Machine learning

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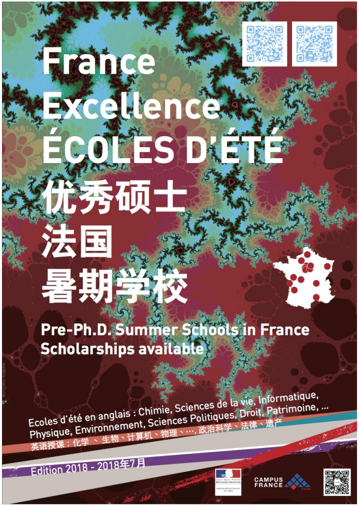
Outline



1. **Introduction**
2. **Optimal discrimination**
   - Bayes limit
   - Multivariate discriminant
3. **Machine learning**
   - Supervised and unsupervised learning
4. **Multivariate discriminants**
   - Quadratic and linear discriminants
   - Support vector machines
   - Decision trees
   - Neural networks
   - Deep networks

Introduction

Typical problems in HEP

- Classification of objects
  - separate real and fake leptons/jets/etc.
- Signal enhancement relative to background
- Regression: best estimation of a parameter
  - lepton energy, $\not{E}_{\mathrm{T}}$ value, invariant mass, etc.

Discrimination of signal from background in HEP

- Event level (Higgs searches, ...)
- Cone level (tau-vs-jet reconstruction, ...)
- Lifetime and flavour tagging (*b*-tagging, ...)
- Track level (particle identification, ...)
- Cell level (energy deposit from hard scatter/pileup/noise, ...)

Introduction

Input information from various sources

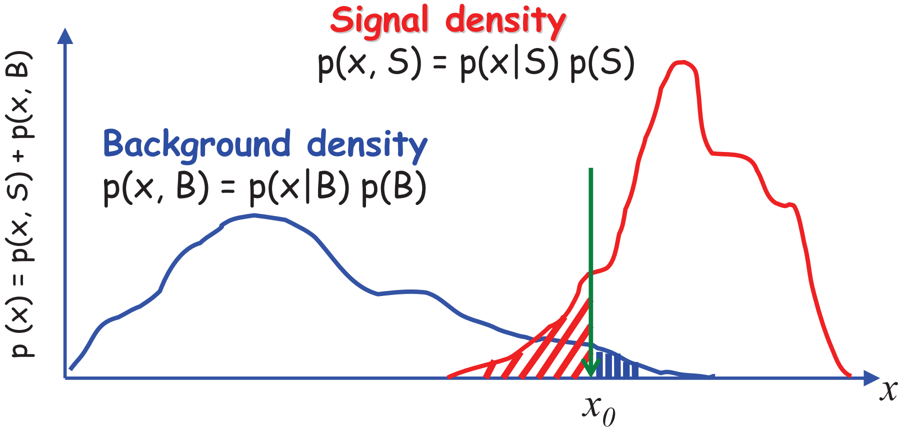
- Kinematic variables (masses, momenta, decay angles, ...)
- Event properties (jet multiplicity, sum of charges, brightness ...)
- Event shape (sphericity, aplanarity, ...)
- Detector response (silicon hits, dE/dx, Cherenkov angle, shower profiles, muon hits, ...)

Most data are (highly) multidimensional

- Use dependencies between $x = \{x_1, \cdots, x_n\}$ discriminating variables
- Approximate this n-dimensional space with a function $f(x)$ capturing the essential features
- f is a multivariate discriminant
- For most of these lectures, use binary classification:
    - an object belongs to one class (e.g. signal) if $f(x) > q$, where q is some threshold,
    - and to another class (e.g. background) if $f(x) \leq q$

Optimal discrimination: 1-dimension case

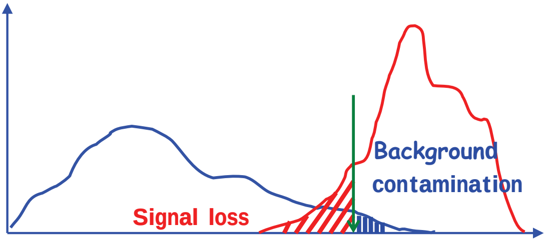
- Where to place a cut x_0 on variable x?



- Optimal choice: minimum misclassification cost at decision boundary $x = x_0$

$$C(x_0) = C_S \int H(x_0 - x)p(x,S)dx \quad \text{signal loss}$$
$$+ \; C_B \int H(x - x_0)p(x,B)dx \quad \text{background contamination}$$

C_S = cost of misclassifying signal as background
C_B = cost of misclassifying background as signal



- $H(x)$: Heaviside step function
- $H(x) = 1$ if $x > 0$, 0 otherwise

- Optimal choice: when cost function C is minimum

Optimal discrimination: Bayes discriminant

Minimising the cost

- Minimise
  $C(x_0) = C_S \int H(x_0 - x)p(x,S)dx + C_B \int H(x - x_0)p(x,B)dx$
  with respect to the boundary x_0:

$$\begin{aligned} 0 &= C_S \int \delta(x_0 - x)p(x,S)dx - C_B \int \delta(x - x_0)p(x,B)dx \\ &= C_S p(x_0,S) - C_B p(x_0,B) \end{aligned}$$

- This gives the Bayes discriminant:

$$BD = \frac{C_B}{C_S} = \frac{p(x_0,S)}{p(x_0,B)} = \frac{p(x_0|S)p(S)}{p(x_0|B)p(B)}$$

Probability relationships

- $p(A,B) = p(A|B)p(B) = p(B|A)p(A)$
- Bayes theorem: $p(A|B)p(B) = p(B|A)p(A)$
- $p(S|x) + p(B|x) = 1$

Optimal discrimination: Bayes limit

Generalising to multidimensional problem

- The same holds when x is an n-dimensional variable:

$$BD = B\frac{p(S)}{p(B)} \quad \text{where} \quad B = \frac{p(x|S)}{p(x|B)}$$

- B is the Bayes factor, identical to the likelihood ratio when class densities $p(x|S)$ and $p(x|B)$ are independent of unknown parameters

Bayes limit

- $p(S|x) = BD/(1+BD)$ is what should be achieved to minimise cost, achieving classification with the fewest mistakes
- Fixing relative cost of background contamination and signal loss $q = C_B/(C_S + C_B)$, $q = p(S|x)$ defines decision boundary:
  - signal-rich if $p(S|x) \geq q$
  - background-rich if $p(S|x) < q$
- Any function that approximates conditional class probability $p(S|x)$ with negligible error reaches the Bayes limit

Optimal discrimination: using a discriminant

How to construct p(S|x)?

- $k = p(S)/p(B)$ typically unknown
- Problem: $p(S|x)$ depends on k!
- Solution: it's not a problem…
- Define a multivariate discriminant:

$$D(x) = \frac{s(x)}{s(x) + b(x)} = \frac{p(x|S)}{p(x|S) + p(x|B)}$$

- Now:

$$p(S|x) = \frac{D(x)}{D(x) + (1 - D(x))/k}$$

- Cutting on $D(x)$ is equivalent to cutting on $p(S|x)$, implying a corresponding (unknown) cut on $p(S|x)$

Machine learning: learning from examples

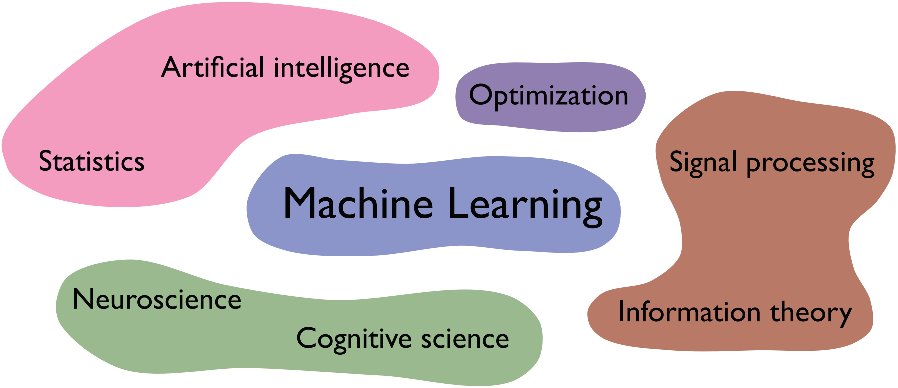
Several types of problems

- Classification/decision:
  - signal or background
  - type Ia supernova or not
  - will pay his/her credit back on time or not
- Regression (mostly ignored in these lectures)
- Clustering (cluster analysis):
  - in exploratory data mining, finding features

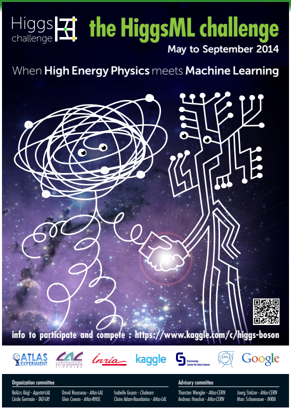
Our goal

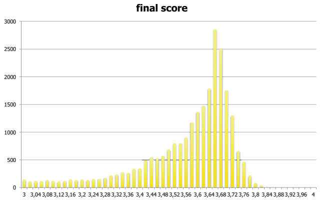
- Teach a machine to learn the discriminant $f(x)$ using examples from a training dataset
- Be careful to not learn too much the properties of the training sample
  - no need to memorise the training sample
  - instead, interested in getting the right answer for new events
    $\Rightarrow$ generalisation ability

Machine learning and connected fields



Machine learning and HEP





HiggsML challenge

- Put ATLAS Monte Carlo samples on the web ($H \to \tau\tau$ analysis)
- Compete for best signal–bkg separation
- 1785 teams (most popular challenge ever)
- 35772 uploaded solutions
- See ▸ Kaggle web site and ▸ more information

#	Δrank	Team Name ‡ model uploaded * in the money		Score	Entries	Last Submission UTC (Best – Last Submission)
1	↑1	Gábor Melis ‡ *	7000$	3.80581	110	Sun, 14 Sep 2014 09:10:04 (-0h)
2	↑1	Tim Salimans ‡ *	4000$	3.78913	57	Mon, 15 Sep 2014 23:49:02 (-40.6d)
3	↑1	nhlx5haze ‡ *	2000$	3.78682	254	Mon, 15 Sep 2014 16:50:01 (-76.3d)
4	↑38	ChoKo Team		3.77526	216	Mon, 15 Sep 2014 15:21:36 (-42.1h)
5	↑35	cheng chen		3.77384	21	Mon, 15 Sep 2014 23:29:29 (-0h)
6	↑16	quantify		3.77086	8	Mon, 15 Sep 2014 16:12:48 (-7.3h)
7	↑1	Stanislav Semenov & Co (HSE Yandex)		3.76211	68	Mon, 15 Sep 2014 20:19:03
8	↓7	Luboš Motl's team		3.76050	589	Mon, 15 Sep 2014 08:38:49 (-1.6h)
9	↑8	Roberto-UCIIIM		3.75864	292	Mon, 15 Sep 2014 23:44:42 (-44d)
10	↑2	Davut & Josef		3.75838	161	Mon, 15 Sep 2014 23:24:32 (-4.5d)
45	↑5	crowwork ‡	HEP meets ML award Free trip to CERN	3.71885	94	Mon, 15 Sep 2014 23:45:00 (-5.1d)
782	↓149	Eckhard	TMVA expert, with TMVA improvements	3.49945	29	Mon, 15 Sep 2014 07:26:13 (-46.1h)
991	↑4	Rem.		3.20423	2	Mon, 16 Jun 2014 21:53:43 (-30.4h)
		simple TMVA boosted trees		3.19956		

Machine learning: (un)supervised learning

Supervised learning

- Training events are labelled: N examples $(x, y)_1, (x, y)_2, \ldots, (x, y)_N$ of (discriminating) feature variables x and class labels y
- The learner uses example classes to know how good it is doing

Reinforcement learning

- Instead of labels, some sort of reward system (e.g. game score)
- Goal: maximise future payoff
- May not even "learn" anything from data, but remembers what triggers reward or punishment

Unsupervised learning

- e.g. clustering: find similarities in training sample, without having predefined categories (how Amazon is recommending you books...)
- Discover good internal representation of the input
- Not biased by pre-determined classes $\Rightarrow$ may discover unexpected features!

Finding the multivariate discriminant $y = f(x)$

- Given our N examples $(x, y)_1, \ldots, (x, y)_N$ we need
  - a function class $\mathbb{F} = \{f(x, w)\}$ (w: parameters to be found)
  - a constraint $Q(w)$ on $\mathbb{F}$
  - a loss or error function $L(y, f)$, encoding what is lost if f is poorly chosen in $\mathbb{F}$ (i.e., $f(x, w)$ far from the desired $y = f(x)$)
- Cannot minimise L directly (would depend on the dataset used), but rather its average over a training sample, the empirical risk:

$$R(w) = \frac{1}{N} \sum_{i=1}^{N} L\big(y_i, f(x_i, w)\big)$$

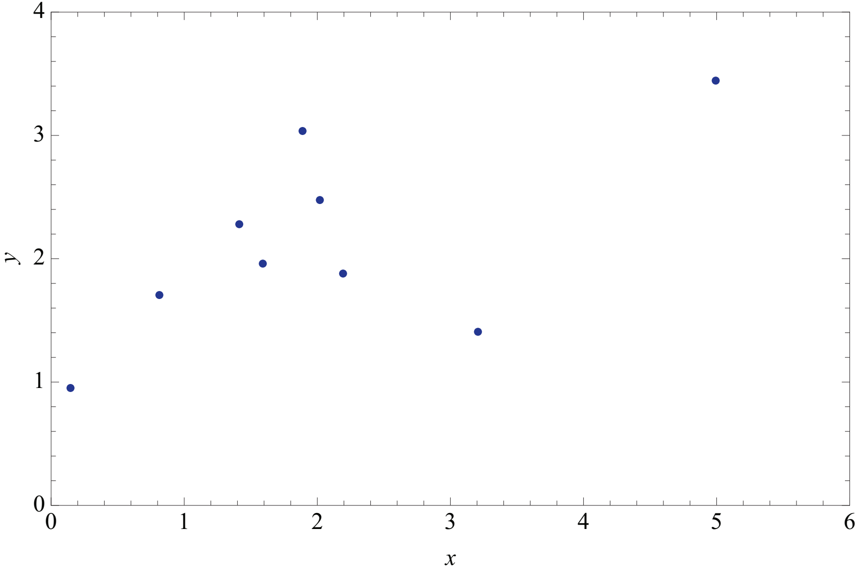
subject to constraint $Q(w)$, so we minimise the cost function:

$$C(w) = R(w) + \lambda Q(w)$$

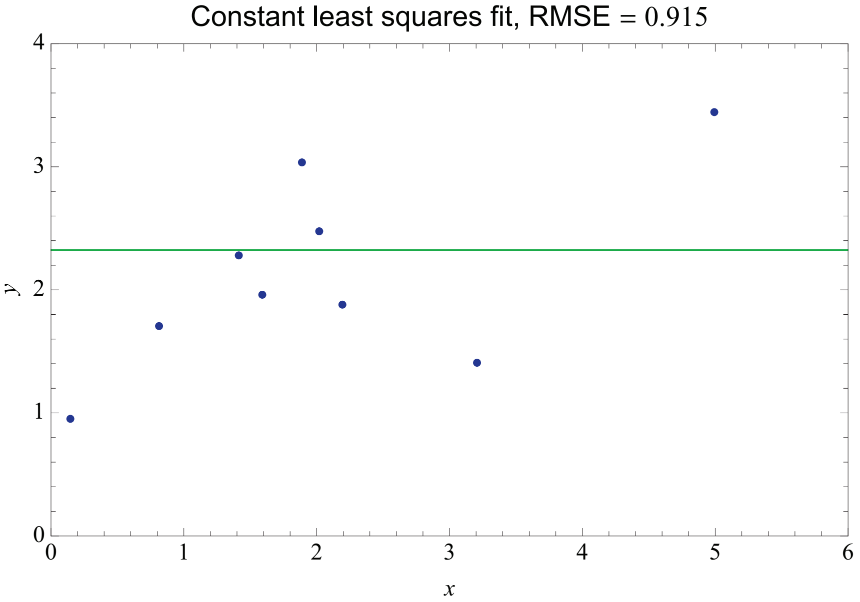
- At the minimum of $C(w)$ we select $f(x, w_*)$, our estimate of $y = f(x)$

Choice of function class: training

Data generated from an unknown function with unknown noise



Choice of function class: training



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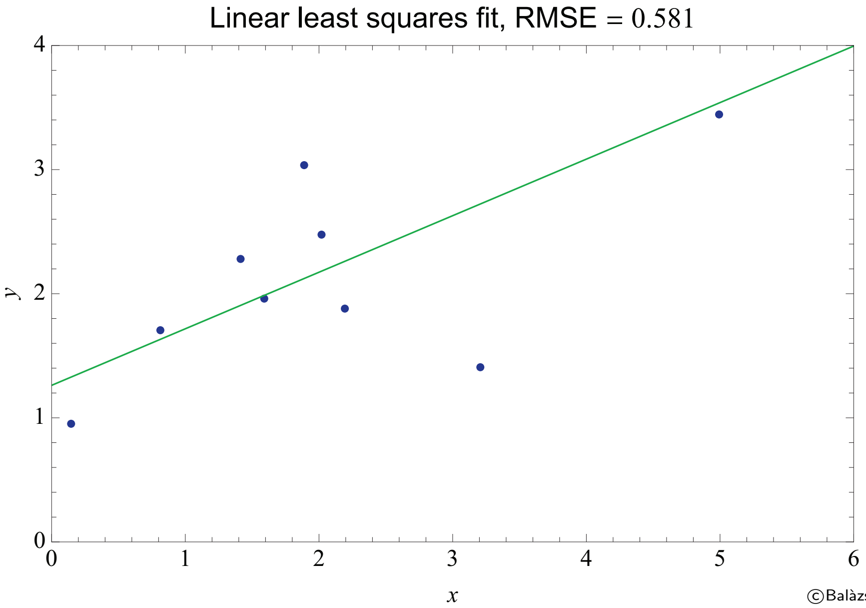

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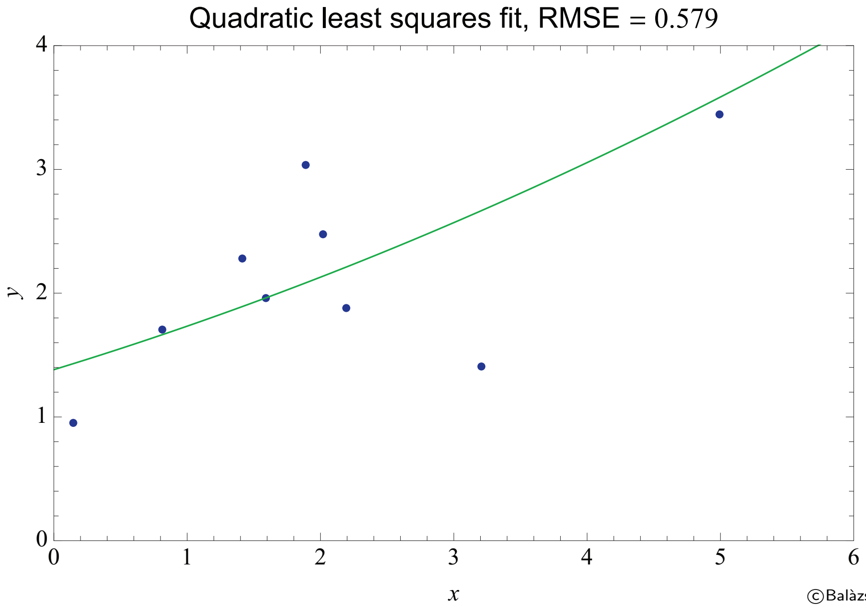

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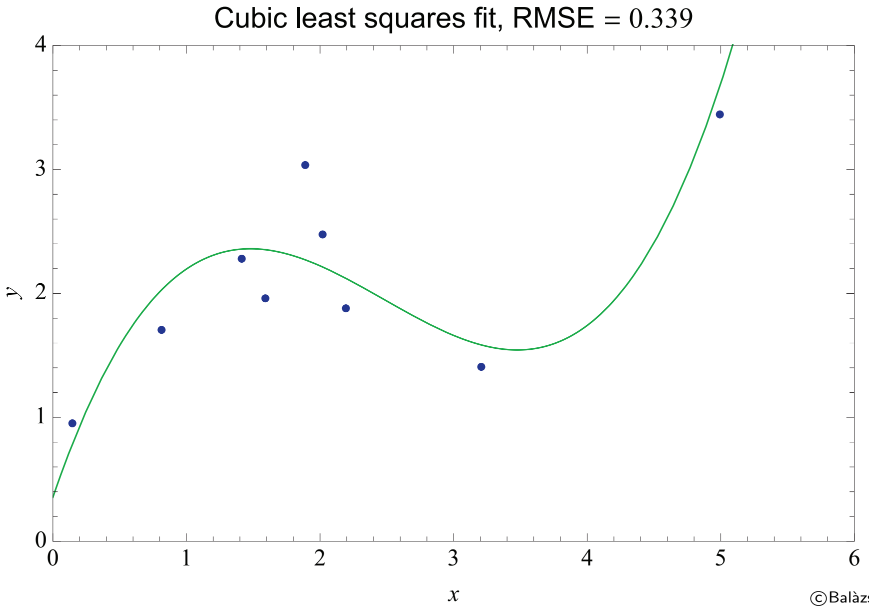

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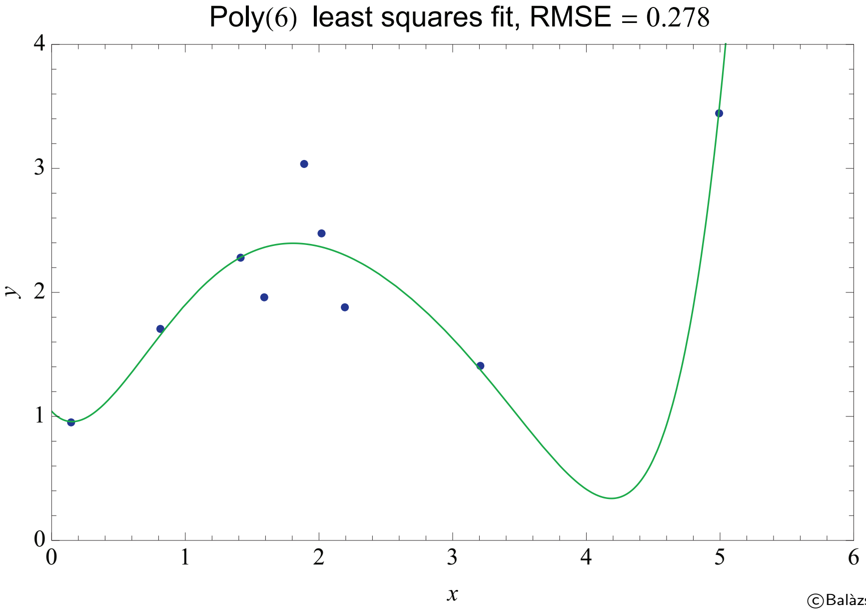

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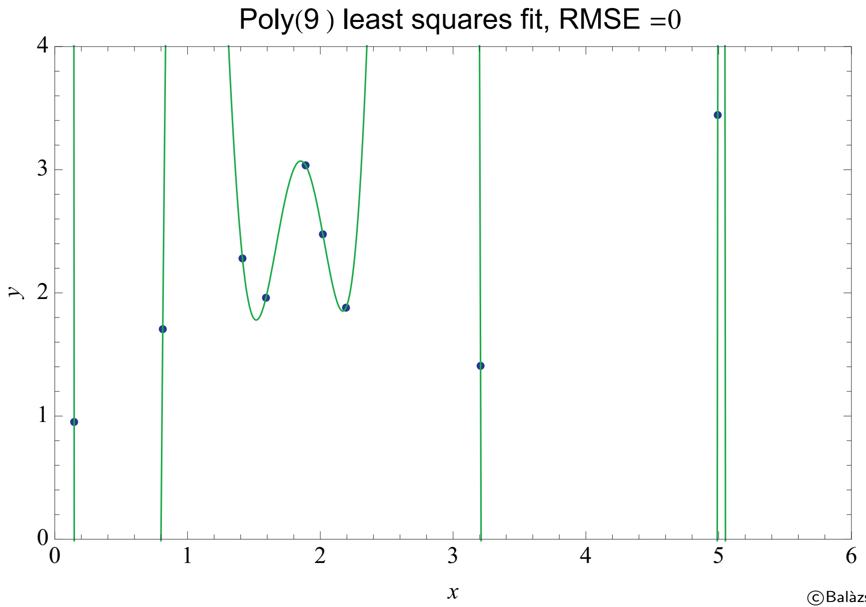
Choice of function class: training



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Choice of function class

Quality of fit

- Increasing degree of polynomial increases flexibility of function
- Higher degree $\Rightarrow$ can match more features
- If degree = # points, polynomial passes through each point: perfect match!

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Is it meaningful?

- It could be:
  - if there is no noise or uncertainty in the measurement
  - if the true distribution is indeed perfectly described by such a polynomial
- . . . not impossible, but not very common. . .

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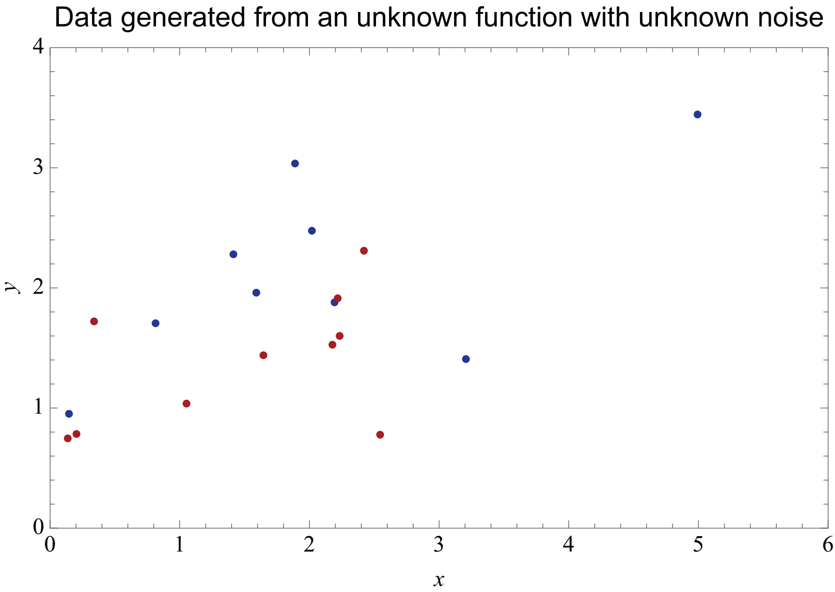
Solution: testing sample

- Use independent sample to validate the result
- Expected: performance will also increase, go through a maximum and decrease again, while it keeps increasing on the training sample

Choice of function class: testing



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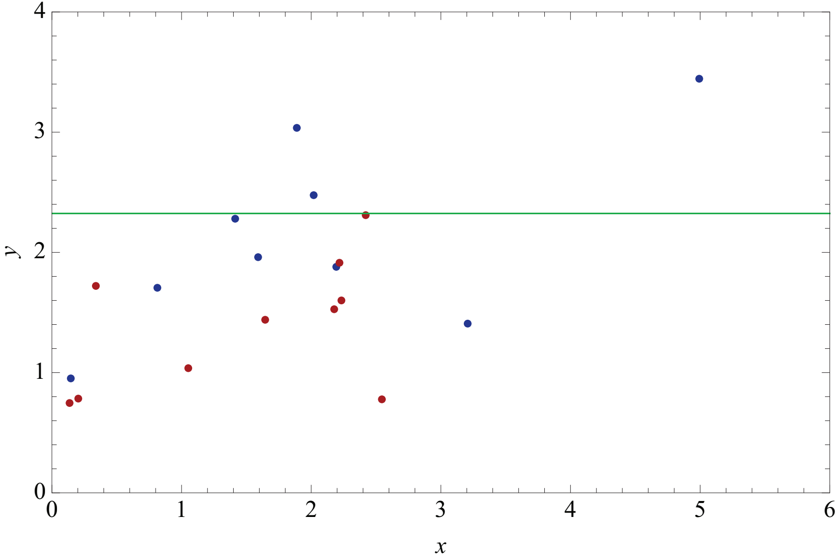
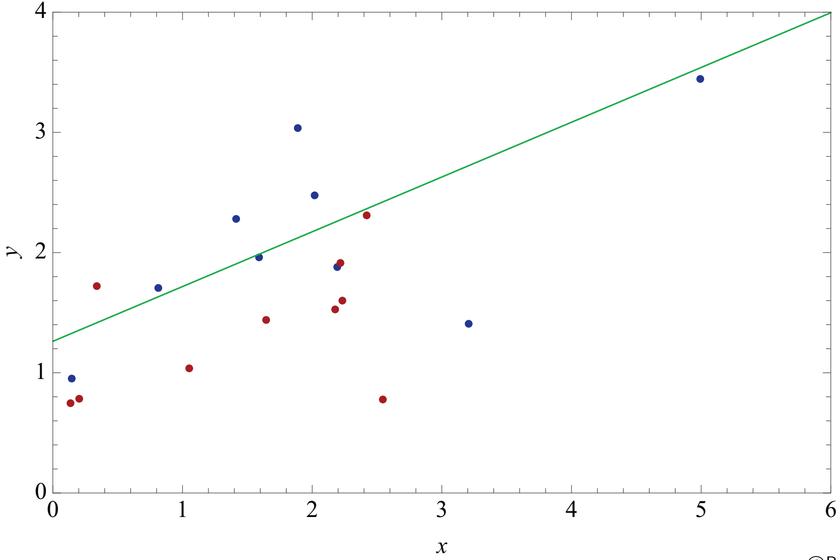
Choice of function class: testing

Const. least squares fit, training RMSE = 0.915, test RMSE = 1.067



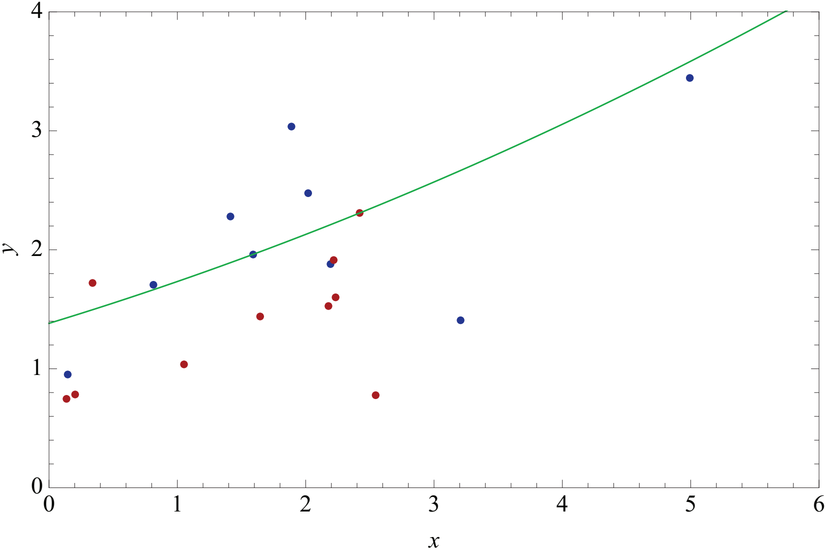
Choice of function class: testing

Linear least squares fit, training RMSE $= 0.581$, test RMSE $= 0.734$



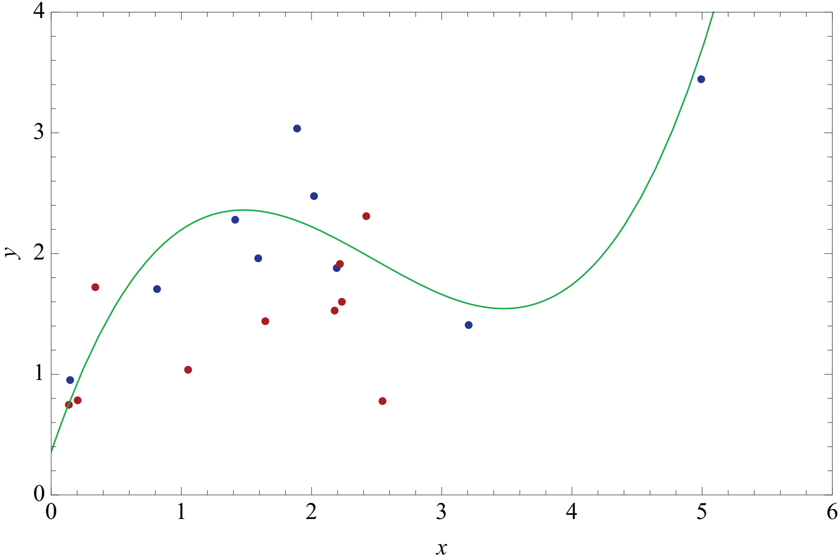
Choice of function class: testing

Quadr. least squares fit, training RMSE = 0.579, test RMSE = 0.723



Choice of function class: testing

Cubic least squares fit, training RMSE = 0.339, test RMSE = 0.672



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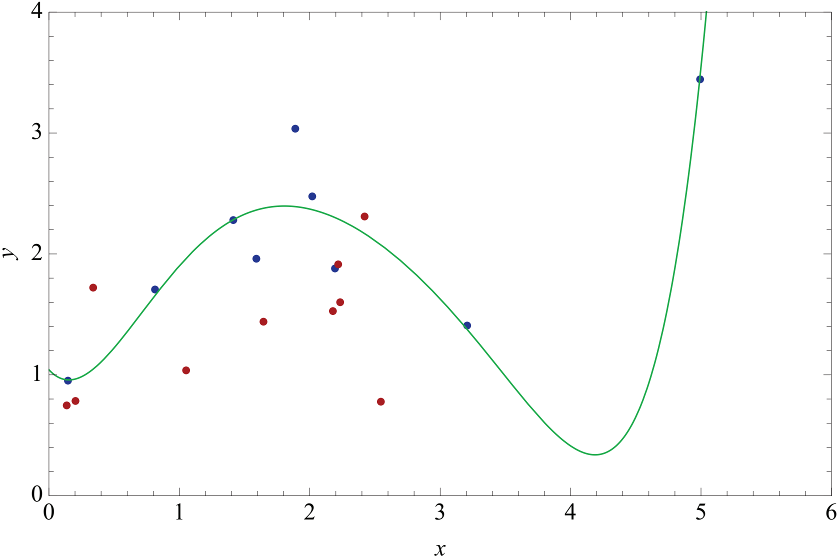
Choice of function class: testing

Poly(6) least squares fit, training RMSE $= 0.278$, test RMSE $= 0.72$



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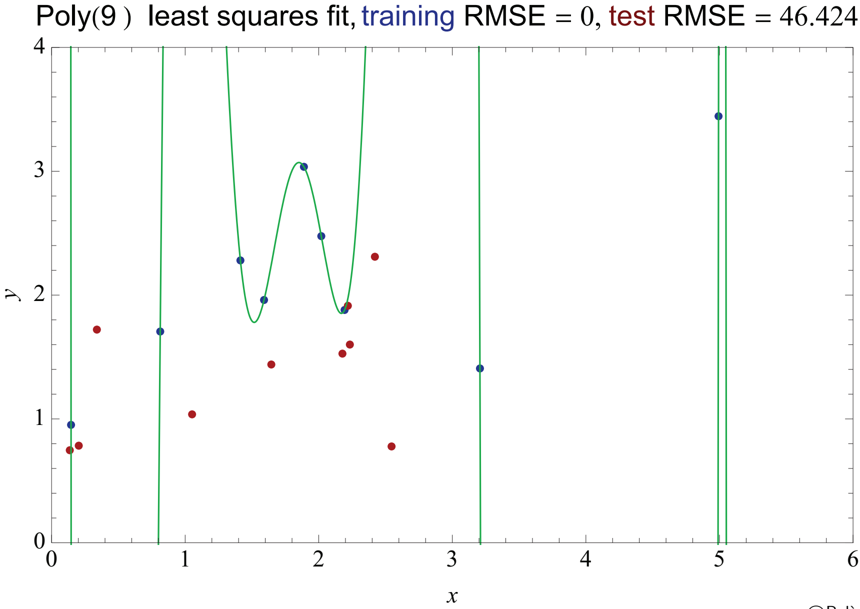
Choice of function class: testing



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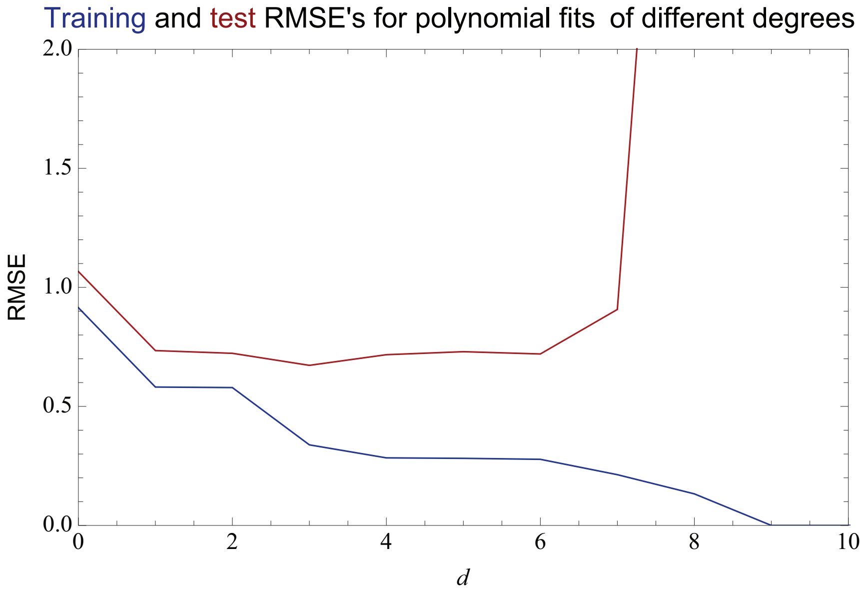
Choice of function class



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Choice of function class

Non-parametric fit

- Minimising the training cost (here, RMSE) does not work if the function class is not fixed in advance (e.g. fix the polynomial degree): complete loss of generalisation capability!
- But if you do not know the correct function class, you should not fix it! Dilemma...

Capacity control and regularisation

- Trade-off between approximation error and estimation error
- Take into account sample size
- Measure (and penalise) complexity
- Use independent test sample
- In practice, no need to correctly guess the function class, but need enough flexibility in your model, balanced with complexity cost

Multivariate discriminants

Reminder

- To solve binary classification problem with the fewest number of mistakes, sufficient to compute the multivariate discriminant:

$$D(x) = \frac{s(x)}{s(x) + b(x)}$$

where:

  - $s(x) = p(x|S)$ signal density
  - $b(x) = p(x|B)$ background density

- Cutting on $D(x)$ is equivalent to cutting on probability $p(S|x)$ that event with x values is of class S

Which approximation to choose?

- Best possible choice: cannot beat Bayes limit (but usually impossible to define)
- No single method can be proven to surpass all others in particular case
- Advisable to try several and use the best one

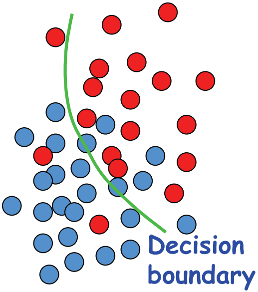
- Suppose densities $s(x)$ and $b(x)$ are multivariate Gaussians:

$$\text{Gaussian}(x|\mu,\Sigma) = \frac{1}{\sqrt{(2\pi)^n|\Sigma|}} \exp^{\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)}$$

  with vector of means μ and covariance matrix Σ

- Then Bayes factor $B(x) = s(x)/b(x)$ (or its logarithm) can be expressed explicitly:

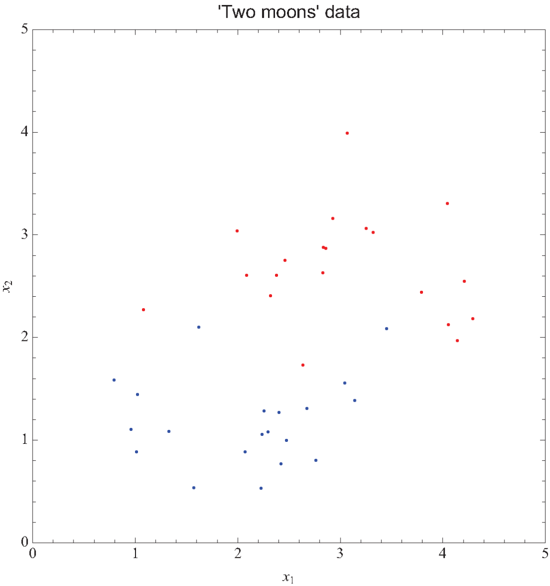
$$\ln B(x) = \lambda(x) \equiv \chi^2(\mu_B,\Sigma_B) - \chi^2(\mu_S,\Sigma_S)$$



with $\chi^2(\mu,\Sigma) = (x-\mu)^T\Sigma^{-1}(x-\mu)$

- Fixed value of $\lambda(x)$ defines a quadratic hypersurface partitioning the n-dimensional space into signal-rich and background-rich regions
- Optimal separation if $s(x)$ and $b(x)$ are indeed multivariate Gaussians

Quadratic discriminant



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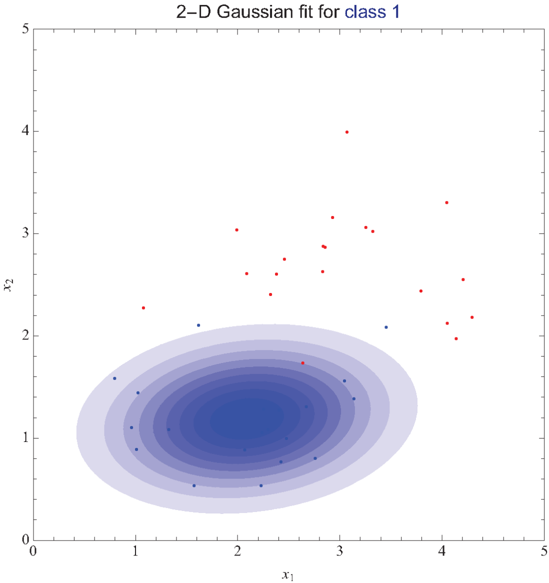
Quadratic discriminant



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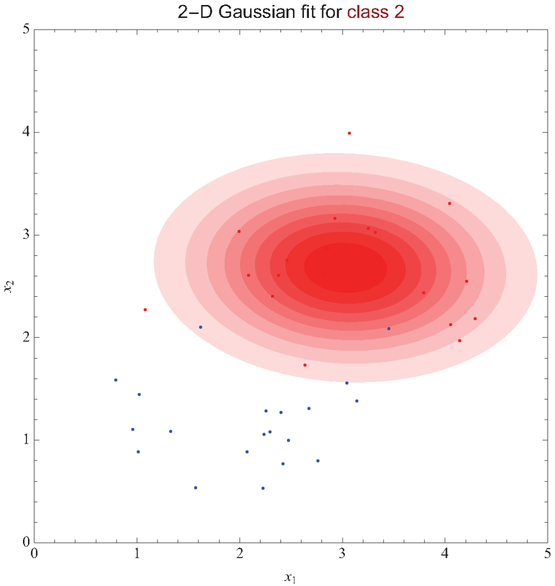
Quadratic discriminant



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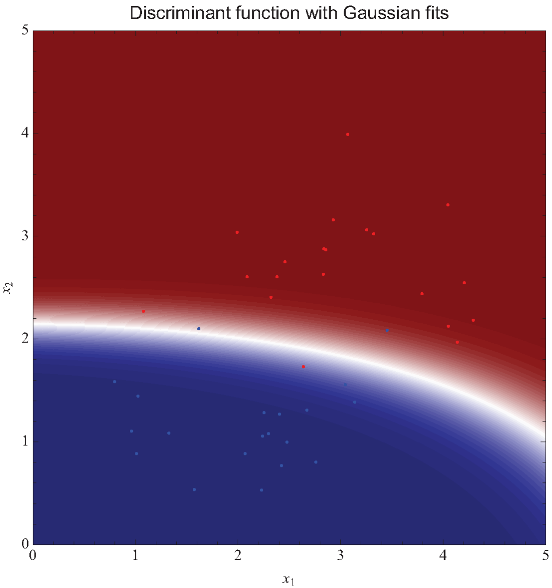
Quadratic discriminant



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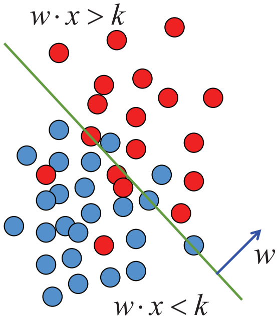
Linear discriminant: Fisher's discriminant

- If in $\lambda(x)$ the same covariance matrix is used for each class (e.g. $\Sigma = \Sigma_S + \Sigma_B$) one gets Fisher's discriminant:

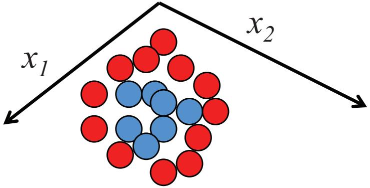
$$\lambda(x) = w \cdot x \quad \text{with} \quad w \propto \Sigma^{-1}(\mu_S - \mu_B)$$

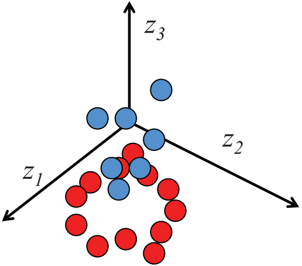


- Optimal linear separation
- Works only if signal and background have different means!
- Optimal classifier (reaches the Bayes limit) for linearly correlated Gaussian-distributed variables

Support vector machines

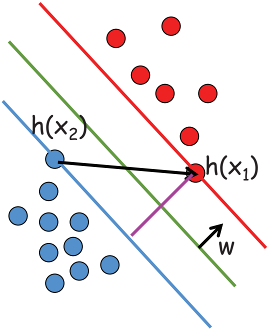
- Fisher discriminant: may fail completely for highly non-Gaussian densities
- But linearity is good feature $\Rightarrow$ try to keep it
- Generalising Fisher discriminant: data non-separable in n-dim space $\mathbb{R}^n$, but better separated if mapped to higher dimension space $\mathbb{R}^H$: $h : x \in \mathbb{R}^n \rightarrow z \in \mathbb{R}^H$
- Use hyper-planes to partition higher dim space: $f(x) = w \cdot h(x) + b$
- Example:$h : (x_1, y_2) \rightarrow (z_1, z_2, z_3) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$





- Consider separable data in $\mathbb{R}^H$, and three parallel hyper-planes:

$$\begin{aligned} w \cdot h(x) + b &= 0 \text{ (separating hyper-plane between red and blue)} \\ w \cdot h(x_1) + b &= +1 \text{ (contains } h(x_1)\text{)} \\ w \cdot h(x_2) + b &= -1 \text{ (contains } h(x_2)\text{)} \end{aligned}$$



- Subtract blue from red: $w \cdot \left(h(x_1) - h(x_2)\right) = 2$
- With unit vector $\hat{w} = w/\|w\|$: $\hat{w} \cdot \left(h(x_1) - h(x_2)\right) = 2/\|w\| = m$
- Margin m is distance between red and blue planes
- Best separation: maximise margin
- $\Rightarrow$ empirical risk margin to minimise: $R(w) \propto \|w\|^2$

Support vector machines: constraints

- When minimising $R(w)$, need to keep signal and background separated
- Label red dots $y = +1$ ("above" red plane) and blue dots $y = -1$ ("below" blue plane)
- Since:

$$\begin{aligned} w \cdot h(x) + b &> 1 \text{ for red dots} \\ w \cdot h(x) + b &< -1 \text{ for blue dots} \end{aligned}$$

  all correctly classified points will satisfy constraints:

$$y_i\big(w \cdot h(x_i) + b\big) \geq 1,\ \forall i = 1, \ldots, N$$

- Using Lagrange multipliers $\alpha_i > 0$, cost function can be written:

$$C(w, b, \alpha) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{N} \alpha_i \big[y_i\big(w \cdot h(x_i) + b\big) - 1\big]$$

Support vector machines

Minimisation

- Minimise cost function $C(w, b, \alpha)$ with respect to w and b:

$$C(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \left(h(x_i) \cdot h(x_j)\right)$$

- At minimum of $C(\alpha)$, only non-zero α_i correspond to points on red and blue planes: support vectors

Kernel functions

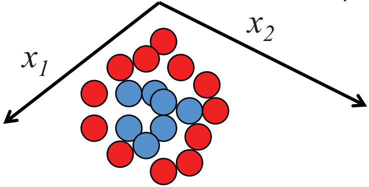
- Issues:
  - need to find h mappings (potentially of infinite dimension)
  - need to compute scalar products $h(x_i) \cdot h(x_j)$
- Fortunately $h(x_i) \cdot h(x_j)$ are equivalent to some kernel function $K(x_i, x_j)$ that does the mapping and the scalar product:

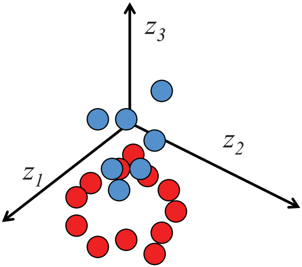
$$C(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$

Support vector machines: example

- $h : (x_1, x_2) \to (z_1, z_2, z_3) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$

$$\begin{aligned} h(x)\cdot h(y) &= (x_1^2, \sqrt{2}x_1x_2, x_2^2)\cdot(y_1^2, \sqrt{2}y_1y_2, y_2^2) \\ &= (x\cdot y)^2 \\ &= K(x,y) \end{aligned}$$



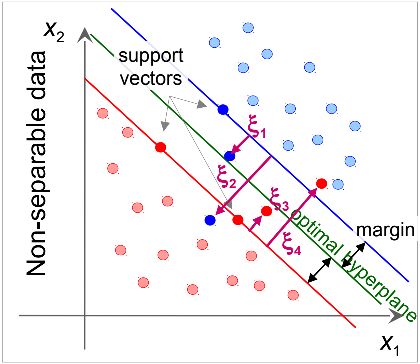


- In reality: do not know a priori the right kernel
- $\Rightarrow$ have to test different standard kernels and use the best one

Support vector machines: non-separable data

- Even in infinite dimension space, data are often non-separable
- Need to relax constraints:

$$y_i\left(w \cdot h(x_i) + b\right) \geq 1 - \xi_i$$



with slack variables $\xi_i > 0$

- $C(w, b, \alpha, \xi)$ depends on ξ, modified $C(\alpha, \xi)$ as well
- Values determined during minimisation

Decision trees

Decision tree origin

- Machine-learning technique, widely used in social sciences.
  Originally data mining/pattern recognition, then medical diagnostic, insurance/loan screening, etc.

L. Breiman *et al.*, "Classification and Regression Trees" (1984)

Basic principle

- Extend cut-based selection
  - many (most?) events do not have *all* characteristics of signal or background
  - try not to rule out events failing a particular criterion
- Keep events rejected by one criterion and see whether other criteria could help classify them properly

Binary trees

- Trees can be built with branches splitting into many sub-branches
- In this lecture: mostly binary trees

Tree building algorithm

Start with all events (signal and background) = first (root) node

- sort all events by each variable
- for each variable, find splitting value with best separation between two children
  - mostly signal in one child
  - mostly background in the other
- select variable and splitting value with best separation, produce two branches (nodes)
  - events failing criterion on one side
  - events passing it on the other

Keep splitting

- Now have two new nodes. Repeat algorithm recursively on each node
- Can reuse the same variable
- Iterate until stopping criterion is reached
- Splitting stops: terminal node = leaf

Algorithm example

- Consider signal (s_i) and background (b_j) events described by 3 variables: p_T of leading jet, top mass M_t and scalar sum of p_T's of all objects in the event H_T

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    - $p_T^{s_1} \leq p_T^{b_{34}} \leq \cdots \leq p_T^{b_2} \leq p_T^{s_{12}}$
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  - best split (arbitrary unit):
    - $p_T < 56$ GeV, separation $= 3$
    - $H_T < 242$ GeV, separation $= 5$
    - $M_t < 105$ GeV, separation $= 0.7$

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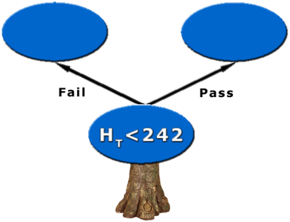

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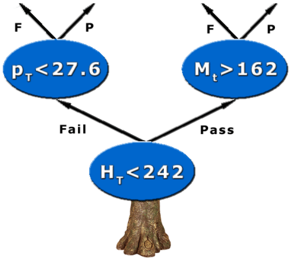

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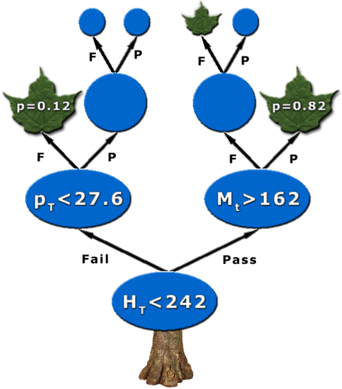
  - split events in two branches: pass or fail $H_T < 242$ GeV
- Repeat recursively on each node
- Splitting stops: e.g. events with $H_T < 242$ GeV and $M_t > 162$ GeV are signal like ($p = 0.82$)



Decision tree output

Run event through tree

- Start from root node
- Apply first best cut
- Go to left or right child node
- Apply best cut for this node
- ...Keep going until...
- Event ends up in leaf

DT Output

- Purity $\left(\frac{s}{s+b}\right.$, with weighted events$\left.\right)$ of leaf, close to 1 for signal and 0 for background
- or binary answer (discriminant function $+1$ for signal, -1 or 0 for background) based on purity above/below specified value (e.g. $\frac{1}{2}$) in leaf
- E.g. events with $H_T < 242$ GeV and $M_t > 162$ GeV have a DT output of 0.82 or $+1$

Tree instability: training sample composition

- Small changes in sample can lead to very different tree structures
- Performance on testing events may be as good, or not
- Not optimal to understand data from DT rules
- Does not give confidence in result:
  - DT output distribution discrete by nature
  - granularity related to tree complexity
  - tendency to have spikes at certain purity values (or just two delta functions at ± 1 if not using purity)

Pruning a tree

Why prune a tree?

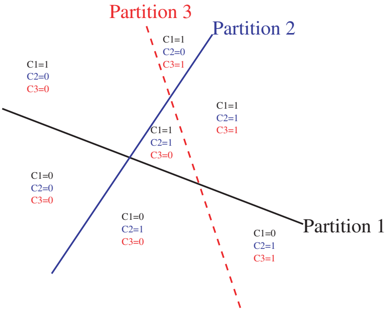
- Possible to get a perfect classifier on training events
- Mathematically misclassification error can be made as little as wanted
- E.g. tree with one class only per leaf (down to 1 event per leaf if necessary)
- Training error is zero
- But run new independent events through tree (testing or validation sample): misclassification is probably > 0, overtraining
- Pruning: eliminate subtrees (branches) that seem too specific to training sample:
  - a node and all its descendants turn into a leaf

Pruning algorithms

- Pre-pruning (early stopping condition like min leaf size, max depth)
- Expected error pruning (based on statistical error estimate)
- Cost-complexity pruning (penalise "complex" trees with many nodes/leaves)

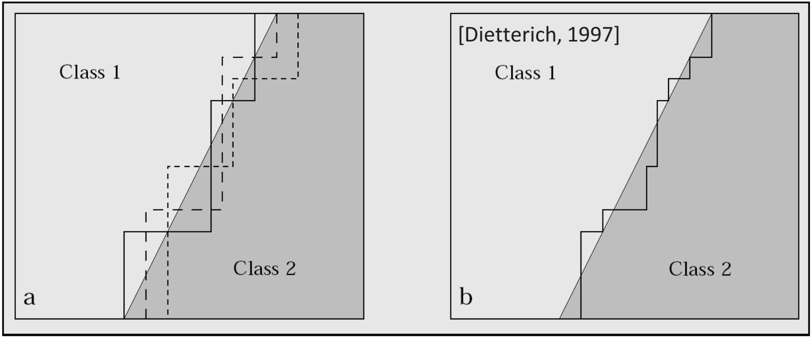
Tree (in)stability: distributed representation

- One tree:
  - one information about event (one leaf)
  - cannot really generalise to variations not covered in training set (at most as many leaves as input size)
- Many trees:
  - distributed representation: number of intersections of leaves exponential in number of trees
  - many leaves contain the event ⇒ richer description of input pattern



Tree (in)stability solution: averaging

- Build several trees and average the output



- K-fold cross-validation (good for small samples)
  - divide training sample $\mathcal{L}$ in K subsets of equal size: $\mathcal{L} = \bigcup_{k=1..K} \mathcal{L}_k$
  - Train tree T_k on $\mathcal{L} - \mathcal{L}_k$, test on $\mathcal{L}_k$
  - DT output $= \frac{1}{K} \sum_{k=1..K} T_k$
- Bagging, boosting, random forests, etc.

Boosting: a brief history

First provable algorithm by Schapire (1990)

- Train classifier T_1 on N events
- Train T_2 on new N-sample, half of which misclassified by T_1
- Build T_3 on events where T_1 and T_2 disagree
- Boosted classifier: $\text{MajorityVote}(T_1, T_2, T_3)$

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When it really picked up in HEP

- MiniBooNe compared performance of different boosting algorithms and neural networks for particle ID (2005)
- D0 claimed first evidence for single top quark production (2006)
- CDF copied (2008). Both used BDT for single top observation

Principles of boosting

What is boosting?

- General method, not limited to decision trees
- Hard to make a very good learner, but easy to make simple, error-prone ones (but still better than random guessing)
- Goal: combine such weak classifiers into a new more stable one, with smaller error

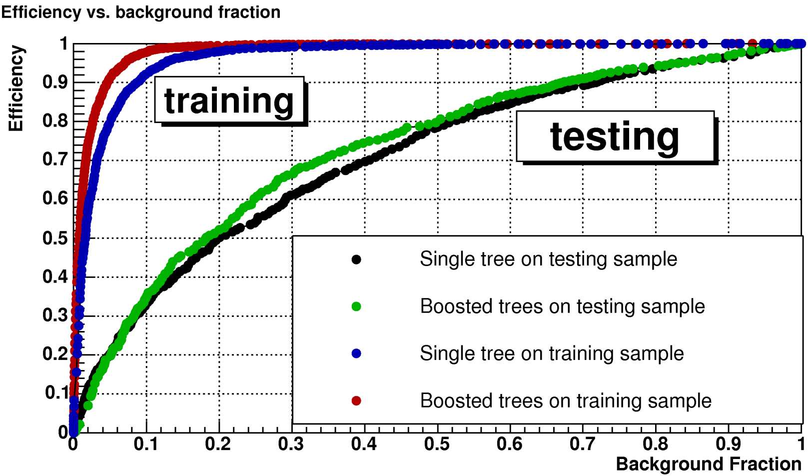
Algorithm

- Training sample $\mathbb{T}_k$ of N events. For i^{th} event:
  - weight w_i^k
  - vector of discriminative variables x_i
  - class label $y_i = +1$ for signal, -1 for background
- Pseudocode:

```
Initialise 𝕋_1
for k in 1..N_tree
  train classifier T_k on 𝕋_k
  assign weight α_k to T_k
  modify 𝕋_k into 𝕋_{k+1}
```

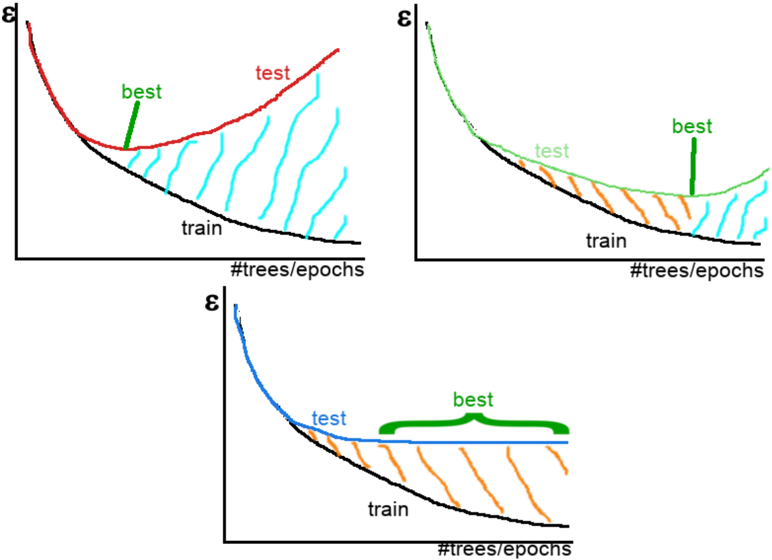
- Boosted output: $F(T_1, .., T_{N_{tree}})$

Training and generalisation error



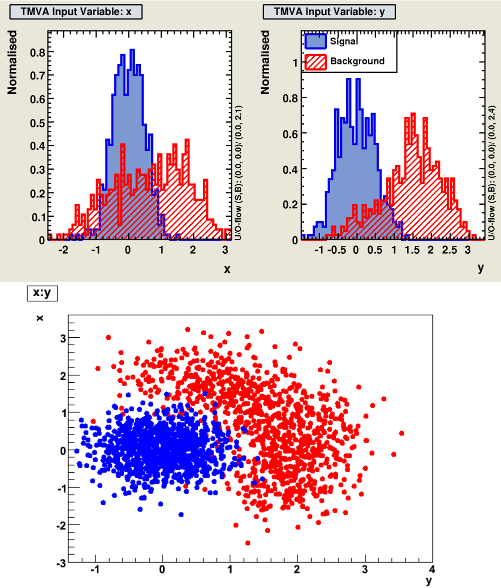
- Clear overtraining, but still better performance after boosting

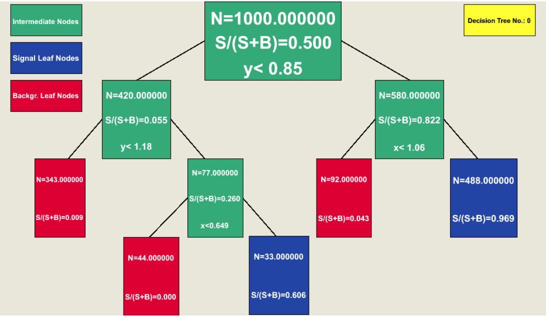
Overtraining estimation: good or bad?



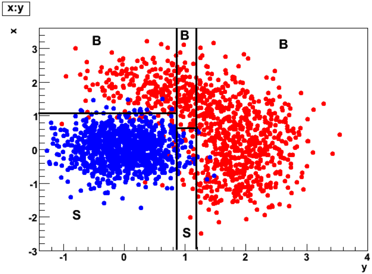
"good" overtraining / "bad" overtraining

Concrete example



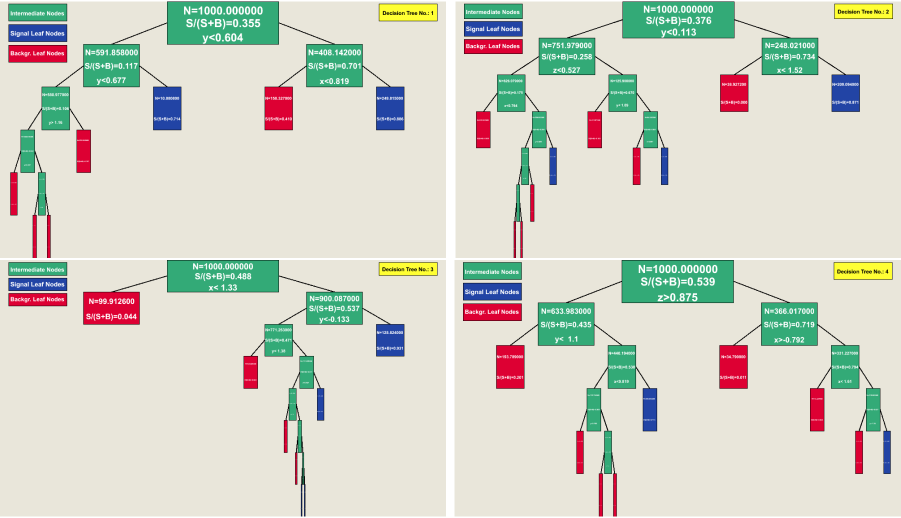


Intermediate Nodes
Signal Leaf Nodes
Backgr. Leaf Nodes
Decision Tree No.: 0
N=1000.000000
S/(S+B)=0.500
y< 0.85
N=420.000000
S/(S+B)=0.055
y< 1.18
N=580.000000
S/(S+B)=0.822
x< 1.06
N=343.000000
S/(S+B)=0.009
N=77.000000
S/(S+B)=0.260
x<0.649
N=92.000000
S/(S+B)=0.043
N=488.000000
S/(S+B)=0.969
N=44.000000
S/(S+B)=0.000
N=33.000000
S/(S+B)=0.606



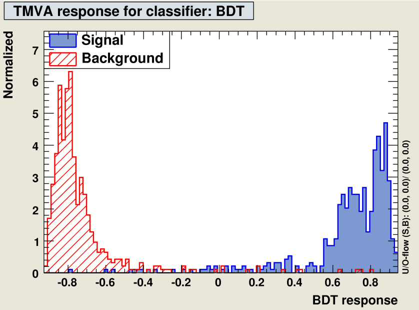
x:y
x
y
B
B
B
S
S

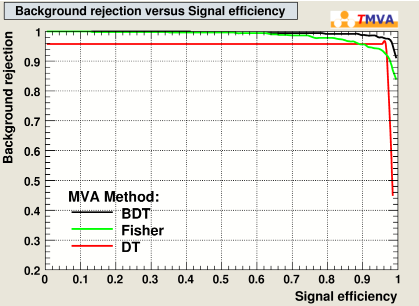
Concrete example



- Specialised trees

Concrete example





Other averaging techniques

Bagging (Bootstrap aggregating)

- Before building tree T_k take random sample of N events from training sample with replacement
- Train T_k on it
- Events not picked form "out of bag" validation sample

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Random forests

- Same as bagging
- In addition, pick random subset of variables to consider for each node split
- Two levels of randomisation, much more stable output

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Trimming

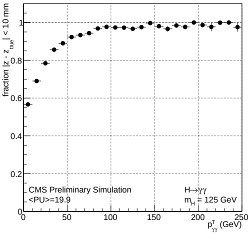
- Not exactly the same. Used to speed up training
- After some boosting, very few high weight events may contribute
- $\Rightarrow$ ignore events with too small a weight

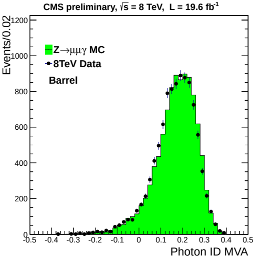
BDT in HEP: CMS H $\to \gamma\gamma$ result

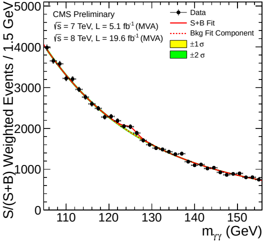
CMS-PAS-HIG-13-001

Hard to use more BDT in an analysis:

- vertex selected with BDT
- 2nd vertex BDT to estimate probability to be within 1cm of interaction point
- photon ID with BDT
- photon energy corrected with BDT regression
- event-by-event energy uncertainty from another BDT
- several BDT to extract signal in different categories



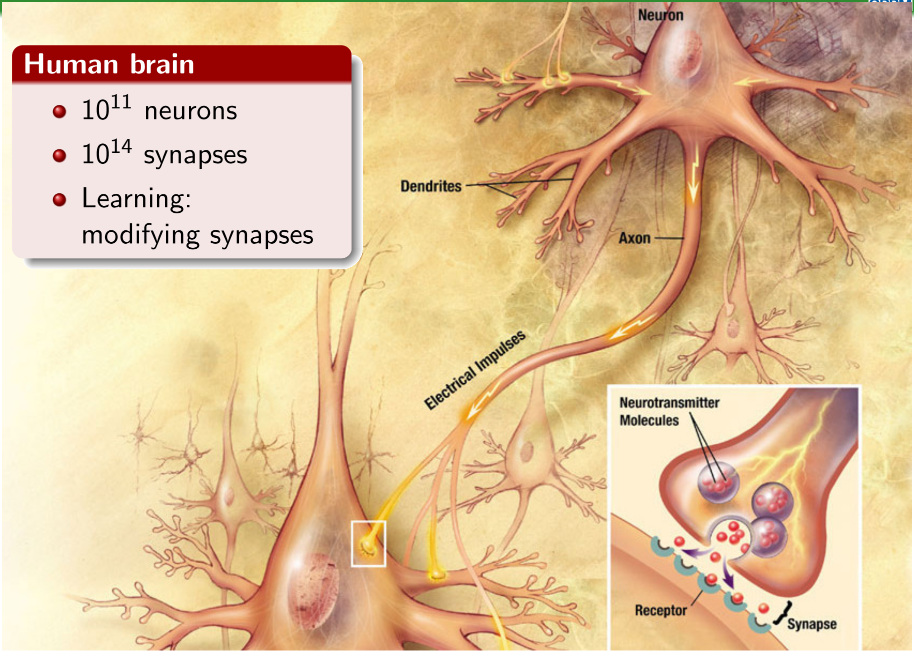




Neural networks

Human brain

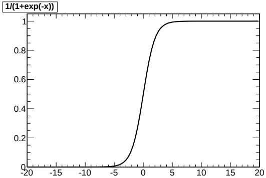
- 10^{11} neurons
- 10^{14} synapses
- Learning:
  modifying synapses



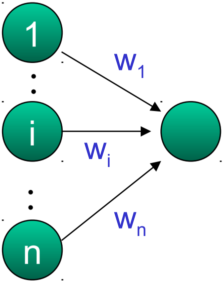
Brief history of artificial neural networks

- 1943: W. McCulloch and W. Pitts explore capabilities of networks of simple neurons
- 1958: F. Rosenblatt introduces perceptron (single neuron with adjustable weights and threshold activation function)
- 1969: M. Minsky and S. Papert prove limitations of perceptron (linear separation only) and (wrongly) conjecture that multi-layered perceptrons have same limitations
  $\Rightarrow$ ANN research almost abandoned in 1970s!!!
- 1986: Rumelhart, Hinton and Williams introduce "backward propagation of errors": solves (partially) multi-layered learning
- Next: focus on multilayer perceptron (MLP)

- Remember linear separation (Fisher discriminant): $\lambda(x) = w \cdot x = \sum_{i=1}^{n} w_i x_i + w_0$
- Boundary at $\lambda(x) = 0$
- Replace threshold boundary by sigmoid (or tanh):



$$\lambda \rightarrow \sigma(\lambda) = \frac{1}{1 + e^{-\lambda}}$$



- $\sigma(\lambda)$ is neuron activity, λ is activation
- Neuron behaviour completely controlled by weights $w = \{w_0, \ldots, w_n\}$
- Training: minimisation of error/loss function (quadratic deviations, entropy [maximum likelihood]), via gradient descent or stochastic approximation

Theorem

Let $\sigma(.)$ be a non-constant, bounded, and monotone-increasing continuous function. Let $\mathcal{C}(I_n)$ denote the space of continuous functions on the n-dimensional hypercube. Then, for any given function $f \in \mathcal{C}(I_n)$ and $\varepsilon > 0$ there exists an integer M and sets of real constants w_j, w_{ij} where $i = 1, \ldots, n$ and $j = 1, \ldots, M$ such that

$$y(x, w) = \sum_{j=1}^{M} w_j \sigma \left(\sum_{i=1}^{n} w_{ij} x_i + w_{0j} \right)$$

is an approximation of $f(.)$, that is $|y(x) - f(x)| < \varepsilon$

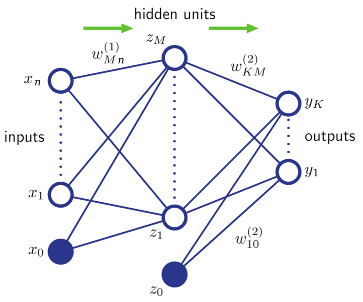
Interpretation

- You can approximate any continuous function to arbitrary precision with a linear combination of sigmoids
- Corollary 1: can approximate any continuous function with neurons!
- Corollary 2: a single hidden layer is enough
- Corollary 3: a linear output neuron is enough

Multilayer perceptron: feedforward network

- Neurons organised in layers
- Output of one layer becomes input to next layer

$$y_k(x, w) = \sum_{j=0}^{M} w_{kj}^{(2)} \, \sigma \underbrace{\left(\sum_{i=0}^{n} w_{ji}^{(1)} x_i \right)}_{z_j}$$



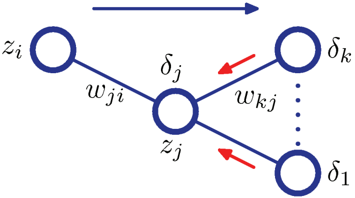
Backpropagation

- Training means minimising error function $E(w)$
- For single neuron: $\frac{dE}{dw_k} = (y - t)x_k$
- One can show that for a network:

$$\frac{dE}{dw_{ji}} = \delta_j z_i, \text{ where}$$

$$\begin{aligned} \delta_k &= (y_k - t_k) \text{ for output neurons} \\ \delta_j &\propto \sum_k w_{kj}\delta_k \text{ otherwise} \end{aligned}$$

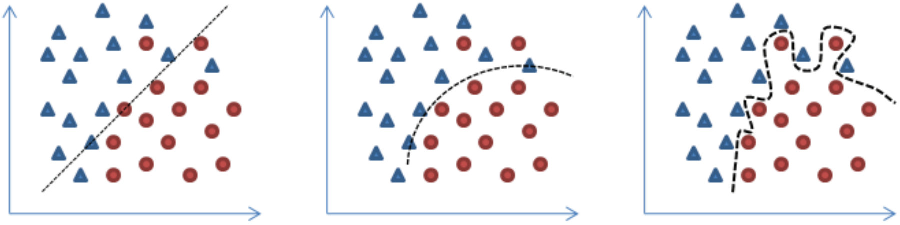
- Hence errors are propagated backwards



Neural network training

- Minimise error function $E(w)$
- Gradient descent: $w^{(k+1)} = w^{(k)} - \eta \frac{dE^{(k)}}{dw}$
- $\frac{\partial E}{\partial w_j} = \sum_{n=1}^{N} -(t^{(n)} - y^{(n)})x_j^{(n)}$ with target $t^{(n)}$ (0 or 1), so $t^{(n)} - y^{(n)}$ is the error on event n
- All events at once (batch learning):
  - weights updated all at once after processing the entire training sample
  - finds the actual steepest descent
  - takes more time
- or one-by-one (online learning):
  - speeds up learning
  - may avoid local minima with stochastic component in minimisation
  - careful: depends on the order of training events
- One epoch: going through the training data once

Neural network overtraining

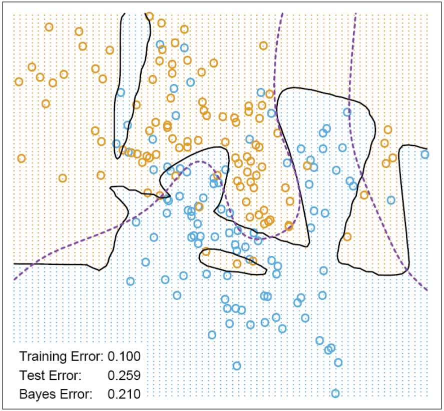


- Diverging weights can cause overfitting
- Mitigate by:
  - early stopping (after a fixed number of epochs)
  - monitoring error on test sample
  - regularisation, introducing a "weight decay" term to penalise large weights, preventing overfitting:

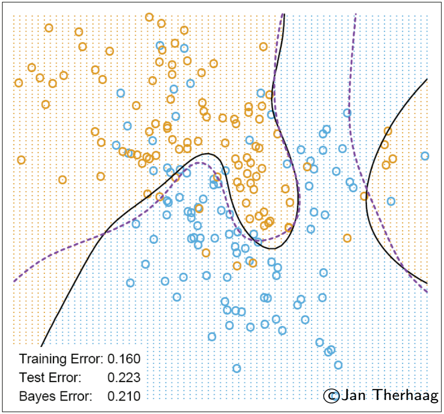
$$\tilde{E}(w) = E(w) + \frac{\alpha}{2} \sum_i w_i^2$$

Regularisation

10 hidden nodes



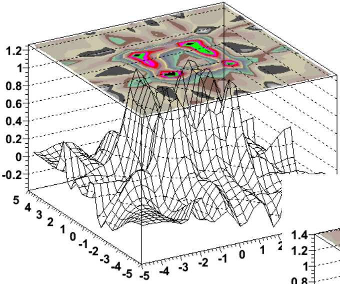
10 hidden nodes and $\alpha = 0.04$



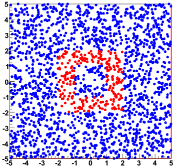
- Much less overfitting, better generalisation properties

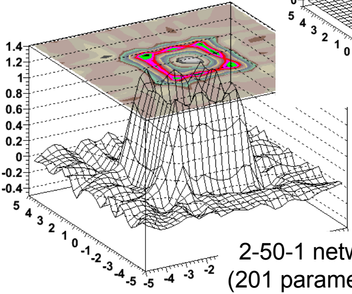
- Preprocess data:
  - if relevant, provide e.g. x/y instead of x and y
  - subtract the mean because the sigmoid derivative becomes negligible very fast (so, input mean close to 0)
  - normalise variances (close to 1)
  - shuffle training sample (order matters in online training)
- Initial random weights should be small to avoid saturation
- Batch/online training: depends on the problem
- Regularise weights to minimise overtraining. May also help select good variables via Automatic Relevance Determination (ARD)
- Make sure the training sample covers the full parameter space
- No rule (not even guestimates) about the number of hidden nodes (unless using constructive algorithm, adding resources as needed)
- A single hidden layer is enough for all purposes, but multiple hidden layers may allow for a solution with fewer parameters

Adding a hidden layer

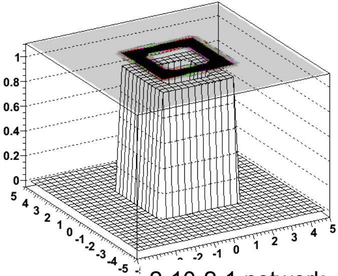


2-20-1 network
(81 parameters)





2-50-1 network
(201 parameters)



2-10-2-1 network
(55 parameters)

Deep learning

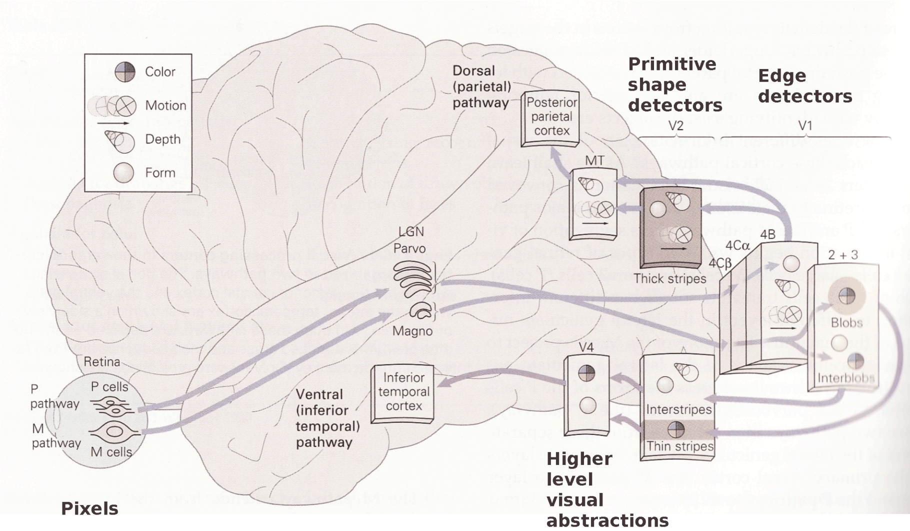
What is learning?

- Ability to learn underlying and previously unknown structure from examples
  $\Rightarrow$ capture variations
- Deep learning: have several hidden layers (> 2) in a neural network

Motivation for deep learning

- Just like in the brain!
- Humans organise ideas hierarchically, through composition of simpler ideas
- Heavily unsupervised training, learning simpler tasks first, then combined into more abstract ones
- Learn first order features from raw inputs, then patterns in first order features, then etc.

Deep architecture in the brain



Deep learning in artificial intelligence

Mimicking the brain

- About 1% of neurons active simultaneously in the brain: distributed representation
  - activation of small subset of features, not mutually exclusive
  - more efficient than local representation
  - distributed representations necessary to achieve non-local generalization, exponentially more efficient than 1-of-N enumeration
  - example: integers in 1..N
    - local representation: vector of N bits with single 1 and N-1 zeros
    - distributed representation: vector of $\log_2 N$ bits (binary notation), exponentially more compact
- Meaning: information not localised in particular neuron but distributed across them

Deep architecture

- Insufficient depth can hurt
- Learn basic features first, then higher level ones
- Learn good intermediate representations, shared across tasks

Deep learning revolution

Deep networks were unattractive

- One layer is theoretically enough for everything
- Used to perform worse than shallow networks with 1 or 2 hidden layers
- Apparently difficult/impossible to train (using random initial weights and supervised learning with backpropagation)
- Backpropagation issues:
  - requires labelled data (usually scarce and expensive)
  - does not scale well, getting stuck in local minima
  - "vanishing gradient": gradients getting very small further away from output $\Rightarrow$ early layers do not learn much, can even penalise overall performance

Deep learning revolution

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Breakthroughs around 2006 (Bengio, Hinton, LeCun)

- Try to model structure of input, $p(x)$ instead of $p(y|x)$
- Can use unlabelled data (a lot of it), with unsupervised training
- Train each layer independently (pre-train and stack)
- New activation functions (e.g. rectified linear unit ReLU)
- Possible thanks to algorithmic innovations, computing resources, data!

Greedy layer-wise pre-training

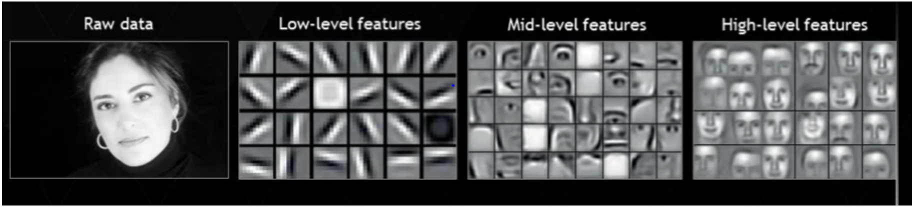
Algorithm

- Take input information
- Train feature extractor
- Use output as input to training another feature extractor
- Keep adding layers, train each layer separately
- Finalise with a supervised classifier, taking last feature extractor output as input
- All steps above: pre-training
- Fine-tune the whole thing with supervised training (backpropagation)
  - initial weights are those from pre-training

Feature extractors

- Restricted Boltzmann machine (RBM), auto-encoder, sparse auto-encoder, denoising auto-encoder, etc.
- Note: important to not use linear activation functions in hidden layers. Combination of linear functions still linear, so equivalent to single hidden layer

Learning feature hierarchy



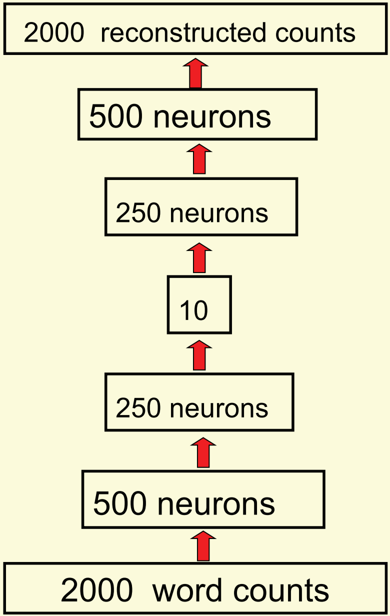
Auto-encoders

Approximate the identity function

- Build a network whose output is similar to its input
- Sounds trivial? Except if imposing constraints on network (e.g., # of neurons, locally connected network) to discover interesting structures
- Can be viewed as lossy compression of input

Finding similar books

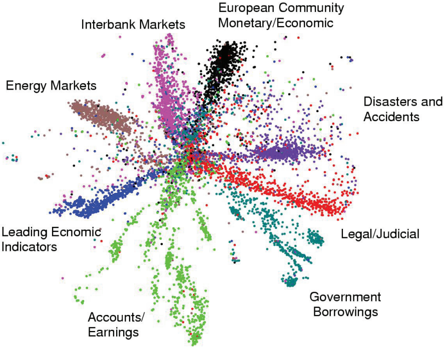
- Get count of 2000 most common words per book
- "Compress" to 10 numbers



Auto-encoders

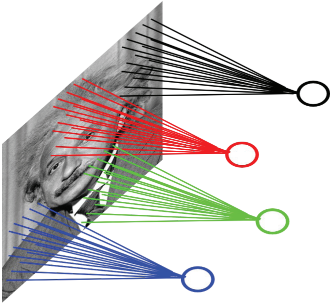
With PCA

With autoencoder

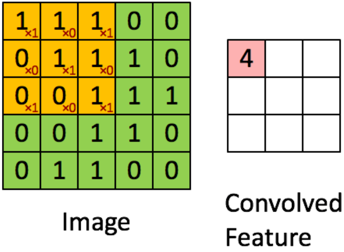


Convolutional networks

- Images are stationary: can learn feature in one part and apply it in another



- Images are stationary: can learn feature in one part and apply it in another
- Use e.g. small patch sampled randomly, learn feature, convolve with full image



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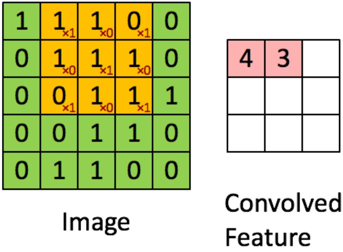

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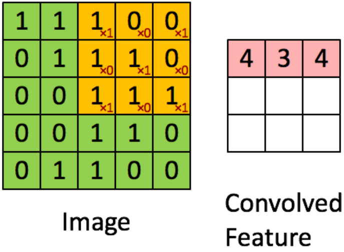

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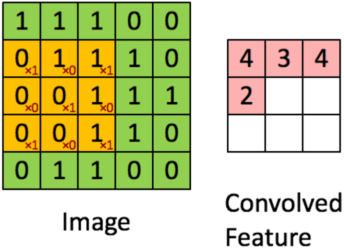

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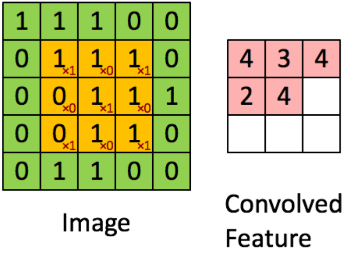

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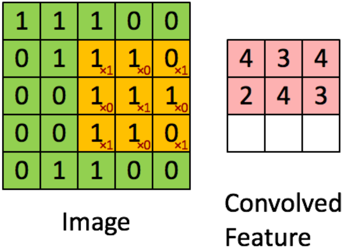

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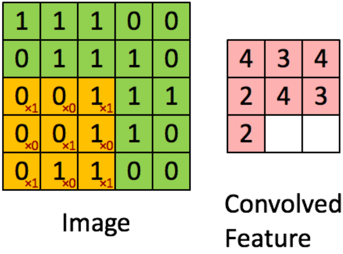

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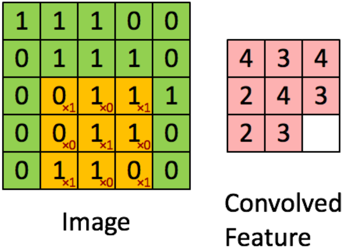

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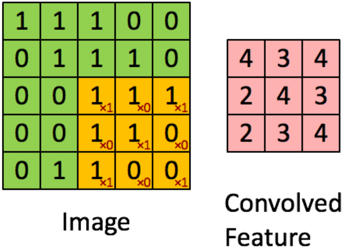
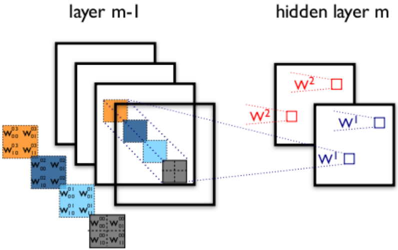


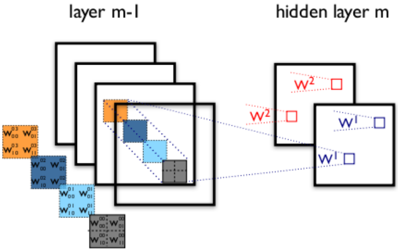
Convolutional networks

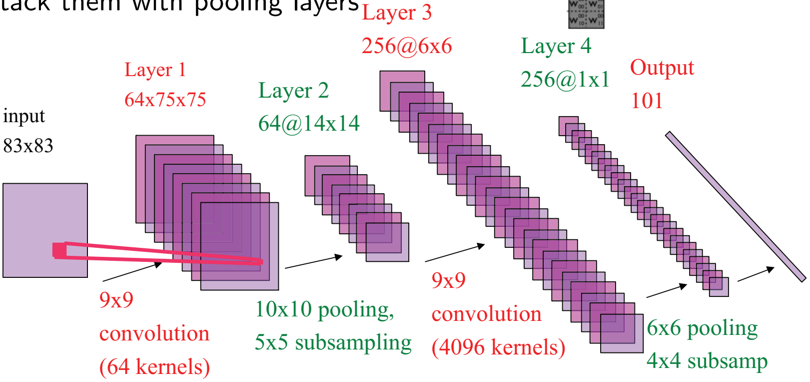
- Images are stationary: can learn feature in one part and apply it in another
- Use e.g. small patch sampled randomly, learn feature, convolve with full image
- Build several “feature maps”



Convolutional networks

- Images are stationary: can learn feature in one part and apply it in another
- Use e.g. small patch sampled randomly, learn feature, convolve with full image
- Build several "feature maps"
- Stack them with pooling layers





Why does unsupervised training work?

Optimisation hypothesis

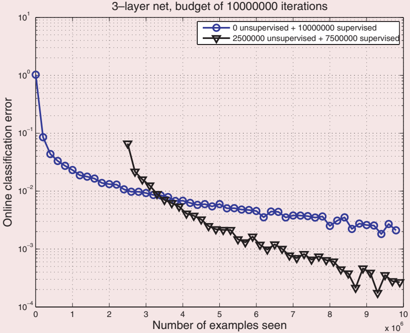
- Training one layer at a time scales well
- Backpropagation from sensible features
- Better local minimum than random initialisation, local search around it

Overfitting/regularisation hypothesis

- More info in inputs than labels
- No need for final discriminant to discover features
- Fine-tuning only at category boundaries

Example

- Stacked denoising auto-encoders
- 10 million handwritten digits
- First 2.5 million used for unsupervised pre-training



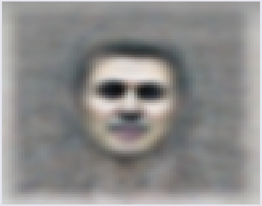
- Worse with supervision: eliminates projections of data not useful for local cost but helpful for deep model cost

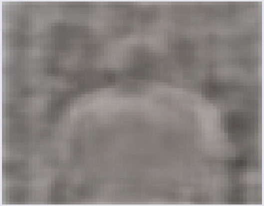
A "giant" neural network

- At Google they trained a 9-layered NN with 1 billion connections
  - trained on 10 million 200×200 pixel images from YouTube videos
  - on 1000 machines (16000 cores) for 3 days, unsupervised learning
- Sounds big? The human brain has 100 billion (10^{11}) neurons and 100 trillion (10^{14}) connections...

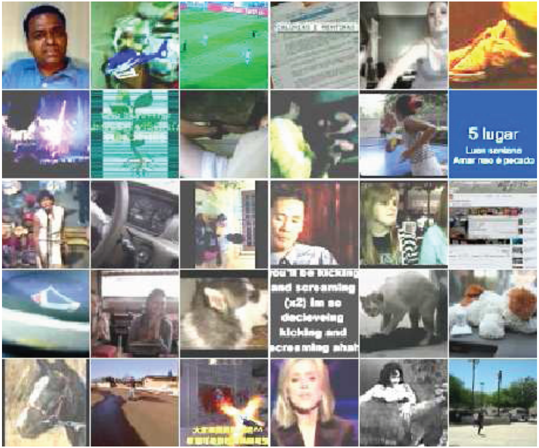
What it did

- It learned to recognise faces, one of the original goals
- ...but also cat faces (among the most popular things in YouTube videos) and body shapes





Google's research on building high-level features



- Features extracted from such images
- Results shown to be robust to
  - colour
  - translation
  - scaling
  - out-of-plane rotation

Deep learning: looking forward

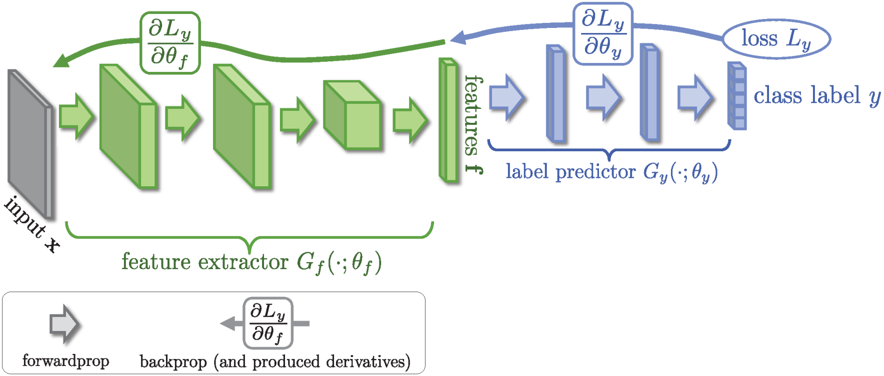
- Very active field of research in machine learning and artificial intelligence
  - not just at universities (Google, Facebook, Microsoft, NVIDIA, etc...)
- Training with curriculum:
  - what humans do over 20 years, or even a lifetime
  - learn different concepts at different times
  - solve easier or smoothed version first, and gradually consider less smoothing
  - exploit previously learned concepts to ease learning of new abstractions
- Influence learning dynamics can have big impact:
  - order and selection of examples matters
  - choose which examples to present first, to guide training and possibly increase learning speed (called shaping in animal training)
- Combination of deep learning and reinforcement learning
  - still in its infancy, but already impressive results
- Domain adaptation and adversarial training
  - e.g. train in parallel network that produces difficult examples
  - learn discrimination (s vs. b) and difference between training and application samples (e.g. Monte Carlo simulation and real data)

Domain adaptation and adversarial training

- Typical training
  - signal and background from simulation
  - results compared to real data to make measurement
- Requires good data–simulation agreement

http://arxiv.org/abs/1409.7495

http://arxiv.org/abs/1505.07818



- Typical training
  - signal and background from simulation
  - results compared to real data to make measurement
- Requires good data–simulation agreement
- Possibility to use adversarial training and domain adaptation to account for discrepancies/systematic uncertainties

http://arxiv.org/abs/1409.7495

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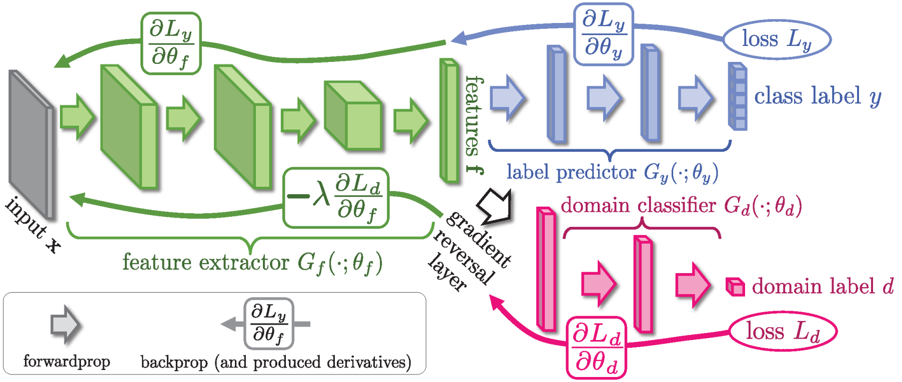


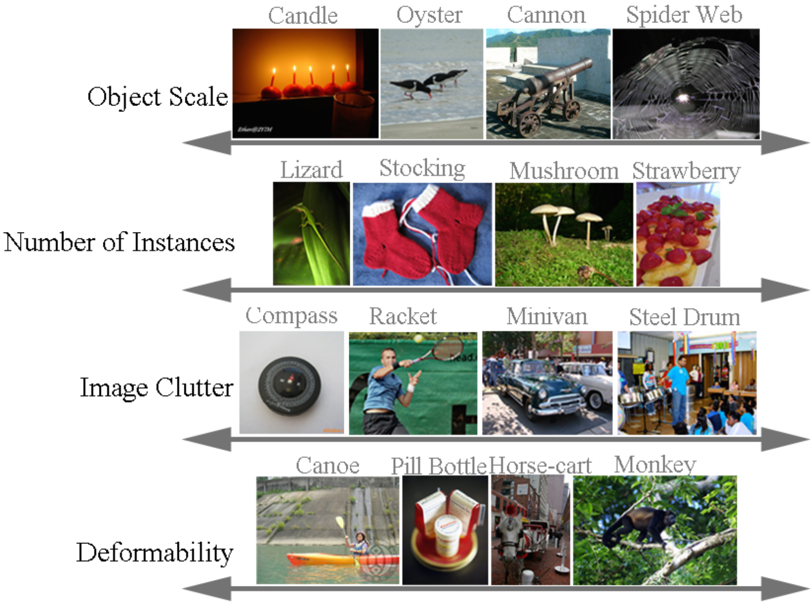
ILSVRC 2014

Summary paper

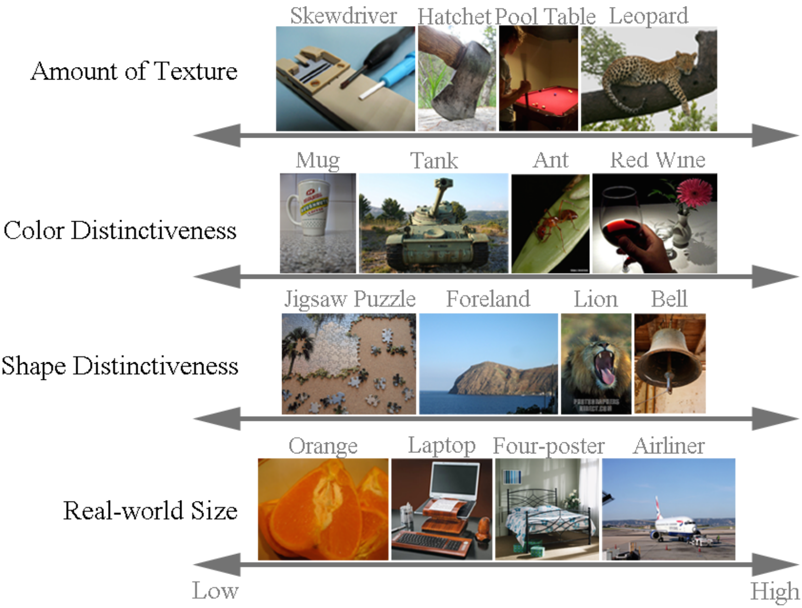
ImageNet Large Scale Visual Recognition Challenge

- ImageNet: database with 14 million images and 20k categories
- Used 1000 categories and about 1.3 million manually annotated images

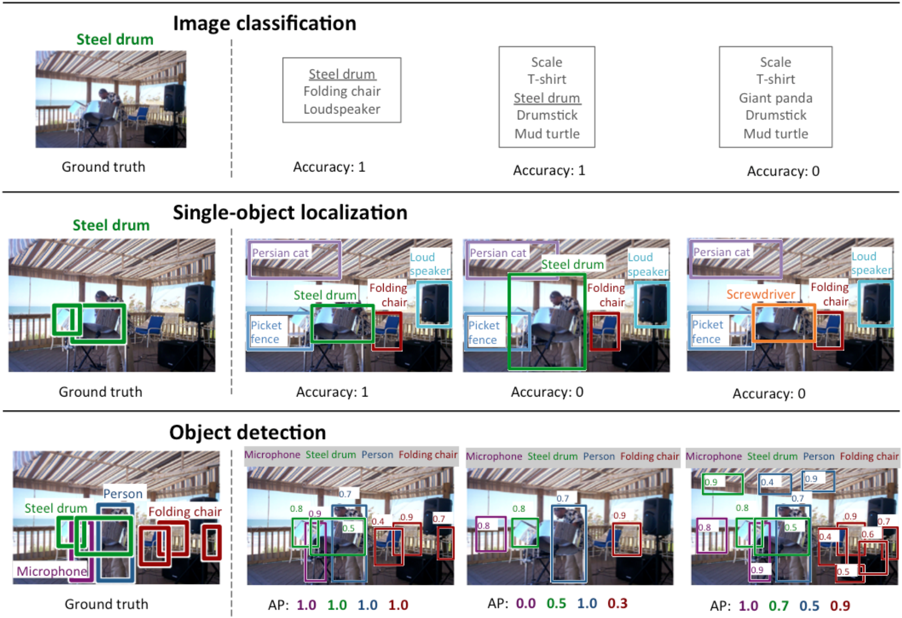
ILSVRC 2014 images



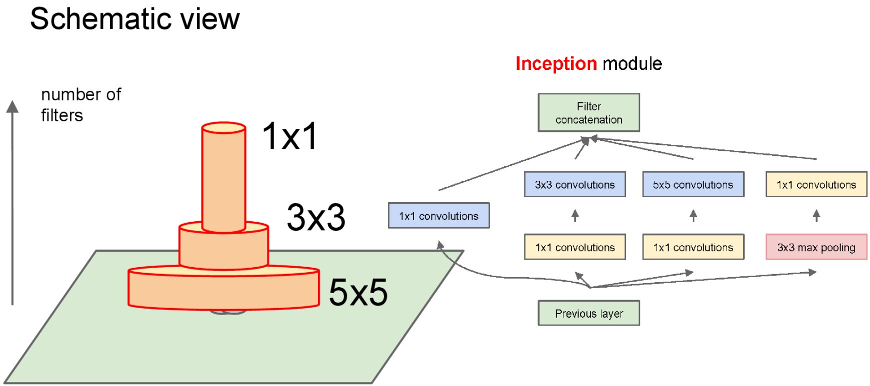
ILSVRC 2014 images



ILSVRC 2014 tasks



- Google of course! (first time)
- GoogLeNet:



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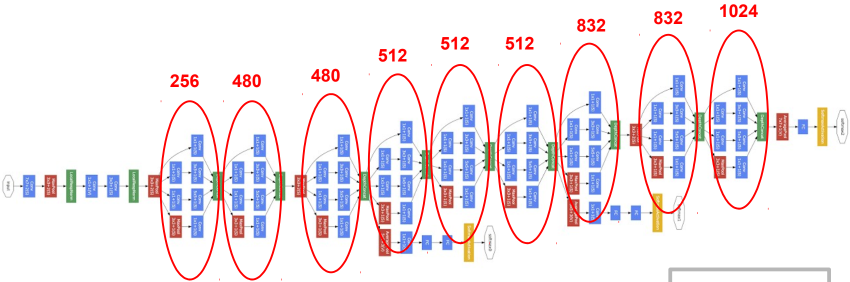


9 **Inception** modules

Network in a network in a network...

Convolution
Pooling
Softmax
Other

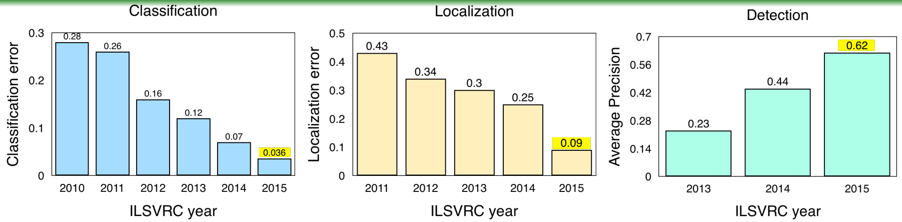
Classification failure cases

Groundtruth: **Police car**

GoogLeNet:

- **laptop**
- **hair drier**
- **binocular**
- **ATM machine**
- **seat belt**

ILSVRC 2010–2016

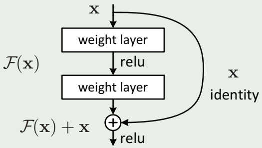


2010–14: 4.2x reduction   1.7x reduction   1.9x increase

ILSVRC 2015 (same dataset as 2014)

▸ arXiv:1512.03385

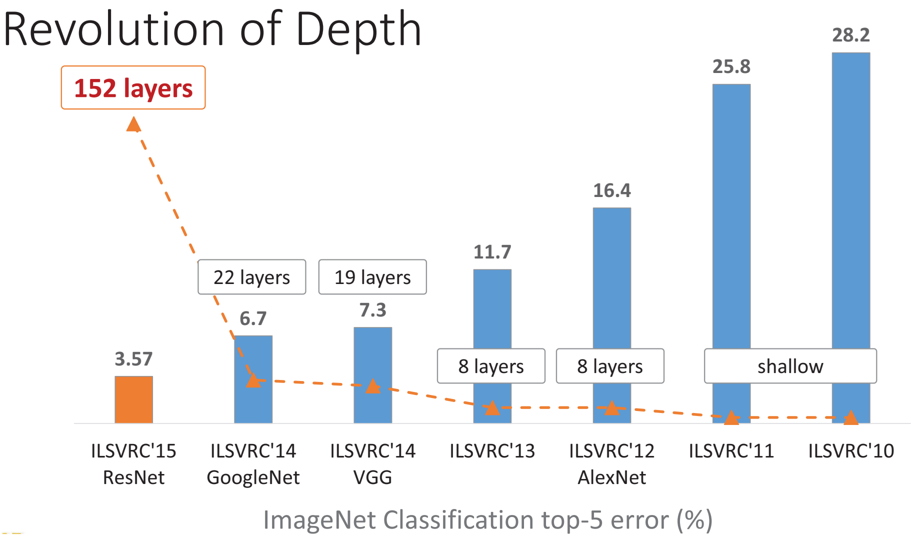
- Winner: MSRA (Microsoft Research in Beijing)
- Deep residual networks with > 150 layers
- Classification error: 6.7% → 3.6% (1.9x)
- Localisation error: 26.7% → 9.0% (2.8x)
- Object detection: 43.9% → 62.1% (1.4x)



ILSVRC 2016

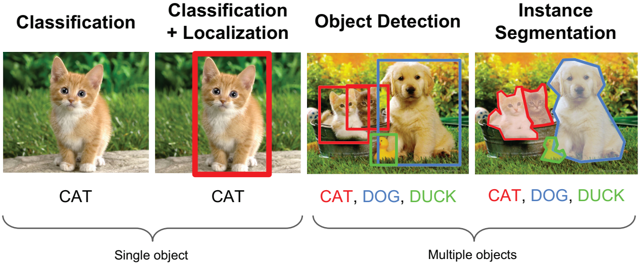
▸ http://image-net.org/challenges/LSVRC/2016

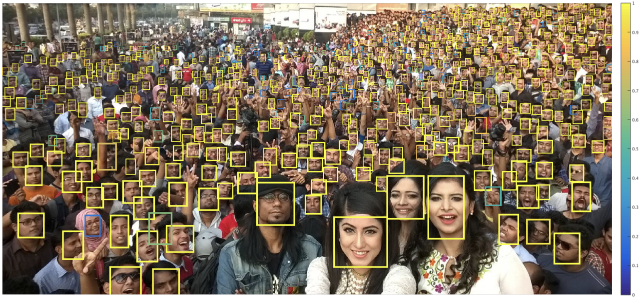
- Mostly ResNets. Classification: 0.030; localisation: 0.08; detection: 0.66


Revolution of Depth
152 layers
22 layers
19 layers
8 layers
8 layers
shallow
3.57
6.7
7.3
11.7
16.4
25.8
28.2
ILSVRC'15 ResNet
ILSVRC'14 GoogleNet
ILSVRC'14 VGG
ILSVRC'13
ILSVRC'12 AlexNet
ILSVRC'11
ILSVRC'10
ImageNet Classification top-5 error (%)

Going further

- More and more refinement (segmentation)
- More objects, in real time on video1/video2/video3



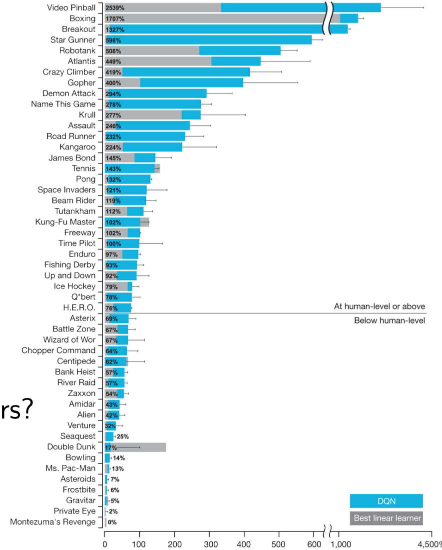


- Learning to play 49 different Atari 2600 games
- No knowledge of the goals/rules, just 84x84 pixel frames
- 60 frames per second, 50 million frames (38 days of game experience)
- Deep convolutional network with reinforcement: DQN (deep Q-network)
    - action-value function $Q^*(s,a) = \max_\pi \mathbb{E}[r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \ldots | s_t = s, a_t = a, \pi]$
    - maximum sum of rewards r_t discounted by γ at each timestep t, achievable by a behaviour policy $\pi = P(a|s)$, after making observation s and taking action a
- Tricks for scalability and performance:
    - experience replay (use past frames)
    - separate network to generate learning targets (iterative update of Q)
- Outperforms all previous algorithms, and professional human player on most games

Google DeepMind: training&performance

Algorithm 1: deep Q-learning with experience replay.

Initialize replay memory D to capacity N
Initialize action-value function Q with random weights θ
Initialize target action-value function $\hat{Q}$ with weights $\theta^- = \theta$
For episode $= 1, M$ **do**
  Initialize sequence $s_1 = \{x_1\}$ and preprocessed sequence $\phi_1 = \phi(s_1)$
  For $t = 1$,T **do**
    With probability ε select a random action a_t
    otherwise select $a_t = \text{argmax}_a Q(\phi(s_t), a; \theta)$
    Execute action a_t in emulator and observe reward r_t and image x_{t+1}
    Set $s_{t+1} = s_t, a_t, x_{t+1}$ and preprocess $\phi_{t+1} = \phi(s_{t+1})$
    Store transition $(\phi_t, a_t, r_t, \phi_{t+1})$ in D
    Sample random minibatch of transitions $(\phi_j, a_j, r_j, \phi_{j+1})$ from D
    Set $y_j = \begin{cases} r_j & \text{if episode terminates at step } j+1 \\ r_j + \gamma \max_{a'} \hat{Q}(\phi_{j+1}, a'; \theta^-) & \text{otherwise} \end{cases}$
    Perform a gradient descent step on $\left(y_j - Q(\phi_j, a_j; \theta)\right)^2$ with respect to the network parameters θ
    Every C steps reset $\hat{Q} = Q$
  End For
End For



- What about Breakout or Space invaders?

Google DeepMind: mastering Go

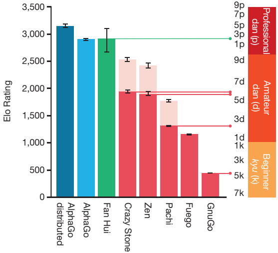
Nature 529, 484 (2016)

- Game of Go considered very challenging for AI
- Board games: can be solved with search tree of b^d possible sequences of moves (b = breadth [number of legal moves], d = depth [length of game])
- Chess: $b \approx 35$, $d \approx 80 \rightarrow$ go: $b \approx 250$, $d \approx 150$
- Reduction:
  - of depth by position evaluation (replace subtree by approximation that predicts outcome)
  - of breadth by sampling actions from probability distribution (policy $p(a|s)$) over possible moves a in position s
- 19×19 image, represented by CNN
- Supervised learning policy network from expert human moves, reinforcement learning policy network on self-play (adjusts policy towards winning the game), value network that predicts winner of games in self-play.

Google DeepMind: AlphaGo

Nature 529, 484 (2016)

- AlphaGo: 40 search threads, simulations on 48 CPUs, policy and value networks on 8 GPUs. Distributed AlphaGo: 1020 CPUs, 176 GPUs
- AlphaGo won 494/495 games against other programs (and still 77% against Crazy Stone with four handicap stones)
  - Fan Hui: 2013/14/15 European champion
  - Distributed AlphaGo won 5–0
  - AlphaGo evaluated thousands of times fewer positions than Deep Blue (first chess computer to bit human world champion) ⇒ better position selection (policy network) and better evaluation (value network)

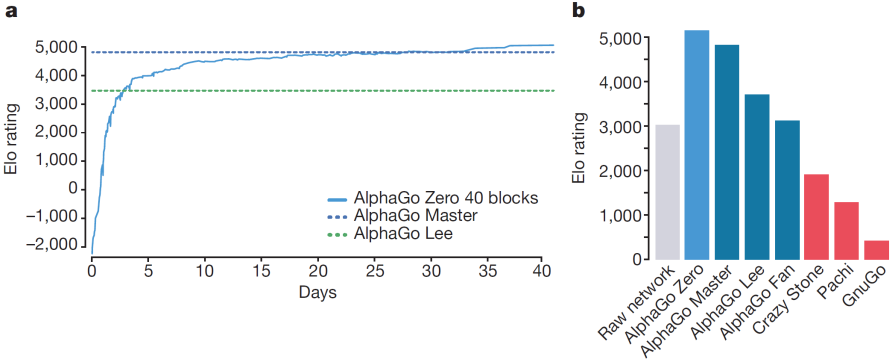


- Then played Lee Sedol (top Go play in the world over last decade) in March 2016 ⇒ won 4–1. AlphaGo given honorary professional ninth dan, considered to have “reach a level ‘close to the territory of divinity’ ”
- Ke Jie (Chinese world #1): “Bring it on!”. Last May 2017: 3–0 win for AlphaGo. New comment: “I feel like his game is more and more like the ‘Go god’. Really, it is brilliant”

DeepMind AlphaGo Zero

Nature 550, 354 (2017)

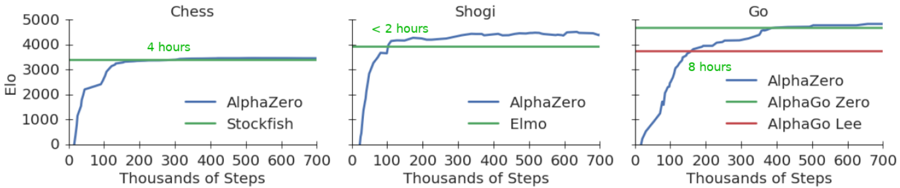
- Learn from scratch, just from the rules and random moves
- Reinforcement learning from self-play, no human data/guidance
- Combined policy and value networks
- 4.9 million self-play games
- Beats AlphaGo Lee (several months of training) after just 36 hours
- Single machine with four TPU



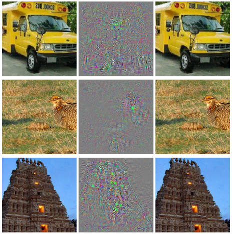
DeepMind AlphaZero

arXiv:1712.01815 [cs.AI]

- Same philosophy as AlphaGo Zero, applied to chess, shogi and go
- Changes:
  - not just win/loss, but also draw or other outcomes
  - no additional training data from game symmetries
  - using always the latest network to generate self-play games rather than best one
  - tree search: 80k/70M for chess AlphaZero/Stockfish, 40k/35M for shogi AlphaZero/Elmo

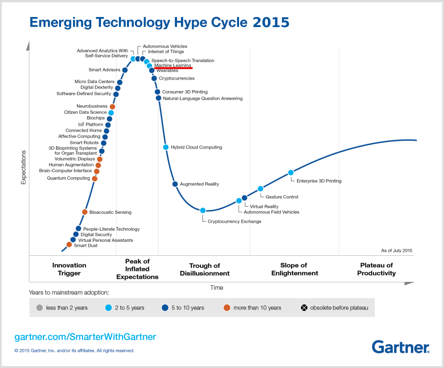


- Playing poker
  - Libratus (AI developed by Carnegie Mellon University) defeated four of the world's best professional poker players (Jan 2017)
  - After 120,000 hands of Heads-up, No-Limit Texas Hold'em, led the pros by a collective $1,766,250 in chips
  - Learnt to bluff, and win with incomplete information and opponents' misinformation
- Lip reading ▸ arXiv:1611.05358 [cs.CV]
  - human professional: deciphers less than 25% of spoken words
  - CNN+LSTM trained on television news programs: 50%
- Limitations ▸ arXiv:1312.6199 [cs.CV]



- left: correctly classified image
- middle: difference between left image and adversarial image (x10)
- right: adversarial image, classified as ostrich

Hype cycle



Emerging Technology Hype Cycle 2015
Expectations
Advanced Analytics With Self-Service Delivery
Autonomous Vehicles
Internet of Things
Speech-to-Speech Translation
Machine Learning
Wearables
Smart Advisors
Cryptocurrencies
Micro Data Centers
Digital Dexterity
Software-Defined Security
Consumer 3D Printing
Natural-Language Question Answering
Neurobusiness
Citizen Data Science
Biochips
IoT Platform
Connected Home
Affective Computing
Smart Robots
3D Bioprinting Systems for Organ Transplant
Volumetric Displays
Human Augmentation
Brain-Computer Interface
Quantum Computing
Hybrid Cloud Computing
Augmented Reality
Enterprise 3D Printing
Gesture Control
Virtual Reality
Autonomous Field Vehicles
Cryptocurrency Exchange
Bioacoustic Sensing
People-Literate Technology
Digital Security
Virtual Personal Assistants
Smart Dust
As of July 2015
Innovation Trigger
Peak of Inflated Expectations
Trough of Disillusionment
Slope of Enlightenment
Plateau of Productivity
Time
Years to mainstream adoption:
less than 2 years
2 to 5 years
5 to 10 years
more than 10 years
obsolete before plateau
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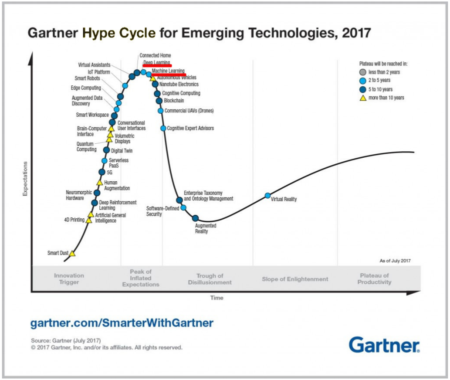

Gartner Hype Cycle for Emerging Technologies, 2017
Expectations
Connected Home
Deep Learning
Machine Learning
Autonomous Vehicles
Nanotube Electronics
Cognitive Computing
Blockchain
Commercial UAVs (Drones)
Cognitive Expert Advisors
Virtual Assistants
IoT Platform
Smart Robots
Edge Computing
Augmented Data Discovery
Smart Workspace
Conversational User Interfaces
Brain-Computer Interface
Volumetric Displays
Quantum Computing
Digital Twin
Serverless PaaS
5G
Human Augmentation
Neuromorphic Hardware
Deep Reinforcement Learning
Artificial General Intelligence
4D Printing
Smart Dust
Enterprise Taxonomy and Ontology Management
Software-Defined Security
Augmented Reality
Virtual Reality
Plateau will be reached in:
less than 2 years
2 to 5 years
5 to 10 years
more than 10 years
As of July 2017
Innovation Trigger
Peak of Inflated Expectations
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Plateau of Productivity
Time
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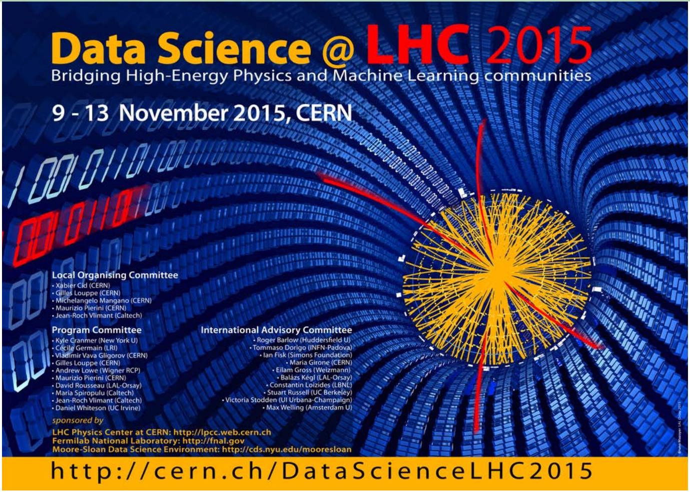
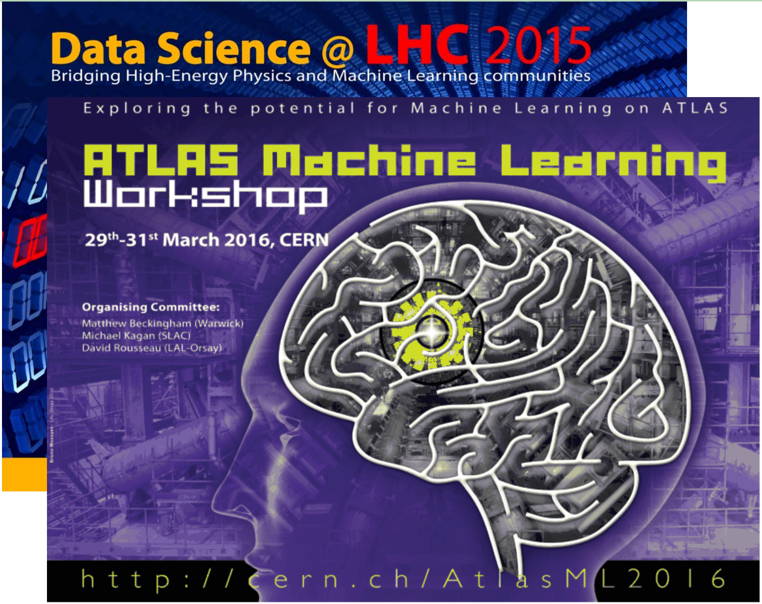
Gartner

Machine learning and particle physics



http://opendata.cern.ch

Machine learning and particle physics



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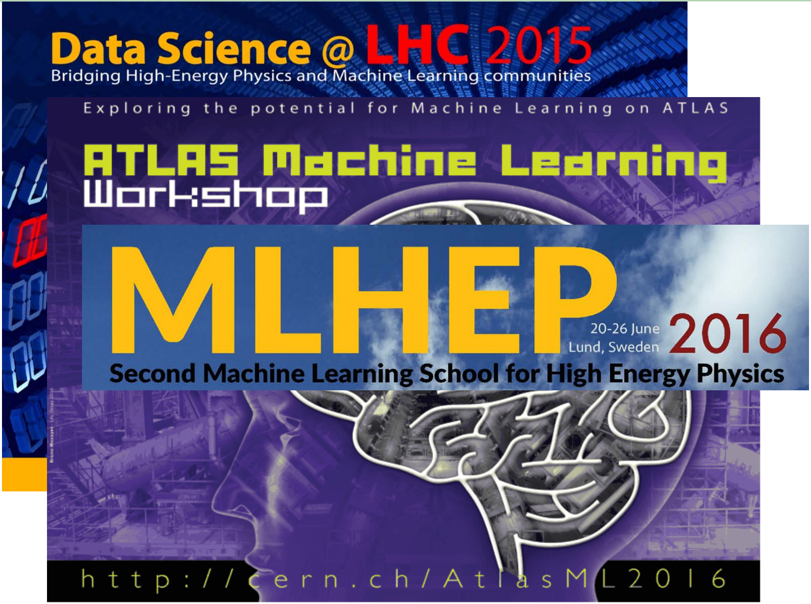
Machine learning and particle physics



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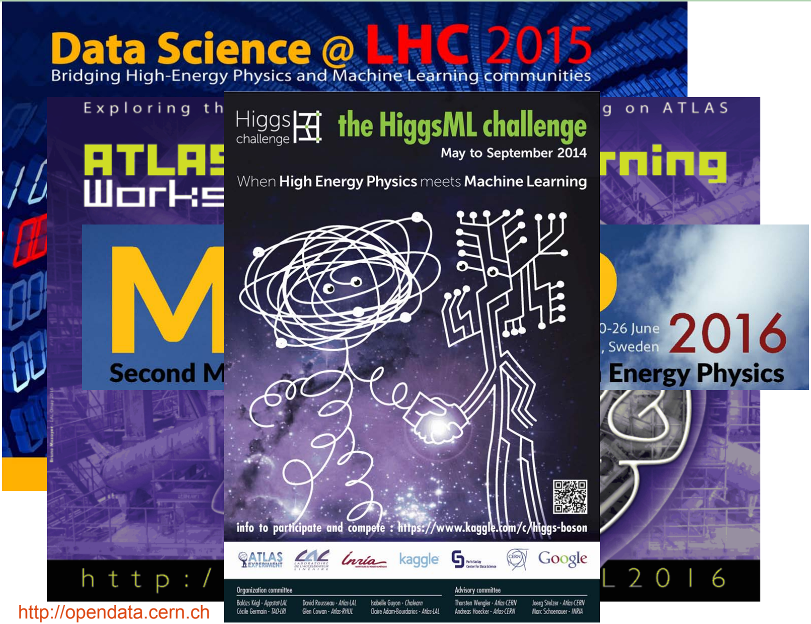
Machine learning and particle physics



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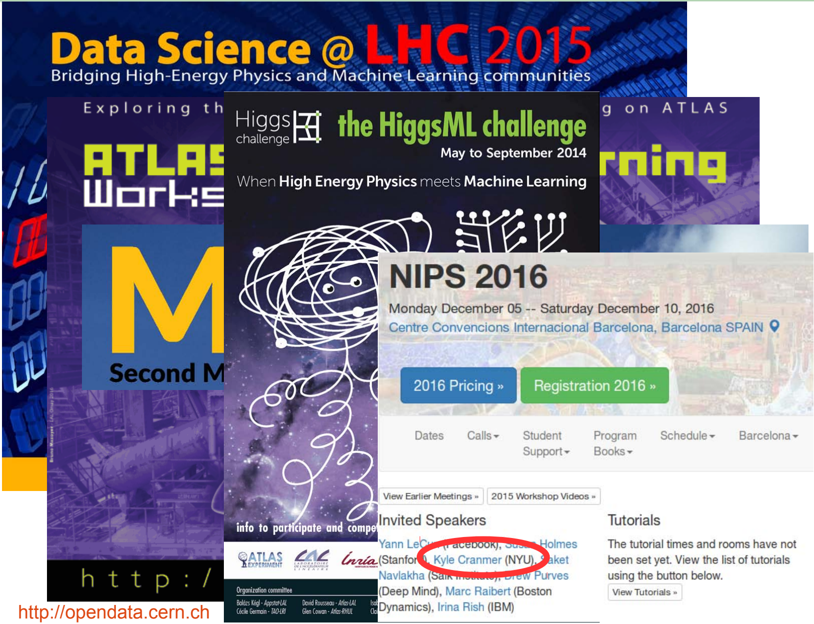


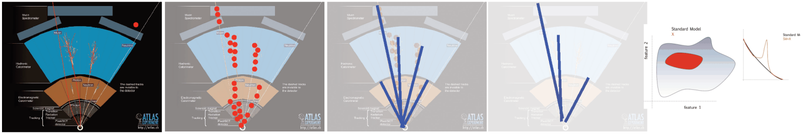
http://opendata.cern.ch

Machine learning and particle physics

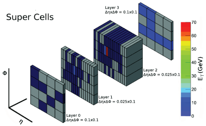
http://opendata.cern.ch

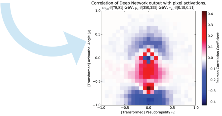
- Going to lower level features ▸ arXiv:1410.3469

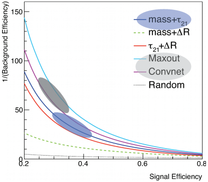
Raw	Sparsified	Reco	Select	Physics	Ana
1e7	1e4	100-ish*	50	10	1



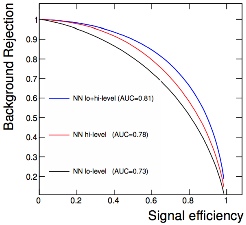
- Transforming inputs into images ▸ arXiv:1511.05190

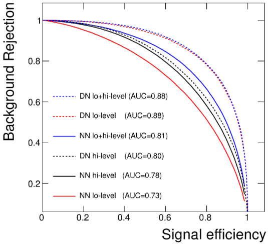






- Going to lower level features [arXiv:1410.3469]





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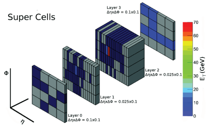
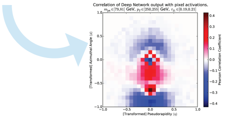
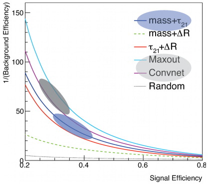






Conclusion

- When trying to achieve optimal discrimination one can try to approximate

$$D(x) = \frac{s(x)}{s(x) + b(x)}$$

- Many techniques and tools exist to achieve this
- (Un)fortunately, no one method can be shown to outperform the others in all cases.
- One should try several and pick the best one for any given problem
- Latest machine learning algorithms (e.g. deep networks) require enormous hyperparameter space optimisation...
- Machine learning and multivariate techniques are at work in your everyday life without your knowning and can easily outsmart you for many tasks

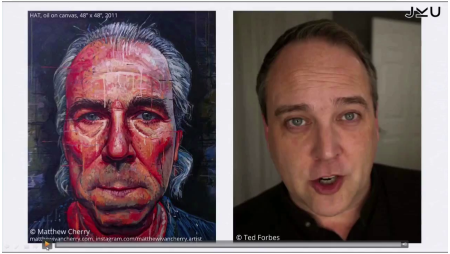
Deep networks and art

- Learning a style ▸ arXiv:1508.06576 [cs.CV] ▸ Neural-style

- Computer dreams ▸ Google original ▸ deepdream

- Face Style ▸ http://facestyle.org

▸ http://dcgi.fel.cvut.cz/home/sykorad/facestyle.html



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Backup

Tree construction parameters

Normalization of signal and background before training

- same total weight for signal and background events ($p = 0.5$, maximal mixing)

Selection of splits

- list of questions ($variable_i < cut_i$?, "Is the sky blue or overcast?")
- goodness of split (separation measure)

Decision to stop splitting (declare a node terminal)

- minimum leaf size (for statistical significance, e.g. 100 events)
- insufficient improvement from further splitting
- perfect classification (all events in leaf belong to same class)
- maximal tree depth (like-size trees choice or computing concerns)

Assignment of terminal node to a class

- signal leaf if purity > 0.5, background otherwise

Splitting a node

Impurity measure i(t)

- maximal for equal mix of signal and background
- symmetric in p_{signal} and $p_{background}$
- minimal for node with either signal only or background only
- strictly concave $\Rightarrow$ reward purer nodes (favours end cuts with one smaller node and one larger node)

Optimal split: figure of merit

- Decrease of impurity for split s of node t into children t_P and t_F (goodness of split): $\Delta i(s,t) = i(t) - p_P \cdot i(t_P) - p_F \cdot i(t_F)$
- Aim: find split s^* such that:

$$\Delta i(s^*,t) = \max_{s \in \{\text{splits}\}} \Delta i(s,t)$$

Stopping condition

- See previous slide
- When not enough improvement ($\Delta i(s^*,t) < \beta$)
- Careful with early-stopping conditions

- Maximising $\Delta i(s,t) \equiv$ minimizing overall tree impurity

Splitting a node: examples

Node purity

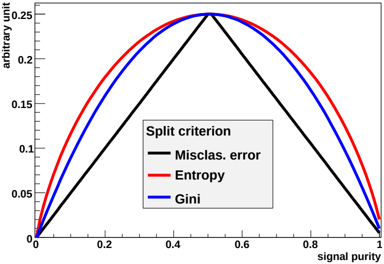
- Signal (background) event i with weight w_s^i (w_b^i)

$$p = \frac{\sum_{i \in signal} w_s^i}{\sum_{i \in signal} w_s^i + \sum_{j \in bkg} w_b^j}$$

- Signal purity (= purity)
  $p_s = p = \frac{s}{s+b}$
- Background purity
  $p_b = \frac{b}{s+b} = 1 - p_s = 1 - p$

Common impurity functions

- misclassification error
  $= 1 - max(p, 1-p)$
- (cross) entropy
  $= -\sum_{i=s,b} p_i \log p_i$
- Gini index



- Also cross section ($-\frac{s^2}{s+b}$) and excess significance ($-\frac{s^2}{b}$)

Splitting a node: Gini index of diversity

Defined for many classes

- $\text{Gini} = \sum_{i,j \in \{\text{classes}\}}^{i \neq j} p_i p_j$

Statistical interpretation

- Assign random object to class i with probability p_i.
- Probability that it is actually in class j is p_j
- $\Rightarrow$ Gini = probability of misclassification

For two classes (signal and background)

- $i = s, b$ and $p_s = p = 1 - p_b$
- $\Rightarrow \text{Gini} = 1 - \sum_{i=s,b} p_i^2 = 2p(1-p) = \frac{2sb}{(s+b)^2}$
- Most popular in DT implementations
- Usually similar performance to e.g. entropy

Variable selection I

Reminder

- Need model giving good description of data

Variable selection I

Reminder

- Need model giving good description of data

Playing with variables

- Number of variables:
  - not affected too much by "curse of dimensionality"
  - CPU consumption scales as $nN \log N$ with n variables and N training events
- Insensitive to duplicate variables (give same ordering $\Rightarrow$ same DT)
- Variable order does not matter: all variables treated equal
- Order of training events is irrelevant (batch training)
- Irrelevant variables:
  - no discriminative power $\Rightarrow$ not used
  - only costs a little CPU time, no added noise
- Can use continuous and discrete variables, simultaneously

Variable selection II

Transforming input variables

- Completely insensitive to the replacement of any subset of input variables by (possibly different) arbitrary strictly monotone functions of them:
  - let $f : x_i \rightarrow f(x_i)$ be strictly monotone
  - if $x > y$ then $f(x) > f(y)$
  - ordering of events by x_i is the same as by $f(x_i)$
  - $\Rightarrow$ produces the same DT
- Examples:
  - convert MeV $\rightarrow$ GeV
  - no need to make all variables fit in the same range
  - no need to regularise variables (e.g. taking the log)
- $\Rightarrow$ Some immunity against outliers

Variable selection II

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Note about actual implementation

- The above is strictly true only if testing all possible cut values
- If there is some computational optimisation (e.g., check only 20 possible cuts on each variable), it may not work anymore.

Pruning a tree II

Pre-pruning

- Stop tree growth during building phase
- Already seen: minimum leaf size, minimum separation improvement, maximum depth, etc.
- Careful: early stopping condition may prevent from discovering further useful splitting

Expected error pruning

- Grow full tree
- When result from children not significantly different from result of parent, prune children
- Can measure statistical error estimate with binomial error $\sqrt{p(1-p)/N}$ for node with purity p and N training events
- No need for testing sample
- Known to be "too aggressive"

Pruning a tree III: cost-complexity pruning

- Idea: penalise "complex" trees (many nodes/leaves) and find compromise between good fit to training data (larger tree) and good generalisation properties (smaller tree)
- With misclassification rate $R(T)$ of subtree T (with N_T nodes) of fully grown tree T_{max}:

$$\text{cost complexity } R_\alpha(T) = R(T) + \alpha N_T$$

$\alpha =$ complexity parameter

- Minimise $R_\alpha(T)$:
  - small α: pick T_{max}
  - large α: keep root node only, T_{max} fully pruned
- First-pass pruning, for terminal nodes t_L, t_R from split of t:
  - by construction $R(t) \geq R(t_L) + R(t_R)$
  - if $R(t) = R(t_L) + R(t_R)$ prune off t_L and t_R

Pruning a tree IV: cost-complexity pruning

- For node t and subtree T_t:
  - if t non-terminal, $R(t) > R(T_t)$ by construction
  - $R_\alpha(\{t\}) = R_\alpha(t) = R(t) + \alpha \; (N_T = 1)$
  - if $R_\alpha(T_t) < R_\alpha(t)$ then branch has smaller cost-complexity than single node and should be kept
  - at critical $\alpha = \rho_t$, node is preferable
  - to find ρ_t, solve $R_{\rho_t}(T_t) = R_{\rho_t}(t)$, or: $\rho_t = \dfrac{R(t) - R(T_t)}{N_T - 1}$
  - node with smallest ρ_t is *weakest link* and gets pruned
  - apply recursively till you get to the root node
- This generates sequence of decreasing cost-complexity subtrees
- Compute their true misclassification rate on validation sample:
  - will first decrease with cost-complexity
  - then goes through a minimum and increases again
  - pick this tree at the minimum as the best pruned tree

Note: best pruned tree may not be optimal in a forest

AdaBoost algorithm

- Check which events of training sample $\mathbb{T}_k$ are misclassified by T_k:
  - $\mathbb{I}(X) = 1$ if X is true, 0 otherwise
  - for DT output in $\{\pm 1\}$: $\text{isMisclassified}_k(i) = \mathbb{I}\big(y_i \times T_k(x_i) \leq 0\big)$
  - or $\text{isMisclassified}_k(i) = \mathbb{I}\big(y_i \times (T_k(x_i) - 0.5) \leq 0\big)$ in purity convention
  - misclassification rate:

$$R(T_k) = \varepsilon_k = \frac{\sum_{i=1}^{N} w_i^k \times \text{isMisclassified}_k(i)}{\sum_{i=1}^{N} w_i^k}$$

- Derive tree weight $\alpha_k = \beta \times \ln((1 - \varepsilon_k)/\varepsilon_k)$
- Increase weight of misclassified events in $\mathbb{T}_k$ to create $\mathbb{T}_{k+1}$:

$$w_i^k \to w_i^{k+1} = w_i^k \times e^{\alpha_k}$$

- Train T_{k+1} on $\mathbb{T}_{k+1}$
- Boosted result of event i:

$$T(i) = \frac{1}{\sum_{k=1}^{N_{\text{tree}}} \alpha_k} \sum_{k=1}^{N_{\text{tree}}} \alpha_k T_k(i)$$

AdaBoost by example

- Assume $\beta = 1$

Not-so-good classifier

- Assume error rate $\varepsilon = 40\%$
- Then $\alpha = \ln \frac{1-0.4}{0.4} = 0.4$
- Misclassified events get their weight multiplied by $e^{0.4}$=1.5
- $\Rightarrow$ next tree will have to work a bit harder on these events

Good classifier

- Error rate $\varepsilon = 5\%$
- Then $\alpha = \ln \frac{1-0.05}{0.05} = 2.9$
- Misclassified events get their weight multiplied by $e^{2.9}$=19 (!!)
- $\Rightarrow$ being failed by a good classifier means a big penalty:
  - must be a difficult case
  - next tree will have to pay much more attention to this event and try to get it right

AdaBoost error rate

Misclassification rate ε on training sample

- Can be shown to be bound:
$$\varepsilon \leq \prod_{k=1}^{N_{tree}} 2\sqrt{\varepsilon_k(1-\varepsilon_k)}$$
- If each tree has $\varepsilon_k \neq 0.5$ (i.e. better than random guessing):

  the error rate falls to zero for sufficiently large N_{tree}

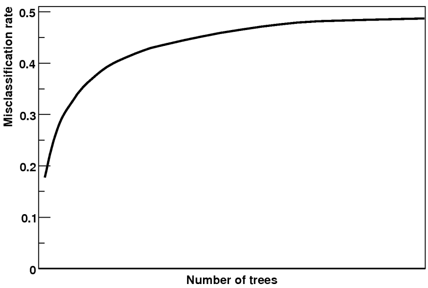
- Corollary: training data is over fitted

Overtraining?

- Error rate on test sample may reach a minimum and then potentially rise. Stop boosting at the minimum.
- In principle AdaBoost *must* overfit training sample
- In many cases in literature, no loss of performance due to overtraining
  - may have to do with fact that successive trees get in general smaller and smaller weights
  - trees that lead to overtraining contribute very little to final DT output on validation sample

Clues to boosting performance

Misclassification rate for each tree



Tree weight α_k