Univariate $P = 1$

$$p(x|\mu,\sigma^2) = (2\pi\sigma^2)^{-1/2}\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] \tag{1.7}$$

Standardized central univariate, $\mu = 0$ and $\sigma = 1$

$$p(x) = (2\pi)^{-1/2}\exp\left(-\frac{x^2}{2}\right). \tag{1.8}$$

## 1.2 Wishart and $\chi^2$ distributions

The central Wishart distribution for $\mathbf{M}(P \times P)$ where $M$ can be regarded as a degree of freedom parameter (Mardia et al., 1979, equation 3.8.1) (Conradsen, 1984, section 2.5)

$$p(\mathbf{M}|\mathbf{\Sigma}, M) = \frac{1}{2^{MP/2}\pi^{P(P-1)/4}|\mathbf{\Sigma}|^{M/2}\prod_p^P \Gamma[\frac{1}{2}(M+1-p)]}|\mathbf{M}|^{(M-P-1)/2}\exp\left[-\frac{1}{2}\mathrm{tr}(\mathbf{\Sigma}^{-1}\mathbf{M})\right] \quad (1.9)$$

The central Wishart distribution on standard form with $\mathbf{\Sigma} = \mathbf{I}$

$$p(\mathbf{M}|M) = \frac{1}{2^{MP/2}\pi^{P(P-1)/4}\prod_p^P \Gamma[\frac{1}{2}(M+1-p)]}|\mathbf{M}|^{(M-P-1)/2}\exp\left[-\frac{1}{2}\mathrm{tr}(\mathbf{M})\right] \quad (1.10)$$

With a one dimensional $P = 1$ central Wishart distribution on standard form the $\mathbf{M} = y \sim \chi^2$ ("chi-square") distribution is attained. The sum of the square of $M$ independently standardized normal distribution random variables is also $\chi^2$ distributed. The $\chi^2$ probability density function (Mardia et al., 1979, section B.3)

$$p_{\chi^2}(y|M) = \left\{2^{M/2}\Gamma(M/2)\right\}^{-1} y^{M/2-1}\exp(-y/2) \quad (1.11)$$

The cumulative distribution function is

$$P(y) = \frac{1}{\Gamma(P/2)}\gamma(y/2, P/2) \quad (1.12)$$

where $\gamma$ is the lower incomplete gamma function, see section 4.1.

## 1.3 Generalized matrix $T$, multivariate Student's $t$ and Cauchy distributions

The type I generalized matrix $T$ distribution (Triantafyllopoulos, 2002, p. 72+), (Triantafyllopoulos, 2003)

$$p(\mathbf{T}|\mathbf{M}, \mathbf{\Omega}, \mathbf{\Sigma}, \mathbf{D}) \propto \left|\mathbf{D}^{1/2}\mathbf{\Omega}\mathbf{D}^{1/2} + (\mathbf{T}-\mathbf{M})\mathbf{\Sigma}^{-1}(\mathbf{T}-\mathbf{M})^\mathsf{T}\right|^{-[\mathrm{tr}(\mathbf{D})/P+N+P-1]/2}, \quad (1.13)$$

where $\mathbf{D}$ is a matrix of degrees of freedom. The matrix $T$ distribution is obtained with $\nu = \mathrm{tr}(\mathbf{D})/P +$ constant and rescaling $\mathbf{\Omega}$. With $\mathbf{X}(N \times P) \sim N_P(\mathbf{M}, \mathbf{\Sigma})$ and $\mathbf{B} \sim W_N(\mathbf{\Omega}, \nu)$ then $\mathbf{T}(N \times P) = \mathbf{B}^{-1/2}\mathbf{X}$ is a matrix distributed with the matrix $T$ distribution (Hedibert Freitas Lopes) (Dickey, 1967) ??? (Triantafyllopoulos, 2002, p. 235)

$$p(\mathbf{T}|\mathbf{M}, \mathbf{\Omega}, \mathbf{\Sigma}, \nu) = \pi^{-NP/2}\prod_{p=1}^{P}\frac{\Gamma[(\nu+P-p+1)/2]}{\Gamma[(\nu-p+1)/2]}|\mathbf{\Omega}|^{-\nu/2}|\mathbf{\Sigma}|^{-N/2}\left|\mathbf{\Omega}^{-1} + (\mathbf{T}-\mathbf{M})\mathbf{\Sigma}^{-1}(\mathbf{T}-\mathbf{M})^\mathsf{T}\right|^{-(\nu+P)/2} \quad (1.14)$$

The multivariate $t$ distribution is attained with $N = 1$ and $\mathbf{\Omega} = \mathbf{I} = 1$ (Mardia et al., 1979, section 2.6.5), (O'Hagan, 1994, section 9.5)

$$p_t(\mathbf{t}|\boldsymbol{\mu}, \mathbf{\Sigma}, \nu) = (\pi\nu)^{-P/2}\frac{\Gamma(\frac{\nu+P}{2})}{\Gamma(\nu/2)}\frac{|\mathbf{\Sigma}|^{-1/2}}{\left[1+\nu^{-1}(\mathbf{t}-\boldsymbol{\mu})^\mathsf{T}\mathbf{\Sigma}^{-1}(\mathbf{t}-\boldsymbol{\mu})\right]^{(\nu+P)/2}} \quad (1.15)$$

where $P$ is the dimension of $\mathbf{t}$. The multivariate Cauchy distribution is obtained with the degrees of freedom parameter $\nu = 1$

$$p_{\mathrm{Ca}}(\mathbf{t}|\boldsymbol{\mu}, \mathbf{\Sigma}) = \pi^{-P/2}\frac{\Gamma(\frac{1+P}{2})}{\Gamma(1/2)}\frac{|\mathbf{\Sigma}|^{-1/2}}{\left[1+(\mathbf{t}-\boldsymbol{\mu})^\mathsf{T}\mathbf{\Sigma}^{-1}(\mathbf{t}-\boldsymbol{\mu})\right]^{(1+P)/2}} \quad (1.16)$$

For the univariate $P = 1$ Cauchy distribution the probability density is

$$p_{\mathrm{Ca}}(t|\mu, \sigma^2) = \frac{1}{\pi\sigma} \frac{1}{1 + (\frac{t-\mu}{\sigma})^2} \tag{1.17}$$

The central standardized univariate Cauchy distribution $\mu = 0$ and $\sigma^2 = 1$

$$p_{\mathrm{Ca}}(t|0, 1) = \frac{1}{\pi} \frac{1}{1 + t^2} \tag{1.18}$$

## 1.4 Normal-inverse Wishart and normal-inverse gamma distribution

Posterior distribution for joint posterior with an information (natural) conjugate normal-inverse Wishart prior (Mardia et al., 1979, exercise 4.3.2)

$$p(\boldsymbol{\mu}, \boldsymbol{\Sigma}|\mathbf{X}, \boldsymbol{\phi}, \mathbf{G}, M) = p(\boldsymbol{\mu}, \boldsymbol{\Sigma}|\bar{\mathbf{x}}, \mathbf{S}, \boldsymbol{\phi}, \mathbf{G}, N, M) \tag{1.19}$$

$$\propto |\boldsymbol{\Sigma}|^{-(N+M+1)/2} \mathrm{etr}\left(-\frac{1}{2}\boldsymbol{\Sigma}^{-1}\left[N\mathbf{S} + \mathbf{G} + (\boldsymbol{\mu} - \boldsymbol{\phi})(\boldsymbol{\mu} - \boldsymbol{\phi})^\mathsf{T} + N(\boldsymbol{\mu} - \bar{\mathbf{x}})(\boldsymbol{\mu} - \bar{\mathbf{x}})^\mathsf{T}\right]\right), \tag{1.20}$$

where etr$(\cdot)$ is the exponential of the trace: $\exp(\mathrm{tr}(\cdot))$.

The normal-inverse gamma distribution is used as the informative (natural) conjugate prior distribution for the parameters in a normal linear model ($\mathbf{y} = \mathbf{X}\mathbf{b} + \mathbf{u}, u \sim N_1(0, \sigma^2)$) in Bayesian inference (O'Hagan, 1994, equation 9.5 and 9.8), (Hansen et al., 2002), (Hansen et al., 2003, eq. 1.6)

$$p_{\mathrm{NIG}}(\mathbf{b}, \sigma^2|a, D, P, \mathbf{m}, \mathbf{V}) = \frac{(a/2)^{D/2}}{(2\pi)^{P/2}|\mathbf{V}|^{1/2}\Gamma(D/2)}(\sigma^2)^{-(D+P+2)/2} \exp\left\{-\frac{1}{2\sigma^2}\left[(\mathbf{b} - \mathbf{m})^\mathsf{T}\mathbf{V}^{-1}(\mathbf{b} - \mathbf{m}) + a\right]\right\} \tag{1.21}$$

$$\propto (\sigma^2)^{-(D+P+2)/2} \exp\left\{-\frac{1}{2\sigma^2}\left[(\mathbf{b} - \mathbf{m})^\mathsf{T}\mathbf{V}^{-1}(\mathbf{b} - \mathbf{m}) + a\right]\right\} \tag{1.22}$$

where $P$ is the dimension of $\mathbf{V}$. The distribution is usually denoted NIG$(a, D, \mathbf{m}, \mathbf{V})$. The marginal distribution of $\mathbf{b}$ is the multivariate $t$ distribution $t(\mathbf{m}, a\mathbf{V}, D)$. The marginal distribution of $\sigma^2$ is the inverse gamma distribution.

Somewhat similar is a distribution for $\theta \equiv \mathbf{b}$ and $\sigma$ (not $\sigma$ *squared*) (Box and Tiao, 1992, eq. 2.4.6)

$$p(\theta, \sigma|\mathbf{x}) = \sqrt{\frac{N}{2\pi}}\left[\frac{1}{2}\Gamma\left(\frac{\nu}{2}\right)\right]^{-1}\left(\frac{\nu s^2}{2}\right)^{\nu/2} \sigma^{-(N+1)} \exp\left\{-\frac{1}{2\sigma^2}\left[\nu s^2 + N(\theta - \bar{x})^2\right]\right\} \tag{1.23}$$

## 1.5 Inverse cosh distribution or hyperbolic secant distribution

The inverse hyperbolic cosine, hyperbolic secant distribution or Perks' distribution that is used in independent component analysis (ICA) is heavy-tailed (Smyth, 1994)

$$p(x|\beta) = \frac{1}{2^{\beta-1}B(\beta/2, \beta/2)}\mathrm{sech}^\beta(x), \tag{1.24}$$

where $B$ is the beta function. Standardized $\beta = 1$

$$p(x) = \frac{1}{\pi}\mathrm{sech}(x) \tag{1.25}$$

For $\beta = 2$ there is also a nice normalization factor

$$p(x|\beta = 2) = \frac{1}{2}\mathrm{sech}^2(x) \tag{1.26}$$

## 1.6 Multinomial distribution including binomial and Bernoulli

The discrete multinomial distribution for a discrete variate $\mathbf{n} = [n_1, \ldots, n_P]^\mathsf{T}$ containing counts (Mardia et al., 1979, page 44)

$$P(\mathbf{n}|\mathbf{a}, n) = \frac{n!}{n_1! \ldots n_P!} \prod_p^P a_p^{n_p}, \qquad \sum_p^P n_p = n \tag{1.27}$$

The parameters $\mathbf{a}$ are restricted to be probabilities: $a_p \geq 0$ and $\sum_p^P a_p = 1$. The binomial distribution is obtained with $P = 2$

$$P_{\text{Bin}}(\mathbf{n}|\mathbf{a}, n) = \frac{n!}{n_1! n_2!} \prod_{p=1}^2 a_p^{n_p} = \frac{n!}{n_1! n_2!} a_1^{n_1} (1 - a_1)^{n_2} = \frac{n!}{n_1!(n - n_1)!} a_1^{n_1} (1 - a_1)^{n - n_1} \tag{1.28}$$

$$= \binom{n}{n_1} a_1^{n_1} (1 - a_1)^{n - n_1} \tag{1.29}$$

The Bernoulli distribution appears with $n = 1$, and then $n_1 \in \{0, 1\}$

$$P_{\text{Ber}}(\mathbf{n}|\mathbf{a}) = P(n_1|a_1) = a_1^{n_1} (1 - a_1)^{1 - n_1}. \tag{1.30}$$

...And the important uninomial distribution with $P = 1$

$$P(n|a) = 1, \qquad a = 1 \tag{1.31}$$

## 1.7 Dirichlet distribution including beta and uniform distributions

The Dirichlet distribution is a kind of "inverse" distribution compared to the multinomial distribution on the bounded continuous variate $\mathbf{x} = [x_1, \ldots, x_P]$ (Mardia et al., 1979, p. 44)

$$p(\mathbf{x}|\boldsymbol{\alpha}) = \frac{\Gamma\left(\sum_p^P \alpha_p\right)}{\prod_p^P \Gamma(\alpha_p)} \prod_p^P x_p^{\alpha_p - 1} \tag{1.32}$$

The beta type I distribution is obtained with a bivariate Dirichlet distribution $P = 2$, $x_1 = x$ and $x_2 = 1 - x$ (Mardia et al., 1979, p. 488)

$$p(x|\alpha_1, \alpha_2) = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1)\Gamma(\alpha_2)} x^{\alpha_1 - 1} (1 - x)^{\alpha_2 - 1} \tag{1.33}$$

A uniform distribution with limits between 0 and 1 is obtained with $\alpha = \alpha_1 = \alpha_2 = 1$

$$p(x|\alpha) = 1, \qquad \alpha = 1 \tag{1.34}$$

## 1.8 Multivariate hypergeometric distribution

$$P(\mathbf{n}|\mathbf{m}) = \frac{\prod_{p=1}^P \binom{m_p}{n_p}}{\binom{m}{n}} \tag{1.35}$$

where $\mathbf{m} = [m_1, m_2 \ldots m_P]$, $\mathbf{n} = [n_1, n_2 \ldots n_P]$, $m = m_1 + m_2 + \ldots + m_P$ and $n = n_1 + n_2 + \ldots + n_P$. With $P = 2$ this is the ordinary hypergeometric distribution.

## 1.9 Normal linear model distribution

The multivariate regression model is (Box and Tiao, 1992, page 439)

$$\mathbf{Y} = \mathbf{X}\mathbf{B} + \mathbf{U} \tag{1.36}$$

With the noise as central matrix normal $\mathbf{U}^{\vee} \sim N_{N\times P}(\mathbf{0}, \mathbf{\Sigma} \otimes \mathbf{\Omega})$ ?

$$\mathbf{B}^{\vee}|\mathbf{X}, \mathbf{Y}, \mathbf{\Sigma}, \mathbf{\Omega} \sim ?N_{Q\times P}\left([\mathbf{X}^{-}\mathbf{Y}]^{\vee}, \mathbf{\Sigma} \otimes \left[\mathbf{X}^{-}\mathbf{\Omega}(\mathbf{X}^{-})^{\mathsf{T}}\right]\right) \tag{1.37}$$

With $\mathbf{U}$ distributed as the white noise matrix normal the maximum likelihood estimates are

$$\widehat{\mathbf{B}} = (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{Y} = \mathbf{X}^{-}\mathbf{Y} \tag{1.38}$$

$$\widehat{\mathbf{\Sigma}} = (\mathbf{Y} - \mathbf{X}\widehat{\mathbf{B}})^{\mathsf{T}}(\mathbf{Y} - \mathbf{X}\widehat{\mathbf{B}})/N \tag{1.39}$$

With **non-informative** Jeffrey's priors a posterior for $\mathbf{B}$ is the matrix $T$ distribution (Box and Tiao, 1992, page 440), (Mardia et al., 1979, page 180)

$$p(\mathbf{B}|\mathbf{X}, \mathbf{Y}) \propto |N\widehat{\mathbf{\Sigma}} + (\mathbf{B} - \widehat{\mathbf{B}})^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{X}(\mathbf{B} - \widehat{\mathbf{B}})|^{-N/2} \tag{1.40}$$

**Conjugate priors**

$$p(\mathbf{b}|\mathbf{\Sigma}) = N_P(\mathbf{m}, \mathbf{W}) \tag{1.41}$$

$$p(\mathbf{\Sigma}|\mathbf{b}) = W_P \tag{1.42}$$

Posterior of parameters $\mathbf{b}$ for known variance of the residual is a multinormal $\mathbf{\Sigma}_u = \sigma^2$ (O'Hagan, 1994, page 264) (Goutte et al., 2000, equation 6)

$$p(\mathbf{b}|\mathbf{X}, \mathbf{y}, \mathbf{m}, \mathbf{W}, \sigma^2) \propto \exp\left[-\frac{1}{2\sigma^2}(\mathbf{b} - \widehat{\mathbf{b}})^{\mathsf{T}}\widehat{\mathbf{W}}^{-1}(\mathbf{b} - \widehat{\mathbf{b}})\right] \tag{1.43}$$

where the maximum a posteriori (MAP) estimates are

$$\widehat{\mathbf{b}} = (\mathbf{W}^{-1} + \sigma^{-2}\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}(\mathbf{W}^{-1}\mathbf{m} + \sigma^{-2}\mathbf{X}^{\mathsf{T}}\mathbf{y}), \tag{1.44}$$

$$\widehat{\mathbf{W}} = (\mathbf{W}^{-1} + \sigma^{-2}\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1} \tag{1.45}$$

## 1.10 Gaussian mixture distributions

Gaussian mixture distributions or Mixture of Gaussian (MoG) with a fixed number $K$ of mixtures where $\mathbf{M} = [\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K]^{\mathsf{T}}$ and a data matrix $\mathbf{X}(N \times P)$

$$p(\mathbf{X}|\mathbf{M}, \mathbf{\Sigma}_1, \ldots, \mathbf{\Sigma}_K) = \prod_n^N \sum_k^K p(\mathbf{x}_n|\boldsymbol{\mu}_k, \mathbf{\Sigma}_k)\, P(k) \tag{1.46}$$

Heterogeneous isotropic variance (Bishop, 1995, equation 2.77)

$$p(\mathbf{X}|\mathbf{M}, \sigma_1^2, \ldots, \sigma_K^2) = \prod_n^N \sum_k^K (2\pi\sigma_k^2)^{-P/2} \exp\left[-\frac{(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathsf{T}}(\mathbf{x}_n - \boldsymbol{\mu}_k)}{2\sigma_k^2}\right] P(k) \tag{1.47}$$

Equal isotropic variances $\sigma^2 = \sigma_k^2$ with equal mixture weights $P(k) = 1/K$. Number of parameters is $P \times K + 1$.

$$p(\mathbf{X}|\mathbf{M}, \sigma^2) = \frac{1}{K} \prod_n^N \sum_k^K (2\pi\sigma^2)^{-P/2} \exp\left[-\frac{(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathsf{T}}(\mathbf{x}_n - \boldsymbol{\mu}_k)}{2\sigma^2}\right] \tag{1.48}$$

with hard assignment where $\boldsymbol{\mu}_n$ is the mixture component $\boldsymbol{\mu}_k$ assigned exclusively for the $\mathbf{x}_n$ data point, and where $\mathbf{k}(N \times 1)$ contains the assignment indicators for all $N$ objects

$$p(\mathbf{X}|\mathbf{M}, \sigma^2, \mathbf{k}) = \prod_n^N \frac{1}{K} (2\pi\sigma^2)^{-P/2} \exp\left[ -\frac{(\mathbf{x}_n - \boldsymbol{\mu}_n)^{\mathsf{T}}(\mathbf{x}_n - \boldsymbol{\mu}_n)}{2\sigma^2} \right] \tag{1.49}$$

### 1.10.1 Ad hoc variances

The variance can be computed with a maximum likelihood estimate

$$\sigma^2_{\text{ML}} = \frac{1}{NP} \sum_k^K \sum_n^{N_k} ||\mathbf{x}_n - \boldsymbol{\mu}_k||^2. \tag{1.50}$$

Another "unbiased" form (that is not unbiased!)

$$\sigma^2_{\text{UB}} = \frac{1}{P} \sum_k^K \frac{1}{N_k - 1} \sum_n^{N_k} ||\mathbf{x}_n - \boldsymbol{\mu}_k||^2. \tag{1.51}$$

This estimate does, however, not work in practice since there might be a small number of objects in a specific cluster such that $N_k = 1$. An *ad hoc* fix with "modified unbiased estimator"

$$\sigma^2_{\text{MUB}} = \frac{1}{P} W \sum_k^K \begin{cases} \frac{1}{N_k - 1} \sum_n^{N_k} ||\mathbf{x}_n - \boldsymbol{\mu}_k||^2 & \text{if } N_k > 1 \\ 0 & \text{if } N_k \leq 1 \end{cases} \tag{1.52}$$

Where $W$ is "some weight" most simply taken as $W = 1$

$$\tag{1.53}$$

### 1.10.2 Univariate Gaussian mixture models

The symmetric subgaussian Pearson mixture model as seen in (Lee et al., 1999): $p(s|\mu, \sigma^2) = 1/2\left(N(\mu, \sigma^2) + N(-\mu, \sigma^2)\right)$

$$p(s|\mu, \sigma^2) = \frac{1}{4\pi\sigma^2} \left[ \exp\left( -\frac{(s-\mu)^2}{2\sigma^2} \right) + \exp\left( -\frac{(s+\mu)^2}{2\sigma^2} \right) \right] \tag{1.54}$$

## 1.11 Hyperbolic secant mixture distribution

The univariate hyperbolic secant mixture distribution is used in independent component analysis to model both heavy-tailed distributions and bimodal distributions (Lee et al., 1999, equation 2.29)

$$p(s|\mu) \propto \operatorname{sech}^2(s - \mu) + \operatorname{sech}^2(s + \mu) \tag{1.55}$$

## 1.12 Dirichlet-multinomial distribution

With a data matrix $\mathbf{N}(N \times P)$ with $N$ independent distributed samples from a Dirichlet-multinomial distribution where an infinite number of multinomial is mixed and weighted by a Dirichlet distribution

$$P(\mathbf{N}|\boldsymbol{\alpha}, n) = \prod_n^N \int p_{\text{mul}}(\mathbf{N}|\mathbf{a})\, p_{\text{Dir}}(\mathbf{a}|\boldsymbol{\alpha})\, d\mathbf{a} \tag{1.56}$$

Here $\mathbf{a} \geq 0$ contains the parameters for the multinomial(s) and $\boldsymbol{\alpha}$ contains the Dirichlet parameters, i.e., a hyperparameter for the multinomial distribution. Minka calls the Dirichlet-multinomial a "Polya distribution" (Minka, 2003b). The model has been applied in text analysis (Madsen et al., 2005).

### 1.12.1 Beta-binomial mixture distribution

The beta-binomial mixture distribution (BBM) is continuously mixing via a beta distribution (Griffith, 1973; Erdfelder, 1993), Anders Hald?

$$P(\mathbf{n}|n, \boldsymbol{\alpha}) = P(n_1|n, \boldsymbol{\alpha}) = \int_0^1 P_{\text{Bin}}(\mathbf{n}|a_1, n)\, p_{\text{Dir}}(a_1|\boldsymbol{\alpha})\, da_1 \tag{1.57}$$

$$= \binom{n}{n_1} \frac{B(n_1 + \alpha_1, n - n_1 + \alpha_2)}{B(\alpha_1, \alpha_2)}, \tag{1.58}$$

where $\mathbf{n} = [n_1, n_2]^\mathsf{T}$ and $n = n_1 + n_2$. It might be said not to be a mixture distribution since the beta distribution could be regarded as a Bayesian prior distribution (that in this case is the natural conjugate prior) where $\boldsymbol{\alpha}$ is the hyperparameters. Applications appear in (Lowe, 1999a; Lowe, 1999b).

## 1.13 Gaussian ratio distribution

The univariate Gaussian ratio distribution constructed from two correlated Gaussian distributions: $p(x|\mu_x, \sigma_x)$ and $p(y|\mu_y, \sigma_y)$ with correlation coefficient $\rho$. The distribution of the ratio $z = x/y$ is given as (Hinkley, 1969, equations 1 and 2)

$$p(z|\mu_x, \mu_y, \sigma_x, \sigma_y, \rho) = \frac{b(z)d(z)}{\sqrt{2\pi}\sigma_x\sigma_y a^3(z)} \left[ \Phi\left\{ \frac{b(z)}{\sqrt{1-\rho^2}a(z)} \right\} - \Phi\left\{ -\frac{b(z)}{\sqrt{1-\rho^2}a(z)} \right\} \right] \tag{1.59}$$

$$+ \frac{\sqrt{1-\rho^2}}{\pi\sigma_x\sigma_y a^2(z)} \exp\left\{ -\frac{c}{2(1-\rho^2)} \right\}, \tag{1.60}$$

$$a(z) = \left( \frac{z^2}{\sigma_x^2} - \frac{2\rho z}{\sigma_x\sigma_y} + \frac{1}{\sigma_y^2} \right)^{\frac{1}{2}}, \tag{1.61}$$

$$b(z) = \frac{\mu_x z}{\sigma_x^2} - \frac{\rho(\mu_x + \mu_y z)}{\sigma_x\sigma_y} + \frac{\mu_y}{\sigma_y^2}, \tag{1.62}$$

$$c = \frac{\mu_x^2}{\sigma_x^2} - \frac{2\rho\mu_x\mu_y}{\sigma_1\sigma_y} + \frac{\mu_y^2}{\sigma_y^2}, \tag{1.63}$$

$$d(z) = \exp\left\{ \frac{b^2(z) - ca^2(z)}{2(1-\rho^2)a^2(z)} \right\}, \tag{1.64}$$

$$\Phi(u) = \int_{-\infty}^{u} \phi(v)\, dv, \qquad \text{where} \qquad \phi(v) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}v^2}. \tag{1.65}$$

With the form of (Pham-Gia et al., 2006) with a confluent hypergeometric function

$$p(z|\mu_x, \mu_y, \sigma_x, \sigma_y, \rho) = K_2 \frac{2(1-\rho^2)\sigma_x^2\sigma_y^2}{\sigma_y^2 z^2 - 2\rho\sigma_x\sigma_y z + \sigma_x^2} \left[ {}_1F_1\left(1, 1/2, \theta_2(z)\right) \right] \tag{1.66}$$

$$\theta_2(z) = \frac{\left[ \sigma_y^2\mu_x z - \rho\sigma_x\sigma_y(\mu_y z - \mu_x) + \mu_y\sigma_x^2 \right]^2}{\sigma_x\sigma_y 2(1-\rho^2)(\sigma_y^2 z^2 - 2\rho\sigma_x\sigma_y z + \sigma_x^2)} \tag{1.67}$$

$$K_2 = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}} \exp\left( -\frac{\sigma_y^2\mu_x^2 - 2\rho\sigma_x\sigma_y\mu_x\mu_y + \mu_y^2\sigma_x^2}{2(1-\rho^2)\sigma_x^2\sigma_y^2} \right) \tag{1.68}$$

### 1.13.1 Gaussian ratio distribution with no correlation

With correlation coefficient set to zero $\rho = 0$ in (Hinkley, 1969, equations 1 and 2)

$$p(z|\mu_x, \mu_y, \sigma_x, \sigma_y, \rho = 0) = \frac{b(z)d(z)}{\sqrt{2\pi}\sigma_x\sigma_y a^3(z)} \left[\Phi\left\{\frac{b(z)}{a(z)}\right\} - \Phi\left\{-\frac{b(z)}{a(z)}\right\}\right] + \frac{1}{\pi\sigma_x\sigma_y a^2(z)} \exp\left\{-\frac{c}{2}\right\} \quad (1.69)$$

$$a(z) = \left(\frac{z^2}{\sigma_x^2} + \frac{1}{\sigma_y^2}\right)^{\frac{1}{2}} \quad (1.70)$$

$$b(z) = \frac{\mu_x z}{\sigma_x^2} + \frac{\mu_y}{\sigma_y^2} \quad (1.71)$$

$$c = \frac{\mu_x^2}{\sigma_x^2} + \frac{\mu_y^2}{\sigma_y^2} \quad (1.72)$$

$$d(z) = \exp\left\{\frac{b^2(z) - ca^2(z)}{2a^2(z)}\right\} \quad (1.73)$$

With the form of (Pham-Gia et al., 2006) with confluent hypergeometric function

$$p(z|\mu_x, \mu_y, \sigma_x, \sigma_y, \rho = 0) = \frac{K_1}{\sigma_y^2 z^2 + \sigma_x^2} \left[{}_1F_1\left(1, 1/2, \theta_1(z)\right)\right] \quad (1.74)$$

$$\theta_1(z) = \frac{1}{2\sigma_x^2\sigma_y^2} \frac{\left(\sigma_y^2\mu_x z + \mu_y\sigma_x^2\right)^2}{\sigma_y^2 z^2 + \sigma_x^2} \quad (1.75)$$

$$K_1 = \frac{\sigma_x\sigma_y}{\pi} \exp\left(-\frac{1}{2}\frac{\mu_x^2}{\sigma_x^2} + \frac{\mu_y^2}{\sigma_y^2}\right) \quad (1.76)$$

### 1.13.2 Gaussian ratio distribution with no mean

With correlation coefficient set to zero $\rho = 0$ and no means $\mu_x = 0$, $\mu_y = 0$ in (Hinkley, 1969, equations 1 and 2)

$$p(z|\mu_x = 0, \mu_y = 0, \sigma_x, \sigma_y, \rho = 0) = \frac{1}{\pi\sigma_x\sigma_y a^2(z)} \quad (1.77)$$

$$a(z) = \left(\frac{z^2}{\sigma_x^2} + \frac{1}{\sigma_y^2}\right)^{\frac{1}{2}} \quad (1.78)$$

$$b(z) = 0 \quad (1.79)$$

$$c = 0 \quad (1.80)$$

$$d(z) = 1 \quad (1.81)$$

$$p(z|\mu_x = 0, \mu_y = 0, \sigma_x, \sigma_y, \rho = 0) = \frac{1}{\pi} \frac{\sigma_x/\sigma_y}{z^2 + (\sigma_x/\sigma_y)^2} \quad (1.82)$$

... and this is the Cauchy distribution with zero mean. If $\rho \neq 0$

$$p(z|\mu_x = 0, \mu_y = 0, \sigma_x, \sigma_y, \rho) = \frac{\sqrt{1-\rho^2}}{\pi \sigma_x \sigma_y a^2(z)} \tag{1.83}$$

$$a(z) = \left( \frac{z^2}{\sigma_x^2} - \frac{2\rho z}{\sigma_x \sigma_y} + \frac{1}{\sigma_y^2} \right)^{\frac{1}{2}} \tag{1.84}$$

$$b(z) = 0 \tag{1.85}$$

$$c = 0 \tag{1.86}$$

$$d(z) = 1 \tag{1.87}$$

$$p(z|\mu_x = 0, \mu_y = 0, \sigma_x, \sigma_y, \rho) = \frac{1}{\pi} \frac{\beta}{(z-\alpha)^2 + \beta^2}, \tag{1.88}$$

$$\text{where,} \qquad \alpha = \rho \frac{\sigma_x}{\sigma_y} \tag{1.89}$$

$$\beta = \frac{\sigma_x}{\sigma_y} \sqrt{1-\rho^2}, \tag{1.90}$$

i.e., the Cauchy distribution with non-zero mean (Curtiss, 1941, page 411).

## 1.14 Finite binomial mixture distribution

The finite binomial mixture distribution is a finite discrete mixture distribution, sometimes refered to as finite binomial mixture (FBM) (Gelfand and Solomon, 1974), (Emrick, 1971)?, Poisson? Pearson (1915)? also discussed in (Everitt and Hand, 1981, pp. 89–97), (Titterington et al., 1985) with $K$ components

$$p(x|N, \mathbf{p}, \boldsymbol{\lambda}) = \sum_{k=1}^{K} \lambda_k P_{\text{bin}}(x|N, p_k); \tag{1.91}$$

where $x \in \{0, \ldots, N\}$ and $0 \leq \lambda_k \leq 1$, $\sum_k^K \lambda_k = 1$ are the mixing proportions. The parameters are identifiable with $N \geq 2K - 1$. The likelihood can be written with another sufficient statistics $\mathbf{c}$

$$p(\mathbf{c}|N, \mathbf{p}, \boldsymbol{\lambda}) = \prod_{m=0}^{M} \left[ \sum_{k=1}^{K} \lambda_k P_{\text{bin}}(m|N, p_k) \right]^{c_m} \tag{1.92}$$

where $c_m = \sum_{n=1, x_n = m}^{N} 1$ and $m = 0 \ldots M$. This might be more efficient to work with if $M$ is small.

$$\tag{1.93}$$

## 1.15 Multinomial mixture distribution

A data matrix $\mathbf{X}(N \times P)$ with $N$ independent samples from a multinomial mixture distribution with $\mathbf{A}$ containing parameters for the multinomial distributions and $\mathbf{q}$ containing the weighting parameters between the multinomials

$$P(\mathbf{X}|\mathbf{A}, \mathbf{q}) = \prod_n^N \sum_k^K q_k \frac{(\sum_p^P x_{np})!}{\prod_p^P x_{np}!} \prod_p^P a_{kp}^{x_{np}} \tag{1.94}$$

There are several applications of this model in text analysis, e.g., (Rigouste et al., 2005; Nigam et al., 2000).

## 1.16 Mixture of matrix hypergeometric distributions

With $K$ mixtures and $N$ objects

$$P(\mathbf{X}|\mathbf{Z}, \mathbf{q}) = \prod_n^N \sum_k^K \frac{\prod_p^P \binom{z_{kp}}{x_{np}}}{\binom{\sum_p^P z_{kp}}{\sum_p^P x_{np}}} q_k. \tag{1.95}$$

# Chapter 2

# Statistical tests and other

## 2.1 Correlation coefficient

With the correlation coefficient

$$r = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_i (x_i - \bar{x})^2 \sum_i (y_i - \bar{y})^2)}} \tag{2.1}$$

And the hypotheses

$$\begin{array}{lccc} H_0 & : & r_{xy} & = & 0 \\ H_1 & : & r_{xy} & \neq & 0 \end{array} \tag{2.2}$$

The test statistic is

$$t = r\sqrt{\frac{N-2}{1-r^2}} \tag{2.3}$$

and distributed with a $t$-distribution with $N-2$ degrees of freedom if $x$ and $y$ are identical and independent Gaussian distributed (Gaussian iids).

## 2.2 Partial correlation coefficient

The partial correlation coefficient between $x$ and $y$ with $z$ as the nuisance

$$r_{xy|z} = \frac{r_{xy} - r_{xz}r_{yz}}{\sqrt{(1-r_{xz}^2)(1-r_{yz}^2)}} \tag{2.4}$$

The test statistic is formed as

$$t = r\sqrt{\frac{N-2-K}{1-r^2}} \tag{2.5}$$

Where $K$ is the size of the subspace factored out and N is the number of samples. For Gaussian distributed signals (Gaussian iids) this can be compared to a $t$-distribution with $N-2-K$ degrees of freedom.

## 2.3 Effect sizes

Hedges $g$ for the effect size between two groups (Hedges and Olkin, 1985)

$$g = \frac{\bar{x}_1 - \bar{x}_2}{s} \qquad \text{where} \qquad s = \sqrt{\frac{(n_1-1)s_1^2 + (n_2-1)s_2^2}{n_1+n_2-2}}, \tag{2.6}$$

With

$$n^* = n_1 + n_2 - 2 \qquad \text{and} \qquad \tilde{n} = \frac{n_1 n_2}{n_1 + n_2}, \tag{2.7}$$

the population value

$$\delta = \frac{\mu_1 - \mu_2}{\sigma}, \tag{2.8}$$

and the bias correction factor

$$J(a) = \frac{\Gamma(a/2)}{\sqrt{a/2}\Gamma((a-1)/2)} \approx 1 - \frac{3}{4a-1} \tag{2.9}$$

then under Gaussianity of the data $\sqrt{\tilde{n}}g$ follows a noncentral $t$-distribution with $n^*$ degress of freedom and the noncentrality parameter $\delta\sqrt{\tilde{n}}$, so the expection and variance of $g$ are (Hedges and Olkin, 1985, p. 104)

$$E(g) = \delta / J(n^*) \tag{2.10}$$

$$\approx \delta + \frac{3\delta}{4(n_1+n_2)-9} \tag{2.11}$$

$$\text{Var}(g) = \frac{n^*}{(n^*-2)\tilde{n}} + \delta^2 \left( \frac{n^*}{n^*-2} - \frac{1}{[J(n^*)]^2} \right) \tag{2.12}$$

$$\approx \frac{1}{n^*} + \delta^2 \frac{1}{2(n_1+n_2-3.94)} \tag{2.13}$$

## 2.4 Combining mean and standard deviation

A data set consisting of two parts where the mean and standard deviation is known for the two part: What are the mean and standard deviation for the full data set?

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{bmatrix}. \tag{2.14}$$

The two means combined in a weighted fashion to the full mean

$$\bar{\mathbf{x}}_1 = \frac{1}{n_1} \sum_i^{n_1} \mathbf{x}_{1,i} \tag{2.15}$$

$$\bar{\mathbf{x}}_2 = \frac{1}{n_2} \sum_j^{n_2} \mathbf{x}_{2,j} \tag{2.16}$$

$$\mathbf{x} = \frac{1}{n} \sum_k^{n} \mathbf{x}_k = \frac{\bar{\mathbf{x}}_1 n_1 + \bar{\mathbf{x}}_2 n_2}{n_1 + n_2} \tag{2.17}$$

Unbiased standard deviations

$$\mathbf{S}_1 = \frac{1}{n_1 - 1} \sum_i^{n_1} (\mathbf{x}_{1,i} - \bar{\mathbf{x}}_1)(\mathbf{x}_{1,i} - \bar{\mathbf{x}}_1)' \tag{2.18}$$

$$\mathbf{S}_2 = \frac{1}{n_2 - 1} \sum_j^{n_2} (\mathbf{x}_{2,j} - \bar{\mathbf{x}}_2)(\mathbf{x}_{2,j} - \bar{\mathbf{x}}_2)' \tag{2.19}$$

$$s^2 = \frac{1}{n-1} \left[ s_1(n_1-1) + s_2(n_2-1) + n_1\bar{x}_1^2 + n_2\bar{x}_2^2 - n\bar{x}^2 \right] \tag{2.20}$$

$$\mathbf{S} = \frac{1}{n-1} \left[ \mathbf{S}_1(n_1-1) + \mathbf{S}_2(n_2-1) + n_1\bar{\mathbf{x}}_1\bar{\mathbf{x}}_1' + n_2\bar{\mathbf{x}}_2\bar{\mathbf{x}}_2' - n\bar{\mathbf{x}}\bar{\mathbf{x}}' \right] \tag{2.21}$$

# Chapter 3

# Matrices

## 3.1 Definition

A matrix is a 2-dimensional table/array of numbers (elements). The numbers can be complex or real. Usually all the elements should be defined, though in some statistical applications one allows for "missing values", — in R denoted by NA ("not available").

## 3.2 Types of matrices

The matrix can be ordered according to several criteria (from the Matrix Market):

- Non-zero structure: Full, diagonal, tridiagonal, block diagonal, sparse, (lower/upper) triangular.
- Shape: Square, non-square, (row/column) vector, scalar
- Element type: Complex, real, integer, non-negative, positive, binary.
- Numerical symmetric: Hermitian, symmetric, positive definite, ...

### 3.2.1 Monomial

A *monomial* matrix (also called a *generalized permutation* matrix) contains exactly one non-zero entry in each row and column, i.e. is of full-ranked (Berman and Plemmons, 1994, p. 67). A non-singular monomial matrix has exactly one non-zero entry in each column Thus permutation and identity matrices are specializations.

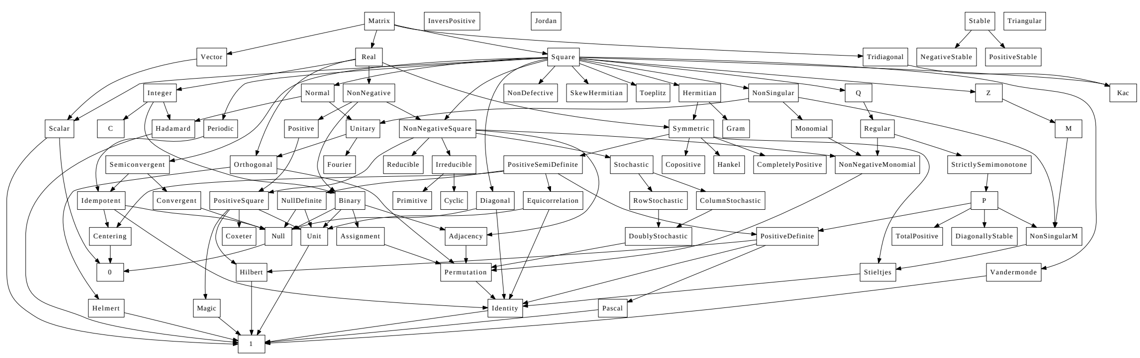



Figure 3.1: Matrix taxonomy

### 3.2.2 Semiconvergent and convergent matrices

For a *semiconvergent* matrix $\mathbf{C}$ the following applies (Berman and Plemmons, 1994, p. 152)

$$\lim_{k\to\infty} \mathbf{C}^k \text{ exists.} \tag{3.1}$$

A *convergent* matrix $\mathbf{B}$ satisfies (Berman and Plemmons, 1979, p. 9)

$$\lim_{k\to\infty} \mathbf{B}^k = \mathbf{0} \tag{3.2}$$

In both case the convergence is related to the spectral radius: For a convergent $\rho(\mathbf{B}) < 1$.

### 3.2.3 Z-matrices

A real square matrix is a $Z$-matrix if all its off-diagonal elements are non-positive (Guo, 2003), and it can be written as

$$\mathbf{A} = s\mathbf{I} - \mathbf{B}, \qquad \mathbf{B} \geq \mathbf{0}. \tag{3.3}$$

#### M-matrices

An $M$-matrix is square and has nonnegative diagonal elements and nonpositive off-diagonal elements (Graham, 1987, chapter 5). An $M$-matrix $\mathbf{A}$ can be decomposed into an positive scaled identity matrix ($s\mathbf{I}$, $s > 0$) and a nonnegative matrix $\mathbf{B}$

$$\mathbf{A} = s\mathbf{I} - \mathbf{B}. \tag{3.4}$$

(Guo, 2003) relates the spectral radius $\rho(\cdot)$ to $s$: A $Z$-matrix is an $M$-matrix if $s \geq \rho(\mathbf{B})$, a singular $M$-matrix if $s = \rho(\mathbf{B})$ and a non-singular $M$-matrix if $s > \rho(\mathbf{B})$. The inverse of such a non-singular M-matrix is non-negative (Guo, 2003).[1]

### 3.2.4 Nonnegative matrices

A *nonnegative matrix* $\mathbf{A}(N \times M)$ is a matrix where all the element are greater than or equal to zero

$$\mathbf{A} \geq \mathbf{0} \qquad \equiv \qquad \forall_{ij} a_{ij} \geq 0 \tag{3.5}$$

And similarly a *positive* matrix $\mathbf{B}(N \times M)$ is a matrix where all the elements are greater than zero

$$\mathbf{B} > 0. \tag{3.6}$$

#### Doubly nonnegative

A doubly nonnegative square matrix is both nonnegative and positive semi-definite. A doubly nonnegative matrix $\mathbf{A}$ that is *completely positive* can be decomposed with a (not necessarily square) nonnegative matrix $\mathbf{B}$ (Berman and Plemmons, 1994, p. 304)

$$\mathbf{A} = \mathbf{B}\mathbf{B}^\mathsf{T} \qquad \mathbf{A} \geq \mathbf{0},\ \mathbf{B} \geq \mathbf{0}. \tag{3.7}$$

#### Inverse nonnegative matrices

Some non-negative matrices have an inverse that is an M-matrix. Other classes of inverse nonnegative matrices are *strictly ultrametric matrices* (SUM) and *generalized ultrametric matrices* (GUM) (Berman and Plemmons, 1994, p. 306–307).

For a non-singular non-negative matrix $\mathbf{A}$ its inverse $\mathbf{A}^{-1}$ is only non-negative if (and only if) $\mathbf{A}$ is (non-negative) monomial (Berman and Plemmons, 1994, chapter 3, exercise 6.7).

An example of a simple inverse non-negative matrix is

$$\mathbf{A} = \mathbf{A}^{-1} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{3.8}$$

and this is monomial.

[1] Is Graham's and Guo's $M$-matrix the same?

### 3.2.5 Normal matrices

(Graham, 1987, p. 86+).

$$\mathbf{A}^*\mathbf{A} = \mathbf{A}\mathbf{A}^* \tag{3.9}$$

### 3.2.6 Hermitian

A complex matrix is *Hermitian* if the following applies

$$\mathbf{A}^* = \mathbf{A}, \tag{3.10}$$

where $^*$ denotes the conjugate transpose (*tranjugate*) (Graham, 1987, p. 67).

#### Symmetric

A real hermitian matrix is symmetric

$$\mathbf{A}^\mathsf{T} = \mathbf{A}, \tag{3.11}$$

i.e., a symmetric matrix is *real*.

### 3.2.7 Unitary matrices

A complex square matrix $\mathbf{U}(N \times N)$ is unitary if it satisfy (Graham, 1987, p. 67)

$$\mathbf{U}^*\mathbf{U} = \mathbf{I} = \mathbf{U}\mathbf{U}^*, \tag{3.12}$$

"Special unitary matrices" are unitary matrices with $\det(\mathbf{X}) = 1$.

#### Orthogonal matrices

A real matrix $\mathbf{P}$ that is unitary satisfy (Graham, 1987, p. 68)

$$\mathbf{P}^\mathsf{T}\mathbf{P} = \mathbf{P}\mathbf{P}^\mathsf{T} = \mathbf{I} \tag{3.13}$$

$$\det(\mathbf{P}) = \pm 1 \tag{3.14}$$

$$\mathbf{P}^{-1} = \mathbf{P}^\mathsf{T} \tag{3.15}$$

#### Givens matrices

Givens matrices are rotation matrices.

#### Helmert matrix

A Helmert matrix $\mathbf{A}(N \times N)$ can be used to decorrelate random variables.

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_{(1)} \\ \vdots \\ \mathbf{a}_{(N)} \end{bmatrix}, \qquad \mathbf{a}_{(n)} = \begin{cases} \left[1/\sqrt{N}, \ldots, 1/\sqrt{N}\right] & \text{if } n = 1 \\ \left[\underbrace{\sqrt{(n-1)n}, \ldots, \sqrt{(n-1)n}}_{(n-1)\text{ elements}}, \quad \underbrace{0, \ldots, 0}_{(N-n)\text{ elements}}\right] & \text{otherwise} \end{cases} \tag{3.16}$$

#### Permutation matrices

A *permutation matrix* $\mathbf{P}$ is a matrix that can be used to interchange the rows (with $\mathbf{PA}$) or columns (with $\mathbf{AP}$) of an other matrix (here $\mathbf{A}$). An example is (Graham, 1987, p. 43)

$$\mathbf{P} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix} \tag{3.17}$$

Permutation matrices are orthogonal and binary matrices.

## 3.3 Arithmetic operations

The row sum of $\mathbf{A}(N \times M)$ gives a column vector $\mathbf{r}(N \times 1)$

$$\mathbf{r} = \sum_m^M a_{nm} = \mathbf{A}\mathbf{1}_M. \tag{3.18}$$

Strangely, in matlab the multiplication '`X*ones(size(X,2),1)`' is faster than a "simple" sum '`sum(X,2)`', — perhaps because of poor cache management (Minka, 2003a).

## 3.4 Vectorization

A matrix $\mathbf{X}(N \times P)$

$$\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_P] \tag{3.19}$$

Vectorization of $\mathbf{X}$ into a column vector $\mathbf{X}^{\vee}(NP \times 1)$

$$\mathbf{X}^{\vee} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_P \end{bmatrix}. \tag{3.20}$$

Arithmetric operations with $\mathbf{A}(I \times J)$ and $\mathbf{B}(J \times K)$

$$(\mathbf{ABC})^{\vee} = (\mathbf{C}^{\mathsf{T}} \otimes \mathbf{A})\mathbf{B}^{\vee}, \tag{3.21}$$

$$(\mathbf{AB})^{\vee} = (\mathbf{I}_K \otimes \mathbf{A})\mathbf{B}^{\vee} \tag{3.22}$$

$$= (\mathbf{B}^{\mathsf{T}} \otimes \mathbf{I}_I)\mathbf{A}^{\vee}. \tag{3.23}$$

## 3.5 Function with scalar output

### 3.5.1 Norms

The rank of a matrix is the number of non-zero singular values

$$\mathrm{rank}(\mathbf{A}) = \sum_i \delta(\sigma_i(\mathbf{A}) \neq 0). \tag{3.24}$$

The ordinary norm (spectral norm or 2-norm) is the largest singular value.

$$\|\mathbf{A}\|_2 = \sqrt{\max_i(\lambda_i(\mathbf{A}^{\mathsf{H}}\mathbf{A}))}. \tag{3.25}$$

If the matrix is symmetric it is the largest eigenvalue

$$\|\mathbf{A}\|_2 = \max_i(\lambda_i(\mathbf{A})), \tag{3.26}$$

Frobenius norm (Golub and Van Loan, 1996, section 2.3)

$$\|\mathbf{A}\|_F = \sqrt{\sum\sum |a_{ij}|^2} \tag{3.27}$$

$$= \sqrt{\sum_k \sigma_k^2(\mathbf{A})} \tag{3.28}$$

$$= \sqrt{\sum_k \lambda_k(\mathbf{A}^{\mathsf{T}}\mathbf{A})} = \sqrt{\sum_k \lambda_k(\mathbf{A}\mathbf{A}^{\mathsf{T}})} \tag{3.29}$$

$$= \sqrt{\mathrm{tr}(\mathbf{A}^{\mathsf{T}}\mathbf{A})} = \sqrt{\mathrm{tr}(\mathbf{A}\mathbf{A}^{\mathsf{T}})} \tag{3.30}$$

where the $\sigma_k$'s are the singular values, and the $\lambda_k$'s are the eigenvalues.

In some tasks of least squares the cost function is the Frobenius norm and in certain cases it may be faster to compute the cost function in a different way. In the case where the number of columns in $\mathbf{A}$ is large and the number of columns in $\mathbf{B}$ the following may result in fewer computation during an iterative algorithm where $\mathbf{B}$ and $\mathbf{C}$ are optimized:

$$\|\mathbf{A} - \mathbf{BC}\|_F^2 = \text{tr}\left[(\mathbf{A} - \mathbf{BC})(\mathbf{A} - \mathbf{BC})^\mathsf{T}\right] \tag{3.31}$$

$$= \text{tr}\left[\mathbf{A}\mathbf{A}^\mathsf{T}\right] - 2\text{tr}\left[\mathbf{B}\left(\mathbf{C}\mathbf{A}^\mathsf{T}\right)\right] + \text{tr}\left[\mathbf{B}\left(\mathbf{C}\mathbf{C}^\mathsf{T}\right)\mathbf{B}^\mathsf{T}\right] \tag{3.32}$$

$$= \|\mathbf{A}\|_F^2 - 2\text{tr}\left[\mathbf{B}\left(\mathbf{C}\mathbf{A}^\mathsf{T}\right)\right] + \text{tr}\left[\mathbf{B}\left(\mathbf{C}\mathbf{C}^\mathsf{T}\right)\mathbf{B}^\mathsf{T}\right] \tag{3.33}$$

The scalar term $\|\mathbf{A}\|_F^2$ only needs to be computed once during the iterations.

### 3.5.2 Spectral radius

The spectral radius $\rho(\mathbf{A})$ is the largest of the absolute values of the eigenvalues

$$\rho(\mathbf{A}) = \max_i(|\lambda_i(\mathbf{A})|) \tag{3.34}$$

## 3.6 Inversion

The inverse $\mathbf{A}^{-1}$ of a *square and non-singular* matrix $\mathbf{A}$ satisfies

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{I}. \tag{3.35}$$

$$a\mathbf{C} + a^2\mathbf{C}^2 + a^3\mathbf{C}^3 + \ldots + a^k\mathbf{C}^k = (\mathbf{I} - a\mathbf{C})^{-1} - \mathbf{I}, \tag{3.36}$$

which is used in a recursive centrality index computation (Katz, 1953).

### 3.6.1 Properties

Some properties, see, e.g., (Mardia et al., 1979, section A.2.4) and the matrix cookbook

$$\mathbf{A}^{-\mathsf{T}} = (\mathbf{A}^\mathsf{T})^{-1} = (\mathbf{A}^{-1})^\mathsf{T} \tag{3.37}$$

$$(c\mathbf{A})^{-1} = c^{-1}\mathbf{A}^{-1} \tag{3.38}$$

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1} \tag{3.39}$$

$$\mathbf{A}\mathbf{B}^\mathsf{T} = \left(\mathbf{B}^{-\mathsf{T}}\mathbf{A}^{-1}\right)^{-1} \tag{3.40}$$

Kronecker product

$$(\mathbf{A} \otimes \mathbf{B})^{-1} = \mathbf{A}^{-1} \otimes \mathbf{B}^{-1} \tag{3.41}$$

### 3.6.2 Matrix inversion lemma

'Matrix inversion lemma' or ((Bartlett-)Sherman-)Morrison-Woodbury formula (Mardia et al., 1979, equation A.2.4f), (Golub and Van Loan, 1996, section 2.1.3)

$$(\mathbf{A} + \mathbf{BCD})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{B}(\mathbf{C}^{-1} + \mathbf{D}\mathbf{A}^{-1}\mathbf{B})^{-1}\mathbf{D}\mathbf{A}^{-1} \tag{3.42}$$

In simplified versions

$$(\mathbf{A} + \mathbf{BD})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{B}(\mathbf{I} + \mathbf{D}\mathbf{A}^{-1}\mathbf{B})^{-1}\mathbf{D}\mathbf{A}^{-1} \tag{3.43}$$

$$(\mathbf{A} + \mathbf{a}\mathbf{b}^\mathsf{T})^{-1} = \mathbf{A}^{-1} - (\mathbf{A}^{-1}\mathbf{a}\mathbf{b}^\mathsf{T}\mathbf{A}^{-1})(1 + \mathbf{b}^\mathsf{T}\mathbf{A}^{-1}\mathbf{a})^{-1} \tag{3.44}$$

### 3.6.3 $2 \times 2$ inversion

With a $(2 \times 2)$-matrix

$$\mathbf{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \tag{3.45}$$

the inverse is

$$\mathbf{A}^{-1} = \frac{1}{\det \mathbf{A}} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}, \tag{3.46}$$

i.e., the inversion of a positive (and invertible) $(2 \times 2)$-matrix will always have an inverse in which two of the elements are negative, — either the off-diagonal or (with negative determinant) the on-diagonal elements.

## 3.7 Determinant

A determinant only applies for square matrices. With a square $\mathbf{A}(P \times P)$

$$|c\mathbf{A}| = c^P |\mathbf{A}| \tag{3.47}$$

$$|\mathbf{A}^n| = |\mathbf{A}|^n \tag{3.48}$$

$$|\mathbf{AB}| = |\mathbf{A}|\,|\mathbf{B}| \tag{3.49}$$

$$|\mathbf{A} + \mathbf{BC}| = |\mathbf{A}|\,|\mathbf{I}_P + \mathbf{A}^{-1}\mathbf{BC}| \tag{3.50}$$

$$= |\mathbf{A}|\,|\mathbf{I}_N + \mathbf{CA}^{-1}\mathbf{B}| \tag{3.51}$$

## 3.8 Trace

The trace of a *square* matrix is the sum of the diagonal elements

$$\mathrm{tr}(\mathbf{A}) = \sum_i a_{ii}. \tag{3.52}$$

$$\mathrm{tr}(\mathbf{C}^\mathsf{T}\mathbf{D}) = \sum_i \sum_j c_{ij} d_{ij} \tag{3.53}$$

$$= (\mathbf{C}^\vee)^\mathsf{T} \mathbf{D}^\vee \tag{3.54}$$

$$\mathrm{tr}(\mathbf{A} + \mathbf{B}) = \mathrm{tr}(\mathbf{A}) + \mathrm{tr}(\mathbf{B}) \tag{3.55}$$

For a 'squared' matrix the trace can be computed with the Frobenius norm

$$\mathrm{tr}(\mathbf{C}^\mathsf{T}\mathbf{C}) = \|\mathbf{C}\|_F^2 \tag{3.56}$$

## 3.9 Derivatives

Matrix derivatives are defined as, see, e.g., (Mardia et al., 1979, section A.9)

$$\frac{\partial f(\mathbf{X})}{\partial \mathbf{X}} = \left[ \frac{\partial f(\mathbf{X})}{\partial x_{ij}} \right]. \tag{3.57}$$

### 3.9.1 Determinant

$$\frac{\partial \ln |\mathbf{X}|}{\partial \mathbf{X}} = \left[\mathbf{X}^\mathsf{T}\right]^{-1}. \tag{3.58}$$

## 3.10 Integrals

### 3.10.1 Transformation with Jacobian

Change from one coordinate system $\mathbf{x}$ to another $\mathbf{u}$ by the transformation $\mathbf{x} = \boldsymbol{\phi}(\mathbf{u})$ (Jacobsen, 2004)

$$\int_D f(\mathbf{x})\, d\mathbf{x} = \int_{D'} f(\boldsymbol{\phi}(\mathbf{u}))\, |\det(\mathbf{J})|\, d\mathbf{u}, \tag{3.59}$$

with the Jacobian $\mathbf{J} = \partial\boldsymbol{\phi}(\mathbf{u})/\partial\mathbf{u}$ and the integration region $\boldsymbol{\phi}(D') = D$.

### 3.10.2 Dirac function

Scalar integral involving Dirac delta function (MacKay, 1999, page 3) relevant for 'no-noise' distributions

$$\int \delta(x - vs)\, f(s)\, ds = \frac{1}{|v|} f(x/v), \tag{3.60}$$

and the matrix version

$$\int \prod_j^J \delta(x_j - V_{ji} s_i) \prod_i^I f_i(s_i)\, d^I \mathbf{s} = \frac{1}{|\mathbf{V}|} \prod_i^I f_i(V_{ij}^{-1} x_j)? \tag{3.61}$$

# Chapter 4

# Functions

## 4.1 Gamma function

The gamma function (found in Matlab as `gamma`) defined as

$$\Gamma(x) = \int_0^\infty u^{x-1} e^{-u} \, du \tag{4.1}$$

The faculty function, when $x$ is a positive integer

$$\Gamma(x) = (x-1)! \tag{4.2}$$

The lower incomplete gamma

$$\gamma(x, a) = \int_0^x u^{a-1} e^{-u} \, du \tag{4.3}$$

The lower "standardized" incomplete gamma is computed by Matlab's `gammainc`

$$\gamma(x, a) = 1/\Gamma(a) \int_0^x u^{a-1} e^{-u} \, du \tag{4.4}$$

The generalized gamma function (Box and Tiao, 1992, equation 8.2.22)

$$\Gamma(M, N) = \left[\Gamma\left(\frac{1}{2}\right)\right]^{M(M-1)/2} \prod_m^M \Gamma\left(N + \frac{m+M}{2}\right), \tag{4.5}$$

and since $\Gamma(1/2) = \sqrt{\pi}$

$$\Gamma(M, N) = \pi^{M(M-1)/4} \prod_m^M \Gamma\left(N + \frac{m+M}{2}\right). \tag{4.6}$$

The digamma function

$$\Psi(x) = \psi_0(x) = \frac{\Gamma'(x)}{\Gamma(x)} = \frac{d}{dx} \ln \Gamma(x). \tag{4.7}$$

## 4.2 Basis functions

Chebyshev polynomials of the first kind $T_n(x)$ are orthogonal

$$T_n(x) = \cos\left(n \operatorname{acos}(x)\right) \qquad x \in [-1; 1], \, n = 0 \ldots \tag{4.8}$$

Other orthogonal polynomials are Hermite and Legendre polynomials.

## 4.3 Link functions

Bradley-Terry-Luce $\mathbf{z}(P \times 1)$

$$\mathbf{y} = \frac{\mathbf{z}^{\alpha}}{\sum_p^P z_p^{\alpha}}, \tag{4.9}$$

where $\mathbf{z}^{\alpha}$ is elementwise.

Softmax transformation

$$\mathbf{y} = \frac{\exp(\alpha \mathbf{z})}{\sum_p^P \exp(\alpha z_p)} \tag{4.10}$$

The logit transform

$$y_1 = \frac{\exp(z_1)}{1 + \exp(z_1)} \tag{4.11}$$

# Chapter 5

# Inequalities

## 5.1 Jensen's inequality

$$\log\left(\sum_i \lambda_i x_i\right) \geq \sum_i \lambda_i \log(x_i) \qquad \text{If } \lambda_i \geq 0 \text{ and } \sum_i \lambda_i = 1 \tag{5.1}$$

# Chapter 6

# Optimization

## 6.1 Gradient descent

Gradient descent (also steepest descent)

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \gamma \boldsymbol{\nabla} f(\mathbf{x}_n) \tag{6.1}$$

Gradient ascent

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \gamma \boldsymbol{\nabla} f(\mathbf{x}_n) \tag{6.2}$$

## 6.2 Newton method

Minimization:

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \mathbf{H}_{\mathbf{xx}}^{-1} \boldsymbol{\nabla}_{\mathbf{x}} f(\mathbf{x}_n) \tag{6.3}$$

# Chapter 7

# Information theory

## 7.1 Entropies

Shannon entropy for a discrete random variable

$$H(X) = -\sum_{x \in X} P_X(x) \log_2[P_X(x)]. \tag{7.1}$$

Rényi entropy of order $\alpha$ (Cachin, 1997, page 15)

$$H_\alpha(X) = \frac{1}{1-\alpha} \log \sum_{x \in X} P_X(x)^\alpha, \tag{7.2}$$

where $\alpha \geq 0$ and $\alpha \neq 1$. Rényi entropy of order $\alpha = 2$ aka. quadratic entropy (Torkkola, 2002)

$$H_2(X) = -\log_2 \sum_x [P(x)]^2. \tag{7.3}$$

"Guessing" entropy for ordered probabilities

$$H_G(X) = \log_2 \sum_i i\, p_i. \tag{7.4}$$

Rényi's quadratic entropy for a continuous random variable $X$

$$H_2(X) = -\log_2 \int_{\mathbf{x}} p(\mathbf{x})^2 \, d\mathbf{x}. \tag{7.5}$$

## 7.2 Mutual information

The mutual information is a measure of the dependence between two random variables $\mathbf{x}$ and $\mathbf{y}$, i.e., a generalized form of correlation coefficient.

$$I(\mathbf{x}, \mathbf{y}) = \int\int p(\mathbf{x}, \mathbf{y}) \log \frac{p(\mathbf{x}, \mathbf{y})}{p(\mathbf{x})\, p(\mathbf{y})} \tag{7.6}$$

For independent variables, $p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x})\, p(\mathbf{y})$, and the mutual information is $I = 0$. The measure is symmetric in $\mathbf{x}$ and $\mathbf{y}$

$$I(\mathbf{x}, \mathbf{y}) = I(\mathbf{y}, \mathbf{x}) \tag{7.7}$$

Expectation value of the mutual information for multinomial variables (Hutter, 2002, eq. 15), see also (Wolf and Wolpert, 1996; Wolf and Wolpert, 1993)

$$\mathsf{E}[I] = \frac{1}{n} \sum_{i,j} n_{ij} \left[\psi(n_{ij}+1) - \psi(n_i+1) - \psi(n_j+1) + \psi(n+1)\right] \tag{7.8}$$

# Chapter 8

# Networks

## 8.1 Types of networks

Table 8.1: Types of graphs

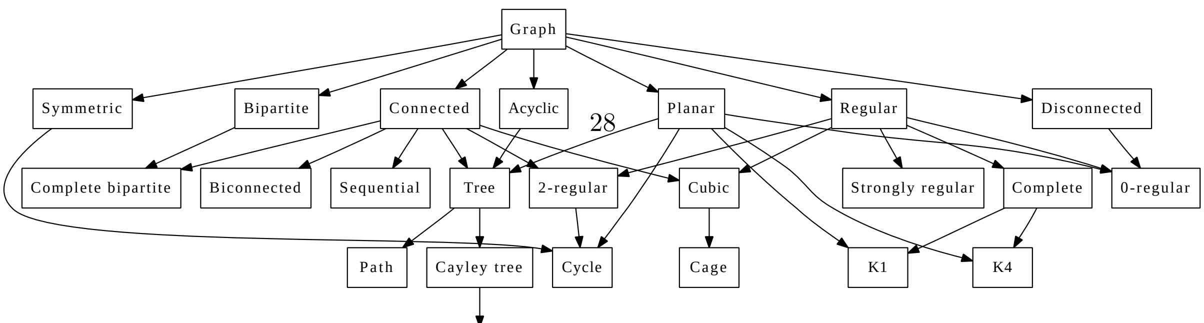
| Name | Description | Reference |
|---|---|---|
| Causal network | DAG | (Ripley, 1988, p. 262) |
| Arborescence | Same as “directed tree” | MathWorld |
| Complete digraph | Digraph with all possible edge | MathWorld |
| Connected digraph | Can either be weakly or strongly connected | Mathworld |
| Forest (undirected) | Acyclic graph | |
| Forest | Polyforest where all nodes have only one parent | David Pennock |
| Functional graph | Digraph in which each vertex has outdegree one | MathWorld |
| Moral graph | Undirected graph constructed from a DAG by turning the directed edges to undirected edges and adding edges between parents | (Ripley, 1988, p. 270) |
| Polyforest | DAG with no undirected cycles | David Pennock |
| Polytree | Single-connected DAG, i.e., a DAG in which only a single path exists between any vertices. A connected polyforest | (Ripley, 1988, p. 247), David Pennock |
| Simple directed graph | Digraph with no loops and no multiple edges | MathWorld |

## 8.2 Graph matrices

A graph can be represented as a matrix in a variaty of ways: Adjacency matrix $\mathbf{A}$, incidens matrix $\mathbf{B}$, cycle matrix $\mathbf{C}$ and cut-set matrix (Fould, 1992, chapter 6).

An incidence matrix $\mathbf{B}(N \times P)$ for a graph $G$ with $N$ nodes and $P$ links can be defined in two ways. In the first case the element are set to one if a link $p$ connects to a node $n$

$$\mathbf{B}_{np} = \begin{cases} 1 & \text{if node } n \text{ and link } p \text{ are incident} \\ 0 & \text{otherwise} \end{cases} \tag{8.1}$$



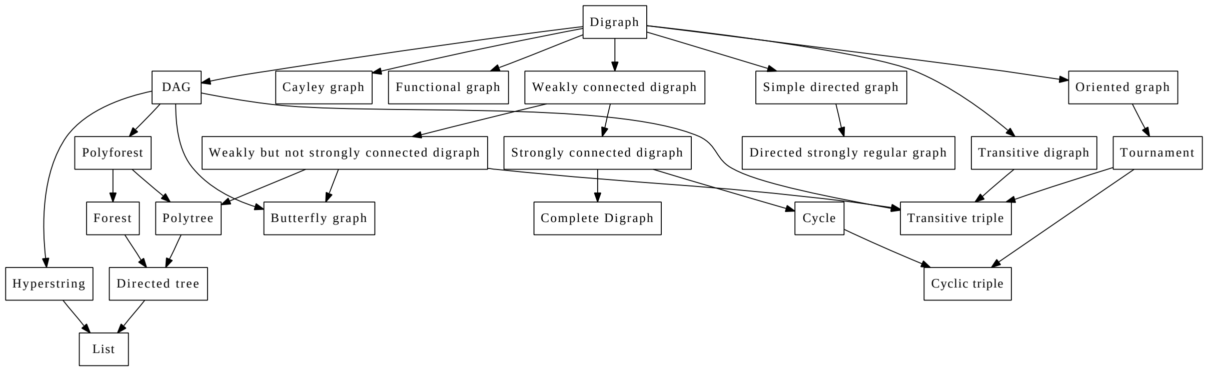



Figure 8.2: Digraph taxonomy

### 8.2.1 Eigenvalues and vectors

The eigenvalues of a graph is the eigenvalues of its adjacency matrix, and similar for the eigenvectors. The graph sepctrum is the set of eigenvalues, e.g., the vector of eigenvalues $\lambda$.

## 8.3 Eccentricity, radius, diameter

The eccentricity for a node $u$ is the maximum of the shortest distance $d$ to all other nodes

$$e(u) = \max_v d(u,v) \tag{8.2}$$

The diameter of a graph is the maximum eccentricity

$$d = \max_u \left[\max_v d(u,v)\right] \tag{8.3}$$

The radius of a graph is the minimum eccentricity

$$r = \min_u \left[\max_v d(u,v)\right] \tag{8.4}$$

The set of nodes with eccentricity equal to the radius is the graph center.

## 8.4 Centralization

While centrality is a local measure for an individual node *centralization* is a global measure considering the distribution of links to nodes, e.g., if there is a single node which receives all links the network has a high degree of centralization. On the other hand regular grids and (Poisson-distributed) random network are examples of networks with no centralization.

In economics and ecology the Lorenz curve has been used to describe centrality. The Gini coefficient (or ratio) is one way of summarizing the Lorenz statistics

$$G = \frac{1}{N^2 \bar{x}} \sum_i^N \sum_j^N |x_i - x_j|. \tag{8.5}$$

Here $x_j$ might be the indegree og the $j$ node.

## 8.5 Spectral gap and expansion

(The **spectral gap** is the smallest non-zero eigenvalue of the Laplacian matrix of a graph.)

## 8.6 Bridge, hinge and articulation

An **articulation node** (also called articulation vertex, articulation point, cut vertex, cutpoint, hinge, point of articulation) is a node which removal will cause the (remaining) graph to become disconnected or increase the number of disconnected subgraphs. The articulation property is also defined for links with names such as articulation edge, bridge, cut edge, isthmus. Others use the word **bridge** to denote a node that connects to peaks. More generally we might speak of a bridge that is connecting two nodes.

# Chapter 9

# Receptor kinetics

An introduction to PET and SPECT neuroreceptor kinetics is (Ichise et al., 2001). A general description of compartmental models is (Gunn et al., 2001).

Table 9.1: Receptor kinetics. Partially from (Maguire and Leenders, 2003). A dagger (†) indicates that the symbol is not widely used.

| Symbol | Unit | Name | Description, Reference |
|---|---|---|---|
| $B_{\max}$ | [mol/l] | Total concentration of receptors | |
| $B'_{\max}$ | [mol/l] | Concentration of available receptors | $B_{\max} - B$ (Innis, 2003, p. 49) |
| $B'_{\max}$ | [fmol/mg] | †Receptor density (after cortical thickness weighting) | The unit is per milligram protein (Forutan et al., 2002) |
| BP | [ ] | Binding potential | |
| $\mathrm{BP_G}$ | [ ] | †Binding potential (graphical) | BP when determined by a "graphical" method, that is the Logan plot (Biver et al., 1994). To distinguish it from, e.g., $\mathrm{BP_{NLR}}$ |
| $C_p$ | [mol/l] | Concentration in plasma | |
| $f_1$ | [ ] | Fraction of free ligand in plasma | $f_1 = c_{\mathrm{free}}/c_{\mathrm{total}} = c_{\mathrm{free}}/(c_{\mathrm{free}} + c_{\mathrm{bound}})$ Some part of total ligand might be bound to proteins in the blood |
| DVR | [ ] | Distribution volume ratio | The ratio between distribution volume in a receptor region and a non-containing receptor (reference) region (Logan et al., 1996) |
| $f_2$ | [ ] | Fraction of free ligand in tissue | |
| $K_1$ | [$\mathrm{min}^{-1}$] | Rate (constant) from blood to tissue | |
| $k_2$ | [$\mathrm{min}^{-1}$] | Rate (constant) from tissue to blood | |
| $k_3$ | [$\mathrm{min}^{-1}$] | Rate (constant) from free ligand in tissue to bound to specific receptor | |
| $k_4$ | [$\mathrm{min}^{-1}$] | Rate (constant) from receptor bound to free ligand | |
| $k_5$ | [$\mathrm{min}^{-1}$] | Rate (constant) from free ligand in tissue to nonreceptor sites (non-specific bound) | |
| $k_6$ | [$\mathrm{min}^{-1}$] | Rate (constant) from nonreceptor sites to free ligand in tissue | |

| Symbol | Unit | Name | Description, Reference |
|---|---|---|---|
| $K_d$ | [nM] | Equilibrium dissociation constant. "Affinity" is $1/K_d$. | $K_d = k_{\text{off}}/k_{\text{on}}$ (Innis, 2003, p. 48) (Lammertsma, 2003, p. 63) |
| $k_{\text{off}}$ | [$\text{min}^{-1}$] | Rate of dissociation | (Innis, 2003, p. 48) |
| $k_{\text{on}}$ | [$\text{nM}^{-1}\ \text{min}^{-1}$] | Rate of association | (Innis, 2003, p. 48) |
| $K_i$ | mol | | |
| $R_I$ | [ ] | "Relative delivery of radiotracer normalized to the cerebellum" | $R_I = K_{1,\text{ROI}}/K_{1,\text{Ref}}$, (Rabiner et al., 2002) |
| SA | [TBq/mmol] | Specific activity | |
| $V_d$ | [ ] | Volume of distribution | Also called "distribution volume" (DV) and the same as the partition coefficient $C_t/C_p$ |

## 9.1 Distribution volume

The "distribution volume" or "volume of distribution" is a ratio between tissue concentration and blood concentration of a ligand and can be found abbreviated as $V_d$ or DV

$$V_d = c_t/c_p \tag{9.1}$$

The blood concentration value can be corrected with the fraction of the ligand that is free (Knudsen, 2003, p. 77)

$$V_d = \frac{c_t}{f_1 c_p} \tag{9.2}$$

For a single-tissue compartment model

$$V_d = K_1/k_2 \tag{9.3}$$

For a two-tissue compartment model

$$V_d = \frac{K_1}{k_2}\left(1 + \frac{k_3}{k_4}\right) \tag{9.4}$$

For a three-tissue compartment model (Lammertsma, 2003, p. 66)

$$V_d = \frac{K_1}{k_2}\left(1 + \frac{k_3}{k_4} + \frac{k_5}{k_6}\right) \tag{9.5}$$

This value was refered to as $K_{\text{NLR}}$ (for estimation with Non-Linear Regression) in (Biver et al., 1994).

The "distribution volume ratio" is actually an estimate of the binding potential.

## 9.2 Binding potential

The binding potential (Lammertsma, 2003, p. 64), Mintun 1984

$$\text{BP} = k_3/k_4 \tag{9.6}$$

$$\text{BP} = f_2 B_{\max}/K_d \tag{9.7}$$

The "SRTM" model (Rabiner et al., 2002, p. 622)

$$\text{BP} = \frac{B_{\max} f_2}{K_D\left(1 + \sum f_i/K_i\right)} \tag{9.8}$$

The **distribution volume ratio** is a estimate of the binding potential using a two-tissue model with a reference region with no specific receptor binding

$$\mathrm{DV}_{\mathrm{ratio}} = \frac{\mathrm{DV}}{\mathrm{DV}_{\mathrm{reference}}}, \tag{9.9}$$

where DV is taken from equation 9.4 (as $V_d$) and the distribution volume of the reference is

$$\mathrm{DV}_{\mathrm{reference}} = \frac{K_1}{k_2}. \tag{9.10}$$

One is substracted to give an estimate of the binding potential

$$\mathrm{BP} = \frac{k_3}{k_4} = \mathrm{DV}_{\mathrm{ratio}} - 1 \tag{9.11}$$

## 9.3 Specific binding ratio

$$\mathrm{SBR} = \frac{\int_{t_1}^{t_2} C(t)\,dt}{\int_{t_1}^{t_2} C_R(t)\,dt} - 1, \tag{9.12}$$

where $C(t)$ is the radioactive concentration at time $t$ for the region of interest and $C_R(t)$ is for the reference region. This appears in, e.g., (Farde et al., 1997; Okubo et al., 1999).

## 9.4 Other values

Incorporation coefficient (Sadzot et al., 1995, p. 789) at time $T$ with plasma activity $C_p$

$$\mathrm{IQ} = \frac{\mathrm{ROI}(T)}{\int_0^T C_p(t)\,dt} \tag{9.13}$$

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