Visualization 1

Applied Multivariate Statistics – Spring 2012
Goals

- Covariance, Correlation (true / sample version)
- Test for zero correlation: Fisher’s z-Transformation
- Scatterplot / Scatterplotmatrix
- Covariance matrix / Correlation matrix
- Multivariate Normal Distribution
- Mahalanobis distance
Visualization in 1d

Histogram of $x$

Boxplot of $x$
Normal distribution in 1d:
Most common model choice

\[
\varphi_{\mu, \sigma^2}(x) = \frac{1}{\sqrt{2\pi \sigma^2}} \exp\left(-\frac{1}{2} \cdot \frac{(x - \mu)^2}{\sigma^2}\right)
\]
Squared Mahalanobis Distance

Sq. Distance from mean in standard deviations

Normal distribution in 1d:
Most common model choice

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\]

\[
\mu = 0, \quad \sigma^2 = 0.2, \quad \mu = 0, \quad \sigma^2 = 1.0, \quad \mu = 0, \quad \sigma^2 = 5.0, \quad \mu = -2, \quad \sigma^2 = 0.5,
\]

\[
\chi = -5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5
\]

\[
\varphi_{\mu, \sigma^2}(x)
\]

\[
\chi
\]
Two variables: Covariance and Correlation

- **Covariance:** \( Cov(X, Y) = E[(X - E[X])(Y - E[Y])] \in [-\infty; \infty] \)

- **Correlation:** \( Corr(X, Y) = \frac{Cov(X,Y)}{\sigma_X \sigma_Y} \in [-1; 1] \)

- **Sample covariance:** \( \hat{Cov}(x, y) = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) \)

- **Sample correlation:** \( r_{xy} = \hat{Corr}(x, y) = \frac{\hat{Cov}(x,y)}{\hat{\sigma_x} \hat{\sigma_y}} \)

- Correlation is invariant to changes in units, covariance is not (e.g. kilo/gram, meter/kilometer, etc.)
Scatterplot: Correlation is scale invariant

Cor = 0.99 - Cov = 1.36

Cor = 0.99 - Cov = 81348.37
Intuition and pitfalls for correlation
Correlation = LINEAR relation
Test for zero correlation: Fisher’s z-Test

- X, Y (bivariate) normal distributed with true correlation $\rho$
- Take n samples
- Compute sample correlation $r$

Compute

$z = \frac{1}{2} \log \left( \frac{1 + r}{1 - r} \right)$

Compute

$\xi = \frac{1}{2} \log \left( \frac{1 + \rho}{1 - \rho} \right)$

- For large n: $\sqrt{n-1}(z - \xi) \sim N(0, 1)$
- Use cor.test() in R to test and get confidence intervals
Many dimensions: Scatterplot matrix

SO2

temp

manu

popul

wind

precip

predays
Covariance matrix / correlation matrix:
Table of pairwise values

- True covariance matrix: $\Sigma_{ij} = Cov(X_i, X_j)$
- True correlation matrix: $C_{ij} = Cor(X_i, X_j)$

- Sample covariance matrix: $S_{ij} = \hat{Cov}(x_i, x_j)$
  Diagonal: Variances
- Sample correlation matrix: $R_{ij} = \hat{Cor}(x_i, x_j)$
  Diagonal: 1
Multivariate Normal Distribution: Most common model choice

\[ f(x; \mu, \Sigma) = \frac{1}{\sqrt{2\pi|\Sigma|}} \exp \left( - \frac{1}{2} \cdot (x - \mu)^T \Sigma^{-1} (x - \mu) \right) \]
Multivariate Normal Distribution: Funny facts

If $X_1, \ldots, X_p$ multivariate normal, then

- every linear combination $Y = a_1 X_1 + \ldots + a_p X_p$ is normally distributed
- every projection on a subspace is multivariate normally distributed

If margins are normally distributed, then it is NOT GUARANTEED that the underlying distribution is multivariate normal

(i.e., “multivariate” is stronger than just normal margins)
Multivariate Normal Distribution: Two examples
1000 random samples

\[
\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]

\[
\mu = \begin{pmatrix} 5 \\ 10 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} 10 & 3 \\ 3 & 2 \end{pmatrix}
\]
Multivariate Normal Distribution: Most common model choice

\[ f(x; \mu, \Sigma) = \frac{1}{\sqrt{2\pi|\Sigma|}} \exp \left( -\frac{1}{2} \cdot (x - \mu)^T \Sigma^{-1} (x - \mu) \right) \]

Sq. Mahalanobis Distance \( \text{MD}^2(x) \)

= Sq. distance from mean in standard deviations IN DIRECTION OF \( X \)
Mahalanobis distance: Example

\[ \mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \]

\[ \Sigma = \begin{pmatrix} 25 & 0 \\ 0 & 1 \end{pmatrix} \]
Mahalanobis distance: Example

\[ \mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \]
\[ \Sigma = \begin{pmatrix} 25 & 0 \\ 0 & 1 \end{pmatrix} \]

\[ \text{MD} = 4 \]

(20,0)
Mahalanobis distance: Example

\[ \mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \]

\[ \Sigma = \begin{pmatrix} 25 & 0 \\ 0 & 1 \end{pmatrix} \]

\( MD = 10 \)
Mahalanobis distance: Example

\[ \mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \]

\[ \Sigma = \begin{pmatrix} 25 & 0 \\ 0 & 1 \end{pmatrix} \]

(10, 7)

MD = 7.3
Concepts to know

- Covariance, Correlation (true / sample version)
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R commands to know

- read.csv, head, str, dim
- colMeans, cov, cor
- mvrnorm, t, solve, %*%