CSCI567 Machine Learning (Spring 2023)
Week 1: Course overview, KNN, ML system

Prof. Yan Liu

University of Southern California

Outline

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What is machine learning?

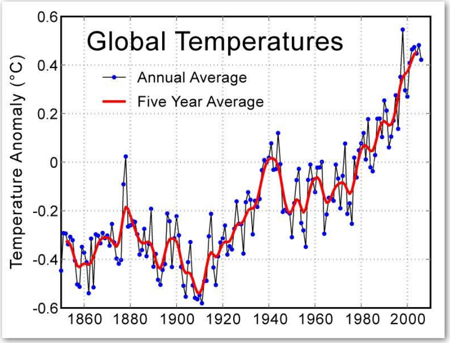
One possible definition[1]

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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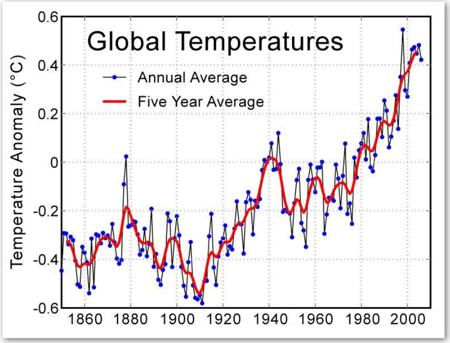
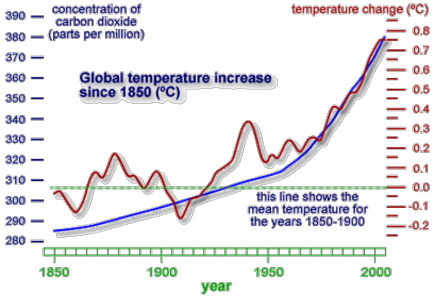


Patterns

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

How do we describe the pattern?

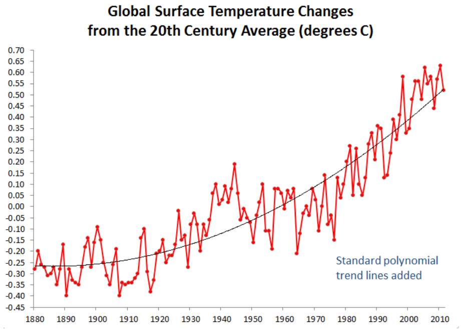
Build a model: fit the data with a polynomial function



- 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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  collected from past observation (we often call them *training data*)
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  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

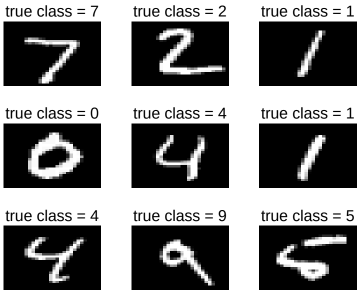
A rich history of applying statistical learning methods

Recognizing flowers (by R. Fisher, 1936)

Types of Iris: setosa, versicolor, and virginica

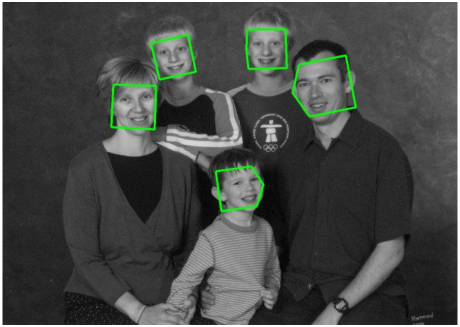
Huge success 20 years ago

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



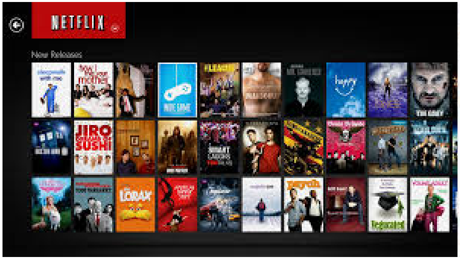
More modern ones, in your social life

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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Different flavors of learning problems

- Supervised learning
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The focus and goal of this course

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

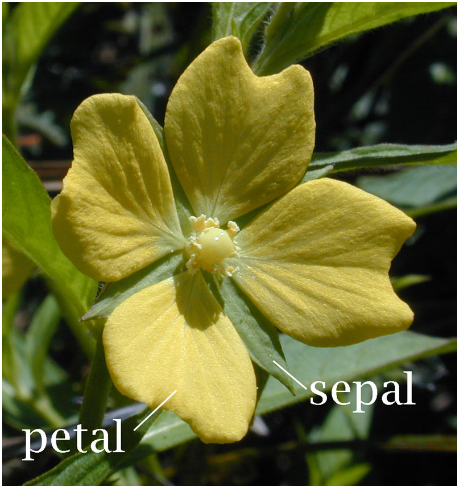
Outline

Recognizing flowers

Types of Iris: setosa, versicolor, and virginica

Measuring the properties of the flowers

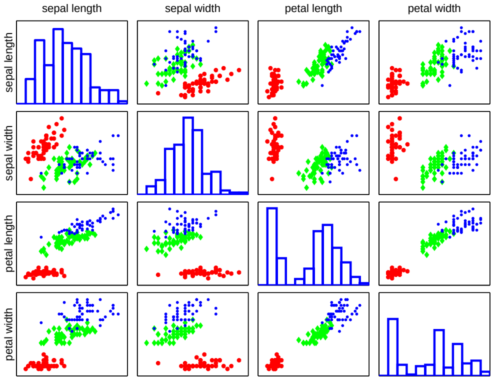
Features and attributes: the widths and lengths of sepal and petal



Pairwise scatter plots of 131 flower specimens

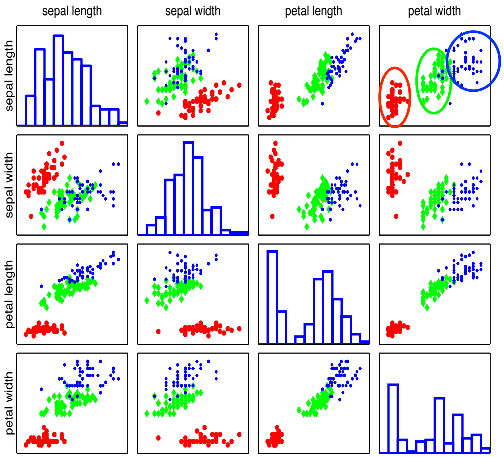
Visualization of data helps identify the right learning model to use

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



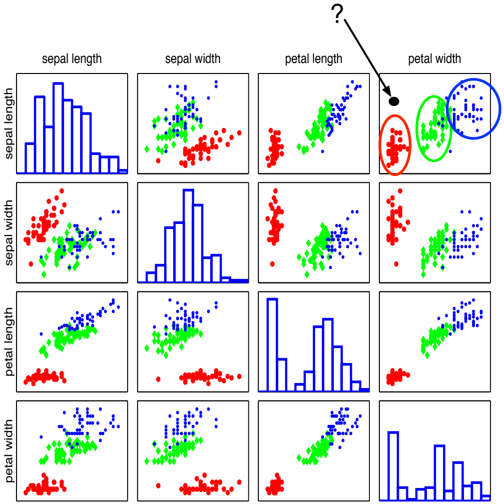
Different types seem well-clustered and separable

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

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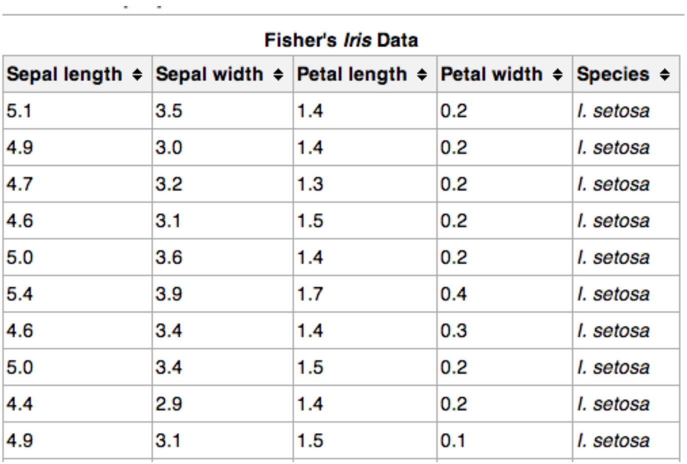
Special case: binary classification

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

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*
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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,

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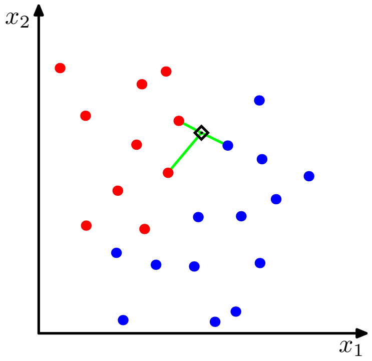
Classification rule

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

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

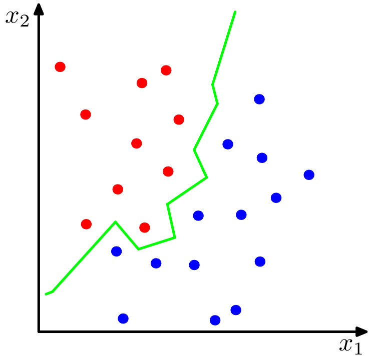
petal width = 1.8 and sepal width = 6.4 (i.e. $\boldsymbol{x} = (1.8, 6.4)$)
Calculating distance $\|\boldsymbol{x} - \boldsymbol{x}_n\|_2 = \sqrt{(x_1 - x_{n1})^2 + (x_2 - x_{n2})^2}$

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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where $\mathbb{I}[\cdot]$ is the indicator function.

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Is this the right measure?

Example

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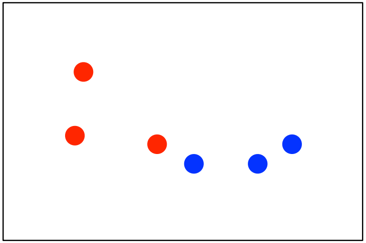

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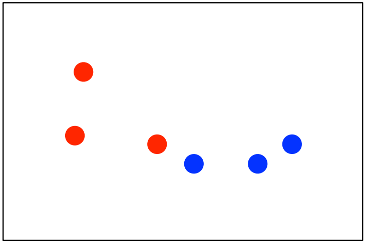

What are A^{TRAIN} and $\varepsilon^{\text{TRAIN}}$?

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

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

Test Error

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- Good measurement of a classifier's performance

Variant 1: measure nearness with other distances

Previously, we use the Euclidean distance

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Many other alternative distances

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

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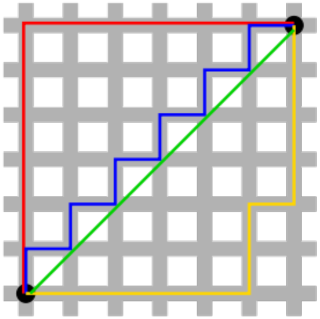

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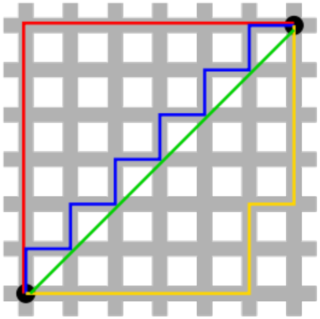
More generally, L_p distance (for $p \geq 1$):

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



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Variant 2: K-nearest neighbor (KNN)

Increase the number of nearest neighbors to use?

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Note: with $\boldsymbol{x}(k) = \boldsymbol{x}_{\mathsf{nn}_k(\boldsymbol{x})}$, we have

$$\|\boldsymbol{x} - \boldsymbol{x}(1)\|_2^2 \leq \|\boldsymbol{x} - \boldsymbol{x}(2)\|_2^2 \cdots \leq \|\boldsymbol{x} - \boldsymbol{x}(K)\|_2^2$$

How to classify with K neighbors?

Classification rule

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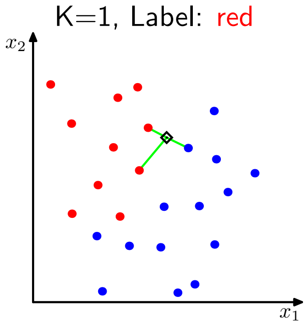
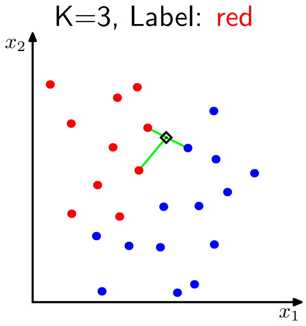
- Predict with the majority

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

Example



(a)



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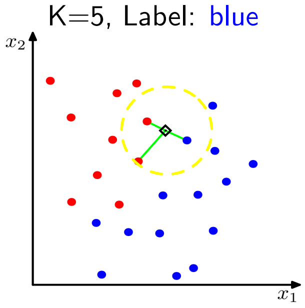
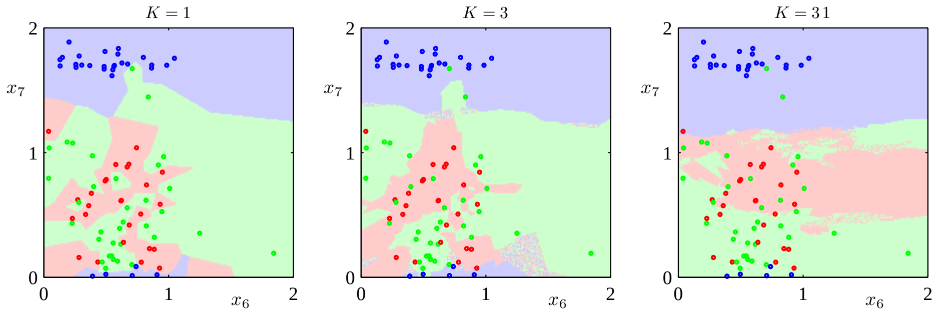


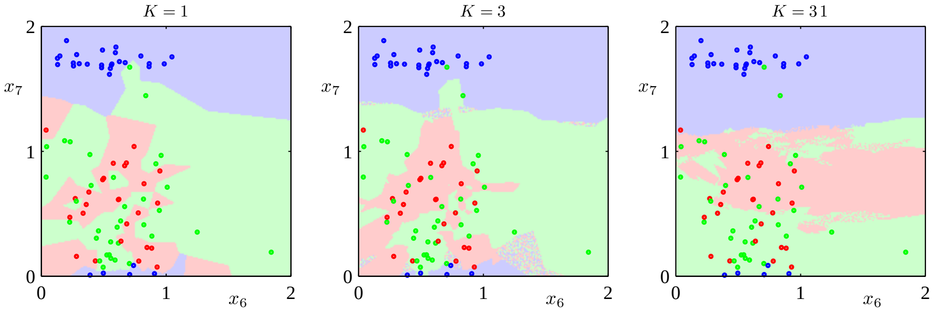
(a)

Decision boundary



When K increases, the decision boundary becomes smoother.

Decision boundary



When K increases, the decision boundary becomes smoother.

What happens when $K = N$?

Variant 3: Preprocessing data

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Example:

- compute the means and standard deviations in each feature

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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)
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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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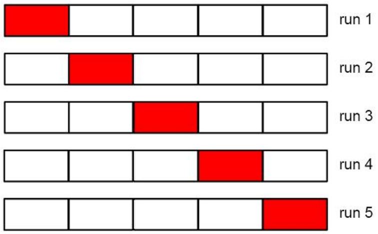
What if we do not have a development set?

- Split the training data into S equal parts.

S $= 5$: 5-fold cross validation



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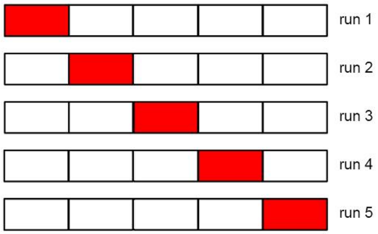

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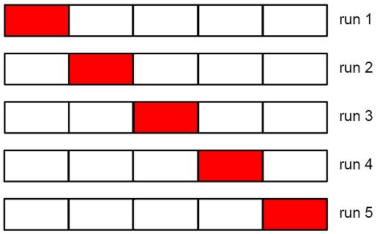

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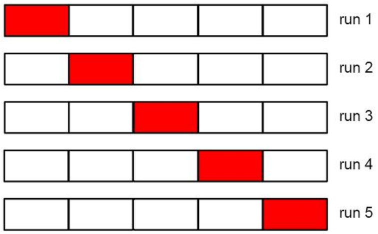

Special case: S $=$ N, called leave-one-out.

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

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

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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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