Module 18 Multivariate Analysis for Genetic data Session 01: Matrix Algebra

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Multivariate Analysis (MVA) and Matrix algebra

- Multivariate analysis is, to a considerable extent, applied matrix algebra.
- A good knowledge of matrix algebra facilitates your understanding of MVA.

Outline

- Vectors
- Matrices
- Quadratic forms
- Matrices commonly used in MVA
- Example data set

Vectors

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \qquad \mathbf{x}' = \begin{bmatrix} x_1, x_2, \dots, x_n \end{bmatrix}$$

Scalar multiplication

Vectors

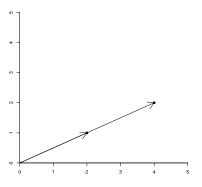
$$\alpha \mathbf{x} = \begin{bmatrix} \alpha x_1 \\ \alpha x_2 \\ \vdots \\ \alpha x_n \end{bmatrix},$$

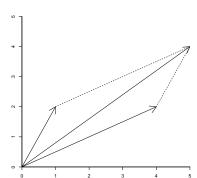
Vectors

Addition

$$\mathbf{x} + \mathbf{y} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_n + y_n \end{bmatrix}$$

Geometric interpretation





Vectors

Introduction

Norm or length

$$\|\mathbf{x}\| = \sqrt{\mathbf{x}'\mathbf{x}} = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}$$

$$\|\alpha \mathbf{x}\| = \alpha \|\mathbf{x}\|$$

Scalar product or inner product:

$$\mathbf{x}'\mathbf{y} = x_1y_1 + x_2y_2 + \cdots + x_ny_n$$

$$\mathbf{x}'\mathbf{y} = \mathbf{0} \leftrightarrow \mathbf{x}$$
 and \mathbf{y} are perpendicular .

Angle:

$$\cos \theta = \frac{\mathbf{x}'\mathbf{y}}{\|\mathbf{x}\|\|\mathbf{y}\|}$$

Notes

Vectors

- The norm is the Euclidean distance from the origin in an n dimensional space
- Let x and y be two centred quantitative variables

$$\cos \theta = \frac{\mathbf{x}' \mathbf{y}}{\|\mathbf{x}\| \|\mathbf{y}\|}$$

$$= \frac{\sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \overline{x})^2} \sqrt{\sum_{i=1}^{n} (y_i - \overline{y})^2}}$$

$$= \frac{s_{xy}}{s_x \cdot s_y}$$

$$= r_{xy}.$$

This property is widely used in biplot interpretation (see later).

Linear combination, linear (in)dependence

Linear combination of n vectors

$$\mathbf{y} = a_1\mathbf{x}_1 + a_2\mathbf{x}_2 + \cdots + a_n\mathbf{x}_n$$

To investigate linear dependence:

$$a_1\mathbf{x}_1 + a_2\mathbf{x}_2 + \dots + a_n\mathbf{x}_n = \mathbf{0} \tag{1}$$

- The set of vectors $\mathbf{x}_1, \mathbf{x}_2, \dots \mathbf{x}_n$ is linearly dependent iff Eq. (1) holds for some set (a_1, a_2, \ldots, a_n) not all zero.
- The set of vectors $\mathbf{x}_1, \mathbf{x}_2, \dots \mathbf{x}_n$ is linearly independent iff Eq. (1) holds only for $(a_1, a_2, ..., a_n) = (0, 0, ..., 0)$.

Investigating linear (in)dependence

Is the following set of vectors linearly independent or not?

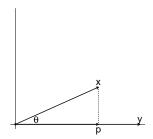
$$\begin{bmatrix} 1 & 5 & -2 \\ 3 & 7 & 2 \\ 2 & 9 & -3 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 5 & -2 \\ 0 & -8 & 8 \\ 0 & -1 & 1 \end{bmatrix}$$

Later:

- determine the rank of the matrix
- compute eigenvalues
- do principal component analysis

Projection

Introduction



$$\cos \theta = \frac{\|\mathbf{p}\|}{\|\mathbf{x}\|}, \quad \|\mathbf{p}\| = \cos \theta \|\mathbf{x}\| = \frac{\mathbf{x}'\mathbf{y}}{\|\mathbf{x}\|\|\mathbf{y}\|} \|\mathbf{x}\| = \frac{\mathbf{x}'\mathbf{y}}{\|\mathbf{y}\|}.$$

• Note that for a given vector **y**, the length of the projection is proportional to the scalar product between the vectors.

Matrix Algebra

• This property is also widely used in biplot interpretation.

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Matrix

Introduction

$$\mathbf{X}_{n \times p} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

About n and p:

- Classical n >> p
- Limiting n = p
- Today often n << p

A duality

$$\mathbf{X}_{n \times p} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_n \end{bmatrix} = \begin{bmatrix} \mathbf{y}_1 \mid \mathbf{y}_2 \mid \cdots \mid \mathbf{y}_p \end{bmatrix}$$

- n points in a p-dimensional space
- p points in a n-dimensional space

Basic matrix operations

Vectors

sum

Introduction

$$C_{n\times p} = A_{n\times p} + B_{n\times p}$$
 $c_{ij} = a_{ij} + b_{ij}$

scalar multiplication

$$\mathbf{C} = \alpha \mathbf{A}_{n \times p}$$
 $c_{ij} = \alpha a_{ij}$

product

$$\mathbf{C}_{n \times p} = \mathbf{A}_{n \times k} \mathbf{B}_{k \times p}$$
 $c_{ij} = \sum_{l=1}^{k} a_{il} b_{lj}$

transposition

$$C = A'$$
 $c_{ii} = a_{ii}$ $E = AB$ $E' = (AB)' = B'A'$

inversion

$$A_{k \times k}$$
 $AB = BA = I$ $B_{k \times k} = A^{-1}$

Some particular cases of matrix multiplication

$$\bullet \ \mathbf{A}_{p\times k}\mathbf{B}_{k\times l}=\mathbf{C}_{p\times l}$$

Introduction

$$\bullet \ \mathsf{A}_{p\times k}\mathsf{x}_{k\times 1}=\mathsf{y}_{p\times 1}$$

$$\bullet \ \mathbf{x}_{1\times p}'\mathbf{A}_{p\times k} = \mathbf{y}_{1\times k}'$$

$$\bullet \ \mathbf{X}_{n \times p} \mathbf{D}_{p \times p} = \left[\ \mathbf{x}_1 d_1 \ \middle| \ \mathbf{x}_2 d_2 \ \middle| \ \cdots \ \middle| \ \mathbf{x}_p d_p \ \right]$$

$$\bullet \ \mathbf{D}_{n\times n} \mathbf{X}_{n\times p} = \begin{bmatrix} \frac{d_1 \mathbf{x}_1}{d_2 \mathbf{x}_2} \\ \vdots \\ \hline d_n \mathbf{x}_n \end{bmatrix}$$

 Pre or post-multiplication of X by a diagonal matrix amounts to weighting observations or variables.

Some special matrices

$$\mathbf{I}_{n} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

$$\mathbf{J}_n = \left| egin{array}{cccc} 1 & 1 & \cdots & 1 \ 1 & 1 & \cdots & 1 \ dots & dots & \ddots & dots \ 1 & 1 & \cdots & 1 \end{array}
ight.$$

$$\mathbf{I}_n = \left[egin{array}{cccc} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{array}
ight] \qquad \mathbf{O}_n = \left[egin{array}{cccc} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{array}
ight]$$

$$\mathbf{J}_n = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{bmatrix} \qquad \mathbf{D}_n = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_n \end{bmatrix}$$

Symmetric and Orthogonal Matrices

• Symmetric matrix: $\mathbf{A} = \mathbf{A}'$

$$\left[\begin{array}{ccc} a & b & c \\ b & d & e \\ c & e & f \end{array}\right]$$

Orthogonal (orthonormal) matrix:

$$AA' = A'A = I$$
 $A' = A^{-1}$

Determinant

Introduction

Matrix property

$$|\mathbf{A}_{k imes k}| = \sum_{j=1}^k \mathsf{a}_{ij} |\mathbf{A}_{ij}| (-1)^{i+j}$$

$$\mathbf{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \qquad |\mathbf{A}| = ad - bc$$

k > 2: by computer.

 $|\mathbf{A}| = 0$ implies linear dependence, and \mathbf{A} is singular.

 $|\mathbf{A}| \neq 0$ implies linear independence, and \mathbf{A} is regular.

Example

Example

Introduction

Calculate the determinant of

$$\mathbf{A} = \left[\begin{array}{rrr} 3 & 2 & 6 \\ 4 & 1 & 0 \\ 5 & 4 & 1 \end{array} \right]$$

$$|\mathbf{A}| = 4 \cdot \begin{vmatrix} 2 & 6 \\ 4 & 1 \end{vmatrix} \cdot (-1)^3 + 1 \cdot \begin{vmatrix} 3 & 6 \\ 5 & 1 \end{vmatrix} \cdot (-1)^4 = 88 - 27 = 61$$

in R

> X <- matrix(c(3,2,6,4,1,0,5,4,1),ncol=3,byrow=TRUE)

> det(X)

[1] 61

Inverse

Introduction

$$A_{k \times k}$$
 $AB = BA = I$ $B_{k \times k} = A^{-1}$

Case 2×2

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

If k > 2 then use a computer. Inverse of a diagonal matrix

$$\mathbf{D} = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_n \end{bmatrix}$$

$$\mathbf{D} = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_n \end{bmatrix} \qquad \mathbf{D}^{-1} = \begin{bmatrix} 1/d_1 & 0 & \cdots & 0 \\ 0 & 1/d_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/d_n \end{bmatrix}$$

Rank

- Row rank = maximum number of linearly independent rows.
- Column rank = maximum number of linearly independent columns.
- "The" rank = row rank = column rank.
- A rank k matrix can be represented exactly in a k dimensional space.
- Example:

$$\begin{bmatrix} 1 & 3 & 5 \\ 0 & 2 & 2 \\ 1 & 1 & 3 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 2 & 4 \\ 0 & 1 & 1 \\ 0 & 2 & 3 \end{bmatrix}$$

have rank 2 and 3 respectively.

Trace

$$\mathbf{A}_{k \times k}$$
 $\operatorname{tr}(\mathbf{A}) = \sum_{i=1}^{k} a_{ii}$

- $tr(\alpha \mathbf{A}) = \alpha tr(\mathbf{A})$
- tr(AB) = tr(BA) tr(ABC) = tr(CAB) = tr(BCA)
- $tr(AA') = \sum_{i=1}^{k} \sum_{j=1}^{k} a_{ij}^2$
- Note the latter trace is a sum-of-squares which is a measure of variability.

Quadratic forms

Introduction

$$4x_1^2 + 5x_2^2 + 3x_3^2 + 2x_1x_2 + 4x_1x_3 + x_2x_3 = \mathbf{x}'\mathbf{A}\mathbf{x}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \mathbf{A} = \begin{bmatrix} 4 & 1 & 2 \\ 1 & 5 & \frac{1}{2} \\ 2 & \frac{1}{2} & 3 \end{bmatrix}$$

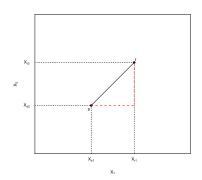
In general

$$\sum_{i=1}^k \sum_{j=1}^k a_{ij} x_i x_j = \mathbf{x}' \mathbf{A} \mathbf{x}$$

- A positive definite x'Ax > 0 for all $x \neq 0$
- A positive semi-definite $\mathbf{x}'\mathbf{A}\mathbf{x} \geq 0$ for all $\mathbf{x} \neq \mathbf{0}$
- A negative definite x'Ax < 0 for all $x \neq 0$
- A negative semi-definite x'Ax < 0 for all $x \neq 0$
- A indefinite

Example

Euclidean Distance

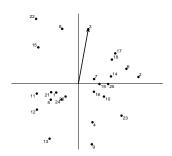


$$d_{rs}^{2} = (x_{r1} - x_{s1})^{2} + (x_{r2} - x_{s2})^{2}$$

= $(\mathbf{x}_{r} - \mathbf{x}_{s})'(\mathbf{x}_{r} - \mathbf{x}_{s})$

Generalizes to p variables.

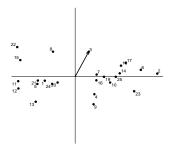
Quadratic forms and distance



- Let x be a single observation written as column vector.
- $\|\mathbf{x}\|^2 = \mathbf{x}'\mathbf{x} = x_1^2 + x_2^2 = \mathbf{x}'\mathbf{A}\mathbf{x}$ with $\mathbf{A} = \mathbf{I}$
- x'Ax is squared Euclidean distance from the origin.
- (x y)'A(x y) is squared Euclidean distance from x to y.

Introduction

Quadratic forms and distance



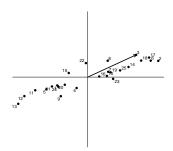
Account for difference in variability:
$$\tilde{\mathbf{x}} = \mathbf{D}^{-1}\mathbf{x}$$
 $\mathbf{D} = \begin{bmatrix} s_1 & 0 \\ 0 & s_2 \end{bmatrix}$

x'Ax is squared Weighted Euclidean distance from the origin.

(x - y)'A(x - y) is squared Weighted Euclidean distance from x to y.

Quadratic forms and distance

Introduction



Account for difference in variability and for correlation: $\tilde{\mathbf{x}} = \mathbf{S}^{-\frac{1}{2}}\mathbf{x}$ Mahalanobis' transformation

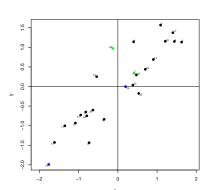
$$\bullet \quad \|\, \tilde{x} \, \|^2 = \tilde{x}' \tilde{x} = x' S^{-1} x = x' A x \text{ with } A = S^{-1} = \left[\begin{array}{cc} s_1^2 & s_{12} \\ s_{21} & s_2^2 \end{array} \right]^{-1}$$

• x'Ax is the squared Mahalanobis distance from the origin.

• (x - y)'A(x - y) is squared Mahalanobis distance from x to y.

Jan Graffelman (SISG 2021)

Mahalanobis distance and Euclidean distance



	D_E	D_{M}
1	1.05	0.84
2	1.98	1.79
3	1.91	1.73
4	0.91	1.25
5	1.43	1.09
6	1.84	1.48
7	0.53	0.42
8	1.21	1.83
9	1.61	1.92
10	0.38	0.80
11	1.69	1.44
12	2.16	1.62
13	2.66	1.99
14	1.14	0.95
15	0.60	1.78
16	0.20	0.46
17	1.96	1.43
18	1.67	1.22
19	0.56	0.56
20	0.88	0.64
21	1.20	0.99
22	0.98	2.49
23	0.56	1.60
24	1.09	0.80
25	0.83	0.83

Introduction

Multivariate statistics: population and sample

Population

(conceptual)

Random vector $\mathbf{X}_{p\times 1}$

Population mean vector

$$\mu_{p\times 1} = E(\mathbf{X})$$

Population covariance matrix

$$\mathbf{\Sigma}_{\mathbf{p} \times \mathbf{p}} = E\left((\mathbf{X} - \mu)(\mathbf{X} - \mu)'\right)$$

Sample

(observed)

Data matrix $\mathbf{X}_{n \times p}$

Sample mean vector

$$\mathbf{m}_{p \times 1} = \frac{1}{p} (\mathbf{1}' \mathbf{X})'$$

Sample covariance matrix

$$\mathbf{S}_{p \times p} = \frac{1}{n-1} \sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{m}) (\mathbf{x}_i - \mathbf{m})'$$

Introduction

Example

Frequently used matrices in MVA

- Data matrix $\mathbf{X}_{n \times n}$
- Sample mean vector $\mathbf{m}_{p\times 1} = (\frac{1}{p}\mathbf{1}'\mathbf{X})'$
- Centered data matrix

$$X_c = X - 1_{n \times 1} m' = X - \frac{1}{n} 11' X = (I - \frac{1}{n} 11') X$$

- Centring matrix $\mathbf{H} = \mathbf{I} \frac{1}{2}\mathbf{1}\mathbf{1}'$ $\mathbf{X}_c = \mathbf{H}\mathbf{X}$
- Standardized data matrix

$$\mathbf{X}_s = \mathbf{X}_c \mathbf{D}_s^{-1}$$
 $\mathbf{D}_s = diag(s_1, s_2, \dots, s_p)$ $\mathbf{X}_s = \mathbf{H} \mathbf{X} \mathbf{D}_s^{-1}$

- Sample covariance matrix $S = \frac{1}{n-1} X'_c X_c$
- Sample correlation matrix $\mathbf{R} = \mathbf{D}_s^{-1} \mathbf{S} \mathbf{D}_s^{-1} = \frac{1}{n-1} \mathbf{X}_s' \mathbf{X}_s$

Sample covariance matrix

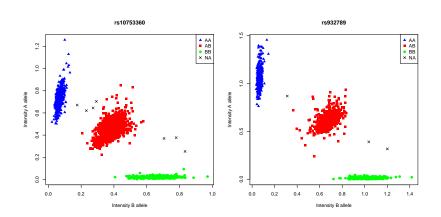
$$\mathbf{S}_{n-1} = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1p} \\ s_{21} & s_{22} & \cdots & s_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ s_{p1} & s_{p2} & \cdots & s_{pp} \end{bmatrix} = \frac{1}{n-1} \mathbf{X}'_{c} \mathbf{X}_{c}$$

$$= \frac{1}{n-1} \sum_{i=1}^{n} (\mathbf{x}_{i} - \mathbf{m}) (\mathbf{x}_{i} - \mathbf{m})'$$

$$\mathbf{S}_{n} = \frac{n-1}{n} \mathbf{S}_{n-1}$$

Sample correlation matrix

$$\mathbf{R} = \begin{bmatrix} 1 & r_{12} & \cdots & r_{1p} \\ r_{21} & 1 & \cdots & r_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ r_{p1} & r_{p2} & \cdots & 1 \end{bmatrix} = \frac{1}{n-1} \mathbf{X}_s' \mathbf{X}_s = \mathbf{D}_s^{-1} \mathbf{S} \mathbf{D}_s^{-1}$$



Data taken from the GENEVA project at UW Biostatistics.

Raw data matrix:

Introduction

	SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB	SNP1	SNP2
1	0.080	0.812	0.070	1.019	0	0
2	0.746	0.022	0.996	0.010	2	2
3	0.402	0.440	0.725	0.569	1	1
4	0.071	0.782	0.057	0.950	0	0
5	0.618	0.028	1.072	0.016	2	2
6	0.362	0.473	0.739	0.564	1	1
7	0.372	0.469	0.752	0.645	1	1
8	0.433	0.455	0.728	0.615	1	1
9	0.364	0.521	0.653	0.646	1	1
10	0.624	0.017	1.056	0.018	2	2
	:	:	:	:	:	

Mean vector:

	SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB
m	0.372	0.426	0 597	0 584

Standard deviations:

	SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB
-	0.220	0.263	0.352	0.377

Centered data matrix:

	SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB
1	-0.292	0.386	-0.527	0.435
2	0.374	-0.404	0.399	-0.574
3	0.030	0.014	0.128	-0.015
4	-0.301	0.356	-0.540	0.366
5	0.246	-0.398	0.475	-0.568
6	-0.010	0.047	0.142	-0.020
7	-0.000	0.043	0.155	0.061
8	0.061	0.029	0.131	0.031
9	-0.008	0.095	0.056	0.062
10	0.252	-0.409	0.459	-0.566
:	:	:	:	:

Mean vector:

	SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB
m	0.000	0.000	0.000	0.000

Standard deviations:

	SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB
s	0.220	0.263	0.352	0.377

Standardized data matrix:

	SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB
1	-1.328	1.467	-1.494	1.154
2	1.700	-1.532	1.134	-1.524
3	0.136	0.055	0.365	-0.040
4	-1.369	1.353	-1.531	0.971
5	1.118	-1.509	1.349	-1.508
6	-0.046	0.180	0.404	-0.054
7	-0.001	0.165	0.441	0.161
8	0.277	0.112	0.373	0.082
9	-0.037	0.362	0.160	0.164
10	1.145	-1.551	1.304	-1.503
	:			:

Mean vector:

	SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB
m	0.000	0.000	0.000	0.000

Standard deviations:

SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB
 1 000	1 000	1 000	1 000

Covariance matrix:

	SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB
SNP1_IA	0.048	-0.052	0.075	-0.078
SNP1_IB	-0.052	0.069	-0.082	0.095
SNP2_IA	0.075	-0.082	0.124	-0.122
SNP2_IB	-0.078	0.095	-0.122	0.142

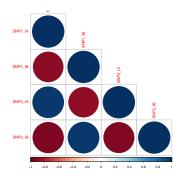
Correlation matrix:

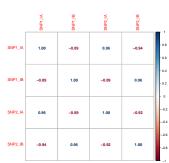
	SNP1_IA	SNP1_IB	SNP2_IA	SNP2_IB
SNP1_IA	1.000	-0.895	0.962	-0.937
SNP1_IB	-0.895	1.000	-0.886	0.962
SNP2_IA	0.962	-0.886	1.000	-0.920
SNP2_IB	-0.937	0.962	-0.920	1.000

Cross table of called genotypes:

	0	1	2	NA
0	512	0	0	0
1	1	949	0	0
2	0	0	470	0
NA	0	4	0	3

Displaying correlations





Bibliography

- Johnson & Wichern, (2002) Applied Multivariate Statistical Analysis, 5th edition, Prentice Hall, Chapters 2 & 3.
- Mardia, K.V. et al. (1979) Multivariate Analysis. Appendix A. Academic press.