CSCI567 Machine Learning (Fall 2018)

Prof. Haipeng Luo

U of Southern California

Aug 22, 2018

Outline

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Enrollment

- There was some delay unfortunately. It is closing by the end of *today*.
- Two offerings: on-campus and DEN. You only need to *attend one*.
- Two sections: a lecture and a discussion section. You need to *attend both*. Discussion section is starting next week.

Teaching staff

- Instructors:

  Lecture: Haipeng Luo
  Discussion: Dr. Victor Adamchik and Dr. Kim Peters
  and a lot of help from Dr. Michael Shindler

- TAs:

  Chin-Cheng Hsu
  Shamim Samadi
  Chi Zhang
  Ke Zhang
  and more...

- More course producers and graders

- Office hours: TBA

Online platforms

A course website:

http://www-bcf.usc.edu/~haipengl/courses/CSCI567/2018_fall

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

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- main discussion forum
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D2L: https://courses.uscden.net/d2l/login

- lecture videos
- submit written assignments
- grade posting

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Required preparation

- Undergraduate courses in probability and statistics, linear algebra, multivariate calculus
- Programming: Python and necessary packages, `git`

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

Slides and readings

Lectures

Lecture slides will be posted before or soon after class.

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Readings

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

Grade

- 15%: 5 written assignments
- 25%: 5 programming assignments
- 60%: 2 exams

Homework assignments

Five, each consists of

- problem set (3%)
  - submit one PDF to D2L (scan copy or typeset with LaTeX etc.)
  - graded based on effort

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- problem set (3%)
    - submit one PDF to D2L (scan copy or typeset with LaTeX etc.)
    - graded based on effort
- programming tasks (5%)
    - submit through GitHub
    - graded by scripts

Policy

Collaboration:

- Allowed, but only at high-level
- Each has to make a separate submission
- State clearly who you collaborated with (or obtained help from)

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Late submissions:

- A total of 5 grace days for the semester
- fill a form to apply within 24 hours of due time
- in place of "excused late" submissions, not in addition to
- no grace period
- late submissions without using grace days will be scored as 0
- your responsibility to keep track

Exams

- One midterm: *10/03, 5:00-7:00 PM*
- One final: *11/28, 5:00-7:00 PM*
- Location: TBA
- Individual effort, closed-book and closed-notes
- *Request for a different date/time must be submitted within first two weeks or asap in case of emergence*

Academic honesty and integrity

Plagiarism and other unacceptable violations

- Neither ethical nor in your self-interest
- Zero-tolerance

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The nature of this course

- Describe basic concepts and tools
- Describe algorithms and their development with intuition and rigor

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Expectation on you

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

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Feel free to interrupt and ask questions!

Important things for you to do

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Questions?

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What is machine learning?

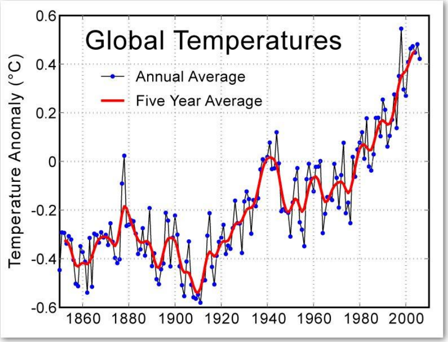
One possible definition[1]

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*

cf. Murphy's book

Example: detect patterns

How the temperature has been changing?



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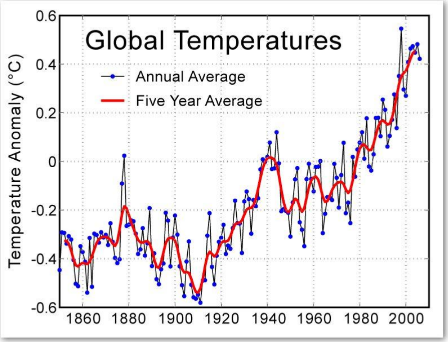
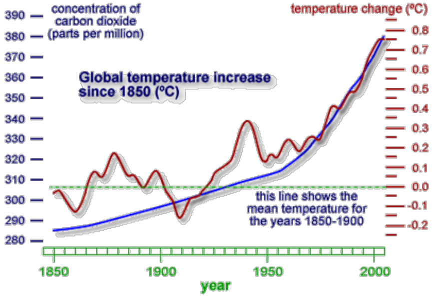


Patterns

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

How do we describe the pattern?

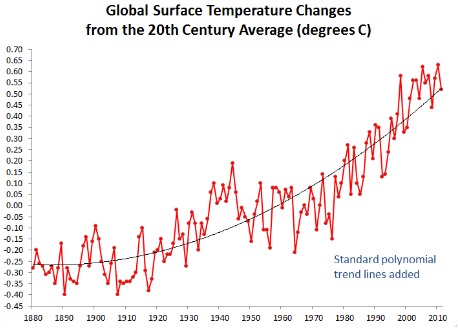
Build a model: fit the data with a polynomial function



- The model is not accurate for individual years
- But collectively, the model captures the major trend
- Still, not able to model the pattern of the *repeated up and down*

Predicting future

What is temperature of 2010?



- Again, the model is not accurate for that specific year
- But then, it is close to the actual one

What we have learned from this example?

Key ingredients in machine learning

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- Modeling
  devised to capture the patterns in the data
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- Prediction
  apply the model to forecast what is going to happen in future

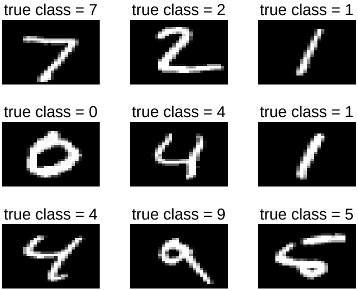
A rich history of applying statistical learning methods

Recognizing flowers (by R. Fisher, 1936)

Types of Iris: setosa, versicolor, and virginica

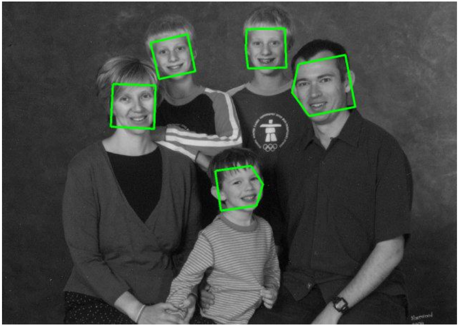
Huge success 20 years ago

Recognizing handwritten zipcodes (AT&T Labs, late 1990s)



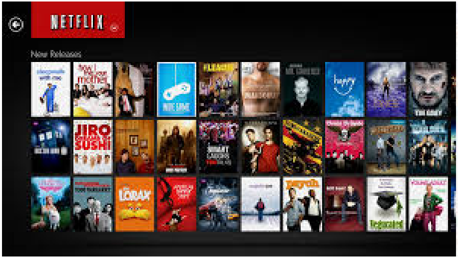
More modern ones, in your social life

Recognizing your friends on Facebook



It might be possible to know about you than yourself

Recommending what you might like



Why is machine learning so hot?

- **Tons of consumer applications**:
  - speech recognition, information retrieval and search, email and document classification, stock price prediction, object recognition, biometrics, etc
  - Highly desirable expertise from industry: Google, Facebook, Microsoft, Uber, Twitter, IBM, Linkedin, Amazon, $\cdots$

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- **Enable scientific breakthrough**
  - Climate science: understand global warming cause and effect
  - Biology and genetics: identify disease-causing genes and gene networks
  - Social science: social network analysis; social media analysis
  - Business and finance: marketing, operation research
  - Emerging ones: healthcare, energy, $\cdots$

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The focus and goal of this course

- Supervised learning (before midterm)
- Unsupervised learning (after midterm)

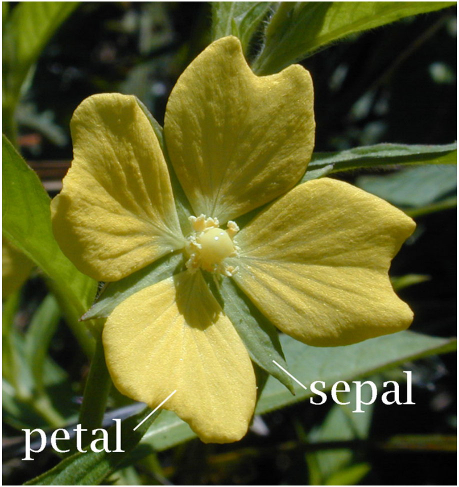
Outline

Recognizing flowers

Types of Iris: setosa, versicolor, and virginica

Measuring the properties of the flowers

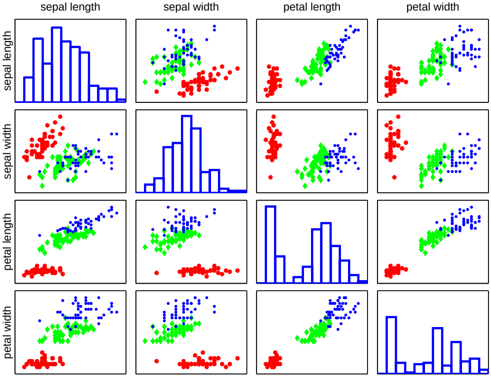
Features and attributes: the widths and lengths of sepal and petal



Pairwise scatter plots of 131 flower specimens

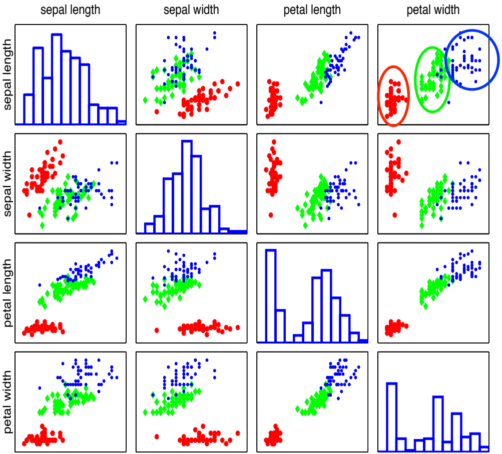
Visualization of data helps identify the right learning model to use

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



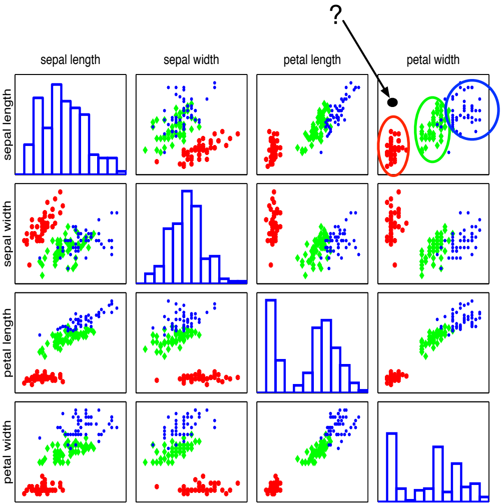
Different types seem well-clustered and separable

Using two features: petal width and sepal length



Labeling an unknown flower type

Closer to red cluster: so labeling it as setosa



General setup for multi-class classification

Training data (set)

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

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Special case: binary classification

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

Often, data is conveniently organized as a table

Ex: Iris data (click here for all data)

- 4 features
- 3 classes

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*
4.6	3.4	1.4	0.3	*I. setosa*
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Nearest neighbor classification (NNC)

Nearest neighbor

$$\boldsymbol{x}(1) = \boldsymbol{x}_{\mathsf{nn}(\boldsymbol{x})}$$

where $\mathsf{nn}(\boldsymbol{x}) \in [\mathsf{N}] = \{1, 2, \cdots, \mathsf{N}\}$, i.e., the index to one of the training instances,

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

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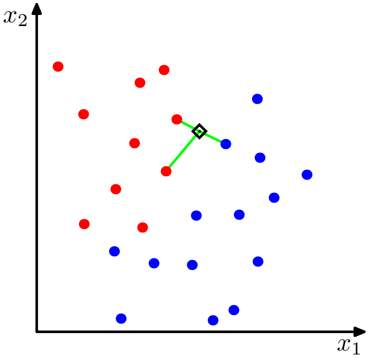
Classification rule

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

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
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Flower with unknown category

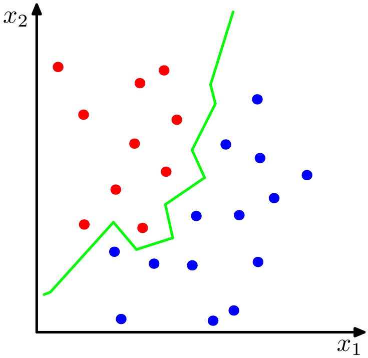
petal width = 1.8 and sepal width = 6.4 (i.e. $\boldsymbol{x} = (1.8, 6.4)$)
Calculating distance $\|\boldsymbol{x} - \boldsymbol{x}_n\|_2 = \sqrt{(x_1 - x_{n1})^2 + (x_2 - x_{n2})^2}$

ID	distance
1	1.75
2	0.72
3	0.76

Thus, the category 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.



(b)

Is NNC doing the right thing for us?

Intuition

We should compute accuracy — the percentage of data points being correctly classified, or the error rate — the percentage of data points being incorrectly classified. (accuracy $+$ error rate $= 1$)

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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?

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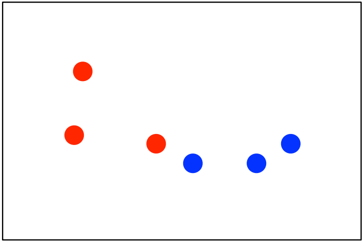

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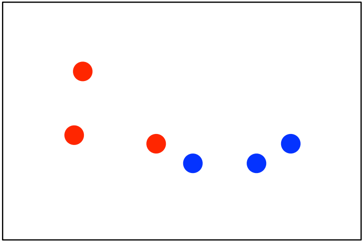

What are A^{TRAIN} and $\varepsilon^{\text{TRAIN}}$?

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

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

Test Error

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- $\mathcal{D}^{\text{TEST}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\mathsf{M}}, y_{\mathsf{M}})\}$
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- Good measurement of a classifier's performance

Variant 1: measure nearness with other distances

Previously, we use the Euclidean distance

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E.g., the following L_1 distance (i.e., city block distance, or Manhattan distance)

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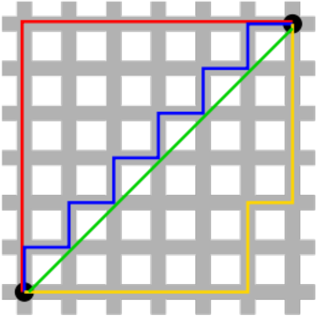

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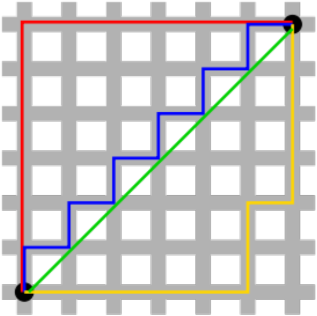
More generally, L_p distance (for $p \geq 1$):

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



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Variant 2: K-nearest neighbor (KNN)

Increase the number of nearest neighbors to use?

- 1-nearest neighbor: $\mathsf{nn}_1(\boldsymbol{x}) = \arg\min_{n\in[\mathsf{N}]} \|\boldsymbol{x} - \boldsymbol{x}_n\|_2$
- 2-nearest neighbor: $\mathsf{nn}_2(\boldsymbol{x}) = \arg\min_{n\in[\mathsf{N}]-\mathsf{nn}_1(\boldsymbol{x})} \|\boldsymbol{x} - \boldsymbol{x}_n\|_2$
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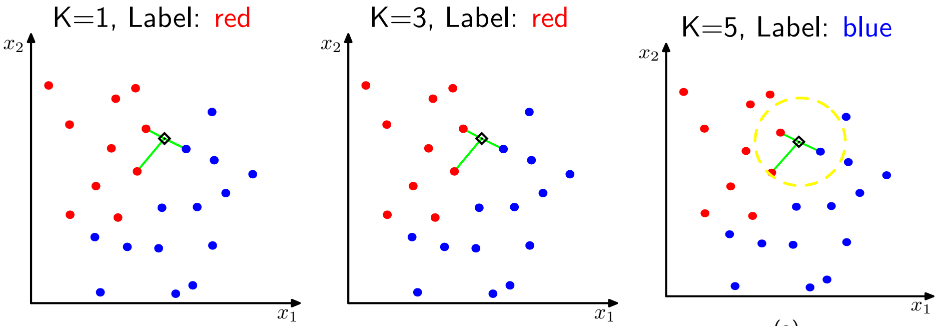
- Predict with the majority

$$y = f(\boldsymbol{x}) = \arg\max_{c \in [\mathsf{C}]} v_c$$

Example



(a) (a) (a)

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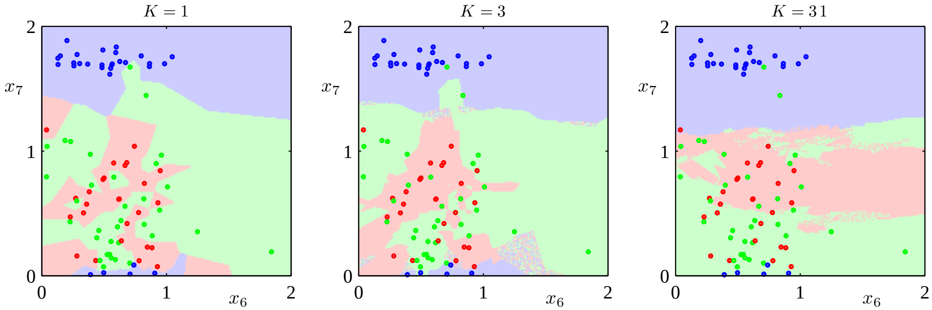

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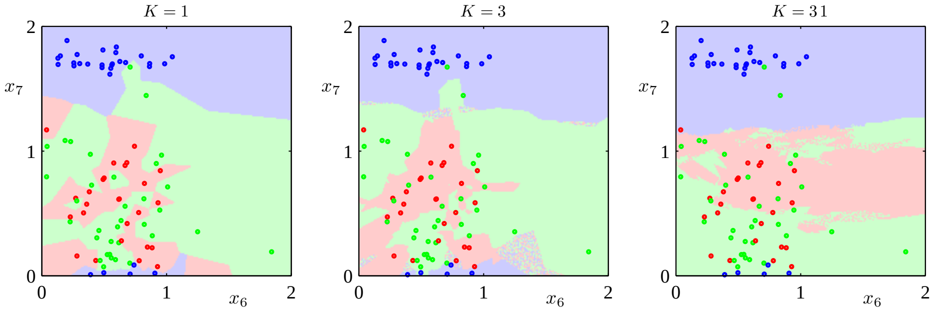

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What happens when $K = N$?

Variant 3: Preprocessing data

One issue of NNC: *distances depend on units of the features!*

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Example:

- compute the means and standard deviations in each feature

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

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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?)
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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 development 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 for learning $f(\cdot)$

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These three sets should *not* overlap!

Recipe

- For each possible value of the hyperparameter (e.g. $K = 1, 3, \cdots$)
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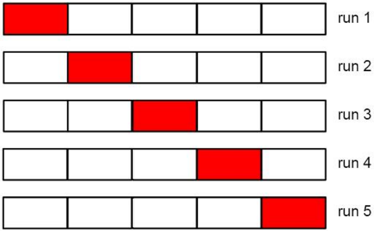
S-fold Cross-validation

What if we do not have a development set?

- Split the training data into S equal parts.

S $= 5$: 5-fold cross validation



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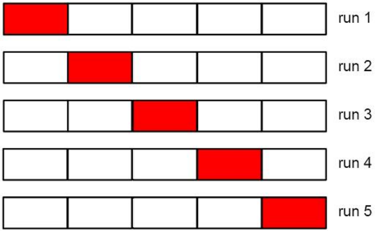

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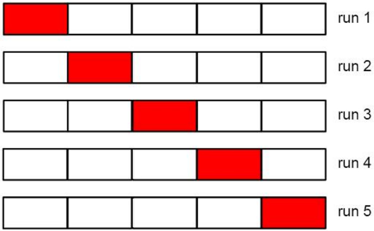

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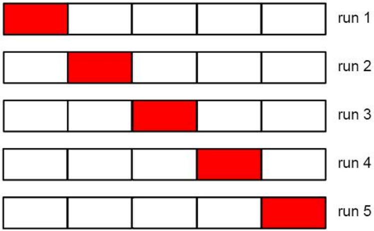

Special case: $\mathsf{S} = \mathsf{N}$, called leave-one-out.

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- Choosing the right hyper-parameters can be involved.

Mini-summary

Typical steps of developing a machine learning system:

- Collect data, split into training, development, 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

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1. Define *more carefully* a performance metric for a 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

More generally, for a loss function $L(y', y)$,

- 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 $\eta(x) = \mathcal{P}(0|x)$, then

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

Comparing NNC to Bayes optimal classifier

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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 $\mathbb{E}[R(f_N)] \to 0$.

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&= \mathbb{E}_{\mathcal{P}_x}\mathbb{E}_{y,y' \overset{i.i.d.}{\sim} \mathcal{P}(\cdot|\boldsymbol{x})}[\mathbb{I}[y' = 0 \text{ and } y = 1] + \mathbb{I}[y' = 1 \text{ and } y = 0]] \\
&= \mathbb{E}_{\mathcal{P}_x}[\eta(x)(1-\eta(x)) + (1-\eta(x))\eta(x)] \\
&= 2\mathbb{E}_{\mathcal{P}_x}[\eta(x)(1-\eta(x))]
\end{aligned}
$$

Proof sketch

Fact: $x(1) \to x$ with probability 1

$$
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&= \mathbb{E}_{\mathcal{P}_x}[\eta(x)(1-\eta(x)) + (1-\eta(x))\eta(x)] \\
&= 2\mathbb{E}_{\mathcal{P}_x}[\eta(x)(1-\eta(x))] \\
&\leq 2\mathbb{E}_{\mathcal{P}_x}[\min\{\eta(x), (1-\eta(x))\}]
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&= 2R(f^*)
\end{aligned}
$$