Who is afraid of non-convex loss functions?

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Convex Shmonvex

- **The NIPS community has suffered of an acute convexivitis epidemic**
  - ML applications seem to have trouble moving beyond logistic regression, SVMs, and exponential-family graphical models.
  - For a new ML model, convexity is viewed as a virtue
  - Convexity is sometimes a virtue
  - But it is often a limitation
  - ML theory has essentially never moved beyond convex models
    - the same way control theory has not really moved beyond linear systems
  - Often, the price we pay for insisting on convexity is an unbearable increase in the size of the model, or the scaling properties of the optimization algorithm [O(n^2), O(n^3)...]
  - SDP-based manifold learning, QP-based kernel method, CRF. MMMN, ...

Convex Shmonvex

- **Other communities aren't as afraid as we are of non-convex optimization**
  - handwriting recognition
    - HMMs and Graph-Transformer-Network-based systems are non-convex
  - speech recognition
    - discriminative HMMs are non convex
- **This is not by choice: non-convex models simply work better**
  - have you tried acoustic modeling in speech with a convex loss?

To solve complicated AI taks, ML will have to go non-convex

- **paraphrasing the deep learning satellite session: Ultimately, complex learning tasks (e.g. vision, speech, language) will be implemented with "deep" hierarchical systems.**
  - To learn hierarchical representations (low-level features, mid-level representations, high-level concepts....), we need "deep architectures".
  - These inevitably lead to non-convex loss functions
- **But wait! don't we have theorems that "shallow" (and convex) kernel methods can learn anything?**
  - Yes. But that says nothing about the efficiency of the representation.
  - For example: there is empirical and theoretical evidence that shallow architectures cannot implement invariant visual recognition tasks efficiently
  - see [Bengio & LeCun 07] "scaling learning algorithms towards AI"

Best Results on MNIST (from raw images: no preprocessing)

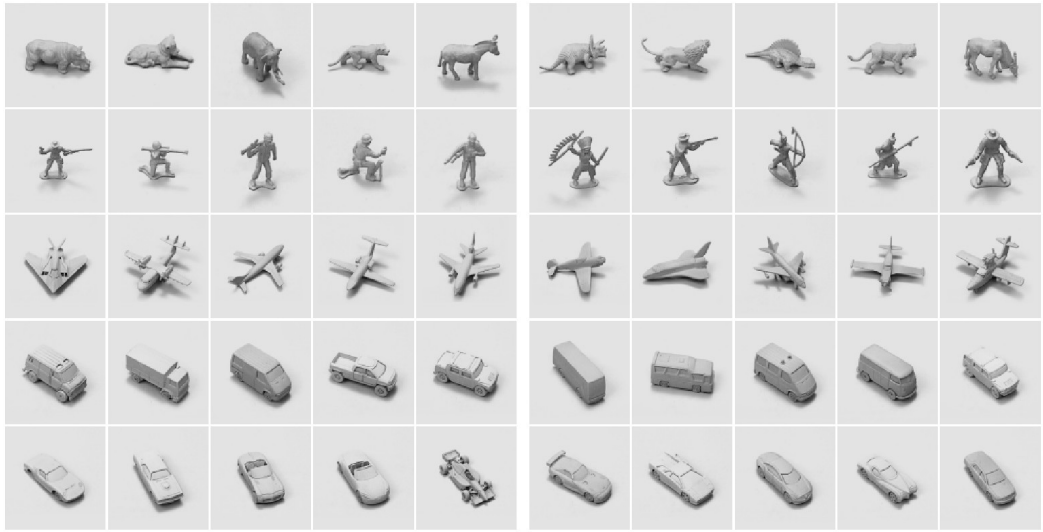
CLASSIFIER	DEFORMATION	ERROR	Reference
Knowledge-free methods			
2-layer NN, 800 HU, CE		1.60	Simard et al., ICDAR 2003
3-layer NN, 500+300 HU, CE, reg		1.53	Hinton, in press, 2005
SVM, Gaussian Kernel		1.40	Cortes 92 + Many others
Unsupervised Stacked RBM + backprop		0.95	Hinton, in press, 2005
Convolutional nets			
Convolutional net LeNet-5,		0.80	LeCun 2005 Unpublished
Convolutional net LeNet-6,		0.70	LeCun 2006 Unpublished
Conv. net LeNet-6- + unsup learning		0.60	LeCun 2006 Unpublished
Training set augmented with Affine Distortions			
2-layer NN, 800 HU, CE	Affine	1.10	Simard et al., ICDAR 2003
Virtual SVM deg-9 poly	Affine	0.80	Scholkopf
Convolutional net, CE	Affine	0.60	Simard et al., ICDAR 2003
Training et augmented with Elastic Distortions			
2-layer NN, 800 HU, CE	Elastic	0.70	Simard et al., ICDAR 2003
Convolutional net, CE	Elastic	0.40	Simard et al., ICDAR 2003
Conv. net LeNet-6- + unsup learning	Elastic	0.38	LeCun 2006 Unpublished

Convexity is Overrated

- **Using a suitable architecture (even if it leads to non-convex loss functions) is more important than insisting on convexity (particularly if it restricts us to unsuitable architectures)**
  - e.g.: Shallow (convex) classifiers versus Deep (non-convex) classifiers
- **Even for shallow/convex architecture, such as SVM, using non-convex loss functions actually improves the accuracy and speed**
  - See "trading convexity for efficiency" by Collobert, Bottou, and Weston, ICML 2006 (best paper award)

Normalized-Uniform Set: Error Rates

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



Training instances Test instances

Normalized-Uniform Set: Learning Times

	SVM	Conv Net				SVM/Conv
test error	11.6%	10.4%	6.2%	5.8%	6.2%	5.9%
train time (min*GHz)	480	64	384	640	3,200	50+
test time per sample (sec*GHz)	0.95	0.03				0.04+
#SV	28%					28%
parameters	σ=2,000 C=40					dim=80 σ=5 C=0.01

SVM: using a parallel implementation by Graf, Durdanovic, and Cosatto (NEC Labs)

Chop off the last layer of the convolutional net and train an SVM on it

Experiment 2: Jittered-Cluttered Dataset

- 291,600 training samples, 58,320 test samples
- SVM with Gaussian kernel — 43.3% error
- Convolutional Net with binocular input: — 7.8% error
- Convolutional Net + SVM on top: — 5.9% error
- Convolutional Net with monocular input: — 20.8% error
- Smaller mono net (DEMO): — 26.0% error
- Dataset available from http://www.cs.nyu.edu/~yann

Jittered-Cluttered Dataset

	SVM	Conv Net			SVM/Conv
test error	43.3%	16.38%	7.5%	7.2%	5.9%
train time (min*GHz)	10,944	420	2,100	5,880	330+
test time per sample (sec*GHz)	2.2	0.04			0.06+
#SV	5%				2%
parameters	σ=10^4 C=40				dim=100 σ=5 C=1

OUCH!

The convex loss, VC bounds and representers theorems don't seem to help

Chop off the last layer, and train an SVM on it it works!

Optimization algorithms for learning

- **Neural nets:**
  - conjugate gradient, BFGS, LM-BFGS, ... don't work as well as stochastic gradient
- **SVM:**
  - "batch" quadratic programming methods don't work as well as SMO. SMO don't work as well as recent on-line methods
- **CRF:**
  - Iterative scaling (or whatever) doesn't work as well as stochastic gradient (Schraudolph et al ICML 2006)
  - The discriminative learning folks in speech and handwriting recognition have known this for a long time
- **Stochastic gradient has no good theoretical guarantees**
  - That doesn't mean we shouldn't use them, because the empirical evidence that it works better is overwhelming

Theoretical Guarantees are overrated

- When Empirical Evidence suggests a fact for which we don't have theoretical guarantees, it just means the theory is inadequate.
- When empirical evidence and theory disagree, the theory is wrong.
- Let's not be afraid of methods for which we have no theoretical guarantee, particularly if they have been shown to work well
- But, let's aggressively look to those theoretical guarantees.
- We should use our theoretical understanding to expand our creativity, not to restrict it.

The visual system is "deep" and learned

- **The primate's visual system is "deep"**
  - It has 10-20 layers of neurons from the retina to the infero-temporal cortex (where object categories are encoded).
  - How does it train itself by just looking at the world?.
- **Is there a magic bullet for visual learning?**
  - The neo-cortex is pretty much the same all over
  - The "learning algorithm" it implements is not specific to a modality (what works for vision works for audition)
  - There is evidence that everything is learned, down to low-level feature detectors in V1
  - Is there a universal learning algorithm/architecture which, given a small amount of appropriate prior structure, can produce an intelligent vision system?
  - Or do we have to keep accumulating a large repertoire of pre-engineered "modules" to solve every specific problem an intelligent vision system must solve?

Do we really need deep architectures?

- **We can approximate any function as close as we want with shallow architecture. Why would we need deep ones?**

$$y = \sum_{i=1}^{P} \alpha_i K(X, X^i) \qquad y = F(W^1.F(W^0.X))$$

  - kernel machines and 2-layer neural net are "universal".

- **Deep learning machines**

$$y = F(W^K.F(W^{K-1}.F(....F(W^0.X)...)))$$

- **Deep machines are more efficient for representing certain classes of functions, particularly those involved in visual recognition**
  - they can represent more complex functions with less "hardware"

- **We need an efficient parameterization of the class of functions that we need to build intelligent machines (the "AI-set")**

Why are Deep Architectures More Efficient?

- **A deep architecture trades space for time**
  - more layers (more sequential computation),
  - but less hardware (less parallel computation).
  - Depth-Breadth tradoff
- **Example1: N-bit parity**
  - requires N-1 XOR gates in a tree of depth log(N).
  - requires an exponential number of gates of we restrict ourselves to 2 layers (DNF formula with exponential number of minterms).
- **Example2: circuit for addition of 2 N-bit binary numbers**
  - Requires O(N) gates, and O(N) layers using N one-bit adders with ripple carry propagation.
  - Requires lots of gates (some polynomial in N) if we restrict ourselves to two layers (e.g. Disjunctive Normal Form).
  - Bad news: almost all boolean functions have a DNF formula with an exponential number of minterms O(2^N).....

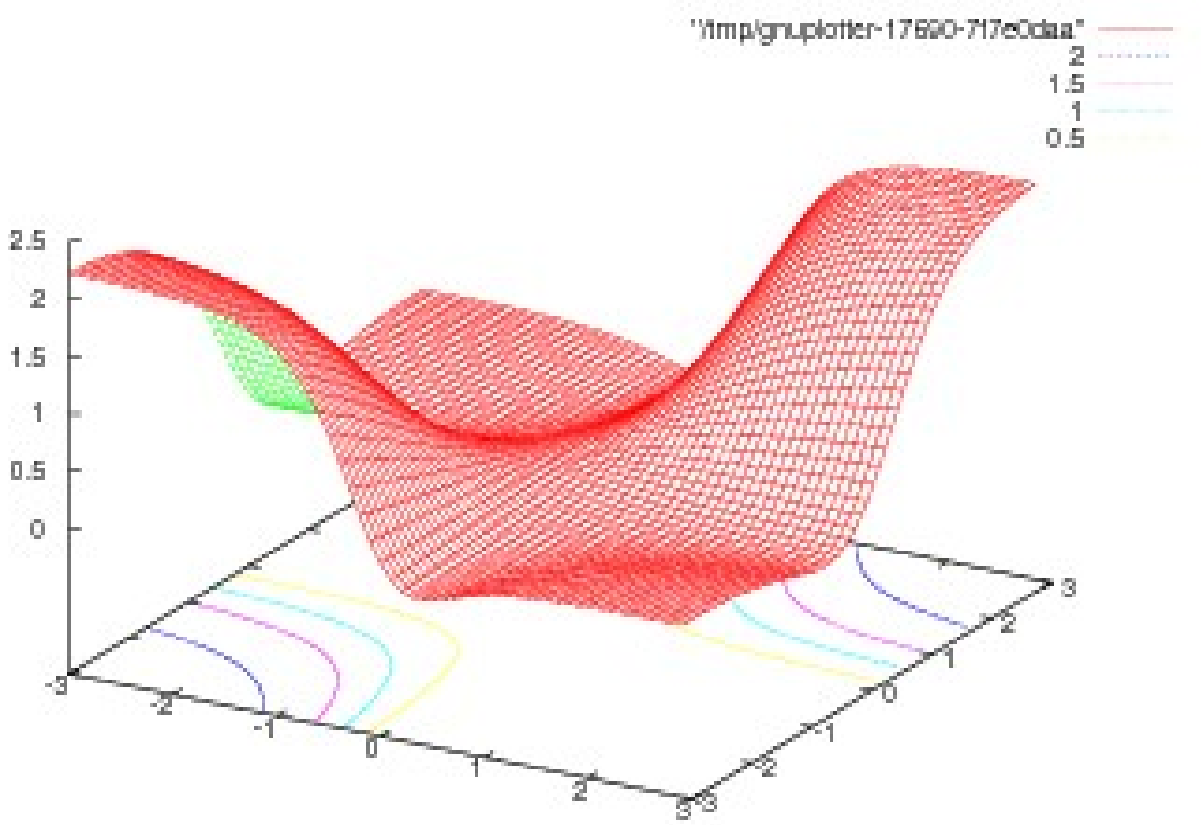
Strategies (after Hinton 2007)

- **Defeatism: since no good parameterization of the AI-set is available, let's parameterize a much smaller set for each specific task through careful engineering (preprocessing, kernel....).**
- **Denial: kernel machines can approximate anything we want, and the VC-bounds guarantee generalization. Why would we need anything else?**
  - unfortunately, kernel machines with common kernels can only represent a tiny subset of functions efficiently
- **Optimism: Let's look for learning models that can be applied to the largest possible subset of the AI-set, while requiring the smallest amount of task-specific knowledge for each task.**
  - There is a parameterization of the AI-set with neurons.
  - Is there an efficient parameterization of the AI-set with computer technology?
- **Today, the ML community oscillates between defeatism and denial.**

Deep Learning is Hard?

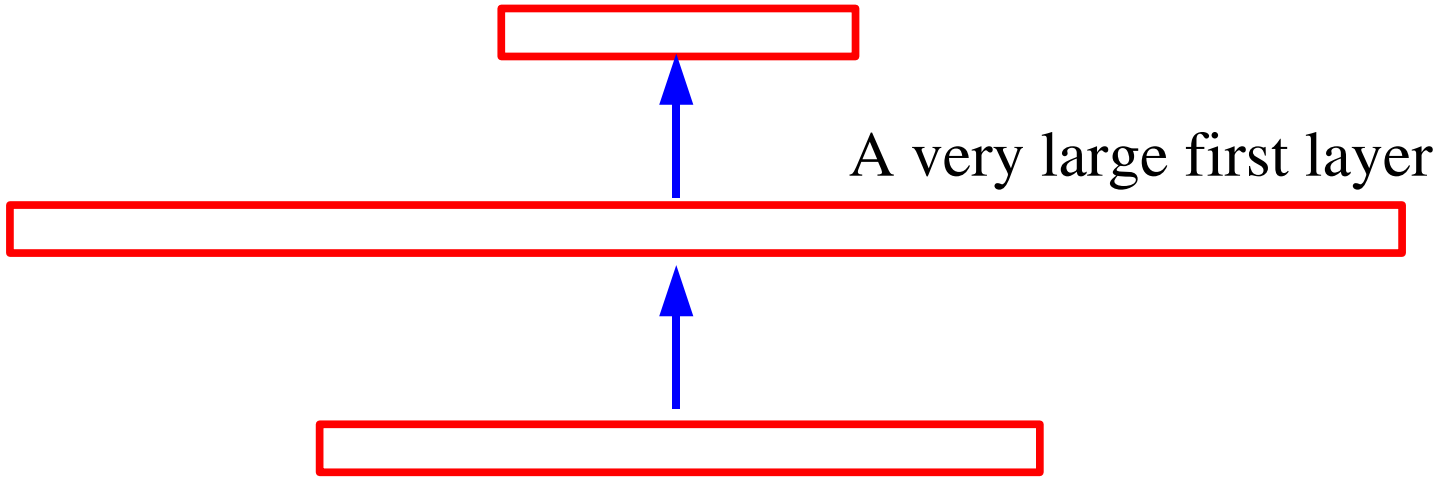
- **Example: what is the loss function for the simplest 2-layer neural net ever**
  - Function: 1-1-1 neural net. Map 0.5 to 0.5 and -0.5 to -0.5 (identity function) with quadratic cost:

$$y = \tanh(W_1 \tanh(W_0.x)) \quad L = (0.5 - \tanh(W_1 \tanh(W_0 0.5)^2$$



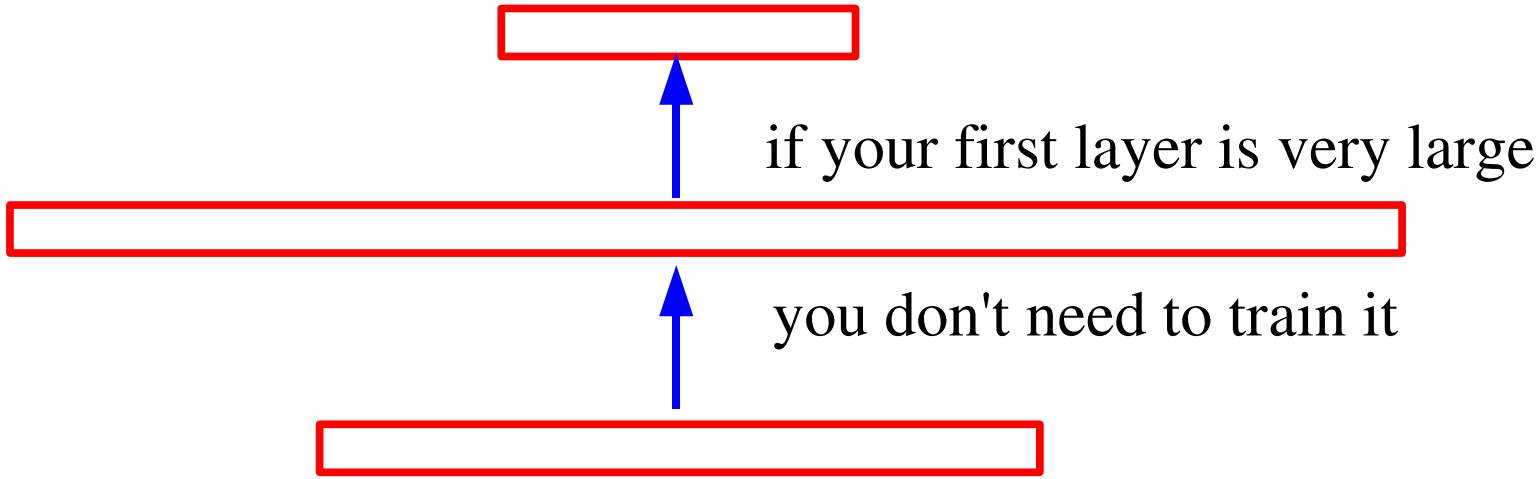
Deep Learning is Hard?

- The loss surface is non-convex, ill-conditioned, has saddle points, has flat spots.....
- For large networks, it will be horrible!
- It will be horrible if the network is tall and skinny.
- It won't be too bad if the network is short and fat.



Shallow models

- **1957: perceptron: fixed/random first layer. Trainable second layer**
- **1985: backprop: both layers are trained. But many people are afraid of the lack of convergence guarantees**
- **1992: kernel machines: large first layer with one template matcher for each training sample. Trainable second layer**
  - sparsity in the second layer with hinge loss helps with efficiency, but not with accuracy



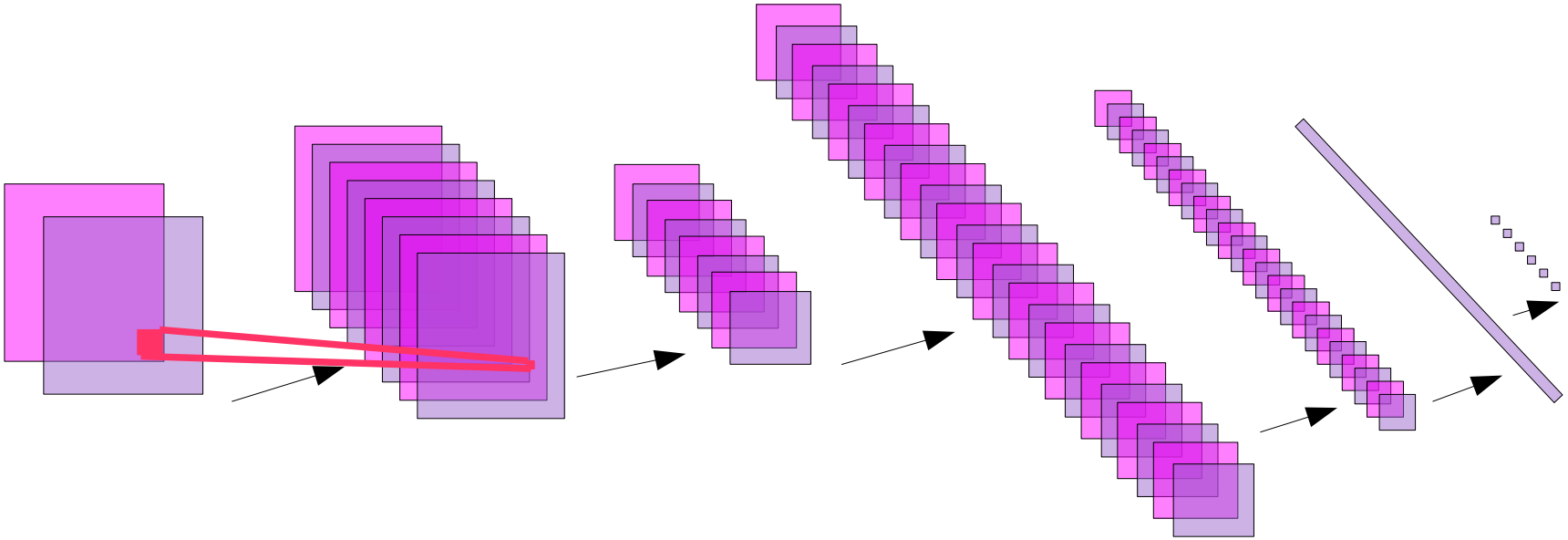
The Problem with Non-Convex Learning

- **None of what you read in the optimization literature applies**
  - (see Leon Bottou's tutorial at NIPS 2007)
- **You need to use stochastic methods to take advantage of the redudancy in the data**
- **stochastic methods have horrible asymptotic properties, but that is irrelevant**
  - they converge very quickly to the "best solution" as measured by the test error
- **the optimization literature does not talk about stochastic methods**
  - forget about conjugate gradient, LM-BFGS, BFGS, Quasi-Newton...
- **the optimization literature deals with problems where O(N^2) is OK**
  - when you have 10^6 parameters, O(N) is all you can afford.

Back-prop learning is not as bad as it seems

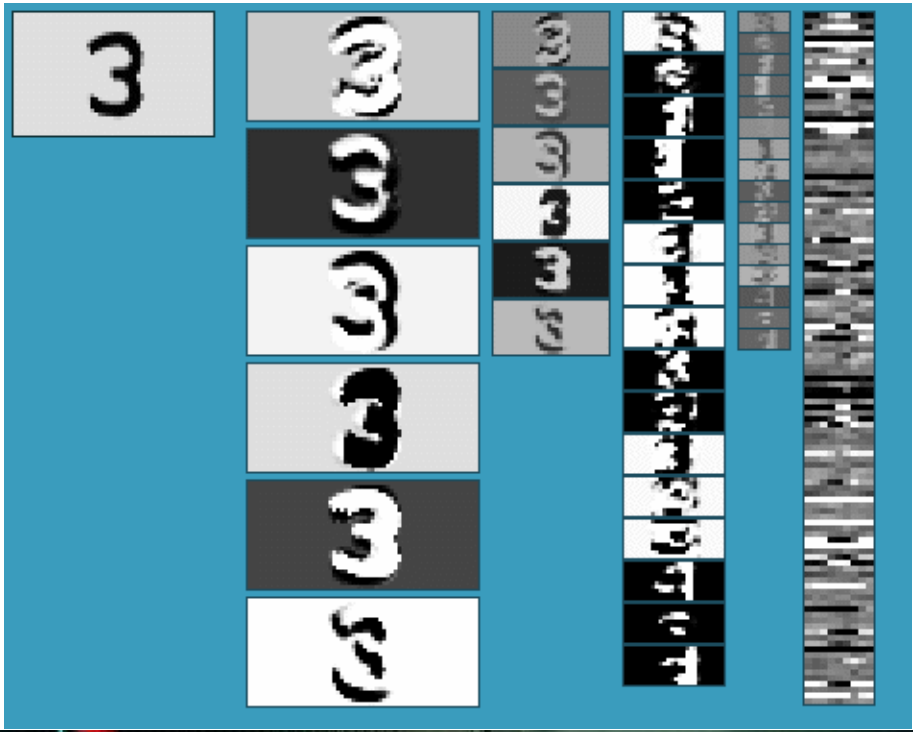
- **gradient descent is unreliable when the network is small, particularly when the network has just the right size to learn the problem**
- **the solution is to make the network much larger than necessary and regularize it (SVM taught us that).**
- **Although there are lots of local minima, many of them are equivalent**
  - it doesn't matter which one you fall into
  - with large nets, back-prop yields very consistent results
- **Many local minima are due to symmetries in the system**
- **Breaking the symmetry in the architecture solves many problems**
  - this may be why convolutional nets work so well

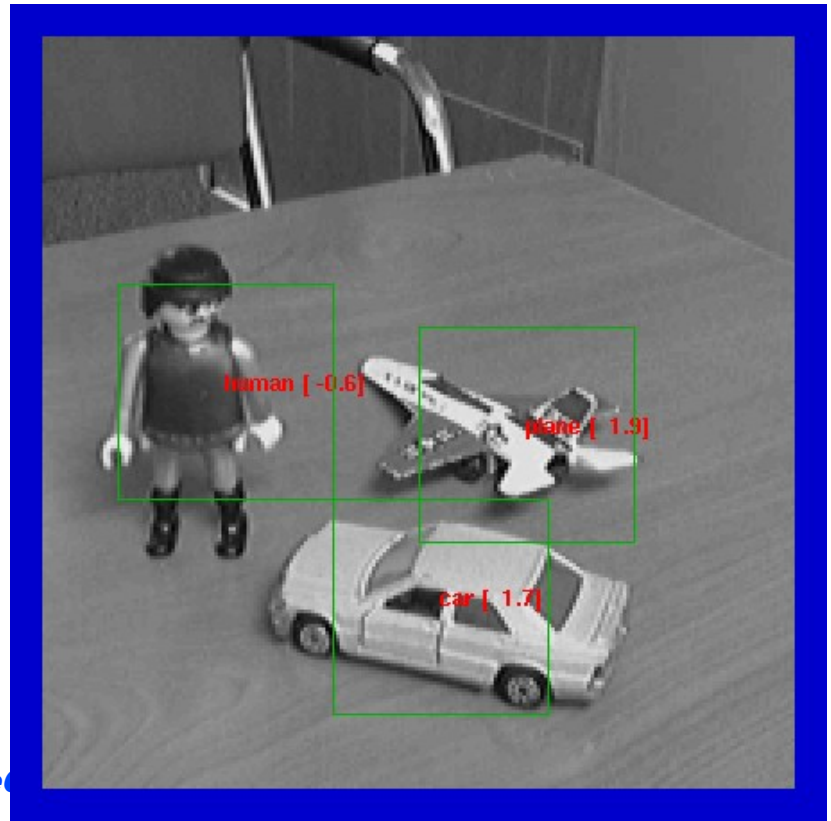
Convolutional Networks

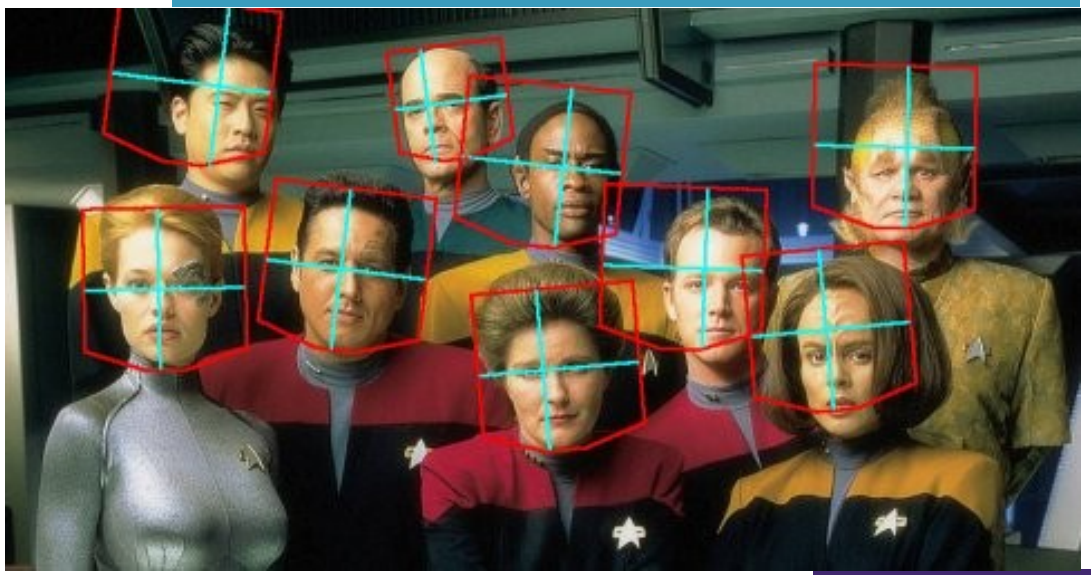


Deep Supervised Learning works well with lots of data

- **Supervised Convolutional nets work very well for:**
  - handwriting recognition(winner on MNIST)
  - face detection
  - object recognition with few classes and lots of training samples





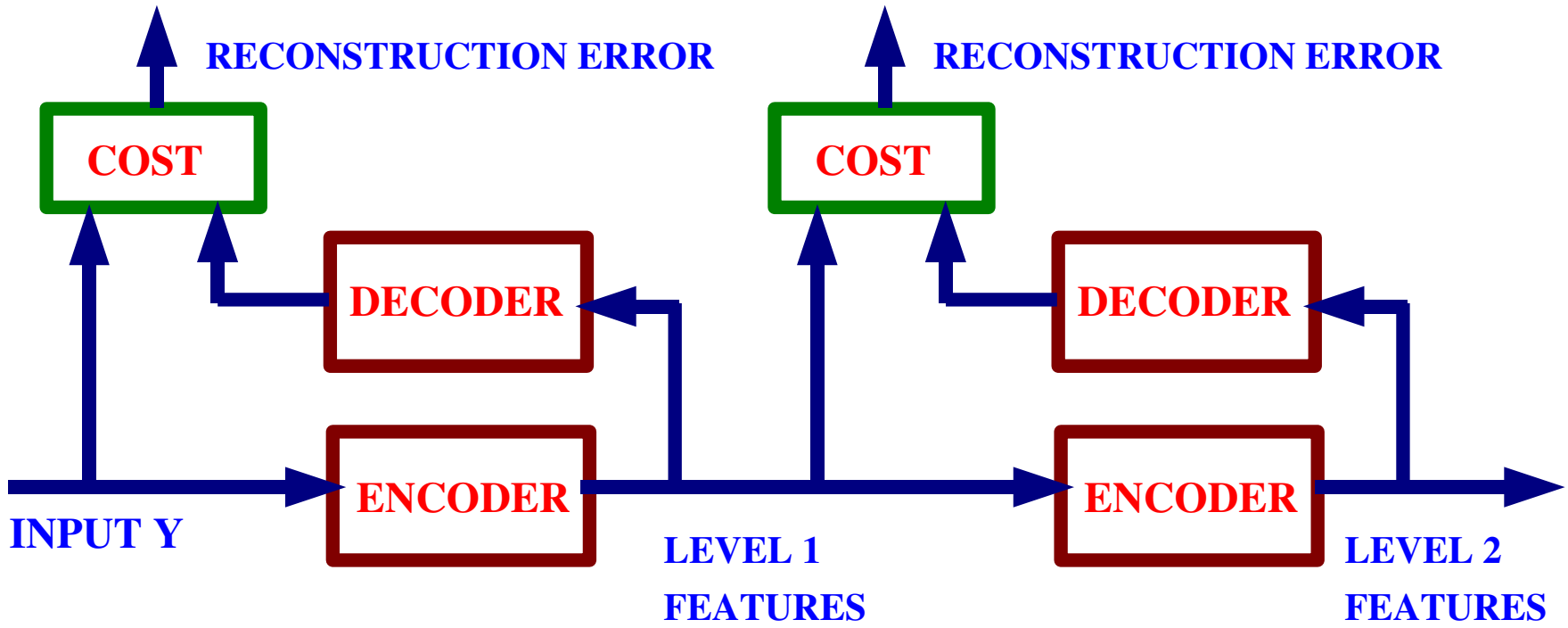


"Only Yann can do it" (NOT!)

- What about Mike O'Neill?
- http://www.codeproject.com/KB/library/NeuralNetRecognition.aspx

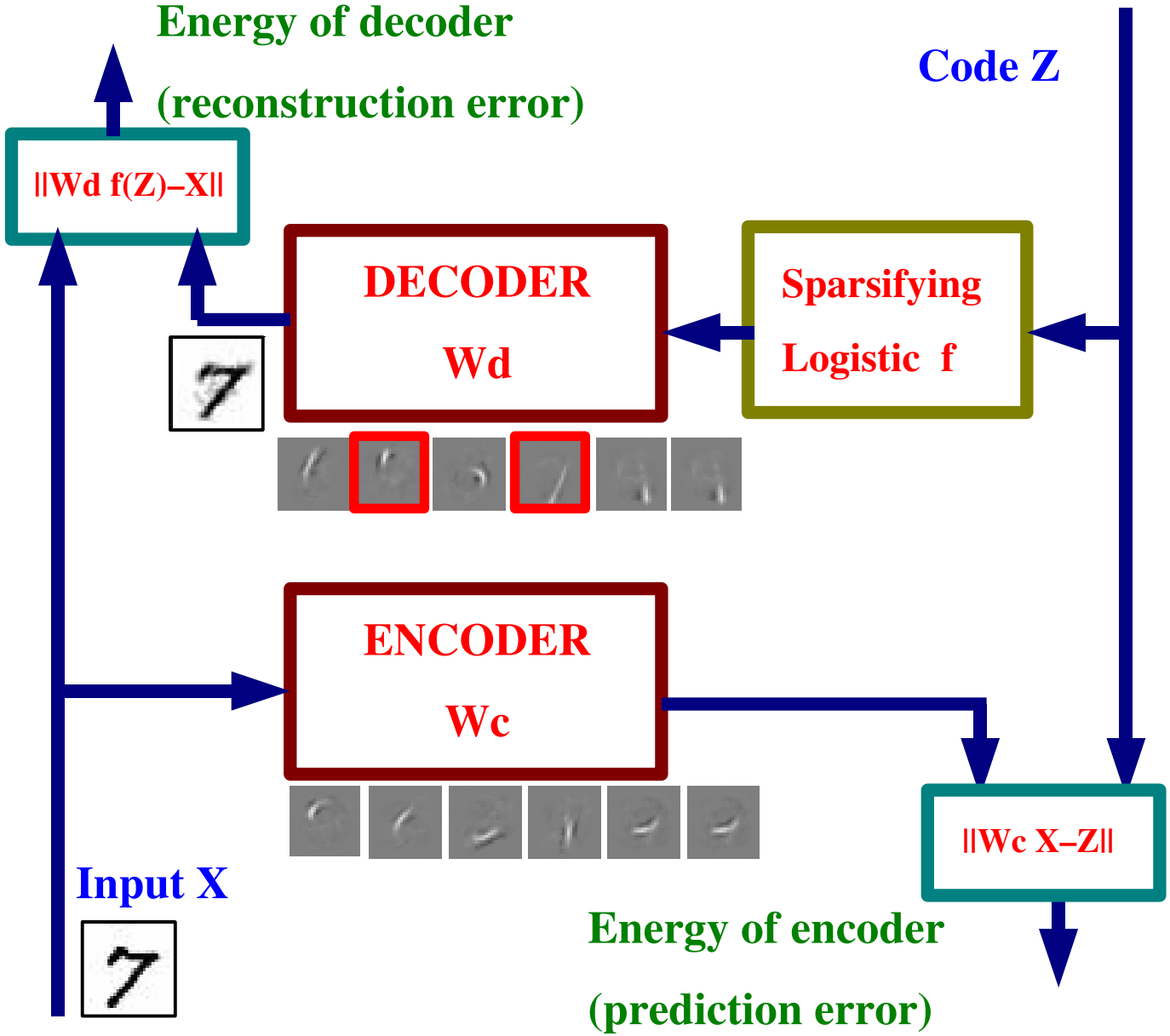
The Basic Idea for Training Deep Feature Hierarchies

- **Each stage is composed of**
  - an encoder that produces a feature vector from the input
  - a decoder that reconstruct the input from the feature vector
    - (RBM is a special case)
- **Each stage is trained one after the other**
  - the input to stage i+1 is the feature vector of stage i.



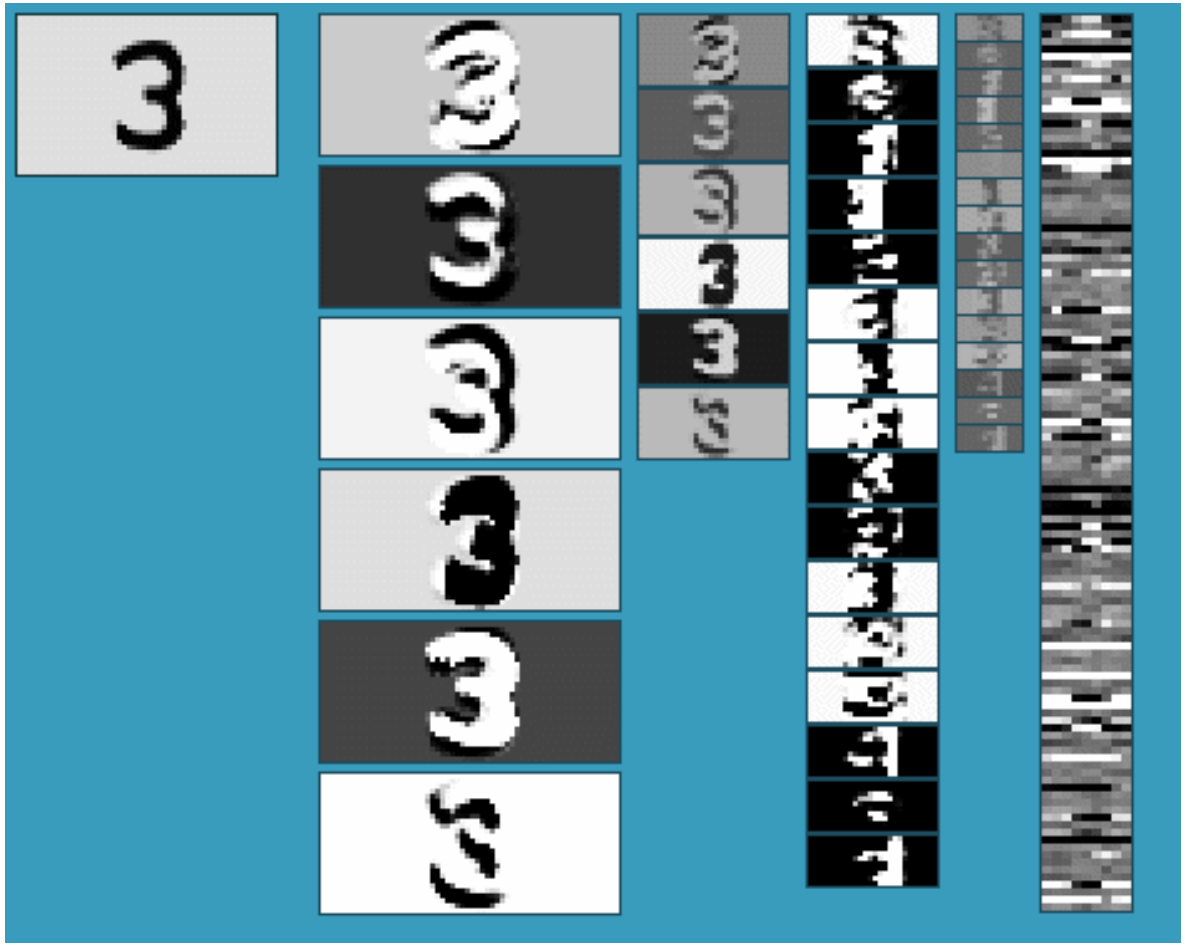
Sparsifying with a high-threshold logistic function

- **Algorithm:**
  - 1. find the code Z that minimizes the reconstruction error AND is close to the encoder output
  - 2. Update the weights of the decoder to decrease the reconstruction error
  - 3. Update the weights of the encoder to decrease the prediction error



The Multistage Hubel-Wiesel Architecture

- **Building a complete artificial vision system:**
  - Stack multiple stages of simple cells / complex cells layers
  - Higher stages compute more global, more invariant features
  - Stick a classification layer on top
  - [Fukushima 1971-1982]
    - neocognitron
  - [LeCun 1988-2007]
    - convolutional net
  - [Poggio 2002-2006]
    - HMAX
  - [Ullman 2002-2006]
    - fragment hierarchy
  - [Lowe 2006]
    - HMAX



Unsupervised Training of Convolutional Filters

CLASSIFICATION EXPERIMENTS

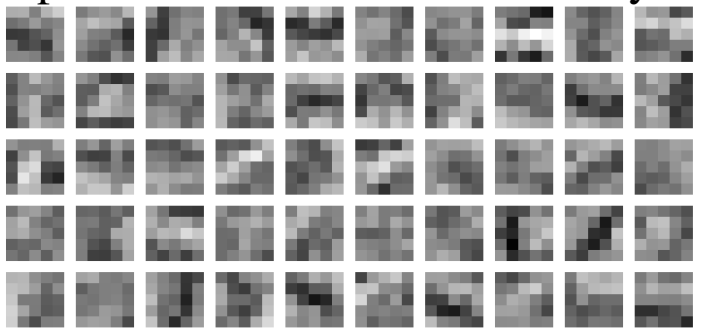
IDEA: improving supervised learning by pre-training with the unsupervised method (*)

sparse representations & *lenet6* (1->50->50->200->10)

- The baseline: *lenet6* initialized randomly

Test error rate: **0.70%**. Training error rate: 0.01%.

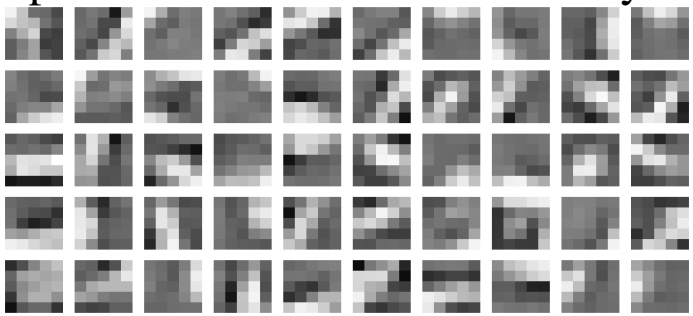
supervised filters in first conv. layer



- *Experiment 1*
  - Train on 5x5 patches to find 50 features
  - Use the scaled filters in the encoder to initialize the kernels in the first convolutional layer

Test error rate: 0.60%. Training error rate: 0.00%.

unsupervised filters in first conv. layer



- *Experiment 2*
  - Same as experiment 1, but training set augmented by elastically distorted digits (random initialization gives test error rate equal to **0.49%**).

Test error rate: 0.39%. Training error rate: 0.23%.

(*)[Hinton, Osindero, Teh "*A fast learning algorithm for deep belief nets*" Neural Computaton 2006]

Best Results on MNIST (from raw images: no preprocessing)

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Learning Invariant Filters in a Convolutional Net

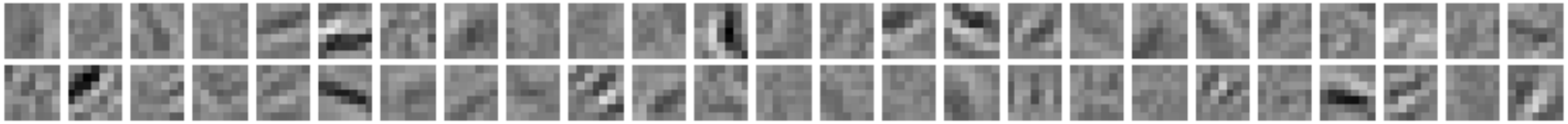


Figure 1: 50 7x7 filters in the first convolutional layer that were learned by the network trained supervised from *random* initial conditions with 600K digits.

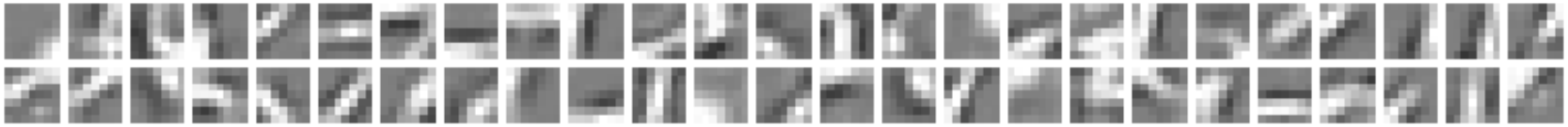


Figure 2: 50 7x7 filters that were learned by the unsupervised method (on 60K digits), and that are used to initialize the first convoltional layer of the network.

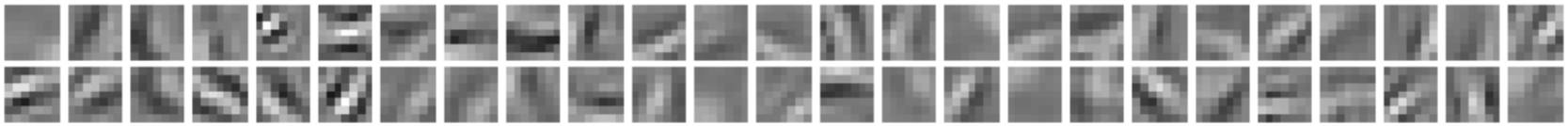
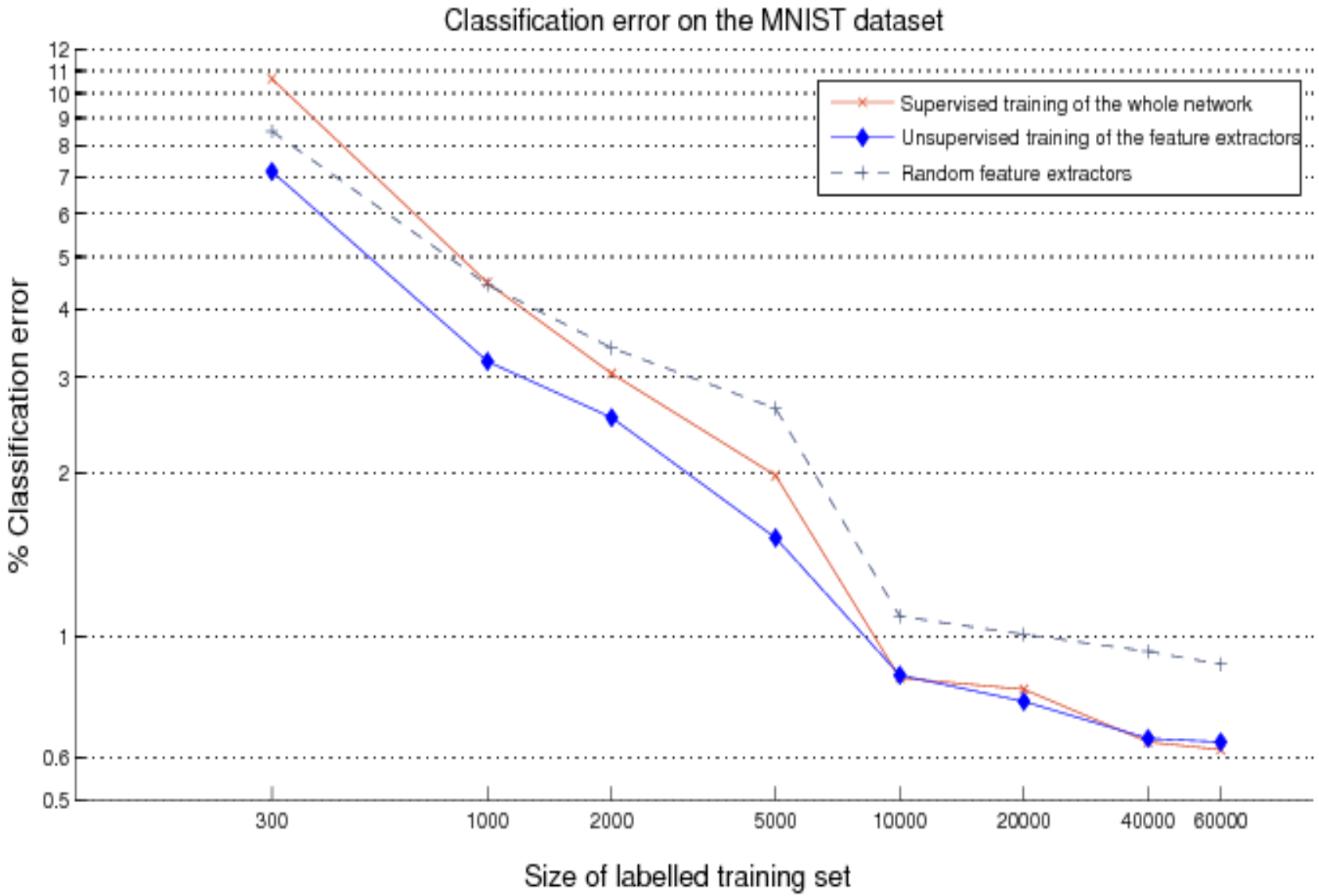


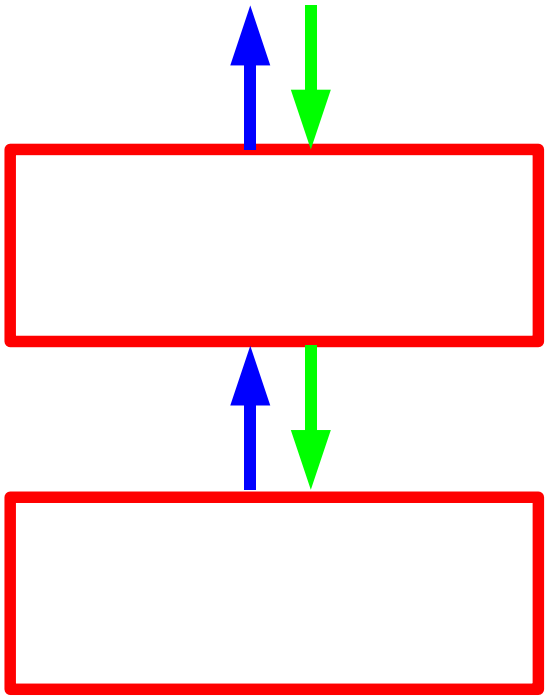
Figure 3: 50 7x7 filters in the first convolutional layer that were learned by the network trained supervised from the initial conditions given by the *unsupervised method* (see fig.2) with 600K digits.

Influence of Number of Training Samples



The right tools: Automatic Differentiation

- **Object-Oriented, module-based AD**
  - [Bottou & Gallinari 1991]
  - Implemented in Lush [Bottou & LeCun]
  - Implemented in Torch [Collobert]
  - Implemented in Monte Python [Memisevic]



module.fprop(input,output)

module.bprop(input,output)

module.bbprop(input,output)

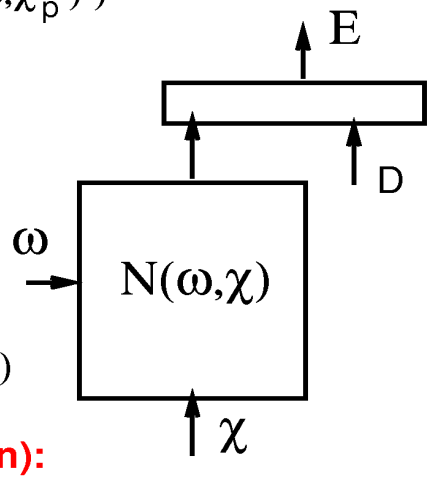
SQUARE JACOBIAN APPROXIMATION FOR GAUSS–NEWTON AND LEVENBERG–MARQUARDT ALGOS.

Assume the cost function is the Mean Square Error:

$$E(\omega) = 1/2 \sum_p (D_p - N(\omega,\chi_p))' (D_p - N(\omega,\chi_p))$$

Gradient:

$$\frac{\partial E(\omega)}{\partial \omega} = -\sum_p (D_p - N(\omega,\chi))' \frac{\partial N(\omega,\chi_p)}{\partial \omega}$$



Hessian:

$$H(\omega) = \sum_p \frac{\partial N(\omega,\chi_p)}{\partial \omega}' \frac{\partial N(\omega,\chi_p)}{\partial \omega} + \sum_p (D_p - N(\omega,\chi))' \frac{\partial^2 N(\omega,\chi_p)}{\partial \omega \partial \omega'}$$

Simplified Hessian (square of the Jacobian):

$$H(\omega) = \sum_p \frac{\partial N(\omega,\chi_p)}{\partial \omega}' \frac{\partial N(\omega,\chi_p)}{\partial \omega}$$

Jacobian: NxO matrix (O: number of outputs)

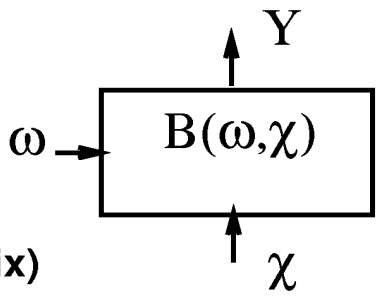
- the resulting approximate Hessian is positive semi–definite
- dropping the second term is equivalent to assuming that the network is a linear function of the parameters

RECIPE for computing the k–th column of the Jacobian:

```
for all training patterns {
  forward prop
  set gradients of output units to 0;
  set gradient of k–th output unit to 1;
  back propagate;   accumulate gradient;
}
```

BACKPROPAGATING SECOND DERIVATIVES

A multilayer system composed of functional blocs. Consider one of the blocs with I inputs, O outputs, and N parameters



Assuming we know $\frac{\partial^2 E}{\partial Y^2}$ (OxO matrix)

what are $\frac{\partial^2 E}{\partial \omega^2}$ (NxN matrix) and $\frac{\partial^2 E}{\partial \chi^2}$ (IxI matrix)

Chain rule for 2nd derivatives:

$$\frac{\partial^2 E}{\partial \omega^2} = \frac{\partial Y'}{\partial \omega}\frac{\partial^2 E}{\partial Y^2}\frac{\partial Y}{\partial \omega} + \frac{\partial E}{\partial Y}\frac{\partial^2 Y}{\partial \omega^2}$$

NxN NxO OxO OxN 1xO OxNxN

ignore this!

The above can be used to compute a bloc diagonal subset of the Hessian

If the term in the red square is dropped, the resulting Hessian estimate will be positive semi–definite

If we are only interested in the diagonal terms, it reduces to:

$$\frac{\partial^2 E}{\partial \omega_{ii}^2} = \sum_k \frac{\partial^2 E}{\partial Y_{kk}^2}\left(\frac{\partial Y_{kk}}{\partial \omega_{ii}}\right)^2$$ (and same with χ instead of ω)

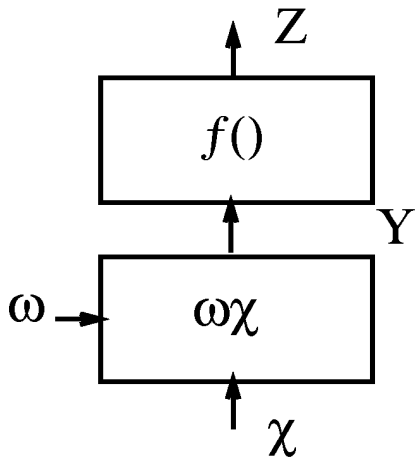
BACKPROPAGATING THE DIAGONAL HESSIAN IN NEURAL NETS

(with the square Jacobian approximation)

[LeCun 87, Becker&LeCun 88, LeCun 89]

Sigmoids (and other scalar functions)

$$\frac{\partial^2 E}{\partial Y_k^2} = \frac{\partial^2 E}{\partial Z_k^2} (f'(Y_k))^2$$



Weighted sums

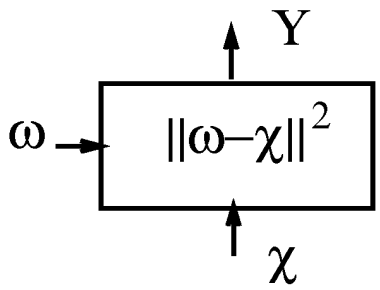
$$\frac{\partial^2 E}{\partial \omega_{ki}^2} = \frac{\partial^2 E}{\partial Y_k^2} \chi_i^2$$

$$\frac{\partial^2 E}{\partial \chi_i^2} = \sum_k \frac{\partial^2 E}{\partial Y_k^2} \omega_{ki}^2$$

RBFs

$$\frac{\partial^2 E}{\partial \omega_{ki}^2} = \frac{\partial^2 E}{\partial Y_k^2} (\chi_i - \omega_{ki})^2$$

$$\frac{\partial^2 E}{\partial \chi_i^2} = \sum_k \frac{\partial^2 E}{\partial Y_k^2} (\chi_i - \omega_{ki})^2$$



(the 2nd derivatives with respect to the weights should be averaged over the training set)

SAME COST AS REGULAR BACKPROP

the "OBD" network pruning techniques uses this procedure [LeCun,Denker&Solla 90]

COMPUTING THE PRODUCT OF THE HESSIAN BY A VECTOR

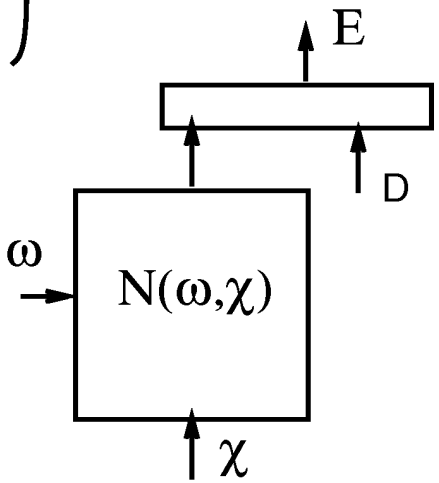
(without computing the Hessian itself)

Finite difference:

$$H\Psi \approx \frac{1}{\alpha}\left(\frac{\partial E}{\partial \omega}(\omega+\alpha\Psi) - \frac{\partial E}{\partial \omega}(\omega)\right)$$

RECIPE for computing the product of a vector Ψ by the Hessian:

1– compute gradient
2– add $\alpha\Psi$ to the parameter vector
3– compute gradient with perturbed parameters
4– subtract result of 1 from 3, divide by α



This method can be used to compute the principal eigenvector and eigenvalue of H by the power method.

By iterating $\Psi \leftarrow H\Psi / \|\Psi\|$

will converge to the principal eigenvector of H and $\|\Psi\|$ to the corresponding eigenvalue [LeCun, Simard&Pearlmutter 93]

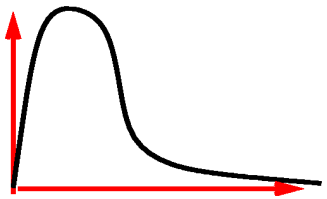
A more accurate method which does not use finite differences (and has the same complexity) has recently been proposed [Pearlmutter 93]

ANALYSIS OF THE HESSIAN IN MULTILAYER NETWORKS

–What does the Hessian of a multilayer network look like?
– How does it change with the architecture and the details of the implementation?

– Typically, the distribution of eigenvalues of a multilayer network looks like this:

a few small eigenvalues, a large number of medium ones, and a small number of very large ones



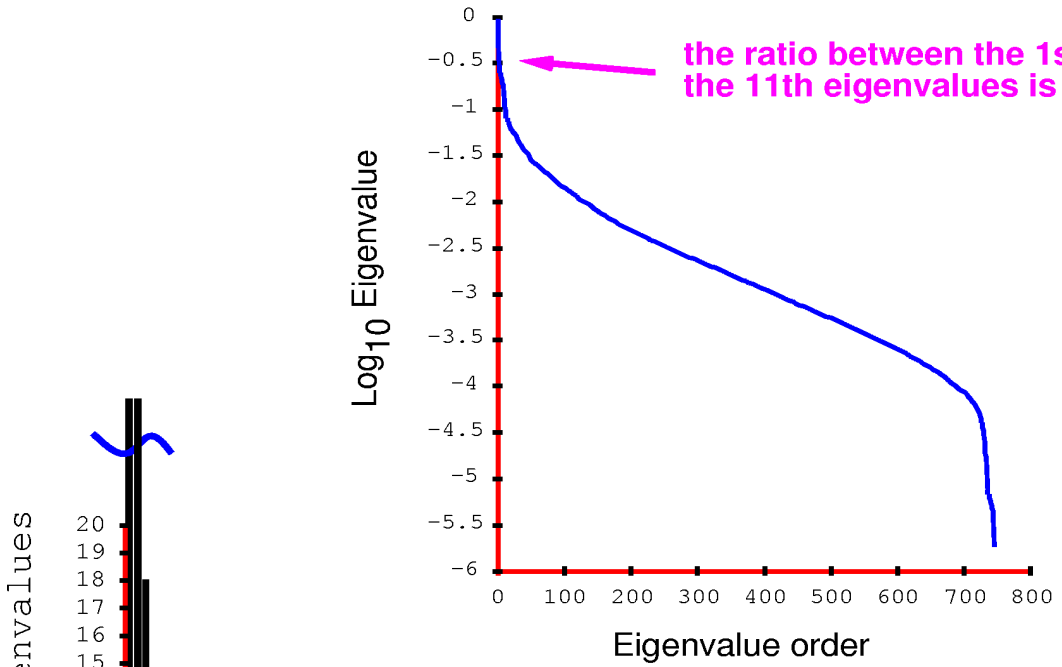
These large ones are the killers

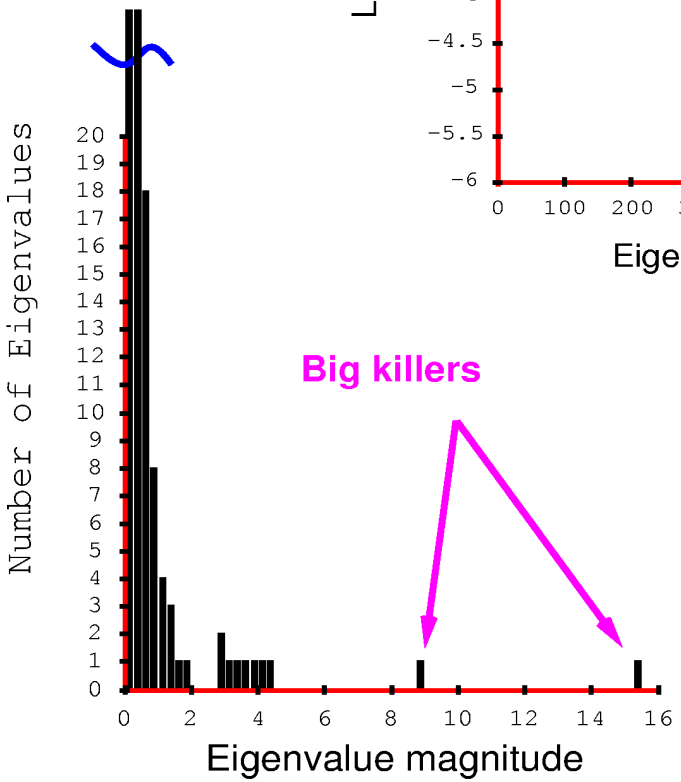
They come from:
– non–zero mean inputs or neuron states
– wide variations second derivatives from layer to layer
– correlations between state variables

for more details see [LeCun, Simard&Pearlmutter 93]
[LeCun, Kanter&Solla 91]

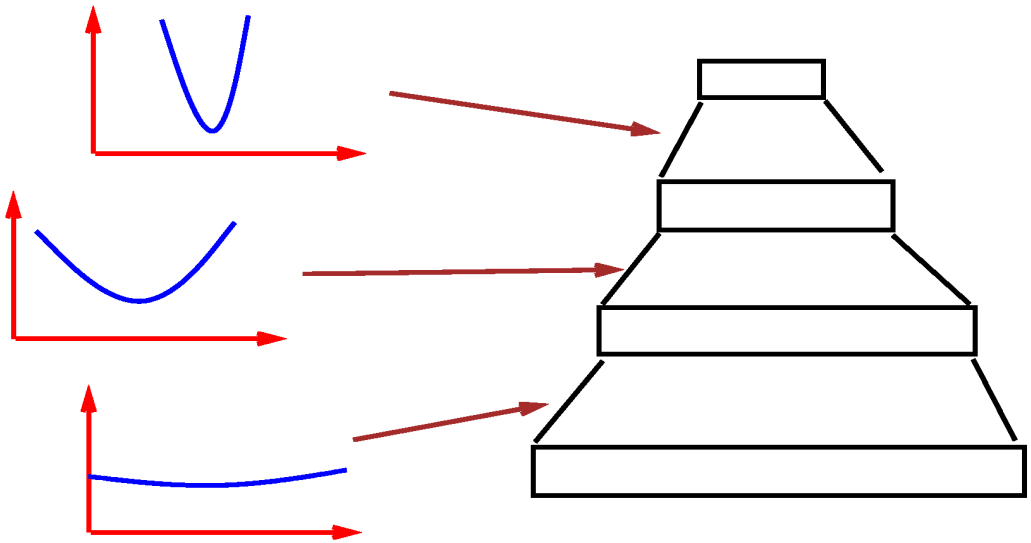
EIGENVALUE SPECTRUM

Network: 256–128–64–10 with local connections and shared weights (around 750 parameters)
Data set: 320 handwritten digits





MULTILAYER NETWORKS HESSIAN

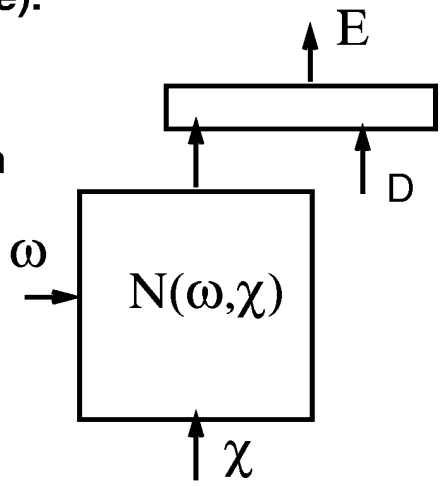


The second derivative is often smaller in lower layers. The first layer weights learn very slowly, while the last layer weights change very quickly.

This can be compensated for using the diagonal 2nd derivatives (more on this later)

GAUSS–NEWTON AND LEVENBERG–MARQUARDT METHODS

These methods only apply to Mean–Square Error objective functions (non–linear least square).



Gauss–Newton algorithm:

like Newton but the Hessian is approximated by the square of the jacobian (which is always positive semidefinite)

$$\Delta\omega = \left(\sum_p \frac{\partial N(\omega,\chi_p)}{\partial \omega}' \frac{\partial N(\omega,\chi_p)}{\partial \omega} \right)^{-1} \nabla E(\omega)$$

Levenberg–Marquardt algorithm:

like Gauss–Newton, but has a safeguard parameter to prevent it from blowing up if some eigenvalues are small

$$\Delta\omega = \left(\sum_p \frac{\partial N(\omega,\chi_p)}{\partial \omega}' \frac{\partial N(\omega,\chi_p)}{\partial \omega} + \mu\, I \right)^{-1} \nabla E(\omega)$$

- Both are O(N^3) algorithms
- they are widely used in statistics for regression
- they are only practical for small numbers of parameters.
- they do not require a line search, so in principle they can be used in stochastic mode (although that has not been tested)

A STOCHASTIC DIAGONAL LEVENBERG–MARQUARDT METHOD

[LeCun 87, Becker&LeCun 88, LeCun 89]

THE MAIN IDEAS:

- use formulae for the backpropagation of the diagonal Hessian (shown earlier) to keep a running estimate of the second derivative of the error with respect to each parameter.
- use these term in a "Levenberg–Marquardt" formula to scale each parameter's learning rate

Each parameter (weight) ω_{ki} has its own learning rate η_{ki} computed as:

$$\eta_{ki} = \frac{\varepsilon}{\frac{\partial^2 E}{\partial \omega_{ki}^2} + \mu}$$

ε is a global "learning rate"

$\frac{\partial^2 E}{\partial \omega_{ki}^2}$ is an estimate of the diagonal second derivative with respect to weight (ki)

μ is a "Levenberg–Marquardt" parameter to prevent η_{ki} form blowing up if the 2nd derivative is small

A STOCHASTIC DIAGONAL LEVENBERG–MARQUARDT METHOD

The second derivatives $\frac{\partial^2 E}{\partial \omega_{ki}^2}$ can be computed using a running average formula over a subset of the training set prior to training:

$$\frac{\partial^2 E}{\partial \omega_{ki}^2} \leftarrow (1-\gamma)\frac{\partial^2 E}{\partial \omega_{ki}^2} + \gamma \frac{\partial^2 E^p}{\partial \omega_{ki}^2}$$

- new estimate of 2nd der.
- previous estimate
- small constant
- instantaneous 2nd der. for pattern p

The instantaneous second derivatives are computed using the formula in the slide entitled:
"BACKPROPAGATING THE DIAGONAL HESSIAN IN NEURAL NETS"

Since the second derivatives evolve slowly, there is no need to reestimate them often.
They can be estimated once at the beginning by sweeping over a few hundred patterns.
Then, they can be reestimated every few epochs.

The additional cost over regular backprop is negligible.

Is usually about 3 times faster than carefully tuned stochastic gradient.

Stochastic Diagonal Levenberg–Marquardt

data set: set–1 (100 examples, 2 gaussians)
network: 1 linear unit, 2 inputs, 1 output.
2 weights, 1 bias.

Learning rates:

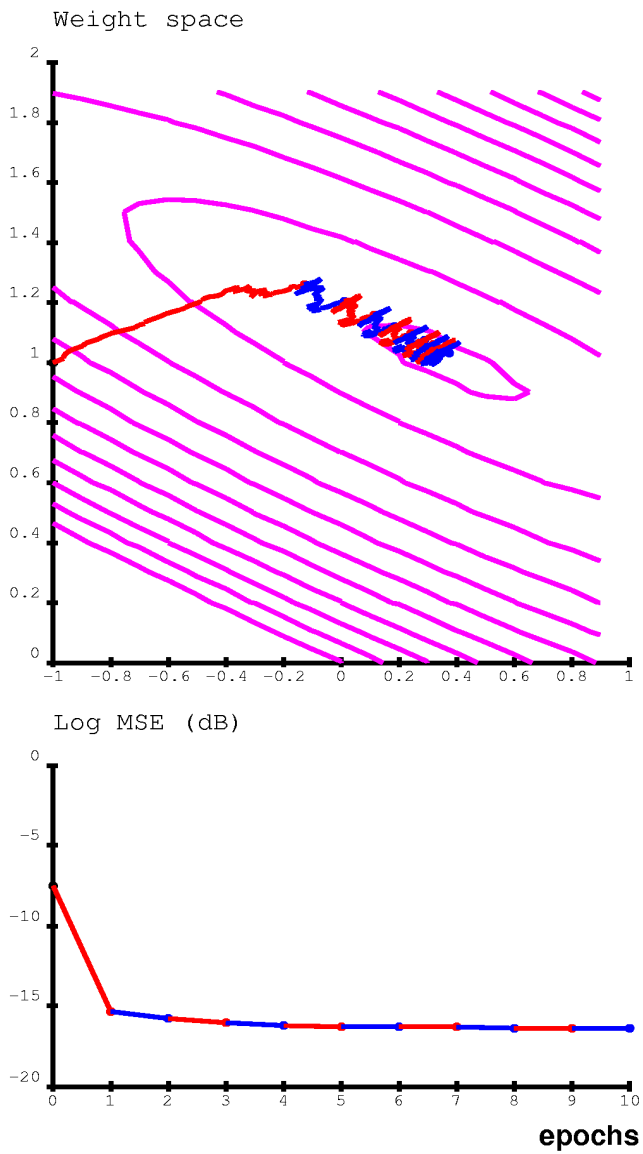
$$\eta 0 = 0.12$$
$$\eta 1 = 0.03$$
$$\eta 2 = 0.02$$

Hessian largest eigenvalue:

$$\lambda_{max} = 0.84$$

Maximum admissible Learning rate (batch):

$$\eta_{max} = 2.38$$



Stochastic Diagonal Levenberg–Marquardt

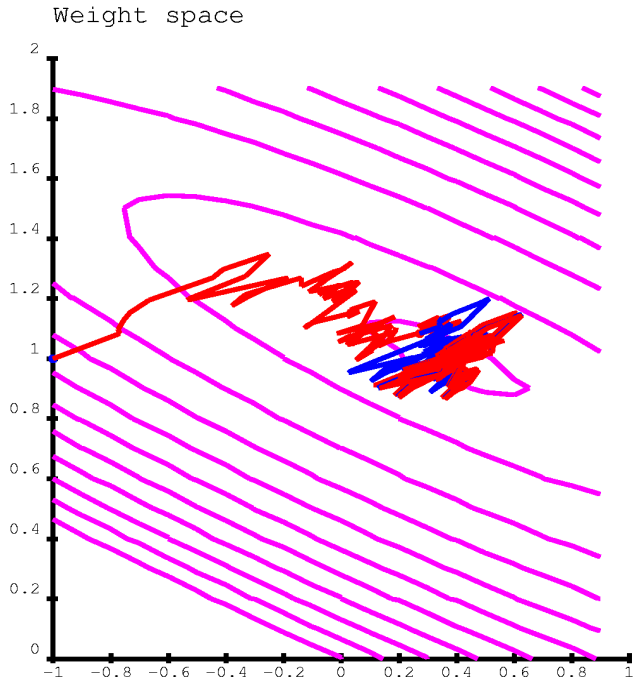
data set: set–1 (100 examples, 2 gaussians)
network: 1 linear unit, 2 inputs, 1 output.
2 weights, 1 bias.

Learning rates:

$$\eta 0 = 0.76$$
$$\eta 1 = 0.18$$
$$\eta 2 = 0.12$$

Hessian largest eigenvalue:

$$\lambda_{max} = 0.84$$



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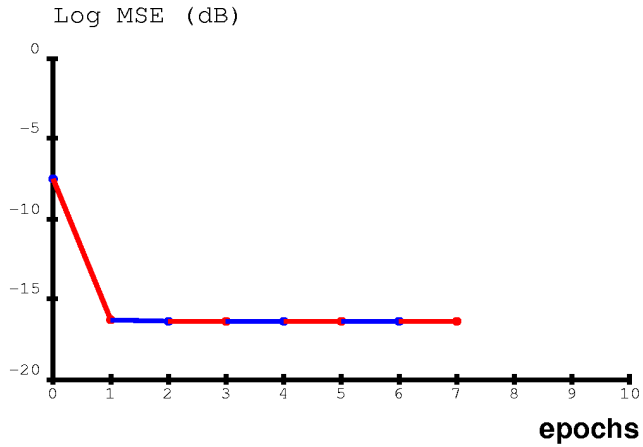


COMPUTING THE PRINCIPAL EIGENVALUE/VECTOR OF THE HESSIAN

without computing the Hessian

IDEA #1 (the power method):

1 – Choose a vector Ψ at random

2 – iterate: $\Psi \leftarrow H \frac{\Psi}{\|\Psi\|}$

OLD ESTIMATE OF EIGENVECTOR

NEW ESTIMATE OF EIGENVECTOR

HESSIAN

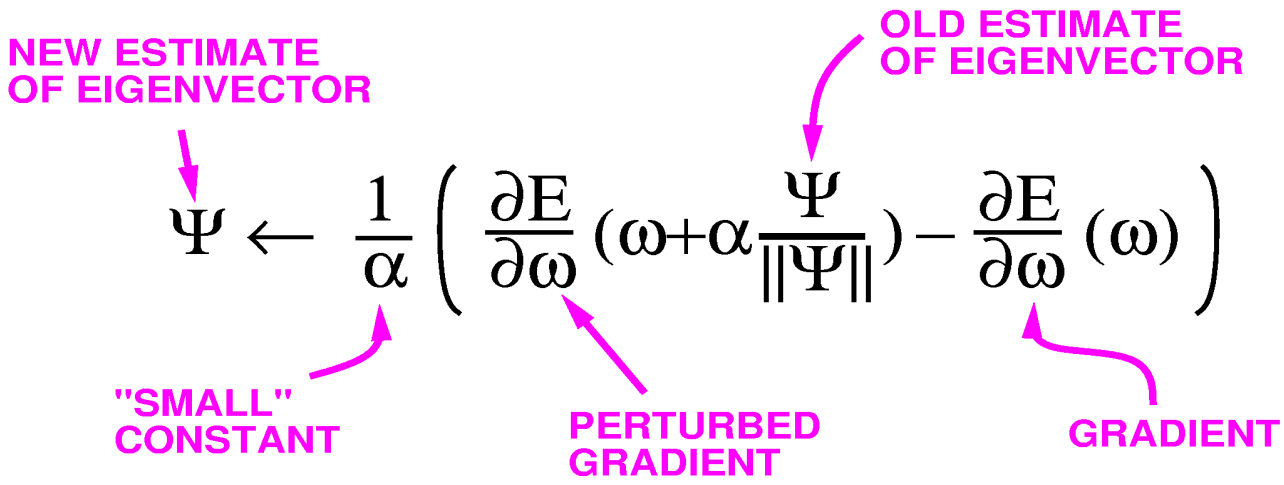
ESTIMATE OF EIGENVALUE

Ψ will converge to the principal eigenvector (or a vector in the principal eigenspace)

$\|\Psi\|$ will converge to the corresponding eigenvalue

COMPUTING THE PRODUCT $H\Psi$

IDEA #2 (Taylor expansion):



One iteration of this procedure requires 2 forward props and 2 backward props for each pattern in the training set.

This converges very quickly to a good estimate of the largest eigenvalue of H

ON–LINE COMPUTATION OF Ψ

IDEA #3 (running average):

NEW ESTIMATE OF EIGENVECTOR

OLD ESTIMATE OF EIGENVECTOR

$$\Psi \leftarrow (1-\gamma)\Psi + \gamma \frac{1}{\alpha}\left(\frac{\partial E^p}{\partial \omega}(\omega + \alpha \frac{\Psi}{\|\Psi\|}) - \frac{\partial E^p}{\partial \omega}(\omega) \right)$$

"SMALL" CONSTANTS

PERTURBED GRADIENT FOR CURRENT PATTERN

GRADIENT FOR CURRENT PATTERN

This procedure converges VERY quickly to the largest eigenvalue of the AVERAGE Hessian.

The properties of the average Hessian determine the behavior of ON–LINE gradient descent (stochastic, or per–sample update).

EXPERIMENT: A shared–weight network with 5 layers of weights, 64638 connections and 1278 free parameters. Training set: 1000 handwritten digits.

Correct order of magnitude is obtained in less than 100 pattern presentations (10% of training set size)

The fluctuations of the average Hessian over the training set are small.

RECIPE

$$\Psi \leftarrow (1-\gamma)\Psi+\gamma \frac{1}{\alpha}\left(\frac{\partial E^p}{\partial \omega}(\omega+\alpha\frac{\Psi}{\|\Psi\|}) - \frac{\partial E^p}{\partial \omega}(\omega) \right)$$

1 – Pick initial eigenvector estimate at random

2 – present input pattern, and desired output.
perform forward prop and backward prop.
Save gradient vector G(w)

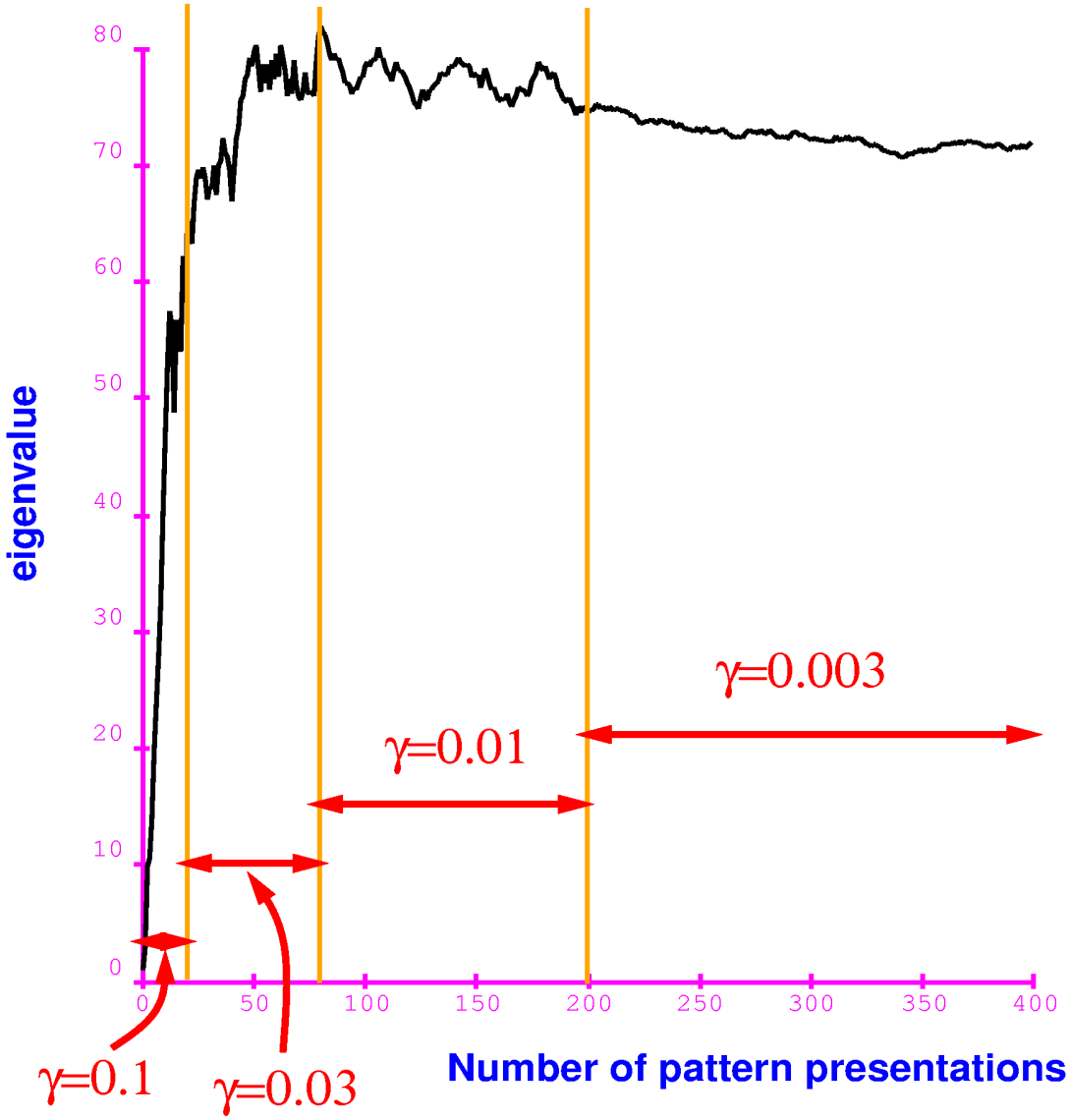
3 – add $\alpha \frac{\Psi}{\|\Psi\|}$ to current weight vector

4 – perform forward prop and backward prop with
perturbed weight vector. Save gradient vector G'(w)

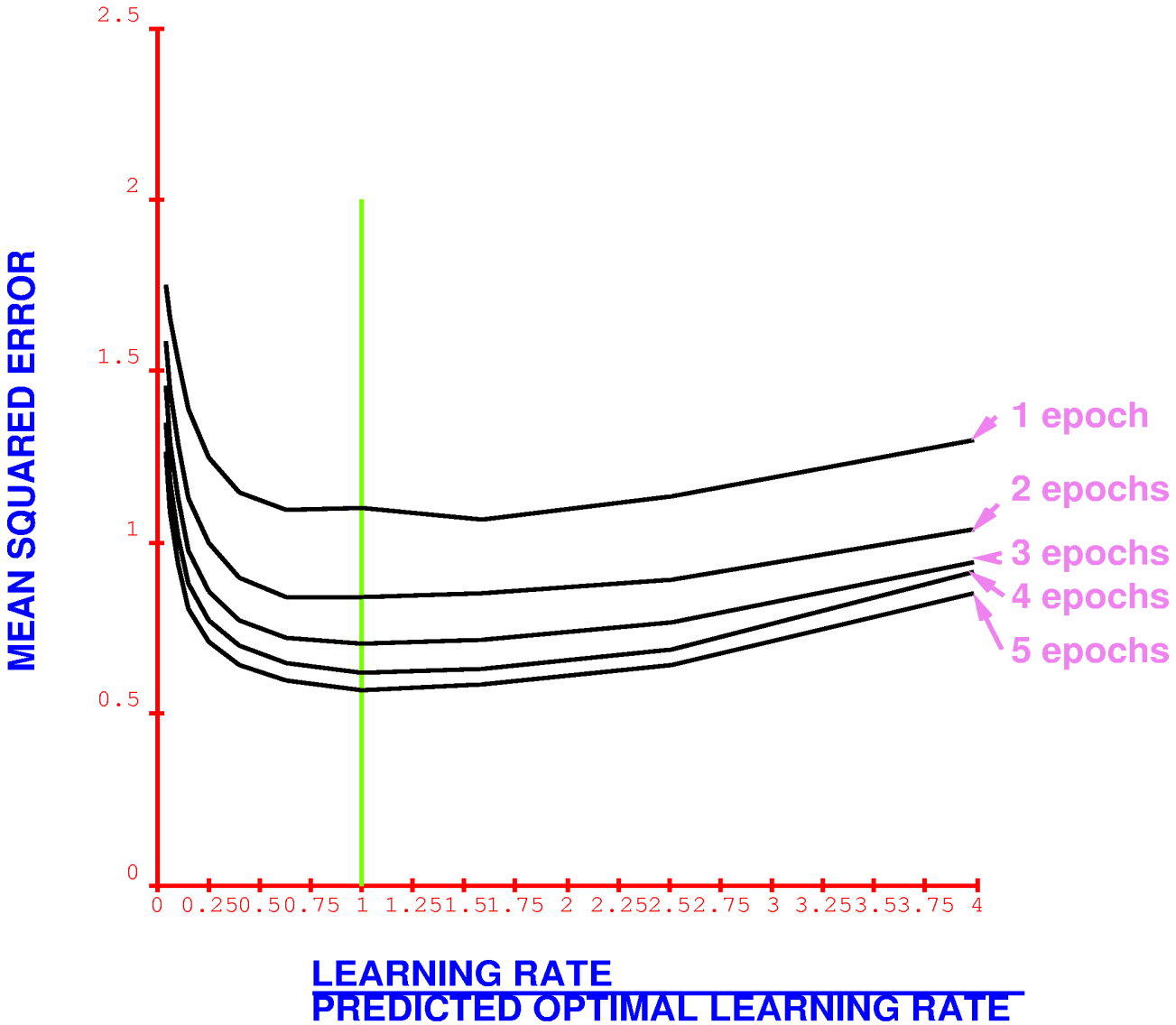
5 – compute difference G'(w)–G(w). and divide by α
update running average of eigenvector
with the result

6 – goto 2 unless a reasonably stable result is obtained

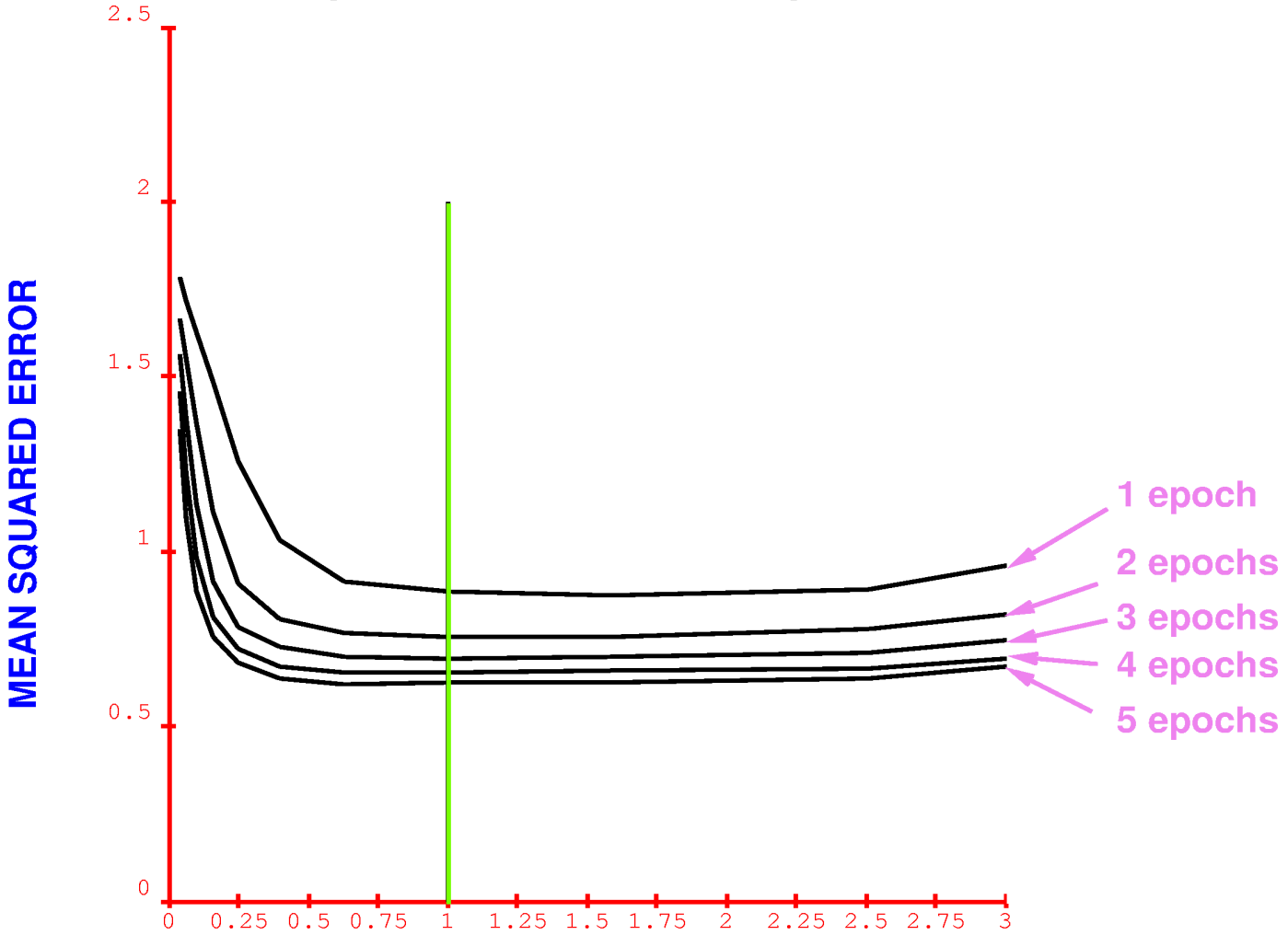
7 – the optimal learning rate is $\frac{1}{\|\Psi\|}$


80
70
60
50
40
30
20
10
0
eigenvalue
0
50
100
150
200
250
300
350
400
Number of pattern presentations
γ=0.003
γ=0.01
γ=0.1
γ=0.03

Network: 784x30x10 fully connected
Training set: 300 handwritten digits



Network: 1024x1568x392x400x100x10
with 64638 (local) connections
and 1278 shared weights
Training set: 1000 handwritten digits



The End