MA8701 Advanced methods in statistical inference and learning

P1W1: Core concepts in statistical decision theory

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Messages to students

Course homepage:
https://wiki.math.ntnu.no/ma8701/2025v/start

- Read before the W1-lecture: ESL 2.2, 2.4, 3 (except 3.2.3, 3.2.4, 3.4, 3.7, 3.8), 4.1-4.5 (except 4.4.4). The only new topic (not taught in recommended courses) is 2.4.
- Work on exercises in the bottom of this page after the W1-lecture.

Learning

Herbert A. Simon (Cognitive science, Nobel Laureate): *Learning results from what the student does and thinks and only from what the student does and thinks. The teacher can advance learning only by influencing what the student does to learn.*

Plan for W1

- Notation (ESL Ch 2.2)
- Regression - should be known from before (ESL Ch 3, except 3.2.3, 3.2.4, 3.4, 3.7, 3.8)
- Statistical decision theoretic framework for regression (ESL 2.4)
- Classification - should be known from before (ESL Ch 4.1-4.5, except 4.4.4)
- Statistical decision theoretic framework for classification (ESL 2.4)

Core concepts

Notation

(mainly from ESL 2.2)

We will only consider supervised methods.

- Response Y (or G): dependent variable, outcome, usually univariate (but may be multivariate)
  - quantitative Y: for regression
  - qualitative, categorical G: for classification, some times dummy variable coding or one-hot coding used (what is the difference?)
- Covariates $X_1, X_2, \ldots, X_p$: "independent variables", predictors, features
  - continuous, discrete: used directly
  - categorical, discrete: often dummy variable coding or one-hot coding used (again, difference?)

We aim to construct a rule, function, learner: $f(X)$, to predict Y (or G).

Random variables and (column) vectors are written as uppercase letters X, and Y, while observed values are written with lowercase (x, y). (Dimensions specified if needed.)

Matrices are presented with uppercase boldface: $\mathbf{X}$, often $N \times (p+1)$. ESL uses boldface also for $\mathbf{x}_j$ being a vector of all N observations of variable j, but in general vectors are not boldface and the vector of observed variables for observation i is just x_i.

Random variables and random vectors

Both the response *and covariates* will be considered to be random, and drawn from some joint distribution
$P(X_1, X_2, \ldots, X_p, Y) = P(X, Y)$ or $P(X, G)$.
Joint to conditional and marginal distribution:
$P(X, Y) = P(Y \mid X)P(X)$ or $P(Y \mid X = x)P(X = x)$ or

$$P(Y = y, X = x) = P(Y = y \mid X = x)P(X = x)$$

Maybe brush up on this?

Resources

- From TMA4268: Module 2 - Random vectors
- From TMA4267: Part 1: Multivariate random variables and the multivariate normal distribution

Training set

(ESL 2.1)

A set of size N of independent pairs of observations (x_i, y_i) is called the *training set* and often denoted $\mathcal{T}$. Here x_i may be a vector. Also $(X, Y) = \mathcal{T}$ is used in articles.

The training data is used to estimate the unknown function f.

Validation and test data

Validation data is used for *model selection* (finding the best model among a candidate set).

Test data is used for *model assessment* (assess the performance of the fitted model on future data).

We will consider theoretical results, and also look at different ways to split or resample available data.

More in ESL Chapter 7.

Group discussion

Two core regression methods are multiple linear regression (MLR) and k-nearest neighbour (kNN).

Choose one of the two methods:

- Set up the formal definition for f, and model assumptions made
- What top results do you remember? Write them down.
- Are there challenges with the method?

Regression and MLR

See also the exercises!

Resources

(mostly what we learned in TMA4267, or ESL Ch 3, except 3.2.3, 3.2.4, 3.4, 3.7, 3.8)

- From TMA4268: Overview and in particular Module 3: Linear regression
- From TMA4315: Overview and in particular Module 2: MLR

For kNN see also Problem 1 of the TMA4268 2018 exam with solutions

Statistical decision theoretic framework for regression

(ESL Ch 2.4, regression part)

is a mathematical framework for developing models f - and assessing optimality.

First, regression:

- $X \in \mathfrak{R}^p$
- $Y \in \mathfrak{R}$
- $P(X, Y)$ joint distribution of covariates and response

Aim: find a function $f(X)$ for predicting Y from some inputs X.

Ingredients: Loss function $L(Y, f(X))$ - for *penalizing errors in the prediction*.

Criterion for choosing f: Expected prediction error (EPE) - later also to be referred to as Err.

$$\mathrm{EPE}(f) = \mathrm{E}_{X,Y}[L(Y, f(X))] = \int_{x,y} L(y, f(x))p(x, y)dxdy$$

Choose f to minimize the EPE(f).

Q: Why do we not involve the distribution of the random variable $f(X)$, but instead the distribution of X?

Law of the unconscious statistican (from our introductory course in statistics): https://en.wikipedia.org/wiki/Law_of_the_unconscious_statistician and Thematics pages TMA4240/45.

What is the most popular loss function for regression?

Squared error loss

$$\mathrm{EPE}(f) = \mathrm{E}_{X,Y}[L(Y, f(X))] = \mathrm{E}_X \mathrm{E}_{Y|X}[(Y - f(X))^2 \mid X]$$

We want to minimize EPE, and see that it is sufficient to minimize $\mathrm{E}_{Y|X}[(Y - f(X))^2 \mid X]$ for each $X = x$ (pointwise):

$$f(x) = \mathrm{argmin}_c \mathrm{E}_{Y|X}[(Y - c)^2 \mid X = x]$$

This gives as result the conditional expectation - the best prediction at any point $X = x$:

$$f(x) = \mathrm{E}[Y \mid X = x]$$

Proof: by differentiating and setting equal 0. See also the exercises!

But, do we know this conditional distribution? In some cases only (which?). In practice: need to estimate f.

What if the joint distribution is multivariate normal?

Conditionally (known from before):
if we assume that $(X, Y) \sim N_{p+1}(\mu, \Sigma)$ then we have seen (TMA4267) that E$(Y \mid X)$ is linear in X and Cov$(Y \mid X)$ is independent of X.
Properties of the mvN
The conditional distributions of the components are (multivariate) normal.

$$\mathbf{X}_2 \mid (\mathbf{X}_1 = \mathbf{x}_1) \sim N_{p2}(\ _2 + \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{x}_1 - \ _1), \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}).$$

Approximate linear model

But, also if we assume an approximate linear model: $f(x) \approx x^T\beta$
Marginally: $\text{argmin}_\beta \mathsf{E}[(Y - X^T\beta)^2]$ gives $\beta = \mathsf{E}[XX^T]^{-1}\mathsf{E}[XY]$ (now random vectors).
We may replace expectations with averages in training data to estimate β.
This is not conditional on X, but we have assumed a linear relationship.

kNN and conditional expectation

Local conditional mean for observations in T close to $\mathbf{x}_0$:

$$\hat{f}(\mathbf{x}_0) = \frac{1}{k} \sum_{i \in N_k(\mathbf{x}_0)} Y_i$$

Absolute loss

Regression with absolute (L1) loss: $L(Y, f(X)) = |Y - f(X)|$ gives $\hat{f}(x) = \text{median}(Y \mid X = x)$.

Proof: for example pages 8-11 of https://getd.libs.uga.edu/pdfs/ma_james_c_201412_ms.pdf

Conclusions - and next step

- What are key take home messages so far?

Continue with the decision theoretic framework for classification.

- Classification - should not be new (ESL Ch 4.1-4.5, except 4.4.4)
- Statistical decision theoretic framework for classification (ESL 2.4)

Statistical decision theoretic framework for classification

(ESL Ch 2.4)

$$\text{EPE}(f) = \text{E}_{X,Y}[L(Y, f(X))] = \int_{x,y} L(y, f(x))p(x, y)dxdy$$

Choose f to minimize the EPE(f).

What changes do we need to do for classifiation?

- $X \in \mathfrak{R}^p$
- $G \in G = \{1, \ldots, K\}$
- $\hat{G}(X) \in G = \{1, \ldots, K\}$ (why f for regression and $\hat{G}$ for classification? strange?)
- $L(G, \hat{G}(X))$ is a function with $K \times K$ possible values where $K = |G|$. We may present this as a matrix with with elements l_{jk} giving the price to pay to misclassify an observation with true class g_j to class g_k.
- Elements on the diagonal of L is 0, and off-diagonal elements are often 1.

We would like to find $\hat{G}$ to minimize the EPE:

$$\mathsf{EPE} = \mathsf{E}_{G,X}[L(G, \hat{G}(X))] = \mathsf{E}_X \mathsf{E}_{G|X}[L(G, \hat{G}(X))]$$

$$= \mathsf{E}_X \{ \sum_{k=1}^{K} L(g_k, \hat{G}(X)) P(G = g_k \mid X = x) \}$$

Also here it is sufficient to minimize the loss for each value of x (pointwise)

$$\hat{G} = \text{argmin}_{g \in G} \sum_{k=1}^{K} L(g_k, \hat{G}(X)) P(G = g_k \mid X = x)$$

In the special case of 0-1 loss (off-diagonal elements in L equal to 1) then all k except the correct class gives loss 1 with probability $P(G = g_k \mid X = x)$. Summing over the wrong classes gives the same as taking 1 minus the conditional probability of the correct class g.

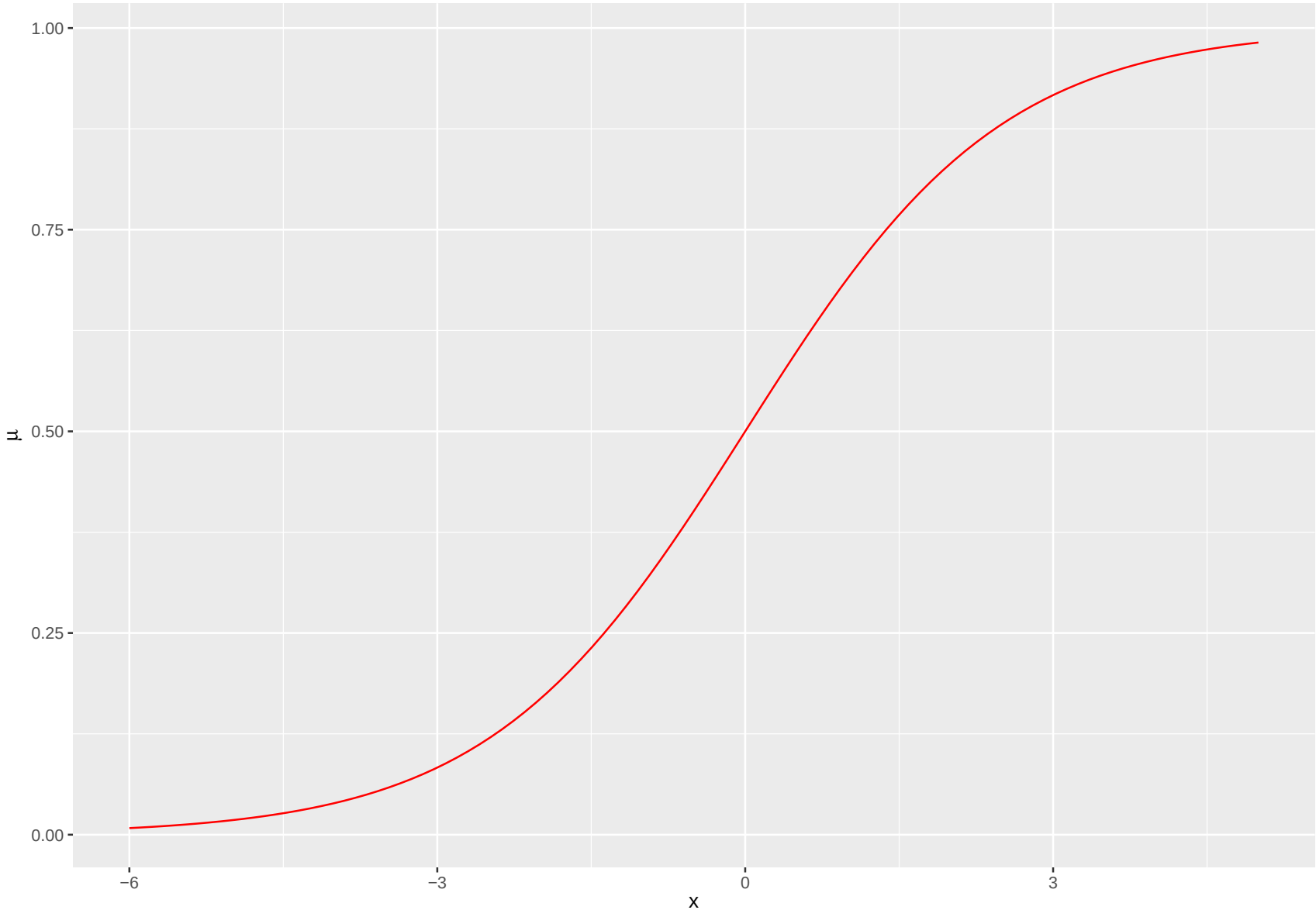
$$\hat{G} = \text{argmin}_{g \in G}[1 - P(G = g \mid X = x)]$$

$$= \text{argmax}_{g \in G} P(G = g \mid X = x)$$

The *Bayes classifier* classifies to the most probable class using the conditional distribution $P(G \mid X)$. The class boundaries are the *Bayes decision boundaries* and the error rate is the *Bayes rate*.

Simple example

Let assume we have $G = 2$, $p = 1$, and know
$P(G = 1 \mid X = x) = \frac{\exp(\beta_0+\beta_1 x)}{1+\exp(\beta_0+\beta_1 x)}$ where $\beta_0 = 0$ and $\beta_1 = 0.8$.
The Bayes classifier classifies to group 1 if $x > 0$, as shown below.



Group discussion

1) What do we know about classification (TMA4268 and TMA4315 mainly, or ESL ch 4.1-4.5, except 4.4.4):

- What is the difference between discrimination and classification?
- What are the sampling vs diagnostic paradigm? Give an example of one method of each type. How does this relate to what we have learned about the optimal solution for the 0/1-loss?
- Give an example of one parametric and one non-parametric classification method.

2) Logistic regression is by many seen as the "most important method in machine learning". What do we remember about logistic regression? (Will be a very important method in Part 2.)

3) What "changes" need to be done to 2) when we have $K > 2$ classes?

Resources

(mostly what we learned in TMA4267, or ESL ch 4.1-4.5, except 4.4.4)

- From TMA4268: Overview and in particular Module 4: Classification and Module 2: Statistical learning
- From TMA4315: Overview and in particular Module 3: Binary regression and for more than two classes: Module 6: Categorical regression.

A look ahead

- But first: one word to describe important statistical theory discussed today!
- Remember to work with the exercises!

Week 2: Working with EPE

Cover new aspects for

- Model selection and assessment (ESL Ch 7.1-7.6, 7.10-7.12). Look through these parts of chapter 7 before the week 2!
- Bias-variance trade-off is here - remind yourself of the derivation for the squared loss.
- We will also look into overparameterized models - where the double descent becomes relevant! (**ISLR2?**) Section 10.8.

Week 3: Missing data

- How to handle missing data in data analyses. (Not in ESL)

Exercises

1: Law of total expectation and total variance

This is to get a feeling of the joint and conditional distributions, so that we understand expected value notation with joint, conditional and marginal distributions.
Give a derivation of the law of total expectation:

$$\mathsf{E}[X] = \mathsf{E}[\mathsf{E}(X \mid Y)]$$

and the law of total variance:

$$\mathsf{Var}[X] = \mathsf{EVar}[X \mid Y] + \mathsf{VarE}[X \mid Y]$$

(There is also a law of total covariance.)

2: Quadratic loss and decision theoretic framework

Show that $f(x) = \mathsf{E}[Y \mid X = x]$ for the quadratic loss.

3: Curse of dimensionality

Read ELS pages 22-23 and then answer Exercise 2.3 - which is to "Derive equation (2.24)."

Solutions to exercises

Please try yourself first, or take a small peek - and try some more - before fully reading the solutions. Report errors or improvements to Mette.Langaas@ntnu.no.

1: Law of total E and Var

Try first yourself

2: Quadratic loss

Page 8 of https://getd.libs.uga.edu/pdfs/ma_james_c_201412_ms.pdf or Mettes notes

3: Curse of dimensionality

2.3

4: Key results from MLR

a) Regression parameter estimator

Both methods are written out in these class notes from TMA4267/8. More on likelihood-version here: TMA4315 GLM Module 2

Reference links

- ESL official errata: and choose “Errata” in the left menu
- ESL solutions to exercises
- ESL solutions from UiO
- Introduction to statistical learning with R, Video playlist
- Introduction to statistical learning with Python, Exercises playlist

Bibliography

Grömping, U. 2007. "Estimators of Relative Importance in Linear Regression Based on Variance Decomposition." *The American Statistician* 61: 139–47.

Hastie, Trevor, Robert Tibshirani, and Jerome Friedman. 2009. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. Vol. 2. Springer series in statistics New York. hastie.su.domains/ElemStatLearn.