An Introduction to Machine Learning

L1: Basics and Probability Theory

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Overview

L1: Machine learning and probability theory
Introduction to pattern recognition, classification, regression, novelty detection, probability theory, Bayes rule, inference

L2: Density estimation and Parzen windows
Nearest Neighbor, Kernels density estimation, Silverman's rule, Watson Nadaraya estimator, crossvalidation

L3: Perceptron and Kernels
Hebb's rule, perceptron algorithm, convergence, feature maps, kernels

L4: Support Vector estimation
Geometrical view, dual problem, convex optimization, kernels

L5: Support Vector estimation
Regression, Quantile regression, Novelty detection, ν-trick

L6: Structured Estimation
Sequence annotation, web page ranking, path planning, implementation and optimization

L1 Introduction to Machine Learning

Data

- Texts, images, vectors, graphs

What to do with data

- Unsupervised learning (clustering, embedding, etc.)
- Classification, sequence annotation
- Regression, autoregressive models, time series
- Novelty detection

What is not machine learning

- Artificial intelligence
- Rule based inference

Statistics and probability theory

- Probability of an event
- Dependence, independence, conditional probability
- Bayes rule, Hypothesis testing

Data

Vectors

- Collections of features
  e.g. height, weight, blood pressure, age, ...
- Can map categorical variables into vectors

Matrices

- Images, Movies
- Remote sensing and satellite data (multispectral)

Strings

- Documents
- Gene sequences

Structured Objects

- XML documents
- Graphs

Optical Character Recognition

Reuters Database


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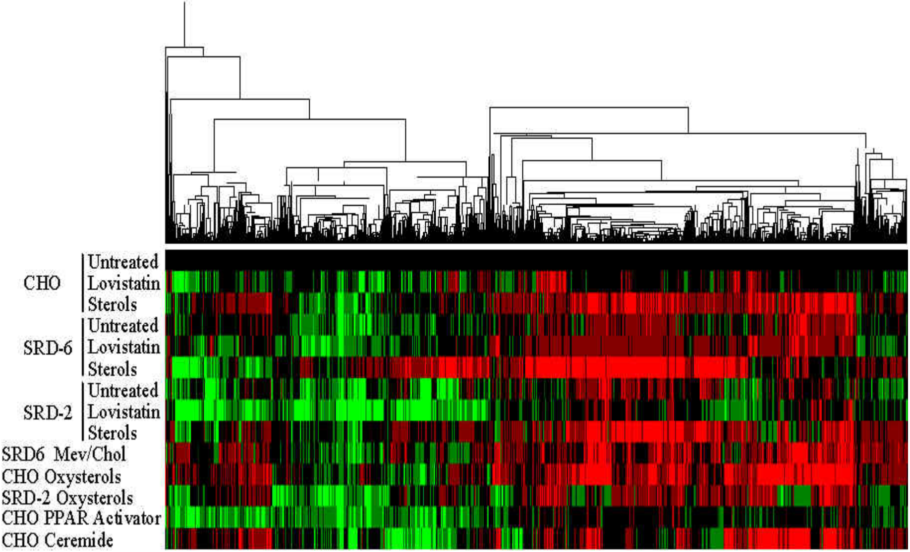
    Revs 32.6 mln vs 24.4 mln
    Year
    Shr 90 cts vs 69 cts
    Net 4,508,000 vs 3,096,000
    Revs 101.0 mln vs 76.9 mln
    Avg shrs 5,029,000 vs 4,464,000
    NOTE: 1986 fiscal year ended Feb 1, 1986
 Reuter
&#3;</BODY></TEXT>
</REUTERS>
```

Faces

More Faces

NATIONAL ICT AUSTRALIA LIMITED

Microarray Data



Biological Sequences

Goal

Estimate function of protein based on sequence information.

Example Data

>0_d1vcaa2 2.1.1.4.1 (1-90) N-terminal domain of vascular cell adhesion molecule-1 (VCAM-1) [human (Homo sapiens)]
FKIETTPESRYLAQIGDSVSLTCSTTGCESPFFSWRTQIDSPLNGKVTNEGTTSTLTMNPVSFGNEHSYL
CTATCESRKLEKGIQVEIYS
>0_d1zxq_2 2.1.1.4.2 (1-86) N-terminal domain of intracellular adhesion molecule-2, ICAM-2 [human (Homo sapiens)]
KVFEVHVRPKKLAVEPKGSLEVNCSTTCNQPEVGGLETSLNKILLDEQAQWKHYLVSNISHDTVLQCHFT
CSGKQESMNSNVSVYQ
>0_d1tlk__ 2.1.1.4.3 Telokin [turkey (Meleagris gallopavo)]
VAEEKPHVKPYFTKTILDMDVVEGSAARFDCKVEGYPDPEVMWFKDDNPVKESRHFQIDYDEEGNCSLTI
SEVCGDDDAKYTCKAVNSLGEATCTAELLVETM
>0_d2ncm__ 2.1.1.4.4 N-terminal domain of neural cell adhesion molecule (NCAM) [human (Homo sapiens)]
RVLQVDIVPSQGEISVGESKFFLCQVAGDAKDKDISWFSPNGEKLSPNQQRISVVWNDDDSSTLTIYNAN
IDDAGIYKCVVTAEDGTQSEATVNVKIFQ
>0_d1tnm__ 2.1.1.4.5 Titin [Human (Homo sapiens), module M5]
RILTKPRSMTVYEGESARFSCDTDGEPVPTVTWLRKGQVLSTSARHQVTTTKYKSTFEISSVQASDEGNY
SVVVENSEGKQEAEFTLTIQK
>0_d1wiu__ 2.1.1.4.6 Twitchin [Nematode (Caenorhabditis elegans)]
LKPKILTASRKIKIKAGFTHNLEVDFIGAPDPTATWTVGDSGAALAPELLVDAKSSTTSIFFPSAKRADS
GNYKLKVKNELGEDEAIFEVIVQ
>0_d1koa_1 2.1.1.4.6 (351-447) Twitchin [Nematode (Caenorhabditis elegans)]
QPRFIVKPYGTEVGEGQSANFYCRVIASSPPVVTWHKDDRELKQSVKYMKRYNGNDYGLTINRVKGDDKG
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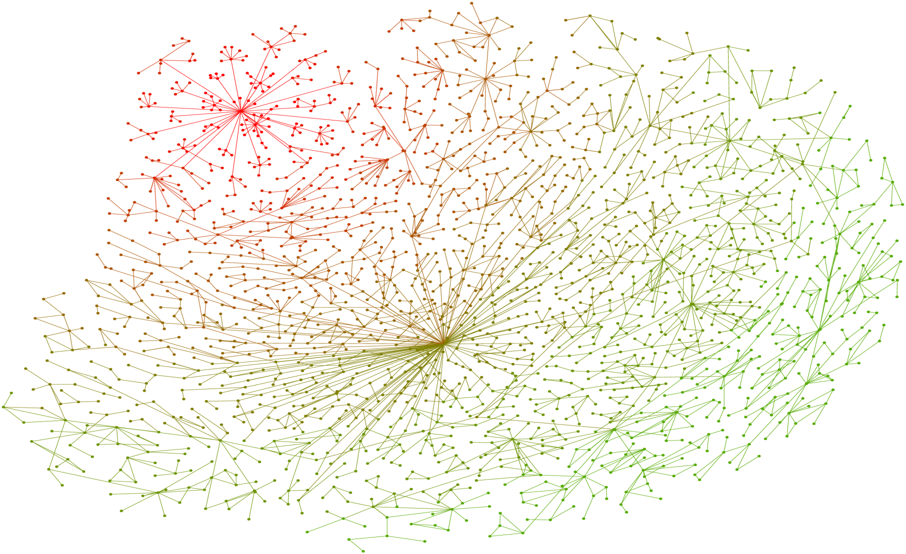
Graphs



Missing Variables

Incomplete Data

- Measurement devices may fail
  E.g. dead pixels on camera, microarray, forms incomplete, ...
- Measuring things may be expensive
  diagnosis for patients
- Data may be censored

How to fix it

- Clever algorithms (not this course ...)
- **Simple mean imputation**
  Substitute in the average from other observations
- Works amazingly well (for starters) ...

Mini Summary

Data Types

- Vectors (feature sets, microarrays, HPLC)
- Matrices (photos, dynamical systems, controllers)
- Strings (texts, biological sequences)
- Structured documents (XML, HTML, collections)
- Graphs (web, gene networks, tertiary structure)

Problems and Opportunities

- Data may be incomplete (use mean imputation)
- Data may come from different sources (adapt model)
- Data may be biased (e.g. it is much easier to get blood samples from university students for cheap).
- Problem may be ill defined, e.g. "find information." (get information about what user really needs)
- Environment may react to intervention (butterfly portfolios in stock markets)

What to do with data

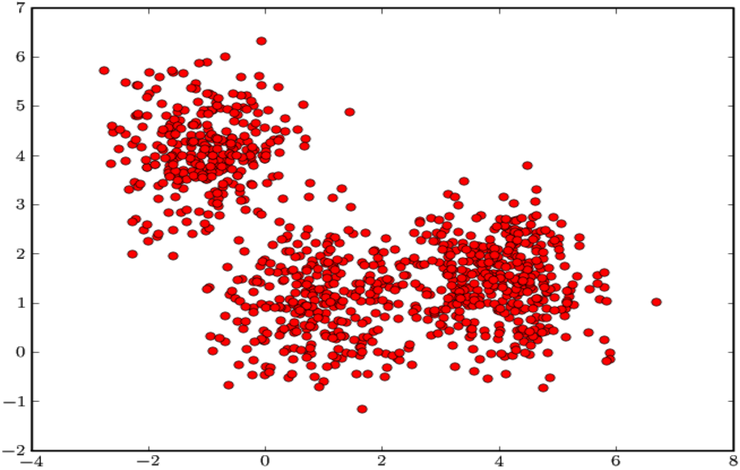
Unsupervised Learning

- Find clusters of the data
- Find low-dimensional representation of the data (e.g. unroll a swiss roll, find structure)
- Find interesting directions in data
- Interesting coordinates and correlations
- Find novel observations / database cleaning

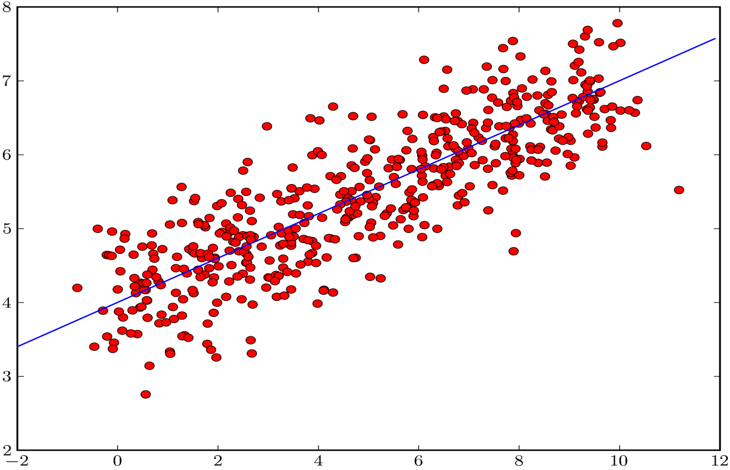
Supervised Learning

- Classification (distinguish apples from oranges)
- Speech recognition
- Regression (tomorrow's stock value)
- Predict time series
- Annotate strings

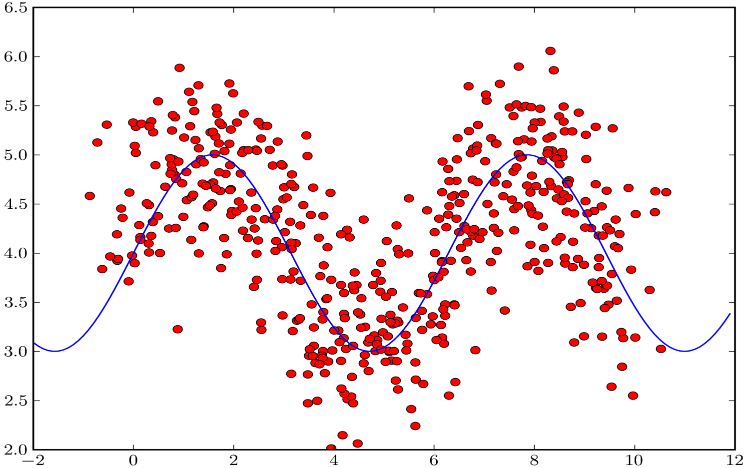
Clustering



Principal Components



Linear Subspace



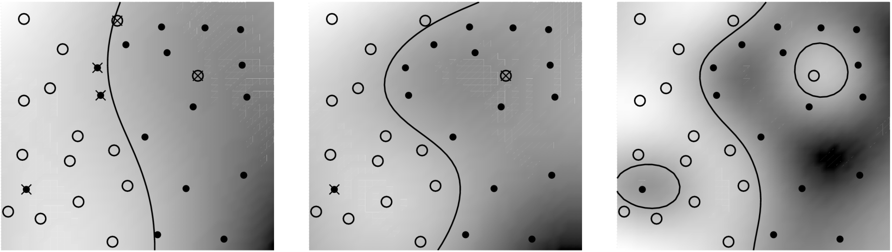
Classification

Data

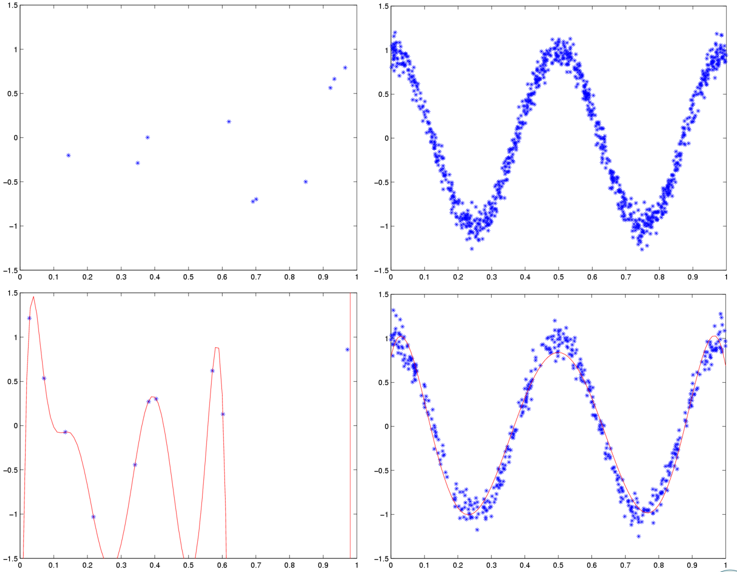
Pairs of observations (x_i, y_i) drawn from distribution
e.g., (blood status, cancer), (credit transactions, fraud), (sound profile of jet engine, defect)

Goal

Estimate $y \in \{\pm 1\}$ **given** x at a new location. Or find a function $f(x)$ that does the trick.



Regression



Regression

Data

Pairs of observations (x_i, y_i) generated from some joint distribution $\Pr(x, y)$, e.g.,

- market index, SP100
- fab parfameters, yield
- user profile, price

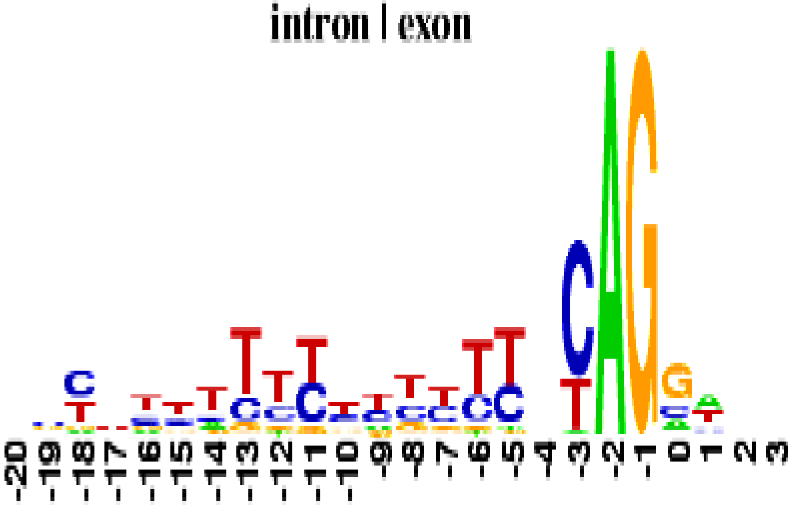
Task

Estimate y, given x, such that some loss $c(x, y, f(x))$ is minimized.

Examples

- Quadratic error between y and $f(x)$, i.e. $c(x, y, f(x)) = \frac{1}{2}(y - f(x))^2$.
- Absolute value, i.e., $c(x, y, f(x)) = |y - f(x))|$.

Annotating Strings



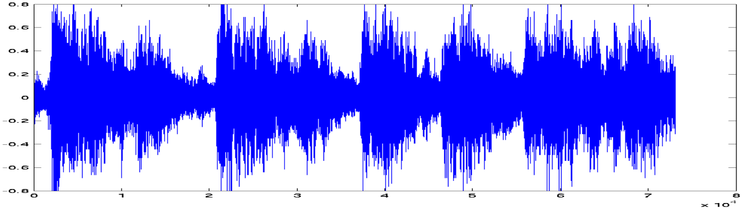
Annotating Audio

Goal

- Possible meaning of an audio sequence
- Give confidence measure

Example (from Australian Prime Minister's speech)

- a stray alien
- Australian



Novelty Detection

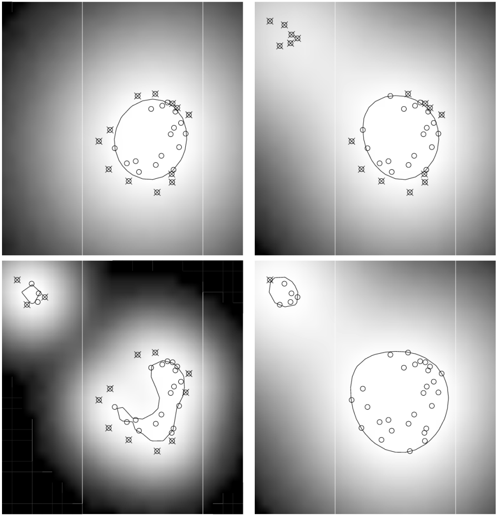
Data

Observations x_i from some $\mathrm{P}(x)$, e.g.,

- network usage patterns
- handwritten digits
- alarm sensors
- factory status

Task

Find unusual events, clean database, distinguish typical examples.



What Machine Learning is **not**

Logic

- If A meets B and B meets C, does A know C?
- Rule satisfaction
- Logical rules from data

Artificial Intelligence

- Understanding of the world
- Meet *Sunny* from *I, Robot*
- Go and get me a bottle of beer
  Robot need not *understand* what it is doing.

Biology and Neuroscience

- Understand the brain by building neural networks?!?
- Model brain and build good systems with that
- Get inspiration from biology but no requirement to build systems like that (e.g. jet planes don't flap wings)

Eliza

Rule based AI dialog system, vintage 1970

I am the psychotherapist. Please, describe your problems.

I am here to learn about giving good talks

Why do you say that?

Because I'm interested in learning that

Is it because you are interested in learning that that you came to me?

Yes, indeed.

Earlier you said you are interested in learning that?

Sure, you stupid computer, this is what I want!

Maybe your plans have something to do with this.

Dammit, sure, that's what i'm trying to say.

I don't understand.

Because you're stupid.

Does it bother you that I am stupid?

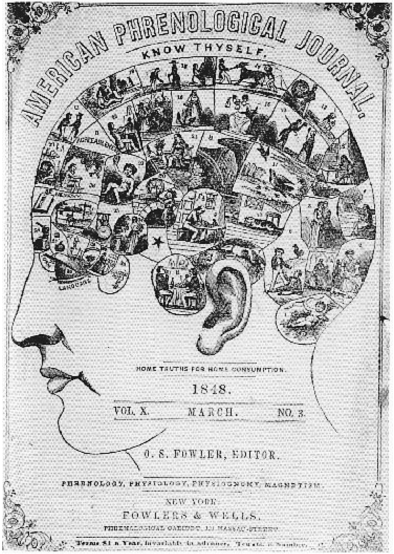
Indeed, it does.

You mentioned that you are interested in learning that?

That's true. And now I want to relax a bit before giving a talk.

Try it out on Emacs using `M-x doctor`.

How the brain doesn’t work



Mini Summary

Structure Extraction

- Clustering
- Low-dimensional subspaces
- Low-dimensional representation of data

Novelty Detection

- Find typical observations (Joe Sixpack)
- Find highly unusual ones (oddball)
- Database cleaning

Supervised Learning

- Regression
- Classification
- Preference relationships (recommender systems)

Statistics and Probability Theory

Why do we need it?

- We deal with **uncertain events**
- Need mathematical formulation for probabilities
- Need to estimate probabilities from data
  (e.g. for coin tosses, we only observe number of heads and tails, not whether the coin is really fair).

How do we use it?

- Statement about probability that an object is an apple (rather than an orange)
- Probability that two things happen at the same time
- Find unusual events (= low density events)
- Conditional events
  (e.g. what happens if A, B, and C are true)

Probability

Basic Idea

We have events in a space of possible outcomes. Then $\Pr(X)$ tells us how likely is that an event $x \in X$ will occur.

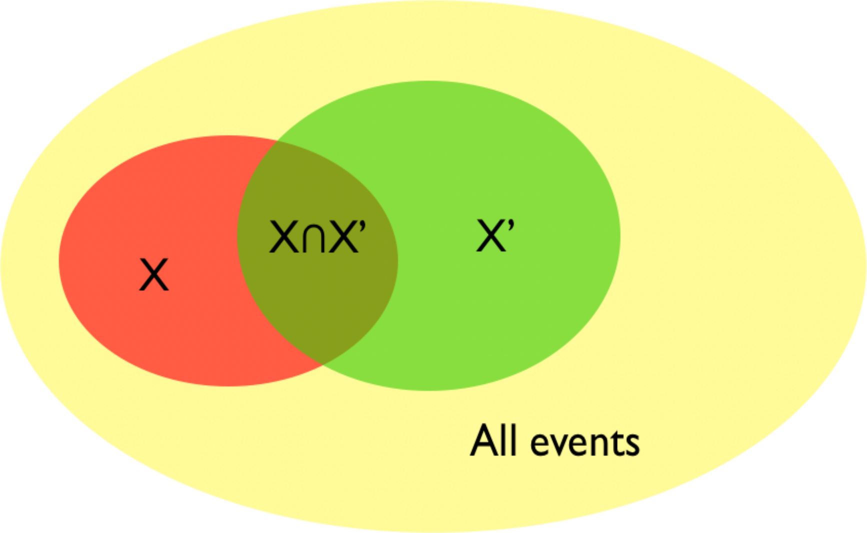
Basic Axioms

- $\Pr(X) \in [0, 1]$ for all $X \subseteq \mathfrak{X}$
- $\Pr(\mathfrak{X}) = 1$
- $\Pr(\cup_i X_i) = \sum_i \Pr(X_i)$ if $X_i \cap X_j = \emptyset$ for all $i \neq j$

Simple Corollary

$$\Pr(X \cup Y) = \Pr(X) + \Pr(Y) - \Pr(X \cap Y)$$

Example



Multiple Variables

Two Sets

Assume that x and y are drawn from a probability measure on the product space of $\mathcal{X}$ and $\mathcal{Y}$. Consider the space of events $(x, y) \in \mathcal{X} \times \mathcal{Y}$.

Independence

If x and y are independent, then for all $X \subset \mathcal{X}$ and $Y \subset \mathcal{Y}$

$$\Pr(X, Y) = \Pr(X) \cdot \Pr(Y).$$

Independent Random Variables

Y
Outcome

X
Astrologist's
Prediction

0.25	0.25
0.25	0.25

Dependent Random Variables

Y
Outcome

X
Physician's
Prediction

	0.49	0.01
	0.01	0.49

Bayes Rule

Dependence and Conditional Probability

Typically, knowing x will tell us something about y (think regression or classification). We have

$$\Pr(Y|X)\Pr(X) = \Pr(Y,X) = \Pr(X|Y)\Pr(Y).$$

- Hence $\Pr(Y,X) \leq \min(\Pr(X), \Pr(Y))$.

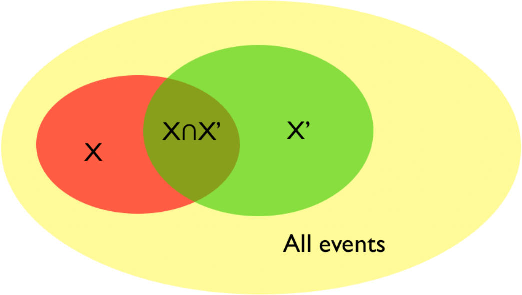
Bayes Rule

$$\Pr(X|Y) = \frac{\Pr(Y|X)\Pr(X)}{\Pr(Y)}.$$

Proof using conditional probabilities

$$\Pr(X,Y) = \Pr(X|Y)\Pr(Y) = \Pr(Y|X)\Pr(X)$$

Example



$$\Pr(X \cap X') = \Pr(X|X')\Pr(X') = \Pr(X'|X)\Pr(X)$$

AIDS Test

How likely is it to have AIDS if the test says so?

- Assume that roughly 0.1% of the population is infected.

$$p(X = \mathrm{AIDS}) = 0.001$$

- The AIDS test reports positive for all infections.

$$p(Y = \text{test positive}|X = \mathrm{AIDS}) = 1$$

- The AIDS test reports positive for 1% healthy people.

$$p(Y = \text{test positive}|X = \text{healthy}) = 0.01$$

We use Bayes rule to infer Pr(AIDS|test positive) via

$$\frac{\Pr(Y|X)\Pr(X)}{\Pr(Y)} = \frac{\Pr(Y|X)\Pr(X)}{\Pr(Y|X)\Pr(X) + \Pr(Y|\mathfrak{X}\backslash X)\Pr(\mathfrak{X}\backslash X)}$$

$$= \frac{1 \cdot 0.001}{1 \cdot 0.001 + 0.01 \cdot 0.999} = 0.091$$

Eye Witness

Evidence from an Eye-Witness

A witness is 90% certain that a certain customer committed the crime. There were 20 people in the bar . . .

Would you convict the person?

- Everyone is presumed innocent until proven guilty:

$$p(X = \text{guilty}) = 1/20$$

- Eyewitness has equal confusion probability

$$p(Y = \text{eyewitness identifies}|X = \text{guilty}) = 0.9$$

$$\text{and } p(Y = \text{eyewitness identifies}|X = \text{not guilty}) = 0.1$$

Bayes Rule

$$\Pr(X|Y) = \frac{0.9 \cdot 0.05}{0.9 \cdot 0.05 + 0.1 \cdot 0.95} = 0.3213 = 32\%$$

But most judges would convict him anyway . . .

Improving Inference

Follow up on the AIDS test:

The doctor performs a followup via a conditionally independent test which has the following properties:

- The second test reports positive for 90% infections.
- The AIDS test reports positive for 5% healthy people.

$$\Pr(\mathrm{T1}, \mathrm{T2}|\mathrm{Health}) = \Pr(\mathrm{T1}|\mathrm{Health}) \Pr(\mathrm{T2}|\mathrm{Health}).$$

A bit more algebra reveals (assuming that both tests are independent): $\frac{0.01 \cdot 0.05 \cdot 0.999}{0.01 \cdot 0.05 \cdot 0.999 + 1 \cdot 0.9 \cdot 0.001} = 0.357.$

Conclusion:

Adding extra observations can improve the confidence of the test considerably.

Different Contexts

Hypothesis Testing:

- Is solution A or B better to solve the problem (e.g. in manufacturing)?
- Is a coin tainted?
- Which parameter setting should we use?

Sensor Fusion:

- Evidence from sensors A and B (AIDS test 1 and 2).
- We have different types of data.

More Data:

- We obtain two sets of data — we get more confident
- Each observation can be seen as an additional test

Mini Summary

Probability theory

- Basic tools of the trade
- Use it to model uncertain events

Dependence and Independence

- Independent events don't convey any information about each other.
- Dependence is what we exploit for estimation
- Leads to Bayes rule

Testing

- Prior probability matters
- Combining tests improves outcomes
- Common sense can be misleading

Estimating Probabilities from Data

Rolling a dice:

Roll the dice many times and count how many times each side comes up. Then assign empirical probability estimates according to the frequency of occurrence.

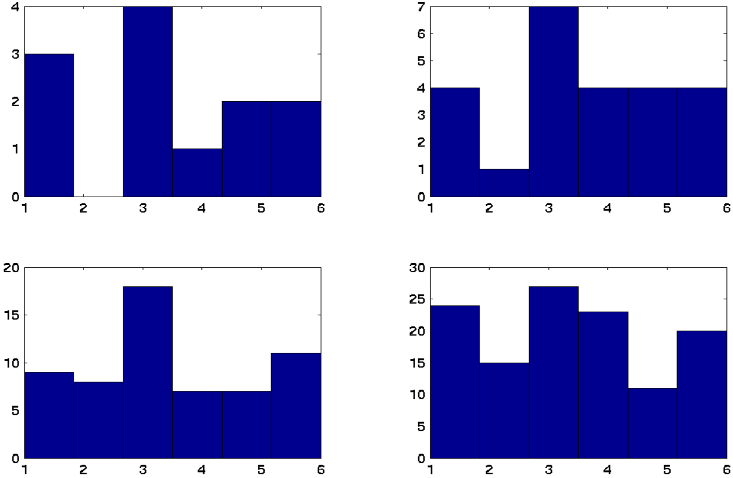
$$\hat{\Pr}(i) = \frac{\#\text{occurrences of } i}{\#\text{trials}}$$

Maximum Likelihood Estimation:

Find parameters such that the observations are *most likely* given the current set of parameters.

This does not check whether the parameters are plausible!

Practical Example



Properties of MLE

Hoeffding's Bound

The probability estimates converge exponentially fast

$$\Pr\{|\pi_i - p_i| > \epsilon\} \leq 2\exp(-2m\epsilon^2)$$

Problem

- For small ϵ this can still take a very long time. In particular, for a fixed confidence level δ we have

$$\delta = 2\exp(-2m\epsilon^2) \Longrightarrow \epsilon = \sqrt{\frac{-\log\delta + \log 2}{2m}}$$

- The above bound holds only for single π_i, **but not uniformly over all i.**

Improved Approach

If we know something about π_i, we should use this extra information: use priors.

Mini Summary

Probability Estimates

- For discrete events, just count occurrences.
- Results can be bad if only few data available.

Maximum Likelihood

- Find parameters which maximize the joint probability of the data occurring.
- Result is not a "real" probability.
- Optimization gives constrained problem, solve using Lagrange function.

Big Guns: Hoeffding and friends

- Use uniform convergence and tail bounds
- Exponential convergence for fixed scale
- Only sublinear convergence, when fixed confidence.

Summary

Data

Vectors, matrices, strings, graphs, ...

What to do with data

Unsupervised learning (clustering, embedding, etc.), Classification, sequence annotation, Regression, ...

Random Variables

Dependence, Bayes rule, hypothesis testing

Estimating Probabilities

Maximum likelihood, convergence, ...