MATH 829: Introduction to Data Mining and Analysis
Graphical Models II - Gaussian Graphical Models

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We will now turn our attention to the special case of a random vector with a multivariate **Gaussian** distribution.

Recall: Multivariate Gaussian/normal distribution

Recall: $X = (X_1, \ldots, X_p) \sim N(\mu, \Sigma)$ where $\mu \in \mathbb{R}^p$ and $\Sigma = (\sigma_{ij}) \in \mathbb{R}^{p \times p}$ is positive definite if

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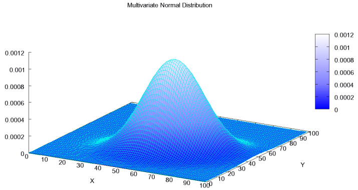

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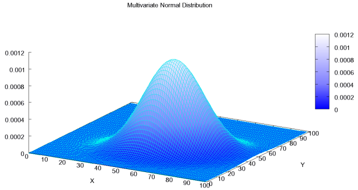

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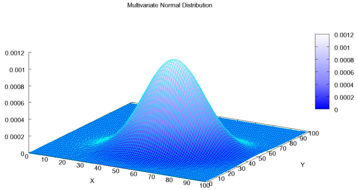

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If $Y = c + BX$, where $c \in \mathbb{R}^p$ and $B \in \mathbb{R}^{m \times p}$, then

$$Y \sim N(c + B\mu, B\Sigma B^T).$$

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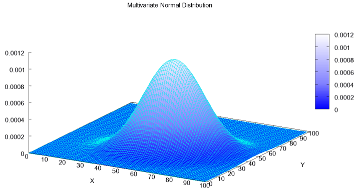

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Note: $\Omega := \Sigma^{-1}$ is called the *precision* matrix or the *concentration* matrix of the distribution.

The Schur complement

Let

$$M := \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

where $A = A_{m\times m}$, $B = B_{m\times n}$, $C = C_{n\times m}$, and $D = D_{n\times n}$.

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1. $\det M = \det D \cdot \det(M/D)$.
2. $M \in \mathbb{P}_{n+m}$ if and only if $D \in \mathbb{P}_n$ and $M/D \in \mathbb{P}_m$.
   where $\mathbb{P}_k =$ denotes the cone of $k \times k$ real symmetric positive semidefinite matrices.

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Proof:

$$M = \begin{pmatrix} I_m & BD^{-1} \\ 0 & I_n \end{pmatrix} \begin{pmatrix} A - BD^{-1}C & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} I_m & 0 \\ D^{-1}C & I_n \end{pmatrix}.$$

Multivariate Gaussian/normal distribution (cont.)

- Conditional distribution: if $A \cup B$ is a partition of $\{1, \ldots, p\}$, then

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Therefore

$$(X_i, X_j)^T \sim N(B\mu, B\Sigma B^T),$$

and

$$B\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \qquad B\Sigma B^T = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}.$$

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Now, suppose

$$X \sim N(\mu, \Sigma)$$

with $\mu \in \mathbb{R}^p$ and $\Sigma = (\sigma_{ij}) \in \mathbb{R}^{p \times p}$ psd.

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where $\rho = \frac{\sigma_{ij}}{\sigma_{ii}\sigma_{jj}}$ is the correlation coefficient between X_i and X_j.

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Therefore $X_i \perp\!\!\!\perp X_j$ iff $\rho = 0$ iff $\sigma_{ij} = 0$.

Proof of (2): Without loss of generality, assume $(i,j) = (1,2)$. Write μ, Σ in block form according to the partition $A = \{1,2\}, B = \{3,\ldots,p\}$:

$$\mu = (\mu_A, \mu_B)^T, \qquad \Sigma = \begin{pmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{pmatrix}.$$

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By part (1), $X_1 \perp\!\!\!\perp X_2 \mid \text{rest}$ iff $(\Sigma_{A|B})_{12} = 0$.

Computing the inverse of a block matrix:

9.1.3 The Inverse

The inverse can be expressed as by the use of

$$\mathbf{C}_1 = \mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21} \qquad (399)$$

$$\mathbf{C}_2 = \mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12} \qquad (400)$$

as

$$\left[\begin{array}{c|c} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \hline \mathbf{A}_{21} & \mathbf{A}_{22} \end{array}\right]^{-1} = \left[\begin{array}{c|c} \mathbf{C}_1^{-1} & -\mathbf{A}_{11}^{-1}\mathbf{A}_{12}\mathbf{C}_2^{-1} \\ \hline -\mathbf{C}_2^{-1}\mathbf{A}_{21}\mathbf{A}_{11}^{-1} & \mathbf{C}_2^{-1} \end{array}\right]$$

$$= \left[\begin{array}{c|c} \mathbf{A}_{11}^{-1} + \mathbf{A}_{11}^{-1}\mathbf{A}_{12}\mathbf{C}_2^{-1}\mathbf{A}_{21}\mathbf{A}_{11}^{-1} & -\mathbf{C}_1^{-1}\mathbf{A}_{12}\mathbf{A}_{22}^{-1} \\ \hline -\mathbf{A}_{22}^{-1}\mathbf{A}_{21}\mathbf{C}_1^{-1} & \mathbf{A}_{22}^{-1} + \mathbf{A}_{22}^{-1}\mathbf{A}_{21}\mathbf{C}_1^{-1}\mathbf{A}_{12}\mathbf{A}_{22}^{-1} \end{array}\right]$$

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Also, we have

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Therefore, $X_i \perp\!\!\!\perp X_j \mid \text{rest}$ iff $(\Sigma^{-1})_{ij} = 0$. □

Estimating the conditional independence structure of a GGM

We have shown that when $X \sim N(\mu, \Sigma)$,

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$$l(\mu, \Sigma) := -\frac{n}{2} \log \det \Sigma - \frac{1}{2} \sum_{i=1}^{n} (x^{(i)} - \mu)^T \Sigma^{-1} (x^{(i)} - \mu) - \frac{np}{2} \log(2\pi).$$

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Classical result: the MLE of (μ, Σ) is given by

$$\hat{\mu} := \frac{1}{n} \sum_{i=1}^{n} x^{(i)}, \qquad S := \frac{1}{n} \sum_{i=1}^{n} (x^{(i)} - \hat{\mu})(x^{(i)} - \hat{\mu})^T.$$

Estimating the CI structure of a GGM (cont.)

- Using $\hat{\mu}$ and $\widehat{\Sigma}$, we can conveniently rewrite the log-likelihood as:

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l(\mu, \Sigma) = &- \frac{n}{2} \log \det \Sigma - \frac{n}{2} \operatorname{Tr}(S\Sigma^{-1}) - \frac{np}{2} \log(2\pi) \\
&- \frac{n}{2} \operatorname{Tr}(\Sigma^{-1}(\hat{\mu} - \mu)(\hat{\mu} - \mu)^T).
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- Note that the last term is minimized when $\mu = \hat{\mu}$ (independently of Σ) since

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(The last inequality holds since Σ^{-1} is positive definite.)

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- Therefore the log-likelihood of $\Omega := \Sigma^{-1}$ is

$$l(\Omega) \propto \log \det \Omega - \operatorname{Tr}(S\Omega) \qquad \text{(up to a constant)}.$$

The Graphical Lasso

The Graphical Lasso (glasso) algorithm (Friedman, Hastie, Tibshirani, 2007), Banerjee et al. (2007), solves the **penalized likelihood** problem:

$$\hat{\Omega}_\rho = \underset{\Omega \text{ psd}}{\operatorname{argmax}} \left[\log\det\Omega - \operatorname{Tr}(S\Omega) - \rho \sum_{i,j=1}^{p} \|\Omega\|_1 \right],$$

where $\|\Omega\|_1 := \sum_{i,j=1}^{p} |\Omega_{ij}|$, and $\rho > 0$ is a fixed regularization parameter.

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- The regularization parameter ρ can be chosen by cross-validation.
- The above problem can be efficiently solved for problems with up to a few thousand variables (see e.g. ESL, Algorithm 17.2).

MLE estimation of a GGM

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- The "graphical MLE" problem can be solved efficiently for up to a few thousand variables (see e.g. ESL, Algorithm 17.1).