Appendices

A.1 Elements of Matrix Algebra

Definitions of vectors and matrices.

$\boldsymbol{X} = \begin{bmatrix} x_1 \\ x_2 \\ \\ x_n \end{bmatrix}$ is an n-variate vector column, where $x_1, x_2, \ldots, x_n$ are components of $\boldsymbol{X}$.

$\boldsymbol{Z} = (x_1, x_2, \ldots, x_n)$ is an n-variate vector row, $\boldsymbol{Z} = \boldsymbol{X}^T$; ^{T} denotes a transpose operation; and n is called a dimensionality of the vectors $\boldsymbol{X}$ and $\boldsymbol{Z}$.

$\mathbf{A} = ((a_{ij}))$, $(i, j = 1, 2, \ldots, n)$ is an $n \times n$ quadratic matrix, a_{ij} are the elements of matrix $\mathbf{A}$. If $a_{ij} = a_{ji}$, the matrix $\mathbf{A}$ is symmetric.

Multiplication of matrices. Let $\mathbf{B} = ((b_{ij}))$, $(i, j = 1, 2, \ldots, n)$ be another $n \times n$ quadratic matrix. Then $\mathbf{AB} = \mathbf{C} = ((c_{ij}))$, is also an $n \times n$ quadratic matrix with elements $c_{ij} = \sum_{s=1}^{n} a_{is} b_{sj}$. If $\boldsymbol{Y} = (y_1, y_2, \ldots, y_n)^T$ is a n-variate vector column, $\boldsymbol{Y}^T \mathbf{A} \boldsymbol{X} = \sum_{j=1}^{n} \sum_{i=1}^{n} a_{ij} y_i x_j$.

A hyperplane is $\boldsymbol{V}^T \boldsymbol{X} + v_0 = 0$, where $\boldsymbol{V}$ is a vector column.

A distance between a vector and the hyperplane $\boldsymbol{V}^T \boldsymbol{X} + v_0 = 0$ is $H = \dfrac{|\boldsymbol{V}^T \boldsymbol{X} + v_0|}{\sqrt{\boldsymbol{V}^T \boldsymbol{V}}}$.

Orthogonal matrices. If $\boldsymbol{Y}^T \boldsymbol{X} = 0$, the vectors $\boldsymbol{Y}$ and $\boldsymbol{X}$ are said to be orthogonal. If, in addition, $\boldsymbol{Y}^T \boldsymbol{Y} = 1$ and $\boldsymbol{X}^T \boldsymbol{X} = 1$, the vectors $\boldsymbol{Y}$ and $\boldsymbol{X}$ are said to be orthonormal. A quadratic matrix $\mathbf{T}$ is said to be orthogonal if $\mathbf{T}\mathbf{T}^T = \mathbf{D} = ((d_{ij}))$

(diagonal matrix). In the diagonal matrix **D**, $d_{ij} = 0$ if $j \neq i$. If all $d_{ii} > 0$, the matrix **D** is positively defined. Its determinant $\det(\mathbf{D}) = \prod_{i=1}^{n} d_{ii} > 0$. If $\mathbf{T}\mathbf{T}^T = \mathbf{I}_n$ (the identity matrix), the matrix **T** is said to be orthonormal. The identity matrix has ones on its diagonal, and zeros outside the diagonal. For orthonormal matrix **T** one can write $\mathbf{T}\mathbf{T}^T = \mathbf{T}^T\mathbf{T} = \mathbf{I}_n$.

Singular value decomposition. The symmetric matrix **A** can be decomposed into a product: $\mathbf{A} = \mathbf{T}\,\mathbf{D}\,\mathbf{T}^T$, where **T** is an orthonormal $n \times n$ matrix such that

$$\mathbf{T}^T\mathbf{A}\mathbf{T} = \mathbf{D} = \begin{bmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & d_n \end{bmatrix}. \qquad \text{(A1.1)}$$

Matrix **T** is called an eigenvectors matrix and diagonal elements of matrix **D** are called eigenvalues of matrix **A**. The matrix **A** is positively defined if all $d_i > 0$.

Inverse of the symmetric quadratic matrix. Let **B** be a quadratic positively defined matrix, such that $\mathbf{B}\mathbf{A} = \mathbf{A}\mathbf{B} = \mathbf{I}$. Then **B** is called an inverse of **A** and denoted by $\mathbf{B} = \mathbf{A}^{-1}$. The representation (A1.1) shows that

$$\mathbf{A}^{-1} = (\mathbf{T}\,\mathbf{D}\,\mathbf{T}^T)^{-1} = (\mathbf{T}^T)^{-1}\mathbf{D}^{-1}\mathbf{T}^{-1} = \mathbf{T}\,\mathbf{D}^{-1}\mathbf{T}^T. \qquad \text{(A1.2)}$$

Pseudo-inversion. If n-r eigenvalues of matrix **A** are equal to zero, the matrix **A** is not positively defined. Its determinant is equal to zero. Let us write the diagonal matrix **D** in a block layout $\mathbf{D} = \begin{bmatrix} \mathbf{d} & 0 \\ 0 & 0 \end{bmatrix}$ in (A1.1), where **d** is an $r \times r$ diagonal matrix composed from non-zero values of **D**. Thus, we can rewrite Equation (A1.1) in a block layout

$$\mathbf{T}^T\mathbf{A}\mathbf{T} = [\mathbf{T}_1\ \mathbf{T}_2]^T\mathbf{A}[\mathbf{T}_1\ \mathbf{T}_2] = \begin{bmatrix} \mathbf{d} & 0 \\ 0 & 0 \end{bmatrix}, \qquad \text{(A1.3)}$$

where we have split the orthogonal matrix $\mathbf{T} = [\mathbf{T}_1\ \mathbf{T}_2]$ into $n \times r$ matrix $\mathbf{T}_1$ and $n \times (n\text{-}r)$ matrix $\mathbf{T}_2$. Then the pseudo-inverse of matrix **A**

$$\mathbf{A}^{+} = \mathbf{T}\begin{bmatrix} \mathbf{d}^{-1} & 0 \\ 0 & 0 \end{bmatrix}\mathbf{T}^T = [\mathbf{T}_1\ \mathbf{T}_2]\begin{bmatrix} \mathbf{d}^{-1} & 0 \\ 0 & 0 \end{bmatrix}[\mathbf{T}_1\ \mathbf{T}_2]^T = \mathbf{T}_1\,\mathbf{d}^{-1}\,\mathbf{T}_1^T. \qquad \text{(A1.4)}$$

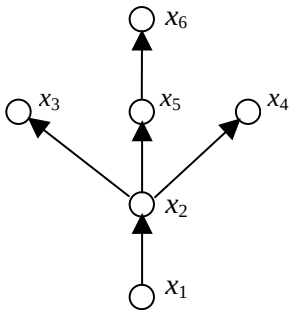
A.2 The First Order Tree Type Dependence Model

The probability density function of the random vector $\boldsymbol{X} = (x_1, x_2, ..., x_n)$ having the first order tree type dependence between the variables can be written in the following form:

$$p(x_1, x_2, ..., x_n) = \prod_{j=1}^{n} p\,(x_j \,|\, x_{m_j}) \quad (0 \le m_j \le n) \tag{A2.1}$$

where a sequence $m_2, ..., m_n$ constitutes a *graph of connections*, $\mathbf{m}$ (an unknown permutation of the integers 1, 2, ... , n), and $p(x_i \,|\, x_0)$, by definition, is equal to $p(x_i)$. In a general case, the covariance matrix has $n \times n$ non-zero elements. An inverse of this matrix $\boldsymbol{\Sigma}^{-1}$ that has to be used in the classifier design, however, has only $2n$-1 diferent non-zero elements. It is a result of the assumption that each component of the vector $\boldsymbol{X}$ depends directly on only one another component.

To depict the dependence relations graphically, the variable is represented by a point on the plane, and if x_i and x_j are two variables such that $j = m_i$, they will be joined by an arrow pointing from x_j to x_i. Figure A2.1 shows an example of a dependence tree with graph $\mathbf{m} = (m_2, m_3, m_4, m_5, m_6) = (1, 2, 2, 2, 5)$.



$$p(\boldsymbol{X}) = p(x_1)\, p(x_2|x_1)\, p(x_3|x_2) p(x_4|x_2) p(x_5|x_2) p(x_6|x_5).$$

Fig. A2.1. An example of the first order dependence tree.

We present an analytical expression of the density for the multivariate Gaussian case. The conditional density function for two Gaussian distributed variables is

$$p(x_i \,|\, x_j) = N(x_i\,,\, m_i + (x_j - m_j)\ \sigma_{jj}^{-1}\sigma_{ij}\,,\ \sigma_{ii} - \sigma_{jj}^{-1}\sigma_{ij}^2\,) \tag{A2.2}$$

where σ_{ij} is an element of the covariance matrix $\boldsymbol{\Sigma}$.

Using (A2.2) in (A2.1) yields a simple analytical expression for the joint probability density function

$$p(x_1, x_2, ..., x_n) = \prod_{j=1}^{n} N(x_j , m_j + (x_{m_j} - m_{m_j})\ \sigma^{-1}_{m_j m_j} \sigma_{j m_j} , \sigma_{jj} - \sigma^{-1}_{m_j m_j} \sigma^2_{j m_j}) =$$

$$\frac{1}{(2\pi)^{n/2}} \prod_{j=1}^{n} (\sigma_{jj} - \sigma^{-1}_{m_j m_j} \sigma^2_{j m_j})^{-1/2}$$

$$\exp\left(-\frac{1}{2} \sum_{j=1}^{n} \frac{[(x_j - m_j) - (x_{mj} - m_{mj})\sigma^{-1}_{mjmj} \sigma_{jmj}]^2}{\sigma_{jj} - \sigma^{-1}_{mjmj} \sigma^2_{jmj}} \right) \qquad \text{(A2.3)}$$

We require that the variables $x_1, x_2, ..., x_n$ be ranked in such a way that $m_j < j$, $j = 2, 3, ..., n$. Then density function (A2.3) may be written in the following form

$$p(x_1, x_2, ..., x_n) = N(\boldsymbol{X}, \boldsymbol{M}, \Sigma),$$

where

$$\Sigma^{-1} = (\mathbf{C}^T \mathbf{C}), \qquad \mathbf{C} = ((c_{ij})), \qquad \text{(A2.4)}$$

$$c_{ij} = \begin{cases} \dfrac{1}{\sqrt{\sigma_{ii}(1 - r^2_{im_i})}} & \text{if} \quad j = i \\ \dfrac{-r_{im_i}}{\sqrt{\sigma_{m_i m_i}(1 - r^2_{im_i})}} & \text{if} \quad j = m_i \\ 0 \quad \text{if} \quad j = i \quad \text{and} \quad j \neq m_i \end{cases} \qquad \text{(A2.5)}$$

$$r_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{jj}\, \sigma_{ii}}}.$$

Example. Let $\sigma_{21} = 0.7$; $\sigma_{32} = -0.3$; $\sigma_{42} = 0.4$; $\sigma_{52} = 0.2$; $\sigma_{65} = -0.6$, and all variances $\sigma_{11} = \sigma_{22} = \sigma_{33} = \sigma_{44} = \sigma_{55} = \sigma_{66} = 1$. Then

$$\mathbf{C} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -0.9802 & 1.4003 & 0 & 0 & 0 & 0 \\ 0 & 0.3145 & 1.0483 & 0 & 0 & 0 \\ 0 & -0.4364 & 0 & 1.0911 & 0 & 0 \\ 0 & -0.2041 & 0 & 0 & 1.0206 & 0 \\ 0 & 0 & 0 & 0 & 0.7500 & 1.2500 \end{bmatrix},$$

$$\Sigma^{-1} = \begin{bmatrix} 1.9608 & -1.3725 & 0 & 0 & 0 & 0 \\ -1.3725 & 2.2918 & 0.3297 & -0.4762 & -0.2083 & 0 \\ 0 & 0.3297 & 1.0989 & 0 & 0 & 0 \\ 0 & -0.4762 & 0 & 1.1905 & 0 & 0 \\ 0 & -0.2083 & 0 & 0 & 1.6042 & 0.9375 \\ 0 & 0 & 0 & 0 & 0.9375 & 1.5625 \end{bmatrix}, \text{ and}$$

$$\Sigma = \begin{bmatrix} 1 & 0.700 & -0.210 & 0.280 & 0.140 & -0.084 \\ 0.700 & 1 & -0.300 & 0.400 & 0.200 & -0.120 \\ -0.210 & -0.300 & 1 & -0.120 & -0.06 & 0.0360 \\ 0.280 & 0.400 & -0.120 & 1 & 0.080 & -0.048 \\ 0.140 & 0.200 & -0.06 & 0.080 & 1 & -0.600 \\ -0.084 & -0.120 & 0.0360 & -0.048 & -0.600 & 1 \end{bmatrix}.$$

When the graph $\mathbf{m} = (m_2, ..., m_n)$ is known, we estimate the inverse covariance matrix from the sample covariance matrix as $\hat{\Sigma}^{-1} = \hat{\mathbf{C}}^T \hat{\mathbf{C}}$, where $\hat{\mathbf{C}}$ is determined by Equation (A2.5) with the elements σ_{ij} substituted by their corresponding sample estimates.

To estimate the graph $\mathbf{m} = (m_2, m_3, \ldots, m_n)$, it is suggested that one uses a stepwise algorithm developed by Kruskal (1956) for the construction of trees of maximum total branch weight. Let $\{|\hat{r}_{12}|, |\hat{r}_{13}|, |\hat{r}_{14}|, ..., |\hat{r}_{n-1\ n}|\}$ be the absolute values of the sample correlation coefficients between the variables. Then, the first step is to select a branch with the greatest weight $|\hat{r}_{st}|$, while the i-th step ($2 \le i \le n$-1) is to choose a branch with the greatest weight $|\hat{r}_{vu}|$ that is different from all the branches selected during the previous steps and does not form a cycle with the previously selected branches. If the multivariate normal density may be represented by the branch $\mathbf{m}$ model, then the sample estimate $\hat{\mathbf{m}}$

of the graph asymptotically (as the sample size N_1, $N_2 \to \infty$ and the dimensionality $n \to \infty$) converges to the true graph $\mathbf{m}$.

When the above model is used to design the linear discriminant function (for the two category case when it is assumed that $\Sigma_2 = \Sigma_1$) then one has to estimate $4n$ - 1 parameters: $2n$ components of the mean vectors, n variances σ_{ii} and n - 1 covariances, as well as n - 1 numbers that compose the graph $\mathbf{m}$.

A.3 Temporal Dependence Models

Let the components $x_1, x_2, ..., x_{n-1}, x_n$ of the multivariate vector be measurements differing in time or in space, and assume they are a stationary random process. Then the covariance matrix has a following structure

$$\Sigma = \begin{bmatrix} \delta_1 & \delta_2 & \delta_3 & ... & \delta_{n-1} & \delta_n \\ \delta_2 & \delta_1 & \delta_2 & ... & \delta_{n-2} & \delta_{n-1} \\ \delta_3 & \delta_2 & \delta_1 & ... & \delta_{n-3} & \delta_{n-2} \\ ... & ... & ... & ... & ... & ... \\ \delta_{n-1} & \delta_{n-2} & \delta_{n-3} & ... & \delta_1 & \delta_2 \\ \delta_n & \delta_{n-1} & \delta_{n-2} & ... & \delta_2 & \delta_1 \end{bmatrix}. \qquad \text{(A3.1)}$$

We see only n parameters $\delta_1, \delta_2, \delta_3, ..., \delta_n$ that describe the dependence between the variables and have to be estimated from the training-set. Let $\boldsymbol{X}_1, \boldsymbol{X}_2, ..., \boldsymbol{X}_N$ be N training-set vectors, $\boldsymbol{X}_j = (x_{j1}, x_{j2}, ..., x_{jN})^T$. Then, the sample estimate

$$\hat{\delta}_l = \frac{1}{N(n-l)} \sum_{j=1}^{N} \sum_{t=1}^{n-l} (x_{jt} - \bar{x}_t)(x_{jt+l} - \bar{x}_t).$$

A number of special models, such as autoregression, moving average, ARMA, and circular, reduce the number of parameters even more.

In the *autoregression model*, we have q + 1 independent parameters, and here the dependence among variables is determined by the equation

$$x_t + a_1 x_{t-1} + ... + a_r x_{t-r} = v_t, \qquad \text{(A3.2)}$$

where random variables $v_t, v_{t-1}, ...$ are supposed to be mutually independent and identically distributed $N(0, 1)$. In this model, the last p-r variables $x_r, x_{r+1}, ..., x_{n-1}$ are linearly dependent on the previous ones. The inverse covariance matrix has a simple form, and can be calculated analytically (Kligiene, 1977)

$$\Sigma^{-1} = \begin{pmatrix} \kappa_{11} & \dots & \kappa_{1r} & \kappa_r & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \kappa_{r1} & \dots & \kappa_{rr} & \kappa_1 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ \kappa_r & \dots & \kappa_1 & \kappa_0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ 0 & .. & 0 & 0 & \kappa_0 & \dots & 0 & 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & 0 & 0 & \dots & \kappa_0 & 0 & 0 & \dots & 0 \\ 0 & \dots & 0 & 0 & 0 & \dots & 0 & \kappa_0 & \kappa_1 & \dots & \kappa_r \\ 0 & \dots & 0 & 0 & 0 & \dots & 0 & \kappa_1 & \kappa_{rr} & \dots & \kappa_{r1} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & 0 & 0 & \dots & 0 & \kappa_r & \kappa_{1r} & \dots & \kappa_{11} \end{pmatrix}, \qquad \text{(A3.3)}$$

where $\kappa_l = \sum_{k=0}^{r-l} a_k a_{k+l}$, $\quad \kappa_{st} = \sum_{k=0}^{\min(s,t)-1} a_k a_{k+|s-t|}$, $\quad s, t = 1, 2, ..., r.$

In the *moving average model*, we have $q + 1$ independent parameters, and here the dependence among variables is determined by the equation

$$x_t = \mu_t + b_0 v_t + b_1 v_{t-1} + ... + b_q v_{t-q}, \qquad \text{(A3.4)}$$

where the variables v_t, v_{t-1}, ... are supposed to be mutually independent and identically distributed $N(0, 1)$. In this model, we have

$$\delta_{q+1} = \delta_{q+2} = \delta_{q+3} = ... = \delta_n = 0; \; q < n.$$

The *circular* covariance matrix has $n/2$ independent parameters and has form

$$\Sigma = \sigma_0 \begin{pmatrix} 1 & \rho_1 & \rho_2 & \rho_3 & \dots & \rho_2 & \rho_1 \\ \rho_1 & 1 & \rho_1 & \rho_2 & \dots & \rho_3 & \rho_2 \\ \rho_2 & \rho_1 & 1 & \rho_1 & \dots & \rho_4 & \rho_3 \\ \rho_3 & \rho_2 & \rho_1 & 1 & \dots & \rho_5 & \rho_4 \\ \rho_4 & \rho_3 & \rho_2 & \rho_1 & \dots & \rho_6 & \rho_5 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \rho_1 & \rho_2 & \rho_3 & \rho_4 & \dots & \rho_1 & 1 \end{pmatrix}. \qquad \text{(A3.5)}$$

This matrix can be transformed into a canonical form by means of the following orthonormal matrix $\mathbf{L} = ((l_{mn}))$ with elements

$$l_{ms} = \sqrt{n}\left(\cos\frac{2\pi}{n}(m-1)(s-1) + \sin\frac{2\pi}{n}(m-1)(s-1) \right), \qquad \text{(A3.6)}$$

such that $\mathbf{L}^T\mathbf{\Sigma}\mathbf{L} = \begin{pmatrix} \sigma_1 & 0 & ... & 0 \\ 0 & \sigma_2 & .. & 0 \\ ... & ... & ... & ... \\ 0 & 0 & ... & \sigma_n \end{pmatrix}$.

Note, the transformation matrix **L** does not depend on **Σ**.

The model of the *additive noise* is typical to physical measurements of the same origin where all variables are influenced by the same systematic Gaussian error N(0, σ_1^2). The original and the inverse covariance matrices are determined only by two parameters:

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_1^2 + \sigma_2^2 & \sigma_1^2 & \sigma_1^2 & \dots & \sigma_1^2 \\ \sigma_1^2 & \sigma_1^2 + \sigma_2^2 & \sigma_1^2 & \dots & \sigma_1^2 \\ \sigma_1^2 & \sigma_1^2 & \sigma_1^2 + \sigma_2^2 & \dots & \sigma_1^2 \\ \dots & \dots & \dots & \dots & \dots \\ \sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \dots & \sigma_1^2 + \sigma_2^2 \end{pmatrix},$$

$$\mathbf{\Sigma}^{-1} = \begin{pmatrix} a & b & b & \dots & b \\ b & a & b & \dots & b \\ b & b & a & \dots & b \\ \dots & \dots & \dots & \dots & \dots \\ b & b & b & \dots & a \end{pmatrix}, \qquad \text{(A3.7)}$$

where

$a = ((n-1)\sigma_1^2 + \sigma_2^2)/(\sigma_2^2(n\sigma_1^2 + \sigma_2^2))$,

$b = -\sigma_1^2/(\sigma_2^2(n\sigma_2^2 + \sigma_2^2))$.

A.4 Pikelis Algorithm for Evaluating Means and Variances of the True, Apparent and Ideal Errors in Model Selection

Let $\hat{\varepsilon}_{v1}, \hat{\varepsilon}_{v2}, ..., \hat{\varepsilon}_{vM}$ be M "inaccurate" (e.g. validation set) performance estimates, and $\hat{\varepsilon}_{t1}, \hat{\varepsilon}_{t2}, ..., \hat{\varepsilon}_{tM}$ be m "accurate" (e.g. large test set) performance estimates, corresponding to M variants (models). We investigate all possible collections composed of m models selected from a pool of M models ($m < M$). We need to estimate the mean values E and variances V of the true, apparent, and ideal errors when we select the best variant from an arbitrary collection composed of m randomly chosen vectors ($\hat{\varepsilon}_{vj}, \hat{\varepsilon}_{tj}$).

1. Input data: M – a total number of variants considered in the experiment,
m – a number of variants in a collection under consideration
M – two-variate vectors $(\hat{\varepsilon}_{vj}, \hat{\varepsilon}_{tj})$, $j = 1, 2, ..., M$. Note, $m << M$.

2. Rank M values $\hat{\varepsilon}_{v1}, \hat{\varepsilon}_{v2}, ..., \hat{\varepsilon}_{vM}$ in increasing order and find order numbers $i_1, i_2, ..., i_M$ of the ranked data.

3. Calculate a number v_j of cases when the value $\hat{\varepsilon}_{vj}$ was the smallest one in each of $J = C_M^m = \frac{M!}{(M - m)!\, m!}$ possible collections composed of r vectors from m ones: $v_1 = m/M$. The following values of v_2, v_3, ... are found using the recursive formula:

$$v_{j+1} = v_j * (M-r-j+1)/(M-j), \quad j = 1, 2, ..., M - m + 1.$$

4. Calculate the means and variances:

$$E\varepsilon_{apparent} = \sum_{j=1}^{M-m+1} v_{i_j} \hat{\varepsilon}_{vi_j}, \qquad V\varepsilon_{apparent\ t} = \sum_{j=1}^{M-m+1} v_{i_j} (\hat{\varepsilon}_{vi_j} - E\varepsilon_{apparent})^2,$$

$$E\varepsilon_{true} = \sum_{j=1}^{M-m+1} v_{i_j} \hat{\varepsilon}_{vi_j}, \qquad V\varepsilon_{true} = \sum_{j=1}^{M-m+1} v_{i_j} (\hat{\varepsilon}_{vi_j} - E\varepsilon_{true})^2.$$

The mean and the variance of the ideal error $E\varepsilon_{ideal}$ can be found in an analogous way. We recommend applying this algorithm for a set of values of m ($m << M$).

A.5 Matlab Codes (the Non-Linear SLP Training, the First Order Tree Dependence Model, and Data Whitening Transformation)

```
% A main program to test for the data whitening by the
% first order tree dependence model and subsequent
% training the nonlinear SLP
% This program generates two p-variate Gaussian classes
% with covariance matrix C having a linear tree
% dependence model structure
% The SLP is trained twice: in original and
% transformed feature spaces.

% AUTHOR: Sarunas Raudys   <raudys@das.mii.lt>

% Example:    dimensionality:  p=30;
% training & valdation sizes   nm=30;nv=500;
% N of iterations:             iter=500;,
% regularization:              lambda=0.001;
% correlation:                 ro=0.5;
% increase in learning step:  gama=1.01 (Section 4.6.6)
CI=eye(p);CI1=ro*eye(p+1);
CI=CI+CI1(2:p+1,1:p)+CI1(1:p,2:p+1);C=inv(CI);
[u,d]=eig(C);G=sqrt(real(d))*real(u);

A= randn(nm,p)*G; % training-data
B=randn(nm,p)*G+ones(nm,1)*[ones(1,10),-ones(1,p-10)];
Av=randn(nv,p)*G; % validation-data
Bv=randn(nv,p)*G+ones(nv,1)*[ones(1,10),-ones(1,p-10)];

% conditions E1, E2 (see Section 4.1.2.1):
M=mean([A;B]);A=A-ones(nm,1)*M;B=B-ones(nm,1)*M;
Av=Av-ones(nv,1)*M;Bv=Bv-ones(nv,1)*M;
CM=0.5*(cov(A)+cov(B));Wstart=zeros(1,p+1);

% training SLP in original feature space:
[W,etest]=slp(A,B,iter,0.1,0.00,Wstart,Av,Bv,gama);

[covt,covtI]=gentree(CM);% search for tree structure
[u,d,v]=svd(covt+lambda);% data whitening
T=u*inv(sqrtm(d));a=A*T;b=B*T;av=Av*T;bv=Bv*T;
% training SLP in transformed (whitened) feature space:

[W,et]=slp(a,b,iter,0.1,0.00,Wstart,av,bv,gama);
figure(1);plot([1:iter],etest,'r-',[1:iter],et,'g-');

%        Try to PRINT:
%disp(covtI(1:7,1:7))a part of inverse of structurised CM
% disp ([min(etest),min(et)]) % minima of
% generalisation error without and with
% whitening data transformation
++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Single layer perceptron

```
% Non-linear single-layer perceptron for 2 classes
% Author S.Raudys  <raudys@das.mii.lt>
% Inputs:
% A, B - training sets from two classes
% rows contains observations, columns - features
% n - number of training iterations
% step - learning step
% target - target value for class A (sigmoid transfer
% function)
% Wstart - initial weight vector
% Aval, Bval - validation set from classes A, B;
% rows contains observations, columns - features
% gama - coefficient to change the learning speed
% after each training  iteration, step=step * gama
% Outputs:  W - weight after the last iteration
% etest - test error after each iteration

function
[W,etest]=slp(A,B,iter,step,target,Wstart,Av,Bv,gama)

[ma k] = size(A);[mb k] = size(B);
[mav k] = size(Av);[mbv k] = size(Bv);

W=Wstart;
stepz=step/(ma+mb);
ta = (1-target) * ones(ma,1);tb = target * ones(mb,1);
oa = ones(ma,1);ob = ones(mb,1);
oav = ones(mav,1);obv = ones(mbv,1);
A=[A,oa];B=[B,ob];Av=[Av,oav];Bv=[Bv,obv];

      for i=1:iter   da = A * W';
db = B * W';
e = (sum(da<0) + sum(db>=0))/(ma+mb);
fa = oa./(oa+exp(-da));
fb = ob./(ob+exp(-db));
za = ((ta-fa).* (fa - fa.*fa))'*A;
zb = ((tb-fb).* (fb - fb.*fb))'*B;
W = W + stepz * (za + zb);
etest(i)=
size([find(W*Av'<0),find(W*Bv'>0)],2)/(mav+mbv);
stepz=stepz*gama;
      end
return
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

% Structurisation of the covariance matrix by
% the first-oder tree-type dependence model
% A main program
% Author: Ausra Saudargiene, ausrsaud@takas.lt
% Department of Data Analysis, Institute of Mathematics
% and Informatics, Akademijos 4, 2600 Vilnius

% Input:   C-covariance matrix
% Outputs: covgen-structured CM, covgenI-inverse of CM

function [covtree,covtreeI]=gentree(C);

[M,S,SS,num]=treev(C);%estimation of the graph,
% weights of the branches, and the new order of
% features

[covtree,covtreeI]=treecov(M,S,SS,num);
%calculation of the tree-type covariance matrix
return

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

% First-order tree-type dependence model
% Estimation of the graph, weights of the branches,
% and the new order of the features
% Author: A.Saudargiene, ausrsaud@takas.lt

% Input:   C-covariance matrix
% Output:
% M - graph of the tree
% S - weights of the branches (covariances)
% SS – variances, num - initial order of the features

function [M,S,SS,num]=treev(C);
[p,ms]=size(C);
%Regularization, if covariance matrix is singular
alfa=0.01;%regularization constant
if det(C)<1e-10, C=C+alfa*eye(p,p); end

%Correlation coefficients
for j=1:p
for i=1:p
     A0(i,j)=C(i,j)/sqrt(C(i,i)*C(j,j));
end
end

A=triu(A0);
Mn(1)=0; M(1)=0;S(1)=0;
k=1;
```

```
M_all=zeros((p*p-p)/2,1);

%Estimating graph of the tree
for ind=2:p % number of branches
   max_A=0;
%finding max value for i-th branch
   for i=1:p
      for j=i+1:p
         ski=0;skj=0;sk=0;
% current A(i,j): checking for common points with the
% previously selected branches
% finding max value
         if abs(A(i,j))>abs(max_A)
            for l=1:k
               if i==M_all(l) ski=1; end
               if j==M_all(l) skj=1; end
            end
            sk=ski+skj;
            if ind==2, sk=1; end
            if sk==1
               max_A=A(i,j);ki=i;kj=j;
               if ski==1
                  Mn(ind)=ki; num(ind)=kj;
               else
                  Mn(ind)=kj; num(ind)=ki;
               end
            end
         end
      end
   end

   S(ind)=C(ki,kj);
   A(ki,kj)=0;
   M_all(k)=ki;k=k+1;M_all(k)=kj;k=k+1;

%Finding initial point
   if ind==2
      if M_all(1)<M_all(2)
         Mn(2)=M_all(1);
num(1)=M_all(1);num(2)=M_all(2);
      else
         Mn(2)=M_all(2);
num(1)=M_all(2);num(2)=M_all(1);
      end
   end
end

% Changing the order of the features
for i=1:p
   for j=1:p
      if Mn(i)==num(j) M(i)=j; end
```

```
      C1(i,j)=C(num(i),num(j));
   end
end
SS=diag(C1)';

return
++++++++++++++++++++++++++++++++++++++++++++++++++++++++
% First-order tree-type dependence model
% Calculation of the covariance matrix (CM)
% Author: A.Saudargiene, ausrsaud@takas.lt
% Inputs: are outputs of  treev.m:
% Outputs: covgen - CM,covgenI - inverse of CM
function [covgen,covgenI]=treecov(M,S,SS,num)

[s1,s2]=size(M);p=s2;
for i=2:p
   r(i)=S(i)/sqrt(SS(i)*SS(M(i)));
end
for i=1:p
   for j=1:p
      C(i,j)=0;
      if j==i
         C(i,j)=1/sqrt(SS(i)*(1-r(i)^2));
      end
      if j==M(i)
         C(i,j)=-r(i)/sqrt(SS(M(i))*(1-r(i)^2));
      end
   end
end
KI=C'*C;d=diag(C);
K=inv(KI);

%Initial order of the features
for i=1:p
   k=find(num==i);
   numret(i)=k;
end

for i=1:p
   for j=1:p
      covgen(i,j)=K(numret(i),numret(j));
      covgenI(i,j)=KI(numret(i),numret(j));
   end
end
return
```

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