Machine learning

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CENTRE DE PHYSIQUE DES PARTICULES DE MARSEILLE CPPM

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Outline

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2. **Optimal discrimination**
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   - Multivariate discriminant
3. **Machine learning**
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4. **Multivariate discriminants**
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   - Genetic algorithms
   - Quadratic and linear discriminants
   - Support vector machines
   - Kernel density estimation
   - Neural networks
   - Bayesian neural networks
   - Deep networks
   - Decision trees
5. **Conclusion**

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

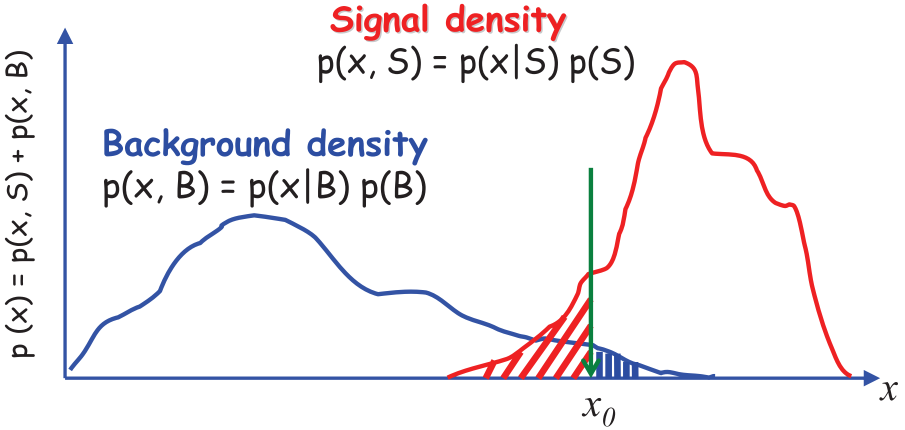
- Kinematic variables (masses, momenta, decay angles, ...)
- Event properties (jet multiplicity, sum of charges, brightness ...)
- Event shape (sphericity, aplanarity, ...)
- Detector response (silicon hits, dE/dx, Cherenkov angle, shower profiles, muon hits, ...)

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

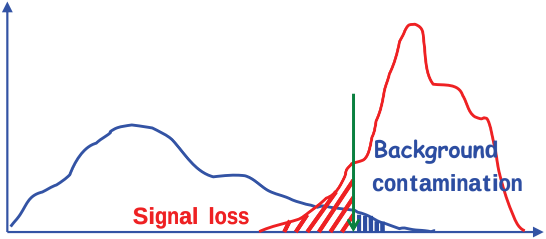
- Where to place a cut x_0 on variable x?



- 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:

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

- 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

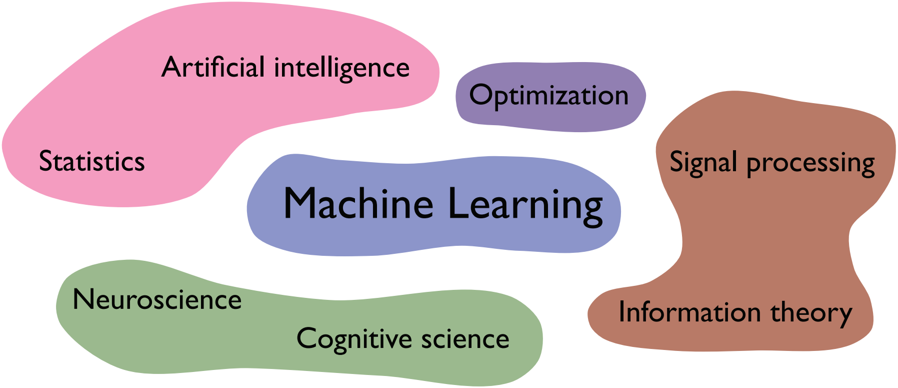
Several types of problems

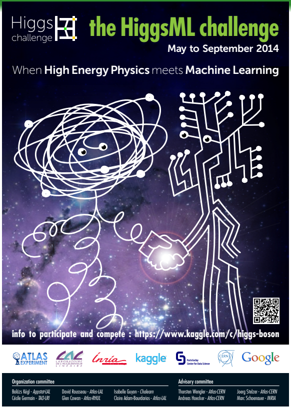
- Classification/decision:
  - signal or background
  - type Ia supernova or not
  - will pay his/her credit back on time or not
- Regression (mostly ignored in these lectures)
- Clustering (cluster analysis):
  - in exploratory data mining, finding features

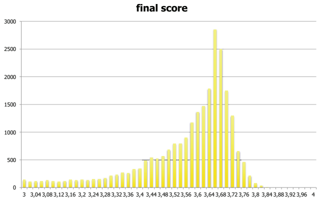
Our goal

- 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







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 $(x, y)_1, (x, y)_2, \dots, (x, y)_N$ 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 $\mathbf{y = f(x)}$

- 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:

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

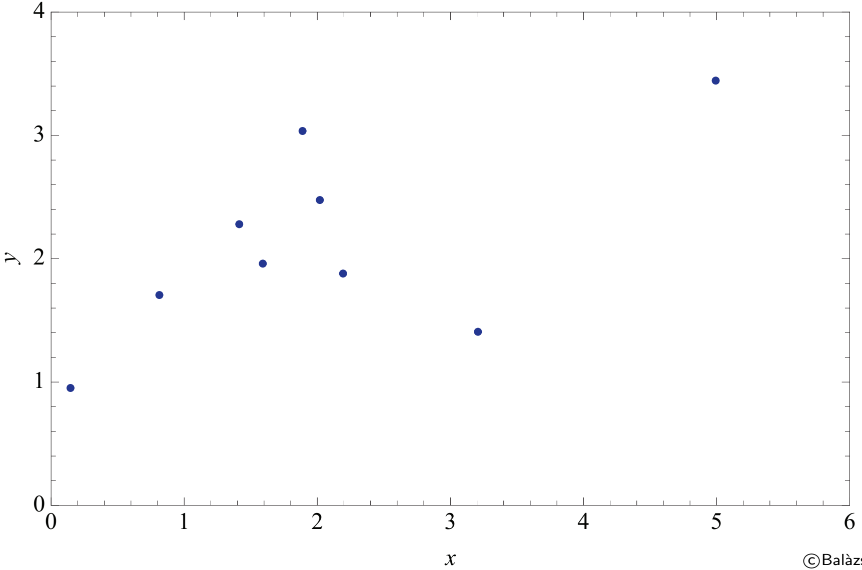
subject to constraint $Q(w)$, so we minimise the cost function:

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

- 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



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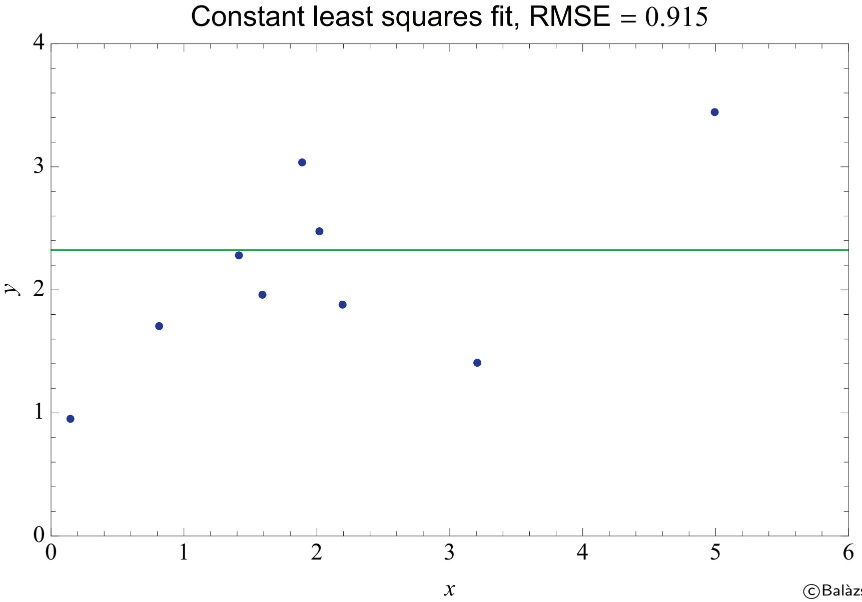

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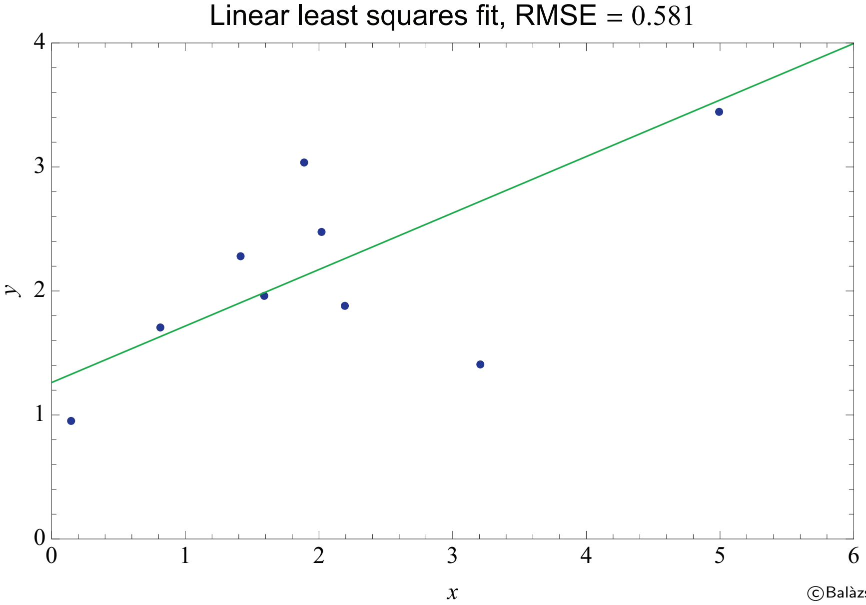

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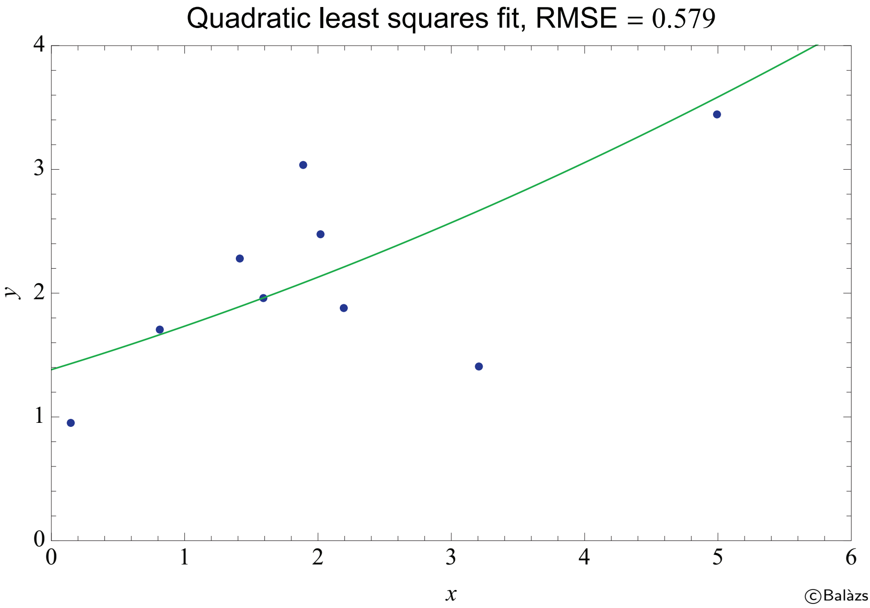

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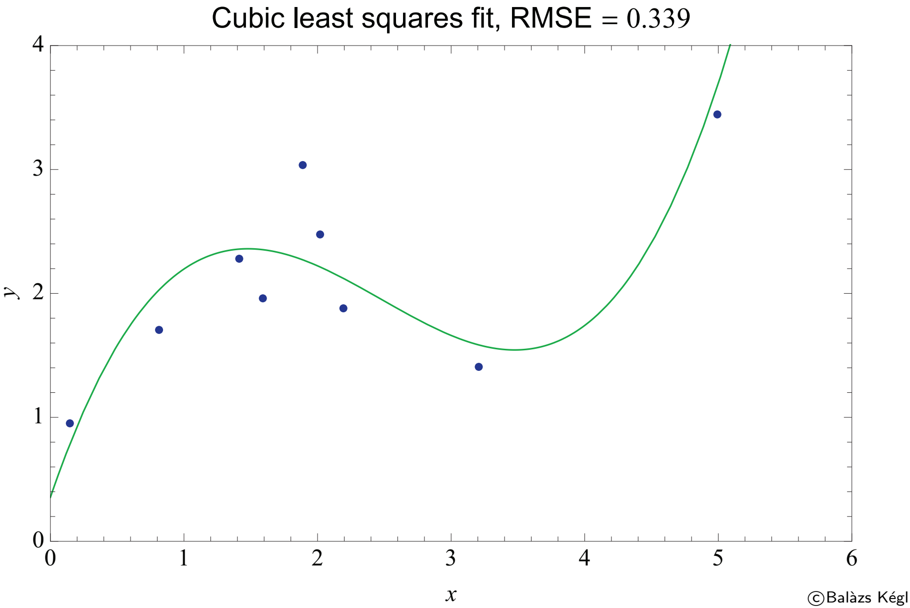
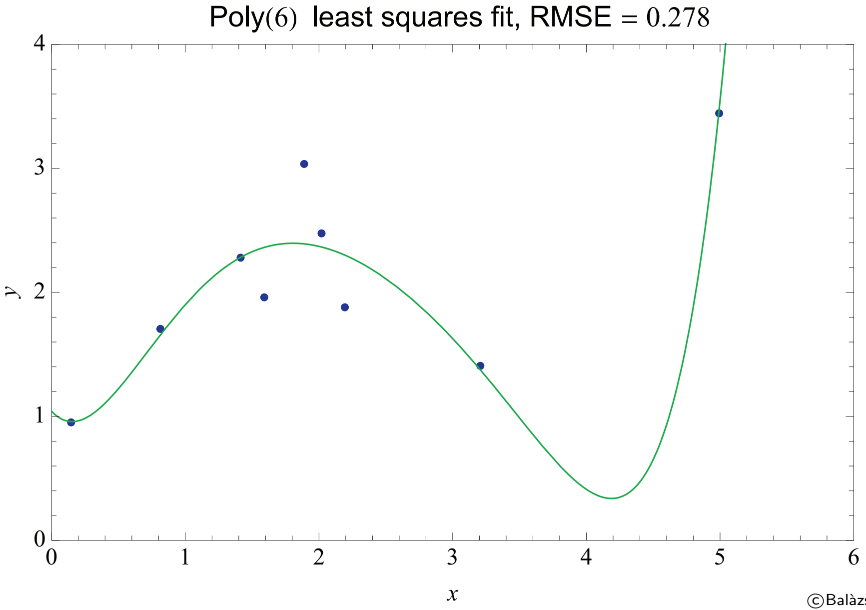


Choice of function class: training



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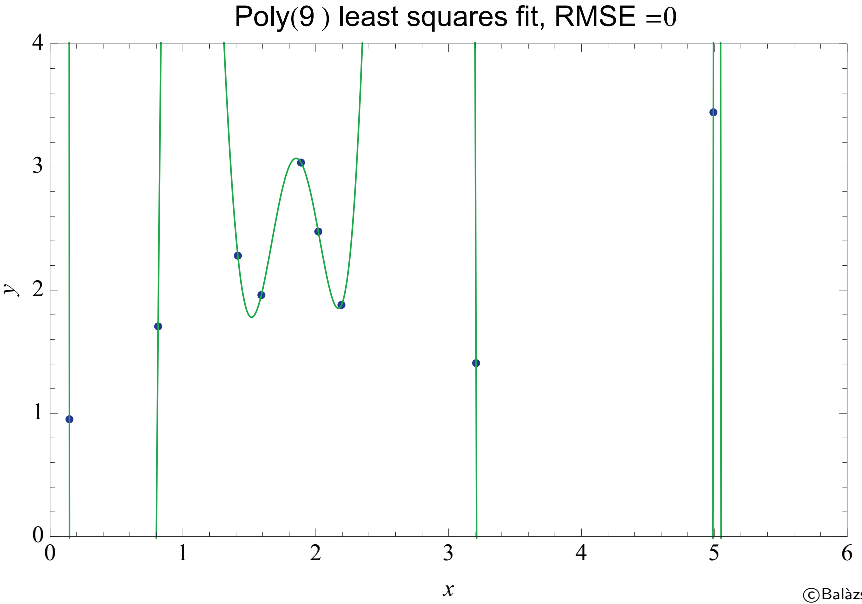
Choice of function class: training



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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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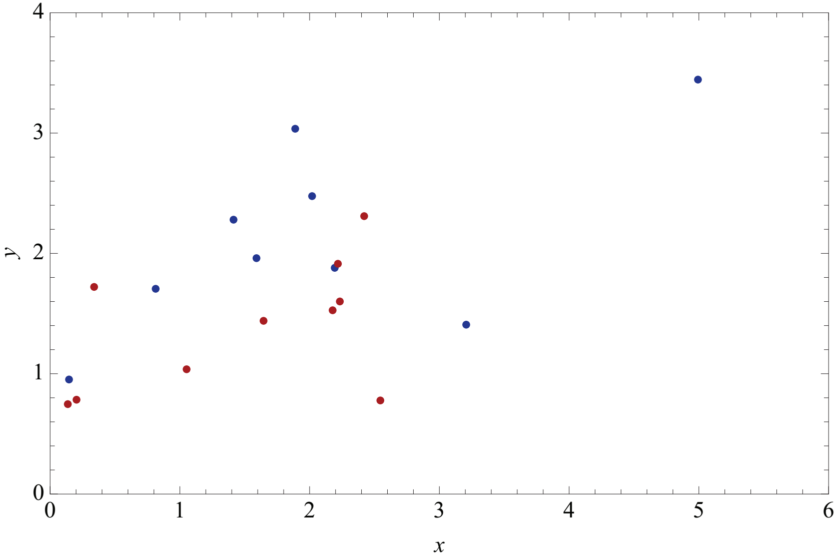
- ... not impossible, but not very common...

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

Data generated from an unknown function with unknown noise



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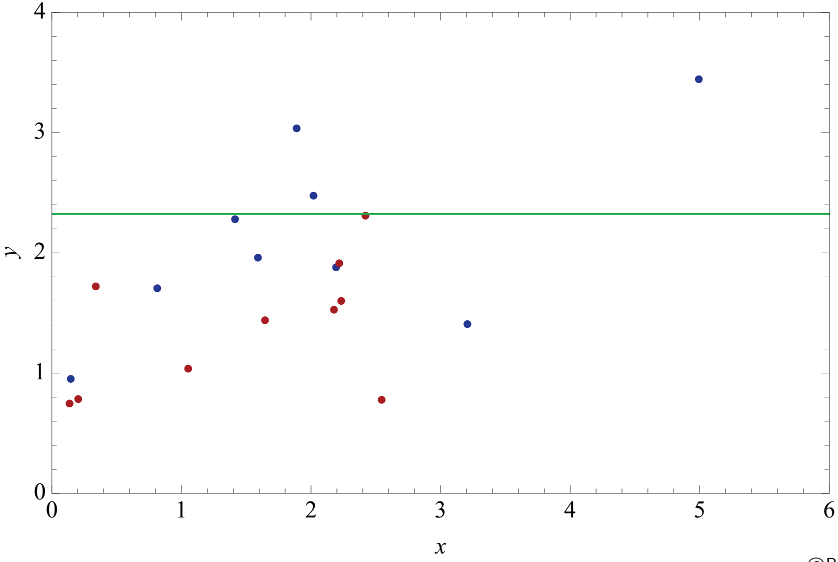
Choice of function class: testing

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



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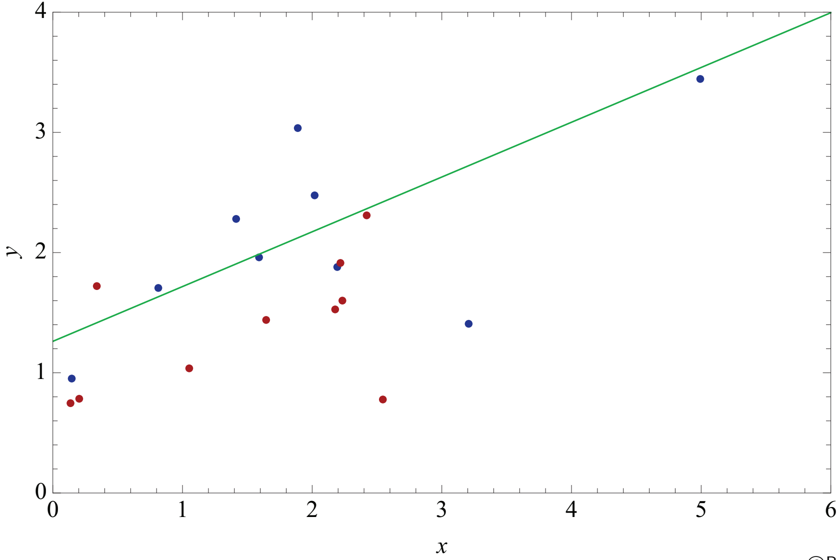
Choice of function class: testing

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



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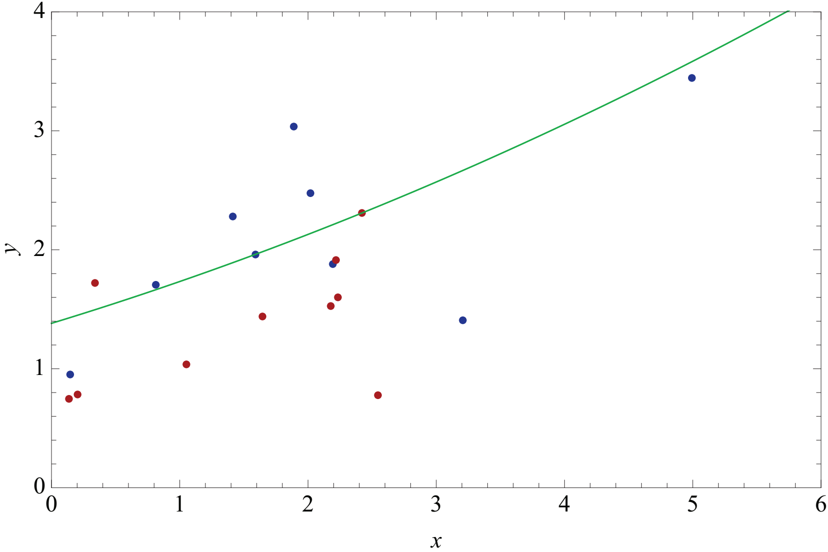
Choice of function class: testing

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



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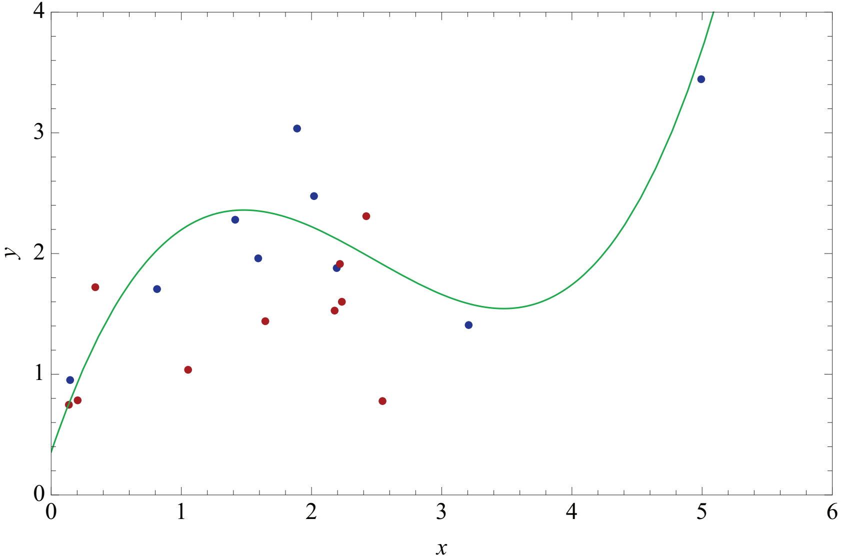
Choice of function class: testing

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



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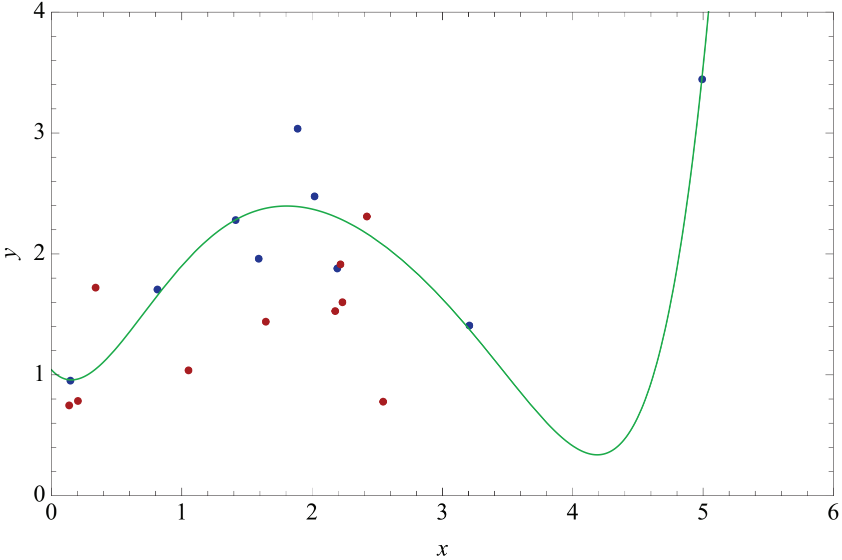
Choice of function class: testing

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



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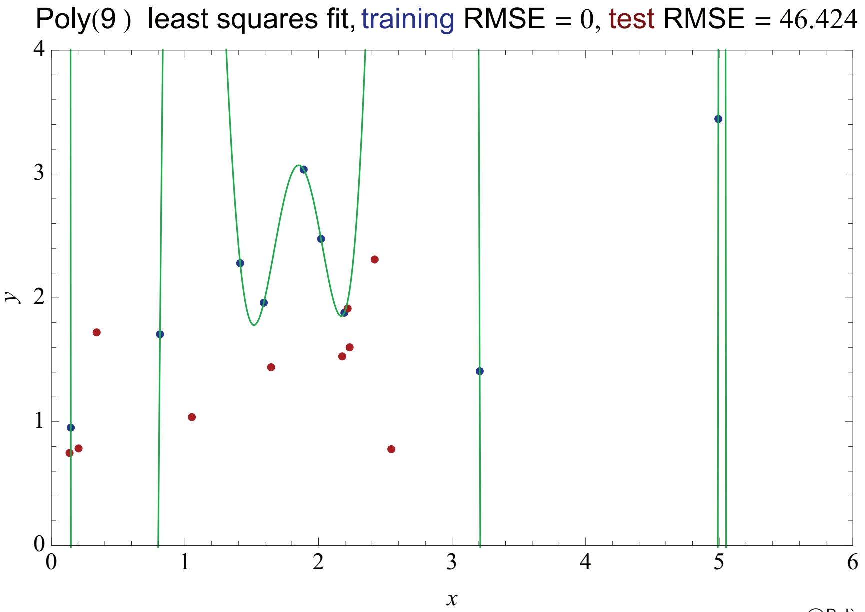
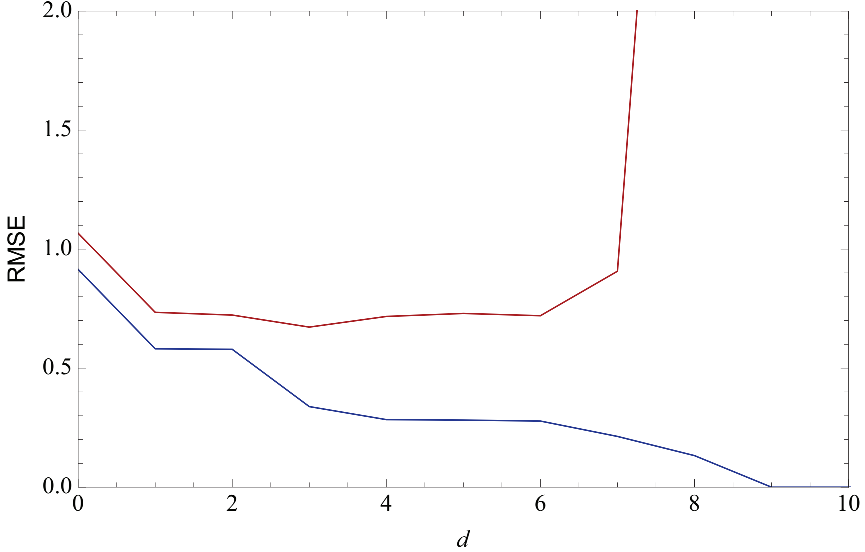
Choice of function class: testing



Choice of function class

Training and test RMSE's for polynomial fits of different degrees



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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

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?

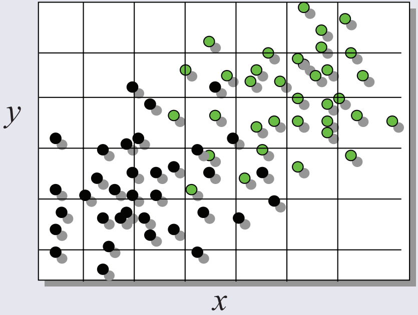
- Best possible choice: cannot beat Bayes limit (but usually impossible to define)
- No single method can be proven to surpass all others in particular case
- Advisable to try several and use the best one

Cut-based analysis and grid search

Cut-based analysis

- Simple approach: cut on each discriminating variable
- Difficulty: how to optimise the cuts?

Grid search



- Split each variable in K values
- Apply cuts at each grid point: $x > x_i$, $y > y_i$
- Number of points scales with K^n: curse of dimensionality

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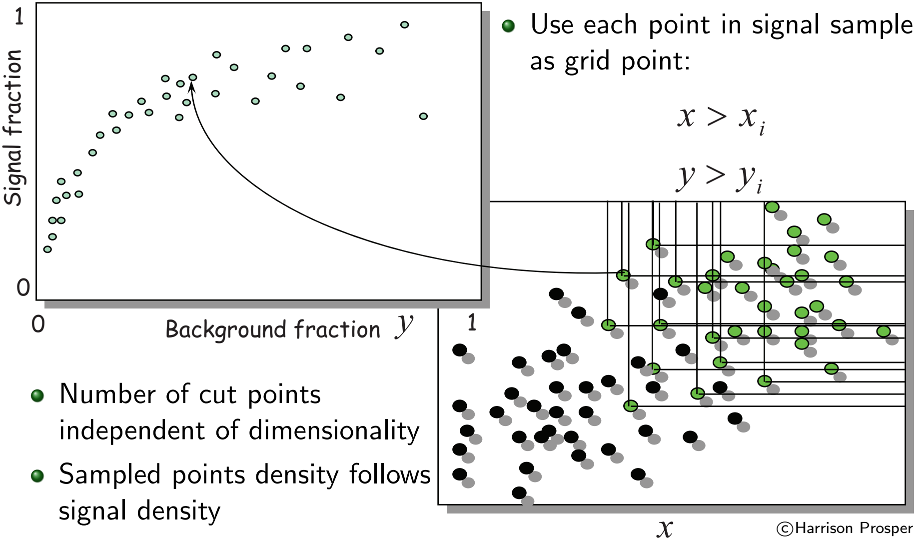
Random grid search



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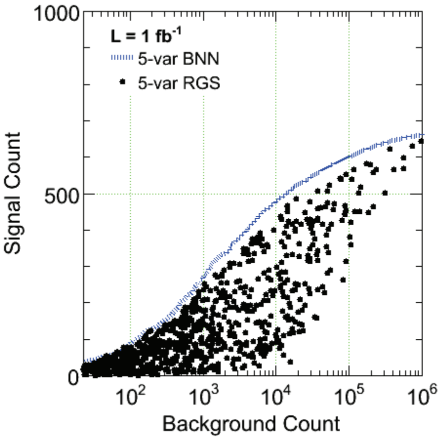
- Use each point in signal sample as grid point:

$$x > x_i$$

$$y > y_i$$

- Number of cut points independent of dimensionality
- Sampled points density follows signal density

Random grid search example



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Comparison to BNN

- Blue: 5-dim Bayesian neural network discriminant (see later)
- Points: each cut point from a 5-dim RGS calculation
- Conclusions:
  - RGS can find very good criteria with high discrimination
  - but it usually cannot compete with a full-blown multivariate discriminant
  - and never outsmarts it

Genetic algorithms: survival of the fittest

- Inspired by biological evolution
- Model: group (population) of abstract representations (genome/discriminating variables) of possible solutions (individuals/list of cuts)
- Typical processes at work in evolutionary processes:
  - inheritance
  - mutation
  - sexual recombination (a.k.a. crossover)
- Fitness function: value representing the individual's goodness, or comparison of two individuals
- For cut optimisation:
  - good background rejection and high signal efficiency
  - compare individuals in each signal efficiency bin and keep those with higher background rejection

Genetic algorithms

- Better solutions more likely to be selected for mating and mutations, carrying their genetic code (cuts) from generation to generation
- Algorithm:
  1. Create initial random population (cut ensemble)
  2. Select fittest individuals
  3. Create offsprings through crossover (mix best cuts)
  4. Mutate randomly (change some cuts of some individuals)
  5. Repeat from 2 until convergence (or fixed number of generations)
- Good fitness at one generation $\Rightarrow$ average fitness in the next
- Algorithm focuses on region with higher potential improvement

Quadratic discriminants: Gaussian problem

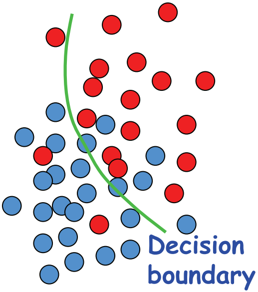
- Suppose densities $s(x)$ and $b(x)$ are multivariate Gaussians:

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

  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:

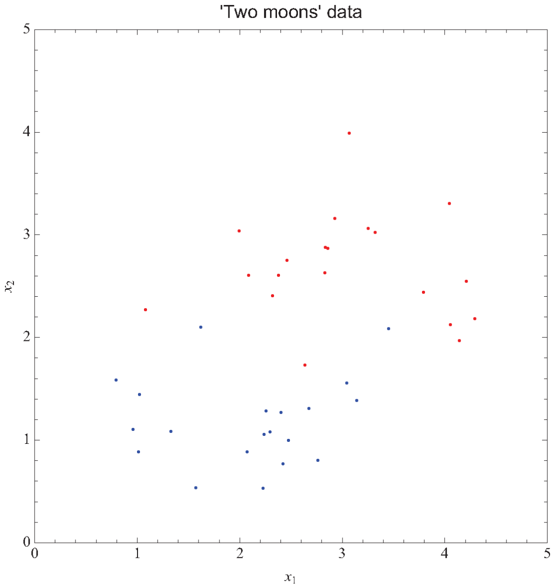
$$\ln B(x) = \lambda(x) \equiv \chi^2(\mu_B, \Sigma_B) - \chi^2(\mu_S, \Sigma_S)$$



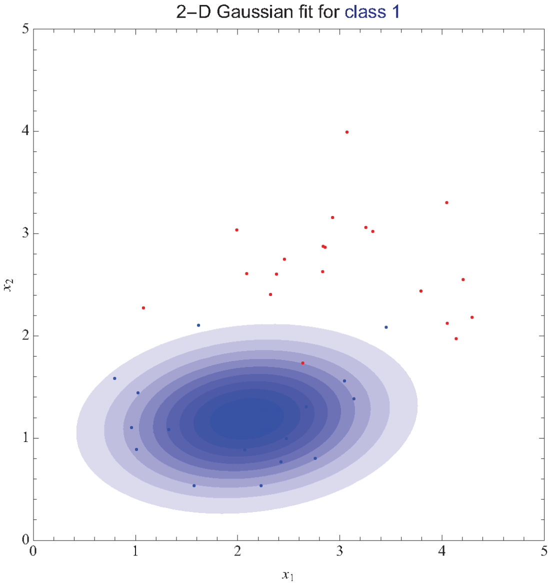
with $\chi^2(\mu, \Sigma) = (x-\mu)^T\Sigma^{-1}(x-\mu)$

- 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



Quadratic discriminant



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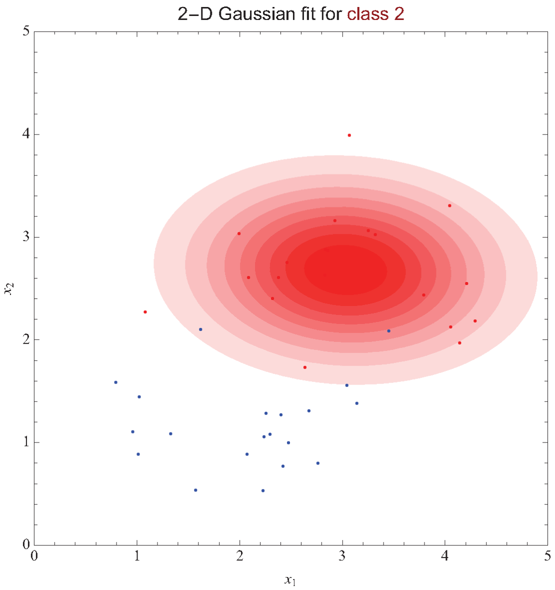
Quadratic discriminant



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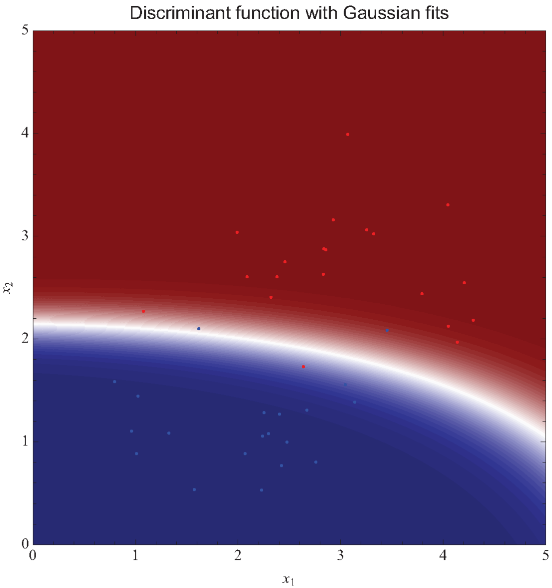
Quadratic discriminant



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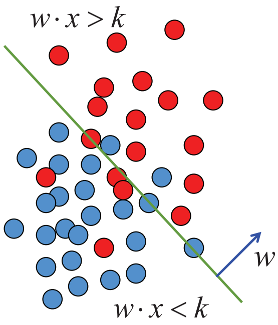
Linear discriminant: Fisher's discriminant

- 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:

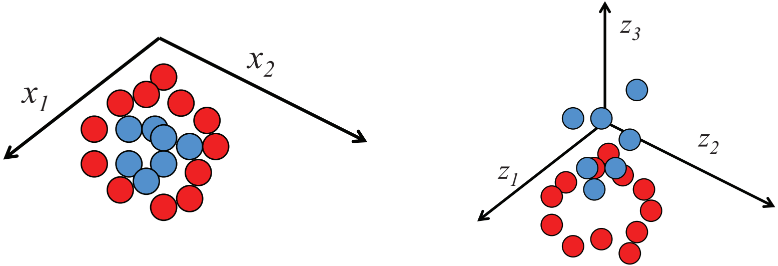
$$\lambda(x) = w \cdot x \quad \text{with} \quad w \propto \Sigma^{-1}(\mu_S - \mu_B)$$



- 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

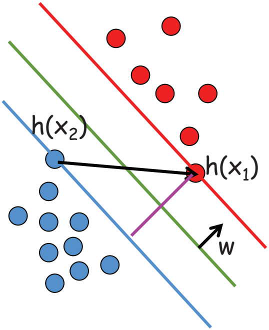
- Fisher discriminant: may fail completely for highly non-Gaussian densities
- But linearity is good feature $\Rightarrow$ try to keep it
- Generalising Fisher discriminant: data non-separable in n-dim space $\mathbb{R}^n$, but better separated if mapped to higher dimension space $\mathbb{R}^H$: $h :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



Support vector machines: separable data

- 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

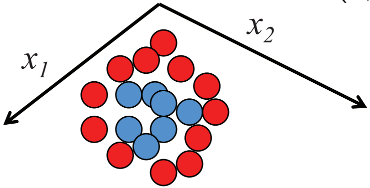
- Issues:
  - need to find h mappings (potentially of infinite dimension)
  - need to compute scalar products $h(x_i) \cdot h(x_j)$
- Fortunately $h(x_i) \cdot h(x_j)$ are equivalent to some kernel function $K(x_i, x_j)$ that does the mapping and the scalar product:

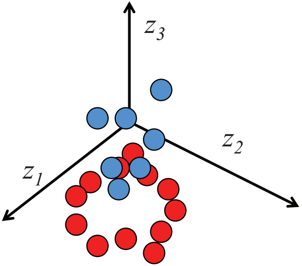
$$C(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$

Support vector machines: example

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

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

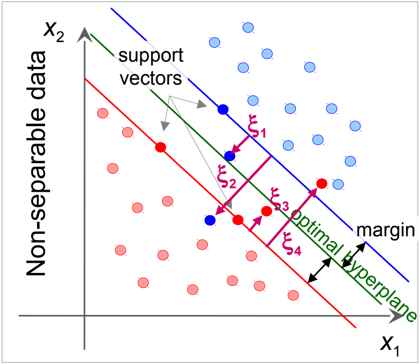




- In reality: do not know a priori the right kernel
- $\Rightarrow$ have to test different standard kernels and use the best one

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

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



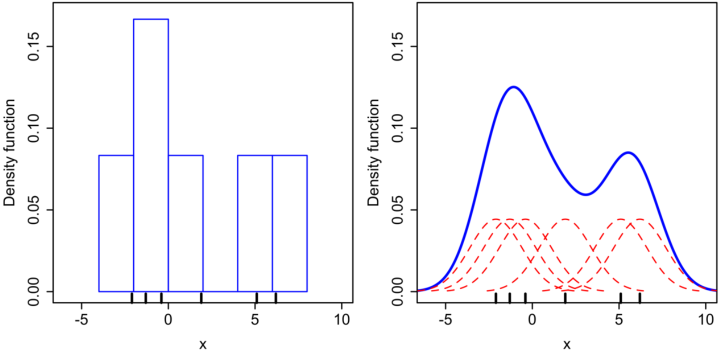
with slack variables $\xi_i > 0$

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

Kernel density estimation (KDE)

- Introduced by E. Parzen in the 1960s
- Place a kernel $K(x, \mu)$ at each training point μ
- Density $p(x)$ at point x approximated by:

$$p(x) \approx \hat{p}(x) = \frac{1}{N} \sum_{j=1}^{N} K(x, \mu_j)$$



Kernel density estimation (KDE)

Choice of kernel

- Any kernel can be used
- In practice, often product of Gaussians:

$$K(x,\mu) = \prod_{i=1}^{n} Gaussian(x_i|\mu, h_i)$$

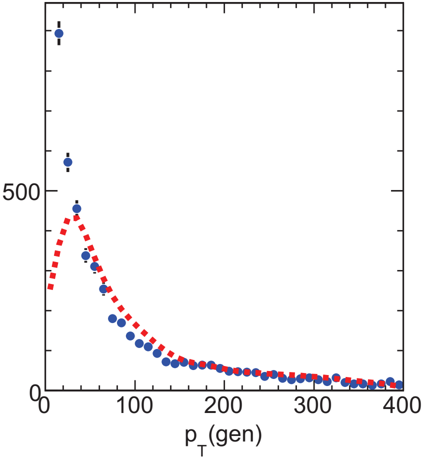
each with bandwidth (width) h_i

Optimal bandwidth

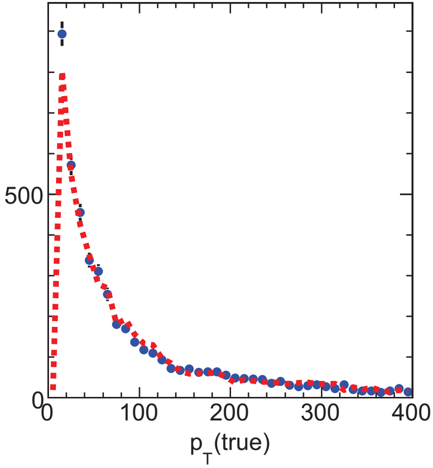
- Too narrow: noisy approximation
- Too wide: loose fine structure
- In principle found by minimising risk function $R(\hat{p}, p) = \int \left(\hat{p}(x) - p(x)\right)^2 dx$
- For Gaussian densities:

$$h = \sigma \left(\frac{4}{(n+2)N}\right)^{1/(n+4)}$$

- Far from optimal for non-Gaussian densities with Gaussian optimal bandwidth



with optimised bandwidth



Kernel density estimation (KDE)

Why does it work?

- When $N \to \infty$:

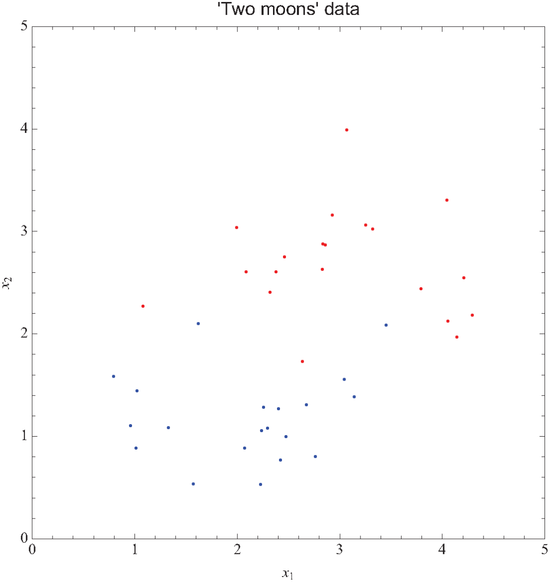
$$\hat{p}(x) = \int K(x,\mu)p(\mu)d\mu$$

- $p(\mu)$: true density of x
- Kernel bandwidth getting smaller with N, so when $N \to \infty$, $K(x,\mu) \to \delta^n(x-\mu)$ and $\hat{p}(x) = p(x)$
- KDE gives consistent estimate of probability density $p(x)$

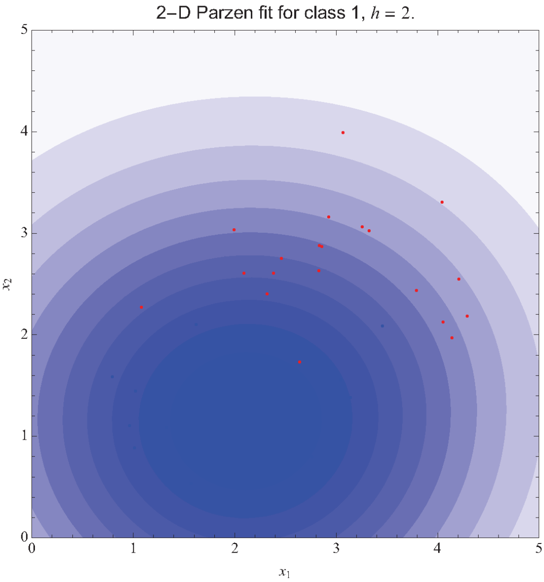
Limitations

- Choice of bandwidth non-trivial
- Difficult to model sharp structures (e.g. boundaries)
- Kernels too far apart in regions of low point density
- (both can be mitigated with adaptive bandwidth choice)
- Requires evaluation of N n-dimensional kernels

Kernel density estimation (KDE)



Kernel density estimation (KDE)



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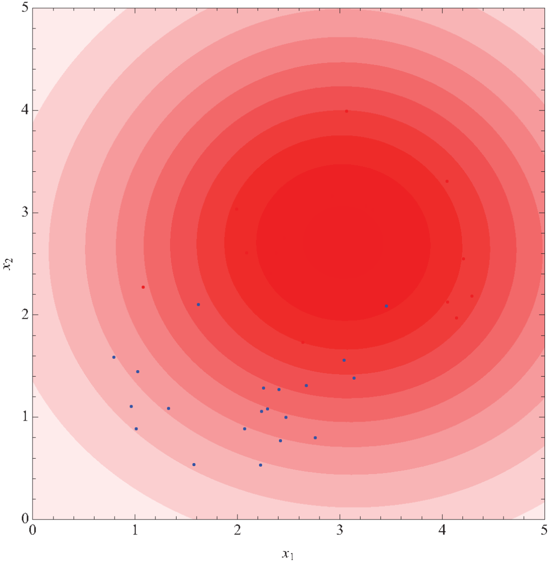
Kernel density estimation (KDE)

2–D Parzen fit for class −1, $h = 2$.



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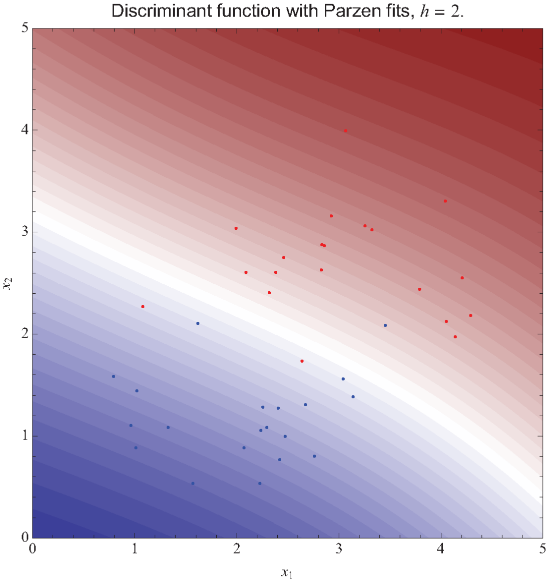
Kernel density estimation (KDE)



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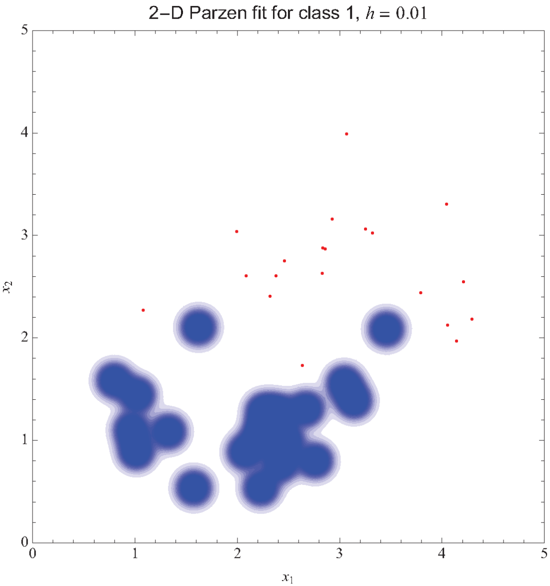
Kernel density estimation (KDE)



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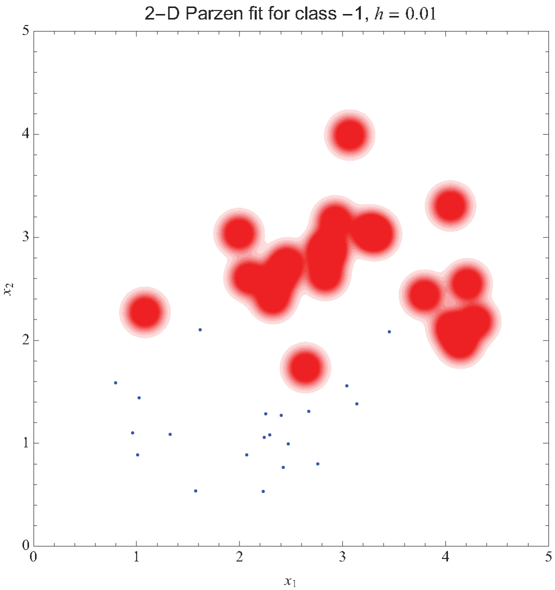
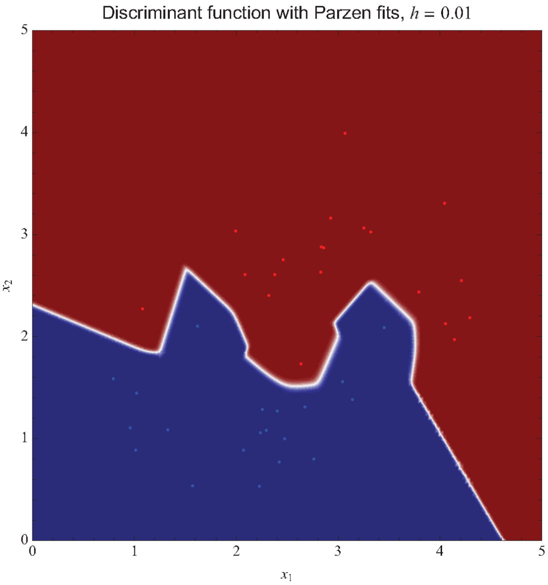
Kernel density estimation (KDE)



Kernel density estimation (KDE)



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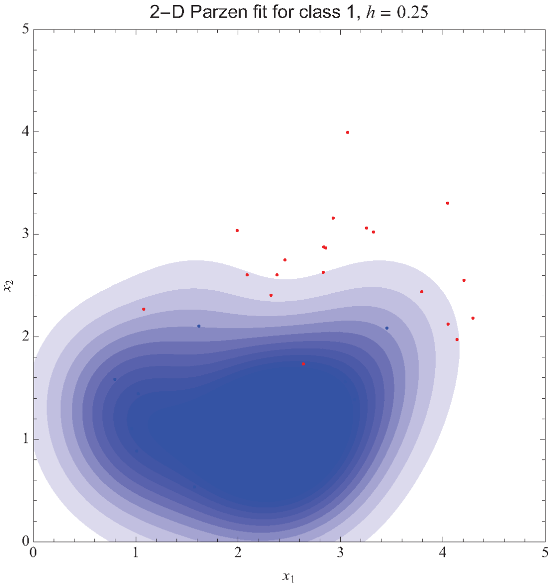
Kernel density estimation (KDE)



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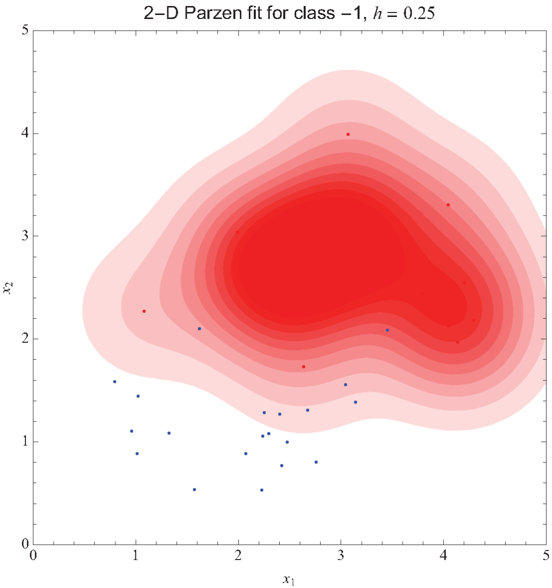
Kernel density estimation (KDE)



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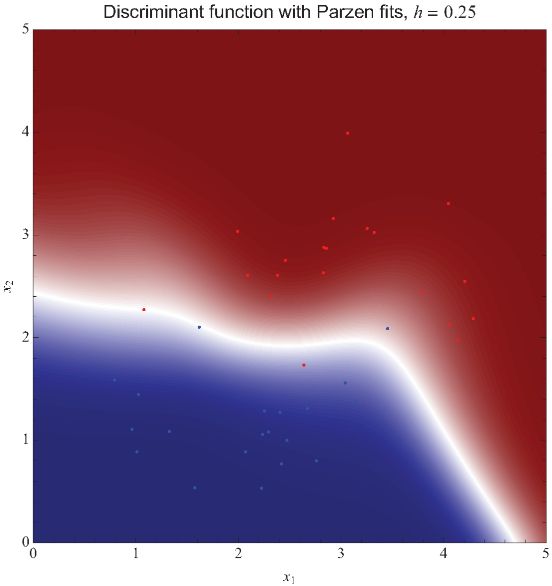
Kernel density estimation (KDE)



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KDE: choice of bandwidth

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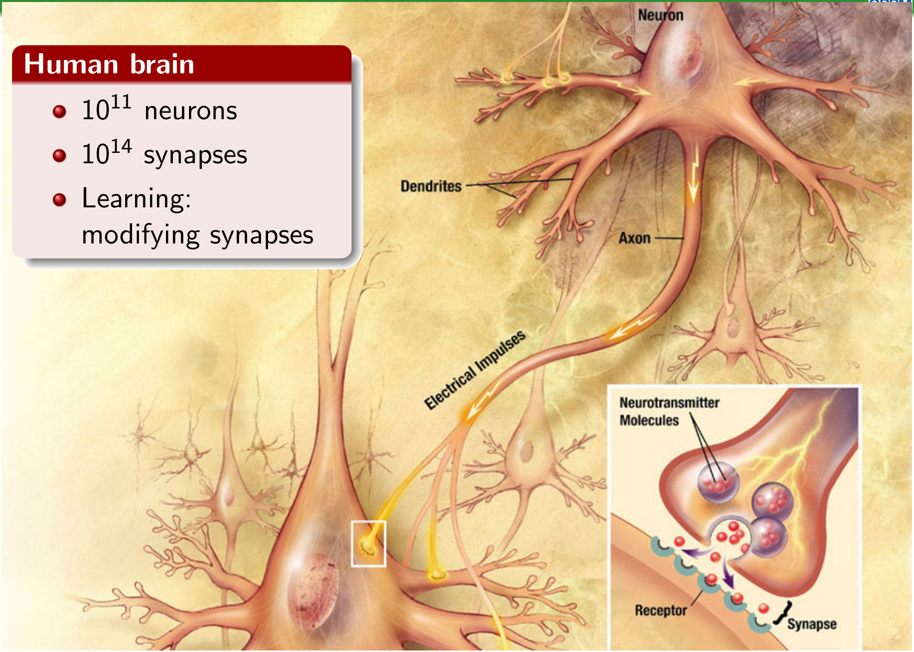
Neural networks

Human brain

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

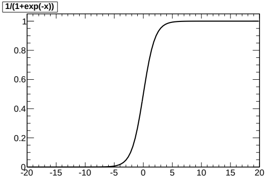


Brief history of artificial neural networks

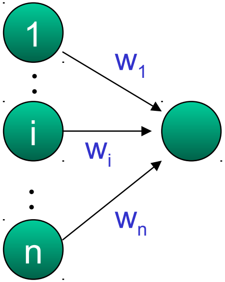
- 1943: W. McCulloch and W. Pitts explore capabilities of networks of simple neurons
- 1958: F. Rosenblatt introduces perceptron (single neuron with adjustable weights and threshold activation function)
- 1969: M. Minsky and S. Papert prove limitations of perceptron (linear separation only) and (wrongly) 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)

Single neuron

- 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):



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



- $\sigma(\lambda)$ 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 $|y(x) - f(x)| < \varepsilon$

Neural networks

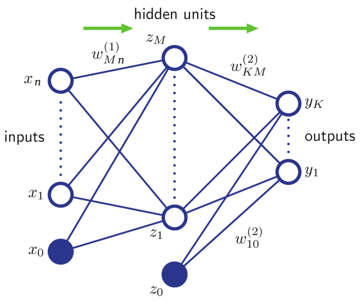
Interpretation

- 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

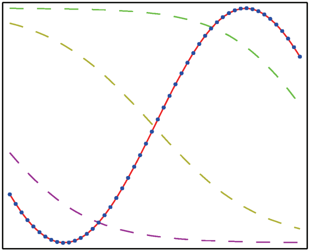
Multilayer perceptron: feedforward network

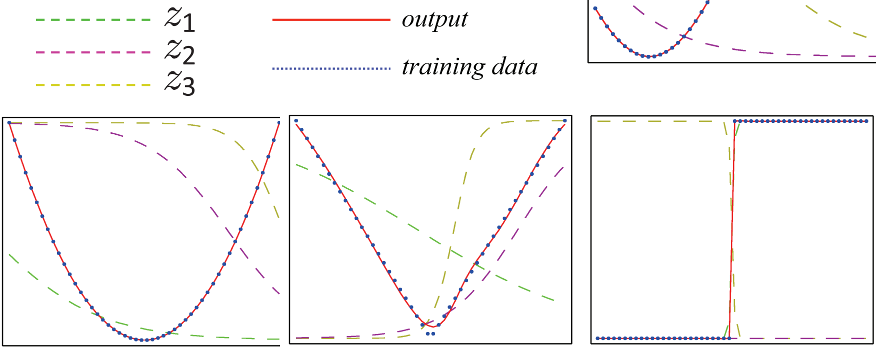
- Neurons organised in layers
- Output of one layer becomes input to next layer

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



- 1 input (training data), 1 output
- 3 hidden neurons on one hidden layer



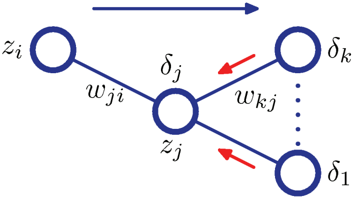


- Training means minimising error function $E(w)$
- For single neuron: $\frac{dE}{dw_k} = (y - t)x_k$
- One can show that for a network:

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

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

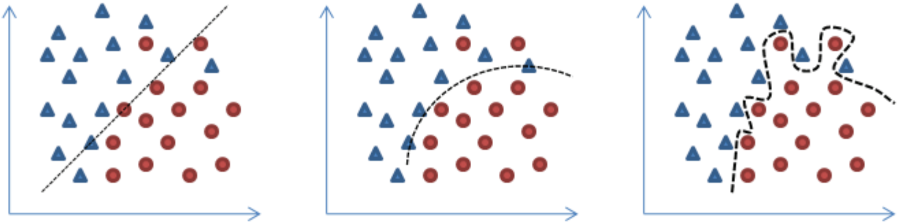
- Hence errors are propagated backwards



Neural network training

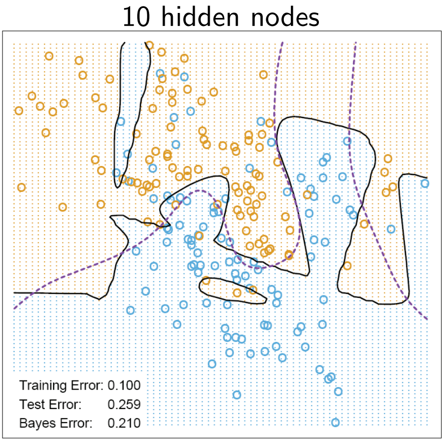
- Minimise error function $E(w)$
- Gradient descent: $w^{(k+1)} = w^{(k)} - \eta \frac{dE^{(k)}}{dw}$
- $\frac{\partial E}{\partial w_j} = \sum_{n=1}^{N} -(t^{(n)} - y^{(n)})x_j^{(n)}$ with target $t^{(n)}$ (0 or 1), so $t^{(n)} - y^{(n)}$ is the error on event n
- All events at once (batch learning):
  - 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

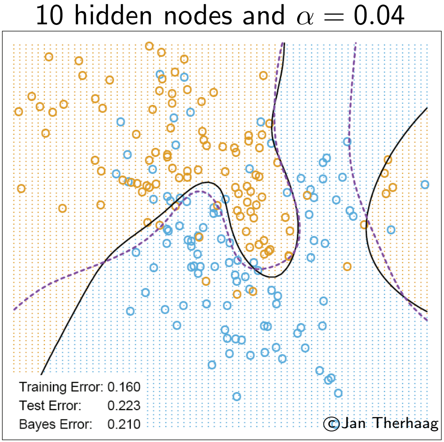
Neural network overtraining



- 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:

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





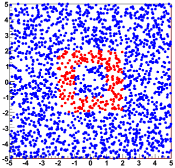
- Much less overfitting, better generalisation properties

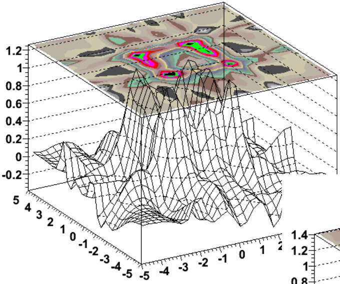
Neural networks: Tricks of the trade

▸ Efficient BackProp

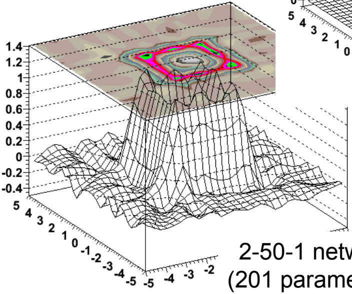
- Preprocess data:
  - if relevant, provide e.g. x/y instead of x and y
  - subtract the mean because the sigmoid derivative becomes negligible very fast (so, input mean close to 0)
  - normalise variances (close to 1)
  - shuffle training sample (order matters in online training)
- Initial random weights 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

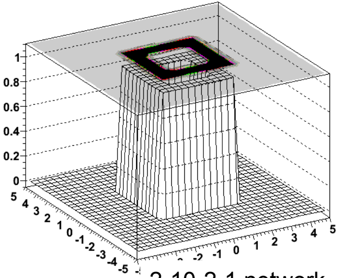




2-20-1 network
(81 parameters)



2-50-1 network
(201 parameters)



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

Bayesian neural networks

- As name says: Bayesian approach, try to *infer* functions $f(x)$
- Training sample T of N examples $(x, y)_1, (x, y)_2, \ldots, (x, y)_N$ of discriminating variables x and class labels y
- Each point w corresponds to a function $f(x, w)$
- Assign probability density $p(w|T)$ to it
- If $p(w_1|T) > p(w_2|T)$, then associated function $f(x, w_1)$ more compatible with training data T than function $f(x, w_2)$
- Posterior density $p(w|T)$ is final result of Bayesian inference
- BNN is the predictive distribution

$$p(y|x, T) = \int p(y|x, w)p(w|T)dw$$

where the function class is class of feedforward neural networks with a fixed structure (inputs, layers, hidden nodes, outputs)

Bayesian neural networks

- Take the mean of the predictive distribution:

$$\begin{aligned} y(x) &= \int z p(z|x,T) dz \\ &= \int f(x,w) p(w|T) dw \end{aligned}$$

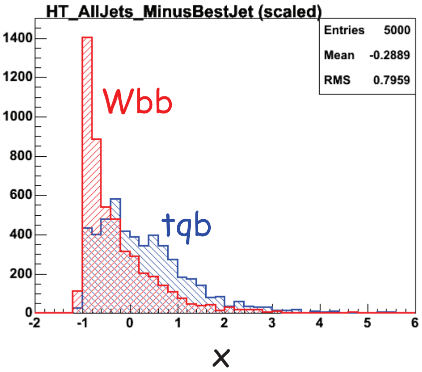
- Why? For classification $p(y|x,w) = f(x,w)^y \left(1 - f(x,w)\right)^{1-y}$
  - for $y = 1$: $p(y|x,w) = f(x,w)$
  - for $y = 0$: $p(y|x,w) = 1 - f(x,w)$
  - so only $f(x,w)$ contributes to the mean
- Example usage:

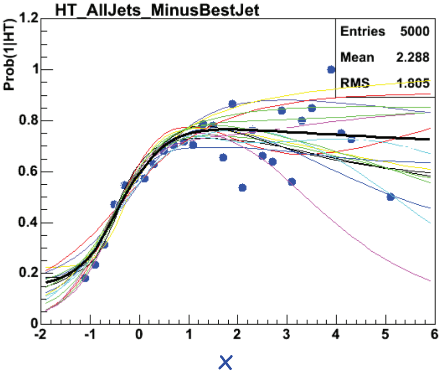
$$\begin{aligned} f(x,w) &= \frac{1}{1+e^{-g(x,w)}} \\ g(x,w) &= b + \sum_{j=1}^{H} v_j \tanh\left(a_j + \sum_{i=1}^{n} u_{ij} x_i\right) \end{aligned}$$

with H hidden nodes

Bayesian neural networks

- Scanning NN parameter space can be daunting
- Can approximate integral in $y(x)$ using Markov chain Monte Carlo method (MCMC)
- Will generate M sample weights $w_1, \ldots, w_M$ from posterior density $p(w|T)$
- $y(x) \approx \frac{1}{M}\sum_{m=1}^{M} f(x, w_m)$
- Use spare subset of MCMC points to avoid correlations
- Start with "reasonable" guesses for parameters (e.g. zero-centred Gaussians)





- points: bin by bin histogram ratio
- thin curves: each $f(x, w_k)$
- thick curve: average, which approximates $D(x)$

Deep learning

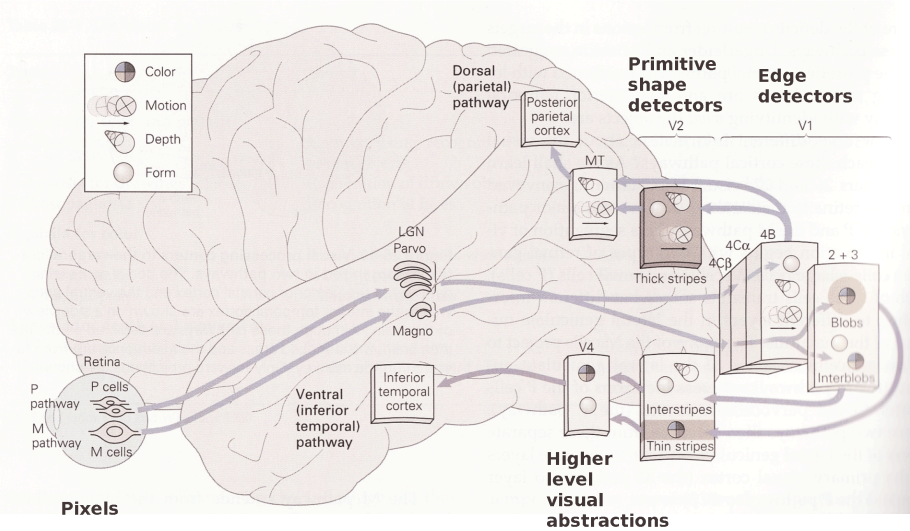
What is learning?

- 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

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 ⇒ early layers do not learn much, can even penalise overall performance

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

Why does unsupervised training work?

Optimisation hypothesis

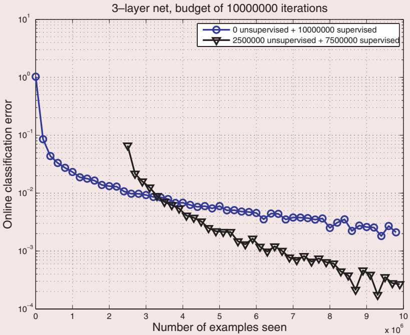
- Training one layer at a time scales well
- Backpropagation from sensible features
- Better local minimum than random initialisation, local search around it

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

An example from Google research team

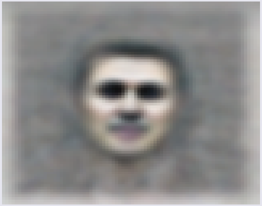
▸ 2011 paper

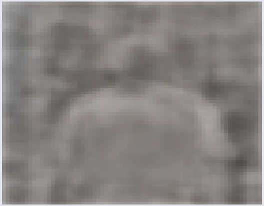
A “giant” neural network

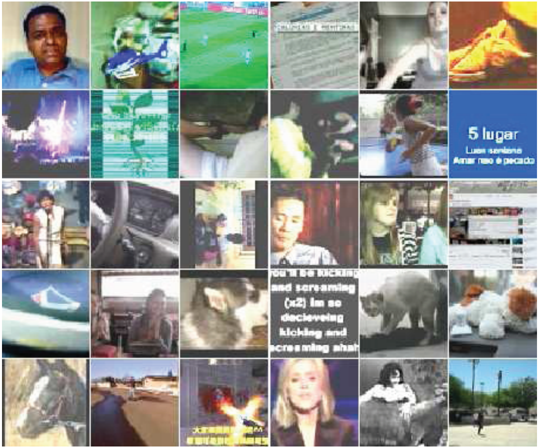
- At Google they trained a 9-layered NN with 1 billion connections
  - trained on 10 million 200×200 pixel images from YouTube videos
  - on 1000 machines (16000 cores) for 3 days, unsupervised learning
- Sounds big? The human brain has 100 billion (10^{11}) neurons and 100 trillion (10^{14}) connections...

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

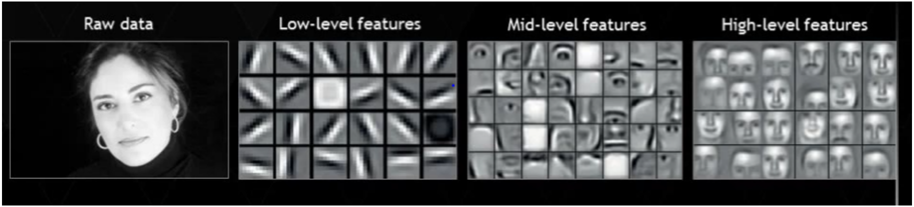






- Features extracted from such images
- Results shown to be robust to
  - colour
  - translation
  - scaling
  - out-of-plane rotation

Learning feature hierarchy



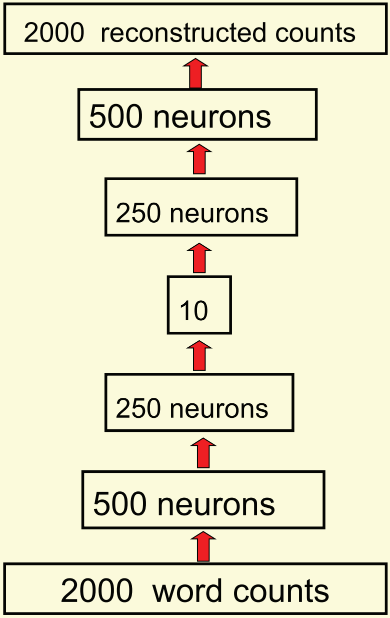
Auto-encoders

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

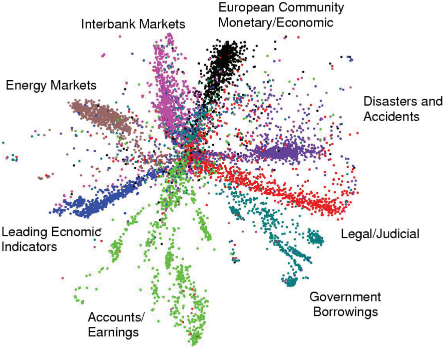
- Get count of 2000 most common words per book
- “Compress” to 10 numbers



Auto-encoders

With principle component analysis (PCA)

With autoencoder

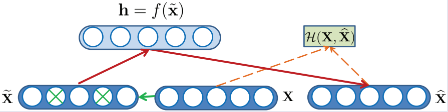


Sparse auto-encoder

- Sparsity: try to have low activation of neurons (like in the brain)
- Compute average activation of each hidden unit over training set
- Add constraint to cost function to make average lower than some value close to 0

Denoising auto-encoder

- Stochastically corrupt inputs
- Train to reconstruct uncorrupted input

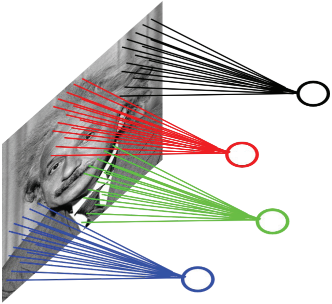


Locally connected auto-encoder

- Allow hidden units to connect only to small subset of input units
- Useful with increasing number of input features (e.g., bigger image)
- Inspired by biology: visual system has localised receptive fields

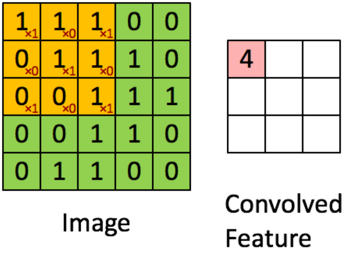
Convolutional networks

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



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



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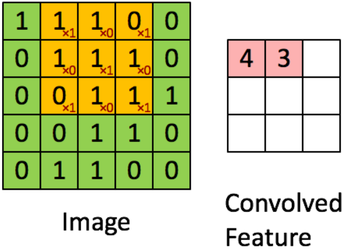

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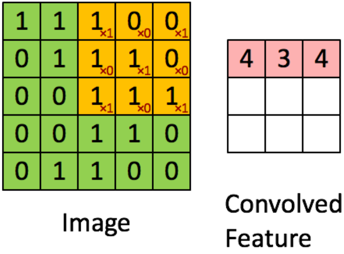

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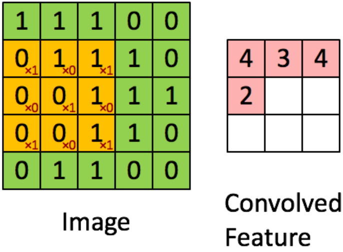

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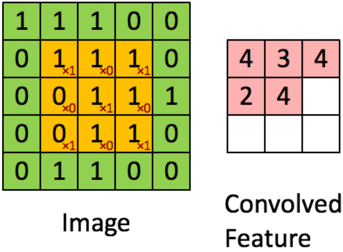

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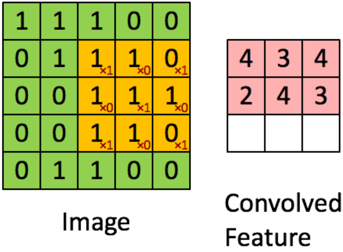

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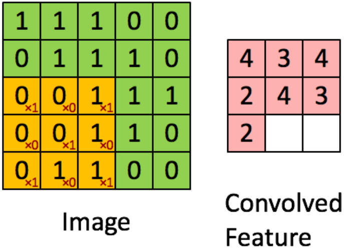

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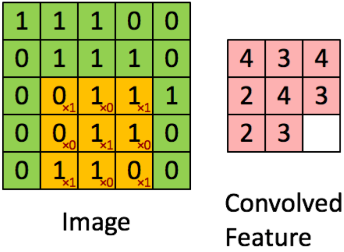

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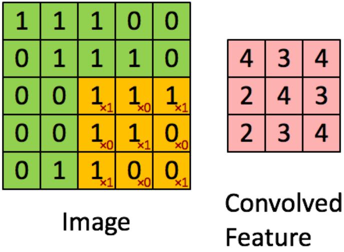
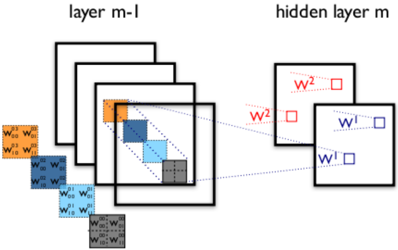


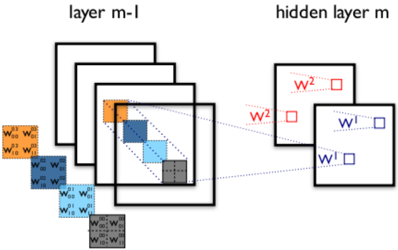
Convolutional networks

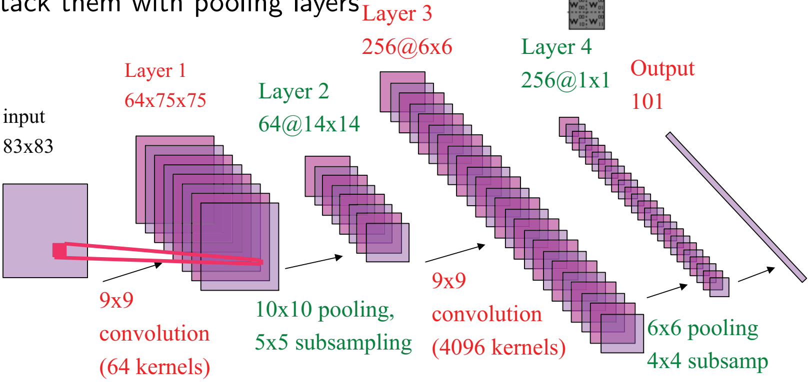
- Images are stationary: can learn feature in one part and apply it in another
- Use e.g. small patch sampled randomly, learn feature, convolve with full image
- Build several "feature maps"



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



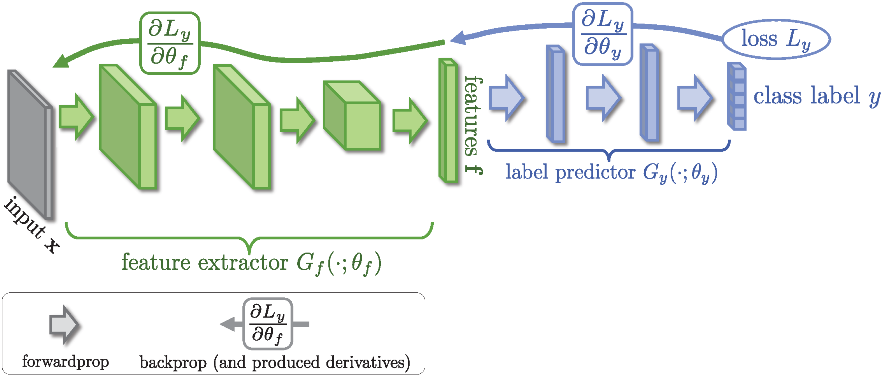


Deep learning: looking forward

- 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)

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

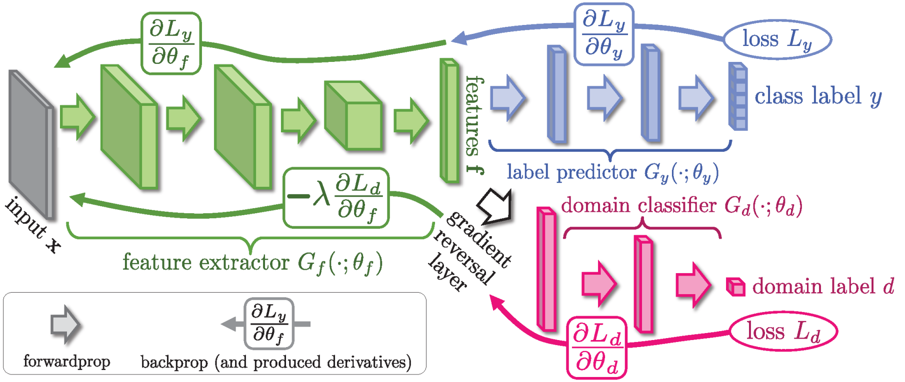
http://arxiv.org/abs/1409.7495
http://arxiv.org/abs/1505.07818



- 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

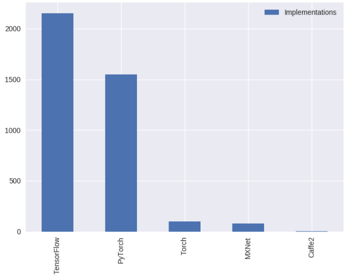
http://arxiv.org/abs/1409.7495

http://arxiv.org/abs/1505.07818

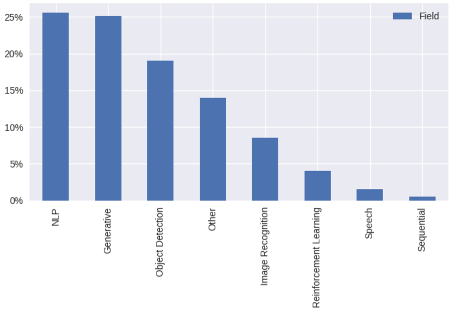


Deep learning: second half of 2018 trends

- Most used software



- Most activity



▸ https://www.kdnuggets.com/2018/12/deep-learning-major-advances-review.html

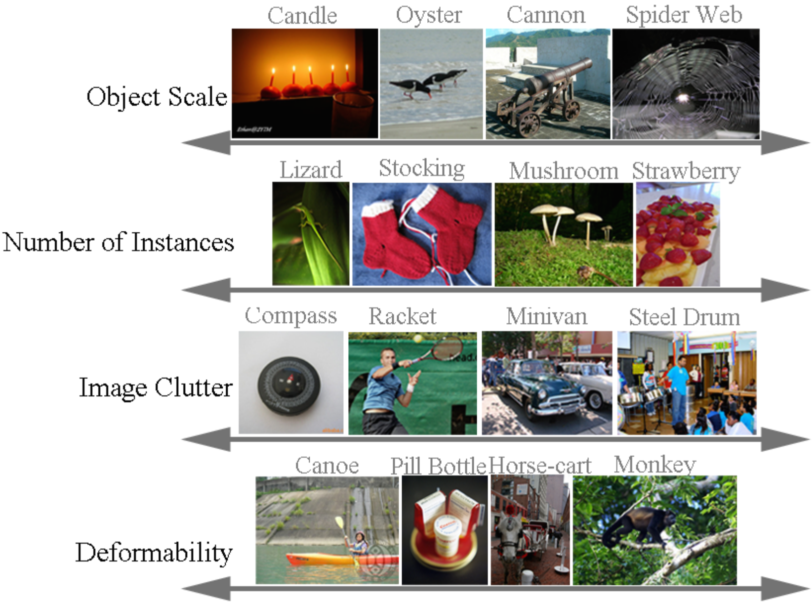
ILSVRC 2014

Summary paper

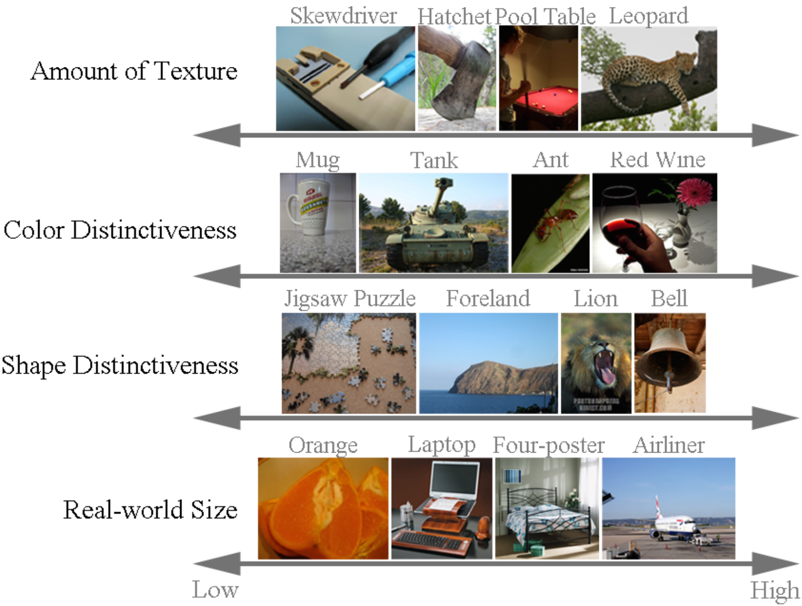
ImageNet Large Scale Visual Recognition Challenge

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

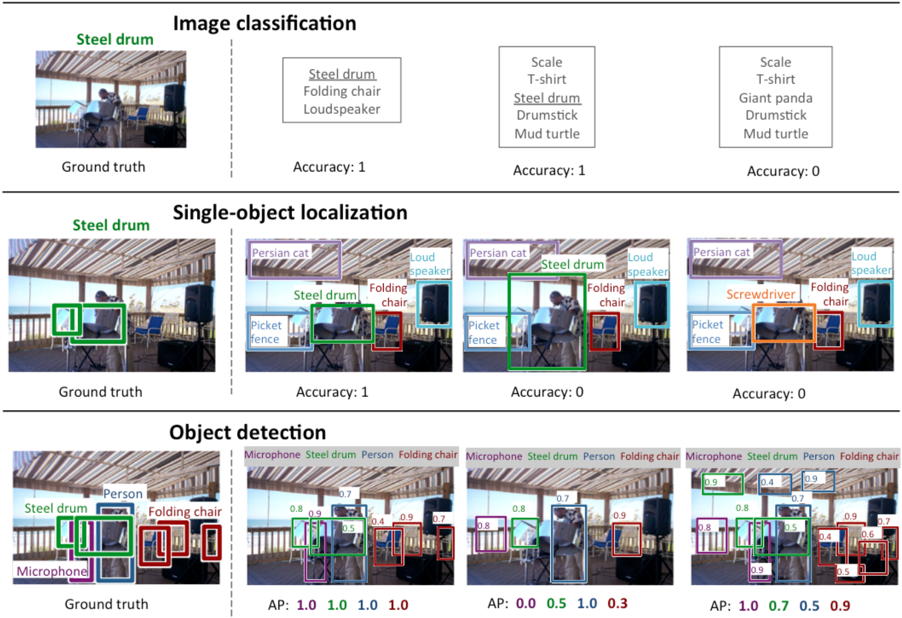
ILSVRC 2014 images



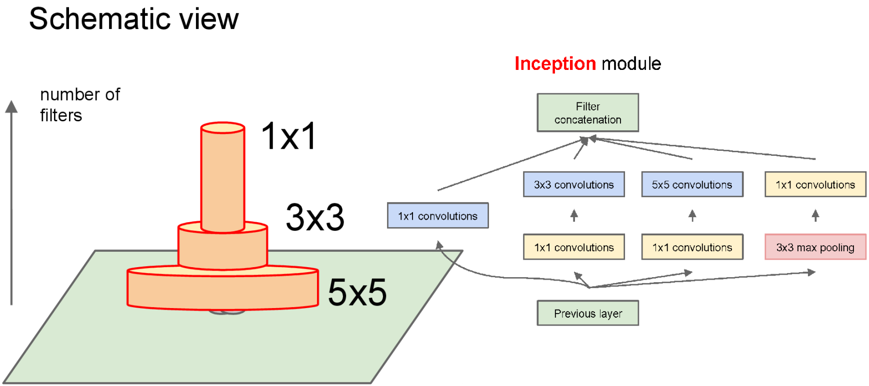
ILSVRC 2014 images



ILSVRC 2014 tasks

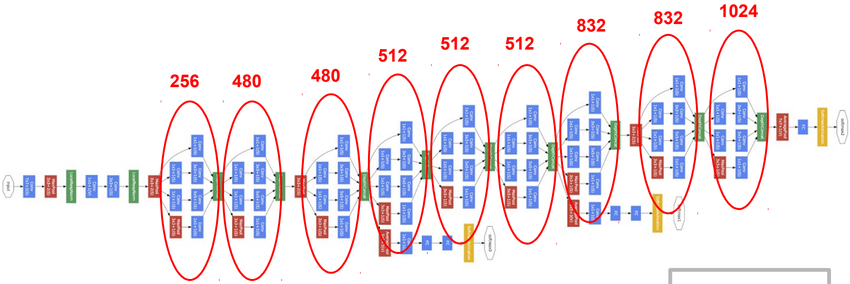


- Google of course! (first time)
- GoogLeNet:



ILSVRC 2014 And the winner is. . .

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



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**

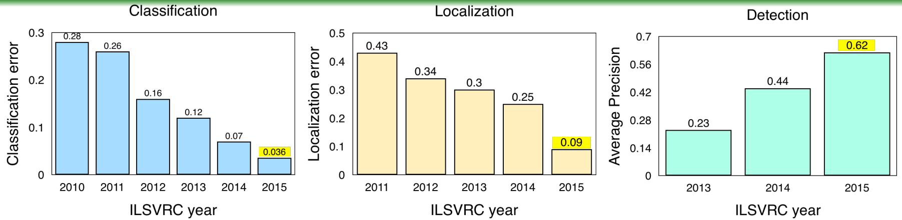
Classification failure cases

Groundtruth: **hay**

GoogLeNet:

- **sorrel (horse)**
- **hartebeest**
- **Arabian camel**
- **warthog**
- **gaselle**

ILSVRC 2010–2016



2010–14: 4.2x reduction

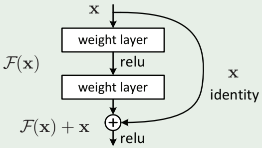
1.7x reduction

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)

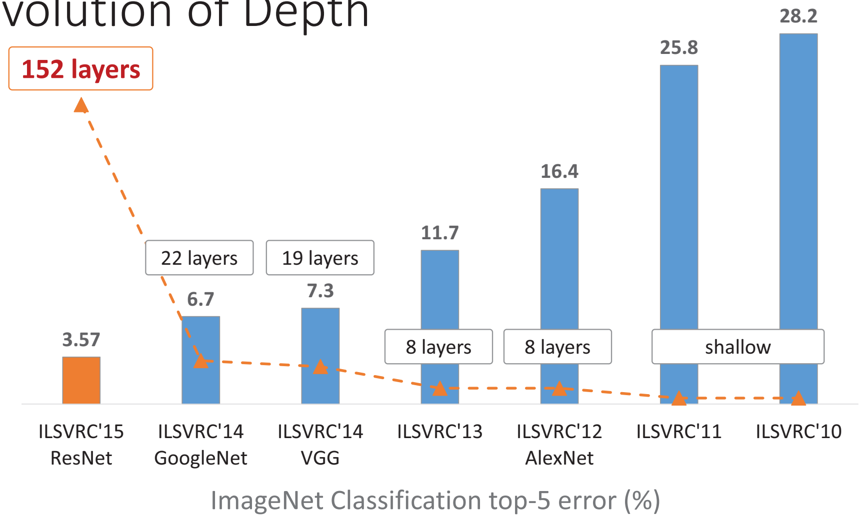


ILSVRC 2016

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

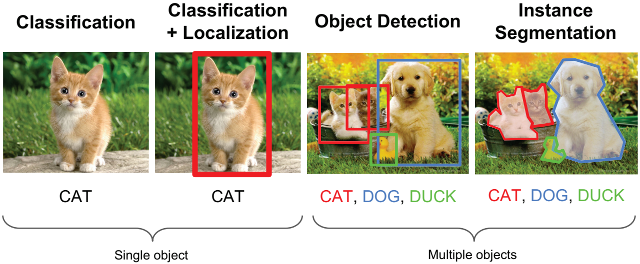
- Mostly ResNets. Classification: 0.030; localisation: 0.08; detection: 0.66

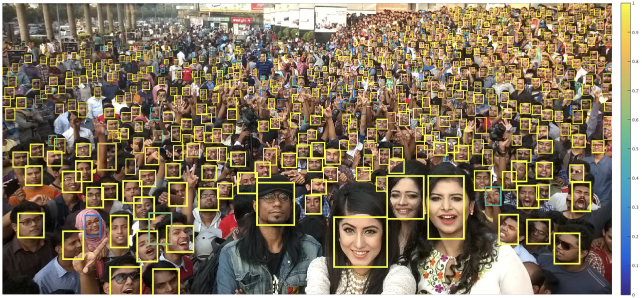
Revolution of Depth



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

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 $a_t = \mathrm{argmax}_a Q(\phi(s_t), a; \theta)$

    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

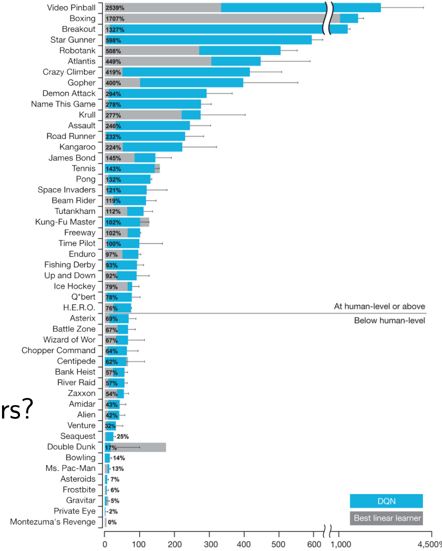
    $$\text{Set } y_j = \begin{cases} r_j & \text{if episode terminates at step j+1} \\ r_j + \gamma \max_{a'} \hat{Q}\left(\phi_{j+1}, a'; \theta^-\right) & \text{otherwise} \end{cases}$$

    Perform a gradient descent step on $\left(y_j - Q\left(\phi_j, a_j; \theta\right)\right)^2$ with respect to the network parameters θ

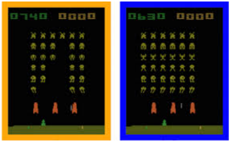
    Every C steps reset $\hat{Q} = Q$

  End For

End For



- What about Breakout or Space invaders?



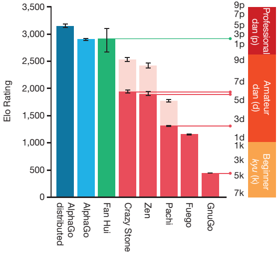
Google DeepMind: mastering Go

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.

▸ Nature 529, 484 (2016)

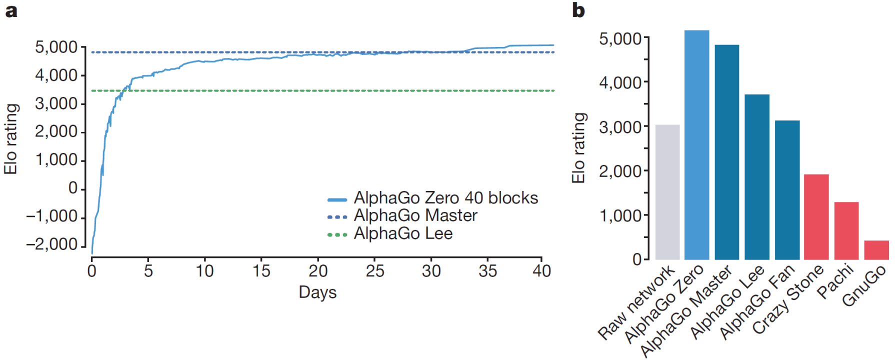
- AlphaGo: 40 search threads, simulations on 48 CPUs, policy and value networks on 8 GPUs. Distributed AlphaGo: 1020 CPUs, 176 GPUs
- AlphaGo won 494/495 games against other programs (and still 77% against Crazy Stone with four handicap stones)
  - Fan Hui: 2013/14/15 European champion
  - Distributed 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)



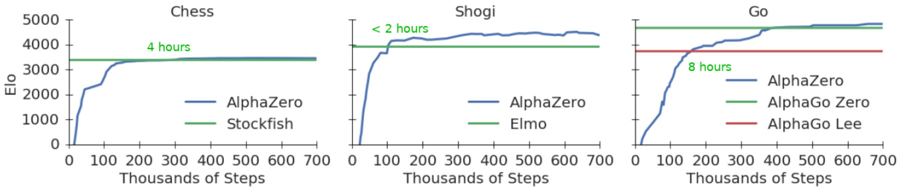
- Then played Lee Sedol (top Go play in the world over last decade) in March 2016 ⇒ won 4–1. AlphaGo given honorary professional ninth dan, considered to have "reach a level 'close to the territory of divinity' "
- Ke Jie (Chinese world #1): "Bring it on!". May 2017: 3–0 win for AlphaGo. New comment: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

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

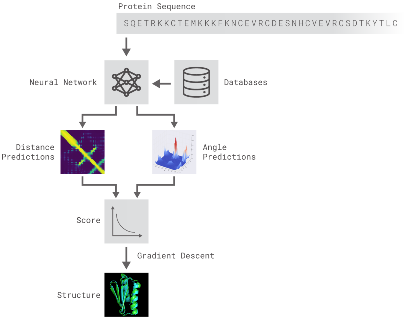


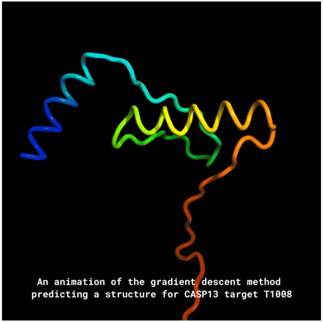
- Same philosophy as AlphaGo Zero, applied to chess, shogi and go
- Changes:
  - not just win/loss, but also draw or other outcomes
  - no additional training data from game symmetries
  - using always the latest network to generate self-play games rather than best one
  - tree search: 80k/70M for chess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



DeepMind AlphaFold

- Trying to tackle scientific problem
- Goal: predict 3D structure of protein based solely on genetic sequence
- Using DNN to predict
  - distances between pairs of amino acids
  - angles between chemical bonds
- Then search DB to find matching existing substructures
- Also train a generative NN to invent new fragments
- Achieved best prediction ever

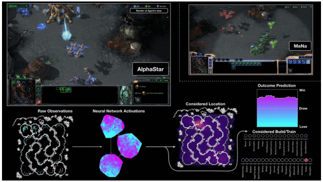




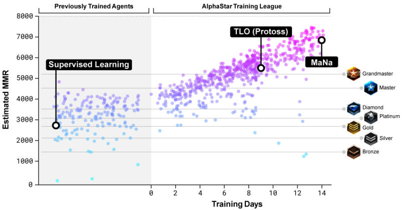
DeepMind AlphaStar

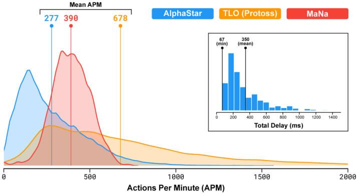
▸ Blog Jan 2019

- Mastering real-time strategy game StarCraft II
- Challenges in game theory (no single best strategy), imperfect information (hidden parts of game), long term planning, real time (continuous flow of actions), large action space (many units/buidings)
- Using DNN trained
  - directly on raw data games
  - supervised learning on human games
  - reinforcement learning (continuous league)



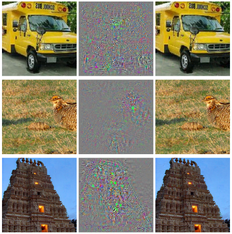
- DNN output: list of actions
- Trained for 14 days; each agent: up to 200 years of real-time play
- Runs on single desktop GPU
- Defeated 5–0 one of best pro-players





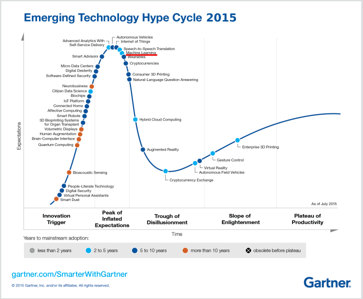
Deep networks: new results all the time

- 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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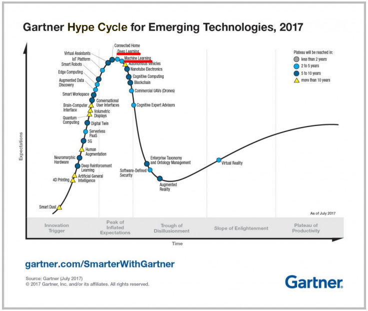

Gartner Hype Cycle for Emerging Technologies, 2017
Expectations
Connected Home
Deep Learning
Machine Learning
Autonomous Vehicles
Nanotube Electronics
Cognitive Computing
Blockchain
Commercial UAVs (Drones)
Cognitive Expert Advisors
Virtual Assistants
IoT Platform
Smart Robots
Edge Computing
Augmented 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
Trough of Disillusionment
Slope of Enlightenment
Plateau of Productivity
Time
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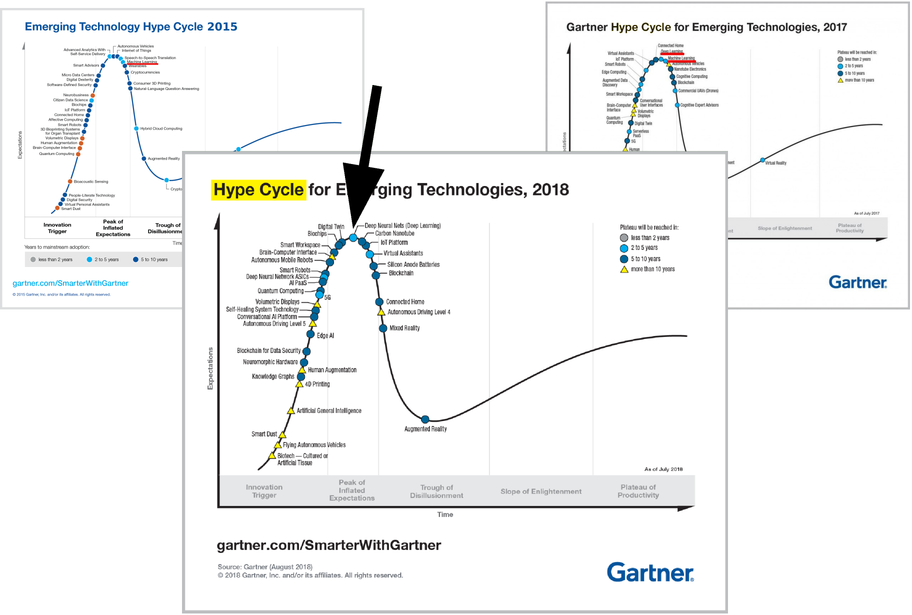
Hype cycle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Gartner
Hype Cycle for E…rging Technologies, 2018
Digital Twin
Biochips
Deep Neural Nets (Deep Learning)
Carbon Nanotube
IoT Platform
Smart Workspace
Brain-Computer Interface
Autonomous Mobile Robots
Virtual Assistants
Silicon Anode Batteries
Blockchain
Smart Robots
Deep Neural Network ASICs
AI PaaS
Quantum Computing
5G
Volumetric Displays
Self-Healing System Technology
Conversational AI Platform
Autonomous Driving Level 5
Connected Home
Autonomous Driving Level 4
Mixed Reality
Edge AI
Blockchain for Data Security
Neuromorphic Hardware
Human Augmentation
Knowledge Graphs
4D Printing
Artificial General Intelligence
Smart Dust
Flying Autonomous Vehicles
Biotech — Cultured or Artificial Tissue
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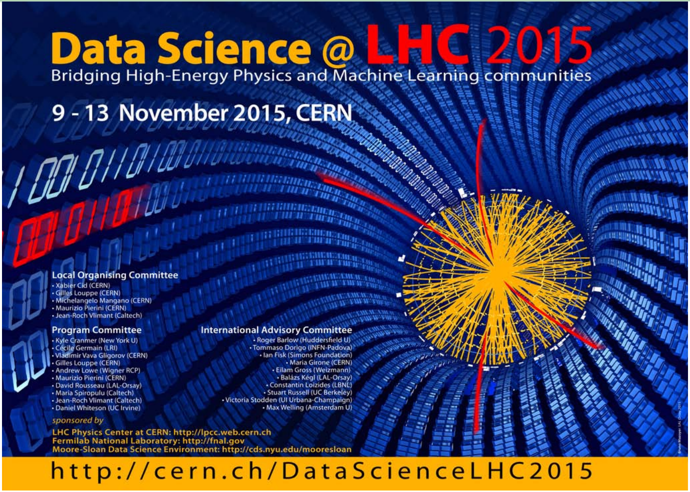
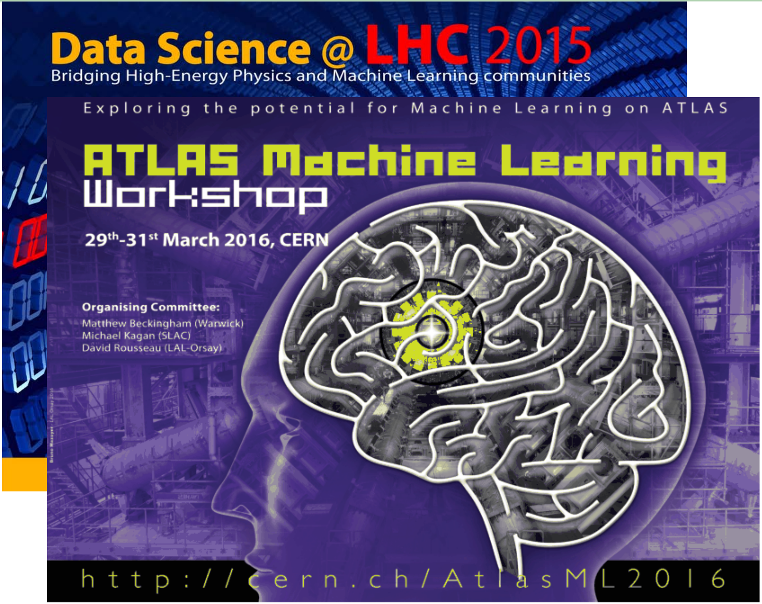


http://opendata.cern.ch

Machine learning and particle physics



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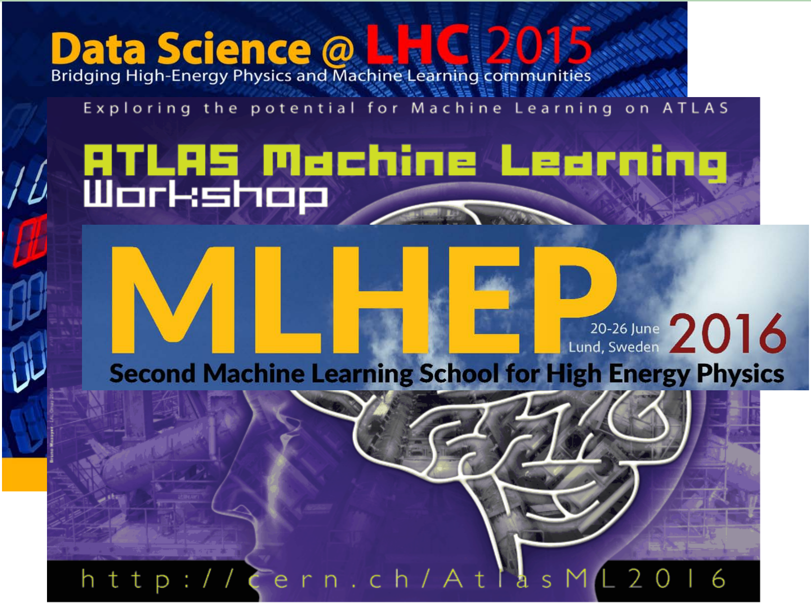
Machine learning and particle physics



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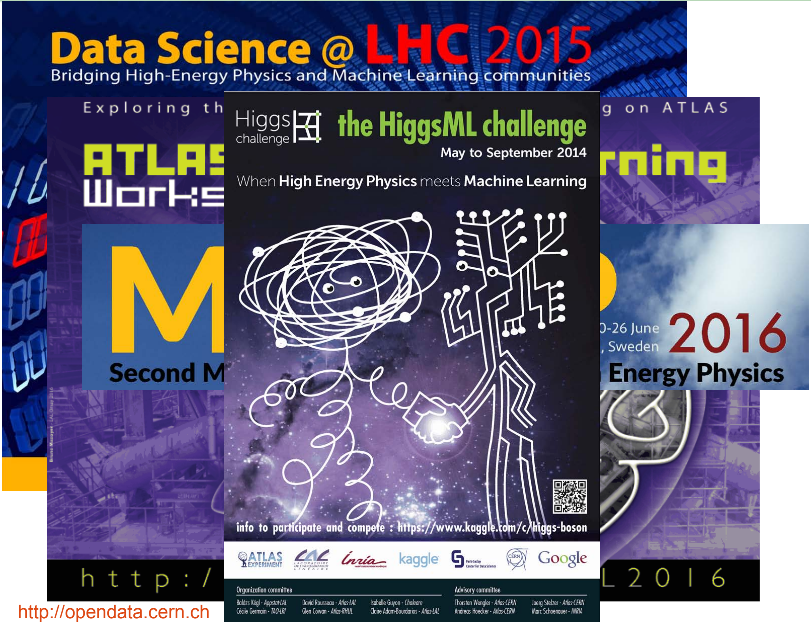

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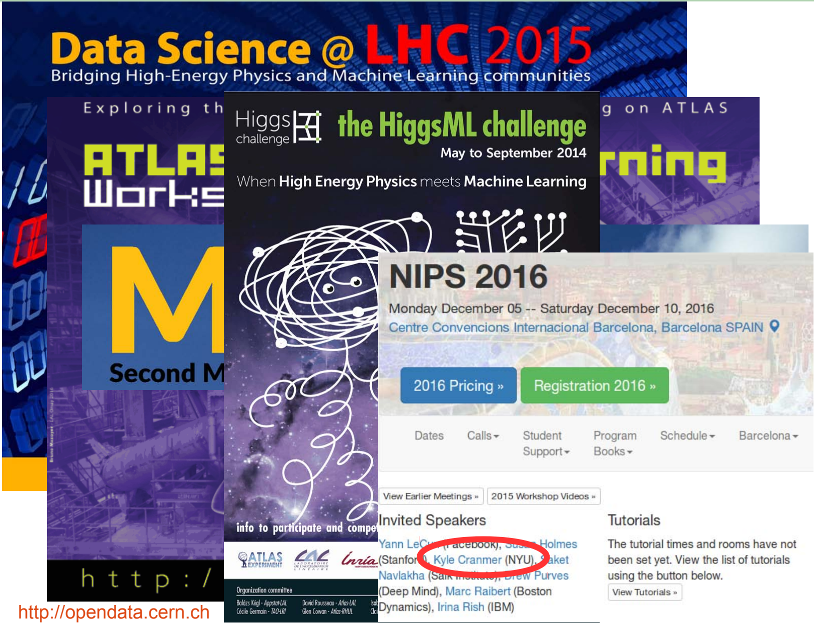
Machine learning and particle physics



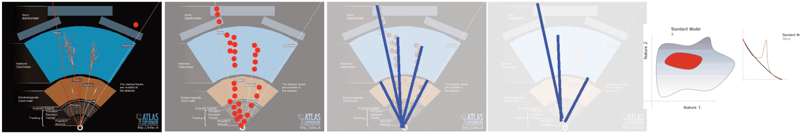
http://opendata.cern.ch

Machine learning and particle physics

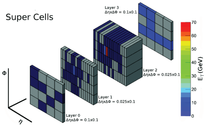
Machine learning and particle physics

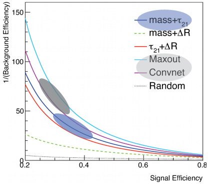
- Going to lower level features ‣ arXiv:1410.3469

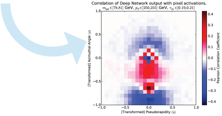
Raw	Sparsified	Reco	Select	Physics	Ana
1e7	1e4	100-ish*	50	10	1



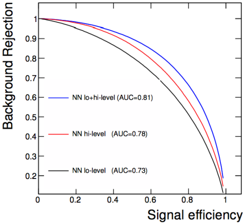
- Transforming inputs into images ‣ arXiv:1511.05190

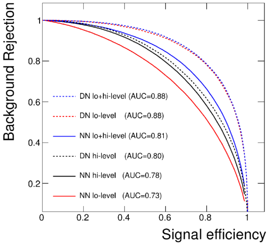






- Going to lower level features [arXiv:1410.3469]





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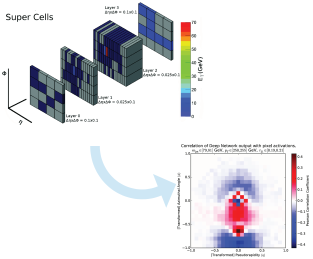
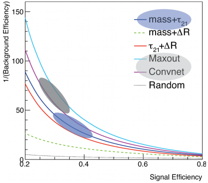
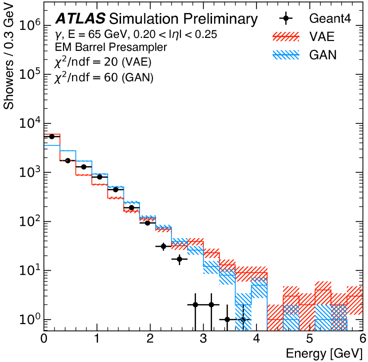
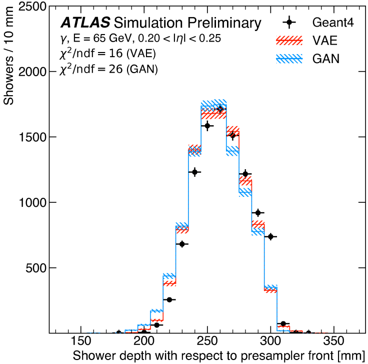




- Generative adversarial networks (GAN) ▸ ATLAS PUB note ATL-SOFT-PUB-2018-001
- Attempts to decrease CPU cost of simulation
  - limiting factor in many analyses already
  - not enough simulated events
- Replace "full simulation" by objects generated automatically by GAN or variational auto-encoders (VAE)





Next lecture

Conclusion

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

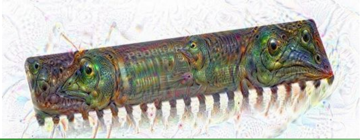
$$D(x) = \frac{s(x)}{s(x) + b(x)}$$

- 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

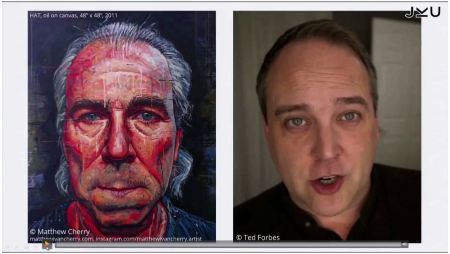
- Learning a style ‣ arXiv:1508.06576 [cs.CV] ‣ Neural-style

- Computer dreams ‣ Google original ‣ deepdream



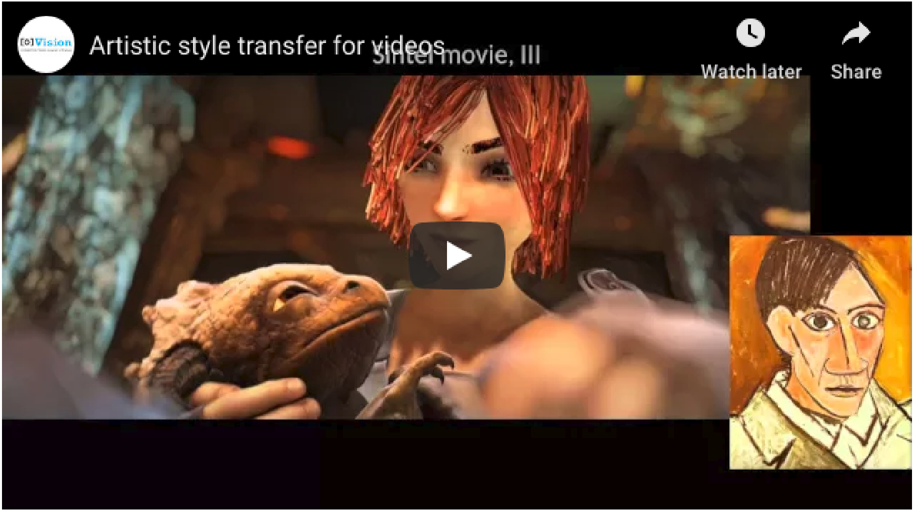
- Face Style ‣ http://facestyle.org

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



Deep networks and art

- Artistic style transfer for videos
  - https://lmb.informatik.uni-freiburg.de/Publications/2018/RDB18/



References I

- V. Vapnik, *The Nature of Statistical Learning Theory*, Springer, New York, 2nd Edition, 2000
- T. Hastie, R. Tibshirani and J. Friedman, *The Elements of Statistical Learning: Data Mining, Inference and Prediction*, Springer-Verlag, New York, 2nd Edition, 2009
- R.M. Neal, *Bayesian Learning of Neural Networks*, Springer-Verlag, New York, 1996
- C.M. Bishop, *Pattern Recognition and Machine Learning*, Springer, New York, 2007
- M. Minsky and S. Papert, “Perceptrons”, M.I.T. Press, Cambridge, Mass., 1969

References II

- H.B. Prosper, "The Random Grid Search: A Simple Way to Find Optimal Cuts", Computing in High Energy Physics (CHEP 95) conference, Rio de Janeiro, Brazil, 1995
- W.S. McCulloch & W. Pitts, "A logical calculus of the ideas immanent in nervous activity", *Bulletin of Mathematical Biophysics*, 5, 115-137, 1943
- F. Rosenblatt, "The Perceptron: A Probabilistic Model for Information Storage & Organization in the Brain", *Psychological Review*, 65, pp. 386-408, 1958
- D.E.Rumelhart et al., "Learning representations by back-propagating errors", *Nature* vol. 323, p. 533, 1986
- K.Hornik et al., "Multilayer Feedforward Networks are Universal Approximators", *Neural Networks*, Vol. 2, pp 359-366, 1989
- Y. LeCun, L. Bottou, G. Orr and K. Muller, "Efficient BackProp", in *Neural Networks: Tricks of the trade*, Orr, G. and Muller K. (Eds), Springer, 1998
- P.C. Bhat and H.B. Prosper, "Bayesian neural networks", in *Statistical Problems in Particles, Astrophysics and Cosmology*, Imperial College Press, Editors L. Lyons and M. Ünel, 2005

References III

- Q.V. Le et al., "Building High-level Features Using Large Scale Unsupervised Learning", in *Proceedings of the 29th International Conference on Machine Learning*, Edinburgh, Scotland, UK, 2012 ▸ http://research.google.com/pubs/pub38115.html
- G.E. Hinton, S. Osindero and Y. Teh, "A fast learning algorithm for deep belief nets", *Neural Computation* 18:1527-1554, 2006
- Y. Bengio, P. Lamblin, D. Popovici and H. Larochelle, "Greedy Layer-Wise Training of Deep Networks", in *Advances in Neural Information Processing Systems 19* (NIPS'06), pages 153–160, MIT Press 2007
- M.A. Ranzato, C. Poultney, S. Chopra and Y. LeCun, in J. Platt et al., "Efficient Learning of Sparse Representations with an Energy-Based Model", in *Advances in Neural Information Processing Systems 19* (NIPS'06), pages 1137–1144, MIT Press, 2007
- Y. Bengio, "Learning deep architectures for AI", *Foundations and Trends in Machine Learning*, Vol. 2, No. 1 (2009) 1–127. Also book at ▸ Now Publishers ▸ http://www.iro.umontreal.ca/ lisa/publications2/index.php/publications/show/239
- I. Goodfellow, Y. Bengio and A. Courville, "Deep Learning", MIT Press (2016) ▸ http://www.deeplearningbook.org