Neural Networks

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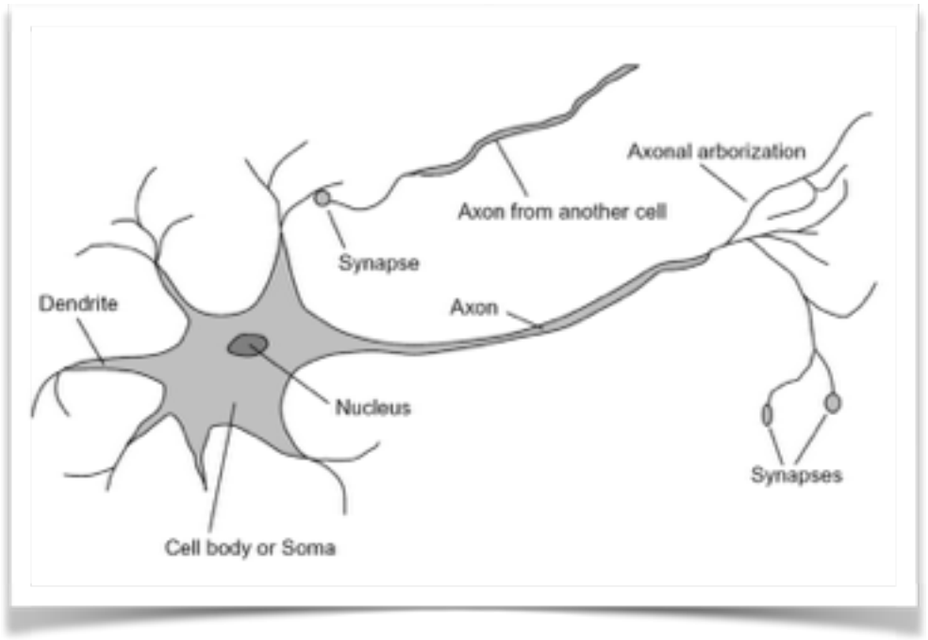
CMPSCI 689: Machine Learning

10 March 2015

12 March 2015

Motivation

- One of the main weakness of linear models is that they are linear
- Decision trees and kNN classifiers can model non-linear boundaries
- Neural networks are yet another non-linear classifier
- Take the biological inspiration further by chaining together perceptrons
- Allows us to use what we learned about linear models:
  - Loss functions, regularization, optimization



neuron

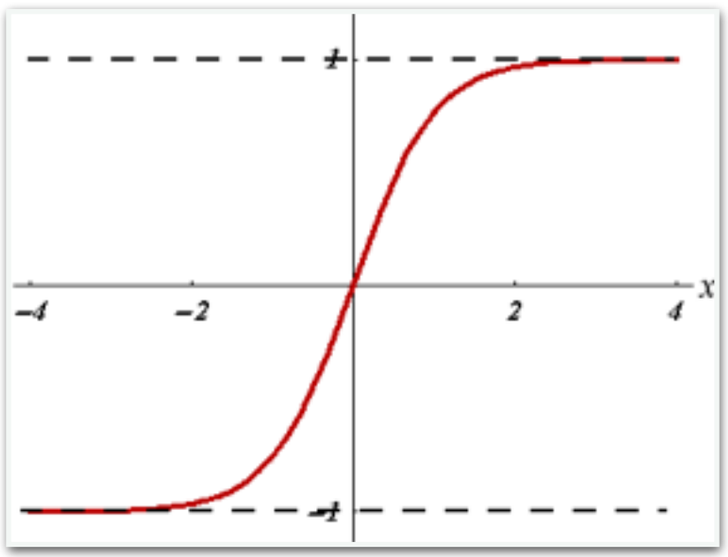
Two-layer network architecture

$$y = \mathbf{v}^T \mathbf{h}$$

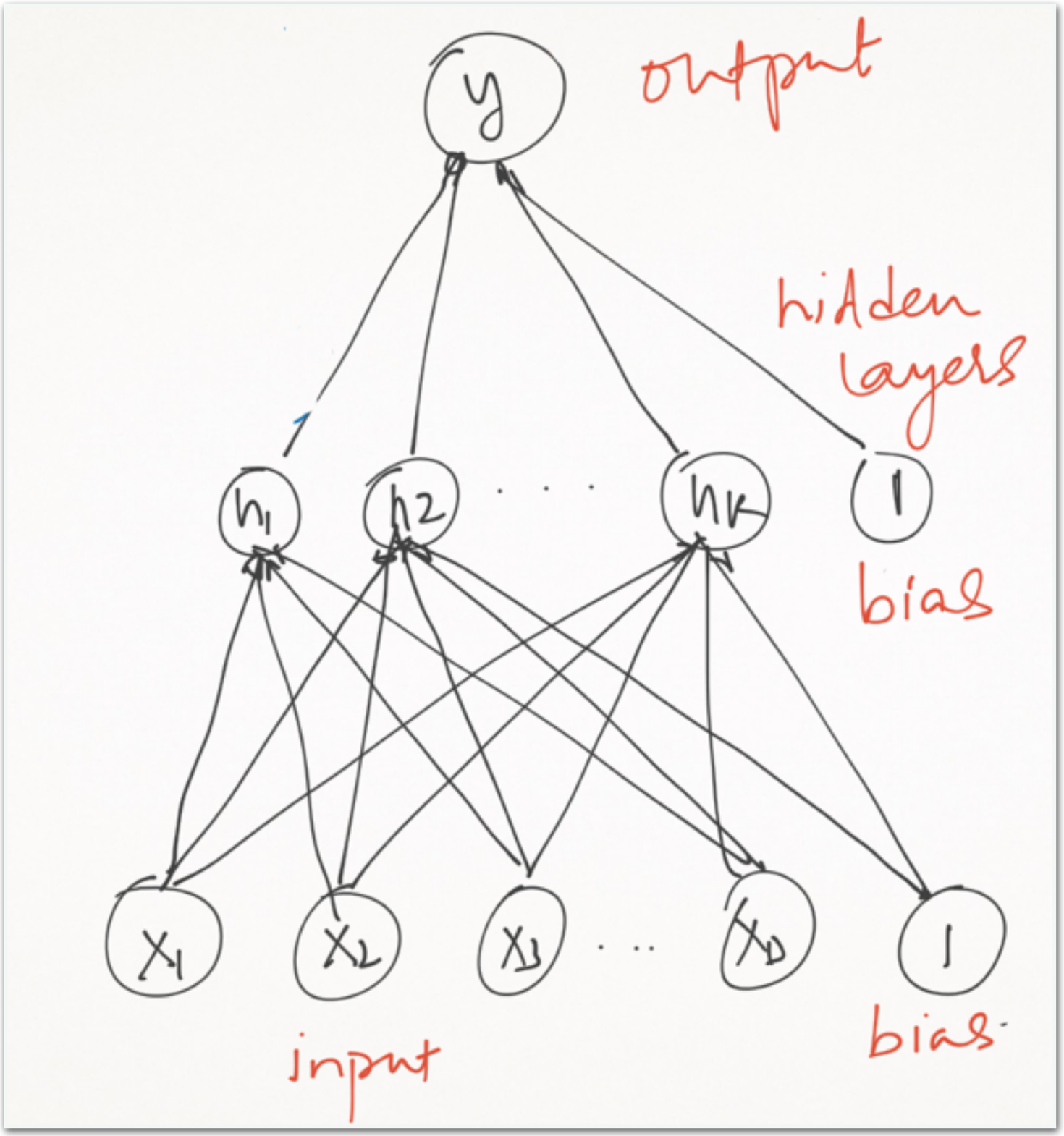
Non-linearity is important

link function

$$h_i = f(\mathbf{w}_i^T \mathbf{x})$$



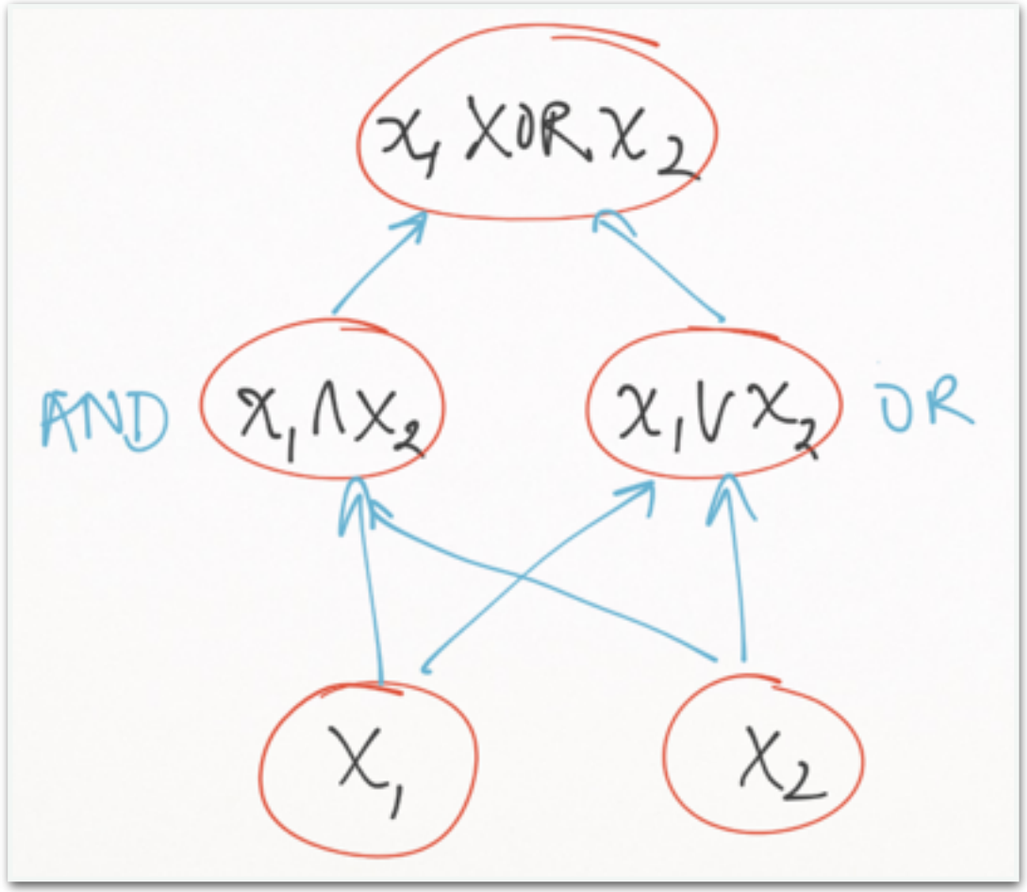
$$\tanh(x) = \frac{1 - e^{-2x}}{1 + e^{-2x}}$$



The XOR function

- We saw that a perceptron cannot learn the XOR function
- **Exercise:** come up with the parameters of a two layer network with two hidden units that computes the XOR function
  - Here is a table with a bias feature for XOR

y	x_0	x_1	x_2
+1	+1	+1	+1
+1	+1	-1	-1
-1	+1	+1	-1
-1	+1	-1	+1



Do we gain anything beyond two layers?

Expressive power of a two-layer network

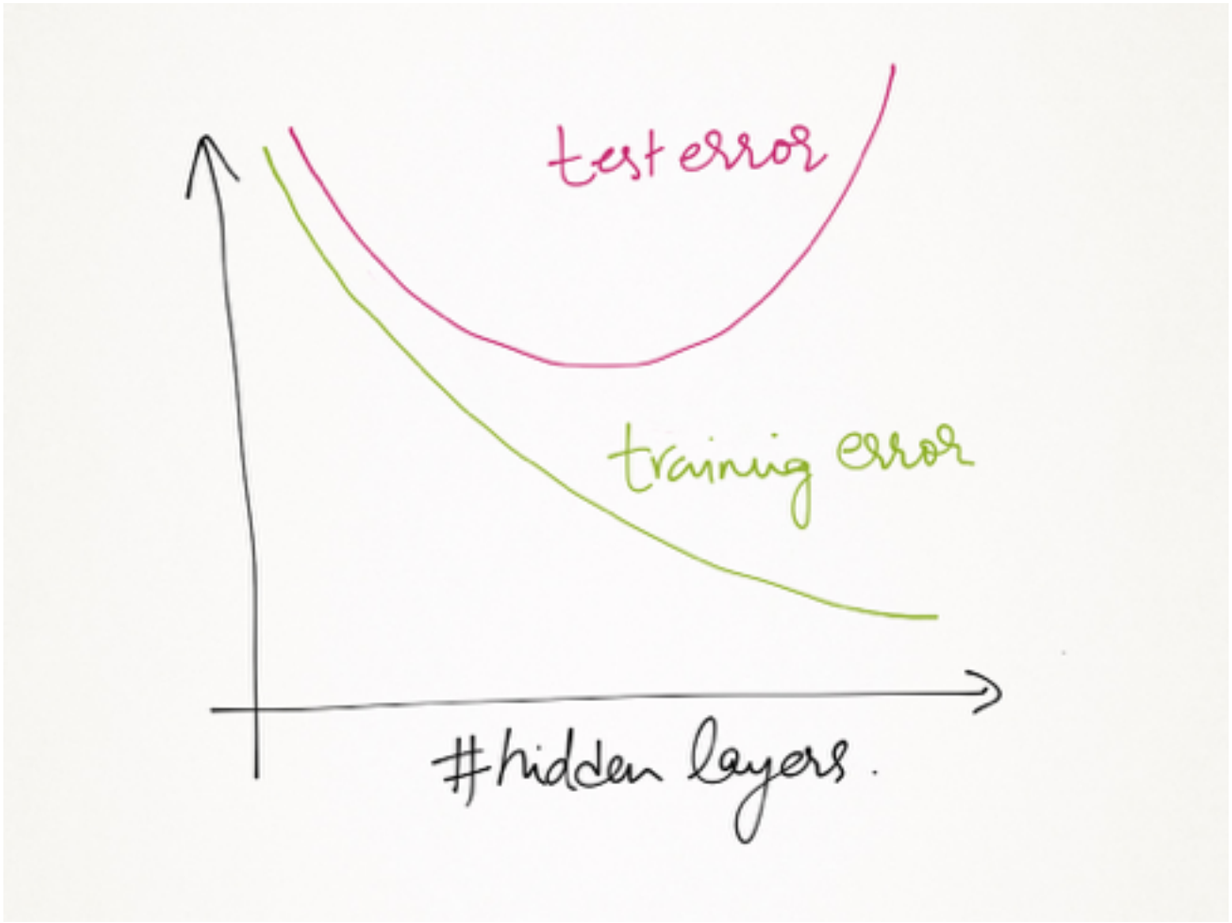
- **Theorem [Kurt Hornik et al., 1989]:** Let F be a continuous function on a bounded subset of D-dimensional space. Then there exists a two-layer network F with finite number of hidden units that approximates $\hat{F}$ arbitrarily well. Namely, for all x in the domain of F, $|F(x)-\hat{F}(x)| < \varepsilon$

- Colloquially “a two-layer network can approximate any function”
  - This is true for arbitrary link function

- Going from one to two layers dramatically improves the representation power of the network

How many hidden units?

- D dimensional data with K hidden units has(D+2)K+1 parameters
  - (D+1)K in the first layer (1 for the bias) and K+1 in the second layer
- With N training examples, set the number of hidden units K ~ N/D to keep the number of parameters comparable to size of training data
- K is both a form of regularization and inductive bias
- Training and test error vs. K



Training a two-layer network

- Optimization framework:

$$\min_{W,v} \sum_n \frac{1}{2} \left(y_n - \sum_i \mathbf{v}_i f(\mathbf{w}_i^T \mathbf{x}_n) \right)^2$$

- Loss minimization: replace squared-loss with any other
- Regularization:
  - Traditionally NN are not regularized (early stopping instead)
  - But you can add a regularization (e.g. l_2-norm of the weights)

- Optimization by gradient descent
  - Highly non-convex problem so no guarantees about optimality

Training a two-layer network

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$$\min_{W,v} \sum_n \frac{1}{2} \left(y_n - \sum_i \mathbf{v}_i f(\mathbf{w}_i^T \mathbf{x}_n) \right)^2$$

or equivalently,

$$\min_{W,v} \sum_n \frac{1}{2} \left(y_n - \mathbf{v}^T \mathbf{h}_n \right)^2$$

$$\mathbf{h}_{i,n} = f(\mathbf{w}_i^T \mathbf{x}_n)$$

- Computing gradients: second layer

$$\frac{dL_n}{d\mathbf{v}} = -\left(y_n - \mathbf{v}^T \mathbf{h}_n \right) \mathbf{h}_n$$

least-squares regression

Training a two-layer network

- Optimization framework:

$$\min_{W,v} \sum_n \frac{1}{2} \left(y_n - \sum_i \mathbf{v}_i f(\mathbf{w}_i^T \mathbf{x}_n) \right)^2$$

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$$\mathbf{h}_{i,n} = f(\mathbf{w}_i^T \mathbf{x}_n)$$

- Computing gradients: first layer
  - Chain rule of derivatives

$$\frac{dL_n}{d\mathbf{w}_i} = \sum_j \frac{dL_n}{d\mathbf{h}_j} \frac{d\mathbf{h}_j}{d\mathbf{w}_i} \longrightarrow \frac{dL_n}{d\mathbf{w}_i} = -\left(y_n - v^T h_n\right) v_i f'(\mathbf{w}_i^T \mathbf{x_n}) \mathbf{x}_n$$

O if $i \neq j$

also called as back-propagation

Practical issues: gradient descent

- Easy to get gradients wrong!
  - One strategy is to learn *v* by fixing *W* (least-squares) and then learn *W* by fixing *v* and iterate between the two steps.
- Use online gradients (or stochastic gradients)

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \frac{dL_n}{d\mathbf{w}}$$

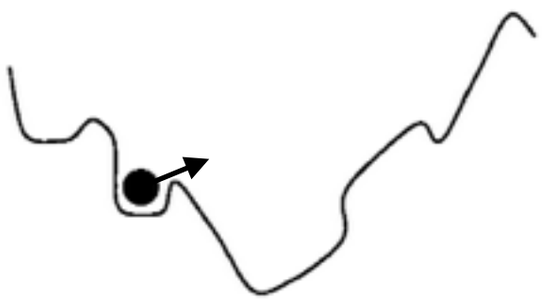
$$\frac{dL}{d\mathbf{w}} = \sum_n \frac{dL_n}{d\mathbf{w}}$$

batch online

- **Learning rate:** start with a high value and reduce it when the validation error stops decreasing
- **Momentum:** move out small local minima
  - Usually set to a high value: $\beta = 0.9$

$$\Delta\mathbf{w}^{(t)} = \beta\Delta\mathbf{w}^{(t-1)} + (1-\beta)\left(-\eta\frac{dL_n}{d\mathbf{w}^{(t)}}\right)$$

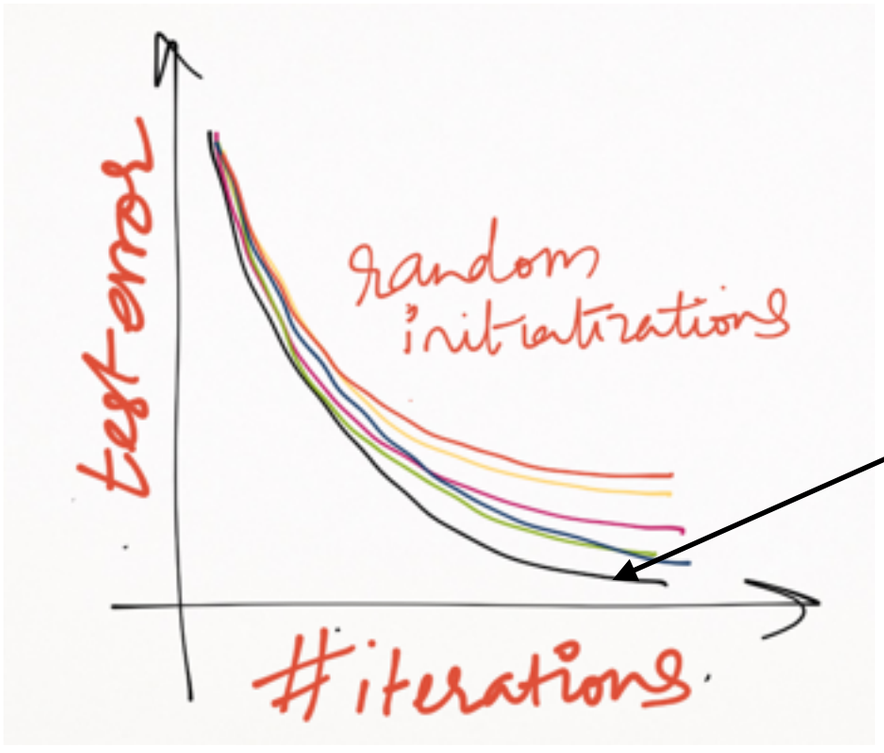
$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{t} + \Delta\mathbf{w}^{(t)}$$



Practical issues: initialization

- Initialization didn't matter for linear models
  - Guaranteed convergence to global minima as long as step size is suitably chosen since the objective is convex
- Neural networks are sensitive to initialization
  - Many local minima
  - **Symmetries:** reorder the hidden units and change the weights accordingly to get another network that produces identical outputs

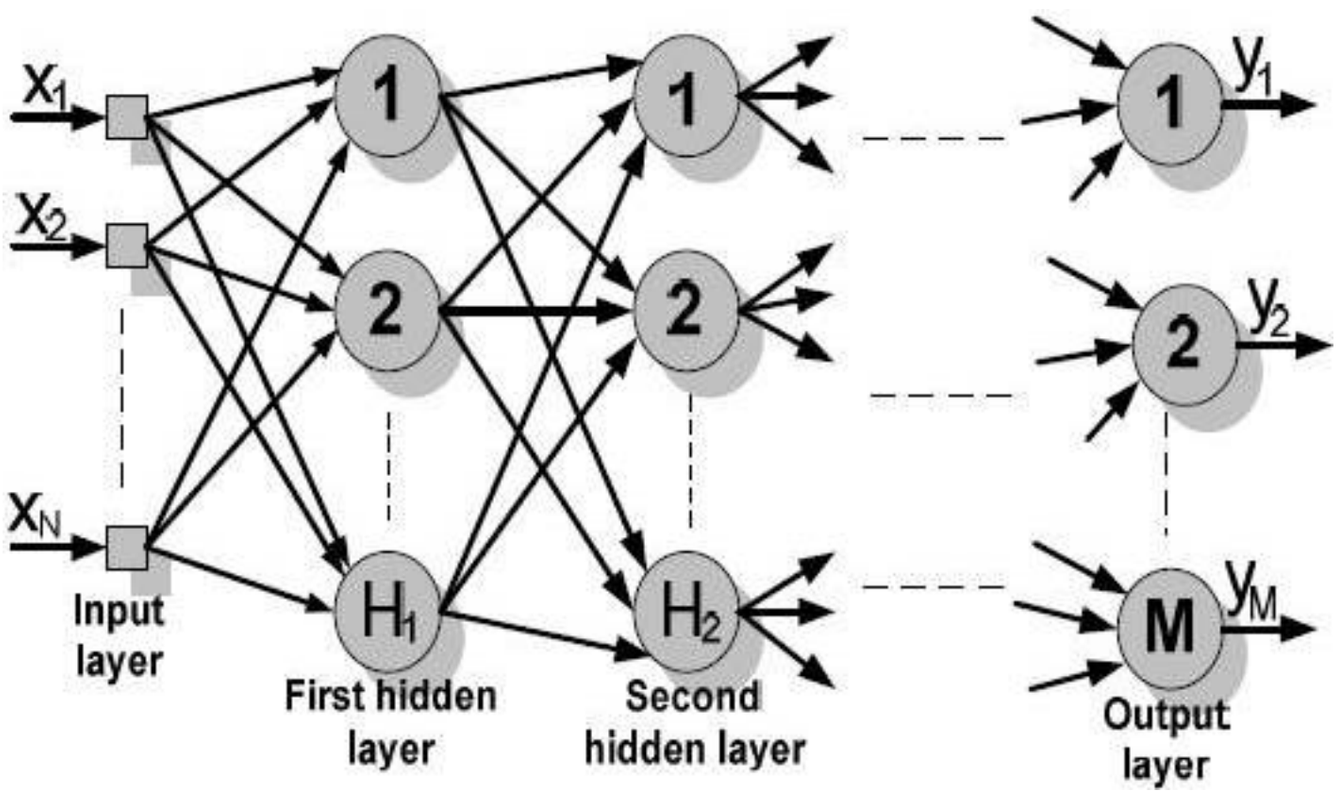
- Train multiple networks with randomly initialized weights



Beyond two layers

- The architecture generalizes to any directed acyclic graph (DAG)
  - For example a multi-layer network
  - One can order the vertices in a DAG such that all edges go from left to right (topological sorting)

prediction: forward propagation



gradients: backward propagation

Breadth vs. depth

- Why train deeper networks?
- We will borrow ideas from theoretical computer science
  - A boolean circuit is a DAG where each node is either an input, an AND gate, an OR gate, or a NOT gate. One of these is designated as an output gate.
  - Circuit complexity of a boolean function f is the size of the smallest circuit (i.e., with the fewest nodes) that can compute f.

- **The parity function:** the number of 1s is even or odd

$$\text{parity}(\mathbf{x}) = \left(\sum_d x_d \right) \mod 2$$

- **[Håstad, 1987]** A depth-*k* circuit requires $\exp\left(n^{\frac{1}{k-1}}\right)$ to compute the parity function of *n* inputs

Breadth vs. depth

- Why **not** train deeper networks?
- Selecting the architecture is daunting
  - How many hidden layers
  - How many units per hidden layer
- Vanishing gradients
  - Gradients shrink as one moves away from the output layer
  - Convergence is slow
- Training deep networks is an active area of research
  - Layer-wise initialization (perhaps using unsupervised data)
  - Engineering: GPUs to train on massive labelled datasets

Two-layer network as kNN classifier

- Can a two-layer network learn a kNN classifier?
- Replace the link function with a Gaussian

$$h_i = \tanh(\mathbf{w}_i^T \mathbf{x}) \longrightarrow h_i = \exp\left(-\gamma(\mathbf{w}_i - \mathbf{x})^2\right)$$

- The output has the form:

$$f(\mathbf{x}) = \sum_i v_i \exp\left(-\gamma(\mathbf{w}_i - \mathbf{x})^2\right)$$

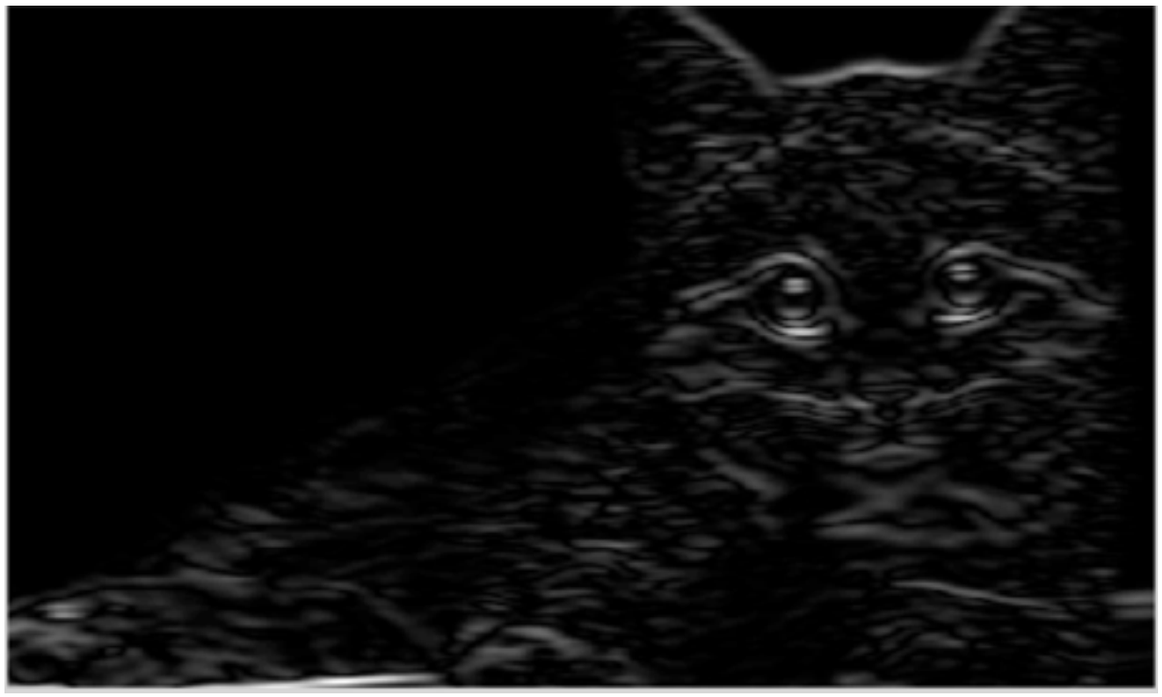
- By setting $\mathbf{w}_i$ as $\mathbf{x}_i$ and v_i as y_i for the i^{th} hidden node, we obtain a
  - distance-weighted kNN classifier, and equivalently a
  - kernel density classifier with a Gaussian kernel.
- The advantage is that we can learn the centers ($\mathbf{w}_i$), widths (γ) and weights (v_i) by back-propagation

Convolutional neural networks

- Images are not just a collection of pixels
  - Lots of local structure: edges, corners, etc
  - These statistics are translation invariant
- The convolution operation:

filter: horizontal edge

image



absolute value of the output of convolution of the image and filter

Convolutional neural networks

- Images are not just a collection of pixels
  - Lots of local structure: edges, corners, etc
  - These statistics are translation invariant
- The convolution operation:

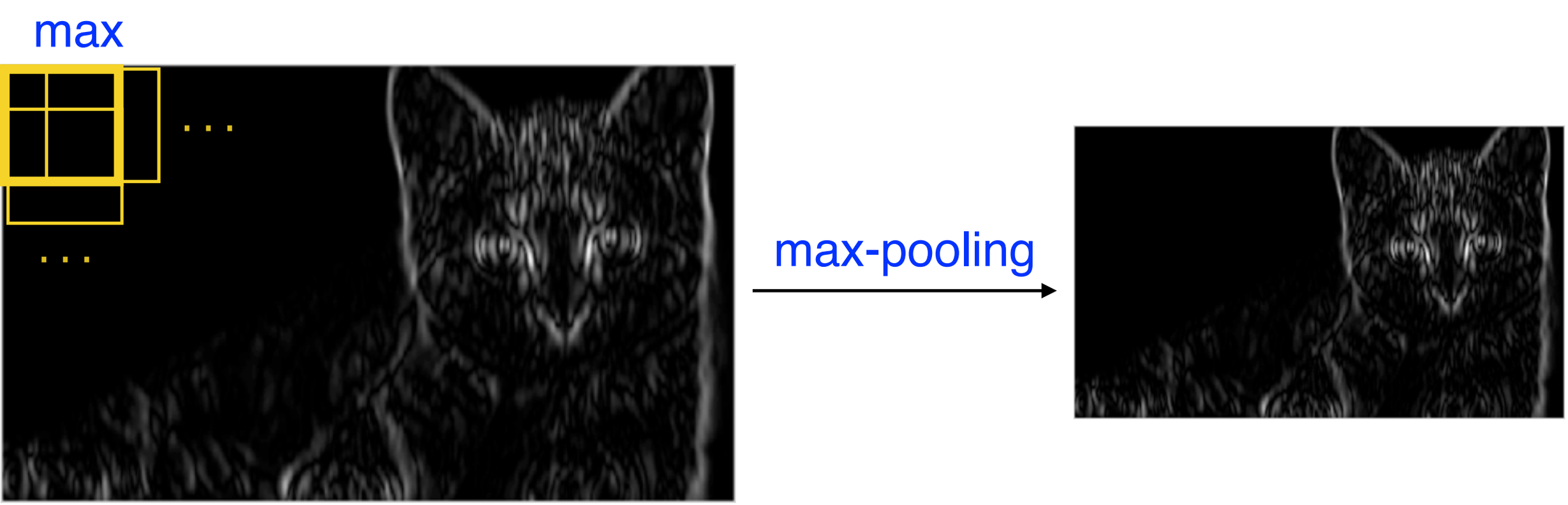
filter: vertical edge

image

absolute value of the output of convolution of the image and filter

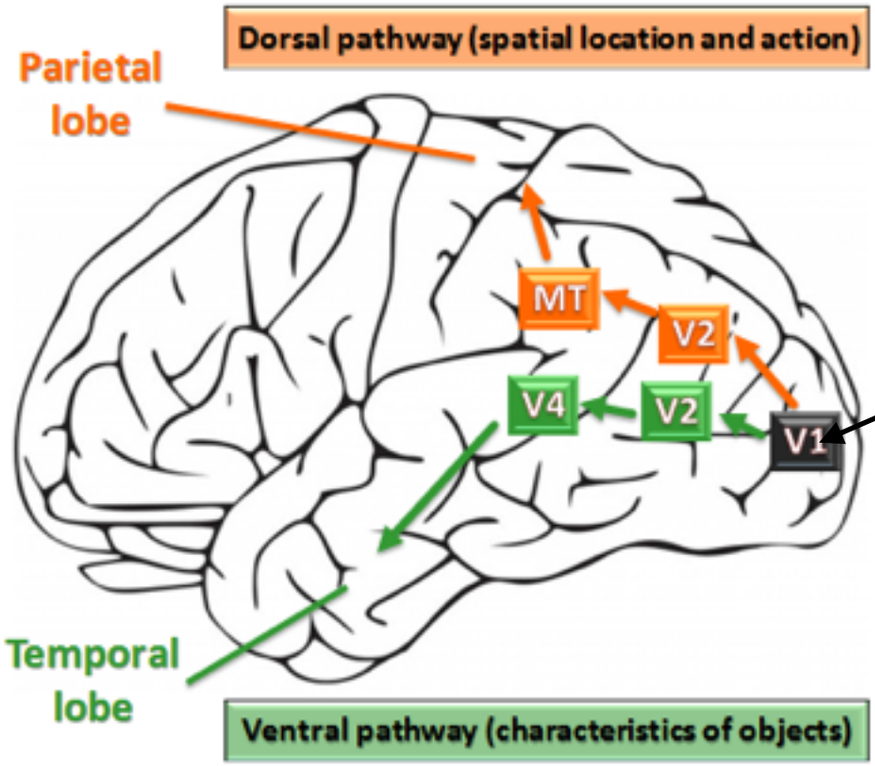
Convolutional neural networks

- Images are not just a collection of pixels
  - Lots of local structure: edges, corners, etc
  - These statistics are translation invariant
- The pooling operation: subsample the output
  - Invariance to small shifts
  - Options: max, sum Parameters: window size, stride



Convolutional neural networks

- A CNN unit contains the following layers:
  1. Convolutional layer containing a set of filters
  2. Pooling layer
  3. Non-linearity
- Deep CNN: a stack of multiple CNN units
  - Inspired by the human visual system (V1, V2, V3 ….)



Hubel and Weisel, 1968
Structure of V1
“simple” cells: edge detectors

Example: LeNet5

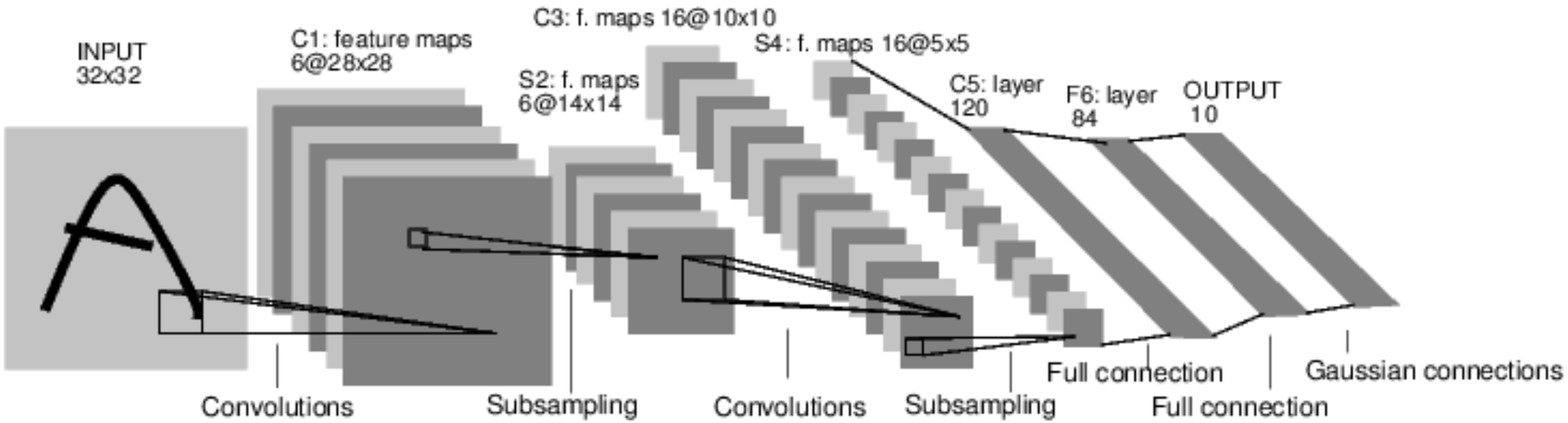


image ⟶ 6 5x5 ⟶ 2x2 ⟶ 16 6x6 ⟶ 2x2 ⟶ 120 5x5 ⟶ full ⟶ full

- C1: Convolutional layer with 6 filters of size 5x5
- Output: 6x28x28
- Number of parameters: (5x5+1)*6 = 156
- Connections: (5x5+1)x(6x28x28) = 122304
- Connections in a fully connected network: (32x32+1)x(6X28x28)

LeCun 98

Example: LeNet5

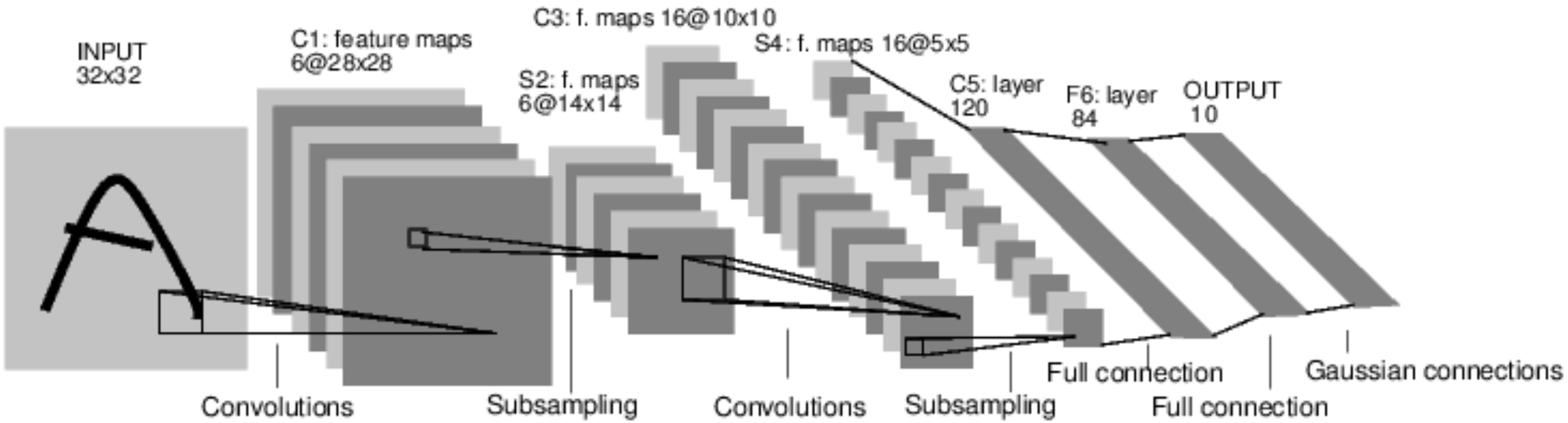


image ⟶ 6 5x5 ⟶ 2x2 ⟶ 16 6x6 ⟶ 2x2 ⟶ 120 5x5 ⟶ full ⟶ full

- S1: Subsampling layer
- Subsample by taking the sum of non-overlapping 2x2 windows
  - Multiply the sum by a constant and add bias
- Number of parameters: 2x6=12
- Pass the output through a sigmoid non-linearity
- Output: 6x14x14

Example: LeNet5

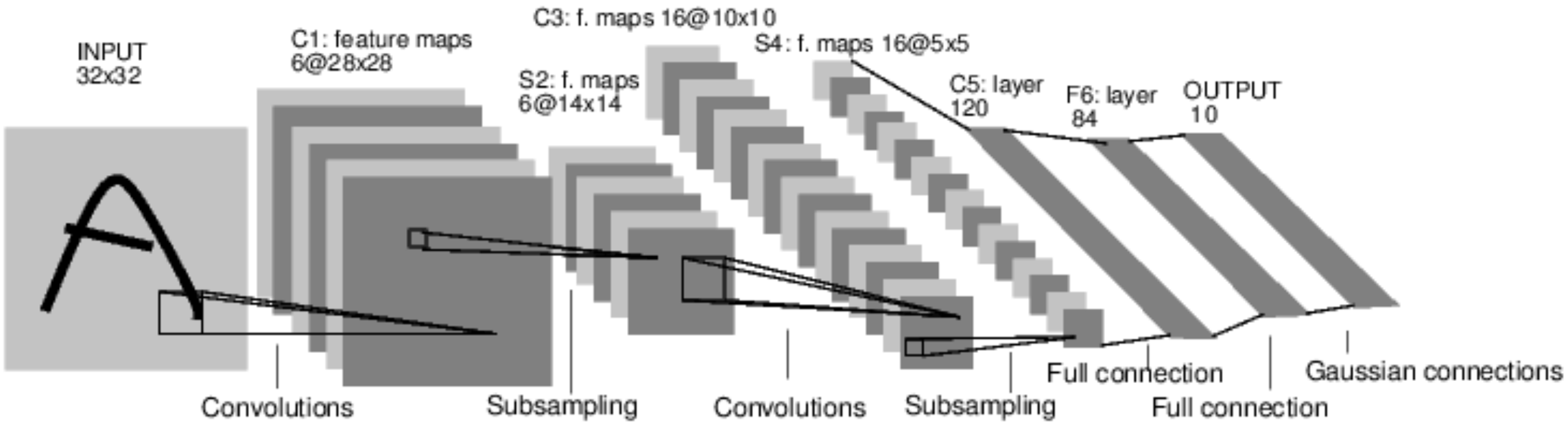


image ⟶ 6 5x5 ⟶ 2x2 ⟶ 16 6x6 ⟶ 2x2 ⟶ 120 5x5 ⟶ full ⟶ full

- C3: Convolutional layer with 16 filters of size 6x6
- Each is connected to a subset:
- Number of parameters: 1,516
- Number of connections: 151,600
- Output: 16x10x10

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	X				X	X	X			X	X	X	X		X	X
1	X	X				X	X	X			X	X	X	X		X
2	X	X	X				X	X	X			X		X	X	X
3		X	X	X			X	X	X	X			X		X	X
4			X	X	X			X	X	X	X		X	X		X
5				X	X	X			X	X	X	X		X	X	X

TABLE I

EACH COLUMN INDICATES WHICH FEATURE MAP IN S2 ARE COMBINED BY THE UNITS IN A PARTICULAR FEATURE MAP OF C3.

Example: LeNet5

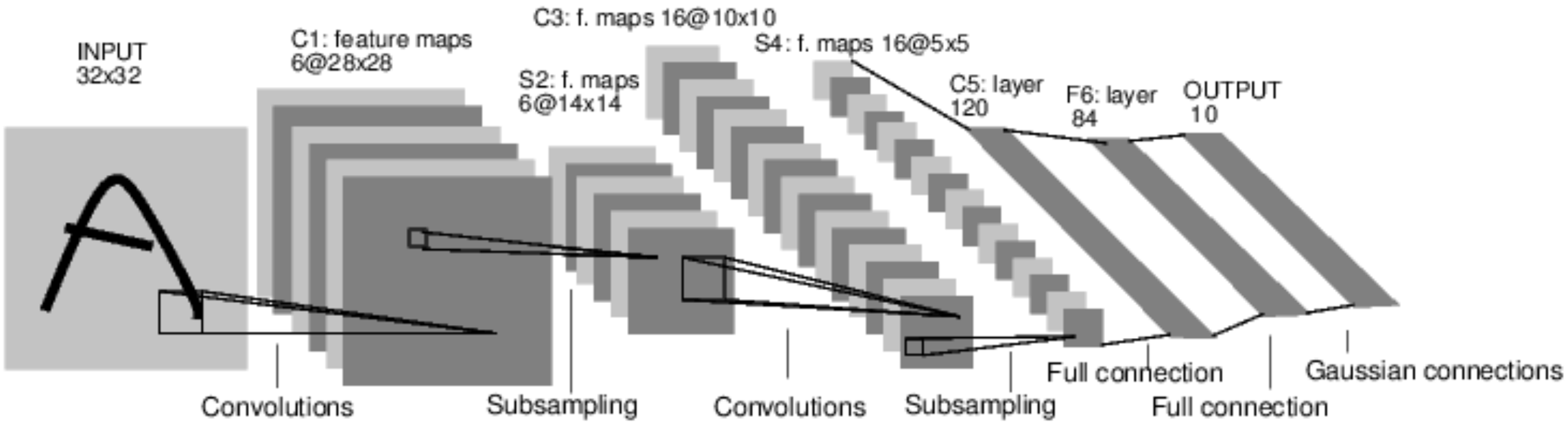


image ⟶ 6 5x5 ⟶ 2x2 ⟶ 16 6x6 ⟶ 2x2 ⟶ 120 5x5 ⟶ full ⟶ full

- S4: Subsampling layer
- Subsample by taking the sum of non-overlapping 2x2 windows
  - Multiply by a constant and add bias
- Number of parameters: 2x16 = 32
- Pass the output through a sigmoid non-linearity
- Output: 16x5x5

Example: LeNet5

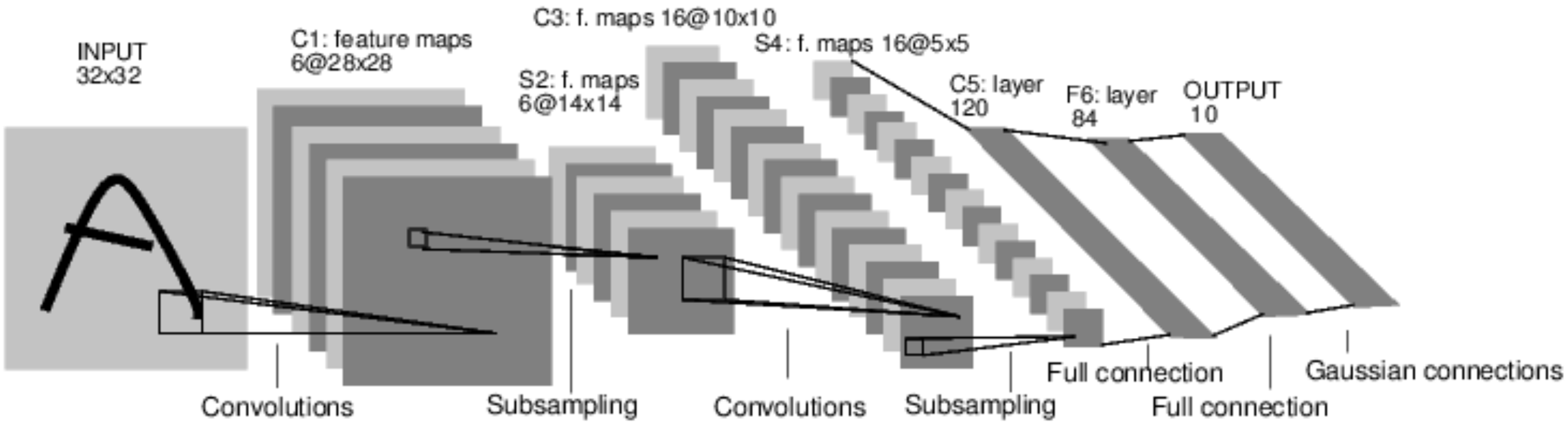


image ⟶ 6 5x5 ⟶ 2x2 ⟶ 16 6x6 ⟶ 2x2 ⟶ 120 5x5 ⟶ full ⟶ full

- C5: Convolutional layer with 120 outputs of size 1x1
- Each unit in C5 is connected to all inputs in S4
- Number of parameters: (16x5x5+1)*120 = 48120

Example: LeNet5

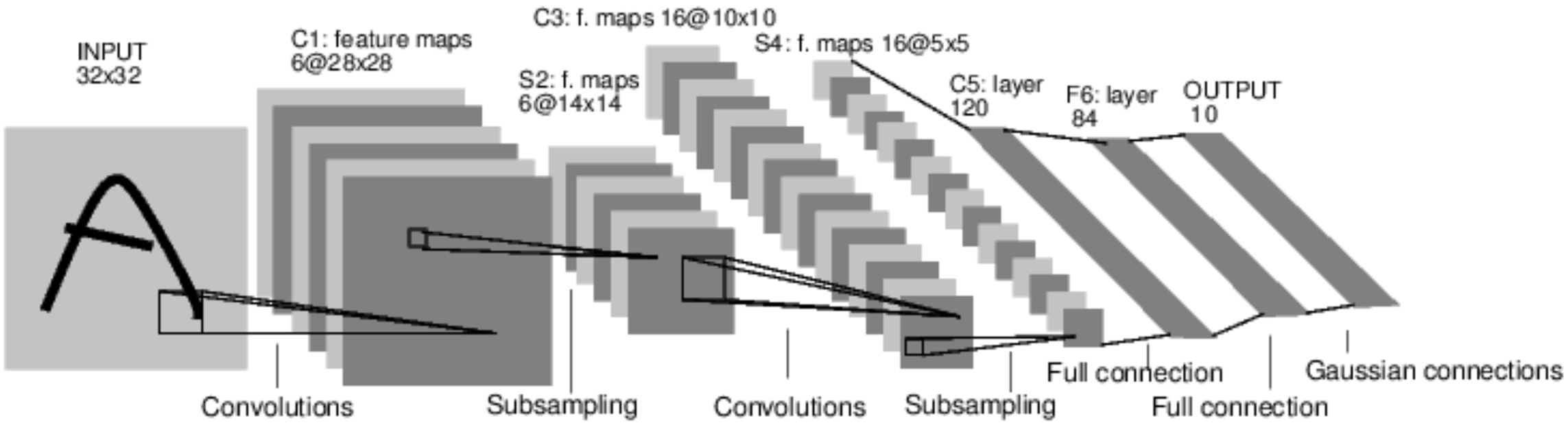


image ⟶ 6 5x5 ⟶ 2x2 ⟶ 16 6x6 ⟶ 2x2 ⟶ 120 5x5 ⟶ full ⟶ full

- F6: fully connected layer
- Output: 1x1x84
- Number of parameters: (120+1)*84 = 10164

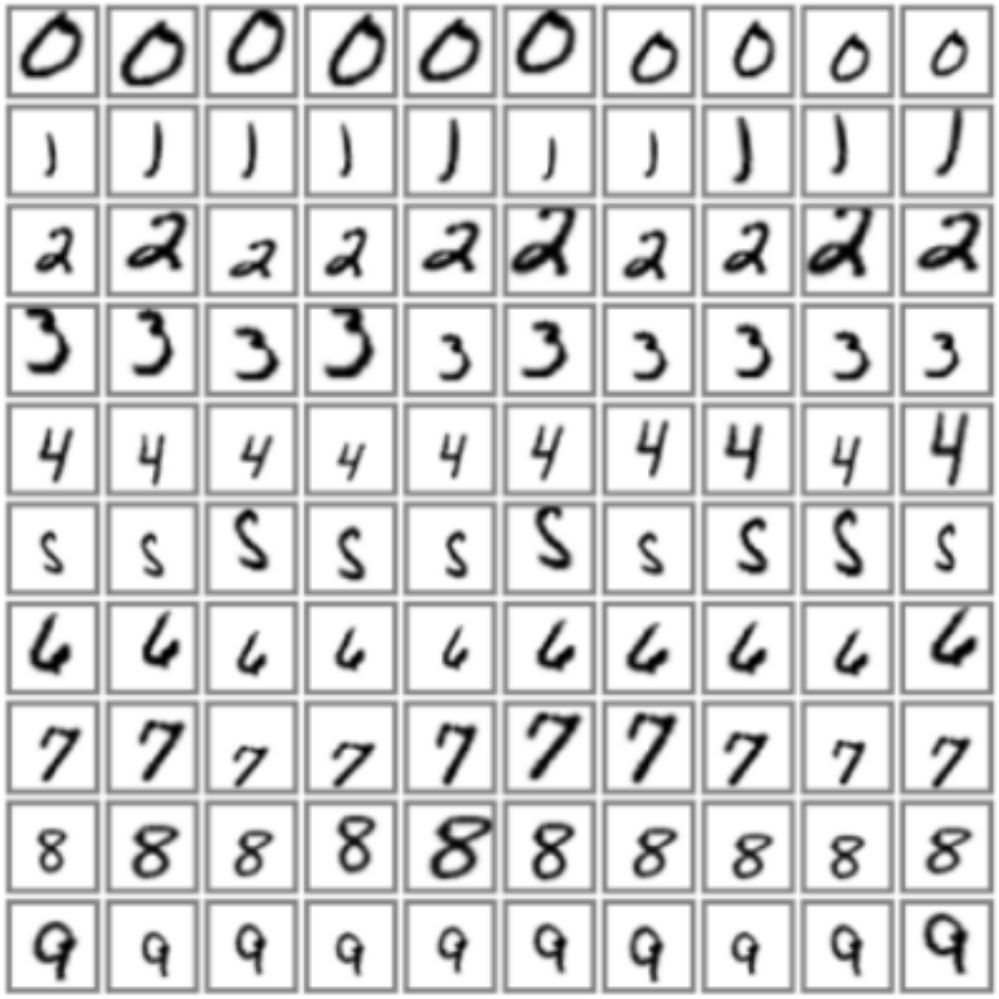
- OUTPUT: 10 Euclidean RBF units (one for each digit class)

$$y_i = \sum_j (x_j - w_{ij})^2.$$

MNIST dataset

60,000 original datasets

Test error: 0.95%



540,000 artificial distortions

+ 60,000 original

Test error: 0.8%

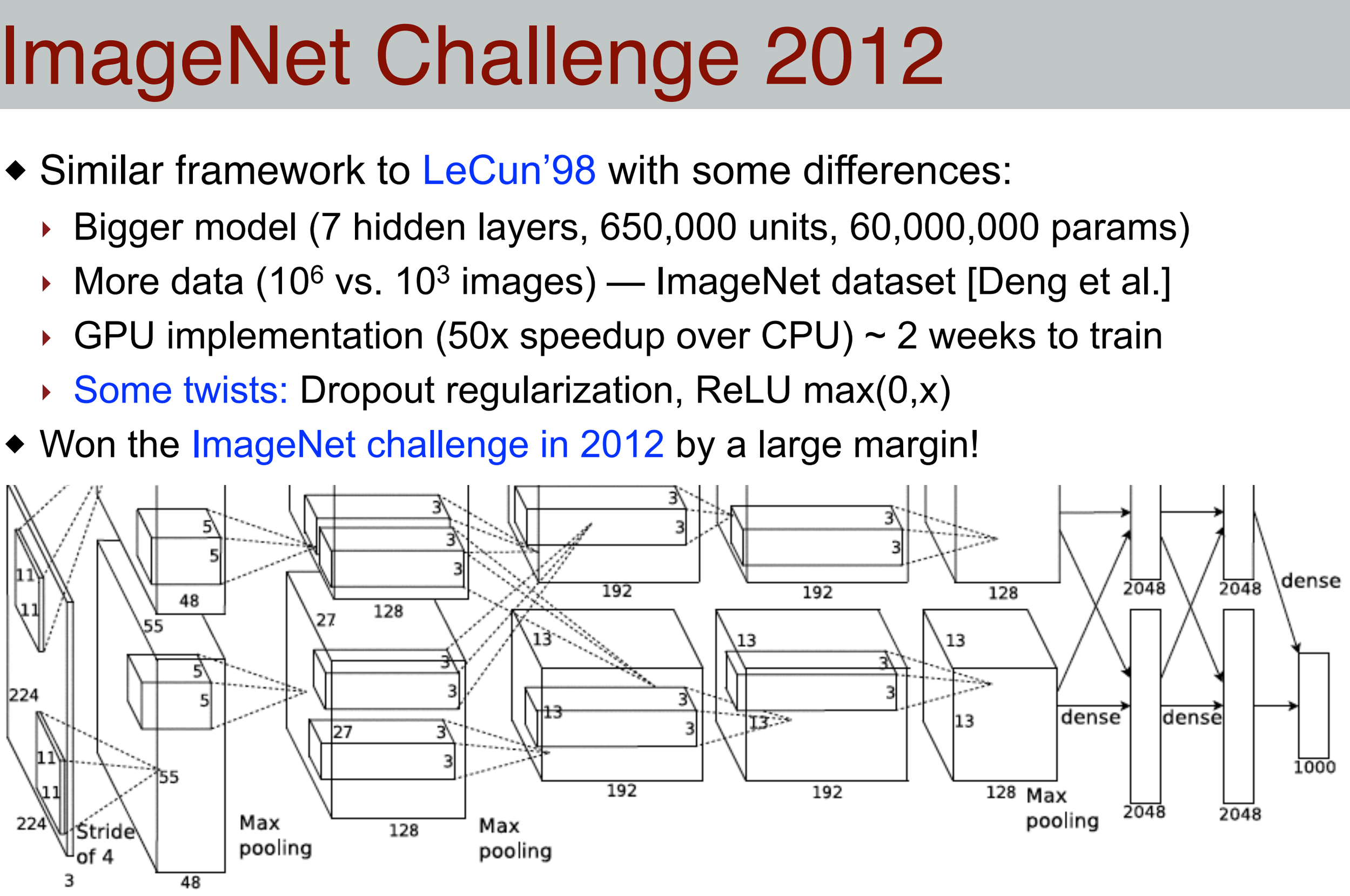
3-layer NN, 300+100 HU [distortions]
Test error: 2.5%

http://yann.lecun.com/exdb/mnist/

MNIST dataset: errors on the test set

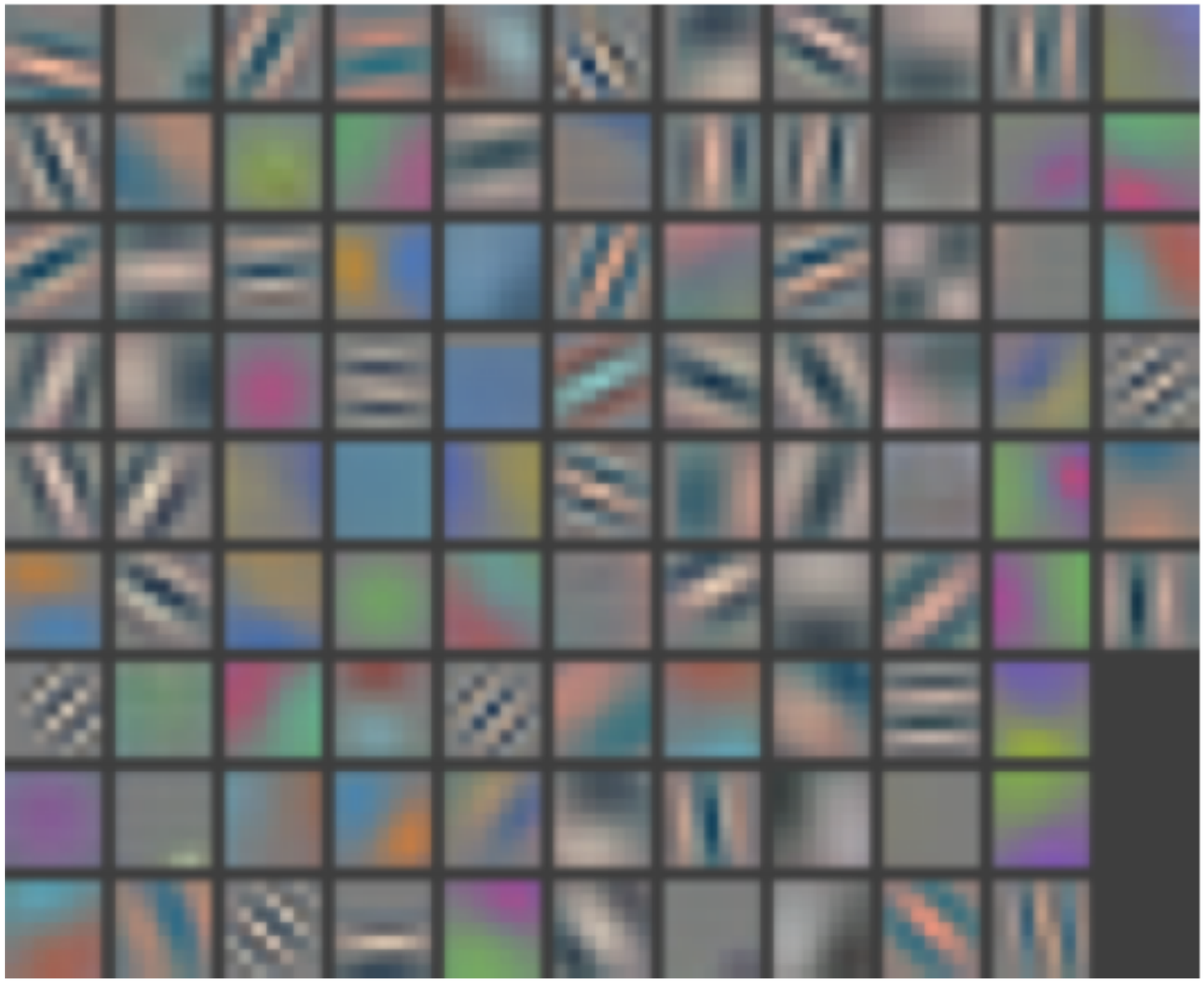
ImageNet Challenge 2012

- Similar framework to LeCun'98 with some differences:
  - Bigger model (7 hidden layers, 650,000 units, 60,000,000 params)
  - More data (10^6 vs. 10^3 images) — ImageNet dataset [Deng et al.]
  - GPU implementation (50x speedup over CPU) ~ 2 weeks to train
  - Some twists: Dropout regularization, ReLU max(0,x)
- Won the ImageNet challenge in 2012 by a large margin!



Krizhevsky, I. Sutskever, and G. Hinton,
ImageNet Classification with Deep Convolutional Neural Networks, NIPS 2012

Layer 1: Learned filters



similar to “edge” and “blob” detectors

Layer 1: Top-9 Patches

- Patches from validation images that give maximal activation of a given feature map

Layer 2: Top-9 Patches

Layer 3: Top-9 Patches

Layer 4: Top-9 Patches

Layer 5: Top-9 Patches

Summary

- Motivation: non-linearity
- Ingredients of a neural network
  - hidden units, link functions
- Training by back-propagation
  - random initialization, chain rule, stochastic gradients, momentum
  - Practical issues: learning, network architecture
- Theoretical properties:
  - A two-layer network is a universal function approximator
  - However, deeper networks can be more efficient at approximating certain functions
- Convolutional neural networks:
  - Good for vision problems where inputs have local structure
  - Shared structure of weights leads to significantly fewer parameters

Slides credit

- Multilayer neural network figure source:
  - http://www.ibimapublishing.com/journals/CIBIMA/2012/525995/525995.html
- Cat image: http://www.playbuzz.com/abbeymcneill10/which-cat-breed-are-you
- More about the structure of the visual processing system
  - http://www.cns.nyu.edu/~david/courses/perception/lecturenotes/V1/lgn-V1.html
- ImageNet visualization slides are by Rob Fergus @ NYU/Facebook
  http://cs.nyu.edu/~fergus/presentations/nips2013_final.pdf
- LeNet5 figure from: http://yann.lecun.com/exdb/publis/pdf/lecun-98.pdf
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