Neural networks and optimization

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13/11/12

Foreword

- I'm here for you, I already know that stuff
- It's better to look silly than to stay so
- Ask questions if you don't understand !

Goal : classification and regression

- Medical imaging : cancer or not ? Classification
- Autonomous driving : optimal wheel position Regression
- Kinect : where are the limbs ? Regression
- OCR : what are the characters ? Classification

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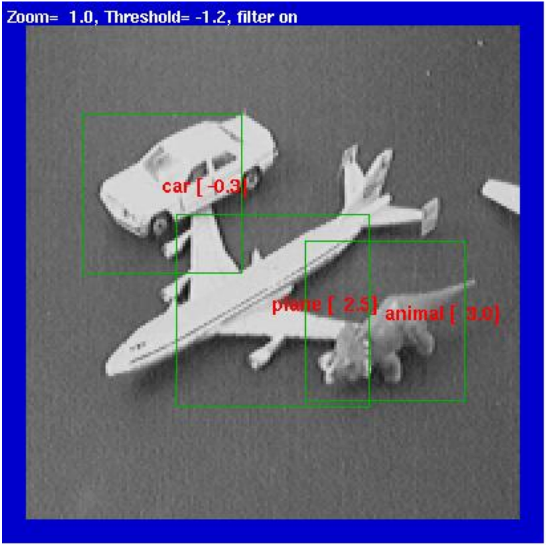
Regression and classification are similar problems

Goal : real-time object recognition



Linear classifier

- Dataset : $\left(X^{(i)}, Y^{(i)}\right)$ pairs, $i = 1, \ldots, N$.
- $X^{(i)} \in \mathbb{R}^n$, $Y^{(i)} \in \{-1, 1\}$.
- Goal : Find w and b such that $\mathrm{sign}(w^\top X^{(i)} + b) = Y^{(i)}$.

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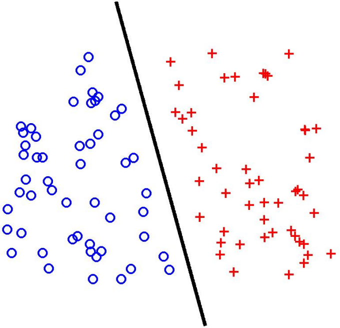
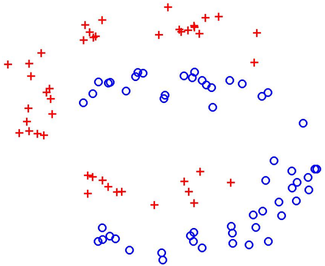


Perceptron algorithm (Rosenblatt, 57)

- $w_0 = 0$, $b_0 = 0$
- $\widehat{Y}^{(i)} = \mathrm{sign}(w^\top X^{(i)} + b)$
- $w_{t+1} \leftarrow w_t + \sum_i \left(Y^{(i)} - \widehat{Y}^{(i)}\right) X^{(i)}$
- $b_{t+1} \leftarrow b_t + \sum_i \left(Y^{(i)} - \widehat{Y}^{(i)}\right)$

Movie `linearly_separable_perceptron.avi`

Some data are not separable



The Perceptron algorithm is NOT convergent for non linearly separable data.

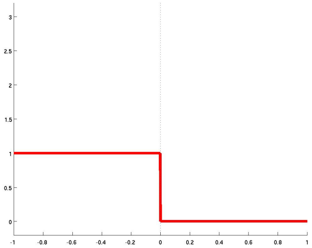
Non convergence of the perceptron algorithm

Movie `non_linearly_separable_perceptron.avi`

- We need an algorithm which works both on separable and non separable data.

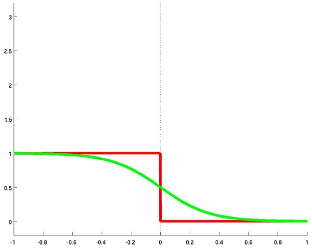
Cost function

- Classification error is not smooth.



Cost function

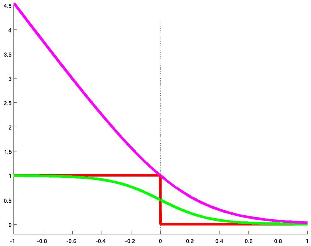
- Classification error is not smooth.
- Sigmoid is smooth but not convex.



- Convexity guarantees the same solution every time.
- In practice, it is not always crucial.

Convex cost functions

- Classification error is not smooth.
- Sigmoid is smooth but not convex.
- Logistic loss is a convex upper bound.



Convex cost functions

- Classification error is not smooth.
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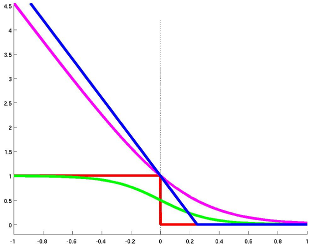
- Logistic loss is a convex upper bound.
- Hinge loss (SVMs) is very much like logistic.



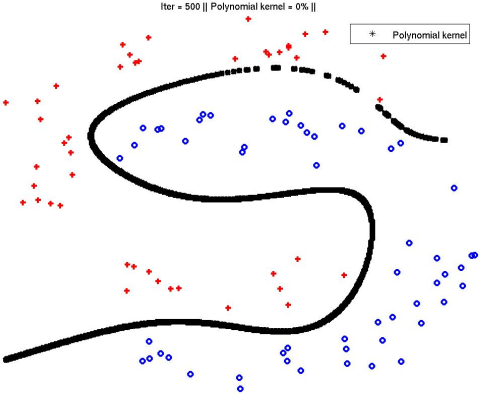
Solving separable AND non-separable problems

Movie `non_linearly_separable_logistic.avi` Movie `linearly_separable_logistic.avi`

Non-linear classification

Movie `non_linearly_separable_poly_kernel.avi`

Non-linear classification



- Features : $X_1, X_2 \to$ linear classifier
- Features : $X_1, X_2, X_1X_2, X_1^2, \ldots \to$ non-linear classifier

Choosing the features

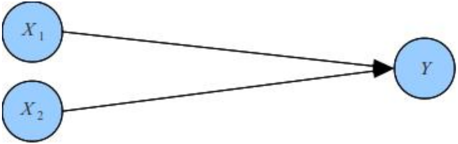
- To make it work, I created lots of extra features :
- $(X_1, X_2, X_1 X_2, X_1^2 X_2, X_1 X_2^2)^{(1,2,3,\ldots,10)}$

Choosing the features

- To make it work, I created lots of extra features :
- $(X_1, X_2, X_1X_2, X_1^2X_2, X_1X_2^2)^{(1,2,3,\ldots,10)}$
- Would it work with fewer features ?
- Test with $(X_1, X_2, X_1X_2, X_1^2X_2, X_1X_2^2)^{(1,2)}$

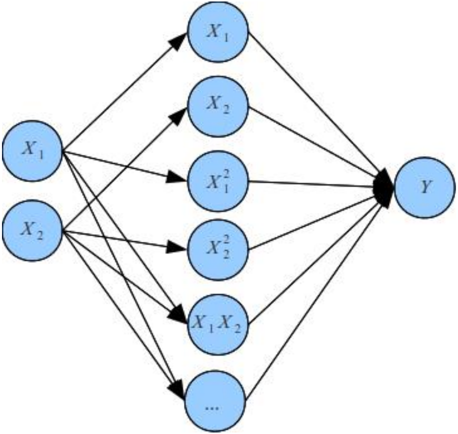
  Movie `non_linearly_separable_poly_2.avi`

A graphical view of the classifiers



$$f(X) = w_1 X_1 + w_2 X_2 + b$$

A graphical view of the classifiers



$$f(X) = w_1X_1 + w_2X_2 + w_3X_1^2 + w_4X_2^2 + w_5X_1X_2 + \dots$$

Non-linear features

- A linear classifier on a non-linear transformation is non-linear.
- A non-linear classifier relies on non-linear features.
- Which ones do we choose ?

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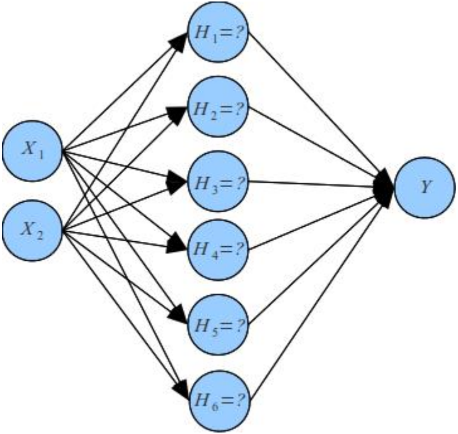
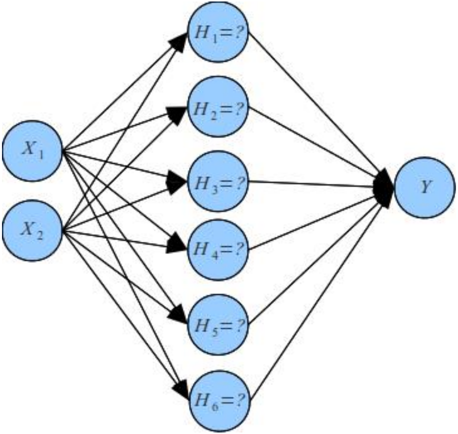
- Which ones do we choose ?
- Example : $H_j = X_1^{p_j} X_2^{q_j}$
- SVM : $H_j = K(X, X^{(j)})$ with K some kernel function
- Do they have to be predefined ?

Neural networks



- A neural network will learn the H_j's

Neural networks



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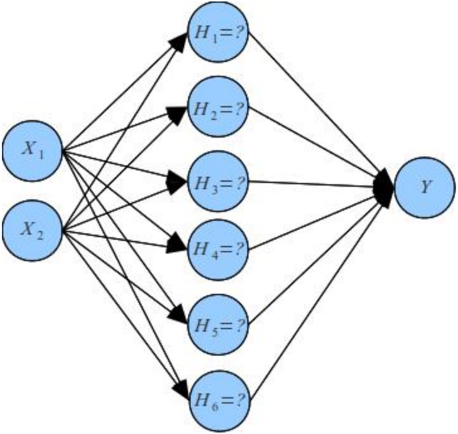
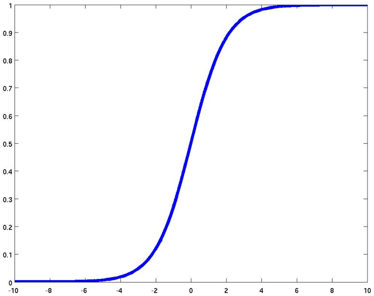


- A neural network will learn the H_j's
- Usually, we use $H_j = g(v_j^\top X)$
- H_j : Hidden unit
- v_j : Input weight
- g : Transfer function

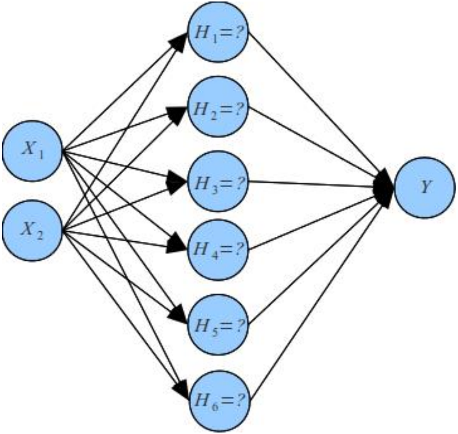
Transfer function

$$f(X) = \sum_j w_j H_j(X) + b = \sum_j w_j g(v_j^\top X) + b$$

- g is the *transfer function*.
- Usually, g is the sigmoid or the tanh.



Neural networks



$$f(X) = \sum_j w_j H_j(X) + b = \sum_j w_j g(v_j^\top X) + b$$

Example on the non-separable problem

Movie `non_linearly_separable_mlp_3.avi`

Training a neural network

- Dataset : $\left(X^{(i)}, Y^{(i)}\right)$ pairs, $i = 1, \ldots, N$.
- Goal : Find w and b such that

$$\operatorname{sign}\left(w^\top X^{(i)} + b\right) = Y^{(i)}$$

Training a neural network

- Dataset : $\left(X^{(i)}, Y^{(i)}\right)$ pairs, $i = 1, \ldots, N$.
- Goal : Find w and b to minimize

$$\sum_i \log\left(1 + \exp\left(-Y^{(i)}\left(w^\top X^{(i)} + b\right)\right)\right)$$

Training a neural network

- Dataset : $\left(X^{(i)}, Y^{(i)}\right)$ pairs, $i = 1, \ldots, N$.
- Goal : Find $v_1, \ldots, v_k$, w and b to minimize

$$\sum_i \log\left(1 + \exp\left(-Y^{(i)}\left[\sum_j w_j g\left(v_j^\top X^{(i)}\right)\right]\right)\right)$$

Neural network - 8 hidden units

Movie `non_linearly_separable_mlp_8.avi`

Neural network - 5 hidden units

Movie `non_linearly_separable_mlp_5.avi`

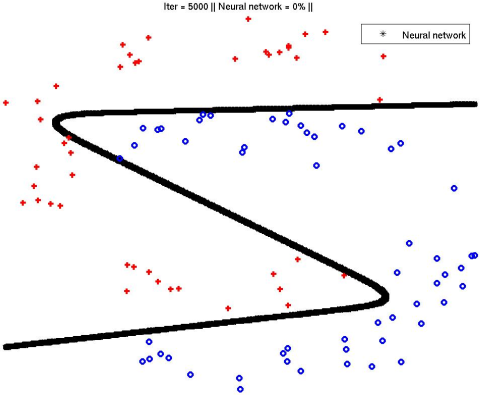
Neural network - 3 hidden units

Movie `non_linearly_separable_mlp_3.avi`

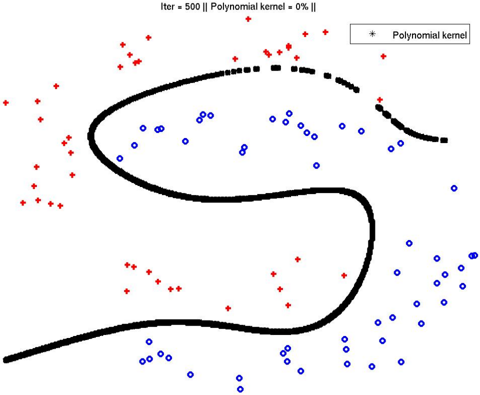
Neural network - 2 hidden units

Movie `non_linearly_separable_mlp_2.avi`

Non-linear classification



Non-linear classification



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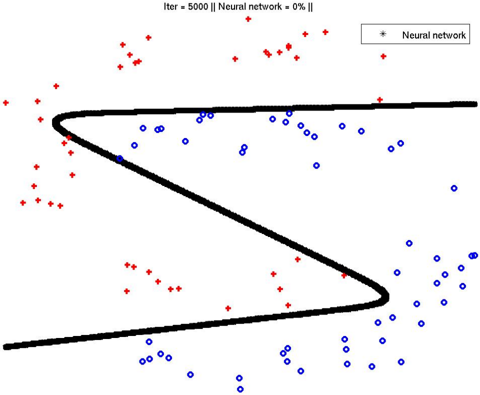


Cost function

s = cost function (logistic loss, hinge loss, ...)

$$\begin{aligned}\ell(v, w, b, X^{(i)}, Y^{(i)}) &= s\left(\widehat{Y}^{(i)}, Y^{(i)}\right)\\ &= s\left(\sum_j w_j H_j(X^{(i)}), Y^{(i)}\right)\\ &= s\left(\sum_j w_j g\left(v_j^\top X^{(i)}\right), Y^{(i)}\right)\end{aligned}$$

Backpropagation - Output weights

s = cost function (logistic loss, hinge loss, ...)

$$\widehat{Y}^{(i)} = \sum_j w_j H_j(X^{(i)})$$

$$\begin{aligned}\frac{\partial \ell(v, w, b, X^{(i)}, Y^{(i)})}{\partial w_j} &= \frac{\partial \ell(v, w, b, X^{(i)}, Y^{(i)})}{\partial \widehat{Y}^{(i)}} \frac{\partial \widehat{Y}^{(i)}}{\partial w_j} \\ &= \frac{\partial \ell(v, w, b, X^{(i)}, Y^{(i)})}{\partial \widehat{Y}^{(i)}} H_j(X^{(i)})\end{aligned}$$

Backpropagation - Input weights

s = cost function (logistic loss, hinge loss, ...)

$$\widehat{Y}^{(i)} = \sum_j w_j H_j(X^{(i)})$$
$$H_j(X^{(i)}) = g\left(v_j^\top X^{(i)}\right)$$

$$\begin{aligned}
\frac{\partial \ell(v, w, b, X^{(i)}, Y^{(i)})}{\partial v_j} &= \frac{\partial \ell(v, w, b, X^{(i)}, Y^{(i)})}{\partial H_j(X^{(i)})} \frac{\partial H_j(X^{(i)})}{\partial v_j} \\
&= \frac{\partial \ell(v, w, b, X^{(i)}, Y^{(i)})}{\partial \widehat{Y}^{(i)}} \frac{\partial \widehat{Y}^{(i)}}{\partial H_j(X^{(i)})} \frac{\partial H_j(X^{(i)})}{\partial v_j} \\
&= \frac{\partial \ell(v, w, b, X^{(i)}, Y^{(i)})}{\partial \widehat{Y}^{(i)}} w_j X^{(i)} g'\left(v_j^\top X^{(i)}\right)
\end{aligned}$$

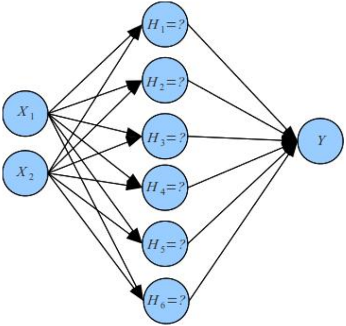
Training neural networks - Summary

- For each datapoint, compute the gradient of the cost with respect to the weights.
- Done using the backpropagation of the gradient.
- Convex with respect to the output weights (linear classifier).
- NOT convex with respect to the input weights : POTENTIAL PROBLEMS !

Neural networks - Summary

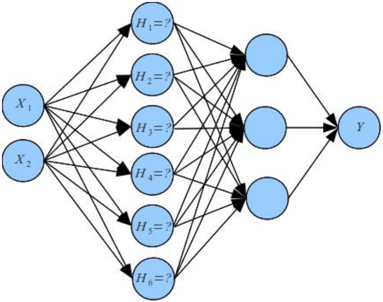
- A linear classifier in a feature space can model non-linear boundaries.
- Finding a good feature space is essential.
- One can design the feature map by hand.
- One can learn the feature map, using fewer features than if it done by hand.
- Learning the feature map is potentially HARD (non-convexity).

Neural networks - Not summary



- Linear combination of the output of soft classifiers.
- This is a non-linear classifier.
- One can take a linear combination of these.

Neural networks - Not summary



- Linear combination of the output of soft classifiers.
- This is a non-linear classifier.
- One can take a linear combination of these.
- This becomes a neural network with two hidden layers.

Advantages of neural networks

- They can learn anything.
- Extremely fast at test time (computing the answer for a new datapoint) because fewer features.
- Complete control over the power of the network (by controlling the hidden layers sizes).

Problems of neural networks

- Highly non-convex $\rightarrow$ many local minima
- Can learn anything but have more parameters $\rightarrow$ need tons of examples to be good.

Take-home messages

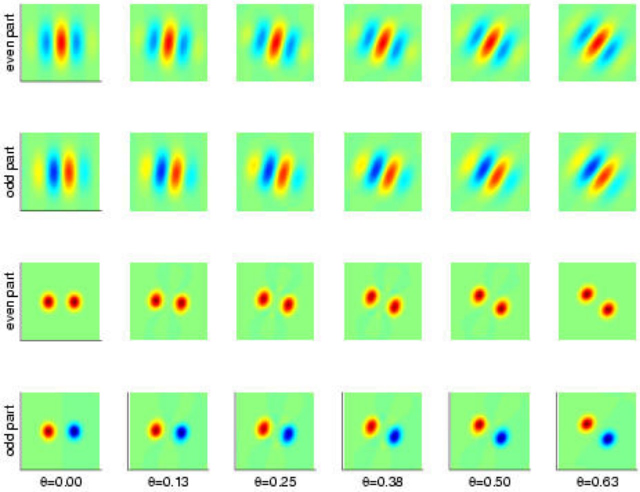
- Neural networks are potentially extremely efficient.
- But it is HARD to train them !
- If you wish to use them, be smart (or ask someone who knows) !
- If you have a huge dataset, they CAN be awesome !

v_j's for images

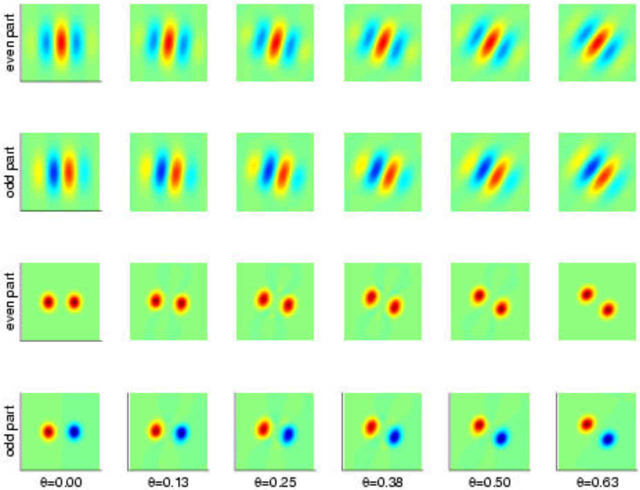
$$f(X) = \sum_j w_j H_j(X) + b = \sum_j w_j g(v_j^\top X) + b$$

- If X is an image, v_j is an image too.
- v_j acts as a filter (presence or absence of a pattern).
- What does v_j look like ?

v_j's for images - Examples



v_j's for images - Examples



- Filters are mostly local

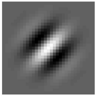
Basic idea of convolutional neural networks

- Filters are mostly local.
- Instead of using image-wide filters, use small ones over patches.
- Repeat for every patch to get a response image.
- Subsample the response image to get local invariance.

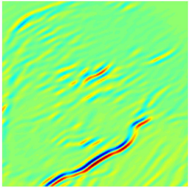
Filtering - Filter 1

Original image

Filter



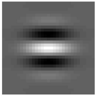
Output image



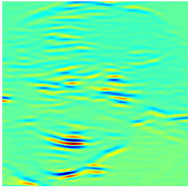
Filtering - Filter 2

Original image

Filter



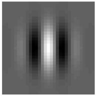
Output image



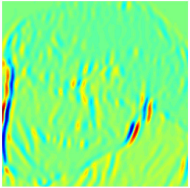
Filtering - Filter 3

Original image

Filter



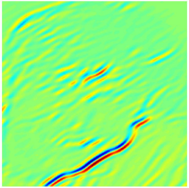
Output image



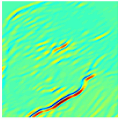
Pooling - Filter 1

Original image

Output image



Subsampled image



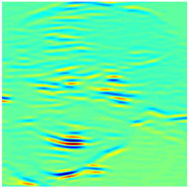
How to do 2x subsampling-pooling :

- Output image = O, subsampled image = S.
- $S_{ij} = \max_{k \text{ over window around } (2i,2j)} O_k$.

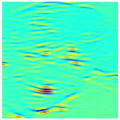
Pooling - Filter 2

Original image

Output image



Subsampled image



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Pooling - Filter 3

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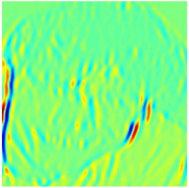
Output image



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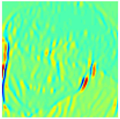

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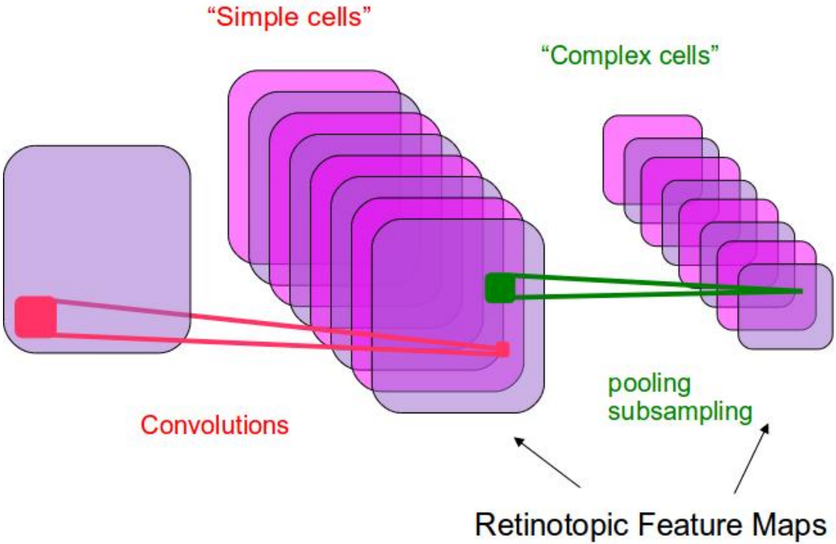
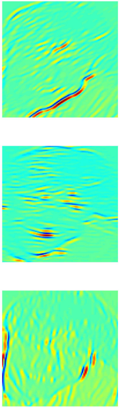
A convolutional layer



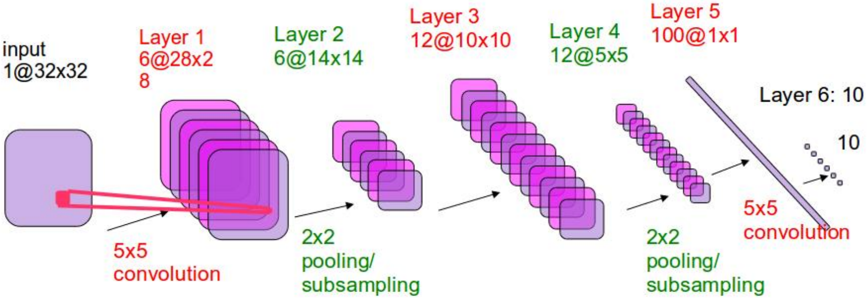
Transforming the data with a layer

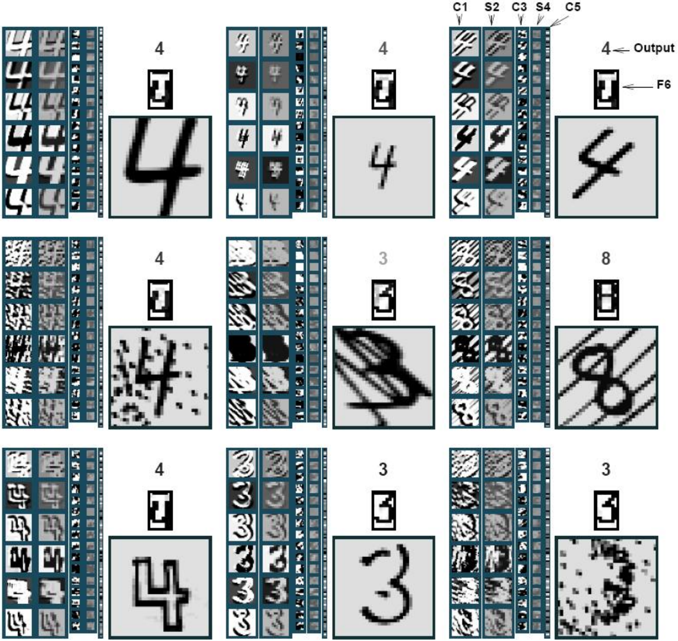
Original datapoint

New datapoint



A convolutional network




C1
S2
C3
S4
C5
4
4
4
Output
F6
4
3
8
4
3
3

Face detection

Face detection

NORB dataset

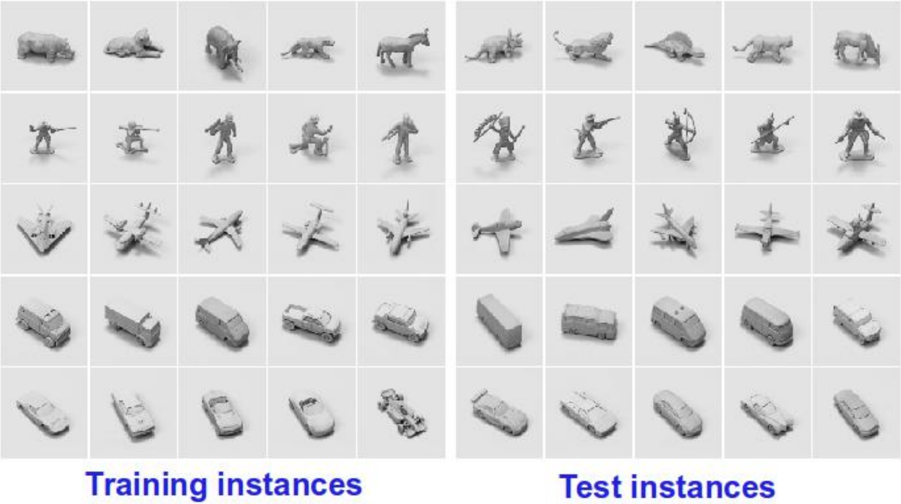
- 50 toys belonging to 5 categories
  - animal, human figure, airplane, truck, car
- 10 instance per category
  - 5 instances used for training, 5 instances for testing
- Raw dataset
  - 972 stereo pairs of each toy. 48,600 image pairs total.

NORB dataset - 2

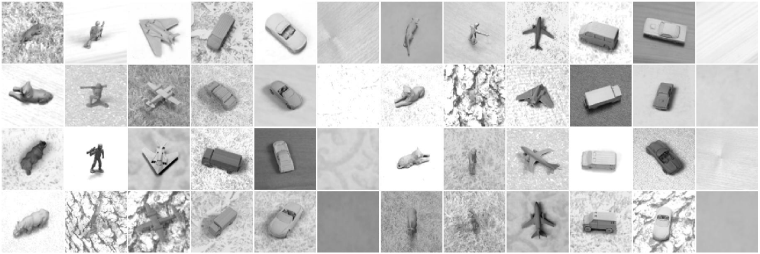
For each instance :

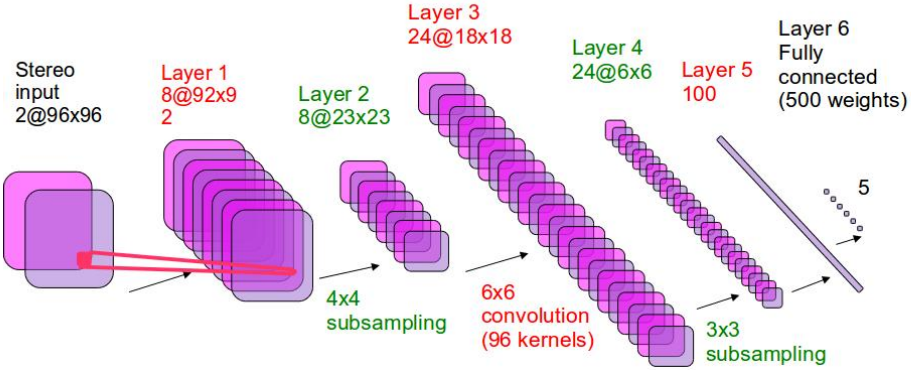
- 18 azimuths
- 0 to 350 degrees every 20 degrees
- 9 elevations
- 30 to 70 degrees from horizontal every 5 degrees
- 6 illuminations
- on/off combinations of 4 lights
- 2 cameras (stereo), 7.5 cm apart
- 40 cm from the object

NORB dataset - 3



Textured and cluttered versions





- 90,857 free parameters, 3,901,162 connections.
- The entire network is trained end-to-end (all the layers are trained simultaneously).

Normalized-Uniform set

Method	Error
Linear Classifier on raw stereo images	30.2%
K-Nearest-Neighbors on raw stereo images	18.4%
K-Nearest-Neighbors on PCA-95	16.6%
Pairwise SVM on 96x96 stereo images	11.6%
Pairwise SVM on 95 Principal Components	13.3%
Convolutional Net on 96x96 stereo images	5.8%

Jittered-Cluttered Dataset

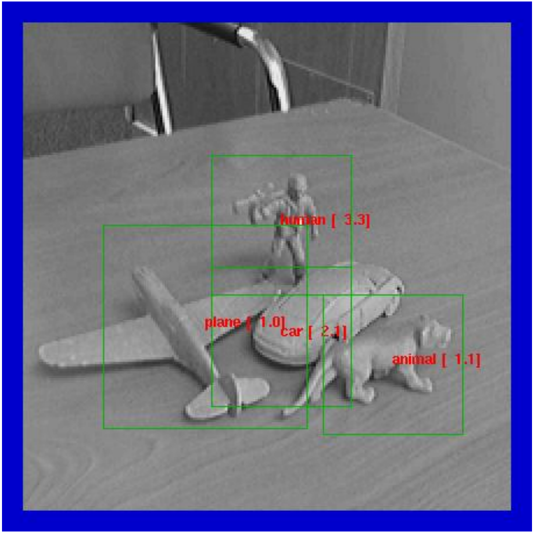
- 291,600 stereo pairs for training, 58,320 for testing
- Objects are jittered
  - position, scale, in-plane rotation, contrast, brightness, backgrounds, distractor objects,...
- Input dimension : 98x98x2 (approx 18,000)

Jittered-Cluttered Dataset - Results

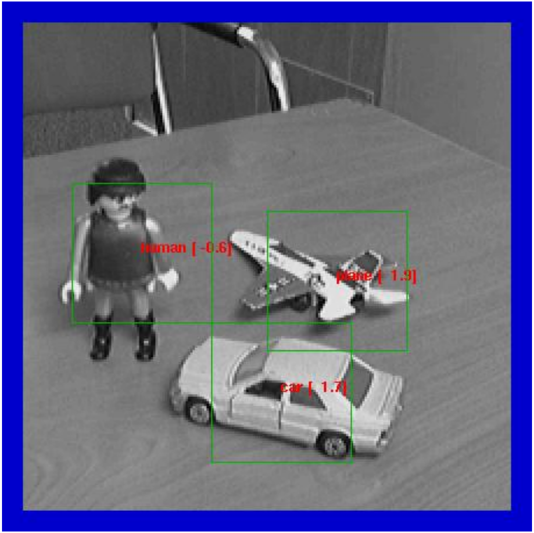
Method	Error
SVM with Gaussian kernel	43.3%
Convolutional Net with binocular input	7.8%
Convolutional Net + SVM on top	5.9%
Convolutional Net with monocular input	20.8%
Smaller mono net (DEMO)	26.0%

Dataset available from `http://www.cs.nyu.edu/~yann`

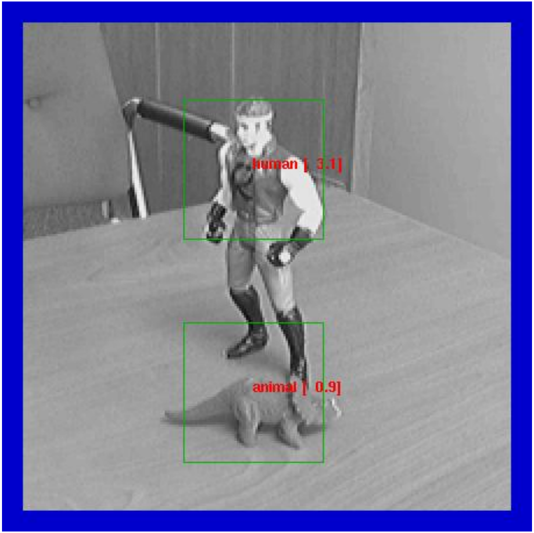
NORB recognition - 1



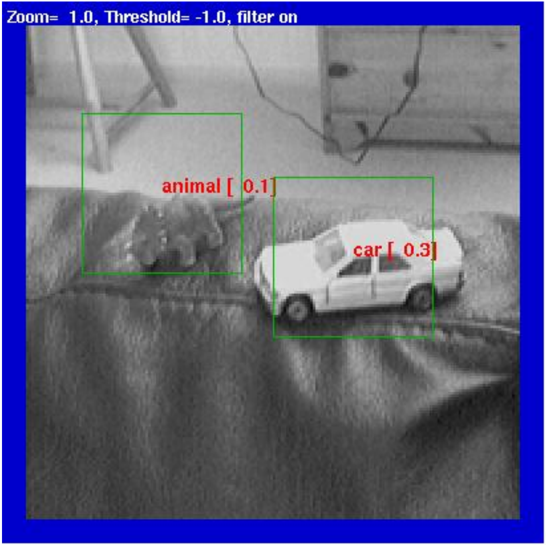
NORB recognition - 2



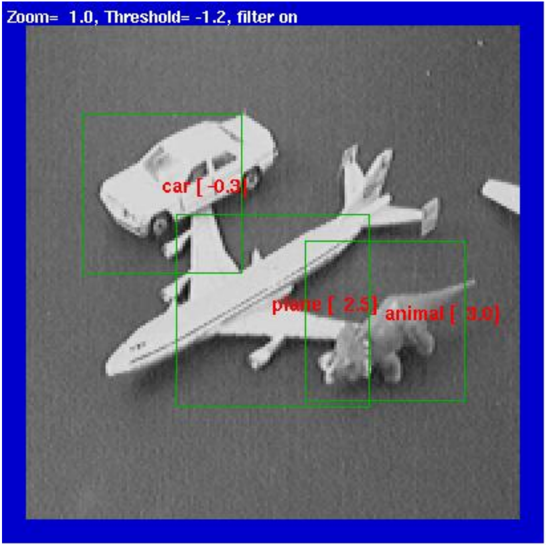
NORB recognition - 3



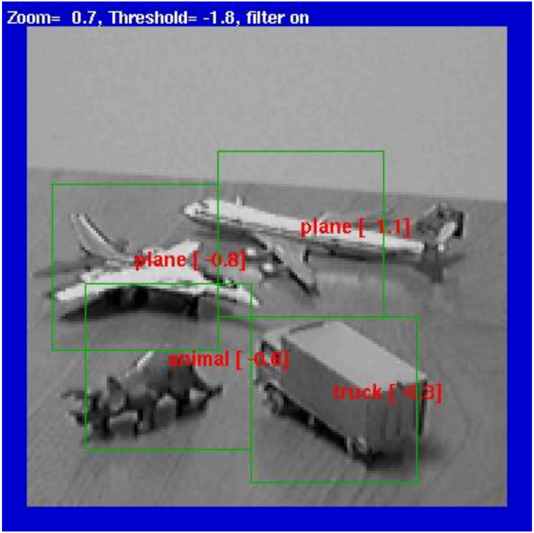
NORB recognition - 4



NORB recognition - 5



NORB recognition - 6



Summary

- With complex problems, it is hard to design features by hand.
- Neural networks circumvent this problem.
- They can be hard to train (again...).
- Convolutional neural networks use knowledge about locality in images.
- They are much easier than standard networks.
- And they are FAST (again...).

What has not been covered

- In some cases, we have lots of data, but without the labels.
- *Unsupervised* learning.
- There are techniques to use these data to get better performance.
- E.g. : *Task-Driven Dictionary Learning*, Mairal et al.

The need for fast learning

- Neural networks may need many examples (several millions or more).
- We need to be able to use them quickly.

Batch methods

$$L(\theta) = \frac{1}{N}\sum_i \ell(\theta, X^{(i)}, Y^{(i)})$$

$$\theta_{t+1} \to \theta_t - \frac{\alpha_t}{N}\sum_i \frac{\partial \ell(\theta, X^{(i)}, Y^{(i)})}{\partial \theta}$$

- To compute one update of the parameters, we need to go through all the data.
- This can be very expensive.
- What if we have an infinite amount of data ?

Potential solutions

1. Discard data.
   - Seems stupid
   - Yet many people do it

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1. Discard data.
   - Seems stupid
   - Yet many people do it
2. Use approximate methods.
   - Update = average of the updates for all datapoints.
   - Are these update really different ?
   - If not, how can we learn faster ?

Stochastic gradient descent

$$L(\theta) = \frac{1}{N}\sum_i \ell(\theta, X^{(i)}, Y^{(i)})$$

$$\theta_{t+1} \to \theta_t - \frac{\alpha_t}{N}\sum_i \frac{\partial \ell(\theta, X^{(i)}, Y^{(i)})}{\partial \theta}$$

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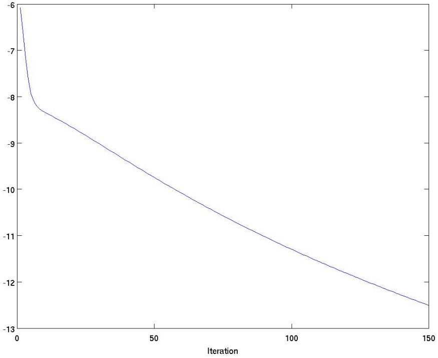
What do we lose when updating the parameters to satisfy just one example ?

Disagreement



- $\|\mu\|^2/\sigma^2$ during optimization (log scale)
- As optimization progresses, disagreement increases
- Early on, one can pick one example at a time
- What about later ?

Training vs test

Standard learning paradigm :

- We want to solve a task on new datapoints.
- We have a training set.
- We hope that the performance on the training set is informative of the performance on new datapoints.

Can we know when we start overfitting ?

Overfitting

- When all gradients disagree, stochastic error stalls.
- When all gradients disagree, training and test error part.

IT DOES NOT MATTER IF ONE DOES NOT REACH THE MINIMUM OF THE TRAINING ERROR !

Decomposition of the error

$$
\begin{aligned}
E(\tilde{f}_n) - E(f^*) = {} & E(f^*_{\mathcal{F}}) - E(f^*) \text{ Approximation error} \\
& + E(f_n) - E(f^*_{\mathcal{F}}) \text{ Estimation error} \\
& + E(\tilde{f}_n) - E(f_n) \text{ Optimization error}
\end{aligned}
$$

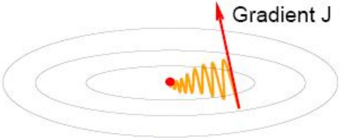
Questions :

1. Do we optimize the training error to decrease $E(\tilde{f}_n) - E(f_n)$?
2. Do we increase n to decrease $E(f_n) - E(f^*_{\mathcal{F}})$?

Gradient Descent (GD)

Iterate

- $w_{t+1} \leftarrow w_t - \eta \frac{\partial E_n(f_{w_t})}{\partial w}$



Best speed achieved with fixed learning rate $\eta = \frac{1}{\lambda_{\max}}$.
(e.g., Dennis & Schnabel, 1983)

	Cost per iteration	Iterations to reach ρ	Time to reach accuracy ρ	Time to reach $E(\tilde{f}_n) - E(f^*_{\mathcal{F}}) < \varepsilon$
GD	$\mathcal{O}(nd)$	$\mathcal{O}\left(\kappa \log \frac{1}{\rho}\right)$	$\mathcal{O}\left(nd\kappa \log \frac{1}{\rho}\right)$	$\mathcal{O}\left(\frac{d^2\kappa}{\varepsilon^{1/\alpha}} \log^2 \frac{1}{\varepsilon}\right)$

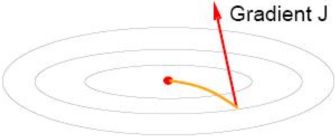
– In the last column, n and ρ are chosen to reach ε as fast as possible.
– Solve for ε to find the best error rate achievable in a given time.
– Remark: abuses of the $\mathcal{O}()$ notation

Slide from Léon Botton

Second Order Gradient Descent (2GD)

Iterate

- $w_{t+1} \leftarrow w_t - H^{-1} \dfrac{\partial E_n(f_{w_t})}{\partial w}$



We assume H^{-1} is known in advance.
Superlinear optimization speed (e.g., Dennis & Schnabel, 1983)

	Cost per iteration	Iterations to reach ρ	Time to reach accuracy ρ	Time to reach $E(\tilde{f}_n) - E(f^*_{\mathcal{F}}) < \varepsilon$
2GD	$\mathcal{O}(d(d+n))$	$\mathcal{O}\left(\log\log\frac{1}{\rho}\right)$	$\mathcal{O}\left(d(d+n)\log\log\frac{1}{\rho}\right)$	$\mathcal{O}\left(\frac{d^2}{\varepsilon^{1/\alpha}}\log\frac{1}{\varepsilon}\log\log\frac{1}{\varepsilon}\right)$

– Optimization speed is much faster.
– Learning speed only saves the condition number κ.

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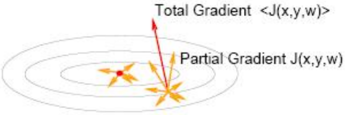
Stochastic Gradient Descent (SGD)

Iterate

- Draw random example (x_t, y_t).
- $w_{t+1} \leftarrow w_t - \frac{\eta}{t} \frac{\partial \ell(f_{w_t}(x_t), y_t)}{\partial w}$



Best decreasing gain schedule with $\eta = \frac{1}{\lambda_{\min}}$.
(see Murata, 1998; Bottou & LeCun, 2004)

	Cost per iteration	Iterations to reach ρ	Time to reach accuracy ρ	Time to reach $E(\tilde{f}_n) - E(f^*_{\mathcal{F}}) < \varepsilon$
SGD	$\mathcal{O}(d)$	$\frac{\nu k}{\rho} + o\left(\frac{1}{\rho}\right)$	$\mathcal{O}\left(\frac{d \nu k}{\rho}\right)$	$\mathcal{O}\left(\frac{d \nu k}{\varepsilon}\right)$

With $1 \leq k \leq \kappa^2$

- Optimization speed is *catastrophic*.
- Learning speed does not depend on the statistical estimation rate α.
- Learning speed depends on condition number κ but *scales very well*.

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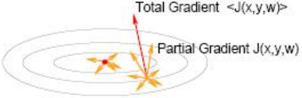
Second order Stochastic Descent (2SGD)

Iterate

- Draw random example (x_t, y_t).
- $w_{t+1} \leftarrow w_t - \frac{1}{t} H^{-1} \frac{\partial \ell(f_{w_t}(x_t), y_t)}{\partial w}$



Replace scalar gain $\frac{\eta}{t}$ by matrix $\frac{1}{t} H^{-1}$.

	Cost per iteration	Iterations to reach ρ	Time to reach accuracy ρ	Time to reach $E(\tilde{f}_n) - E(f^*_{\mathcal{F}}) < \varepsilon$
2SGD	$\mathcal{O}(d^2)$	$\frac{\nu}{\rho} + o\left(\frac{1}{\rho}\right)$	$\mathcal{O}\left(\frac{d^2\,\nu}{\rho}\right)$	$\mathcal{O}\left(\frac{d^2\,\nu}{\varepsilon}\right)$

– Each iteration is d times more expensive.
– The number of iterations is reduced by κ^2 (or less.)
– Second order only changes the constant factors.

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In practice :

- You will ALMOST ALWAYS have enough data.
- You will ALMOST ALWAYS lack time.
- You must ALMOST ALWAYS use stochastic methods.
- How to use accelerated techniques remains to be seen.