CSCI567 Machine Learning (Spring 2025)

Haipeng Luo

University of Southern California

Jan 17, 2025

Outline

1. About this course
2. Overview of machine learning
3. Classification and Nearest Neighbor Classifier (NNC)
4. Theory of NNC (or an example of what are beyond this course...)

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Overview

Nature of this course

- Covers both classical machine learning methods and recent advancements (supervised learning, unsupervised learning, reinforcement learning, etc.), in a systemic and rigorous way
- Particular focuses are on the conceptual understanding and derivation of these methods

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Learning objectives:

- Hone skills on grasping abstract concepts and thinking critically to solve problems with ML techniques
- Solidify your knowledge with hand-on programming tasks
- Prepare you for studying advanced ML techniques

Teaching logistics

Lectures: Friday, 1:00-3:20pm

Discussions: Friday, 3:30-4:20pm (by TAs, same locations)

Online platforms

Web: https://haipeng-luo.net/courses/CSCI567/2025_spring

- general information (schedule, slides, homework, etc.)

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- recorded lectures/discussions

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- submit homework

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Vocareum: https://www.vocareum.com/

- programming project

Teaching staff

4 TAs

- Dongze Ye
- Xiao Fu
- Soumita Hait
- Robby Costales

2 graders (for grading homework only)

- Joonyoung (Aaron) Bae
- Mounika Mukkamalla

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- note: location for office hours might vary during the semester

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- Undergraduate level training in **probability and statistics, linear algebra, (multivariate) calculus**

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  not an intro-level CS course, no training of basic programming skills.

Slides and readings

Lectures

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Readings

- No required textbooks
- Main recommended readings:
  - Probabilistic Machine Learning: An Introduction by Kevin Murphy
  - Elements of Statistical Learning by Hastie, Tibshirani and Friedman
- More: see course website

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Structure:

- 40%: 4 written assignments
- 40%: 2 quizzes
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Important: final cut-offs will NOT be released. If adjusted they could only be LOWER.

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- A two-day window for re-grading (regarding *factual errors*)

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- the project is available throughout the semester (*due on 05/13*, no late days)

Academic honesty and integrity

Zero tolerance for plagiarism and other unacceptable violations:

- finding solutions online, including using chatbots such as ChatGPT
- uploading any material from the course to the Internet

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Bottom line: *help us help you by asking informative questions!*

Outline

Machine learning: the driving force of AI

Recent amazing AI advances: generative AI

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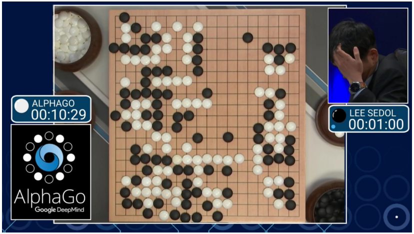
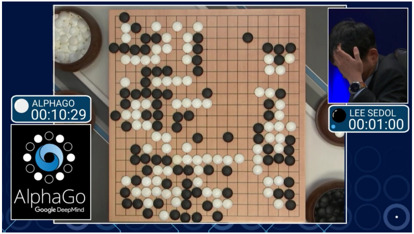
Machine learning: the driving force of AI

Recent amazing AI advances: intelligent planning



Machine learning: the driving force of AI

Recent amazing AI advances: intelligent planning



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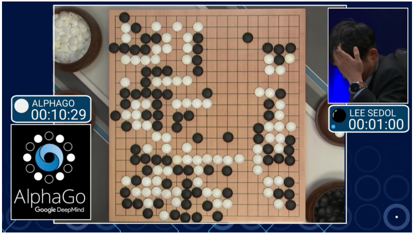

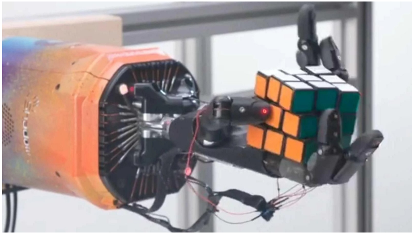

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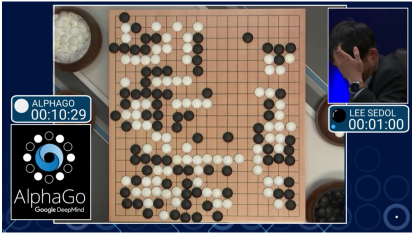

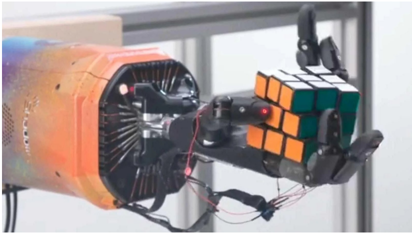

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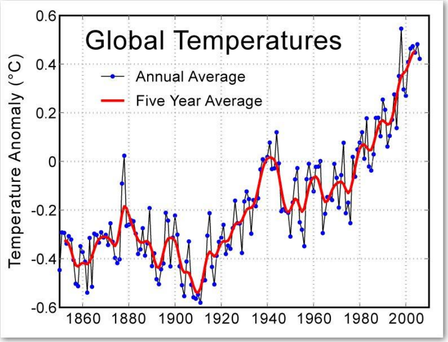
What is machine learning?

One possible definition (cf. Murphy's book)
a set of methods that can automatically *detect patterns* in data, and then use the uncovered patterns to *predict future data*, or to perform other kinds of *decision making under uncertainty*

Example: detect patterns

How the temperature has been changing?



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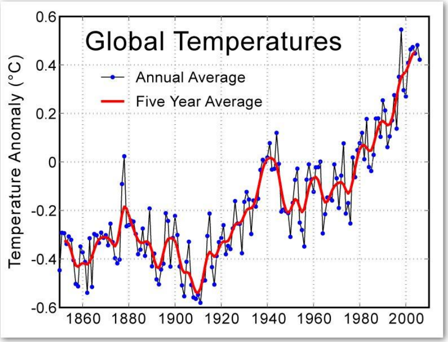
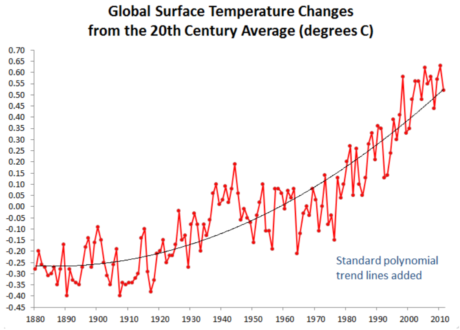


Patterns

- Seems going up
- Repeated periods of going up and down.

How do we describe the pattern?

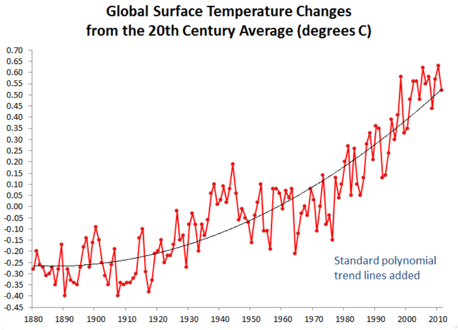
Build a model: fit the data with a polynomial function



- The model is not accurate for individual years
- But collectively, the model captures the major trend

Predicting future

What is temperature of 2030?



- Again, the model is probably inaccurate for that specific year
- But it might be close enough

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Key ingredients in machine learning

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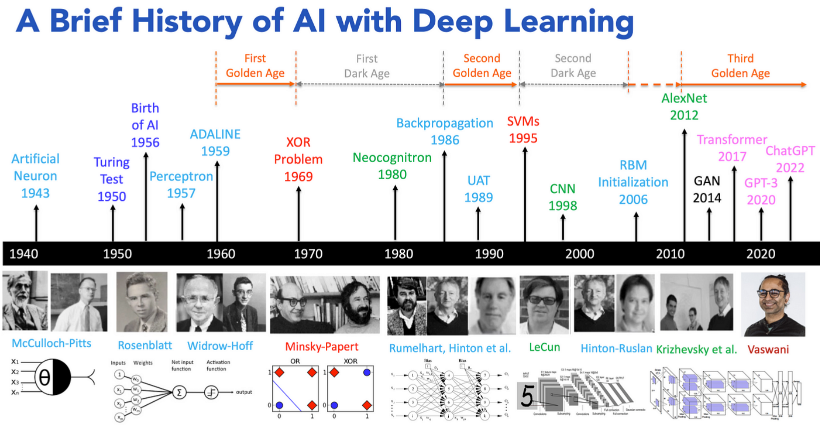
  devised to capture the patterns in the data
  - The model does not have to be true — "All models are wrong, but some are useful" by George Box.
- Prediction
  apply the model to forecast what is going to happen in future

A rich history of applying statistical learning methods

Recognizing flowers (by R. Fisher, 1936)

Types of Iris: setosa, versicolor, and virginica

Huge success with the rise of “deep” learning



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The main focus and goal of this course

- Supervised learning (before Quiz 1)
- Unsupervised learning and reinforcement learning (after Quiz 1)

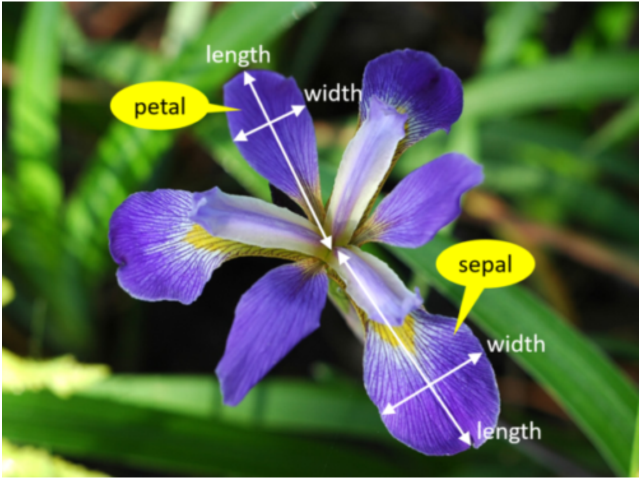
Outline

Recognizing flowers

Types of Iris: setosa, versicolor, and virginica

Measuring the properties of the flowers

Features and attributes: the widths and lengths of sepal and petal



Often, data is conveniently organized as a table

Fisher's *Iris* Data

Sepal length ♦	Sepal width ♦	Petal length ♦	Petal width ♦	Species ♦
5.1	3.5	1.4	0.2	*I. setosa*
4.9	3.0	1.4	0.2	*I. setosa*
4.7	3.2	1.3	0.2	*I. setosa*
4.6	3.1	1.5	0.2	*I. setosa*
5.0	3.6	1.4	0.2	*I. setosa*
5.4	3.9	1.7	0.4	*I. setosa*
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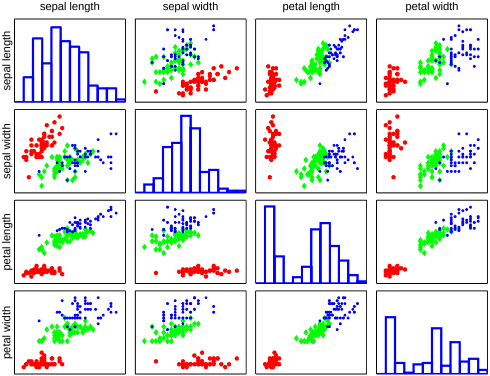
4.4	2.9	1.4	0.2	*I. setosa*
4.9	3.1	1.5	0.1	*I. setosa*

Pairwise scatter plots of 131 flower specimens

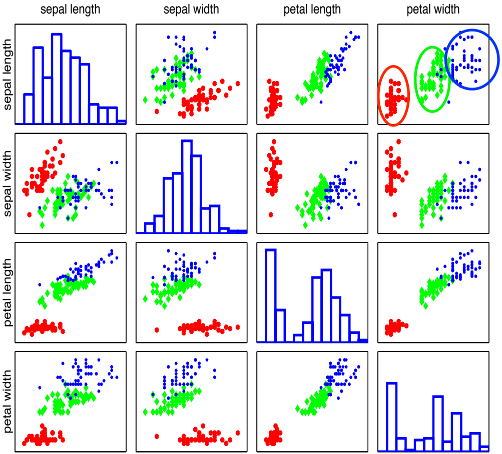
Visualization of data helps identify the right learning model to use

Each colored point is a flower specimen: setosa, versicolor, virginica



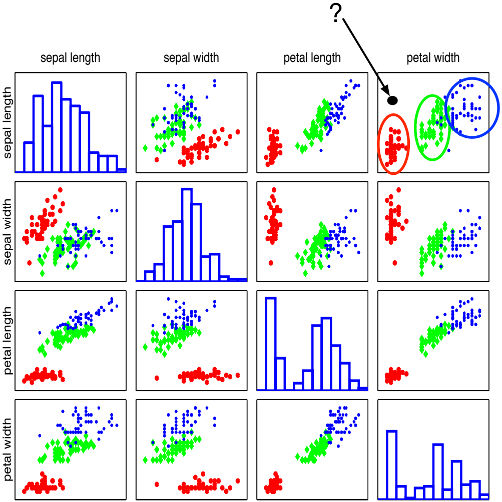
Different types seem well-clustered and separable

Using two features: petal width and sepal length



Labeling an unknown flower type

Closer to red cluster: so predict setosa



General setup for multi-class classification

Training data (set)

- N samples/instances: $\mathcal{D}^{\text{TRAIN}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\mathsf{N}}, y_{\mathsf{N}})\}$

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Special case: binary classification

- Number of classes: $\mathsf{C} = 2$
- Conventional labels: $\{0, 1\}$ or $\{-1, +1\}$ (instead of $\{1, 2\}$)

Nearest neighbor classification (NNC)

The index of the **nearest neighbor** of a point $\boldsymbol{x}$ is

$$\mathsf{nn}(\boldsymbol{x}) = \operatorname*{argmin}_{n \in [\mathsf{N}]} \|\boldsymbol{x} - \boldsymbol{x}_n\|_2 = \operatorname*{argmin}_{n \in [\mathsf{N}]} \sqrt{\sum_{d=1}^{\mathsf{D}} (x_d - x_{nd})^2}$$

where $\|\cdot\|_2$ is the L_2/Euclidean distance.

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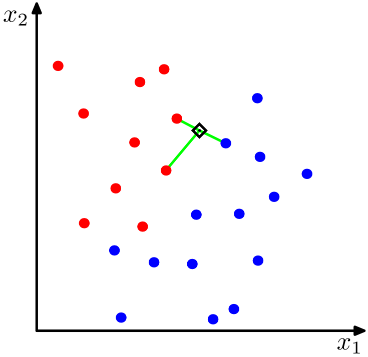
Classification rule

$$f(\boldsymbol{x}) = y_{\mathsf{nn}(\boldsymbol{x})}$$

Visual example

In this 2-dimensional example, the nearest point to $\boldsymbol{x}$ is a red training instance, thus, $\boldsymbol{x}$ will be labeled as red.



(a)

Example: classify Iris with two features

Training data

ID (n)	petal width (x_1)	sepal length (x_2)	category (y)
1	0.2	5.1	setoas
2	1.4	7.0	versicolor
3	2.5	6.7	virginica
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A new specimen with unknown category:

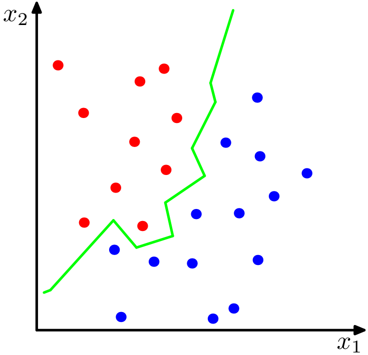
petal width = 1.8 and sepal length = 6.4 (i.e. $\boldsymbol{x} = (1.8, 6.4)$)
Calculating distance $\|\boldsymbol{x} - \boldsymbol{x}_n\|_2 = \sqrt{(x_1 - x_{n1})^2 + (x_2 - x_{n2})^2}$

ID	distance
1	2.06
2	0.72
3	0.76

Thus, the prediction is *versicolor*.

Decision boundary

For every point in the space, we can determine its label using the NNC rule. This gives rise to a *decision boundary* that partitions the space into different regions.



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Is NNC doing the right thing for us?

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$$A^{\text{TRAIN}} = \frac{1}{\mathsf{N}} \sum_n \mathbb{I}[f(\boldsymbol{x}_n) == y_n], \quad \varepsilon^{\text{TRAIN}} = \frac{1}{\mathsf{N}} \sum_n \mathbb{I}[f(\boldsymbol{x}_n) \neq y_n]$$

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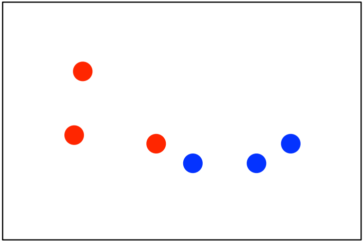
Is this the right measure?

Example

Training data



What are A^{TRAIN} and $\varepsilon^{\mathrm{TRAIN}}$?

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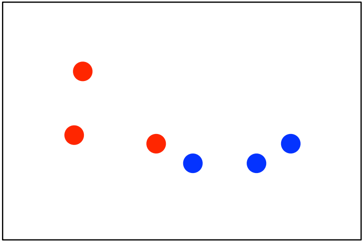

What are A^{TRAIN} and $\varepsilon^{\mathrm{TRAIN}}$?

$$A^{\mathrm{TRAIN}} = 100\%, \quad \varepsilon^{\mathrm{TRAIN}} = 0\%$$

For every training data point, its nearest neighbor is itself.

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- Good measurement of a classifier's performance

Variant 1: measure nearness with other distances

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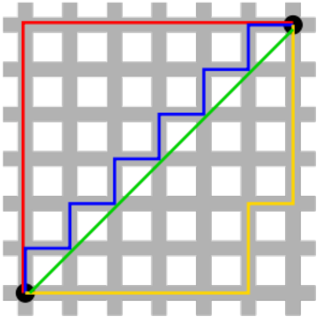

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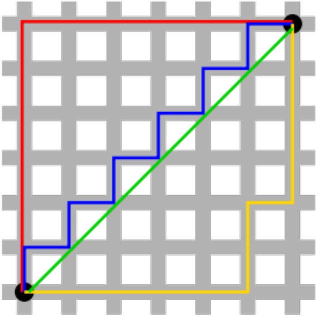
More generally, L_p distance (for $p \geq 1$):

$$\|\boldsymbol{x} - \boldsymbol{x}_n\|_p = \left(\sum_d |x_d - x_{nd}|^p \right)^{1/p}$$



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Variant 2: K-nearest neighbor (KNN)

Increase the number of nearest neighbors to use?

- 1st-nearest neighbor: $\mathsf{nn}_1(\boldsymbol{x}) = \operatorname{argmin}_{n \in [\mathsf{N}]} \|\boldsymbol{x} - \boldsymbol{x}_n\|_2$
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Note: we have

$$\|\boldsymbol{x} - \boldsymbol{x}_{\mathsf{nn}_1(\boldsymbol{x})}\|_2 \leq \|\boldsymbol{x} - \boldsymbol{x}_{\mathsf{nn}_2(\boldsymbol{x})}\|_2 \cdots \leq \|\boldsymbol{x} - \boldsymbol{x}_{\mathsf{nn}_K(\boldsymbol{x})}\|_2$$

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Classification rule

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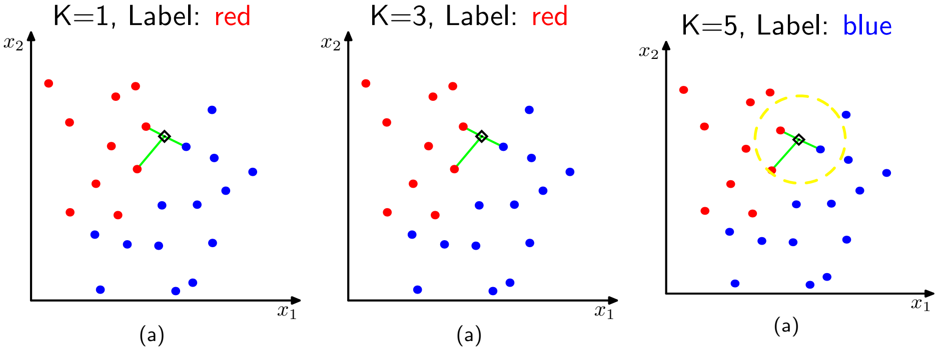
- Predict with the majority

$$f(\boldsymbol{x}) = \operatorname*{argmax}_{c \in [\mathsf{C}]} v_c$$

Example



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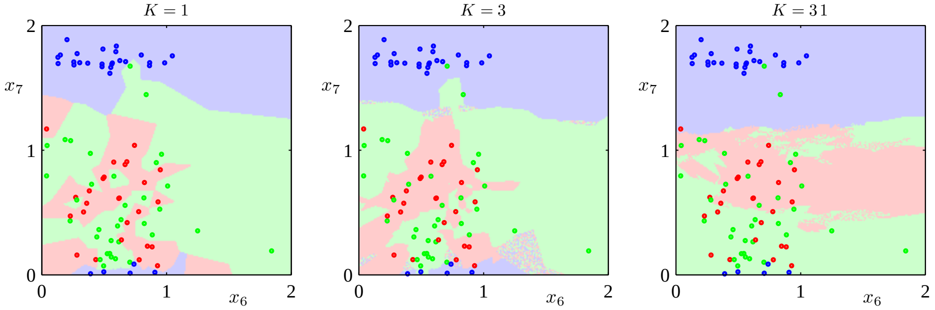

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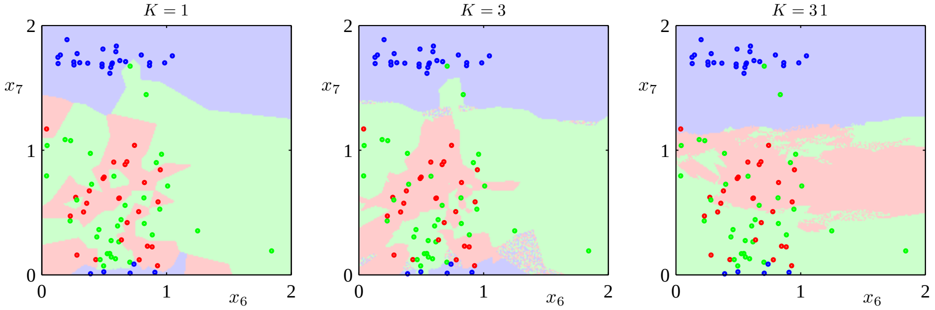

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What happens when $K = N$?

Variant 3: Preprocessing data

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Example:

- compute the means and standard deviations in each feature

$$\bar{x}_d = \frac{1}{\mathsf{N}} \sum_n x_{nd}, \qquad s_d^2 = \frac{1}{N} \sum_n (x_{nd} - \bar{x}_d)^2$$

- Scale the feature accordingly

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Many other ways of normalizing data.

Which variants should we use?

Hyper-parameters in NNC

- The distance measure (e.g. the parameter p for L_p norm)
- K (i.e. how many nearest neighbor?)
- Different ways of preprocessing

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- Different ways of preprocessing

Most algorithms have hyper-parameters. Tuning them is a significant part of applying an algorithm.

Tuning via a validation dataset

Training data

- N samples/instances: $\mathcal{D}^{\text{TRAIN}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_\mathsf{N}, y_\mathsf{N})\}$
- They are used to learn $f(\cdot)$

Test data

- M samples/instances: $\mathcal{D}^{\text{TEST}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_\mathsf{M}, y_\mathsf{M})\}$
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These three sets should *not* overlap!

Recipe

- For each possible value of the hyperparameter (e.g. $K = 1, 3, \cdots$)
  - Train a model using $\mathcal{D}^{\text{TRAIN}}$
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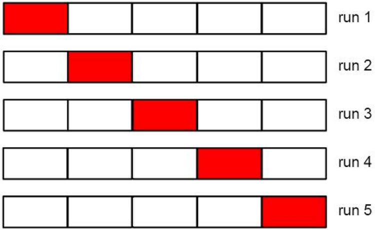
S-fold Cross-validation

What if we do not have a validation set?

- Split the training data into S equal parts.

S $= 5$: 5-fold cross validation



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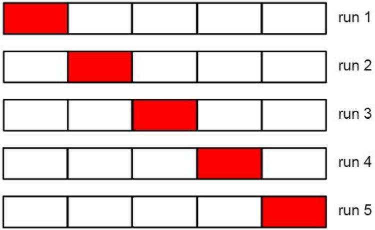

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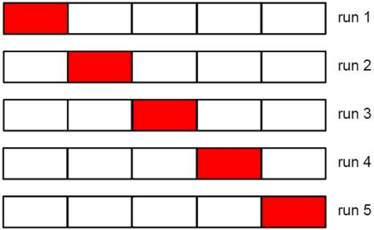

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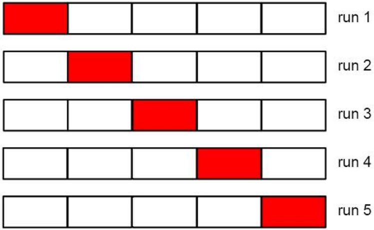

Special case: S = N, called leave-one-out.

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- Choosing the right hyper-parameters can be involved.

Summary

Typical steps of developing a machine learning system:

- Collect data, split into training, validation, and test sets.
- Train a model with a machine learning algorithm. Most often we apply cross-validation to tune hyper-parameters.
- Evaluate using the test data and report performance.
- Use the model to predict future/make decisions.

Outline

1. About this course
2. Overview of machine learning
3. Classification and Nearest Neighbor Classifier (NNC)
4. Theory of NNC (or an example of what are beyond this course...)
   - Step 1: Expected risk
   - Step 2: The ideal classifier
   - Step 3: Comparing NNC to the ideal classifier

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3. Compare NNC to the ideal one.

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Need a more "certain" measure of performance (so it's easy to compare different classifiers for example).

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What about the expectation of training error? Is training error a good proxy of expected error?

Expected risk

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- e.g. $L(y', y) = \mathbb{I}[y' \neq y]$, called *0-1 loss*.
- many more other losses as we will see.

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For special case $C = 2$, let $\eta(\boldsymbol{x}) = \mathcal{P}(0|\boldsymbol{x})$, then

$$R(f^*) = \mathbb{E}_{\boldsymbol{x}\sim\mathcal{P}_{\boldsymbol{x}}}[\min\{\eta(\boldsymbol{x}), 1 - \eta(\boldsymbol{x})\}].$$

Comparing NNC to Bayes optimal classifier

Come back to the question: how good is NNC?

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Theorem (Cover and Hart, 1967)

Let f_N be the 1-nearest neighbor binary classifier using N training data points, we have (under mild conditions)

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A pretty strong guarantee.
In particular, $R(f^*) = 0$ implies $\mathbb{E}[R(f_N)] \to 0$.

Proof sketch

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This kind of ML theory is not covered/required in this course!