Module 19 Multivariate Analysis for Genetic data
Session 10 Multivariate Normal Distribution

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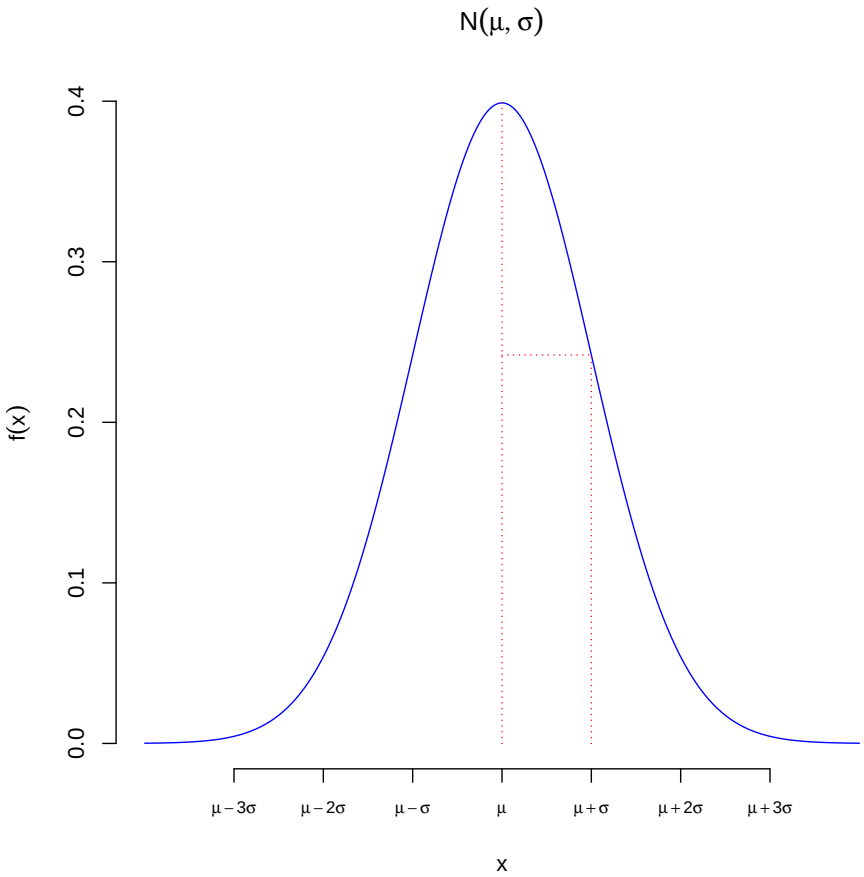
Multivariate Normal Distribution



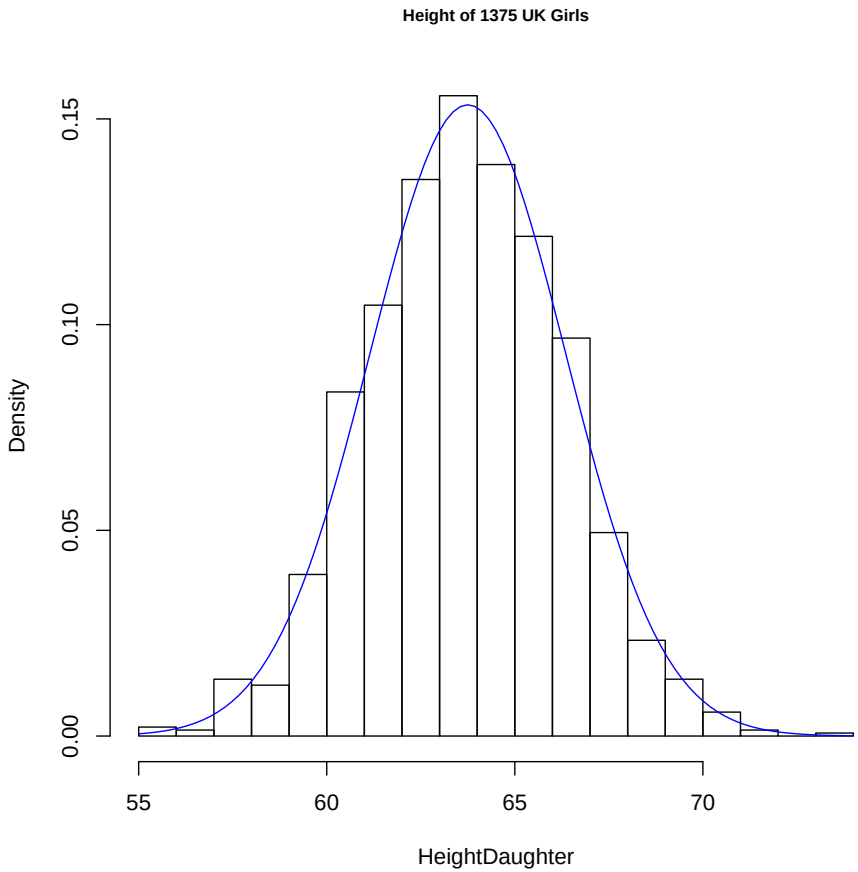
$$X \sim N(\mu, \sigma)$$

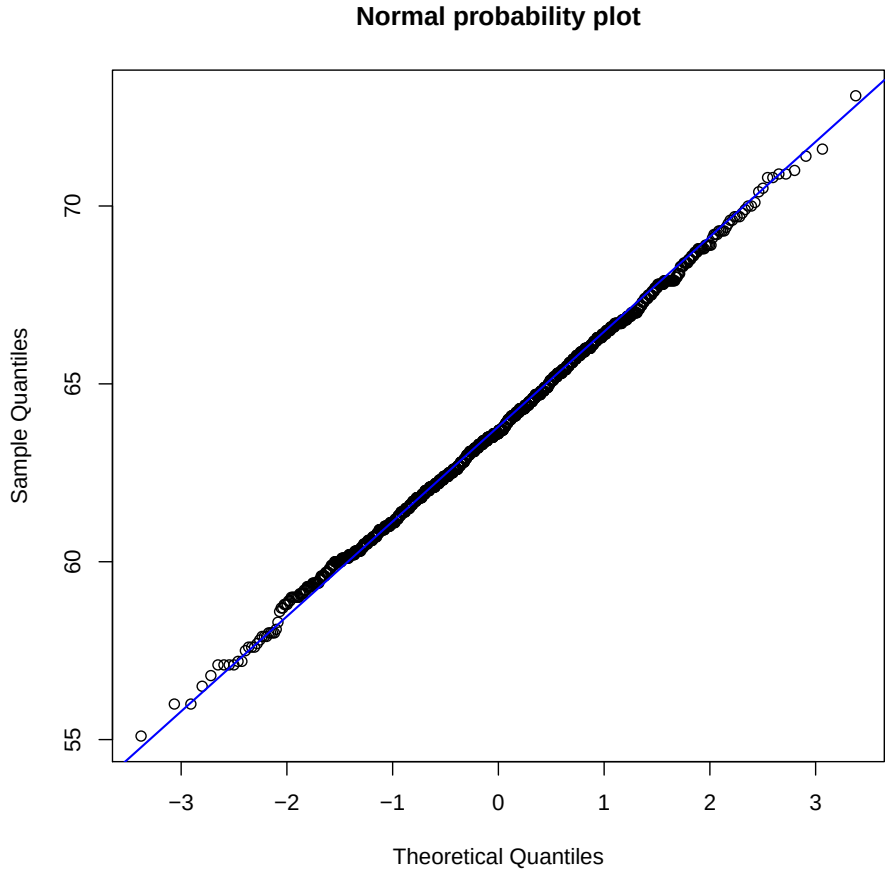
$$f(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

$$E(X) = \mu$$

$$V(X) = \sigma^2$$

Some normal data (Height UK girls in 1903)

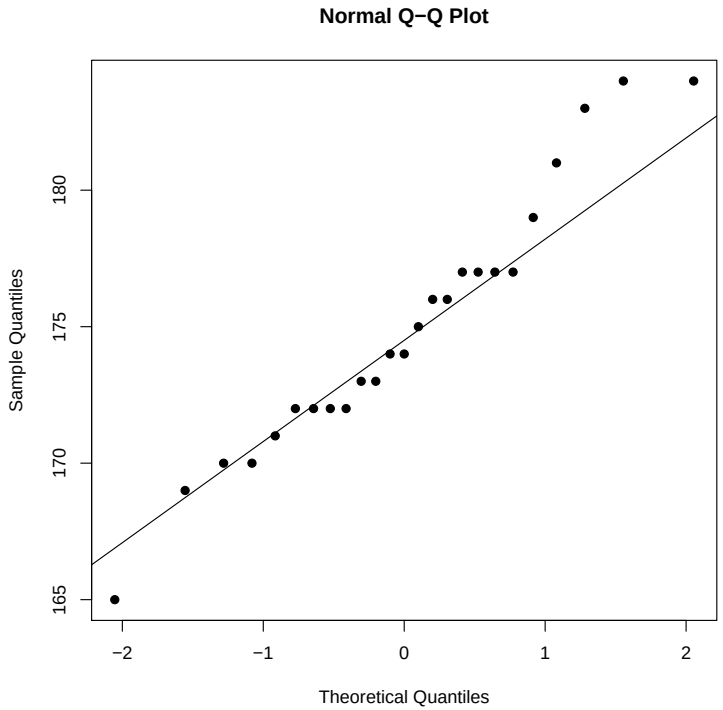




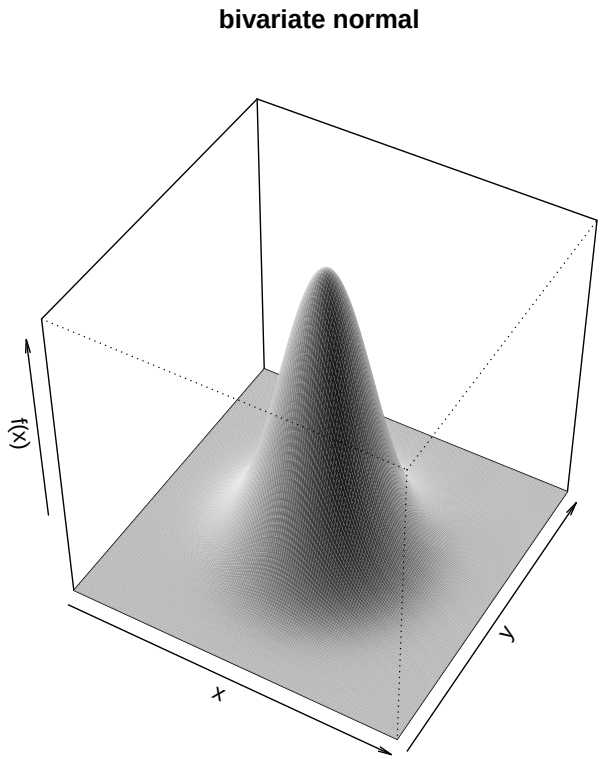
	N	N*	Mean	Stdev	Med	Q1	Q3	Min	Max
Height	1375	0	63.751	2.6	63.6	62	65.6	55.1	73.1

Normal probability plot

i	1	2	3	4	5	6	7	8	9	...	25
Height	172	174	183	175	176	184	177	169	172	...	172
Sorted	165	169	170	170	171	172	172	172	172	...	184
Rank i	1	2	3	4	5	6	7	8	9	...	25
$\frac{i-0.5}{n}$	0.02	0.06	0.10	0.14	0.18	0.22	0.26	0.30	0.34	...	0.98
$z_{(i-0.5)/n}$	-2.05	-1.55	-1.28	-1.08	-0.92	-0.77	-0.64	-0.52	-0.41	...	2.05



Some bivariate normal distributions



Density multivariate normal

$$f(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Exponent univariate normal

$$-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2 = -\frac{1}{2}(x-\mu)(\sigma^2)^{-1}(x-\mu)$$

Exponent multivariate normal

$$-\frac{1}{2}(\mathbf{x}-\mu)'\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu)$$

Multivariate normal distribution

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{\frac{1}{2}}} e^{-\frac{1}{2}(\mathbf{x}-\mu)'\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu)}$$

Parameters:

- Population mean vector:

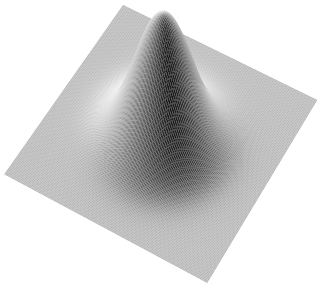
$$\mu = (\mu_1, \mu_2, \ldots, \mu_p)$$

- Population variance-covariance matrix:

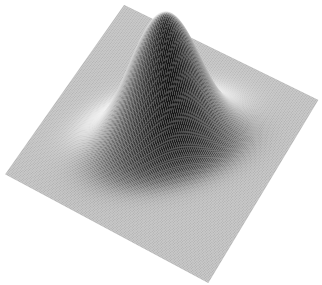
$$Cov(\mathbf{X}) = \mathbf{\Sigma}_{p\times p} = E\left((\mathbf{X}-\mu)(\mathbf{X}-\mu)'\right) = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{p1} & \sigma_{p2} & \cdots & \sigma_{pp} \end{bmatrix}$$

Bivariate normal distribution

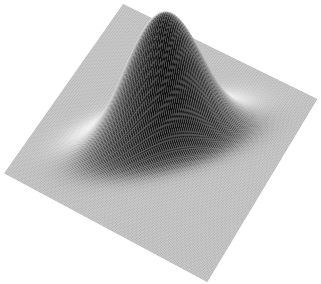
$\rho = 0$



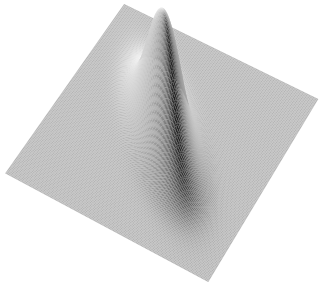
$\rho = 0.5$



$\rho = 0.75$



$\rho = -0.75$



Parameter estimation

Maximum likelihood estimator for μ:

$$\hat{\mu} = \bar{\mathbf{x}} = (\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_p)$$

Maximum likelihood estimator for $\mathbf{\Sigma}$:

$$\hat{\mathbf{\Sigma}} = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})' = \mathbf{S}_n$$

In practice, $\mathbf{S}_{n-1}$ is often used to estimate $\mathbf{\Sigma}$:

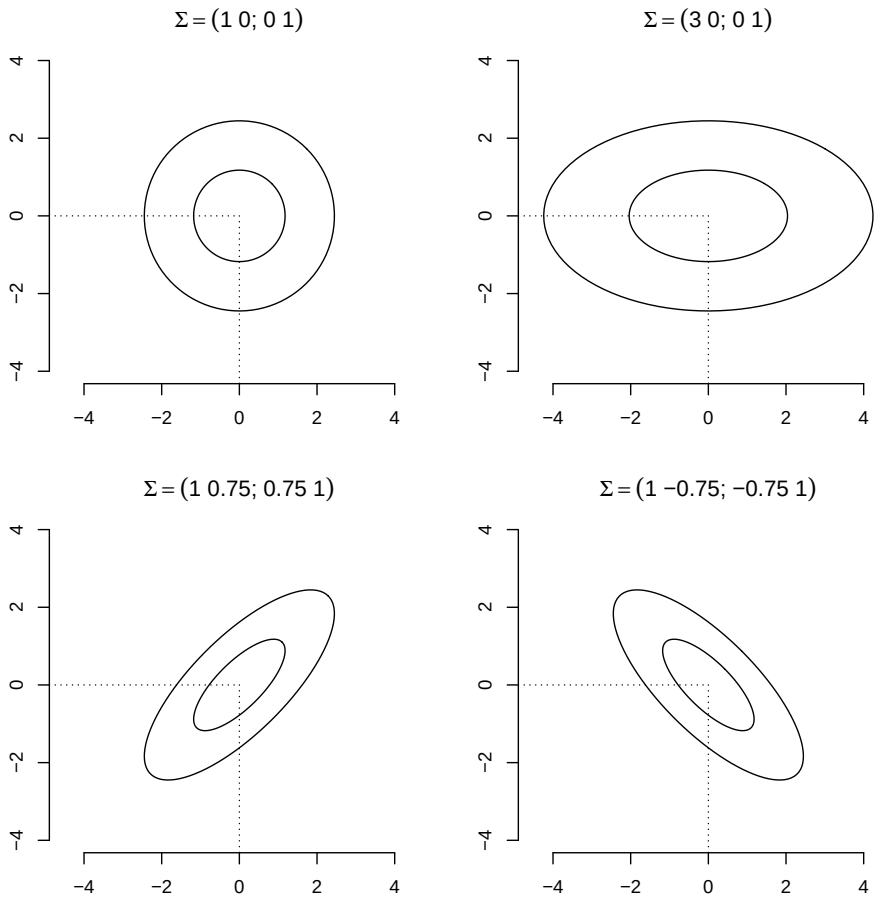
$$\mathbf{S}_{n-1} = \frac{n}{n-1}\mathbf{S}_n$$

Some Properties of MVN random variates

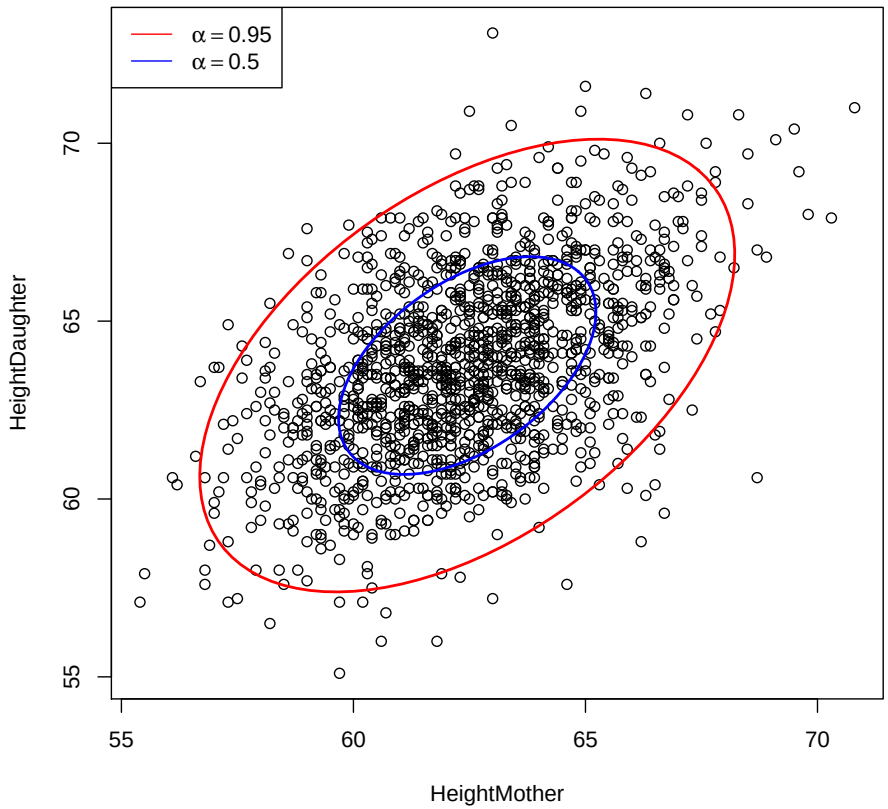
Let $\mathbf{X}$ be a $p \times 1$ random vector, and $\mathbf{X} \sim N_p(\mu, \mathbf{\Sigma})$.

- Linear combinations of the components of $\mathbf{X}$ are normally distributed.
- Basic result: if $\mathbf{X} \sim N_p(\mu, \mathbf{\Sigma})$ and $\mathbf{A}q \times p$, then $\mathbf{AX} \sim N_q(\mathbf{A}\mu, \mathbf{A\Sigma A}')$
- Subsets of components have a (multivariate) normal distribution.
- Components with covariance zero $\Leftrightarrow$ components are independent.
- Conditional distributions of components are (multivariate) normal.

Contours of normal densities (0.50 and 0.95)



Contours for empirical data



Assessing multivariate normality

Some basic ideas:

- Individual variables (marginal distributions) should have bell-shaped (normal) histograms
- Bivariate scatterplots should have clouds of points with an elliptic shape
- Some outliers can be expected, in particular in larger samples

χ^2 plot for multivariate normality

$$(\mathbf{x} - \mu)' \mathbf{\Sigma}^{-1} (\mathbf{x} - \mu) \sim \chi^2_p$$

The ellipsoid traced by $\mathbf{x}$ described by

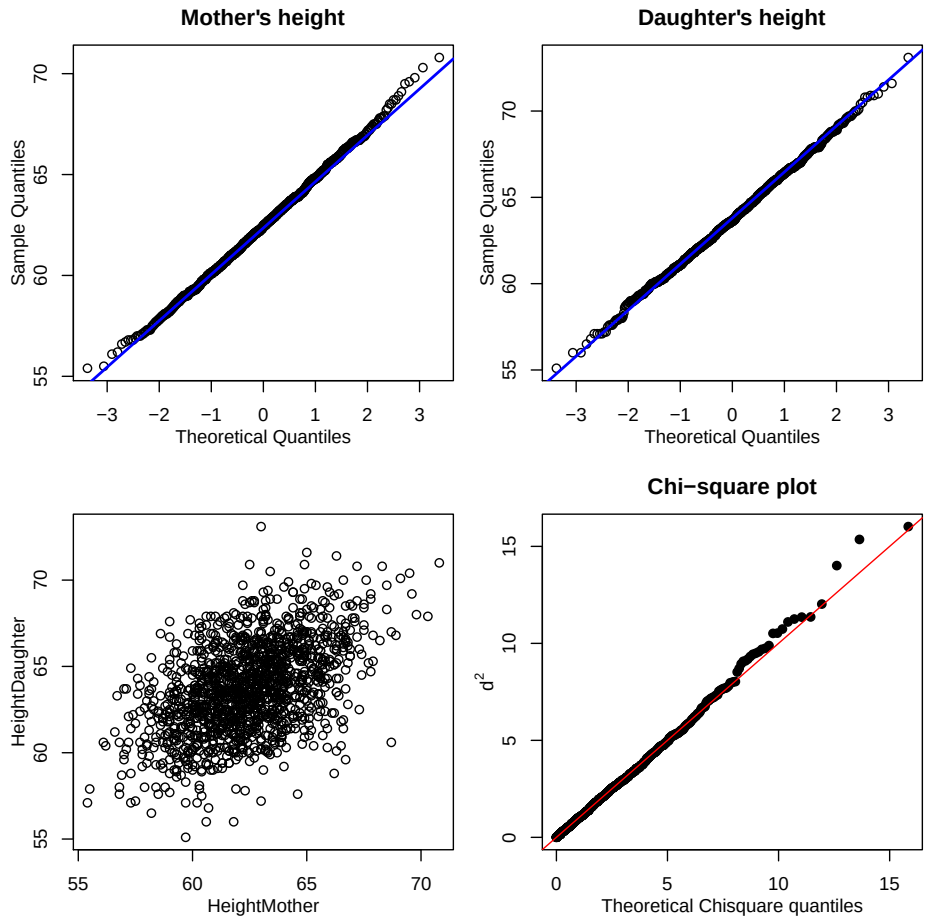
$$(\mathbf{x} - \mu)' \mathbf{\Sigma}^{-1} (\mathbf{x} - \mu) \leq \chi^2_p (1 - \alpha)$$

should contain $100 \cdot (1 - \alpha)\%$ of the observations.

For sample data:

1. Calculate $d_i^2 = (\mathbf{x}_i - \bar{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x}_i - \bar{\mathbf{x}})$
2. Order the distances from small to large
3. Calculate the rank $(i - \frac{1}{2})/n$
4. Calculate corresponding quantiles q_i according to a χ^2_p distribution.
5. Plot (d_i^2, q_i)
6. Compare with a reference line with intercept 0 and slope 1

Example χ^2 plot for multivariate normality



Normality of the NIST STR data

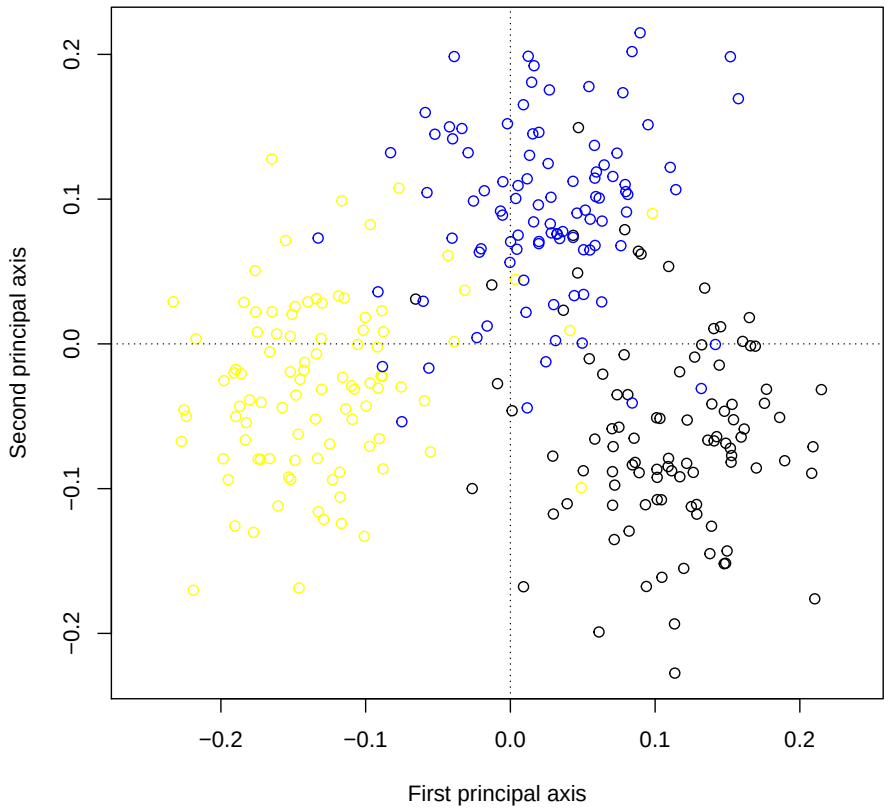
The data:

- 29 autosomal STRs
- Consider individuals with African-American, Asian and Caucasian ancestry
- Sample sizes balanced by subsampling
- STRs coded as binary variables
- Quantification of the data by MDS based on Jaccard metric

The multivariate normality of the MDS principal axis was seen to be important for:

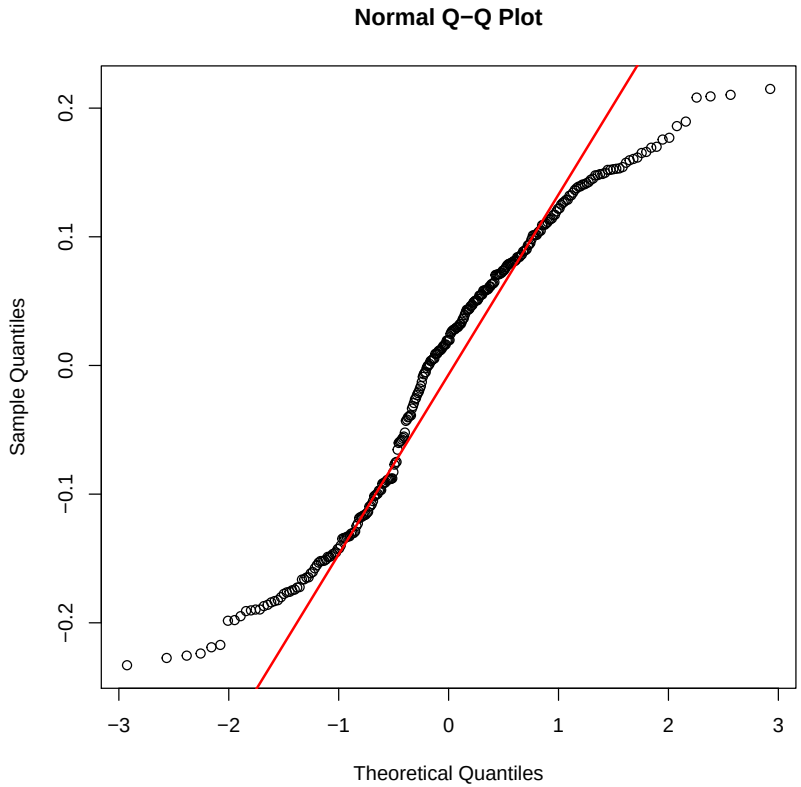
- Model-based clustering
- Linear and quadratic discriminant analysis
- ....

Normality of the NIST STR data

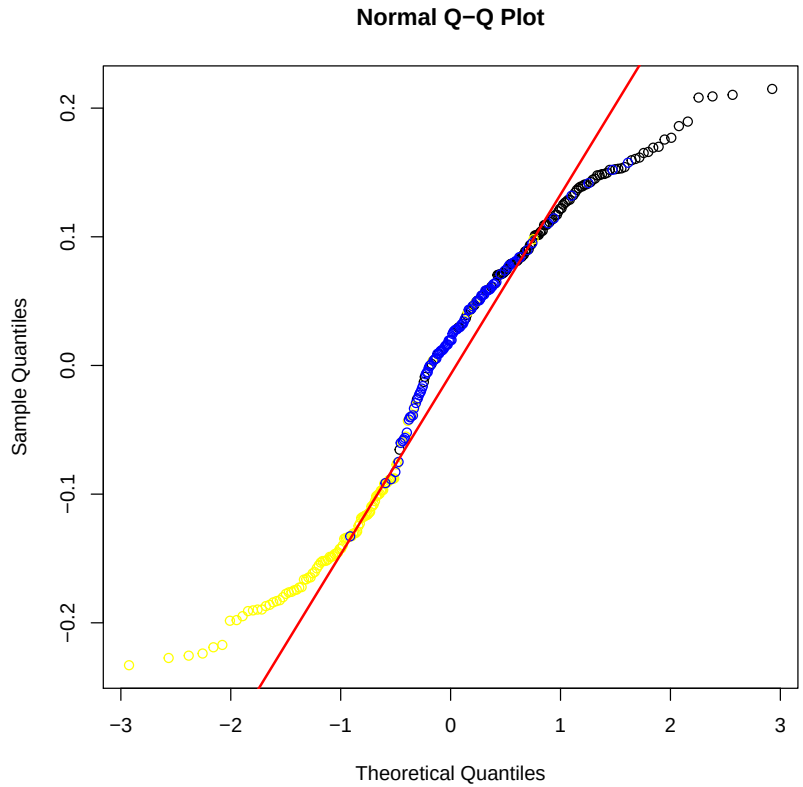


Multivariate normal?

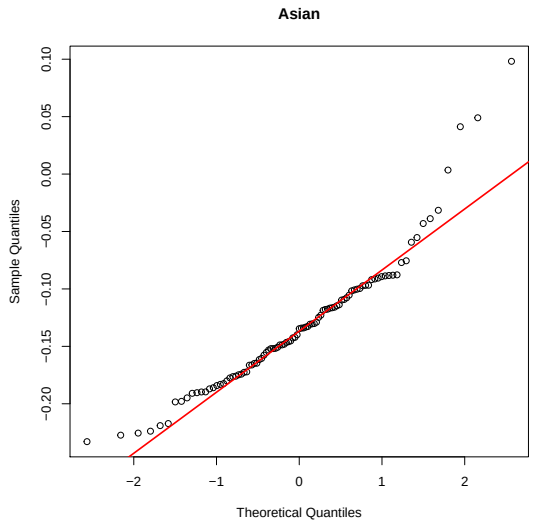
Normality of the NIST STR data

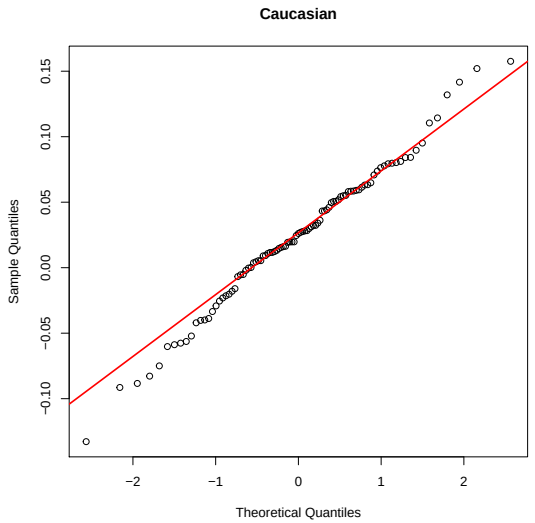


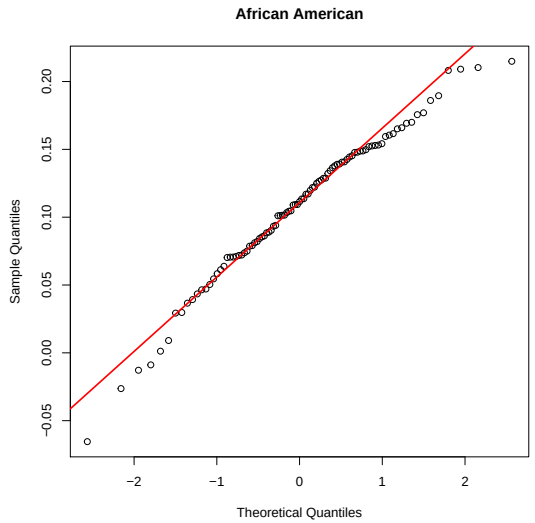
Normality of the NIST STR data



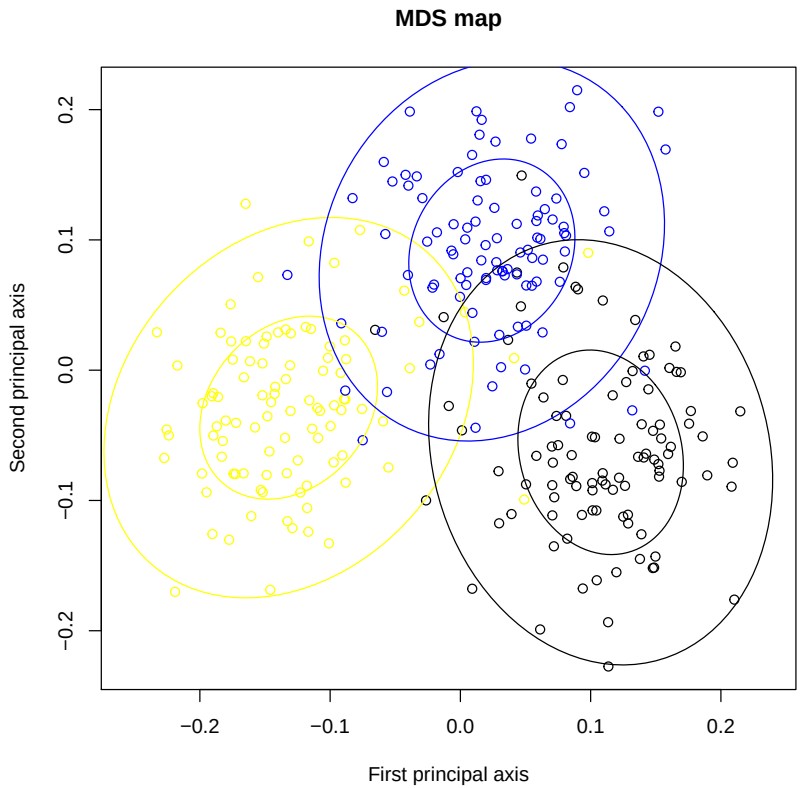
Stratifying





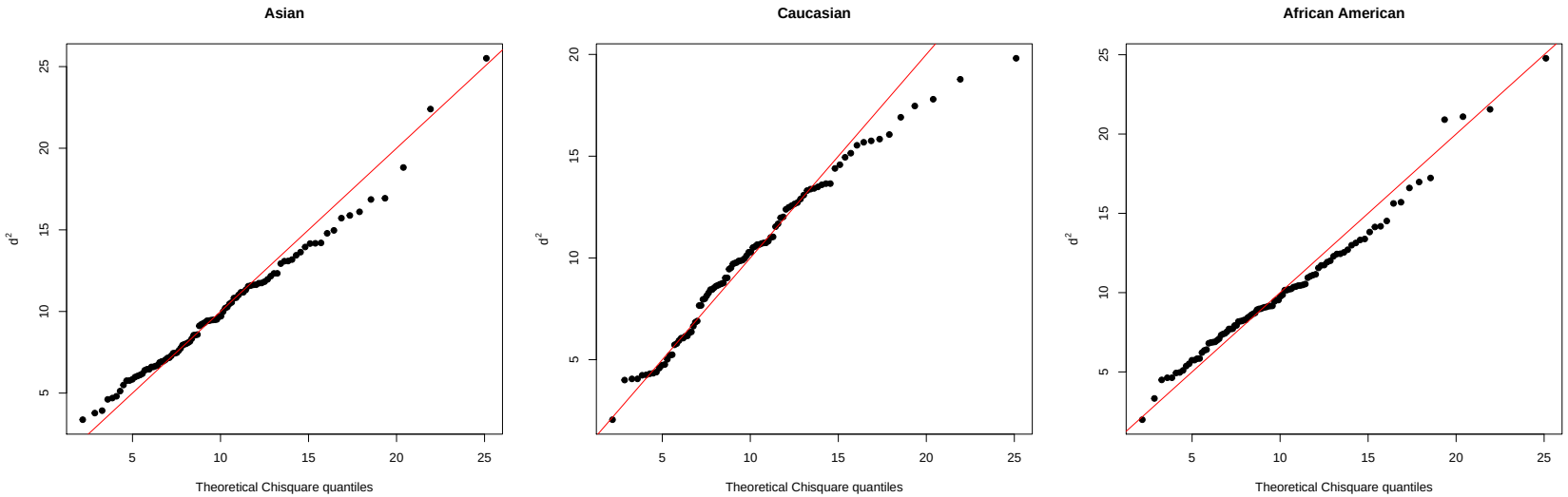


Bivariate exploration



with 0.95 and 0.50 ellipses

Multivariate exploration (χ^2 plots for $p = 10$)



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- Johnson & Wichern, (2002) Applied Multivariate Statistical Analysis, Chapters 4 and 5, 5th edition, Prentice Hall.