

# TTK4260

## Multivariate data analysis and machine learning

by Jan-Øivind Lima

Notes from exam preparation

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### §1. Introductions and motivations

The overarching workflow for data analysis is seen below:

#### Example (The main piece of the data analysis workflow).

- Consider the best approach given the data and objective
- Split the data into training/validation/test
- Decide on preprocessing of the training data; save this procedure for validation and test sets
- Proposing some alternative models
- Estimating the model parameters
- Choosing the best model structure
- Model interpretation given background knowledge (theory, literature, own experience)
- Identify possible outliers and decide whether to take them out or not
- Validating the chosen model(s)
- Estimating the performance of the model, including parameter uncertainties

For modeling there are several strategies to employ, here are a few of them.

- Mechanistic models / physics based models: based on theory, first principles and/or domain knowledge (deduction)

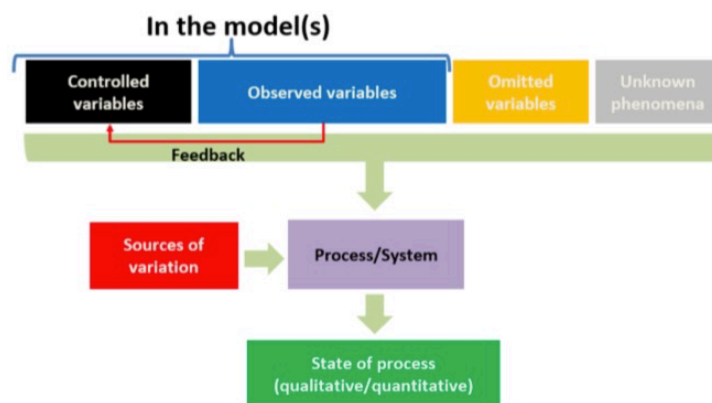


Figure 1: Variables in a system

- Data-driven models: Models based on carefully designed experimental (numerical or physics) data. They can be black box, grey box or white box (induction)
- Meta Modelling / Hybrid Modelling: A combination of the above two.

Some desired characteristics in the modeling approach are:

- Generalizability / Robustness
- Trustworthiness / Transparent / Explainable
- Computational efficiency yet accurate
- Dynamically adapting and evolving

### §1.1. Dimensionality of a model

Most systems are observed with more sensors/variables than the actual underlying dimensionality (rank). Methods based on latent variables will summarize the information in terms of “super variables” and reveal the individual variable’s contribution to these. The rank of a system can mean different things:

- The **numerical** rank (This will for all real data be the smallest dimension of the data table)
- The **statistical** rank (found by some statistical criterion, e.g. the chosen validation scheme or maximum likelihood)
- The **application** specific rank based on experience and interpretation

### §1.2. Redundancy and selectivity

Tool	Symbol	Purpose
TTK4260 Multivariat dataanalyse og maskinl�ring (2025 V�r) Design of experiments (DoE) Full and Fractional Factorial Designs, Optimisation Designs		Gain maximum information from a minimum of experimental effort
Exploratory Data Analysis (EDA)		Find important sample groups or variable relationships in large data sets. Define classes.
Classification/Discrimination		Classify samples. Identify raw materials. Is the process under control (MSPC)?
Regression and Prediction		Predict quality for new samples and/or find out which variables that most influence a process

Figure 2: Tools used in this course

Most sensors are not measuring directly the inherent state or property of a system. Although individual sensors are not selective, we can still use them for observing the system:

- **Qualitative:** Is the system under control?
- **Quantitative:** What is the water content in this rock on Mars?

### §1.3. Typical pitfalls for validation of classification or prediction models

- No independent test set
- Replicates in training and test sets respectively
- Use information in the model that is not present during prediction (for example using time as a variable)
- Selection bias (especially when tuning hyper-parameters)
- Extending sample sets with simulated samples to e.g. handle skewed distributions, then split in training/test
- Feature selection on all data, then split in training/test (see above)
- **And what is not often mentioned: Random training/test when the samples must be stratified due to meta-information**

## §2. Principal Component Analysis (PCA) introduction

PCA is the “mother” of all exploratory multivariate methods, below are some examples demonstrating the need/utility of the exploratory data analysis.

### Example.

- Pattern recognition
- Dimensionality reduction
- Clustering and classification
- Outlier detection
- Condition monitoring and predictive maintenance, e.g. of wind turbines
- Denoising
- Data imputation
- Speed up training of machine learning models (using latent variables)

## §3. Least squares estimators

Introductory definitions:

- $y \in \mathcal{Y}$  : random variable (r.v.) from a probability distribution  $P$ :

$$y \sim P(\theta) \quad \theta \in \Theta$$

(Example:  $y \sim \mathcal{N}(m, \sigma^2)$ )

- $y_1, \dots, y_N = \mathbf{y} \in \mathcal{Y}^N$  : sampled data

#### Definition (statistic)

$$\phi(\mathbf{y}) : \mathcal{Y}^N \mapsto \mathbb{R}^M$$

is a *statistic* of  $\mathbf{y}$  if

- it is measurable
- it does not depend on  $\theta$

Figure 3: Introductory definitions of least squares estimators

### §3.1. Estimator

#### Estimator of $\theta$

- $y \in \mathcal{Y}$  : random variable (r.v.) from a probability distribution  $P$ :

$$y \sim P(\theta) \quad \theta \in \Theta$$

- $y_1, \dots, y_N = \mathbf{y} \in \mathcal{Y}^N$  : sampled data

#### Definition (estimator (of $\theta$ ))

any statistic of  $\mathbf{y}$  with co-domain equal to  $\Theta$ , i.e., any

$$\phi(\mathbf{y}) : \mathcal{Y}^N \mapsto \Theta$$

that

- is measurable
- does not depend on  $\theta$

Figure 4: Estimator

### §3.2. Least squares form geometrical interpretations

First the assumptions:

data generation model:  $y_t = f(u_t; \theta) + v_t$

dataset:  $\mathcal{D} = \{(u_t, y_t)\}_{t=1, \dots, N}$

hypothesis space:  $\theta \in \Theta$

Problem: *find a  $\hat{\theta} \in \Theta$  that "best explains"  $\mathcal{D}$*

Figure 5: Assupptions for model.

This leads to the geometrical interpretation:

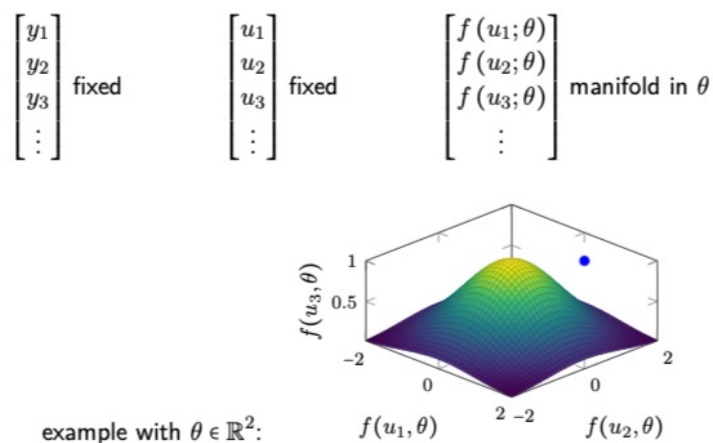


Figure 6: Geometrical interpretation of least squares

## §4. Statistical performance indexes

There are three measures of central tendencies, they are **mode**, **median** and **mean**.

### Example.

- **Mode**: most commonly observed value
- **Median**: midpoint
- **Mean**: average

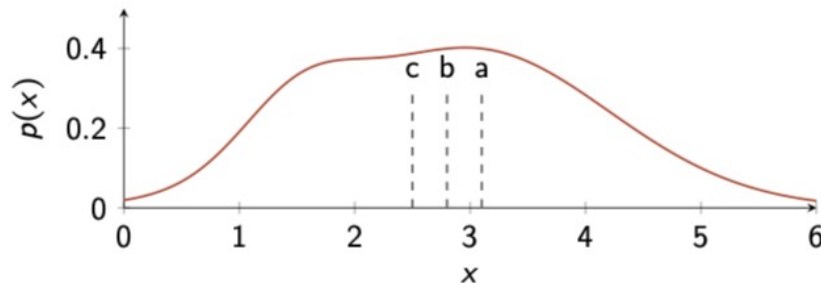


Figure 7: Central tendency

Measures of dispersion are **range**, **variance** and **standard deviation**.

### Example.

- **Range**: maximum - minimum
- **Variance**: mean of the squared differences between the elements of a dataset and their mean
- **Standard deviation**: square root of the variance

Measures of association are **covariance** and **correlation**.

### Example.

- **Covariance**: measure of the joint variability of two random variables

- **Correlation:** measure of the strength and direction of the linear relationship between two random variables

Some other measures are **skewness** and **kurtosis**:

**Example.**

- **Skewness:** how symmetric a probability distribution is
- **Kurtosis:** how tailed a probability distribution is

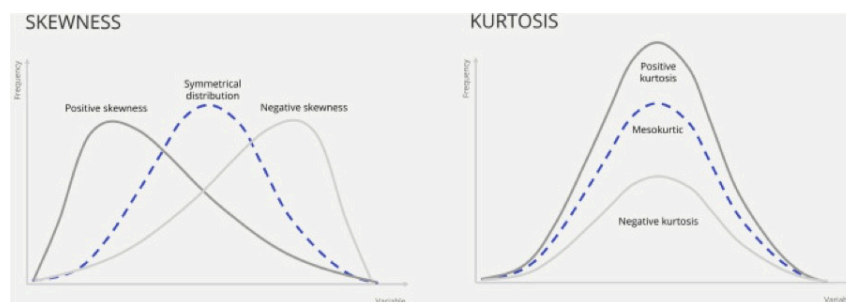


Figure 8: Skewness and kurtosis

Some units discussed in the lecture:

**Example.**

- regression metrics (MAE, MSE, RMSE, R2)
- classification metrics (accuracy, precision, recall, F1-score, sensitivity, specificity, ROC, AUC)
- Computer Vision metrics (PSNR, SSIM, IoU)
- timeseries related metrics (fit)

## §4.1. Regression metrics

Mean absolute Error (MAE) is the average of the absolute differences between predicted and actual values.

**Definition 4.1.1.**

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$$

- $y_i$  = measured value
- $\hat{y}_i$  = predicted value
- $n$  = # of observations

Mean Squared Error (MSE) is the average of the squared differences between predicted and actual values.

**Definition 4.1.2.**

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

- $y_i$  = measured value
- $\hat{y}_i$  = predicted value
- $n$  = # of observations

Root mean squared error (RMSE) is the square root of the mean of the squared differences between predicted and actual values.

**Definition 4.1.3.**

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$$

- $y_i$  = measured value
- $\hat{y}_i$  = predicted value
- $n$  = # of observations

$R^2$  or the coefficient of determination is the proportion of variance in the dependent variable that can be explained by the independent variable(s).

**Definition 4.1.4.**

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y}_i)^2} = 1 - \left( \frac{\mathbb{S}_{\text{res}}}{\mathbb{S}_{\text{tot}}} \right)$$

- $y_i$  = measured value
- $\hat{y}_i$  = predicted value
- $n$  = # of observations
- $\bar{y}_i$  = sample mean of the  $y_i$ 's
- $\mathbb{S}_{\text{res}}$  = residual sum of squares
- $\mathbb{S}_{\text{tot}}$  = total sum of squares

Comparison of **MSE**, **MAE** and  **$R^2$** :

<b>MSE</b>	<b>MAE</b>	<b><math>R^2</math></b>
based on square error	based on the absolute value	based on correlation between actual and predicted value
value lies between 0 and $+\infty$	value lies between 0 and $+\infty$	value lies between $-\infty$ and 1
most sensitive to outliers	least sensitive to outliers	in-between sensitive to outliers
small value indicates better model	small value indicates better model	value near 1 indicates better model

## §4.2. Classification metrics

When performing classification we have different outcomes, they can be seen in the Figure 9. An important definition is the types of errors that can occur:

**Example.**

- False positive (**FP**): incorrectly predicted positive class (**Type I error**)
- False negative (**FN**): incorrectly predicted negative class (**Type II error**)

		actual condition	
		true	false
test outcome	positive	true positive	false positive
	negative	false negative	true negative

Figure 9: False positive and false negative etc...

## §4.3. Accuracy, recall, precision and F1-score

Accuracy is the ratio of correctly predicted instances to the total instances.

**Definition 4.3.1 (Accuracy).**

$$\text{Accuracy} = \frac{TP + TN}{\sum(TP + TN + FP + FN)}$$

Recall (*or sensitivity*) is the ratio of correctly predicted positive observations to all actual positive observations.

**Definition 4.3.2 (Recall/sensitivity).**

$$\text{Recall} = \frac{\sum TP}{\sum(TP + FN)}$$

Precision is the ratio of correctly predicted positive observations to the total predicted positive observations.

**Definition 4.3.3 (Precision).**

$$\text{Precision} = \frac{\sum TP}{\sum(TP + FP)}$$

F1-score is the weighted average of precision and recall.

**Definition 4.3.4 (F1-score).**



$$\text{F1-score} = \frac{2 * (\text{Precision} * \text{Recall})}{\text{Precision} + \text{Recall}}$$

When designing the classifier there are some rules of thumb to follow:

**Example.**

- **recall:** maximize this if false negatives are more costly
- **precision:** maximize this if false positives are more costly
- **F1 score:** maximize this if costs are similar and you want a balanced performance

We can visualize this with a ROC-curve<sup>1</sup>:

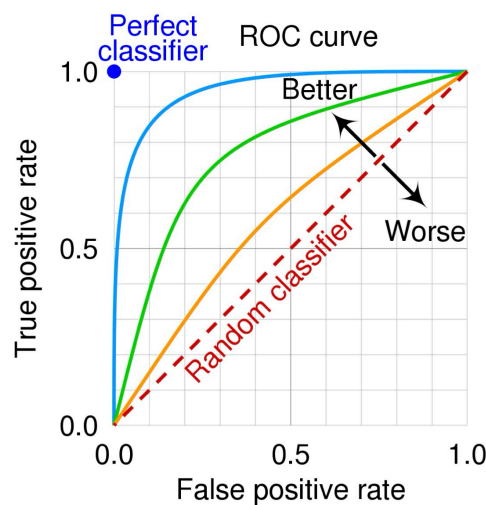


Figure 10: ROC-curve

**Example.**

- **High Sensitivity & Low Specificity:** you capture most positive instances but might misclassify many negative instances as positive. Appropriate only when detecting all positive instances is crucial, even if it raises false alarms
- **High Specificity & Low Sensitivity:** you correctly identify negative instances but might miss many positive instances. Appropriate when avoiding false positives is crucial, even if it means increasing the false negatives
- **High Sensitivity & High Specificity:** you rock!

#### §4.4. Metrics for computer vision

In computer vision we have some other metrics that are used. They are **PSNR**, **SSIM** and **IoU**.

Peak signal-to-noise ratio (PSNR) is a *maximum possible power of a signal / power of the noise that corrupts the signal*. The formula for PSNR is:

<sup>1</sup>ROC: receiver operating characteristic

**Definition 4.4.1 (PSNR).**

$$\text{PSNR} = 10 * \log_{10} \left( \frac{\text{MAX}^2}{\text{MSE}} \right)$$

- MAX = maximum possible pixel value of the image (usually 255 for 8-bit images)
- MSE = Mean Squared Error between the original and the compressed image

SSIM (Structural Similarity Index) is a *type of similarity between two images; intuitively, prediction of the quality of the second image as a distorted version of the first one, intended as distortion-free* The formula for SSIM is:

**Definition 4.4.2 (SSIM).**

$$\text{SSIM} = \frac{(2\mu_x\mu_y + c_1)(2\sigma_{xy} + c_2)}{(\mu_x^2 + \mu_y^2 + c_1)(\sigma_x^2 + \sigma_y^2 + c_2)}$$

- $\mu_x, \mu_y$  = average pixel intensity of the two images
- $\sigma_x^2, \sigma_y^2$  = variance of the two images
- $\sigma_{xy}$  = covariance between the two images
- $c_1, c_2$  = constant used to stabilize the division

Intersection over Union (IoU) is a metric used to evaluate the performance of an object detection model. It measures the overlap between the predicted bounding box and the ground truth bounding box. The formula for IoU is:

**Definition 4.4.3 (IoU).**

$$\text{IoU} = \frac{\text{Area of overlap}}{\text{Area of union}} = \frac{TP}{TP + FP + FN}$$

- Area of overlap = area of the intersection between the predicted and ground truth bounding boxes
- Area of union = area of the union between the predicted and ground truth bounding boxes

## §4.5. Metrics for time series

In addition to MSE, RMSE and MAE we also have (goodness of) fit.

**Definition 4.5.1 (Fit).**

$$\text{fit} = 100 \cdot \left( 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i y_i^2} \right)$$

## §5. Maximum likelihood

**Why something more than least squares?**

- (I.e., why do we introduce maximum likelihood estimators?)

**answer:** to include information about the statistical distribution of the measurement noise (and also to facilitate quantification of uncertainties)

**caveat:** by extending LS into ML, we “inject” assumptions. If the assumptions are good then ok, if they are bad then “not so ok”

### §5.1. Types of probability distributions

**Example.**

- Uniform
- Exponential
- Poisson
- Gamma
- Beta
- Binomial
- Log-normal
- Normal

**Definition 5.1.1 (Uniform).**

$$f(x|a, b) = \begin{cases} \frac{1}{b-a} & \text{if } a \leq x \leq b \\ 0 & \text{otherwise} \end{cases}$$

**Definition 5.1.2 (Exponential).**

$$f(x|\lambda) = \lambda e^{-\lambda x}$$

**Definition 5.1.3 (Binomial).**

$$f(x|n, p) = \frac{n!}{(n-x)!x!} p^x (1-p)^{n-x}$$

- n = number of trials
- x = number of successes
- p = probability of success for each trial

**Definition 5.1.4 (Poisson).**

$$f(x|\lambda) = \frac{\lambda^x e^{-\lambda}}{x!}$$

**Definition 5.1.5 (Beta).**

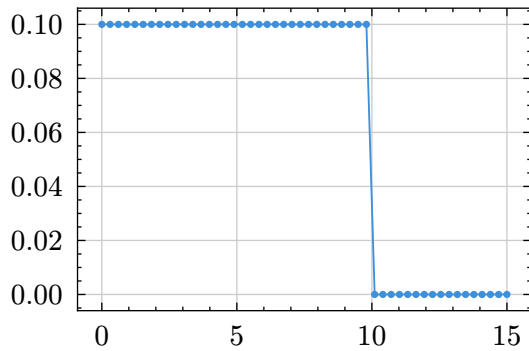
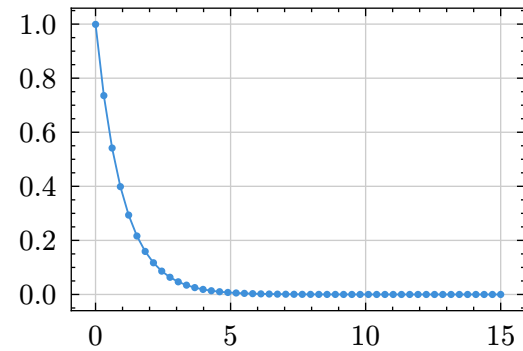
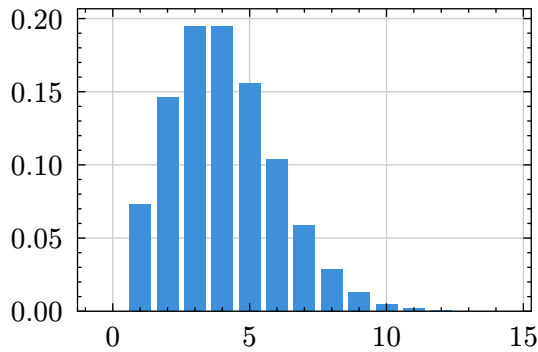
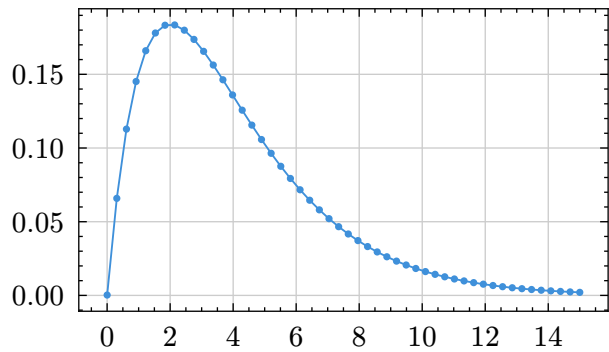
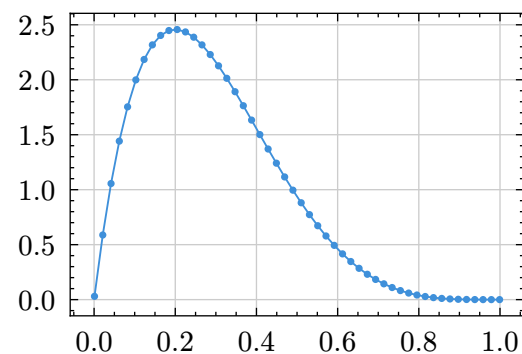
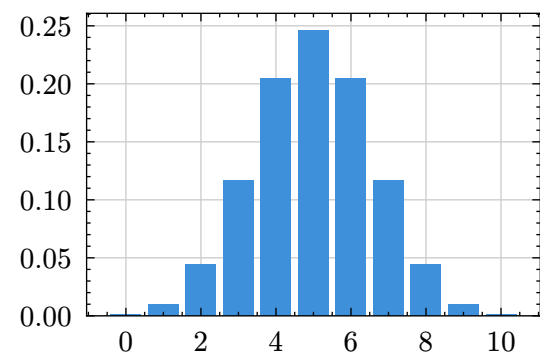
$$f(x|\alpha, \beta) = \frac{1}{B(\alpha, \beta)} (x^{\alpha-1} (1-x)^{\beta-1})$$

- $\alpha$  and  $\beta$  = shape parameters
- $B(\cdot, \cdot)$  = beta function

**Definition 5.1.6 (Normal).**

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

- $\mu$  = mean
- $\sigma$  = standard deviation

Figure 11: Uniform Distribution  $U(0, 10)$ Figure 12: Exponential Distribution  $\lambda = 1$ Figure 13: Poisson Distribution  $\lambda \approx 4$ Figure 14: Gamma Distribution  $k=2, \theta=2$ Figure 15: Beta Distribution  $\alpha=2, \beta=5$  (scaled)Figure 16: Binomial Distribution  $n=10, p=0.5$

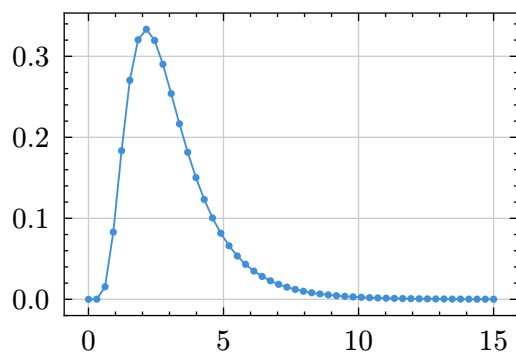


Figure 17: Log-normal Distribution  $\mu=1$ ,  $\sigma=0.5$

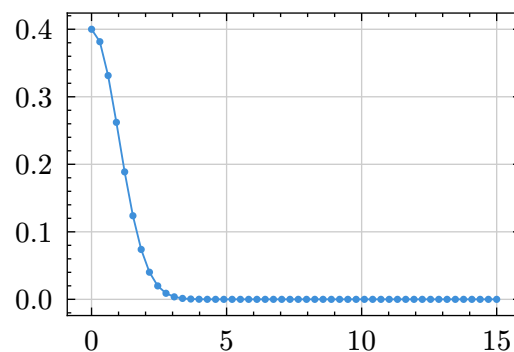


Figure 18: Normal Distribution  $\mu=0$ ,  $\sigma=1$

## §5.2. Probability vs. likelihood

## §6. Potential exam questions (*provided on BlackBoard*)

### Q&A 6.1.

- *What do we mean with internal and external validity? May you make some practical examples?*
  - Internal validity refers to the degree to which a study accurately identifies a causal relationship between variables, by controlling for confounders. For example, a lab experiment with randomized groups. External validity refers to the generalizability of findings to other populations or settings, e.g., applying lab results to real-world patients.

### Q&A 6.2.

- *What are least squares estimators? What is the geometrical intuition behind them? And how can they be formulated mathematically?*
  - Least squares estimators minimize the sum of squared differences between observed and predicted values. Geometrically, this corresponds to projecting the observation vector onto the space spanned by the regressors. Mathematically:  $\hat{\vartheta} = (X^T X)^{-1} X^T y$ .

### Q&A 6.3.

- *What are maximum likelihood estimators? What is the probabilistic intuition behind them? And how can they be formulated mathematically?*
  - Maximum likelihood estimators choose parameters that make the observed data most probable. The idea is to find the parameter  $\vartheta$  that maximizes the likelihood function  $L(\vartheta|\text{data})$ . For independent samples, this often involves maximizing the product (or log-sum) of densities.

### Q&A 6.4.

- *Why should one divide a dataset into training, test, and validation sets? And how should one select such sets from the original dataset?*

- Splitting data ensures that the model is trained, tuned, and tested on separate sets to avoid overfitting and evaluate generalization. Randomly shuffle and divide data, or use stratified sampling if class imbalance exists.

#### Q&A 6.5.

- *What does cross validation mean? How should it be used? And why should one use a cross validation approach instead of using a training, test, and validation sets based approach?*
  - Cross-validation involves dividing data into  $k$  folds, training on  $k-1$  and testing on the remaining one, iteratively. It gives a robust estimate of model performance and is preferred when limited data makes a fixed split unreliable.

#### Q&A 6.6.

- *What are maximum a posteriori estimators? What is the probabilistic intuition behind them? And how can they be formulated mathematically?*
  - MAP estimators maximize the posterior probability of parameters, combining prior beliefs and observed data. It's like MLE but includes a prior:  $\hat{\vartheta} = \operatorname{argmax} P(\vartheta|\text{data}) \propto P(\text{data}|\vartheta)P(\vartheta)$ .

#### Q&A 6.7.

- *What are the conditions about existence and uniqueness of the LS, ML and MAP estimates?*
  - LS and ML estimates require full column rank in the design matrix for a unique solution. MAP adds a prior, which can ensure uniqueness even in ill-posed problems if the prior is well-formed.

#### Q&A 6.8.

- *Derive the maximum likelihood estimator for the separable problem  $y_i = \vartheta u_i + v_i$  with  $v_i \sim N(0, \sigma^2)$  with  $\sigma^2$  known,  $\vartheta$  unknown and deterministic*
  - The likelihood is a product of Gaussians. Taking the log, differentiating, and solving gives  $\hat{\vartheta} = (\sum u_i^2)^{-1} \sum u_i y_i$ , which minimizes squared residuals, same as LS here.

#### Q&A 6.9.

- *Derive and comment the bias-variance tradeoff*
  - Expected error = bias<sup>2</sup> + variance + irreducible noise. Complex models have low bias, high variance (overfit); simple models have high bias, low variance (underfit). The goal is a balanced model minimizing total error.

#### Q&A 6.10.

- *What do we expect to see when training and testing different estimators with different model order complexities? How should we account for the effects that we see on the statistical performance indexes?*
  - As complexity increases, training error typically decreases, but test error may rise due to overfitting. This is seen as a U-shaped curve in validation error. Use cross-validation and penalized metrics (e.g., AIC, BIC) to choose optimal complexity.

**Q&A 6.11.**

- *Which statistical performance indexes would you consider when dealing with a regression problem? And which peculiarities / usages do they have?*
  - MSE and RMSE measure average error; MAE is less sensitive to outliers;  $R^2$  indicates explained variance. Choose based on robustness or interpretability needs.

**Q&A 6.12.**

- *Which statistical performance indexes would you consider when dealing with a classification problem? And which peculiarities / usages do they have?*
  - Accuracy, precision, recall, F1 score. Precision-recall better for imbalanced data. ROC AUC shows tradeoff over thresholds.

**Q&A 6.13.**

- *What does “design of experiments” mean? And “factorial design”? Which alternative factorial-design based alternatives do you know, and what are the tradeoffs among them?*
  - DOE is planning experiments to extract information efficiently. Full factorial tests all variable combinations. Alternatives like fractional factorial reduce experiments at cost of detail.

**Q&A 6.14.**

- *What does PCA mean from a geometrical point of view? How is it formulated mathematically, and how does it connect with SVD?*
  - PCA finds directions (principal components) of maximal variance. Mathematically via eigendecomposition or SVD of the data matrix. PCs are orthogonal axes of variation.

**Q&A 6.15.**

- *What are the uses of PCA? And how can its results be interpreted?*
  - PCA is used for dimensionality reduction, denoising, and visualization. Loadings show how variables contribute; scores show sample projections.

**Q&A 6.16.**

- *What are the uses of the loadings plots and scores plots, in a PCA?*
  - Loadings plot shows how variables contribute to PCs. Scores plot shows patterns or clusters among samples in the reduced space.

**Q&A 6.17.**

- *How can one decide how many components should be used when analysing some data through PCA? And how can one decide whether a sample is an outlier or not, through PCA?*
  - Use scree plots or cumulative explained variance. Outliers are samples with high score distance or reconstruction error.

**Q&A 6.18.**

- *How does the Ockham's razor principle connect with the model order selection problem? Which alternative strategies can be used to solve the model order selection problem?*
  - Prefer the simplest model that explains the data well. Strategies include AIC, BIC, cross-validation, and hypothesis testing.

**Q&A 6.19.**

- *What does "rotated PCA" mean? How does this concept connect with PCA, from both geometrical and mathematical points of view?*
  - Rotation (e.g., varimax) simplifies interpretation by redistributing variance across PCs while keeping orthogonality. Enhances variable grouping.

**Q&A 6.20.**

- *Which type of problems does the ICA algorithm solve? Which assumptions does it require? And how does it work, from intuitive perspectives?*
  - ICA separates mixed signals into independent sources (e.g., blind source separation). Assumes statistical independence and non-Gaussianity.

**Q&A 6.21.**

- *What does "total least squares" mean? How does this concept connect with least squares, from both geometrical and mathematical points of view?*
  - TLS accounts for noise in both X and y. Geometrically, it minimizes orthogonal distances to the model plane, unlike LS which only minimizes vertical distance.

**Q&A 6.22.**

- *What does ANOVA mean? Which type of analyses does this approach serve? How is it formulated mathematically, and how can one use it in practice?*



- ANOVA tests differences between group means. It partitions variance into within- and between-group components and uses F-tests for inference.

#### Q&A 6.23.

- *What does PLS mean? Which type of analyses does this approach serve? How is it formulated mathematically, and how can one use it in practice?*
  - PLS projects X and y to latent variables that maximize covariance. Useful when predictors are many and collinear. Combines features of PCA and regression.

#### Q&A 6.24.

- *What does MLR mean? Which type of analyses does this approach serve? How is it formulated mathematically, and how can one use it in practice?*
  - MLR models the linear relation between multiple inputs and an output.  $y = X\beta + \epsilon$ , estimated by LS. Used for prediction and inference.

#### Q&A 6.25.

- *What does PCR mean? Which type of analyses does this approach serve? How is it formulated mathematically, and how can one use it in practice?*
  - PCR uses PCA to reduce dimensionality of X, then applies regression on components. Helps when predictors are correlated.

#### Q&A 6.26.

- *How do PLS, MLR, and PCR relate to each other? In which cases does one expect one of them to work better than the other ones, and viceversa?*
  - MLR works if predictors are uncorrelated. PCR reduces dimensions blindly. PLS considers both X and y and often performs best with collinearity or few samples.

#### Q&A 6.27.

- *What is the NIPALS algorithm? How does it work, from a graphical perspective? Which advantages does it bring over SVD, when used to compute a PCA?*
  - NIPALS computes components iteratively, one at a time. Useful for large or incomplete datasets. More flexible than full SVD.

#### Q&A 6.28.

- *What does metamodeling mean? When would one want to use a metamodeling approach? What are the potential shortcomings of a metamodel?*
  - Metamodels approximate complex models using simpler ones. Useful for simulation or optimization. Downsides: potential inaccuracy, limited extrapolation.

**Q&A 6.29.**

- What do “stationarity” and “ergodicity” mean? Why are these two concepts important when dealing with statistical analyses of time series? And what would the lack of stationarity and ergodicity imply in practice?
  - Stationarity: statistical properties don’t change over time. Ergodicity: averages over time  $\approx$  averages over ensemble. Lack of these breaks model assumptions.

**Q&A 6.30.**

- Which LTI model structures do you know that are suitable to do control-oriented modelling of discrete time MISO systems?
  - ARX, ARMAX, OE, and Box-Jenkins. Choice depends on noise and model goals. ARX is simplest, BJ most flexible.

**Q&A 6.31.**

- What is the principle behind prediction error methods? When should the focus be on prediction errors, when identifying a dynamical model?
  - PEM minimizes the difference between observed and predicted outputs. Focus on prediction errors when the model is used for forecasting or simulation.

**Q&A 6.32.**

- What are the implications of choosing an ARX, instead of an ARMAX, instead of an OE model structure when doing system identification? And what are the implications of choosing different model orders? How should one choose a specific structure and order?
  - ARX is fast but sensitive to noise. ARMAX models noise more accurately. OE assumes noise-free input. Choose structure by validation and orders via AIC/BIC.

**Q&A 6.33.**

- What are Hammerstein Wiener models, and what are their usages?
  - They model nonlinear dynamics via static nonlinearity + linear dynamic blocks. Useful for control systems with known nonlinearity.

**Q&A 6.34.**

- What is a  $p$  value? How should it be computed? What is its usage for? And its drawbacks?
  - $p$ -value is the probability of seeing data as extreme as observed, under  $H_0$ . Computed from test statistic distribution. Misuse includes binary cutoff thinking.

**Q&A 6.35.**

- What is a statistical test? How can it be interpreted from geometrical perspectives? And from mathematical perspectives?

- A statistical test evaluates hypotheses using data. Geometrically, compares projections. Mathematically, tests whether a statistic lies in a rejection region.

**Q&A 6.36.**

- *What are the statistical performance indexes associated to a statistical test? And which concepts may one use to say that a test is “better” than another one?*
  - Power, significance level, Type I/II error rates. Better tests have higher power for fixed significance. UMP tests are optimal under specific conditions.

**Q&A 6.37.**

- *What are the differences between simple and composite hypotheses? How do the formulations of hypothesis testing algorithms change, depending on which type of hypothesis is considered?*
  - Simple: fully specified distributions. Composite: parameters unknown. Composite tests often require approximations or likelihood ratios.

**Q&A 6.38.**

- *What does the Linear Discriminant Analysis algorithm do? How? Which advantages and disadvantages does it have?*
  - LDA finds projection that separates classes based on class means and shared covariance. Works well with Gaussian data, struggles with nonlinear boundaries.

**Q&A 6.39.**

- *What does the Partial least squares discriminant analysis algorithm do? How? Which advantages and disadvantages does it have?*
  - PLS-DA adapts PLS for classification, modeling latent structures in predictors to distinguish classes. Good with multicollinearity, less interpretable.

**Q&A 6.40.**

- *What does the logistic regression algorithm do? How? Which advantages and disadvantages does it have?*
  - Models class probabilities using a sigmoid function over linear combinations. Interpretable but limited to linear decision boundaries.

**Q&A 6.41.**

- *What does the Support Vector Classification algorithm do? How? Which advantages and disadvantages does it have?*
  - SVC finds hyperplanes maximizing class margins. Effective in high dimensions. Requires tuning and can be slow for large datasets.

**Q&A 6.42.**

- *What is the kernel trick? Where may one use it, and why?*
  - Maps data to high dimensions via kernels without explicit computation. Enables nonlinear classification or PCA efficiently.

**Q&A 6.43.**

- *What does the K-means algorithm do? How? Which advantages and disadvantages does it have?*
  - K-means partitions data into k clusters by minimizing within-cluster variance. Simple and fast, but assumes spherical clusters and needs k known.

**Q&A 6.44.**

- *What does the DBSCAN algorithm do? How? Which advantages and disadvantages does it have? What are its differences with the k-means algorithm?*
  - Density-based clustering; identifies noise and arbitrarily shaped clusters. Unlike k-means, doesn't require number of clusters but sensitive to parameters.

**Q&A 6.45.**

- *What do decision trees and random forests do? How? Which advantages and disadvantages do they have?*
  - Trees split data based on features. Forests average over many trees to reduce overfitting. Trees are interpretable, forests are more accurate.

**Q&A 6.46.**

- *What is the need for features selection? And what are the differences between feature engineering and selection?*
  - Reduces overfitting and improves interpretability. Selection chooses from existing features; engineering creates new informative features.

**Q&A 6.47.**

- *What are the pros and cons of using a wrapper method for feature selection, or an embedded method for the same sake?*
  - Wrappers use model feedback, often more accurate but slower. Embedded methods (e.g., Lasso) are faster but model-dependent.

**Q&A 6.48.**

- *Why is categorical cross entropy loss used instead of mean squared error as a cost function in classification problems as against the regression problems?*

- Cross-entropy measures divergence between predicted and true class probabilities, offering better gradients and performance than MSE in classification.

**Q&A 6.49.**

- *Which regularization technique is more effective in feature selection? And why?*
  - L1 (Lasso) is better than L2 (Ridge) for selection because it shrinks some coefficients to zero, effectively removing features.