## Statistical Machine Learning

https://cvml.ist.ac.at/courses/SML_W20

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## Stastical Machine Learning Course - Formalities

## Goals:

- learn the principles of (mainly supervised) machine learning
- get an overview of some core techniques
- not:hands-on experience in solving real-world tasks using machine learning


## Target Audience:

- anyone interest in machine learning as a research topic.
- not: anyone who wants to apply machine learning to their own problems


## Prerequisites:

- mathematics: set notation, linear algebra, multi-dimensional calculus, probabilities
- programming skills: in a language that allows numeric computation, e.g. Python


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## Caveat:

- rumor is, the course is quite some work for its 3 ECTS


## Evaluation criteria:

- 50\% homework, $50 \%$ final project


## Homework:

- every Monday there is a new homework sheet
- exercises are mainly theoretical/analytical, but also some practicals
- return your answers via email to the TAs before the next Monday lecture
- homeworks must be handed in individually
- group discussion about homeworks is permitted and encouraged
- cut-and-paste solutions are not permitted and will be sanctioned (1st offence: no points for sheet, 2nd offence: fail course)


## Final Team Project:

- starting two weeks before the end of the course (approx. Nov 1)
- teams should have two participants
- you can use any method and software you want
- teams present their approaches during the "exam week" (Nov 13, Nov 15)


## Overview (tentative)

| Date |  | no. | Topic |
| :--- | :---: | :---: | :--- |
| Oct 05 | Mon | 1 | A Hands-On Introduction |
| Oct 07 | Wed | 2 | Bayesian Decision Theory, Generative Probabilistic Models |
| Oct 12 | Mon | 3 | Discriminative Probabilistic Models |
| Oct 14 | Wed | 4 | Maximum Margin Classifiers, Generalized Linear Models |
| Oct 19 | Mon | 5 | Estimators; Overfitting/Underfitting, Regularization, Model Selection |
| Oct 21 | Wed | 6 | Bias/Fairness, Domain Adaptation |
| Oct 26 | Mon | - | no lecture (public holiday) |
| Oct 28 | Wed | 7 | Learning Theory I |
| Nov 02 | Mon | 8 | Learning Theory II |
| Nov 04 | Wed | 9 | Deep Learning I |
| Nov 09 | Mon | 10 | Deep Learning II |
| Nov 11 | Wed | 11 | Unsupervised Learning |
| Nov 16 | Mon | 12 | project presentations |
| Nov 18 | Wed | 13 | buffer |

## What is Machine Learning

## Definition (Mitchell, 1997)

A computer program is said to learn from experience $E$ with respect to some class of tasks $T$ and performance measure $P$, if its performance at tasks in $T$, as measured by $P$, improves with experience $E$.

## What is Machine Learning

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## Example: Backgammon

- T)ask: Play backgammon.
- E)xperience: Games playes against itself
- P)erformance Measure: Games won against human players.


## What is Machine Learning

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A computer program is said to learn from experience $E$ with respect to some class of tasks $T$ and performance measure $P$, if its performance at tasks in $T$, as measured by $P$, improves with experience $E$.

## Example: Spam classification

- T)ask: determine if emails are Spam or non-Spam.
- E)xperience: Incoming emails with human classification
- P)erformance Measure: percentage of correct decisions


## Definition (Mitchell, 1997)

A computer program is said to learn from experience $E$ with respect to some class of tasks $T$ and performance measure $P$, if its performance at tasks in $T$, as measured by $P$, improves with experience $E$.

## Example: Stock market predictions

- T)ask: predict the price of some shares
- E)xperience: past prices
- P)erformance Measure: money you win or lose


## Notation

## Task:

- $\mathcal{X}$ : input set, set of all possible inputs
- $\mathcal{Y}$ : output set, set of all possible outputs
- $f: \mathcal{X} \rightarrow \mathcal{Y}:$ prediction function,
- e.g. $\mathcal{X}=\{$ all possible emails $\}, \mathcal{Y}=\{$ spam, ham $\}$ $f$ spam filter: for new email $x \in \mathcal{X}: f(x)=$ spam or $f(x)=$ ham.


## Performance:

- $\ell: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ : loss function
- e.g. $\ell\left(y, y^{\prime}\right)$ is cost of predicting $y^{\prime}$ if $y$ is correct.
- $\ell\left(y, y^{\prime}\right)$ can be asymmetric: spam $\rightarrow$ ham is annoying, but no big deal.
- ham $\rightarrow$ spam can cause serious problems.

Experience: task-dependent, many different scenarios

- Supervised learning: a labeled training set examples from $\mathcal{X}$ with outputs provided by an expert, $\mathcal{D}=\left\{\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)\right\} \subset \mathcal{X} \times \mathcal{Y}$
- A person goes through his/her $n$ emails and marks each one whether it is spam or not.


## What is Machine Learning

Many other variants on how to formalize experience exist:

- Unsupervised Learning: $\mathcal{D}=\left\{x^{1}, \ldots, x^{n}\right\}$, only observing, no input from an expert/teacher
- Semi-supervised Learning: $\mathcal{D}=\left\{\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)\right\} \cup\left\{x^{n+1}, \ldots, x^{n+l}\right\}$ : only a subset of examples has labels
- spam: quite common, nobody wants to label every email in their inbox
- Reinforcement Learning: $\mathcal{D}=\left\{\left(x^{1}, r^{1}\right), \ldots,\left(x^{n}, r^{n}\right)\right\}$ with $r^{i} \in \mathbb{R}$ : actions and feedback how good the action was
- backgammon: nobody tells you the best move, but eventually you observe a win or loss
- Active Learning: $\mathcal{D}=\left\{x^{1}, \ldots, x^{n}\right\}$, but the algorithms may ask for labels
- spam: email program can ask the user, if its not too often
- Zero-Shot Learning: $\mathcal{D}=\left\{\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)\right\} \subset \mathcal{X} \times \mathcal{Y}$ but only a subset of all classes actually shows up in the training data.

In this course, we don't look at these (except a little bit at unsupervised learning).

## Supervised Learning

## Definition

- A supervised learning system (or learner), $L$, is a (computable) function from the set of (finite) training sets to the set of prediction functions:

$$
\begin{array}{ll} 
& L: \mathbb{P}^{<\infty}(\mathcal{X} \times \mathcal{Y}) \rightarrow \mathcal{Y}^{\mathcal{X}} \\
\text { i.e. } & L: \mathcal{D} \mapsto f
\end{array}
$$

If presented with a training set $\mathcal{D} \subset \mathcal{X} \times \mathcal{Y}$, it provides a decision rule/function $f: \mathcal{X} \rightarrow \mathcal{Y}$.

## Definition

Let $L$ be a learning system.

- The process of computing $f=L(\mathcal{D})$ is called training (phase).
- Applying $f$ to new data is called prediction, or testing (phase).


## Machine Learning: A very practical introduction:

We will look at examples of classical learning algorithms, to get a feeling what problems a learning system faces.

- Decision Trees
- Nearest Neighbor Classifiers
- Perceptron
- Boosting
- Artificial Neural Networks

Caveat: for each of these are there more advanced, often better, variants. Here, we look at the only as prototypes, not as guideline what to actually use in real life.

## Decision Trees - analysis: Breiman 1980s

Task: decide what to do today


Classifier has a tree structure:

- each interior node makes a decision: it picks an attribute within $x$, branches for each possible value
- each leaf assigns an (output) label
- to classify a new example, we
- put it into the root node,
- follow the decisions until we reach a leaf.
- use the leaf value as the prediction

Decisions trees ('expert systems') are popular especially for non-experts:

- efficient, easy to use, and interpretable.


## How to automatically build a decision tree

Given: training set $\mathcal{D}=\left\{\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)\right\}$.
Convention:

- each node contains a subset of examples,
- its label is the majority label of the examples in this node (any of the majority labels, if there's a tie)


## Decision Tree - Training

initialize: put all examples in root node
mark root as active

## repeat

pick active node with largest number of misclassified examples
mark the node as inactive
for each attributes, check error rate of splitting along this attribute
keep the split with smallest error, if any, and mark children as active until no more active nodes.

## Decision Tree - Classification

input decision tree, example $x$ assign $x$ to root node
while $x$ not in leaf node do
move $x$ to child according to the test in node end while
output label of the leaf that $x$ is in

## Decision Trees Example - Training

- We have a personalized dating agency, our only customer is Zoe.
- Task: For new customers registering, predict if Zoe should date them.
- Performance Measure: If Zoe is happy with the decision.
- Experience: We show Zoe a catalog of previous custemers and she tells us whether she would have like to date them or not.
- Let $x \in \mathcal{X}$ be a collection of values or properties, $x=\left(x_{1}, \ldots, x_{d}\right)$.

| property | possible values |
| :---: | :---: |
| eye color | blue/brown/green |
| handsome | yes/no |
| height | short/tall |
| sex | male (M)/female (F) |
| soccer fan | yes/no |

Preparation: you give Zoe a set of profiles to see whom she would like to date (none of these people really have to exists...)

Here's her answers, which we'll use as training data:

| $\mathcal{X}$ |  |  |  |  |  | Y |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| person | eyes | handsome | height | sex | soccer | date? |
| Apu | blue | yes | tall | $M$ | no | yes |
| Bernice | brown | yes | short | $F$ | no | no |
| Carl | blue | no | tall | M | no | yes |
| Doris | green | yes | short | $F$ | no | no |
| Edna | brown | no | short | $F$ | yes | no |
| Prof. Frink | brown | yes | tall | $M$ | yes | no |
| Gil | blue | no | tall | $M$ | yes | no |
| Homer | green | yes | short | $M$ | no | yes |
| Itchy | brown | no | short | $M$ | yes | yes |

(this table is also on the exercise sheet)

Step 1: put all all training examples into the root node

$$
\text { root }=\{(A, y),(B, n),(C, y),(D, n),(E, n),(F, n),(G, n),(H, y),(1, y)\}
$$

For each feature, check the classification accuracy of this single feature:


Total accuracy eyes: 6/9

Step 1: put all all training examples into the root node

$$
\operatorname{root}=\{(A, y),(B, n),(C, y),(D, n),(E, n),(F, n),(G, n),(H, y),(1, y)\}
$$

For each feature, check the classification accuracy of this single feature:


Total accuracy handsome: 5/9

Step 1: put all all training examples into the root node

$$
\operatorname{root}=\{(\mathrm{A}, \mathrm{y}),(\mathrm{B}, \mathrm{n}),(\mathrm{C}, \mathrm{y}),(\mathrm{D}, \mathrm{n}),(\mathrm{E}, \mathrm{n}),(\mathrm{F}, \mathrm{n}),(\mathrm{G}, \mathrm{n}),(\mathrm{H}, \mathrm{y}),(\mathrm{l}, \mathrm{y})\}
$$

For each feature, check the classification accuracy of this single feature:

| feature | $\rightarrow$ total |  |
| :---: | :---: | :---: |
| eyes | blue: $(2 / 3)$, brown: $(3 / 4)$, green: $(1 / 2)$ | $\rightarrow$ total: $(6 / 9)$ |
| handsome | yes: $(3 / 5)$, no: $(2 / 4)$ | $\rightarrow$ total: $(5 / 9)$ |
| height | tall: $(2 / 4)$, short: $(3 / 5)$ | $\rightarrow$ total: $(5 / 9)$ |
| sex | male: $(4 / 6)$, female: $(3 / 3)$ | $\rightarrow$ total: $(7 / 9)$ |
| soccer | yes: $(3 / 4)$, no: $(3 / 6)$ | $\rightarrow$ total: $(6 / 9)$ |

Best feature: sex.

Step 1 result: first split ist along sex feature


Right node: no mistakes, no more splits Left node: run checks again for remaining data

Step 2:

| person | eyes | handsome | height | sex | soccer | date? |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Apu | blue | yes | tall | male | no | yes |
| Carl | blue | no | tall | male | no | yes |
| Frink | brown | yes | tall | male | yes | no |
| Gil | blue | no | tall | male | yes | no |
| Homer | green | yes | short | male | no | yes |
| Itchy | brown | no | short | male | yes | yes |


| feature | accuracies | $\rightarrow$ total |
| :---: | :---: | :---: | :---: |
| eyes | blue: $(2 / 3)$, brown: $(1 / 2)$, green: $(1 / 1)$ | $\rightarrow$ total: $(4 / 6)$ |
| handsome | yes: $(2 / 3)$, no: $(2 / 3)$ | $\rightarrow$ total: $(4 / 6)$ |
| height | tall: $(2 / 4)$, short: $(2 / 2)$ | $\rightarrow$ total: $(4 / 6)$ |
| sex | male: $(4 / 6)$ | $\rightarrow$ total: $(4 / 6)$ |
| soccer | yes: $(2 / 3)$, no: $(3 / 3)$ | $\rightarrow$ total: $(5 / 6)$ |

Best feature: soccer.

Step 2 result: second split ist along soccer feature


Left node: no mistakes, no more splits Right node: run checks again for remaining data

Step 3:

| person | eyes | handsome | height | sex | soccer | date? |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Frink | brown | yes | tall | male | yes | no |
| Gil | blue | no | tall | male | yes | no |
| Itchy | brown | no | short | male | yes | yes |


| feature | accuracies | $\rightarrow$ total |
| :---: | :---: | :---: |
| eyes | blue: $(1 / 1)$, brown: $(1 / 2)$, green: $(0 / 0)$ | $\rightarrow$ total: $(2 / 3)$ |
| handsome | yes: $(1 / 1)$, no: $(1 / 2)$ | $\rightarrow$ total: $(2 / 3)$ |
| height | tall: $(2 / 2)$, short: $(1 / 1)$ | $\rightarrow$ total: $(3 / 3)$ |
| sex | male: $(2 / 3)$ | $\rightarrow$ total: $(2 / 3)$ |
| soccer | yes: $(2 / 3)$ | $\rightarrow$ total: $(2 / 3)$ |

Best feature: height.

Decision Trees Example - Training phase
Step 3 result: third split ist along height feature


Left node: no mistakes, no more splits Right node: no mistakes, no more splits

Step 3 result: third split ist along height feature


Left node: no mistakes, no more splits Right node: no mistakes, no more splits
$\rightarrow$ Decision tree learning complete.

```
Decision Trees Example - How good is this classifier?
```

Training example 1: correct

| person | eyes | handsome | height | sex | soccer | date? |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Apu | blue | yes | tall | male | no | yes |



Decision Trees Example - How good is this classifier?

Training example 2: correct

| person | eyes | handsome | height | sex | soccer | date? |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Bernice | brown | yes | short | F | no | no |



Decision Trees Example - How good is this classifier?

Training example 3: correct

| person | eyes | handsome | height | sex | soccer | date? |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Carl | blue | no | tall | M | no | yes |



Decision Trees Example - How good is this classifier?

- All training examples are classified correctly!

Decision Trees Example - How good is this classifier?

- All training examples are classified correctly!

Not overly surprising... that's how we constructed the tree.

Decision Trees Example - How good is this classifier?
What if we check on new data of the same kind?

| person | eyes | handsome | height | sex | soccer | date? |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| Jimbo | blue | no | tall | $M$ | no | yes |
| Krusty | green | yes | short | $M$ | yes | no |
| Lisa | blue | yes | tall | $F$ | no | no |
| Moe | brown | no | short | $M$ | no | no |
| Ned | brown | yes | short | $M$ | no | yes |
| Quimby | blue | no | tall | $M$ | no | yes |

Decision Trees Example - How good is this classifier?
What if we check on new data of the same kind?

| person | eyes | handsome | height | sex | soccer | date? | tree |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Jimbo | blue | no | tall | $M$ | no | yes | yes |
| Krusty | green | yes | short | $M$ | yes | no | yes |
| Lisa | blue | yes | tall | $F$ | no | no | no |
| Moe | brown | no | short | $M$ | no | no | yes |
| Ned | brown | yes | short | $M$ | no | yes | yes |
| Quimby | blue | no | tall | $M$ | no | yes | yes |

2 mistakes in 6, hm...

## Observation

Zoe won't care if our tree classifier worked perfectly on the training data. What really matters is how it works on future data: ability to generalize

```
Decision Trees Example - How good is this classifier?
```


## Observation

There is a relation between accuracy during training and accuracy at test time, but it isn't a simple one. Perfect performance on the training set does not guarantee perfect performance on future data!

Why did the tree make a mistake?
Maybe it took the training data too seriously?
Would Zoe really decide that male soccer fans are only datable, if they are short, but not if they are tall?
Let's see what happens in we simplify the tree?

Decision Trees Example - How good is this classifier?
Original four-level tree: 2 mistakes in 6.


Decision Trees Example - How good is this classifier?
Tree with three levels: 1 mistake in 6.


| person | eyes | handsome | height | sex | soccer | date? | tree |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Jimbo | blue | no | tall | M | no | yes | yes |
| Krusty | green | yes | short | M | yes | no | no |
| Lisa | blue | yes | tall | F | no | no | no |
| Moe | brown | no | short | M | no | no | yes |
| Ned | brown | yes | short | M | no | yes | yes |
| Quimby | blue | no | tall | M | no | yes | yes |

Decision Trees Example - How good is this classifier?
Tree with two levels: 2 mistakes in 6 .

| m/ | sex |
| :---: | :---: |
|  | \f |
| label: yes | label: no |


| person | eyes | handsome | height | sex | soccer | date? | tree |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Jimbo | blue | no | tall | $M$ | no | yes | yes |
| Krusty | green | yes | short | $M$ | yes | no | yes |
| Lisa | blue | yes | tall | $F$ | no | no | no |
| Moe | brown | no | short | $M$ | no | no | yes |
| Ned | brown | yes | short | $M$ | no | yes | yes |
| Quimby | blue | no | tall | $M$ | no | yes | yes |

Decision Trees Example - How good is this classifier?
Tree with one level: 3 mistakes in 6 .
label: no

| person | eyes | handsome | height | sex | soccer | date? | tree |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Jimbo | blue | no | tall | $M$ | no | yes | no |
| Krusty | green | yes | short | $M$ | yes | no | no |
| Lisa | blue | yes | tall | $F$ | no | no | no |
| Moe | brown | no | short | $M$ | no | no | no |
| Ned | brown | yes | short | $M$ | no | yes | no |
| Quimby | blue | no | tall | $M$ | no | yes | no |

Decision Trees Example - How good is this classifier?
Error analysis:

| size | training error | test error |
| :---: | :---: | :---: |
| height 1 | $4 / 9$ | $3 / 6$ |
| height 2 | $2 / 9$ | $2 / 6$ |
| height 3 | $1 / 9$ | $1 / 6$ |
| height 4 (full) | $0 / 9$ | $2 / 6$ |

Decision Trees Example - How good is this classifier?
Error analysis:

| size | training error | test error |
| :---: | :---: | :---: |
| height 1 | $4 / 9$ | $3 / 6$ |
| height 2 | $2 / 9$ | $2 / 6$ |
| height 3 | $1 / 9$ | $1 / 6$ |
| height 4 (full) | $0 / 9$ | $2 / 6$ |

Typical behaviour of classical machine learning systems:


## Decision Tree Example - Lessons learned

Classifiers can have different complexity:

- Complexity has impact on both: training error and testing error.
- Training error: usually decreases with increasing complexity
- Test error: first decreases, then might go up again.

Test error behavior is so common that it has its own name:

- too simple models: high test error due to underfitting
- the model cannot absorb the information from the training data
- too complex models: high test error due to overfitting
- the model tries to reproduce idiosyncracies of the training data that future data will not have

Optimal classifier has a complexity somewhere inbetween, but:

- we cannot tell from either training error or test error alone if we underfit, overfit or neither
- seeing the complete curve will tell us!


## Decision Trees - Conclusion

- Categorial data can often be handled nicely by a tree.
- For continuous data, $\mathcal{X}=\mathbb{R}^{d}$, one typically uses splits by comparing any coordinate by a threshold: $\llbracket x_{i} \geq \theta \rrbracket$ ?
- Finding a split consists of checking all $i=1, \ldots, d$ and all (reasonable) thresholds, e.g. all $x_{i}^{1}, \ldots, x_{i}^{n}$
- If $d$ is large, and all dimension are roughly of equal importance (e.g. time series), this is tedious, and the resulting tree might not be good.

Caveat: single decision trees are rarely used for real-world systems these days. But related techniques are, in particular random forests.

## Nearest Neighbor - analysis: Cover\&Thomas, 1967

## Nearest Neighbor - Training

input dataset $\mathcal{D}=\left\{\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)\right\} \subset \mathbb{R}^{d} \times \mathcal{Y}$
store all examples $\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)$.

## Nearest Neighbor - Prediction

input new example $x \in \mathbb{R}^{d}$
for each training example $\left(x^{i}, y^{i}\right)$
compute $\operatorname{dist}_{i}(x)=\left\|x-x^{i}\right\|$ (Euclidean distance)
output $y^{j}$ for $j=\operatorname{argmin}_{j} \operatorname{dist}_{i}(x)$
(if argmin is not unique, pick between possible examples)

Nearest Neighbor - Illustration


Nearest Neighbor - Illustration


Nearest Neighbor - Illustration


Nearest Neighbor - Illustration


Nearest Neighbor - Illustration


Nearest Neighbor - Illustration


Nearest Neighbor - Illustration


Nearest Neighbor - Illustration


## Nearest Neighbor - Illustration




## Definition (Decision Boundary)

Let $f: \mathcal{X} \rightarrow \mathcal{Y}$ be a classifier with discrete $\mathcal{Y}=\{1, \ldots, M\}$. The points where $f$ is discontinuous are called decision boundary.

## Nearest Neighbor

Nearest Neighbor prediction in the real world:

- very natural and intuitive
- we apply it without even considering it "learning" or "prediction"
- very popular in industry under a variety of names, e.g. 'case based reasoning', Example: helpdesk "Similar problems have similar solutions".

From a machine learning point of view:

- consider data as points in a (potentially high-dim.) vector space
- distance between two points tells us their similarity
- Similar points tend to have the same label.

We can also use NN for categorical labels: embed values into $\mathbb{R}^{d}$, e.g.


## $k$-Nearest Neighbor

More general than nearest neighbor:

## $k$-Nearest Neighbor - Training

input dataset $\mathcal{D}=\left\{\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)\right\} \subset \mathbb{R}^{d} \times \mathcal{Y}$
store all examples $\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)$.

## $k$-Nearest Neighbor - Classification

input new example $x$
for each training example $\left(x^{i}, y^{i}\right)$ compute $d_{i}(x)=\left\|x-x^{i}\right\|$ (Euclidean distance) sort $d_{i}$ in increasing order
output majority vote among $y^{i}$ s within the $k$ smallest $d^{i}$

## $k$-Nearest Neighbor

$k=1:$

- original nearest neighbor rule
- any "outlier" influences the decision boundary



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$k=1:$

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- any "outlier" influences the decision boundary



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## $k$-Nearest Neighbor

$$
k=3:
$$

- isolated outliers are ignored
- decision boundary becomes smoother



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$$
k=3:
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$$
k=3:
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- isolated outliers are ignored
- decision boundary becomes smoother



## $k$-Nearest Neighbor

$k=3:$

- isolated outliers are ignored
- decision boundary becomes smoother


Observation: $k$ controls the complexity of the model:

- $k=1$, decisions based on a single (most similar) example at a time, this might have an unreliable label (overfitting).
- $k=n$, all new points are classified with the label (underfitting).
- as before: there's a sweet spot inbetween.


## Perceptron - Rosenblatt, 1957

So far we've seen two classifiers:

- decision tree: picks a few important features to base decision on
- $k$-NN: all features contribute equally (to Euclidean distance)

Often, neither is optimal:

- we have many features, we want to make use of them.
- but some features are more useful or reliable than others.

Idea: learn how important each feature, $x_{j}$, is by a weight, $w_{j}$
Perceptron algorithm: inspired by (early) neuroscience:

- neurons form a weighted sum of their inputs $x=\left(x_{1}, \ldots, x_{d}\right)$
- they output a spike if the result exceeds a threshold, $\theta$

$$
h(x)=\left\{\begin{array}{ll}
+1 & \text { if } \sum_{j} w_{j} x_{j} \geq \theta \\
-1 & \text { otherwise }
\end{array} \quad=\operatorname{sign}(\langle w, x\rangle-\theta) .\right.
$$

## Perceptron - Training (for $\theta=0$ )

input training set $\mathcal{D} \subset \mathbb{R}^{d} \times\{-1,+1\}$
initialize $w=(0, \ldots, 0) \in \mathbb{R}^{d}$.
repeat
for all $(x, y) \in \mathcal{D}$ : do
compute $a:=\langle w, x\rangle \quad$ ('activation')
if $y a \leq 0$ then
$w \leftarrow w+y x$
end if
end for
until $w$ wasn't updated for a complete pass over $\mathcal{D}$

Perceptron - Classification (for $\theta=0$ )
input new example $x$
output $f(x)=\operatorname{sign}\langle w, x\rangle \quad$ by convention, $\operatorname{sign}(0)=-1$

## Perceptron - Example

$$
\left.\mathcal{D}:\left(x^{1}, y^{1}\right)=\left(\binom{3}{1},+1\right),\left(x^{2}, y^{2}\right)=\binom{1}{1},+1\right),\left(x^{3}, y^{3}\right)=\left(\binom{1}{4},-1\right) .
$$

Round 1:

$$
\begin{gathered}
w=\binom{0}{0}, \quad i=1:\left\langle w, x^{1}\right\rangle=0, \quad 1 \cdot 0=0 \leq 0 \quad \rightarrow \quad \text { update } \\
w_{\text {new }}=w_{\text {old }}+1 \cdot\binom{3}{1}=\binom{3}{1}
\end{gathered}
$$

- $w=\binom{3}{1}, \quad i=2:\left\langle w, x^{2}\right\rangle=4 \quad 1 \cdot 4=4 \not \leq 0 \quad \rightarrow$ no change
- $w=\binom{3}{1}, \quad i=3:\left\langle w, x^{3}\right\rangle=7, \quad(-1) \cdot 7=-7 \leq 0 \quad \rightarrow \quad$ update

$$
w_{\text {new }}=w_{\text {old }}+(-1)\binom{1}{4}=\binom{2}{-3}
$$

## Perceptron - Example

$$
\mathcal{D}:\left(x^{1}, y^{1}\right)=\left(\binom{3}{1},+1\right),\left(x^{2}, y^{2}\right)=\left(\binom{1}{1},+1\right),\left(x^{3}, y^{3}\right)=\left(\binom{1}{4},-1\right) .
$$

Round 2:

$$
\begin{aligned}
& w=\binom{2}{-3}, \quad i=1:\left\langle w, x^{1}\right\rangle=3, \quad 1 \cdot 3=3 \not \leq 0 \quad \rightarrow \text { no change } \\
& w=\binom{2}{-3}, \quad i=2:\left\langle w, x^{2}\right\rangle=-1, \quad 1 \cdot(-1)=-1 \leq 0 \\
& \rightarrow \quad w_{\text {new }}=w_{\text {old }}+1\binom{1}{1}=\binom{3}{-2} \\
& w=\binom{3}{-2}, \quad i=3:\left\langle w, x^{3}\right\rangle=-5, \quad(-1) \cdot(-5)=5 \not \leq 0 \\
& \rightarrow \quad \text { no change }
\end{aligned}
$$

## Perceptron - Example

$$
\mathcal{D}:\left(x^{1}, y^{1}\right)=\left(\binom{3}{1},+1\right),\left(x^{2}, y^{2}\right)=\left(\binom{1}{1},+1\right),\left(x^{3}, y^{3}\right)=\left(\binom{1}{4},-1\right) .
$$

Round 3:

$$
\begin{aligned}
& w=\binom{3}{-2}, i=1:\left\langle w, x^{1}\right\rangle=7, \quad 1 \cdot 7=7 \not \leq 0 \\
& w=\binom{3}{-2}, \\
& w=\binom{3}{-2}, i=3:\left\langle w, x^{2}\right\rangle=1, \quad 1 \cdot 1=1 \not \leq 0 \\
&\left.w, x^{3}\right\rangle=-5, \quad(-5) \cdot(-1)=5 \not \leq 0
\end{aligned}
$$

nothing changed for 1 complete round: converged

## Perceptron - Example

$\mathcal{D}:\left(x^{1}, y^{1}\right)=\left(\binom{3}{1},+1\right),\left(x^{2}, y^{2}\right)=\left(\binom{1}{1},+1\right),\left(x^{3}, y^{3}\right)=\left(\binom{1}{4},-1\right)$.
Round 3:

- $w=\binom{3}{-2}, \quad i=1:\left\langle w, x^{1}\right\rangle=7, \quad 1 \cdot 7=7 \not \leq 0$
- $w=\binom{3}{-2}, \quad i=2:\left\langle w, x^{2}\right\rangle=1, \quad 1 \cdot 1=1 \not \leq 0$
- $w=\binom{3}{-2}, \quad i=3:\left\langle w, x^{3}\right\rangle=-5, \quad(-5) \cdot(-1)=5 \not \leq 0$
nothing changed for 1 complete round: converged
Final classifier: $f(x)=\operatorname{sign}\left(3 \cdot x_{1}-2 \cdot x_{2}\right)$
Limitation: always has a linear decision boundary, might not converge


## Learning algorithms come in all kind of forms and flavors:

- tree structured, "expert systems"
- similarity-based, geometric
- linear thresholding function
- weighted combinations of simpler units ( $\rightarrow$ next lecture)
- iterated/stacked combinations of simpler units $(\rightarrow$ next lecture)


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## Machine learning research

- studies their properties
- provides tools for choosing between different methods
- allows constructing new ones (with better properties)

