

UPPSALA UNIVERSITET

FÖRELÄSNINGSKOMMENTARER

Multivariate Methods

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1. INTRODUCTION

Analysis dealing with simultaneous measurements on many variables.

We may want to do some statistical analysis on not only salary, but factor in things such as gender, whether or not one has been to uni etc.

One should always strive to use as much information as possible, you want to remove any chance to miss a pattern.

In general, if you arrive to a conclusion, think of why/what caused this and factor everything in your data and analysis.

1.1. MANOVA.

MANOVA is a method to measure if a data-set shares a similar mean. For example, with different flower types we may want to check if "does sweden has a similar income as norwegian citizens", comparing the sample from sweden to norwegian. We will get different numbers but that is something that we take into analysis.

1.2. Regressionanalysis.

Allows us to predict a variable y from an observation x . $x = \text{bmi}$, while y is your blood pressure.

2. SAMPLE & RANDOM MATRICES

2.1. Slide 3 - Expectation.

For a discrete random variable we use summation, for a continuous random variable we use integrals. What do we use for vectors/matrices?

⇒ We perform the operations elementwise in the matrix. Take $\mathbb{E}(X_{ij})$

2.2. Slide 4 - Covariance Matrix.

Recall

$$\text{Cov}(X, Y) = \mathbb{E}(X - \mathbb{E}(X))(Y - \mathbb{E}(Y)) = \mathbb{E}(XY) - \mathbb{E}(X)\mathbb{E}(Y) \quad (1)$$

for scalars.

What about $\text{Cov} \left(\begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}, \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \right)$?

We can pick any pair (X_i, Y_j) and compute $\text{Cov}(X_i, Y_j)$ leading to the same as (1) but with X_i, Y_j instead.

In the case $\begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}, \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}$, we get a 3×2 matrix where the i, j th elements corresponds to $\text{Cov}(X_i, Y_j)$.

Think of it like

$$XY^T = \begin{pmatrix} X_1Y_1 & X_1Y_2 \\ X_2Y_1 & X_2Y_2 \\ X_3Y_1 & X_3Y_2 \end{pmatrix} \quad (2)$$

Now look at $\mathbb{E}(XY^T)$, same as (2) but $\mathbb{E}(X_iY_j)$.

Then we can easily see that $\text{Cov}(X, Y) = \mathbb{E}(XY^T) - \mu_X \mu_Y^T$

What if X is continuous and Y discrete?

What if $Y = X$?

$$\text{Cov}(X_i, X_i) = \mathbb{E}(X_i^2) - (\mathbb{E}(X_i))^2 = \text{Var}(X_i)$$

2.3. Slide 5 - Covariance Matrix.

Since in the scalar case $\text{Cov}(X_i, X_j) = \text{Cov}(X_j, X_i)$, then $\text{Cov}(X, Y) = \sum = \text{symmetric \& positive definite}$.

Definition/Sats 2.1: Positive & Semi-definite

Definite matrix A :

$$A > 0 \Leftrightarrow x^T A x > 0$$

Semi-definite matrix A :

$$A \geq 0 \Leftrightarrow x^T A x \geq 0$$

2.4. Slide 6 - Linear Combination.

You can view the vector c as regression values for example

2.5. Slide 7 - Linear Combination.

Example:

$$\text{Var}(X_1 + 2X_2 + 4X_3) \sim \text{Var} \left(\begin{pmatrix} 1 & 2 & 4 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \right)$$

A tip for remembering where to put c^T , think of it like matching dimensions of left hand side and right hand side.

We only want to compute expectation for the random stuff, so we can chuck coefficients and constants out.

2.6. Slide 9 - Independence.

For simplicity, we define independence in the continuous case as $f(X, Y) = f(X)f(Y)$ and in the discrete case as $P(X, Y) = P(X)P(Y)$

Anmärkning: Jist because $\text{Cov}(X, Y) = 0$ does not imply independence. Take the unit circle and the contour as pairs over (X, Y) . It is clear that (X, Y) are dependant but their covariance is 0 since for every point on the circle you can reflect the X, Y and therefore, by $\text{Cov}(X, Y) = \mathbb{E}(XY) - \mathbb{E}(X)\mathbb{E}(Y)$, you would be adding a bunch of 0. Same goes for any function that can be reflected.

2.7. Slide 10 - Random Sample.

Example (Scalar case):

Let $\mathbf{x} \sim x_1 x_2 x_3 \dots$ be a random sample from $N(\mu, \sigma^2)$

We look at what it means for scalar random variables to be independent:

$$\begin{aligned} F(X, Y) &= F(X)F(Y) \\ f(x, y) &= f(x)f(y) \\ p(x, y) &= p(x)p(y) \end{aligned}$$

The same principle goes for random vectors, eg:

$$X_{n \times p} = \begin{pmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_n^T \end{pmatrix}$$

Think of each row as a sample from a different place \Rightarrow independence in row \Rightarrow random sample.

Non-example: Looking at the pulse of 1 person is not an independent response since it is only about 1 person. Even if you sampled a bunch of values from the same person into a matrix, that would still be a non-independent sample since we only sample from 1 person.

Non-example: Let us assume there is a competition between Uppsala and Lund in Multivariate Analysis. Everyone in the class at Uppsala has had the same teacher, so the values collected from that class are not independent.

2.8. Slide 12 - Some Notes on Sample Covariance Matrix.

Unbiased becomes biased during non-linear & non-affine transformations.

Even for large n , sometimes you cannot ignore the difference between S_n and S (eg. determining exact distributions)

2.9. Slide 17 - Sample Covariance Matrix.

$$X - \frac{1}{n}\mathbf{1}\mathbf{1}^T X = (I - \frac{1}{n}\mathbf{1}\mathbf{1}^T)X$$

So for $(X - \frac{1}{n}\mathbf{1}\mathbf{1}^T X)^T (X - \frac{1}{n}\mathbf{1}\mathbf{1}^T X)$:

$$X^T (I - \frac{1}{n}\mathbf{1}\mathbf{1}^T)^T (I - \frac{1}{n}\mathbf{1}\mathbf{1}^T) X = X^T \left[I - \frac{1}{n}\mathbf{1}\mathbf{1}^T - \frac{1}{n}\mathbf{1}\mathbf{1}^T - \frac{1}{n}\mathbf{1}\mathbf{1}^T + \frac{1}{n}\mathbf{1}\underbrace{\mathbf{1}^T\mathbf{1}}_{=n}\mathbf{1}^T \right] X$$

$$X^T (I - \frac{1}{n}\mathbf{1}\mathbf{1}^T - \frac{1}{n}\mathbf{1}\mathbf{1}^T + \frac{1}{n}\mathbf{1}\mathbf{1}^T) X = X^T (I - \frac{1}{n}\mathbf{1}\mathbf{1}^T) X$$

$$X^T X - X^T \mathbf{1}\mathbf{1}^T X \Rightarrow S_n = \frac{1}{n} \underbrace{X^T X}_{\text{Data matrix}} - (\frac{1}{n} X^T \mathbf{1}) (\frac{1}{n} \mathbf{1}^T X)$$

$$\text{Cov}(X) = \mathbb{E}(X X^T)^n - \mathbb{E}(X) \mathbb{E}(X)^T$$

Anmärkning:

$\mathbf{1}$ is an $n \times 1$ vector of ones.

3. MULTIVARIATE NORMAL DISTRIBUTION

3.1. Slide 4-5 - From Univariate to Multivariate Normal.

Recall that in the univariate case we had:

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

In the multivariate case, we swap x and μ for vectors instead.

Since variance matrix is expressed by $(x - \mu)^T \Sigma^{-1} (x - \mu)$, instead of σ^2 we have have

$$\frac{1}{\sigma \sqrt{2\pi}} \sim \rightarrow \frac{1}{(2\pi)^{p/2} \sqrt{\det(\Sigma)}}$$

Anmärkning:

Covariance matrix must be positive definite! Not semi.

There is no requirement for slide 4 with Σ

The $(2\pi)^{p/2}$ comes from multiplying $z_1 z_2 \cdots z_p$ p -times.

3.2. Slide 6 - Special Case: Bivariate Normal.

Anmärkning:

ρ denotes the correlation coefficient

σ_{11} & σ_{22} correspond to our variance

σ_{12} & σ_{21} correspond to our covariance

$$\text{Corr}(x_1, x_2) = \frac{\sigma_{12}}{\sqrt{\sigma_{11}\sigma_{22}}}$$

3.3. Slide 7 - Contour of Bivariate Normal Density.

We change the correlation to see what happens.

3.4. Slide 8 - Linear Combinations.

For the univariate case, we had that if we scaled $X \sim N(\mu, \sigma^2)$ with an affine transformation, we got $aX + b \sim N(a\mu, a^2\sigma^2)$.

One thing that is good to keep in the back of the head is that the linear combination/affine transformation of normally distributed random variables will remain normal.

Let us look at what happens when we look at the multivariate case:

$$\begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \quad Y_1 \sim N \quad Y_2 \sim N$$

$$\Rightarrow \begin{pmatrix} x_1 + x_2 \\ x_1 - x_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix} \sim N_2 \left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, A \Sigma A^T \right)$$

From result 4.2, we can get the result of multi-linear combinations

3.5. Slide 10 - Normal and Chi-Square.

If X has a linear combination will it still be p -degrees of freedom? Answer is surprisingly yes!

$$\Sigma^{-1} = \Sigma^{-1/2} \Sigma^{-1/2} \quad X \sim N_p(\mu, \Sigma)$$

$$\Rightarrow Z = \Sigma^{-1/2}(x - \mu) = \underbrace{\Sigma^{-1/2}x}_A \underbrace{- \Sigma^{-1/2}\mu}_d \sim N_p(0, \Sigma^{-1/2} \Sigma \Sigma^{-1/2})$$

$$(x - \mu)^T \Sigma^{-1} (x - \mu) = Z^t Z = \sum_{j=1}^p Z_j^2$$

3.6. Slide 11 - Subset of Variables.

Using result 4.4, we can choose subsets however we want, it will stay normal.

3.7. Slide 12 - Example: Subset of Variables.

From the slide we have the following:

Suppose that:

$$\begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \sim N_2 \left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \right)$$

Find the distribution of $\begin{bmatrix} X_1 \\ X_3 \end{bmatrix}$ as well as the distribution of

$$\begin{bmatrix} X_1 & X_3 \end{bmatrix} \begin{bmatrix} \sigma_{11} & \sigma_{13} \\ \sigma_{31} & \sigma_{33} \end{bmatrix}^{-1} \begin{bmatrix} X_1 \\ X_3 \end{bmatrix}$$

In the first one, what we really essentially are looking for is the following:

$$\begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \sim N_3 \left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \right)$$

If we want $\begin{bmatrix} X_1 \\ X_3 \end{bmatrix}$, then:

$$\begin{bmatrix} X_1 \\ X_3 \end{bmatrix} \sim N_2 \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma_{11} & \sigma_{13} \\ \sigma_{31} & \sigma_{33} \end{bmatrix} \right)$$

So:

$$\begin{bmatrix} X_1 & X_3 \end{bmatrix} \begin{bmatrix} \sigma_{11} & \sigma_{13} \\ \sigma_{31} & \sigma_{33} \end{bmatrix}^{-1} \begin{bmatrix} X_1 \\ X_3 \end{bmatrix} \sim \chi^2_2$$

It is really important to remember that linear combinations of normal variables, are still normal variables. Since linear combinations can be regarded as linear/affine transformations, the "crossing out the X_2 " part of the computation is really just matrix-multiplication, since:

$$\begin{bmatrix} X_1 \\ X_3 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_A \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix}$$

3.8. Slide 13 - Subset of Variables.

Anmärkning:

Since what we really care about is what happens during the transpose, sometimes we write Σ_{12} for $\Sigma_{12} = \Sigma_{21} = 0$

3.9. Slide 15 - Marginal Normal and Joint Distribution.

Usually, if they are independent, they are normal.

3.10. Slide 23 - Likelihood of Normal Random Sample.

$$a^T B a = \text{tr}(a^T B a) = \text{tr}(B a a^T)$$

Of course, in order to maximize the likelihood we sometimes need to find the derivative of the matrix/vector.

Example:

$$\underbrace{\begin{bmatrix} x_1 & x_2 \end{bmatrix}}_{x^T} \underbrace{\begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}}_B \underbrace{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}_x \Rightarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \begin{bmatrix} b_{11}x_1 + b_{12}x_2 \\ b_{21}x_1 + b_{22}x_2 \end{bmatrix}$$

$$\Rightarrow b_{11}x_1^2 + b_{12}x_1x_2 + b_{21}x_1x_2 + b_{22}x_2^2 = f(x_1, x_2)$$

Now we can just collect the partials in a vector (or a matrix if we end up with a matrix):

$$\begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2b_{11}x_1 + b_{12}x_2 + b_{21}x_2 \\ 2b_{22}x_2 + b_{12}x_1 + b_{21}x_1 \end{bmatrix} = \begin{bmatrix} 2b_{11} & b_{12} + b_{21} \\ b_{12} + b_{21} & 2b_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

3.11. Slide 32 - Limit of MLE.

$$\underbrace{\frac{n}{n-1}}_{\substack{n \rightarrow \infty \\ \rightarrow 1}} \underbrace{(\mu_1 - \hat{X}_i)}_{\rightarrow 0} \underbrace{(\hat{X}_k - \mu_k)}_{\rightarrow 0} \rightarrow \frac{1}{n-1} \sum \approx \sigma_{ik}$$

4. INFERENCE FOR SEVERAL SAMPLE

4.1. Slide 3 - Paired Data.

Here, *paired* means 2 tests/observations from the **same** subject x_{j_1} and x_{j_2} are always correlated since they are about the same person.

4.2. Slide 9 - Two Populations.

Different people, but 2 populations (different countries, people, etc).

X_{ij} , where j could be the j :th person in the i :th "country"/group

But different countries may have different amounts in population, what happens to D_i ? Well, we will allow t and define our own \mathbb{E} and Σ

4.3. Slide 10 - Pooled Sample Covariance Matrix.

$$\begin{aligned} X_{11}, \dots, X_{1n} &\sim N(\mu_1, \Sigma) & \text{Estimate of } \Sigma: \hat{\Sigma}_1 &= \frac{1}{n_1 - 1} \sum_{j=1}^{n_1} (X_{1j} - \bar{X}_1)^2 \\ X_{21}, \dots, X_{2n} &\sim N(\mu_2, \Sigma) & \text{Estimate of } \Sigma: \hat{\Sigma}_2 &= \frac{1}{n_2 - 1} \sum_{j=1}^{n_2} (X_{2j} - \bar{X}_2)^2 \end{aligned}$$

Here we are not using all our possible data to get a good approximation/estimate. Sure, $\hat{\Sigma}_1$ may be unbiased, but it can be better:

$$\left. \begin{aligned} \mathbb{E}(\hat{\Sigma}_1) &= (n_1 - 1)\Sigma \\ \mathbb{E}(\hat{\Sigma}_2) &= (n_2 - 1)\Sigma \end{aligned} \right\} \Rightarrow (n_1 + n_2 - 2)\Sigma = S_{\text{pooled}}$$

If $\mu_1 = \mu_2$, then we can estimate Σ using:

$$\left. \frac{\sum_{j=1}^{n_1} (X_{1j} - \bar{Z})^2 + \sum_{j=1}^{n_2} (X_{2j} - \bar{Z})^2}{n_1 + n_2} \right\} \text{ Where } \bar{Z} = \frac{X_1 + \dots + X_{1n} + X_{21} + \dots + X_{2n}}{n_1 + n_2}$$

4.4. Slide 20 - MANOVA Model.

τ_i denotes population i where τ_i is how much that population deviates from the mean. This can be useful, since we can look at some statistic over nordic countries and let μ be the mean over all nordic countries (by adding all statistics from every country and dividing by the nordic population, not by taking the mean of the mean in every country)

A one way MANOVA indicates that we are looking at one category of population, ie nationality. We can of course include things like nationality, race, gender, etc. but then it will be two-way/more MANOVA.

Since we have variations either above or below the average (per definition of the average), some $n_i\tau_i$ will be negative while others might be positive. That is why we set $\sum n_i\tau_i = 0$.

If we do not do this, we might as well write:

$$\begin{aligned} \mu + \tau_{\text{SWE}} &= \mu + c + \tau_{\text{SWE}} - c \\ \mu + \tau_{\text{NOR}} &= \mu + c + \tau_{\text{NOR}} - c \end{aligned}$$

4.5. Slide 28 - Multivariate Two-Way Fixed Effects Model with Interaction.

$$\mu + \underbrace{\tau_l}_{\text{property 1 in nordic}} + \underbrace{\beta_k}_{\text{property 2 in nordic}} + \underbrace{\gamma_{lk}}_{\text{property 1} \wedge \text{property 2 in nordic}} + e_{lkr}$$

A *marginalising parameter* is setting it as a summation index, eg: $\sum_j \gamma_{jk} \rightarrow j$ is marginalised

$\tau, \beta = \text{main effect}$, while γ is called the *interaction term*

4.6. Slide 33 - Test of No Interaction.

It makes no sense (often) to test τ_i since even if $\sum \tau_i = 0$, it may/will have effect on γ_{lk} . This is called *principal of marginality*.

5. REGRESSION

5.1. Slide 6 - Classic Linear Regression.

$$Y = Z^T \beta + e \rightarrow \mathbb{E}(e|Z) = 0$$

$$\mathbb{E}(Y|Z) = \mathbb{E}(Z^T \beta + e|Z) = \underbrace{\mathbb{E}(Z^T \beta|Z)}_{\mathbb{E}(Z^T \beta)} + \underbrace{\mathbb{E}(e|Z)}_{=0}$$

Why is it then called linear when we do not always approximate using linear functions but curves? Well, $Y = Z^T \beta + e = \beta_1 z_1 + \dots + \beta_r z_r$, this is just a *linear* combination of our regression-coefficients.

An example, $Y = \beta_1 z_1 + \beta_2 z_2^2$ is still linear regression, since it is linear in β , what happens with Z is not what we care about.

However, $Y = e^{\beta_1 z_1} / \sin(\beta_2 z_2)$ is not a linear regression.

5.2. Slide 7 - Matrix Notation.

Heteroscedasticity = every observation variance depends on observation. Can also be dependant on Z , so σ_i^2

Estimation methods still valid for heteroscedastic variances, although maybe not optimal.

5.3. Slide 9 - ANOVA With $g = 2$.

Note that we only need 2 columns to find the last rank $\rightarrow 1$ restriction:

$$\sum n_l \tau_l = 0 \Rightarrow \tau_l = 0$$

5.4. Slide 10 - Anova With $g = 2$ and $b = 2$.

Instead of restriction, construct a submatrix with the bad (linearly dependant) columns deleted. Estimation depends on rank.

5.5. Slide 11 - Ordinary Least Squares.

$$-2Z^T(y - Z\beta) = 0 \Leftrightarrow Z^T y = Z^T Z \beta = \hat{\beta}_{\text{OLS}} = (Z^T Z)^{-1} Z^T y$$

5.6. Slide 12 - OLS Estimator.

$$Y = Z\beta + e \quad \mathbb{E}(Y) = Z\beta \quad \hat{Y} = Z\hat{\beta}$$

Residual is given by $\hat{e} = y - Z\hat{\beta} = y - Hy = (I - H)y$

Interesting things:

$$Z^T \hat{e} = Z^T (I - H)y = (Z^T - \underbrace{Z^T Z (Z^T Z)^{-1} Z^T}_H)y = 0$$

We note that the residual is perpendicular to observed values! This makes sense.

$$\hat{y}^T \hat{e} = y^T H (I - H)y = y^T (H - H^2)y = 0$$

$$H^2 = Z Z^T (Z^T Z)^{-1} Z^T Z (Z^T Z)^{-1} Z^T = H \quad (\text{idempotent})$$

Predicted value is perpendicular to \hat{e}

5.7. Slide 15 - Sampling Properties of OLS Estimators.

$\mathbb{E}(\hat{e}^T \hat{e}) = (n - r)\sigma^2$ if e has some distribution of $\mu = 0$ and $\Sigma = \sigma^2 I$

$\frac{1}{n-1}$ comes from $\frac{\hat{e}^T \hat{e}}{n-r}$, since $\underbrace{Z}_{n \times r} \underbrace{\beta}_{r \times 1}$, but for constants/1D we have $r = 1$

$$\begin{aligned} \text{Cov}(\hat{\beta}, \hat{e}) &= \text{Cov}\left(\underbrace{(Z^T Z)^{-1} Z^T y}_A, \underbrace{(I - H) y}_B\right) = (Z^T Z)^{-1} Z^T \sigma^2 I (I - H)^T \\ &\Rightarrow \sigma^2 (Z^T Z)^{-1} Z [I - Z(Z^T Z)^{-1} Z] = \sigma^2 ((Z^T Z)^{-1} Z^T - (Z^T Z)^{-1} Z (Z^T Z)^{-1} Z^T) = 0 \\ &\Rightarrow \text{unbiased} \end{aligned}$$

5.8. Slide 17 - Distribution of Regression Coefficients.

By assuming $e \sim N$ distributed, we could do inference on β

Anmärkning:

- Normal distribution \Rightarrow every marginal distribution is normal
- Sum of squares of normal random variables $\sim \chi^2$
- Standard normal ($N(0, 1)$) divided by χ^2 divided by degrees of freedom $\sim t_{n-r} \rightarrow$ degrees of freedom
- Joint statistics = how many things you chuck in the conf. intern.

5.9. Slide 18 - Confidence Region.

If $\hat{\beta} - \beta \ll 1$, then we are close. We capture this in our test.

5.10. Slide 19 - Confidence interval.

You will get some F distribution (**CHECK**)

Anmärkning:

Some nomenclature:

- *Multiple regression* $r \geq 2, 3, \dots$
- *Multivariate regression* Y is a matrix

5.11. Slide 20 - More Than One Responses.

$\underbrace{Y}_{m \times 1}$ here is for one subject, where m is the amount of responses. If we have n subjects, we get what is on slide 21.

5.12. Slide 22 - Assumptions.

In the second point $e_{(i)} = i$ th thing to compare, eg price/time and not subject such as apartment. $\text{Cov}(e_{(i)}, e_{(k)})$ compares price and time simultaneously.

5.13. Slide 23 - Least Squares.

$$\underbrace{(Y_Z \beta)^T}_{m \times n} \underbrace{(Y_Z \beta)}_{n \times m} \sim m \times m$$

Anmärkning:

- $Y_{(i)}$ = i th column Y_i = i th row
- Wishart = Generalisation of χ^2 in multivariate case

5.14. Slide 27 - Regression Coefficients With Zero Constraints.

When we reduce to $Y_{n \times m} = Z_1 \beta_1 + E$, we can go back to multiple regression by letting $Z = Z_1$, $\beta = \beta_1$

What happens to E ? It never changes, we just use the one that corresponds with the column we test in the multiple regression model.

5.15. Slide 31 - LRT when $m = 1$.

Let w = numerator = $(Y - Z\hat{\beta})^T(Y - Z\hat{\beta})$

Let w_1 = denominator = $(Y - Z_1\hat{\beta}_1)^T(Y - Z_1\hat{\beta}_1)$

Result 7.6 says $\frac{w_1 - w}{w}$ but if $\frac{w}{w_1}$ small, then $\frac{w_1}{w}$ must be big $\Rightarrow \frac{w_1}{w} - 1$ is still big.

F test tests if every β_i is 0 except the intercept.

5.16. Slide 32 - Prediction of Regression Function.

$\beta_{(i)}$ has dimension $1 \times r$ $\hat{\beta}_{(i)}^T$ has dimension $r \times 1$, dimension of z_0 $1 \times r$. This gives us that $\hat{\beta}_{(i)} z_0$ is a scalar $\Rightarrow N_1(\mu, \sigma^2)$

5.17. Slide 34 - Forecast New Response.

$\mathbb{E}(Y)$ is predicting mean, but we want to find/predict Y

6. PRINCIPAL COMPONENT ANALYSIS

6.1. Slide 3 - Motivation.

PCA is mostly used in pre-processing these days, instead of being the actual analysis.

6.2. Slide 4 - Task of Principal Component Analysis (PCA).

\mathbf{a}_3 maximizes $\text{Var}(\mathbf{a}_3^T \mathbf{X})$ and $\text{Cov}(\mathbf{a}_3^T \mathbf{X}, \mathbf{a}_j^T \mathbf{X}) = 0$. In the covariance term, we look at all $j < 3$ and not just $j = 1$. That is, our requirement is that $\text{Cov}(\mathbf{a}_3^T \mathbf{X}, \mathbf{a}_1^T \mathbf{X}) = 0 \wedge \text{Cov}(\mathbf{a}_1^T \mathbf{X}, \mathbf{a}_2^T \mathbf{X}) = 0$

Big variation is good since it covers more cases. Think of it like salary analysis, with low variance you may only have asked the CEO/higher ups and you will not get as great of a picture as if you used the whole wide company.

6.3. Slide 5 - Restriction.

$$\text{Cov}(\mathbf{a}_i^T \mathbf{X}, \mathbf{a}_k^T \mathbf{X}) = \mathbf{a}_i^T \underbrace{\text{Cov}(\mathbf{X}, \mathbf{X})}_{=\Sigma} \mathbf{a}_k \Rightarrow \mathbf{a}_i^T \Sigma \mathbf{a}_k$$

6.4. Slide 6/7 - Principal Components and Two useful Lemmas.

Maximize $\text{Var}(\mathbf{a}_1^T \mathbf{X})$ such that $\mathbf{a}_1^T \mathbf{a}_1 = 1 \Leftrightarrow \text{maximize } f(\mathbf{a}_1) = \text{Var}(\mathbf{a}_1^T \mathbf{X}) - \underbrace{\lambda}_{\text{Lagrange multiplier}} (\mathbf{a}_1^T \mathbf{a}_1 - 1)$

This uses the Lagrange multiplier method.

Adding more constraints, you add more Lagrange multipliers (*KKT condition*)

In order to maximise, we want $\frac{df}{da_1} = 0 \wedge \frac{df}{d\lambda} = 0$

Note that:

$$\begin{aligned} \frac{df}{d\lambda} &= -(a_1^T a_1 - 1) = 0 \wedge \frac{df}{da_1} = 1 \\ &\Rightarrow 2\Sigma a_1 - 2\lambda a_1 = 0 \end{aligned}$$

Zero only when $\Sigma a_1 = \lambda a_1$

6.5. Slide 7 - Two useful Lemmas.

Reason we want to use the largest eigenvalue is because we want to maximise variance:

$$Y_1 = a_1^T X \quad (\Sigma a_1 = \lambda a_1) \rightarrow \text{Var}((Y_1)) = a_1^T \Sigma a_1 = \lambda \underbrace{a_1^T a_1}_{=1} = \lambda$$

First thing (maximise variance) is done, second step:

$$\begin{aligned} \max(\text{Var}(a_2^T X)) &= a_2^T \Sigma a_2 \text{ s.t. } a_2^T a_1 = 1 \quad \underbrace{\text{Cov}(a_2^T X, a_1^T X)}_{\substack{= a_2^T \Sigma a_1 = a_2^T \lambda a_1 = \lambda a_2^T a_1 \\ a_2 \notin \text{span}\{a_1\} \Leftrightarrow a_2^T a_1 = 0}} = 0 \\ &\Rightarrow \max(f(a_2)) = a_2^T \Sigma a_2 - \lambda(a_2^T a_2 - 1) \end{aligned}$$

The whole text under the covariance can be boiled down to implying that a_2 has to be a span of other eigenvectors. Then they will be orthogonal to each other.

For the last row, to $f(a_2)$, we use the second largest eigenvector.

6.6. Slide 9 - Principal Components.

Even if we have eigenvalues with duplicate values this holds.

6.7. Slide 10 - Total Variation Explained by Principal Components.

By having orthogonal Y_i :s (due to eigenvectors), we have reduced dependency from all Y_i :s. Any non-orthogonality yields some correlation between some Y_i and Y_k , and we have now removed that.

Using $\frac{\lambda_k}{\sum \lambda_i}$ gives us the contribution from λ_k , but we can look for say $\frac{\sum_k^j \lambda_k}{\sum \lambda_i}$ until we get a % we are satisfied with.

6.8. Slide 12 - Principal Components From Correlation Matrix.

Reason we standardized is to be able to compare with other data of different scale

$$V = \begin{bmatrix} \sigma_{11} & & \\ & \sigma_{22} & \\ & & \ddots \end{bmatrix}$$

6.9. Slide 14 - Sample Principal Components.

Let Σ be our sample covariance matrix instead. Then we carry out as usual.

Anmärkning:

Centered = mean is 0. Taking away some of the data would yield an almost 0 mean (numerically 0)

7. FACTOR ANALYSIS

7.1. Slide 3 - Latent Variable Modelling.

LVM = factor analysis. Find values such as personality using a proxy. Personality is the factor/latent variable.

In PCA, we had a bunch of values and we wanted to simplify them and keep them as concise as possible while still retaining as much of the information as possible. In factor analysis, we go the other direction, we have some "simplified" data set and we want to draw more conclusions from this.

7.2. Slide 4 - The Model.

i = i th question in questionnaire

$$\underbrace{X_i}_{\text{Math-score/what you know}} = \mu_i + \underbrace{\ell_{i1}}_{\text{Algebra ability/what you want to predict}} + \cdots + \varepsilon \rightarrow \text{math ability still there, but } \varepsilon \text{ may be latent}$$

Depending on application, sometimes we need to find ℓ .

Tasks is usually lower than factors.

In multiple regression we had $X = X\beta + \varepsilon$, but this is for all people/subjects, while $X = \mu + \ell F + \varepsilon$ is for 1 person/subject, like in multivariate multiple regression model, difference is $Y_i = \beta^T \underbrace{X_i}_{\text{observed}} + \varepsilon$

A regressor is values you do not really observe such as IQ, but you still want to build a model using observations.

7.3. Slide 5 - Scale Indeterminacy.

We can redefine scale, continuing with the IQ example, there really is nothing stopping us from saying that the IQ scale should lay inbetween $[-1,1]$ by just compressing the Gaussian.

7.4. Slide 7 - Model Implied Covariance Matrix.

$$\text{Cov}(LF + e) = \text{Cov}(LF, LF) + \underbrace{\text{Cov}(LF, e)}_{L\text{Var}(F)L^T + \text{Var}(e) = LL^T + \psi = \text{Cov}(X)} + \underbrace{\text{Cov}(e, LF)}_{=0} + \text{Cov}(e, e)$$

The reason for the name model implied covariance matrix, is because it is implied by the setup of the model.

Example:

$$\underbrace{\begin{bmatrix} l_{11} & l_{12} \\ l_{21} & l_{22} \\ l_{31} & l_{32} \end{bmatrix}}_L \underbrace{\begin{bmatrix} l_{11} & l_{21} & l_{31} \\ l_{12} & l_{22} & l_{32} \end{bmatrix}}_{L^T} + \begin{bmatrix} \psi_1 & & \\ & \psi_2 & \\ & & \psi_3 \end{bmatrix}$$

$$= \begin{bmatrix} l_{11}^2 + l_{12}^2 + \psi_1 & 0 & 0 \\ 0 & l_{21}^2 + l_{22}^2 + \psi_2 & 0 \\ 0 & 0 & l_{31}^2 + l_{32}^2 + \psi_3 \end{bmatrix}$$

Here $l_{11}^2 + l_{12}^2 + \psi_1 = \text{Var}(X_1)$, $l_{21}^2 + l_{22}^2 + \psi_2 = \text{Var}(X_2)$, $l_{31}^2 + l_{32}^2 + \psi_3 = \text{Var}(X_3)$ Want communality over uniqueness

7.5. Slide 8 - Existence of Decomposition.

Note that the invalid decomposition is invalid due to negative ψ , $\text{Var}(e)$ not as assumption.

Anmärkning: PCA always doable, not the same with factor analysis.

7.6. Slide 9 - Indeterminacy.

Rotation (multiplication by diagonal matrix T) is invariant \Rightarrow indeterminate

7.7. Slide 10 - Scale Invariant.

Curiosity: What happens if $c\mu$ or cz ?

7.8. Slide 11 - Popular Estimation Methods.

Curiosity: What if only one person in our sample has $p + 1 \times 1$?

7.9. Slide 12 - Spectral Decomposition.

Recurring small eigenvalues yields a possibility to find ψ such that ψ is diagonal.

7.10. Slide 14 - Determine Number of Factors.

A factor/factors = things we want to test, while m is the number of things we want to test. Say for example we use the multivariate analysis exam as an example. It might test our knowledge in multivariate analysis ($m = 1$), but might also in addition test our R knowledge ($m = 2$)

Kaiser criterion sucks.

7.11. Inbetween lectures.

We want the RMSEA index < 0.1 . Or rank of the two sample test $> 3 = \text{bad?}$

7.12. Slide 23 - Versus PCA.

Notice that they are very similar. I can do PCA to solve FA.

7.13. Slide 24 - Orthogonal Rotation.

Multiplication will not change anything.

7.14. Slide 26 - Oblique Rotation.

All factors cannot always be orthogonal. For example, say we test English knowledge, then spelling will have some correlation to writing \rightarrow oblique.

If we have the following correlation matrix $\begin{bmatrix} 1 & 0.9 \\ 0.9 & 1 \end{bmatrix}$, then 0.9 (since it is too close to 1), might be the same so we could reduce 1 factor.

7.15. Slide 28 - Bartlett Score.

A factor score is the estimate of F

8. CANONICAL CORRELATION ANALYSIS

Anmärkning:

Tasks is coumns/abilites, such as listening etc

Demean = remove mean, that is if something hsa value $\mu + x$, after demeaning it only has value x

Scores is tranformed data, ie. x -scores = $a^T x$ (values of linear combination of U)

The scores (latent variables) are what we want for further analysis

8.1. Slide 3 - Motivation.

In PCA, we had a lot of variables and we simplified them to less variables, and in factor analysis we did the opposite and were able to draw conclusions from our data.

In CCA, we have 2 sets of variables, and simplify them to have some lower dimension (think PCA on 2 sets of data).

Note that just like FA was the "opposite" of PCA, there is an "opposite" to CCA (not covered) called structural equation modelling.

The intuition is, say $X^{(2)}$ has q entries, and $X^{(1)}$ has p entries. That is $p \cdot q$ scatter plots to read, we want to minimize this number.

In PCA, we maximize $\text{Var} \left(a^T \begin{bmatrix} X^{(1)} \\ X^{(2)} \end{bmatrix} \right)$

8.2. Slide 4 - Task.

When $\text{Cor}(U, V)$ is maxed, we capture as much information from lower dimensions as we do with higher dimensions (ie, adding more dimensions will not yield more data). This can be seen as regression, want U to describe V as good as possible.

8.3. Slide 5 - Correlation Coefficient.

Even if we let a, b blow up, we normalise it in he correlation through the denominator

8.4. Slide 7 - Canonical Variates.

(U_2, V_2) will be orthogonal to (U_1, V_1) , same with (U_k, V_k) , it will be uncorrelated to all the previous ones.

8.5. Slide 9 - Find Canonical Variates.

In PCA we used the Lagrange multipliers in order to maximize, we will do the same but with 2 constraints ($a^T \Sigma_{11} a = 1$ and $b^T \Sigma_{22} b = 1$):

$$\max f = a^T \Sigma_{12} b - \lambda_1 (a^T \Sigma_{11} a - 1) - \lambda_2 (b^T \Sigma_{22} b - 1)$$

Note that usually it will be $(a^T \Sigma_{12} b)$, but we only care about positive values, so we do $(a^T \Sigma_{12} b)$

Maximizing:

$$\begin{aligned} \frac{\partial f}{\partial a} = 0 &= \Sigma_{12} b - \lambda_1 (\Sigma_{11} + \Sigma_{11}^T) a - 2 \Sigma_{11} & \frac{\partial f}{\partial b} = 0 &= \Sigma_{21} a - \lambda_2 (\Sigma_{22} + \Sigma_{22}^T) b - 2 \Sigma_{22} \\ \frac{\partial x^T \Sigma x}{\partial x} &= (\Sigma + \Sigma^T) x & \frac{\partial b^T x}{\partial x} &= b \\ a^T \Sigma_{12} b &= 2 \lambda_1 \underbrace{a^T \Sigma_{11} a}_{=1} \\ b^T \Sigma_{21} a &= a^T \Sigma_{12} b \Rightarrow b^T \Sigma_{21} a = 2 \lambda_2 \underbrace{b^T \Sigma_{22} b}_{=1} \end{aligned} \left. \vphantom{\begin{aligned} \frac{\partial f}{\partial a} = 0 \\ \frac{\partial f}{\partial b} = 0 \\ \frac{\partial x^T \Sigma x}{\partial x} = (\Sigma + \Sigma^T) x \\ \frac{\partial b^T x}{\partial x} = b \\ a^T \Sigma_{12} b = 2 \lambda_1 \underbrace{a^T \Sigma_{11} a}_{=1} \\ b^T \Sigma_{21} a = 2 \lambda_2 \underbrace{b^T \Sigma_{22} b}_{=1} \end{aligned}} \right\} \Rightarrow \lambda_2 = \lambda_1 = \lambda$$

We will see that for $\Sigma_{12}b$ and $\Sigma_{12}a$:

$$\Sigma_{12}b = 2\lambda\Sigma_{11}a$$

$$\Sigma_{21}a = 2\lambda\Sigma_{22}b \Rightarrow b = \frac{1}{2\lambda}\Sigma_{22}^{-1}\Sigma_{21}a \quad (\text{assuming } \Sigma_{22} \text{ is invertible, which it is since it is the covariance matrix})$$

Plugging this definition of b in the first equation yields:

$$\Rightarrow \Sigma_{12} \left(\frac{1}{2\lambda}\Sigma_{22}^{-1}\Sigma_{21}a \right) = 2\lambda\Sigma_{22}b$$

$$\Rightarrow \Sigma_{11}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}a = 4\lambda^2a \Rightarrow a \quad \text{is an eigenvector to } \Sigma_{11}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} \quad \text{with eigenvalue } (2\lambda)^2$$

By the useful lemma on slide 8:

$$\begin{aligned} \Sigma_{11}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} &= \Sigma_{11}^{-1/2}\Sigma_{22}^{-1}\Sigma_{12}^T\Sigma_{11}^{-1/2} \quad \text{since:} \\ &\Sigma_{11}^{1/2}\Sigma_{11}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11}^{-1/2}\Sigma_{11}^{1/2} \\ &= \Sigma_{11}^{-1/2}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11}^{-1/2}(\Sigma_{11}^{1/2}a) = (2\lambda)^2(\Sigma_{11}^{1/2}a) \\ &\Rightarrow \Sigma_{11}^{-1/2}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11}^{-1/2}e = (\rho^*)^2e \quad \rho^* = 2\lambda \\ &e = \Sigma_{11}^{1/2}a \Rightarrow a = \Sigma_{11}^{-1/2}e \\ &b = \frac{1}{2\lambda}\Sigma_{22}^{-1}\Sigma_{21}a \end{aligned}$$

Using $a^T\Sigma_{11}a$:

$$e^T\Sigma_{11}^{-1/2}\Sigma_{11}\Sigma_{11}^{-1/2}e = e^Te = 1$$

Similarly:

$$\begin{aligned} b &= \frac{1}{(2\lambda)^2}a^T\Sigma_{12}\underbrace{\Sigma_{22}^{-1}\Sigma_{22}}_{=1}\Sigma_{22}^{-1}\Sigma_{21}a \\ &\Rightarrow \frac{1}{(2\lambda)^2}a^T\underbrace{\Sigma_{11}\Sigma_{11}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}}_{\substack{\text{add this} \\ =(2\lambda)^2a}}a \end{aligned}$$

Here, we are using $a^T\Sigma_{11}a = 1$ (linear constraint is satisfied and variance is 1)

Now:

$$a^T\Sigma_{12}b = \frac{1}{2\lambda}a^T\Sigma_{11}\Sigma_{11}^{-1}\Sigma_{12}^T\Sigma_{12}^{-1}\Sigma_{12}a \Rightarrow 2\lambda\underbrace{a^T\Sigma_{11}a}_{=1} = 2\lambda$$

Correlation is therefore given by the square root of eigenvalues. Once we know a , we can find b (that is the meaning behind proportionality).

8.6. Slide 12 - Scale Invariant: Coefficient Vector.

Even though it is scale invariant, it is good practice to scale/normalize.

8.7. Slide 14 - Proportion of Explained Variance.

r^2 = how much of the variance that is explained. Sample covariance matrix *or* sample correlation matrix work in slide 9.

8.8. Slide 15 - Sample Canonical Variate Pair.

Sample variance should be one.

Since we use maximum correlation, we can use one set to describe the other

8.9. Slide 19 - Special case: $p = 1$.

α = proportional

8.10. Slide 22 - Almost same thing.

- Demean $\hat{Y} = 0$ $\bar{x}_1 = \bar{x}_2 = \bar{x}_3 = 0$
- $\underbrace{S_{11}^{-1/2} S_{12} S_{22}^{-1} S_{21} S_{11}^{-1/2}}_{\substack{Y \\ \text{mean} = 0}} = \alpha + \sum_i \underbrace{\beta_i x_i}_{\substack{\beta_i x_i \\ \text{mean} = 0}} \Rightarrow$ forces α to be 0

Multiple r -squared = "how much variation/variance in Y is explained by our model"

8.11. Slide 24 - Maximize Covariance.

Multicollinearity is a problem with numerical 0:es, such when trying to invert the following matrix:

$$\begin{bmatrix} 1 & 1e16 \\ 1e16 & 1 \end{bmatrix}$$

Very similar to CCA, difference is how we manage restriction:

$$\max \text{Corr}(a^T X, b^T Y) \stackrel{\text{Var}=1}{=} \text{Cov}(a^T X, b^T Y)$$

Anmärkning:

Restriction can be $a^T \sum_{xx} a = 1$ and $b^T \sum_{yy} b = 1$. In CCA we downgrade dimension of both X, Y in PLS we only downgrade X

8.12. Slide 26 - PLS Regression.

Since t is a vector, $t^T t$ is a scalar, so $(t^T t)^{-1}$ is just the reciprocal.

9. DISCRIMINANT ANALYSIS AND CLASSIFICATION

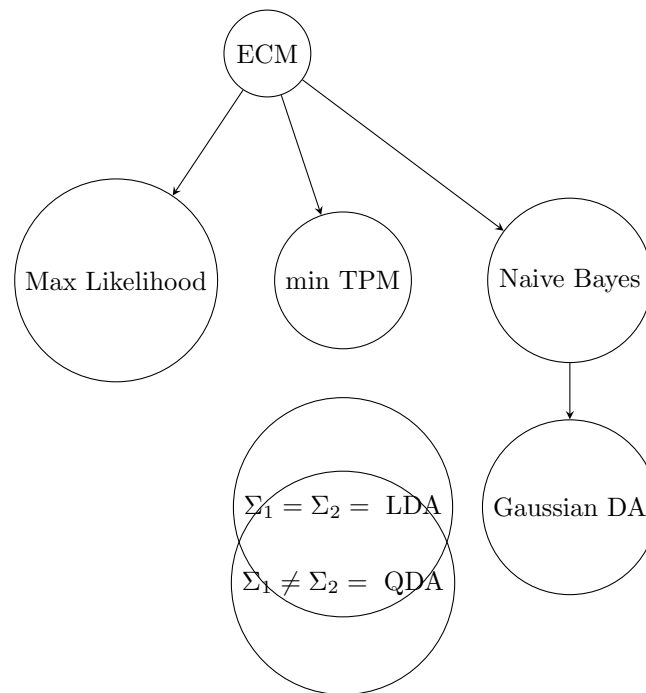


FIGURE 1.

9.1. Slide 3 - Motivation.

Discrimination here means to separate subjects.

Use labeled observations to build a classification rule, means using previous data.

Classes are well defined, that is they are fixed in some sense. Having two classes such as cat and trying to classify a picture of a horse will only lead to the picture of the horse being classified into either cat or dog. It will not "create a new class" just because the data does not match. It will find which class it matches the best in, and sort into there.

9.2. Slide 4 - Two-class problem.

Dividing Ω into two disjoint sets R_1 and R_2 is the discrimination step.

Probabilistic = vague group belonging

Deterministic = you are either in group A or group B

9.3. Slide 6 - Classification Table.

m_{ij} where j = observed, and i = predicted

There is another thing we can compute, accuracy = $\frac{m_{11} + m_{22}}{m_{11} + m_{12} + m_{21} + m_{22}}$

Note that using absolute rates, ie $\frac{m_{12} + m_{21}}{m_{11} + m_{22}}$ does not take into account the cost of misclassification, it cares more about maximizing $m_{12} + m_{21}$

9.4. Slide 7 - F-Score of Binary Classification.

If F-score > 0.5 , then we are good (DIY rule of thumb)

9.5. Slide 8 - Cost of Misclassification.

$$\text{ECM} = \underbrace{c(2|1)}_{\text{cost of misclas.}} \underbrace{P(2|1)}_{\text{prob. of misclas.}} p_1 + \dots$$

Bayesian means "I have some knowledge, I get new data, I update my previous knowledge"

9.6. Slide 9 - Minimizing ECM.

Intuitive idea: If it costs a lot to misclass into class 1, then we "want" to shift our mistake-making into the other class (ie shift such that whenever we misclass it is a higher probability that we misclass into the "less costly" class).

9.7. Slide 10 - An Example Using ECM.

$$\begin{aligned} \pi_1 : X &\sim N(0, \Sigma) & p_1 &= 0.8 & c(2|1) &= 5 \\ \pi_2 : X &\sim N(\mu, \Sigma) & p_2 &= 0.2 & c(1|2) &= 10 \end{aligned}$$

We now have everything we need to compute:

$$R_1 : \frac{f_1(x)}{f_2(x)} = \frac{\frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} \exp\left(-\frac{1}{2}x^T \Sigma^{-1}x\right)}{\frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)\right)} > \frac{1}{2}$$

The cost is subject to your own judgement, can be biased to you/the one who decides what the cost of misclassification is.

9.8. Slide 13 - Special Case III: Highest Posterior Probability.

Assigning class depending on posterior probability.

- Prior: $P(\pi_i)$
- Posterior: $P(\pi_i \underbrace{x}_{\text{data}})$

After reading mail (spam not spam mail problem), I may update my knowledge of the probabilities of belonging to each class.

Naive Bayes does this, after updating probabilities it adds into the class with highest probability.

9.9. Slide 14 - Naive Bayes: Gaussian Discriminant Analysis.

If we do not know something, either estimate or use your own judgement.

Log-likelihood given by:

$$\begin{aligned} \ell = \sum_j^n Z_j &\left[\ln(\phi) - \frac{p}{2} \ln(2\pi) - \frac{1}{2} \ln(|\Sigma|) - \frac{1}{2}(x_j - \mu_1)^T \Sigma^{-1}(x_j - \mu_1) \right] + \\ &(1 - Z_j) \left[\ln(1 - \phi) - \frac{p}{2} \ln(2\pi) - \frac{1}{2} \ln(|\Sigma|) - \frac{1}{2}(x_j - \mu_2)^T \Sigma^{-1}(x_j - \mu_2) \right] \end{aligned}$$

$$\text{Where } \hat{\phi} = \frac{\text{numbers of 1}}{n} = \hat{p}_1 \Rightarrow \hat{p}_2 = 1 - \phi = \frac{\text{number of 2}}{n}$$

MLE: In order to optimize (find $\widehat{\mu}_1$), we can use the optimization lemma from chapter 4 (slide 24):

$$\left. \begin{aligned} \widehat{\mu}_1 &= \frac{\Sigma}{\Sigma Z_j = \frac{1}{n} \text{ part}} \underbrace{\sum_{\substack{\text{if in group 2, } Z=0, \text{ so no contrib.} \\ Z_j}} x_j}_{\text{average of group 1}} \\ \widehat{\mu}_2 &= \frac{\Sigma(1 - Z_j)x_j}{\Sigma(1 - Z_j)} \end{aligned} \right\} \text{average of group 2}$$

Only thing we do not know is Σ , but we use the same lemma from chapter 4.

Anmärkning:

Quadratics are the same trace!

$$\begin{aligned} (x_j - \mu_1)^T \Sigma^{-1} (x_j - \mu_1) &= \text{tr}(\Sigma^{-1} (x_j - \mu_1)(x_j - \mu_1)^T) \\ \Rightarrow -\frac{1}{2} [\Sigma Z_j + \Sigma(1 - Z_j)] \ln(|\Sigma|) - \frac{1}{2} \Sigma \text{tr} &\underbrace{(\Sigma^{-1} Z_j (x_j - \mu_1)(x_j - \mu_1)^T + (1 - Z_j)(x_2 - \mu_2)(x_2 - \mu_2)^T)}_{=A} \\ &= -\frac{1}{2} \text{tr}(\Sigma \Sigma^{-1} (Z_j (x_j - \mu_1) \cdots)) \\ q &= \Sigma Z_j + \Sigma(1 - Z_j) \end{aligned}$$

$$\begin{aligned} P(Z = 1) &= \widehat{p}_1 & X|Z = 1 &\sim N(\widehat{\mu}_1, \widehat{\Sigma}) & P(Z = 0) &= \widehat{p}_2 & X|Z = 0 &\sim N(\widehat{\mu}_2, \widehat{\Sigma}) \\ \Rightarrow P(Z|x_0) &= \frac{P(x_0|Z)P(Z)}{\sum_Z P(x_0|Z)P(Z)} \end{aligned}$$

Given you have cancer, you will observe X . Logistic regression is opposite, given X determine if the patient has cancer.

9.10. Slide 15 - Gaussian Discriminant Analysis: Classification.

The equivalence is same as slide 16, by taking the logarithm

Anmärkning:

Gaussian \Rightarrow only for normally distributed

9.11. Slide 16 - Gaussian Discriminant Analysis: Decision Boundary.

Changing \geq to $=$ yields your *decision boundary*

9.12. Slide 17 - Fishers Linear Discriminant Analysis.

Assuming $\Sigma_1 = \Sigma_2 = \Sigma$ yields linearity. Gaussian discriminant analysis is a type of ECM. Fisher ECM works through projections instead.

9.13. Slide 18 - MANOVA-Like Idea.

W = within group variation

B = between group variation.

Want things in the "within" set to be as close to each other, ie small $a^T W a$ and big $a^T B a$

9.14. Slide 19 - Within Versus Between Variation.

Note that we have not made any assumptions on the distribution.

9.15. Slide 20 - Fishers LDA.

Idea is the same as Guassiam, instead of Σ , we use W and we have "mean - mean" Σ (or W)

9.16. Slide 22 - Case I: $\Sigma_1 = \Sigma_2 = \Sigma$.

The $-\frac{1}{2}(\mu_1 - \mu_2)^T$ looks similar to $\frac{1}{2}(\bar{x}_1 - \bar{x}_2)^T$

9.17. Slide 24 - Connection to Fishers LDA.

Normality yields robust results, but it can be from other distributions and not necessarily normal.

9.18. Slide 26 - Case II: $\Sigma_1 \neq \Sigma_2$.

QDA allows Σ to be different, contrary to LDA where it has to be the same.

9.19. Slide 27 - Logistic Model For Two Populations.

Probabilistic model of X to model probability

9.20. Slide 28 - Maximum Likelihood Estimator.

For Bernoulli! No close method for finding α and β . We can either guess or use some numerical method to find it/approximate it.

9.21. Slide 29 - Penalized Logistic Regression.

Think of α like the intercept and β like the slope coefficients

Maximizing likelihood function is the same as minimizing the likelihood function after you multiply it by -1.

SPLINE approach (yields continuous and differential function)

Recall noise in data, what can happen to complicated models? Well they would end up modelling the noise in their attempt to fit the curve to the data-points.

Doupple descent phenomenon

Example:

$$-\ell(\alpha, \beta) + \lambda[|\beta_1| + |\beta_2|] \Leftrightarrow \max(\ell(\alpha, \beta)) \text{ such that } |\beta_1| + |\beta_2| = t$$

Here t is some number. Tuning t tunes λ . The above example is an example of LASSO. Below is an example of Ridge:

$$\beta_1^2 + \beta_2^2$$

One way to tune λ is by cross validation. 3-fold cross validation works in the following way:

- Find a sequence of lambdas beforehand, testing will yield which λ to pick $(\lambda = 0, \dots, \lambda_{\max})$
somewhere in here
- Split data into 3 disjoint sets
- Use the first 2 parts to predict 3
- Tune accordingly
- Repeat previous 2 steps $\binom{3}{2}$ times

Anmärkning:

10-fold method is the most popular.

9.22. Slide 30 - Limitation.

Kind of like how Newtons method works to find 0:es of a function

9.23. Slide 31 - Euclidean Inner Product.

We replace the estimate $\hat{\beta}$ with $\Sigma d_j x_j$

9.24. Slide 32 - New Features.

Here *features* = covariates. $\delta(x)$ includes "old" features:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \xrightarrow{\delta} \delta \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right) = \begin{bmatrix} x_1 \\ x_2 \\ x_1^2 \\ x_2 x_1 \\ x_2^2 \\ x_1^3 \end{bmatrix}$$

9.25. Slide 33 - Kernel Function and Kernel Matrix.

The output of the function κ is a scalar.

$\delta^T(x)\delta(z)$ = Euclidean inner product of $\delta(x)$ and $\delta(z)$

9.26. Slide 38 - Motivation: Margin.

Idea of a *support vector machine*; if we have multiple ways to pick our decision line, this will give us the best lines.

Y here is some binary set.

9.27. Slide 40 - Hinge Loss: Brief Intro.

Term after hinge loss is the Ridge penalty

9.28. Slide 41 - Hinge Loss Vs Log-Likelihood Loss.

You always lose some with logistic regression. With Hinge loss we will lose more because of how the curve is.

Anmärkning:

In the R code, γ is the inverse of Σ

9.29. Slide 45 - Best Partition.

\hat{p}_{mk} is the proportion of say x_1 in that region.

Purity is about how red is in the black area etc. A very pure area is homogenous and has a small Gini index.

9.30. Slide 47 - A Tree Versus A Forest.

B = the number of trees in the forest.

We cannot mimick the population due to biases, but we can see the data as our population instead and pick out a subset of our data and pretend we are picking out a subset of our population

Line 3 is the bootstrapping method.

9.31. Slide 56 - Linear Discriminants.

x_0 is our new variable \Rightarrow still linear

10. OLD EXAM 2022-01-05

1. a) Remember than any linear combination of normally distributed random variables is normal:

$$AX \sim N(A\mu, A\Sigma A^T)$$

So let $A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$:

$$A \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix} = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \sim N_2(A\mu, A\Sigma A^T)$$

- b) $X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$, then $X_1|X_2 = a \sim N(\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(a - \mu_2), \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})$

In our case,

$$\begin{aligned} X_1 &= \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} & \mu_1 &= \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\ X_2 &= \begin{bmatrix} X_3 \\ X_4 \end{bmatrix} & \mu_2 &= \begin{bmatrix} 1 \\ 1 \end{bmatrix} \end{aligned}$$

$$\begin{aligned} \Sigma_{12} &= \begin{bmatrix} 1/4 & 0 \\ 0 & 0 \end{bmatrix} & \Sigma_{22} &= \begin{bmatrix} 2 & 1/2 \\ 1/2 & 2 \end{bmatrix} \\ \Sigma_{11} &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & \Sigma_{21} = \Sigma_{12}^T &= \begin{bmatrix} 1/4 & 0 \\ 0 & 0 \end{bmatrix} \end{aligned}$$

Anmärkning: Normally distributed variables are independent if and only if the covariance matrix is diagonal

2. a) Two-way MANOVA (CHapter 6).

The measured variables are $\begin{bmatrix} O \\ V \\ C \\ B \end{bmatrix} = \underbrace{X}_{4 \times 1}$, depends on brands of coffee and milk type, so we get:

$$X_{ijk} = \mu + \underbrace{\alpha_i}_{\text{coffee brand}} + \underbrace{\beta_j}_{\text{milk}} + \underbrace{r_{ij}}_{\text{interaction between brand \& milk}} + \underbrace{\varepsilon_{ijk}}_{\text{error}}$$

k = repeated measures. Our model assumptions are assumptions of α, β, r

we need $\sum \alpha_i = 0 \sum \beta_i = \sum r_{ij} = 0$

Error term should be normailly distributed $N_4(0, \Sigma)$

- b) Testing wether interaction is 0 yields $H_0 : r_{ij} = 0$ for any i, j

In that case, the model becomes additive model (how the milk influences coffee is same regardless of brand) i.e $X_{ijk} = \mu + \alpha_i + \beta_i + \varepsilon_{ijk}$

If we want to test wether brand has effect then we test $\alpha_i = 0$

3. a) **Anmärkning:** How do you determine if it is paired data or uncorrolated?

In our case, think of it like this, if we take the sample from the same cup and add oat milk to 1/2 of the sample and cream to the other then it is paired since the coffee comes from the same sample.

In the case of paired data, we can use Hotellings T^2 .

In our case however, we let $X(4 \times 1)$ be the sample tested with cream, and $Y(4 \times 1)$ be tested with oat milk. We have a 2-sample problem.

We test $H_0 : \mu_X = \mu_Y$, in order to do so we need some assumptions about the distributions as well as i.i.d:

- $X \sim N(\mu_X, \Sigma)$ (cream)
- $Y \sim N(\mu_Y, \Sigma)$ (oat milk)

Note that they have the same variance.

- b) For Hotellings T^2 we need our hamburger

Normal	Wishart	Normal
--------	---------	--------

:

$$(\bar{X} - \bar{Y})^T S^{-1} (\bar{X} - \bar{Y})$$

- c) In b), we had S^{-1} which comes from S_{pooled} , which can be estimated by (we can do this since $\Sigma_X = \Sigma_Y$):

$$\frac{(n_1 - 1)S_1 + (n_2 - 1)S_2}{n_1 + n_2 - 2} \quad (3)$$

In order to determine the distribution of our estimation (3), we need to find the distribution of the terms:

- $(n_1 - 1)S_1 = \sum_{i=1}^{n_1} (X_i - \bar{X})(X_i - \bar{X})^T \sim W_4(\Sigma, n_1 - 1)$
- $(n_2 - 1)S_2 = \sum_{i=1}^{n_2} (X_i - \bar{X})(X_i - \bar{X})^T \sim W_4(\Sigma, n_2 - 1)$

We also know that Wishart + Wishart = Wishart if they are independent which we have assumed, so we get

$$(n_1 - 1)S_1 + (n_2 - 1)S_2 \sim W_4(\Sigma, n_1 + n_2 - 2)$$

With a scaling of $\frac{1}{n_1 + n_2 - 2}$ in front.

- d) To estimate S_1 , we need to ask ourselves if we are looking for a biased or unbiased estimate. We arrive at the following:

- *Biased*: $\frac{1}{n_1} \sum_{i=1}^{n_1} (X_i - \bar{X})(X_i - \bar{X})^T$
- *Unbiased*: $\frac{1}{n_1 - 1} \sum_{i=1}^{n_1} (X_i - \bar{X})(X_i - \bar{X})^T$

4. a) Recall that in CCA, the main task is to find linear combinations of $\left. \begin{matrix} U = a^T X \\ V = b^T Y \end{matrix} \right\}$ such that their

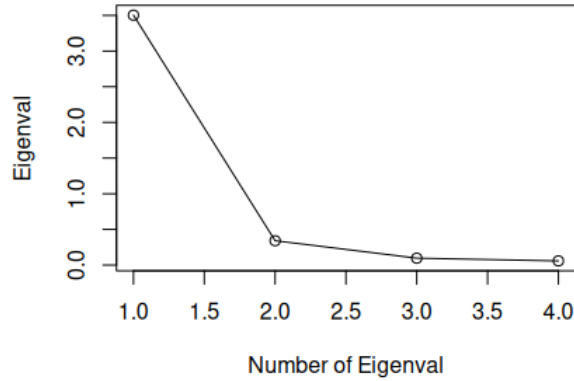
correlation is maximized and $\left. \begin{matrix} \text{Var}(U) = 1 \\ \text{Var}(V) = 1 \end{matrix} \right\}$

- b) In order to find the canonical variates, we can use Result 10.1 but we would need the eigenvalues of $\Sigma_{11}^{-1/2} \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \Sigma_{11}^{-1/2}$ which we can compute using R:

```
eigen() decomposition
$values
[1] 0.5458401879 0.0008598121
```

- c) Notice that the second eigenvalue is numerically 0 (i.e it does not contribute that much).

5. a) A scree plot is essentially a plot of $(x, y) = (\text{number of eigenvalue}, \text{eigenvalue})$. In our case, we can plot it by hand or in R to get the following:



- b) There are numerous methods to decide how many components to include in the study. We can use the elbow-method in the scree plot or we can use the explained variance proportion which is given by:

$$\frac{\sum_{j=1}^k \lambda_j}{\sum_{i=1}^n \lambda_i} = \text{variance explained by the } k\text{th eigenvalues}$$

Personally I would have used 2 components, since this seems to be the elbow in the scree plot. Computing the variance explained yields:

$$\frac{3.50293864 + 0.34142136}{3.50293864 + 0.34142136 + 0.09706136 + 0.05857864} \approx 96\% \text{ explained}$$

- c) By result 8.3, the first component is given by $[, 1]X$, and second component by $[, 2]X$
6. a) This is a matter of classification since we know the classes.
The ECM is given by:

$$p_1 P(2|1) c(2|1) + p_2 P(1|2) c(1|2) = \frac{1}{2} \int_{R_2} f_1(x) dx c + \frac{1}{2} \int_{R_1} f_2(x) dx c$$

- b) & c)

$$R_1 = \left\{ x : \frac{f_1(x)}{f_2(x)} \geq \frac{c(1|2)p_2}{c(2|1)p_1} \right\} \Leftrightarrow \left\{ x : \frac{f_1(x)}{f_2(x)} \geq 2 \right\}$$

8. We have multivariate regression, our assumption is independence.

11. OLD EXAM - TRAINING EXAM

Anmärkning: There are certain questions that have come in the homeworks, see respective homework solution.

4. a) The test problem that has been considered here is if the mean is $\begin{bmatrix} 60 \\ 29 \\ 60 \\ 1000 \end{bmatrix}$. This is a one sample T^2 test where we assume our data is i.i.d and normal.

- b) We know that we can express the T^2 distribution using the F distribution through the following relationship:

$$\left. \begin{matrix} T^2(p, n-1) \\ \text{sigma} \frac{(n-1)p}{n-p} F_{p, n-p} \\ n-p=199 \\ p=4 \end{matrix} \right\} n=403$$

- c) Yes they can if we look individually for each X_i , no if they are joint.
- d) We are not testing any interaction between the data points, only if they have the same value. The MANOVA model is therefore specified through:

$$X_{ij} = \mu + \alpha_i + \varepsilon_{ij} \quad H_0 : \alpha_i = 0 \quad \forall i$$

- e) Our assumptions correspond to the normal MANOVA assumptions, that is ε_{ij} is multivariate normal, data is independent across stations.
- f) We can use 2 methods, either the elbow method (subjective) or we fix an acceptable percentage of explained variance such as 95%.

- g) We sort our n eigenvalues, and then compute the k th component by: $\frac{\sum_{j=1}^k \lambda_j}{\sum_{i=1}^n \lambda_i}$

In our case, this yields $\frac{3}{3 + 0.6 + 0.3 + 0.1} = 75\%$

- h)

$$X = \mu + LF + \varepsilon \quad \text{Cov}(X) = LL^T + \Psi$$

Under rotation, this becomes:

$$L \mapsto LT \Rightarrow (LT)(LT)^T + \Psi = L^T T^T L^T + \Psi$$

We can see here that the matrix T did not disappear, so the communalities after rotations are not the same as the communalities before rotation they need to be rotated as well.

- i) PCA is dimension reduction while FA is environmental/causal stuff.

5. a) Y-axis groups distance, so if three clusters are desired then we pick those top 3 highest Y values $\Rightarrow 29, 6, 12$
- b) Using the max CH-index, we get 3 clusters.
- c) In k -means, the data needs to be standardized and the $nstart$ is too low otherwise it would be unstable.

12. OLD EXAM 2021-01-11

2. a) A useful model could be $\underbrace{X_{ij}}_{4 \times 1} = \mu + \underbrace{\alpha_i}_{\text{brand}} + \varepsilon_{ij}$, here we test if the mean is the same across all $\alpha_i = 0 \quad \forall i$

- b) Mathematically, the testing problem can be expressed as the following:

$$H_0 : \alpha_i = 0 \quad \forall i = 1, 2, 3, 4$$

Identification restriction is given by $\Sigma \alpha_i = 0$

- c)

$$\sum_{i=1}^4 \sum_j (X_{ij} - \bar{X})(X_{ij} - \bar{X})^T = B + W$$

Here the B is the *between* sum of squares (compares observations between groups)

Here the W is the *within* sum of squares (compares observations between each group)

- d) $H = : \mu = \mu_0 \quad X_1, \dots, X_n \sim N(\mu, \Sigma)$. Testing normal mean

3. If $m \neq n$, then we can exclude the "paired data test" directly since they need to have the same dimensions

- a) We are therefore testing $\mu_X = \mu_Y$

- b) Only S_{pooled} is for 2-sample test (which is what we have for this case)

What we do is assume $\Sigma_1 = \Sigma_2$ and estimate by Chapter 6 p.10:

$$S_{\text{pooled}} = \frac{\sum_{j=1}^{n_1} (X_{1j} - \bar{X}_1)(X_{1j} - \bar{X}_1)^T + \sum_{j=1}^{n_2} (X_{2j} - \bar{X}_2)(X_{2j} - \bar{X}_2)^T}{n_1 + n_2 - 2} = \frac{(n_1 - 1)S_1}{n_1 + n_2 - 2} + \frac{(n_2 - 1)S_2}{(n_1 + n_2 - 2)}$$

Before we proceed with showing which distribution, it will be easier if we first do c) and then use the results here

- c)

$$S_1 = \frac{1}{n-1} \sum (X_{ij} - \bar{X})(X_{ij} - \bar{X})^T \quad \text{for unbiased}$$

$$S_1 = \frac{1}{n} \sum (X_{ij} - \bar{X})(X_{ij} - \bar{X})^T \quad \text{for MLE}$$

$$\Rightarrow \sum_{j=1}^n (X_j - \bar{X})(X_j - \bar{X})^T \sim W_p(\Sigma, n-1)$$

$$\Rightarrow S_1 \text{ is Wishart} \Leftrightarrow (n_1 - 1)S_1 \text{ is Wishart}$$

$$\Rightarrow S_{\text{pool}} \sim W_p(\Sigma, n_1 - 1) + W_p(\Sigma, n_2 - 1) \Rightarrow (n_1 + n_2 - 2)S_{\text{pool}} = W_p(\Sigma, n_1 + n_2 - 2)$$

Due to the independance, Wishart + Wishart is still Wishart.

If we test the mean of the first sample, can we get Hotellings T^2 ?

$$\bar{X} \sim N(\mu, \Sigma) \Rightarrow n(\bar{X} - \mu_X) \sim N(0, \Sigma)$$

- d) Σ is common for both samples. We shall use some results from S_{pool} :

$$X_1, \dots, X_{n_1} \sim N\left(\mu_X, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}\right)$$

$$Y_1, \dots, Y_{n_2} \sim N\left(\mu_Y, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}\right)$$

If we only care about Σ_{11} then for every observation we take out the first 2 since:

$$\begin{aligned} \forall X_i \quad \begin{bmatrix} X_{i1} \\ X_{i2} \\ X_{i3} \\ X_{i4} \end{bmatrix} &\rightarrow \begin{bmatrix} X_{i1} \\ X_{i2} \end{bmatrix} \\ \forall Y_i \quad \begin{bmatrix} Y_{i1} \\ Y_{i2} \\ Y_{i3} \\ Y_{i4} \end{bmatrix} &\rightarrow \begin{bmatrix} Y_{i1} \\ Y_{i2} \end{bmatrix} \end{aligned}$$

\Rightarrow the estimator has distribution $W_2(\Sigma_{11}, n_1 + n_2 - 2)$

- e) In order to use $ny^T M^{-1}y \sim T^2(\Sigma, n)$, we need $\bar{x} \sim N(0, \Sigma)$ and $M \sim W(\Sigma, n)$ (where they share Σ):

$$\begin{aligned} \bar{x} &\sim N(\mu, \Sigma_{11}/n) \Rightarrow \sqrt{n}(\bar{x} - \mu_1) \sim N(0, \Sigma_{11}) = y \\ (n_1 + n_2 - 2)S_{\text{pool}} &= M \end{aligned}$$

For two-sample testing:

$$\begin{aligned} (\bar{x} - \bar{y}) &\sim N\left([\mu_{X_1} - \mu_{Y_1}], \left(\frac{1}{n_1} + \frac{1}{n_2}\right) \Sigma_{11}\right) \\ \Rightarrow \frac{1}{\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} [\bar{x} - \bar{y} - (\mu_{X_1} - \mu_{Y_1})] &\sim N(0, \Sigma_{11}) \end{aligned}$$