Lecture 4 – k-Nearest Neighbors, Discriminant Analysis,

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Summary of Lecture 3 (I/VI)

The classification problem amounts to modeling the relationship between the input $\mathbf{x}$ and a **categorical output** y, i.e., the output belongs to one out of M distinct **classes**.

A **classifier** is a prediction model $\widehat{y}(\mathbf{x})$ that maps any input $\mathbf{x}$ into a predicted class $\widehat{y} \in \{1, \ldots, M\}$.

Common classifier predicts each input as belonging to the **most likely class** according to the conditional probabilities

$$p(y = m \,|\, \mathbf{x}) \text{ for } m \in \{1, \ldots, M\}.$$

Summary of Lecture 3 (II/VI)

For binary (two-class) classification, $y \in \{-1, 1\}$, the **logistic regression model** is

$$p(y = 1 \,|\, \mathbf{x}) \approx f(\mathbf{x}) = \frac{e^{\theta^{\mathsf{T}}\mathbf{x}}}{1 + e^{\theta^{\mathsf{T}}\mathbf{x}}}.$$

The model parameters θ are found by maximum likelihood by (numerically) maximizing the log-likelihood function,

$$\log \ell(\theta) = -\sum_{i=1}^{n} \log\left(1 + e^{-y_i \theta^{\mathsf{T}}\mathbf{x}_i}\right).$$

Summary of Lecture 3 (III/VI)

Using the common classifier, we get the prediction model

$$\widehat{y}(\mathbf{x}) = \begin{cases} 1 & \text{if } g(\mathbf{x}) > 0.5 \quad \Leftrightarrow \hat{\theta}^{\mathsf{T}}\mathbf{x} > 0 \\ -1 & \text{otherwise} \end{cases}$$

This attempts to **minimize the total misclassification error**.

More generally, we can use

$$\widehat{y}(\mathbf{x}) = \begin{cases} 1 & \text{if } g(\mathbf{x}) > r, \\ -1 & \text{otherwise} \end{cases}$$

where $0 \leq r \leq 1$ is a **user chosen threshold**.

Summary of Lecture 3 (IV/VI)

Confusion matrix:

		True condition $y=0$	True condition $y=1$	Total
Predicted condition	$\widehat{y}=0$	**TN**	**FN**	**N***
	$\widehat{y}=1$	**FP**	**TP**	**P***
	Total	**N**	**P**	

For the classifier

$$\widehat{y}(\mathbf{x}) = \begin{cases} 1 & \text{if } f(\mathbf{x}) > r, \\ -1 & \text{otherwise} \end{cases}$$

the numbers in the confusion matrix will **depend on the threshold** r.

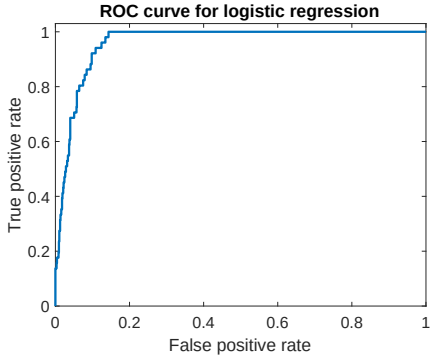
- Decreasing r $\Rightarrow$ **TN**, **FN** decrease and **FP**, **TP** increase.
- Increasing r $\Rightarrow$ **TN**, **FN** increase and **FP**, **TP** decrease.

Summary of Lecture 3 (V/VI)

Some commonly used performance measures are:

- True positive rate: $\mathbf{TPR} = \frac{\mathbf{TP}}{\mathbf{P}} = \frac{\mathbf{TP}}{\mathbf{FN} + \mathbf{TP}} \in [0, 1]$
- False positive rate: $\mathbf{FPR} = \frac{\mathbf{FP}}{\mathbf{N}} = \frac{\mathbf{FP}}{\mathbf{FP} + \mathbf{TN}} \in [0, 1]$
- Precision: $\mathbf{Prec} = \frac{\mathbf{TP}}{\mathbf{P^*}} = \frac{\mathbf{TP}}{\mathbf{FP} + \mathbf{TP}} \in [0, 1]$

Summary of Lecture 3 (VI/VI)



- **ROC: plot of TPR vs. FPR** as r ranges from 0 to 1.
- **Area Under Curve (AUC):** condensed performance measure for the classifier, taking all possible thresholds into account.

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Parametric and non-parametric models

Up to now we have looked at **parametric models**,

- linear regression,
- logistic regression,
- LDA and QDA (later in this lecture)

all of which involve assuming (in all these examples) a Normal distribution and estimating parameters like β, μ and σ.

Another approach is to use a non-parametric model. A model which directly relates the input data to the output data. We make no assumption about how the data is distributed (all models are wrong anyway!).

A simple example of k-nearest neighbors

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i	x_1	x_2	y
1	−1	3	Red
2	2	1	Blue
3	−2	2	Red
4	−1	2	Blue
5	−1	0	Blue
6	1	1	Red

A simple example of k-nearest neighbors

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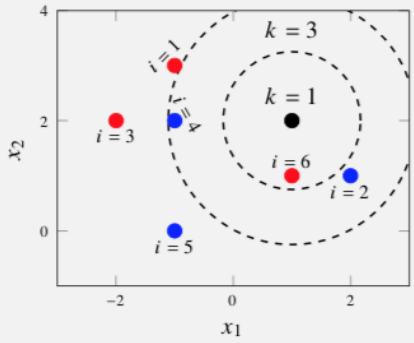
i	$\|\mathbf{x}_i - \mathbf{x}_\star\|$	y_i
6	$\sqrt{1}$	Red
2	$\sqrt{2}$	Blue
4	$\sqrt{4}$	Blue
1	$\sqrt{5}$	Red
5	$\sqrt{8}$	Blue
3	$\sqrt{9}$	Red



A simple example of k-nearest neighbors

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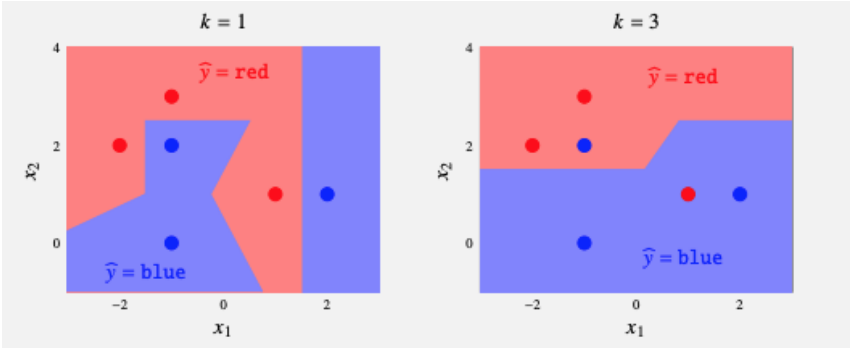


k-nearest neighbors is a non-linear classifier.

Logistic regression is a linear classifier.

k-NN algorithm

The **k-nearest neighbors (k-NN)** classifier is a simple non-parametric method.

Given training data $\mathcal{T} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, for a test input $\mathbf{x}_\star$,

1. Identify the set

$$R_\star = \{i : \mathbf{x}_i \text{ is one of the } k \text{ training data points closest to } \mathbf{x}_\star\}$$

2. Classify $\mathbf{x}_\star$ according to a majority vote within the neighborhood $R_\star$, i.e. assign $\mathbf{x}_\star$ to class m for which

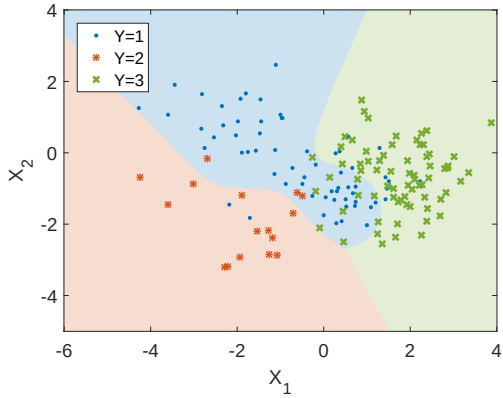
$$\sum_{i \in R_\star} \mathbb{I}\{y_i = m\}$$

is largest.

Good time to start having a look in the book

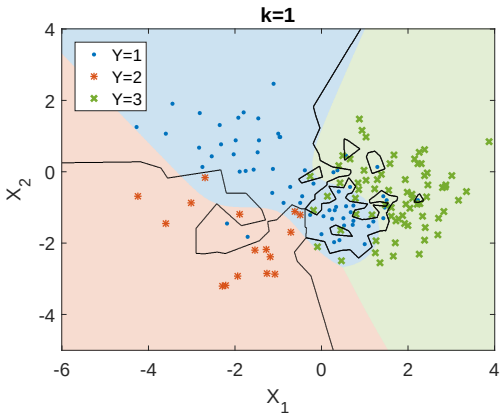
ex) k-NN with three classes

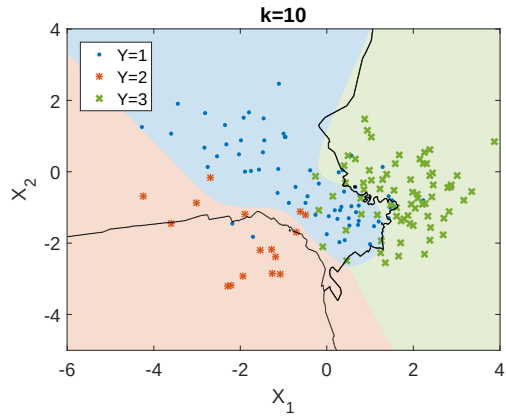
We illustrate the k-NN classifier on a synthetic example where the optimal classifier is known (colored regions).



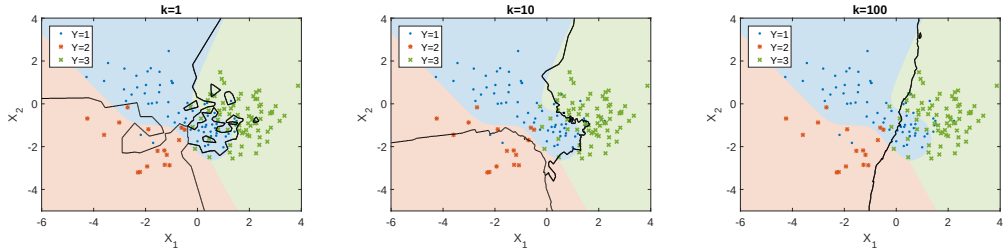
ex) k-NN on a toy model

The decision boundaries for the k-NN classifier are shown as black lines.





ex) k-NN with three classes



The choice of the ***tuning parameter*** k controls the model flexibility:

- Small $k \Rightarrow$ small bias, large variance
- Large $k \Rightarrow$ large bias, small variance

Parametric vs. non-Parametric

Advantages of non-parametric models

- Allow the flexibility of the model to grow with the amount of available data.
- Can be ***very*** flexible (= low bias, see next lecture)
- Intuitive. Less theory involved.

Disadvantages of non-parametric models

- Have very little theoretical support
- Can suffer from overfitting (= high variance, see next lecture)
- Can be computing and memory intensive
- Difficult to interpret what the results mean

The ***bias-variance trade-off*** (next lecture) is going to be a useful tool.

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Bayes' theorem: visually

Bayes' theorem

If A and B are two events with $\Pr(B) > 0$, then

$$\Pr(A \mid B) = \frac{\Pr(B \mid A)\Pr(A)}{\Pr(B)}.$$

Can also be written,

$$\Pr(A \mid B) = \frac{\Pr(B \mid A)\Pr(A)}{\Pr(B \mid A)\Pr(A) + \Pr(B \mid A^C)\Pr(A^C)}.$$

where A^C is the complement of A.

Example of Bayes' theorem

Let A be the event that you have a disease. Let B be the event that a test you have taken is positive.

Assume that the test gives an error 1 in 100 tests., i.e. $\Pr(B|A) = 99/100$ and $\Pr(B|A^C) = 1/100$.

Further assume a randomly selected person has probability 1 in 1000 people of having the disease, i.e. $\Pr(A) = 1/1000$

You have no symptoms but take a test and test positive. What is the probability you have the disease?

Example: worked out

Let A be the event that you have a disease. Let B be the event that a test you have taken is positive: $\Pr(B|A) = 99/100$, $\Pr(B|A^C) = 1/100$ and $\Pr(A) = 1/1000$

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Example of Bayes' theorem

You have no symptoms but take a test and test positive. What is the probability you have the disease?

$$\begin{aligned}
\Pr(A \mid B) &= \frac{\Pr(B \mid A)\Pr(A)}{\Pr(B \mid A)\Pr(A) + \Pr(B \mid A^C)\Pr(A^C)} \\
&= \frac{99/100 \cdot 1/1000}{99/100 \cdot 1/1000 + 1/100 \cdot 999/1000} \\
&\approx 1/11
\end{aligned}$$

!!!!!!

Discriminative vs. Generative models

A **discriminative model** describes how the output y is generated drieectly, i.e. $p(y \mid \mathbf{x})$. This is what we do in logistic regression.

A **generative model** describes how both the output y and the input $\mathbf{x}$ is generated via $p(y, \mathbf{x}) = p(y)p(\mathbf{x} \mid y)$. This is what we do now.

A discriminative model takes the role of $\Pr(A \mid B)$. A generative model is based on $\Pr(B \mid A)$.

Discriminat analysis

We need to complete two steps:

1. The prior class probabilities $Pr(y = m)$, $m \in \{1, \ldots, M\}$.
2. The conditional probability densities of the input $\mathbf{x}$, $p(\mathbf{x} \,|\, y = m)$, for each class m.

We can then use Bayes' theorem to create a discriminative classifier from a generative model:

$$\Pr(y = m \,|\, \mathbf{x}) = \frac{p(\mathbf{x} \,|\, y = m) \Pr(y = m)}{\sum_{j=1}^{K} p(\mathbf{x} \,|\, y = j) \Pr(y = j)}.$$

Discriminant analysis

For the first step, a natural *estimator* is the proportion of training samples in the mth class.

$$\Pr(y = m) \text{ is estimated by } \frac{1}{n}\sum_{i=1}^{n}\mathbb{I}\{y_i = m\} = \frac{n_m}{n}$$

where n is the size of the training set and n_m the number of training samples of class m.

This the idea of an uninformative prior probability: before we use the model the probability it is in any class is proportional to number in that class.

Discriminant analysis

For the **second step**, one model is to *assume* that the pdf of $p(\mathbf{x}|y = m)$ is a multivariate normal density with mean $\boldsymbol{\mu}_m$ and covariance matrix $\boldsymbol{\Sigma}_m$,

$$p(\mathbf{x}|y = m) = \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}_m|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_m)^\mathsf{T}\boldsymbol{\Sigma}_m^{-1}(\mathbf{x} - \boldsymbol{\mu}_m)\right).$$

The parameters of the model are the means

$$\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_M$$

And the variance

$$\boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_M,$$

Multivariate Gaussian density

The p-dimensional Gaussian (normal) probability density function with mean vector $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$ is,

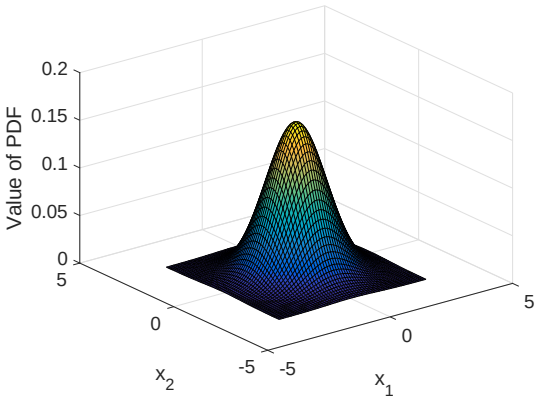
$$\mathcal{N}(\mathbf{x} \,|\, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right),$$

where $\boldsymbol{\mu}$: $p \times 1$ vector and $\boldsymbol{\Sigma}$: $p \times p$ positive definite matrix.

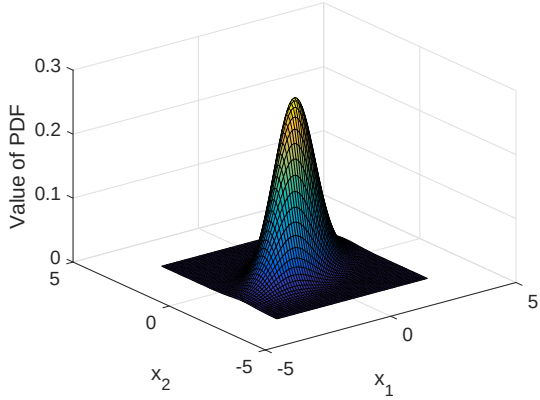
Let $\mathbf{x} = (x_1, \ldots, x_p)^{\mathsf{T}} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$,

- μ_j is the mean of x_j,
- Σ_{jj} is the variance of x_j,
- Σ_{ij} $(i \neq j)$ is the covariance between x_i and x_j.

Multivariate Gaussian density



$$\mathbf{\Sigma} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



$$\mathbf{\Sigma} = \begin{pmatrix} 1 & 0.4 \\ 0.4 & 0.5 \end{pmatrix}$$

Estimating the co-variance matrix

The mean vector $\boldsymbol{\mu}$ is estimated by

$$\widehat{\boldsymbol{\mu}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i, \tag{1}$$

The covariance matrix $\boldsymbol{\Sigma}$ is estimated by

$$\widehat{\boldsymbol{\Sigma}} = \frac{1}{n-1}\sum_{i=1}^{n}(\mathbf{x}-\widehat{\boldsymbol{\mu}})(\mathbf{x}-\widehat{\boldsymbol{\mu}})^{\mathsf{T}}. \tag{2}$$

The element (j,k) of the covariance matrix is equal to the covariance between $\mathbf{x}_j$ and $\mathbf{x}_k$, i.e. the entry has value

$$\frac{1}{n-1}\sum_{i=1}^{n}(x_{ij}-\widehat{\mu}_j)(x_{ik}-\widehat{\mu}_k)$$

Linear discriminant analysis: estimation

Linear discriminant analysis assumes that the means are the same for all classes m

$$\boldsymbol{\Sigma} \stackrel{\text{def}}{=} \boldsymbol{\Sigma}_1 = \cdots = \boldsymbol{\Sigma}_M,$$

the remaining parameters of the model are
These parameters are naturally estimated as the (within class) sample means and sample covariance, respectively:

$$\widehat{\boldsymbol{\mu}}_m = \frac{1}{n_m} \sum_{i:y_i=m} x_i, \qquad m = 1, \ldots, M,$$

$$\widehat{\boldsymbol{\Sigma}} = \frac{1}{n-M} \sum_{m=1}^{M} \sum_{i:y_i=m} (x_i - \widehat{\boldsymbol{\mu}}_m)(x_i - \widehat{\boldsymbol{\mu}}_m)^{\mathsf{T}}.$$

Linear discriminant analysis: classification

The probability (density function) of a point y is in class m is estimated by

$$\frac{\mathcal{N}\left(\hat{\boldsymbol{\mu}_m}, \hat{\boldsymbol{\Sigma}}\right) \frac{n_m}{n}}{\sum_{j=1}^{K} \mathcal{N}\left(\hat{\boldsymbol{\mu}}_j, \hat{\boldsymbol{\Sigma}}\right) \frac{n_j}{n}}.$$

Since the denominator is independent of m we just need to find the value of m for which

$$\mathcal{N}\left(\hat{\boldsymbol{\mu}_m}, \hat{\boldsymbol{\Sigma}}\right) \frac{n_m}{n}$$

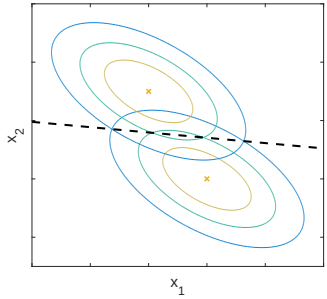
is maximised. Or equivalently, for which the log of this is maximised.
Thus, the LDA classifier assigns a test input $\mathbf{x}$ to class m for which,

$$\widehat{\delta}_m(\mathbf{x}) = \underbrace{\mathbf{x}^\mathsf{T} \widehat{\boldsymbol{\Sigma}}^{-1} \widehat{\boldsymbol{\mu}}_m - \frac{1}{2} \widehat{\boldsymbol{\mu}}_m^\mathsf{T} \widehat{\boldsymbol{\Sigma}}^{-1} \widehat{\boldsymbol{\mu}}_m}_{\text{step 2}} + \underbrace{\log \frac{n_m}{n}}_{\text{step 1}}$$

is largest.

Linear discriminant analysis: decision boundary

Illustration of LDA decision boundary – the level curves of two Gaussian PDFs with **the same covariance matrix** intersect along a straight line, $\widehat{\delta}_1(\mathbf{x}) = \widehat{\delta}_2(\mathbf{x})$.



LDA is a ***linear classifier*** (its decision boundaries are linear).

Quadratic discriminant analysis

Do we have to assume a common covariance matrix?

No! Estimating a separate covariance matrix for each class leads to an alternative method, Quadratic Discriminant Analysis (QDA).

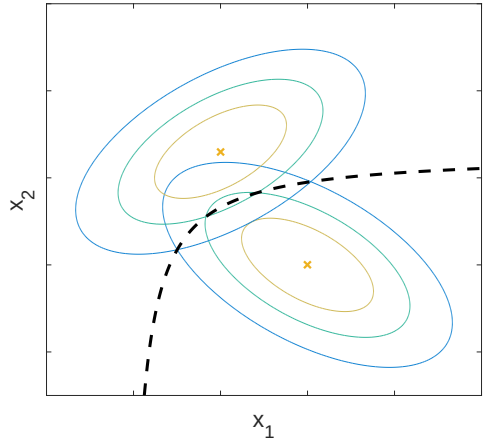
Whether we should choose LDA or QDA has to do with the **bias-variance trade-off**, i.e. the risk of **over- or underfitting**.

Compared to LDA, QDA...

- has more parameters
- is more flexible (lower bias)
- has higher risk of overfitting (larger variance)

ex) QDA decision boundary

Illustration of QDA decision boundary – the level curves of two Gaussian PDFs with **different covariance matrices** intersect along a curved (quadratic) line.



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A few concepts to summarize lecture 4

Generative model: A model that describes both the output y and the input $\mathbf{x}$.

Linear discriminant analysis (LDA): A classifier based on the assumption that the distribution of the input $\mathbf{x}$ is multivariate Gaussian for each class, with different means but the same covariance. LDA is a linear classifier.

Quadratic discriminant analysis (QDA): Same as LDA, but where a different covariance matrix is used for each class. QDA is *not* a linear classifier.

Non-parametric model: A model where the flexibility is allowed to grow with the amount of available training data.

k-NN classifier: A simple non-parametric classifier based on classifying a test input $\mathbf{x}$ according to the class labels of the k training samples nearest to x.