Introduction to Machine Learning
Part I.

Michèle Sebag

TAO: Theme Apprentissage & Optimisation

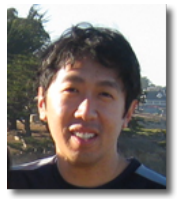
http://tao.lri.fr/tiki-index.php

Sept 4th, 2012

Overview

Examples

- Vision
- Control
- Netflix
- Spam
- Playing Go
- Google



http://ai.stanford.edu/~ang/courses.html

Reading cheques

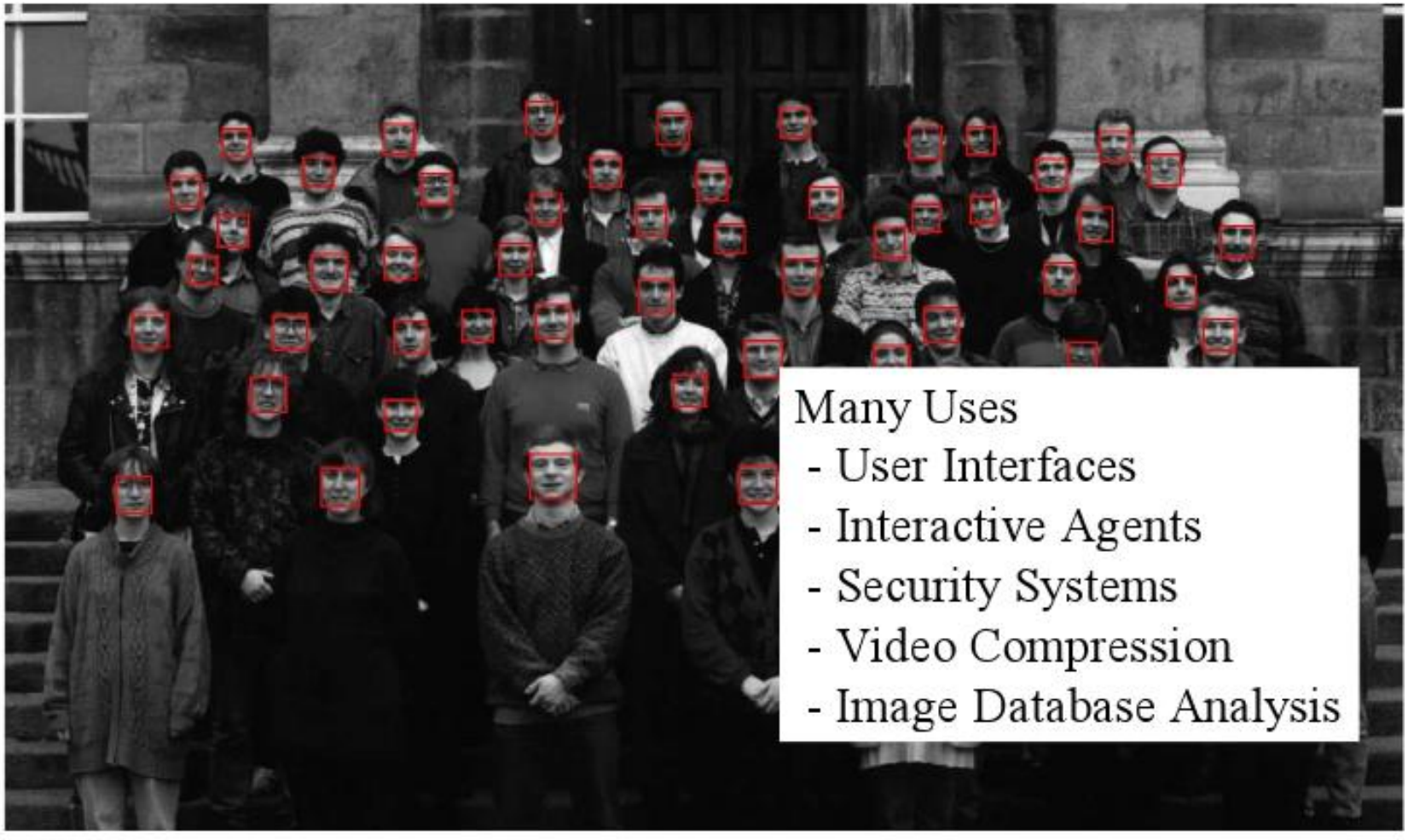
LeCun et al. 1990

MNIST: The drosophila of ML

Fig. 4. Size-normalized examples from the MNIST database.

Classification

Detecting faces



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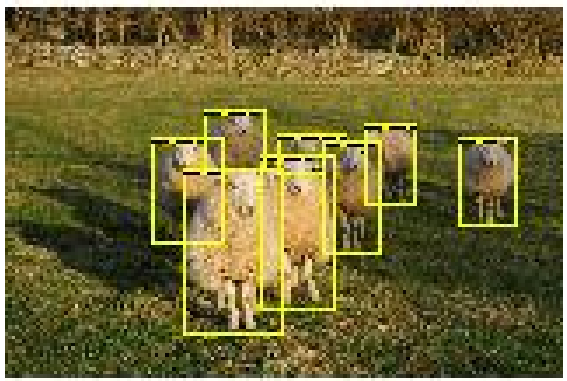
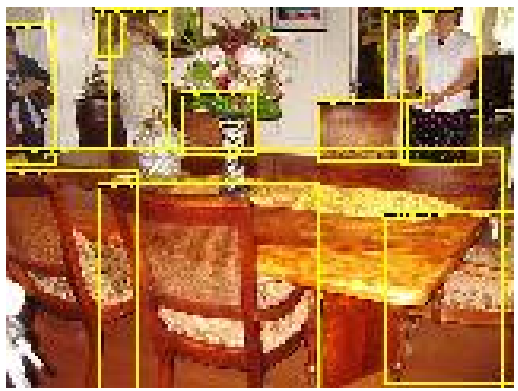
Viola and Jones, Robust object detection using a boosted cascade of simple features, CVPR 2001

The 2005-2012 Visual Object Challenges

A. Zisserman, C. Williams, M. Everingham, L. v.d. Gool


The supervised learning setting

Input: set of $(\mathbf{x}, y)$

- An instance $\mathbf{x}$ e.g. set of pixels, $\mathbf{x} \in \mathbb{R}^D$
- A label y in $\{1, -1\}$ or $\{1, \ldots, K\}$ or $\mathbb{R}$

The supervised learning setting

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Pattern recognition

- Classification Does the image contain the target concept ?

$$h : \{ \text{Images} \} \mapsto \{1, -1\}$$

- Detection Does the pixel belong to the img of target concept?

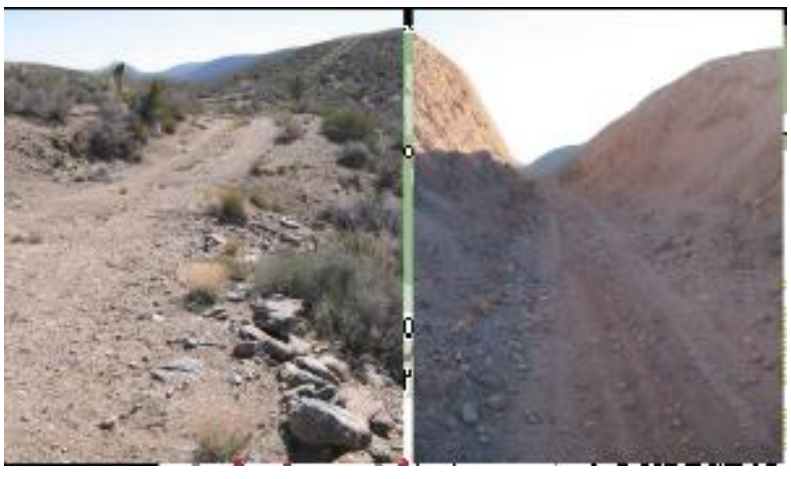
$$h : \{ \text{Pixels in an image} \} \mapsto \{1, -1\}$$

- Segmentation

  Find contours of all instances of target concept in image

The 2005 Darpa Challenge

Thrun, Burgard and Fox 2005



Autonomous vehicle Stanley – Terrains

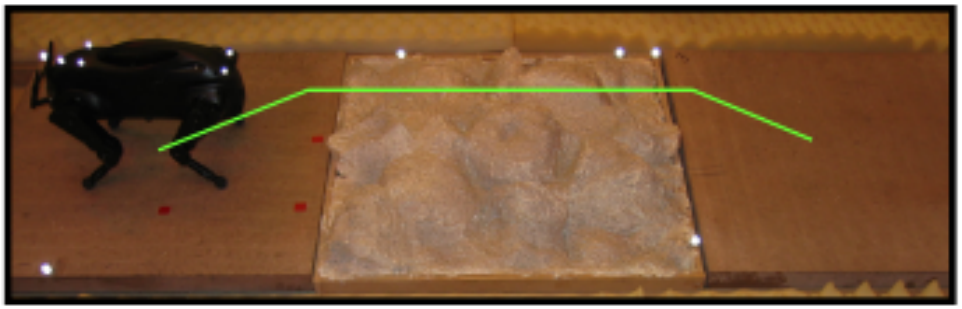
The Darpa challenge and the AI agenda

What remains to be done Thrun 2005

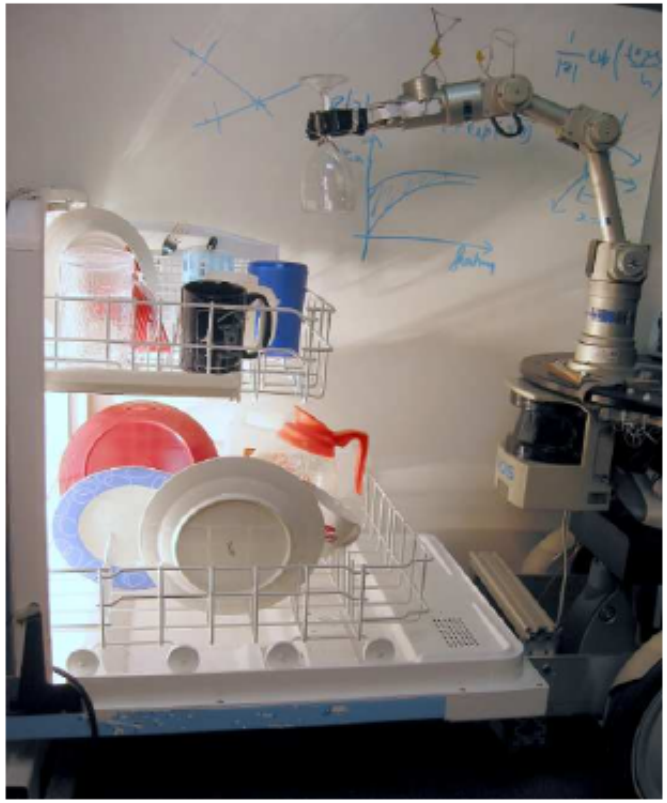
- Reasoning 10%
- Dialogue 60%
- Perception 90%

Robots

Ng, Russell, Veloso, Abbeel, Peters, Schaal, ...



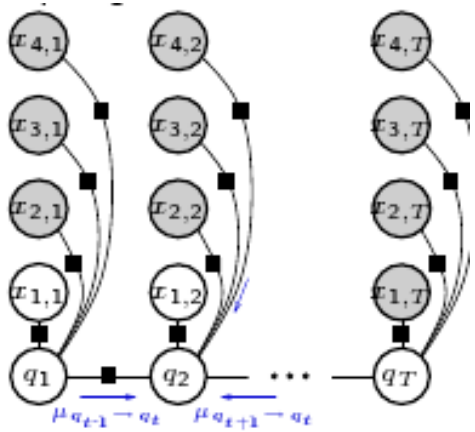
Reinforcement learning



Classification

Robots, 2

Toussaint et al. 2010



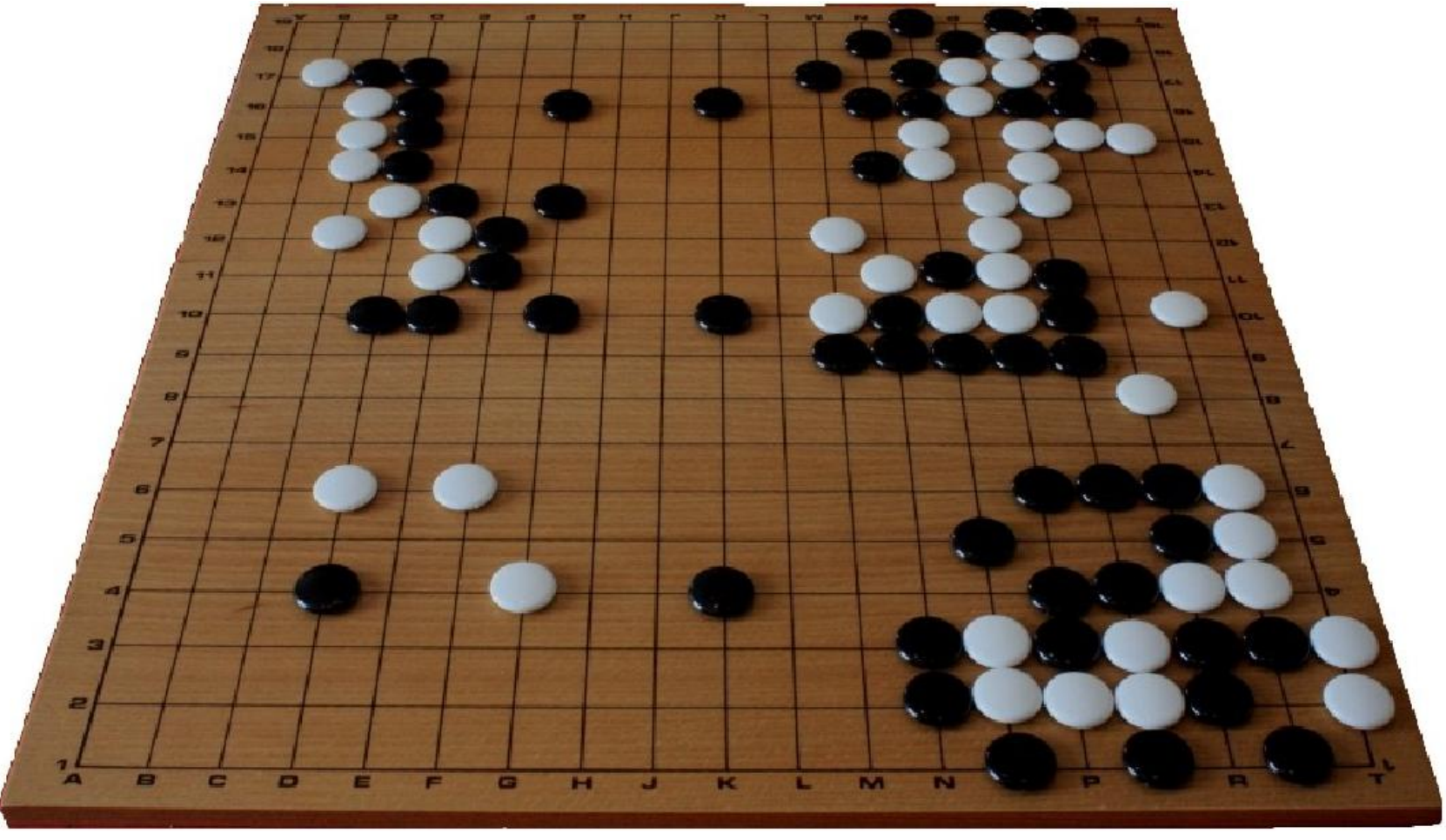
(a) Factor graph modelling the variable interactions

(b) Behaviour of the 39-DOF Humanoid:
Reaching goal under Balance and Collision constraints

Bayesian Inference for Motion Control and Planning

Go as AI Challenge

Gelly Wang 07; Teytaud et al. 2008-2011



Reinforcement Learning, Monte-Carlo Tree Search

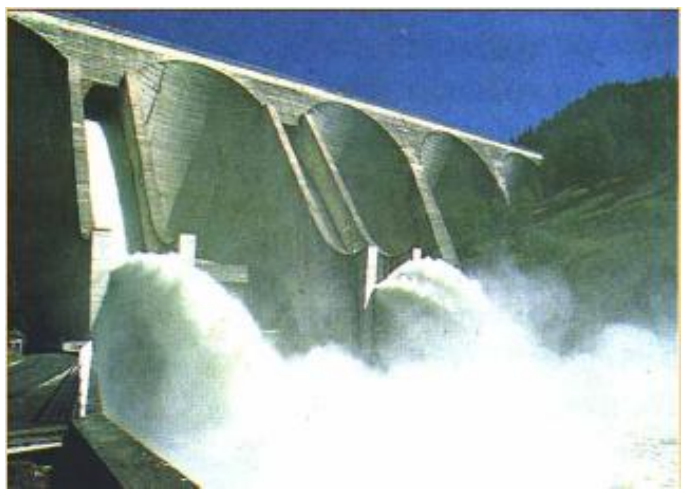
Energy policy

Claim

Many problems can be phrased as optimization in front of the uncertainty.

Adversarial setting	2 two-player game
uniform setting	a single player game

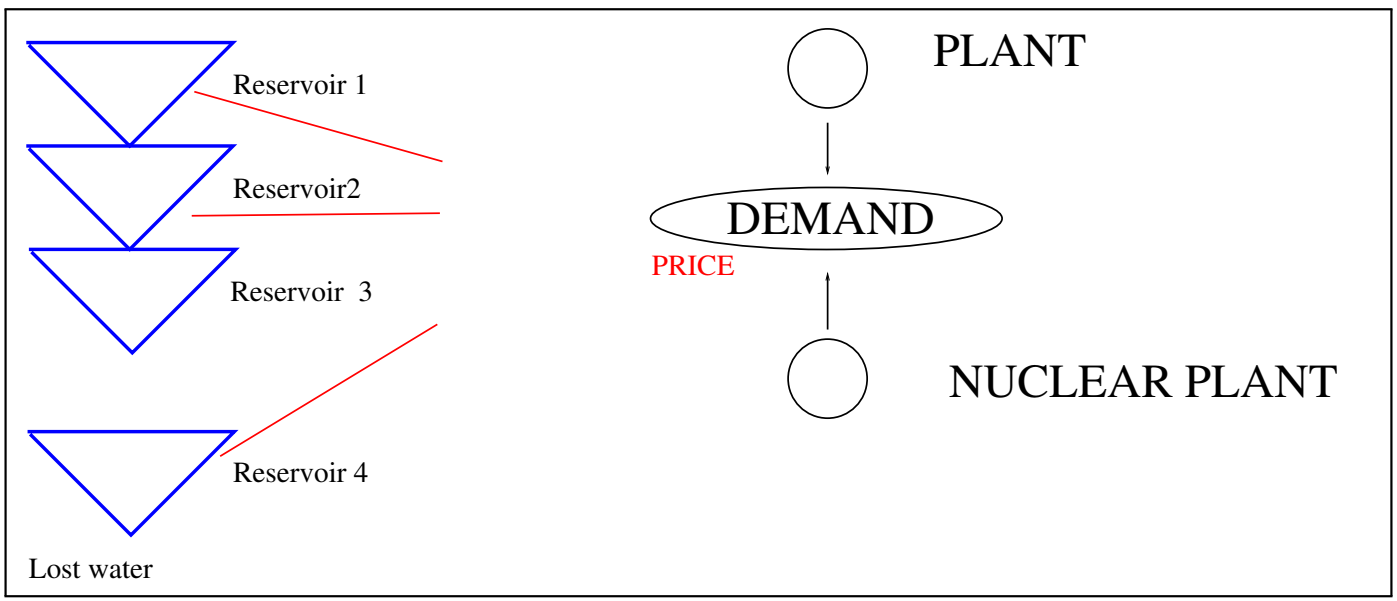
Management of energy stocks under uncertainty



States and Decisions

States

- Amount of stock (60 nuclear, 20 hydro.)
- Varying: price, weather alea or archive
- Decision: release water from one reservoir to another
- Assessment: meet the demand, otherwise buy energy



Netflix Challenge 2007-2008

Collaborative Filtering

Collaborative filtering

Input

- A set of users — n_u, ca 500,000
- A set of movies — n_m, ca 18,000
- A $n_m \times n_u$ matrix: person, movie, rating
  Very sparse matrix: 1%...

Output

- Filling the matrix !

Collaborative filtering

Input

- A set of users — n_u, ca 500,000
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- A $n_m \times n_u$ matrix: person, movie, rating
  Very sparse matrix: 1%...

Output

- Filling the matrix !

Criterion

- (relative) mean square error
- ranking error

Spam – Phishing – Scam

Classification, Outlier detection

The power of big data

- Now-casting outbreak of flu
- Public relations >> Advertizing

Mc Luhan and Google

We shape our tools and afterwards our tools shape us

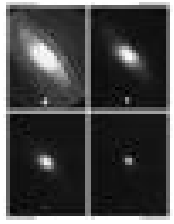
Marshall McLuhan, 1964

First time ever a tool is observed to modify human cognition that fast.

Sparrow et al., Science 2011

Overview

Where we are

Ast. series 

 Pierre de Rosette

World

Natural
phenomenons

Human–related
phenomenons

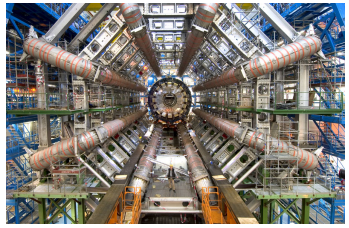
Data / Principles

Maths.
Modelling

Common
Sense

You are here

WHERE WE ARE

Sc. data 

Google

World

Natural phenomenons

Human–related phenomenons

Data / Principles

Maths. Modelling

Common Sense

You are here

Types of Machine Learning problems

WORLD – DATA – USER

Observations	+ Target	+ Rewards
Understand	Predict	Decide
Code	Classification/Regression	Policy
Unsupervised	Supervised	Reinforcement
LEARNING	LEARNING	LEARNING

Data

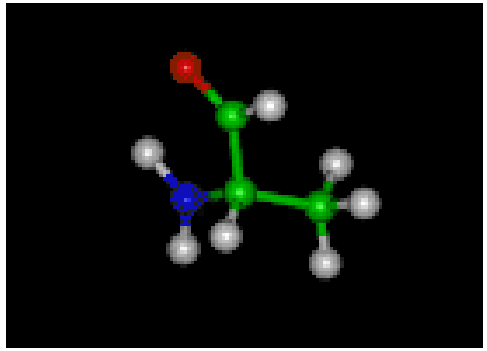
Example

- row : example/ case
- column : feature/variables/attribute
- attribute : class/label

age	employme	education	edun	marital	...	job	relation	race	gender	hour	country	wealth
					...							
39	State_gov	Bachelors	13	Never_mar	...	Adm_cleric	Not_in_fam	White	Male	40	United_Sta	poor
51	Self_emp_	Bachelors	13	Married	...	Exec_man	Husband	White	Male	13	United_Sta	poor
39	Private	HS_grad	9	Divorced	...	Handlers_c	Not_in_fam	White	Male	40	United_Sta	poor
54	Private	11th	7	Married	...	Handlers_c	Husband	Black	Male	40	United_Sta	poor
28	Private	Bachelors	13	Married	...	Prof_speci	Wife	Black	Female	40	Cuba	poor
38	Private	Masters	14	Married	...	Exec_man	Wife	White	Female	40	United_Sta	poor
50	Private	9th	5	Married_sp	...	Other_serv	Not_in_fam	Black	Female	16	Jamaica	poor
52	Self_emp_	HS_grad	9	Married	...	Exec_man	Husband	White	Male	45	United_Sta	rich
31	Private	Masters	14	Never_mar	...	Prof_speci	Not_in_fam	White	Female	50	United_Sta	rich
42	Private	Bachelors	13	Married	...	Exec_man	Husband	White	Male	40	United_Sta	rich
37	Private	Some_coll	10	Married	...	Exec_man	Husband	Black	Male	80	United_Sta	rich
30	State_gov	Bachelors	13	Married	...	Prof_speci	Husband	Asian	Male	40	India	rich
24	Private	Bachelors	13	Never_mar	...	Adm_cleric	Own_child	White	Female	30	United_Sta	poor
33	Private	Assoc_acd	12	Never_mar	...	Sales	Not_in_fam	Black	Male	50	United_Sta	poor
41	Private	Assoc_voc	11	Married	...	Craft_repai	Husband	Asian	Male	40	*MissingV	rich
34	Private	7th_8th	4	Married	...	Transport_	Husband	Amer_Indi	Male	45	Mexico	poor
26	Self_emp_	HS_grad	9	Never_mar	...	Farming_fi	Own_child	White	Male	35	United_Sta	poor
33	Private	HS_grad	9	Never_mar	...	Machine_c	Unmarried	White	Male	40	United_Sta	poor
38	Private	11th	7	Married	...	Sales	Husband	White	Male	50	United_Sta	poor
44	Self_emp_	Masters	14	Divorced	...	Exec_man	Unmarried	White	Female	45	United_Sta	rich
41	Private	Doctorate	16	Married	...	Prof_speci	Husband	White	Male	60	United_Sta	rich
:	:	:	:	:	:	:	:	:	:	:	:	:

Instance space $\mathcal{X}$

- Propositionnal : $\mathcal{X} \equiv \mathbb{R}^d$
- Structured : sequential, spatio-temporal, relational.



aminoacid

Supervised Learning, notations

Context

$$\text{World} \rightarrow \text{Instance } \mathbf{x}_i \rightarrow \begin{array}{c}\text{Oracle}\\ \downarrow \\ y_i\end{array}$$

INPUT $\sim P(\mathbf{x}, y)$

$$\mathcal{E} = \{(\mathbf{x}_i, y_i), x_i \in \mathcal{X}, y_i \in \{0,1\}, i = 1 \ldots n\}$$

HYPOTHESIS SPACE

$$\mathcal{H} \quad h : \mathcal{X} \mapsto \{0,1\}$$

LOSS FUNCTION

$$\ell : \mathcal{Y} \times \mathcal{Y} \mapsto \mathbb{R}$$

OUTPUT

$$h^* = arg\ max\{score(h), h \in \mathcal{H}\}$$

Classification and criteria

Generalization Error

$$Err(h) = E[\ell(y, h(\mathbf{x}))] = \int \ell(y, h(\mathbf{x}))dP(x, y)$$

Empirical Error

$$Err_e(h) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, h(\mathbf{x}_i))$$

Bound structural risk

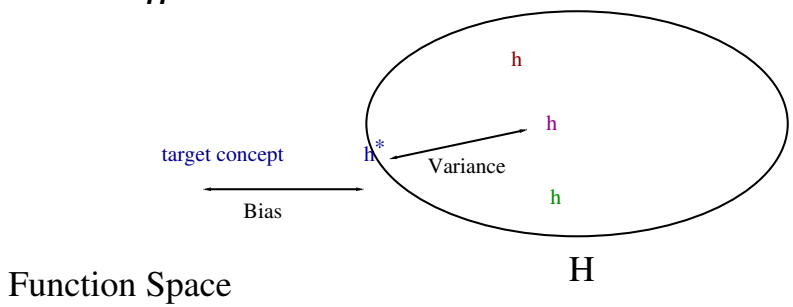
$$Err(h) < Err_e(h) + \mathcal{F}(n, d(\mathcal{H}))$$

$d(\mathcal{H})$ = Vapnik Cervonenkis dimension of $\mathcal{H}$, see later

The Bias-Variance Trade-off

Biais Bias ($\mathcal{H}$): error of the best hypothesis h^* de $\mathcal{H}$

Variance Variance of h_n as a function of $\mathcal{E}$



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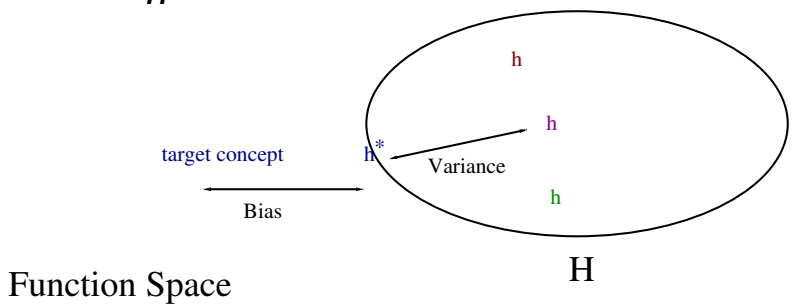
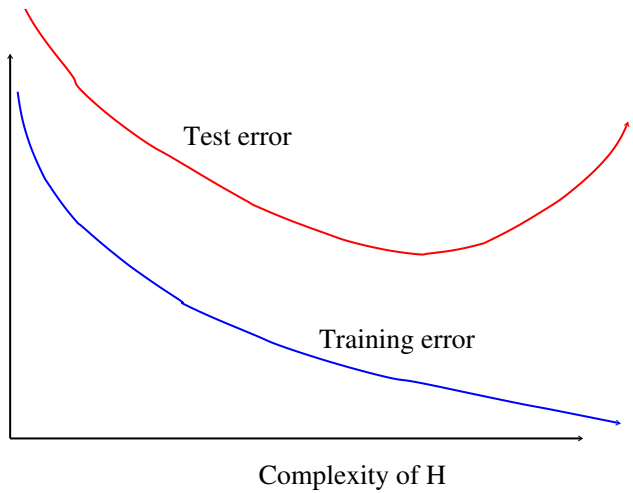


Overfitting



Key notions

- The main issue regarding supervised learning is overfitting.
- How to tackle overfitting:
  - Before learning: use a sound criterion — regularization
  - After learning: cross-validation — **Case studies**

Summary

- Learning is a search problem
- What is the space ? What are the navigation operators ?

Hypothesis Spaces

Logical Spaces

$$\text{Concept} \leftarrow \bigvee \bigwedge \text{Literal,Condition}$$

- Conditions = [color = blue]; [age < 18]
- Condition $f : X \mapsto \{True, False\}$
- Find: disjunction of conjunctions of conditions

- Ex: (unions of) rectangles of the 2D-plane$X$.

Hypothesis Spaces

Numerical Spaces

$$\text{Concept} = (h() > 0)$$

- $h(x) =$ polynomial, neural network, ...
- $h : X \mapsto \mathbb{R}$
- Find: (structure and) parameters of h

Hypothesis Space $\mathcal{H}$

Logical Space

- h covers one example x iff $h(x) = \mathit{True}$.
- $\mathcal{H}$ is structured by a partial order relation

$$h \prec h' \text{ iff } \forall x, h(x) \rightarrow h'(x)$$

Numerical Space $\mathcal{H}$

- $h(x)$ is a real value (more or less far from 0)
- we can define $\ell(h(x), y)$
- $\mathcal{H}$ is structured by a partial order relation

$$h \prec h' \text{ iff } E[\ell(h(x), y)] < E[\ell(h'(x), y)]$$

Hypothesis Space $\mathcal{H}$ / Navigation

	$\mathcal{H}$	operators
Version Space	Logical	spec / gen
Decision Trees	Logical	specialisation
Neural Networks	Numerical	gradient
Support Vector Machines	Numerical	quadratic opt.
Ensemble Methods	–	adaptation $\mathcal{E}$

This course

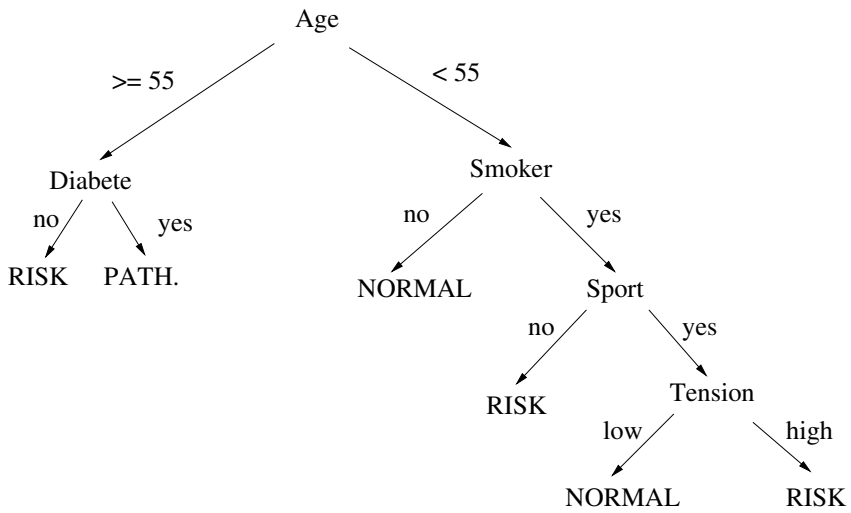
- Decision Trees
- Support Vector Machines
- Ensemble methods

Overview

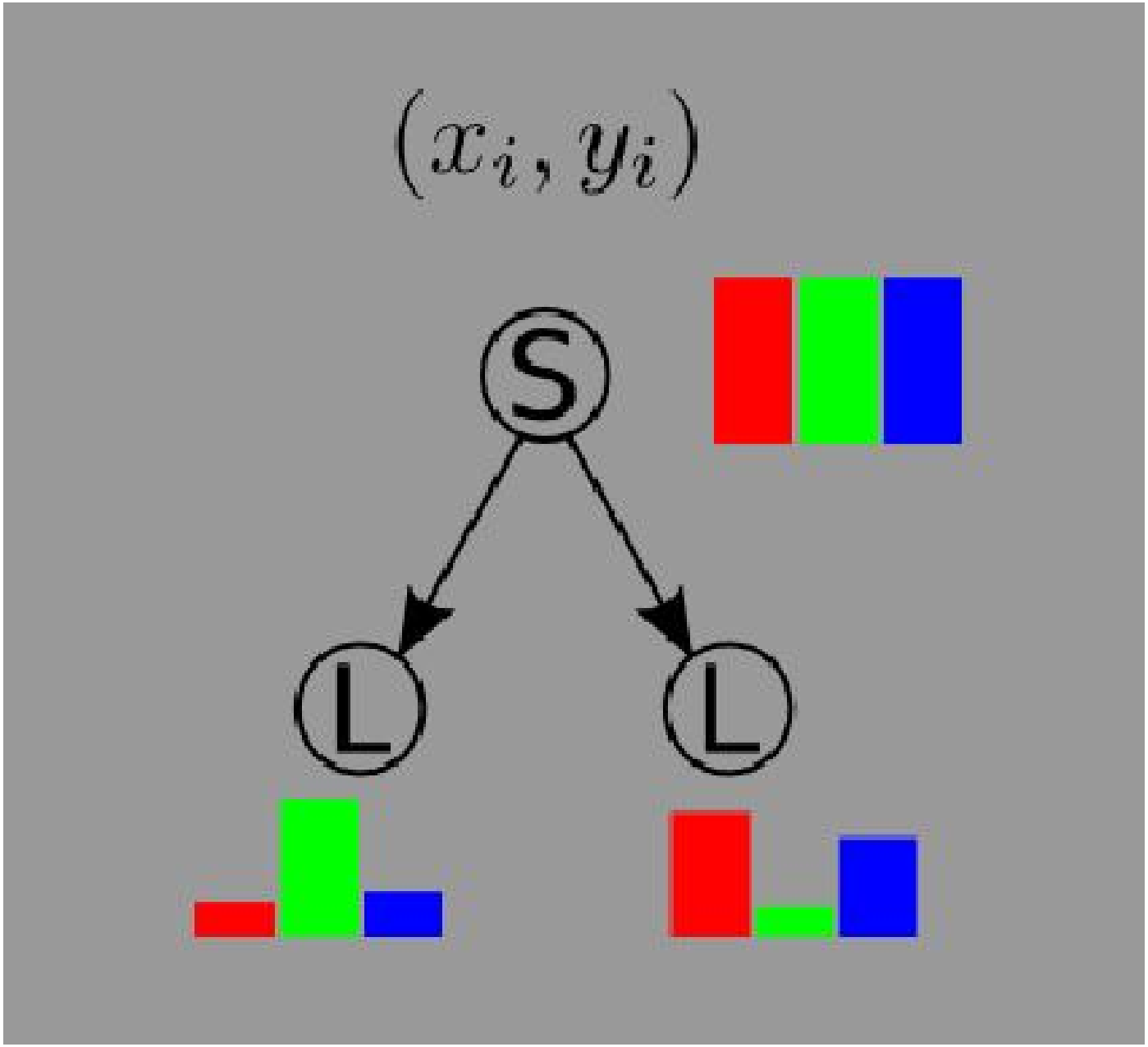
Decision Trees

C4.5 (Quinlan 86)

- Among the most widely used algorithms
- Easy
  - to understand
  - to implelement
  - to use
  - and cheap in CPU time
- J48, Weka, SciKit



Decision Trees



Decision Trees (2)

Procedure DecisionTree($\mathcal{E}$)

1. Assume $\mathcal{E} = \{(x_i, y_i)_{i=1}^n,\ x_i \in \mathbb{R}^D,\ y_i \in \{0, 1\}\}$
   - If $\mathcal{E}$ single-class (i.e., $\forall i, j \in [1, n]; y_i = y_j$), return
   - If n too small (i.e., $<$ threshold), return
   - Else, find the most informative attribute att
2. Forall value val of att
   - Set $\mathcal{E}_{val} = \mathcal{E} \cap [att = val]$.
   - Call DecisionTree($\mathcal{E}_{val}$)

Criterion: information gain

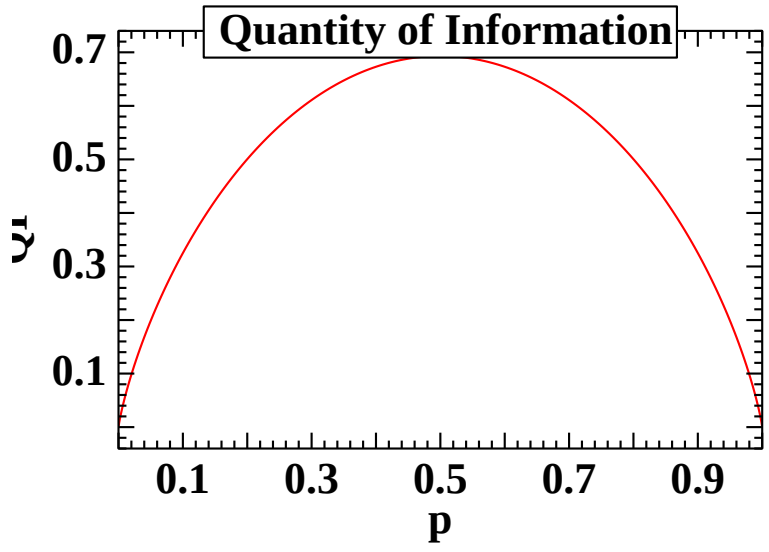
$$\begin{aligned} p &= Pr(Class = 1 | att = val) \\ I([att = val]) &= -p \log p - (1 - p) \log (1 - p) \\ I(att) &= \sum_i Pr(att = val_i).I([att = val_i]) \end{aligned}$$

Decision Trees (3)

Contingency Table

wealth values:	poor	rich
agegroup 10s	2507	3
20s	11262	743
30s	9468	3461
40s	6738	3986
50s	4110	2509
60s	2245	809
70s	668	147
80s	115	16
90s	42	13

Quantity of Information (QI)



Computation

value	p(value)	p(poor | value)	QI (value)	p(value) * QI (value)
[0,10[	0.051	0.999	0.00924	0.000474
[10,20[	0.25	0.938	0.232	0.0570323
[20,30[	0.26	0.732	0.581	0.153715

Decision Trees (4)

Limitations

- XOR-like attributes
- Attributes with many values
- Numerical attributes
- Overfitting

Limitations

Numerical Attributes

- Order the values $val_1 < \ldots < val_t$
- Compute $\mathrm{QI}([att < val_i])$
- $\mathrm{QI}(\mathrm{att}) = \max_i \mathrm{QI}([att < val_i])$

The XOR case

Bias the distribution of the examples

Complexity

Quantity of information of an attribute

$$n \ln n$$

Adding a node

$$D \times n \ln n$$

Tackling Overfitting

Penalize the selection of an already used variable

- Limits the tree depth.

Do not split subsets below a given minimal size

- Limits the tree depth.

Pruning

- Each leaf, one conjunction;
- Generalization by pruning litterals;
- Greedy optimization, QI criterion.

Decision Trees, Summary

Still around after all these years

- Robust against noise and irrelevant attributes
- Good results, both in quality and complexity

Random Forests Breiman 00

Overview

Validation issues

1. What is the result ?
2. My results look good. Are they ?
3. Does my system outperform yours ?
4. How to set up my system ?

Validation: Three questions

Define a good indicator of quality

- Misclassification cost
- Area under the ROC curve

Computing an estimate thereof

- Validation set
- Cross-Validation
- Leave one out
- Bootstrap

Compare estimates: Tests and confidence levels

Which indicator, which estimate: depends.

Settings

- Large/few data

Data distribution

- Dependent/independent examples
- balanced/imbalanced classes

Overview

Performance indicators

Binary class

- h^* the truth
- $\hat{h}$ the learned hypothesis

Confusion matrix

$\hat{h}$ / h^*	1	0	
1	a	b	a + b
0	c	d	c+d
	a+c	b+d	a + b + c + d

Performance indicators, 2

$\hat{h}$ / h^*	1	0	
1	a	b	a + b
0	c	d	c+d
	a+c	b+d	a + b + c + d

- Misclassification rate $\frac{b+c}{a+b+c+d}$
- Sensitivity, True positive rate (TP) $\frac{a}{a+c}$
- Specificity, False negative rate (FN) $\frac{b}{b+d}$
- Recall $\frac{a}{a+c}$
- Precision $\frac{a}{a+b}$

Note: always compare to random guessing / baseline alg.

Performance indicators, 3

The Area under the ROC curve

- ROC: Receiver Operating Characteristics
- Origin: Signal Processing, Medicine

Principle

$$h : X \mapsto \mathbb{R} \qquad h(x) \text{ measures the risk of patient } x$$

h leads to order the examples:

$$+ + + - + - + + + + + - - - + - - - + - - - - - - - - - - - - - -$$

Performance indicators, 3

The Area under the ROC curve

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h leads to order the examples:

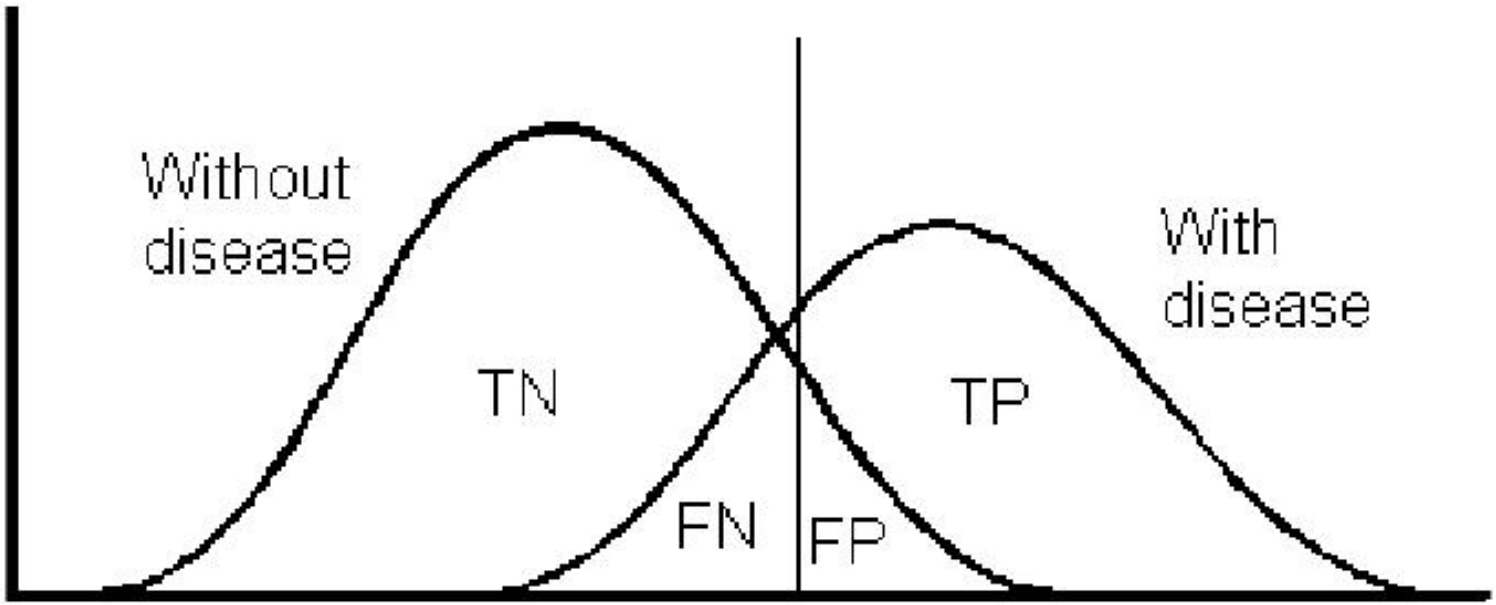
$+ + + - + - + + + + + - - - + - - - + - - - - - - - - - - - - - -$

Given a threshold θ, h yields a classifier: Yes iff $h(x) > \theta$.

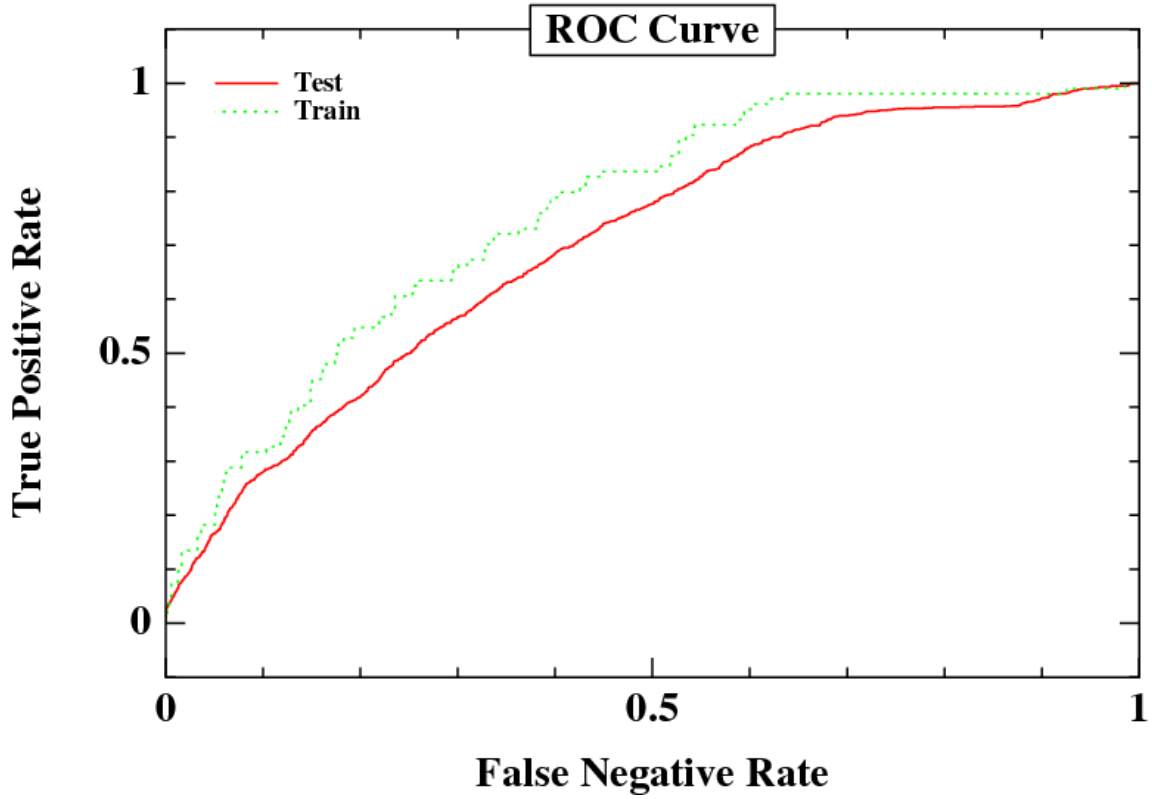
$+ + + - + - + + + ++ \quad | - - - + - - - + - - - - - - - - - - - - - -$

Here, TP (θ)= .8; FN (θ) = .1

ROC



The ROC curve



Ideal classifier: (0 False negative,1 True positive)
Diagonal (True Positive = False negative) ≡ nothing learned.

ROC Curve, Properties

Properties

ROC depicts the trade-off True Positive / False Negative.

Standard: misclassification cost (Domingos, KDD 99)

$$\text{Error} = \#\text{ false positive} + c \times \#\text{ false negative}$$

In a multi-objective perspective, ROC = Pareto front.

Best solution: intersection of Pareto front with $\Delta(-c, -1)$

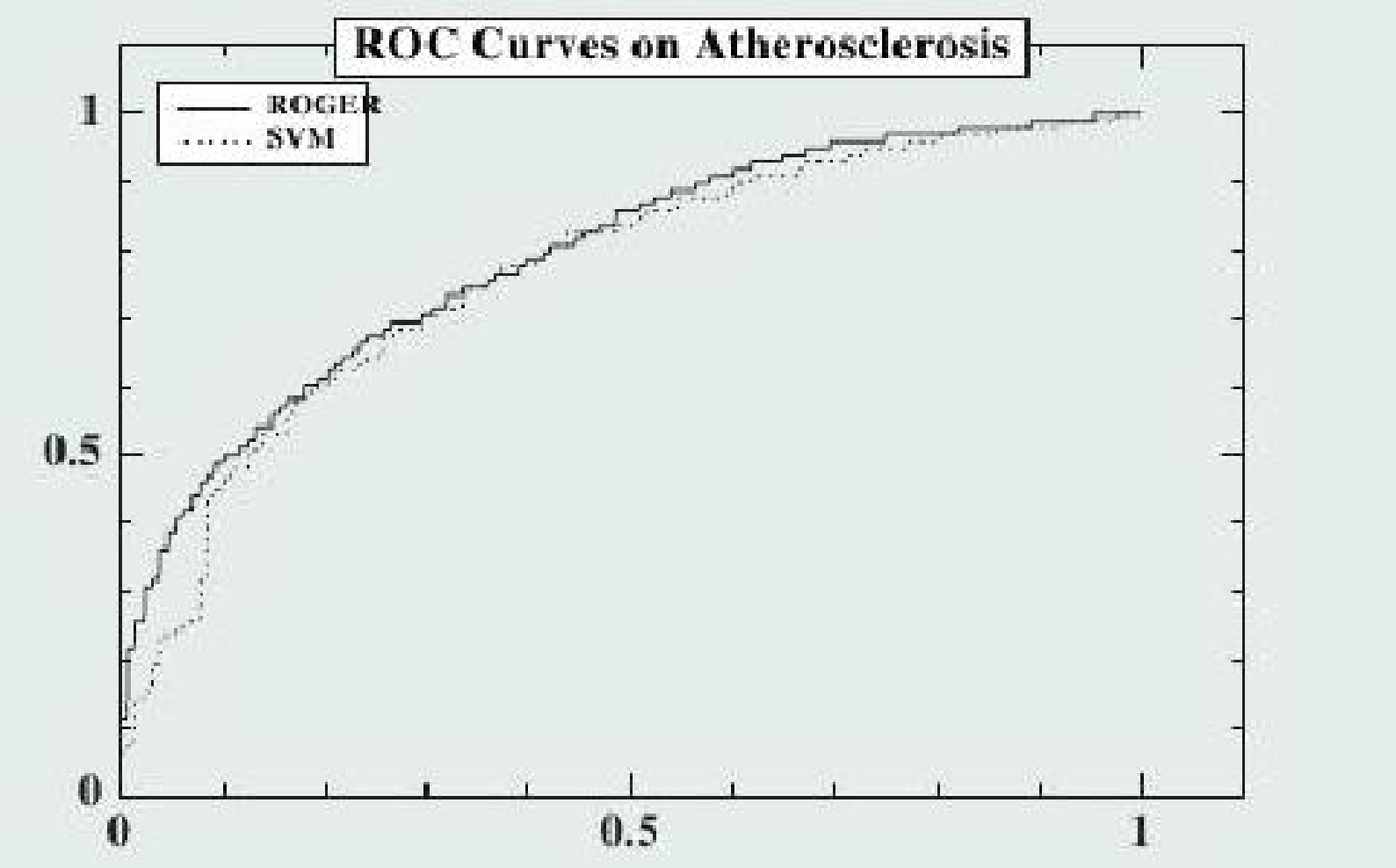
ROC Curve, Properties, foll'd

Used to compare learners Bradley 97

multi-objective-like

insensitive to imbalanced distributions

shows sensitivity to error cost.



Area Under the ROC Curve

Often used to select a learner

Don't ever do this ! Hand, 09

Sometimes used as learning criterion Mann Whitney

Wilcoxon

$$AUC = Pr(h(x) > h(x')|y > y')$$

WHY Rosset, 04

- More stable $\mathcal{O}(n^2)$ vs $\mathcal{O}(n)$
- With a probabilistic interpretation Clemençon et al. 08

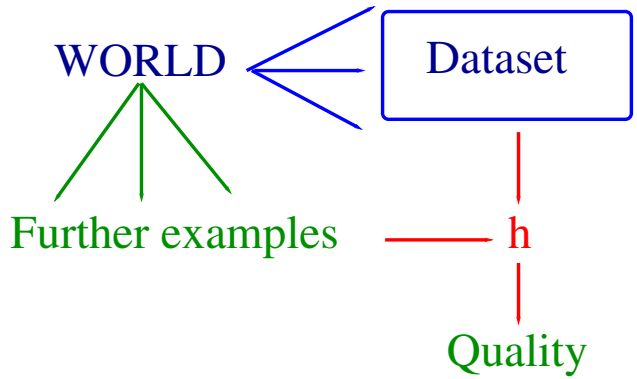
HOW

- SVM-Ranking Joachims 05; Usunier et al. 08, 09
- Stochastic optimization

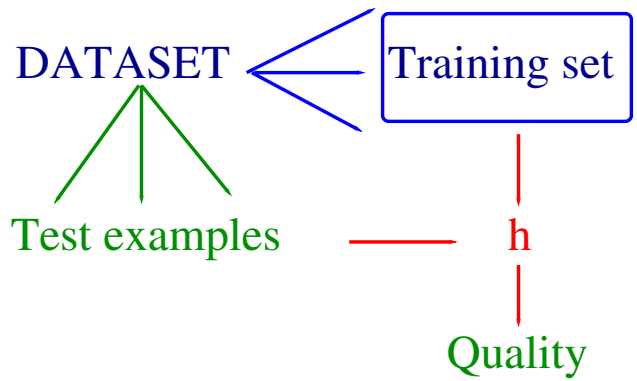
Overview

Validation, principle

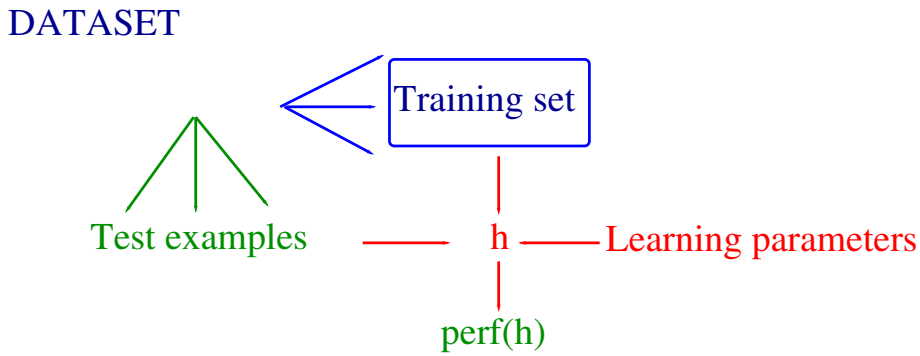
Desired: performance on further instances



Assumption: Dataset is to World, like Training set is to Dataset.



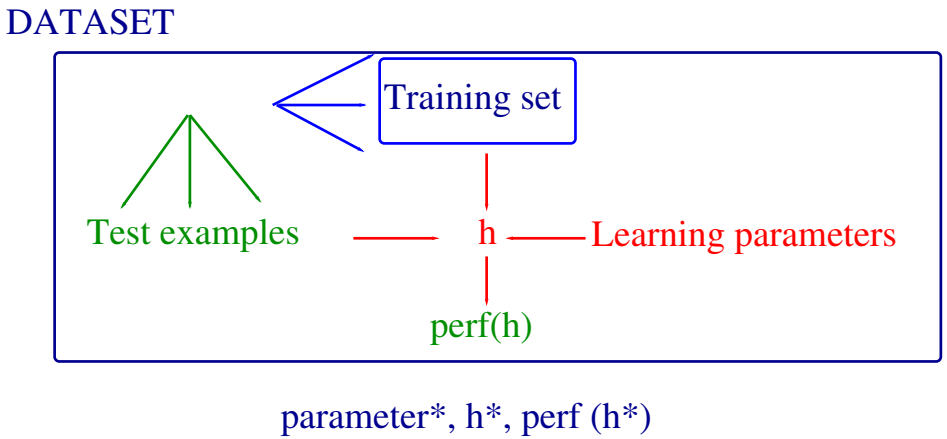
Validation, 2



Unbiased Assessment of Learning Algorithms

T. Scheffer and R. Herbrich, 97

Validation, 2

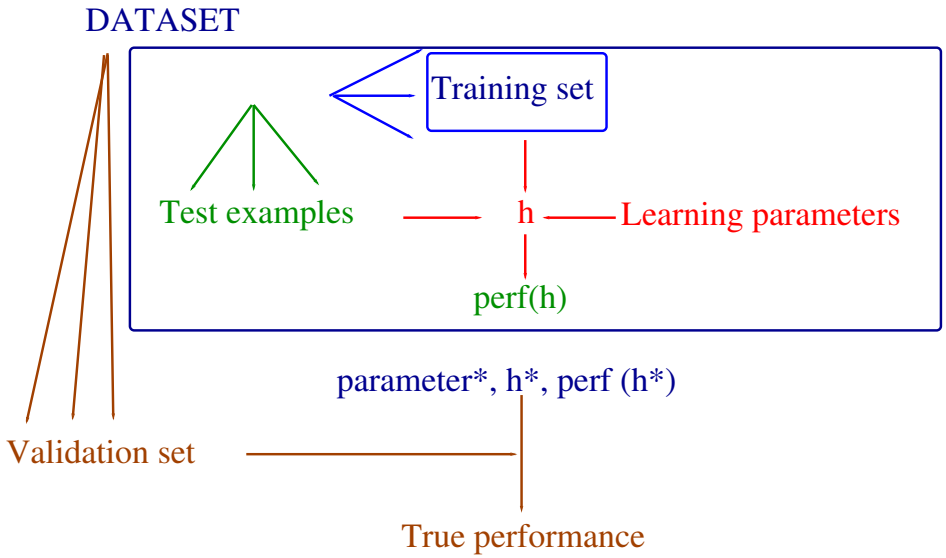


parameter*, h*, perf (h*)

Unbiased Assessment of Learning Algorithms

T. Scheffer and R. Herbrich, 97

Validation, 2



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Overview

Confidence intervals

Definition

Given a random variable X on $\mathbb{R}$, a p%-confidence interval is $I \subset \mathbb{R}$ such that

$$Pr(X \in I) > p$$

Binary variable with probability ϵ

Probability of r events out of n trials:

$$P_n(r) = \frac{n!}{r!(n-r)!}\epsilon^r(1-\epsilon)^{n-r}$$

- Mean: $n\epsilon$
- Variance: $\sigma^2 = n\epsilon(1-\epsilon)$

Gaussian approximation

$$P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} exp^{-\frac{1}{2}\frac{x-\mu}{\sigma}^2}$$

Confidence intervals

Bounds on (true value, empirical value) for n trials, $n > 30$

$$Pr(|\hat{x}_n - x^*| > \underbrace{1.96}_{z} \sqrt{\frac{\hat{x}_n.(1-\hat{x}_n)}{n}}) < \underbrace{.05}_{\varepsilon}$$

Table

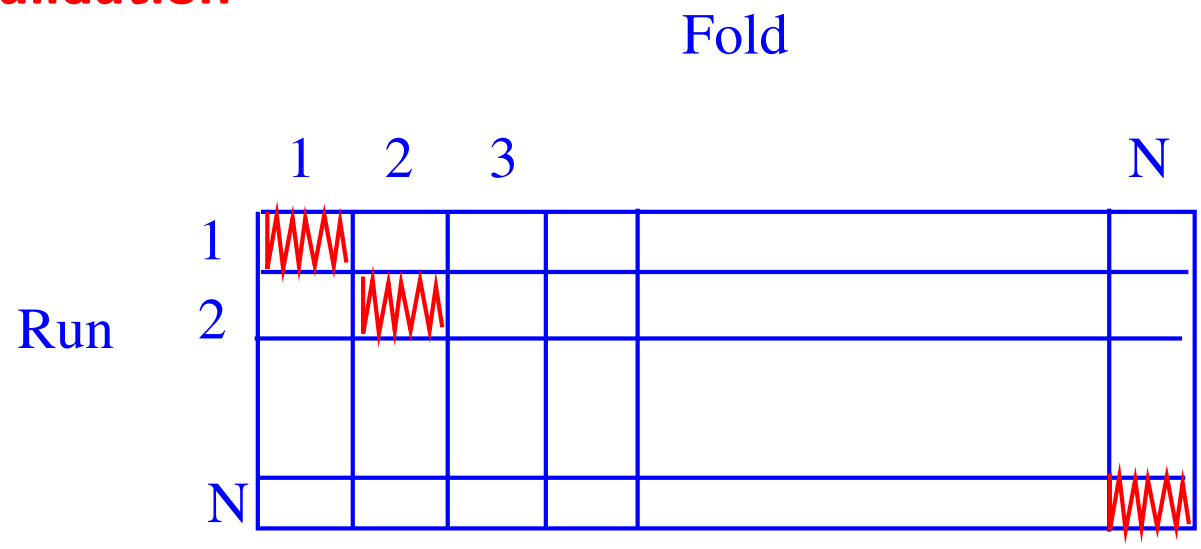
z	.67	1.	1.28	1.64	1.96	2.33	2.58
ε	50	32	20	10	5	2	1

Empirical estimates

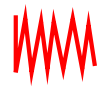
When data abound (MNIST)

Training Test Validation

Cross validation



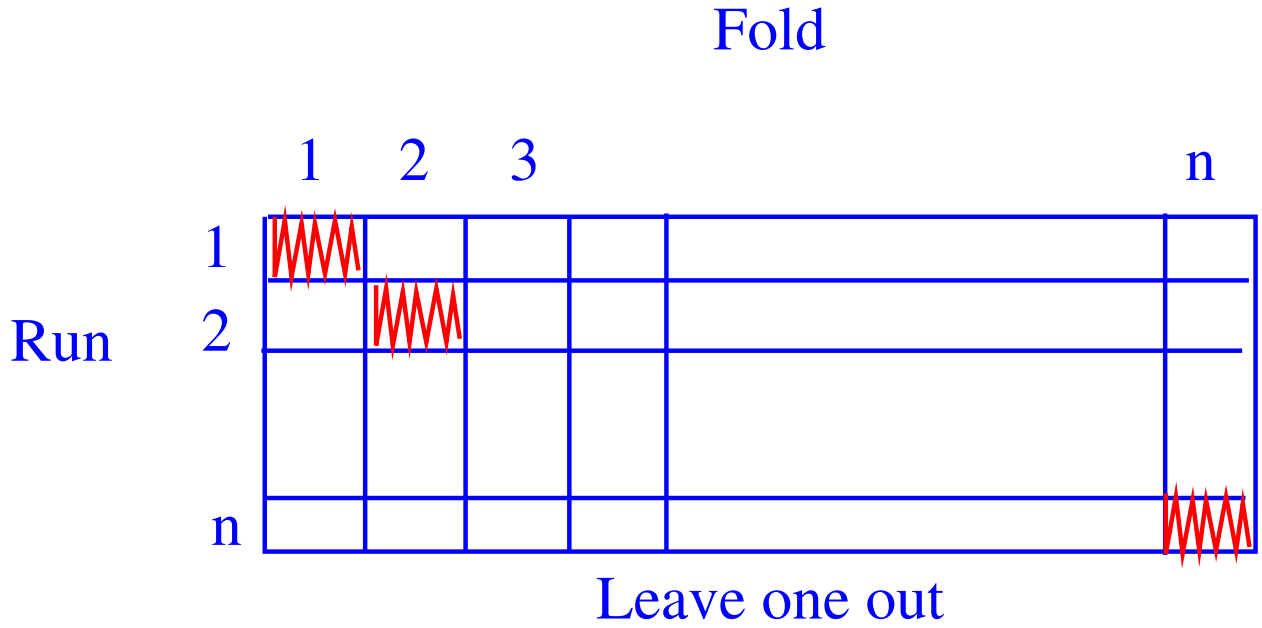
N–fold Cross Validation

Error = Average (error on  of h

learned from )

Empirical estimates, foll'd

Cross validation $\rightarrow$ Leave one out

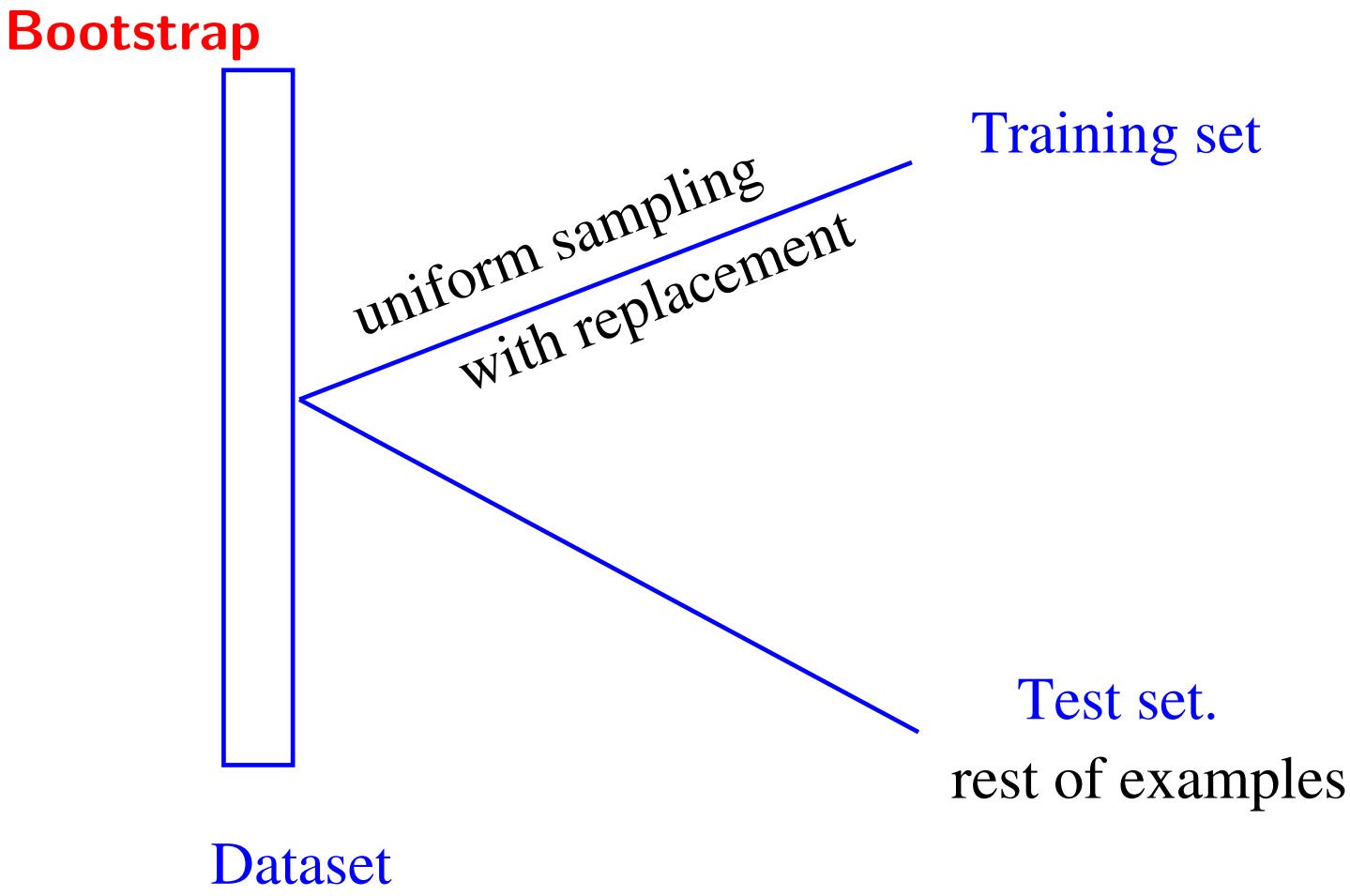


Same as N-fold CV, with N = number of examples.

Properties

Low bias; high variance; underestimate error if data not independent

Empirical estimates, foll'd



Average indicator over all (Training set, Test set) samplings.

Beware

Multiple hypothesis testing

- If you test many hypotheses on the same dataset
- one of them will appear confidently true...

More

- Tutorial slides:
  http://www.lri.fr/ sebag/Slides/Validation_Tutorial_11.pdf
- Video and slides (soon): ICML 2012, Videolectures, Tutorial Japkowicz & Shah
  http://www.mohakshah.com/tutorials/icml2012/

Validation, summary

What is the performance criterion

- Cost function
- Account for class imbalance
- Account for data correlations

Assessing a result

- Compute confidence intervals
- Consider baselines
- Use a validation set

If the result looks too good, don't believe it