ECE408/CS483/CSE408 Fall 2022

Applied Parallel Programming

Lecture 11:

Feed-Forward Networks and Gradient-Based Training

Course Reminders

- Lab 1-4 grades will be posted on Canvas by the end of this week
- Midterm 1 is on Tuesday, October 11th
  - On-line, everybody will be taking it at the same time
    - Tuesday, Oct. 11th 7:00pm-8:20pm US Central time
    - Wednesday, Oct. 12th 8:00am-9:20am Beijing time
  - Includes materials from Lecture 1 through Lecture 10
  - If you have a conflict, please let us know by Friday Sept 30th
- Project Milestone 1: Baseline CPU implementation is due Friday October 14th
  - Project details to be posted this week

Objective

- To learn the basic approach to feedforward neural networks:
  - neural model
  - common functions
  - training through gradient descent

Example: Digit Recognition

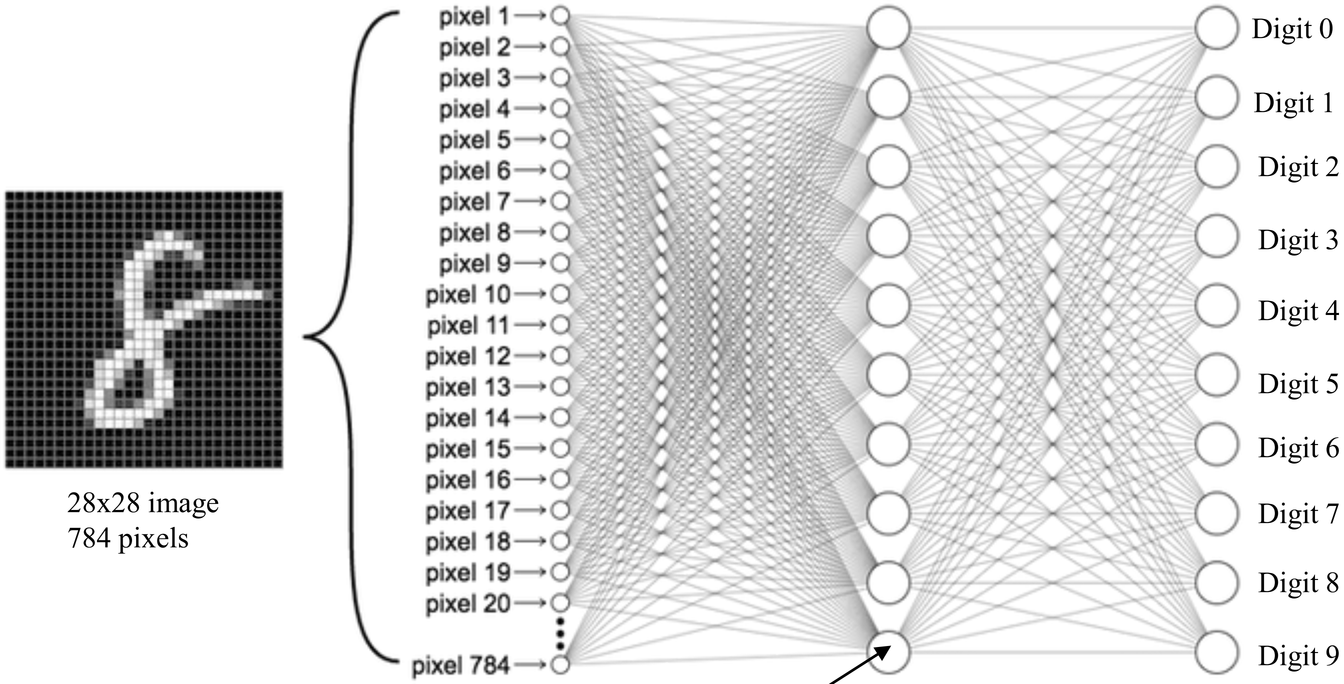
Let's consider an example.

- **handwritten digit recognition**:
- given a **28 × 28 grayscale image**,
- produce a **number from 0 to 9**.

Input dataset

- **60,000** images
- Each labeled by a human with correct answer.

MultiLayer Perceptron (MLP) for Digit Recognition



n_k^1 = activation($\boldsymbol{w}_k\boldsymbol{x}$+$b_k$)

This network would has
- 784 nodes on input layer (L0)
- 10 nodes on hidden layer (L1)
- 10 nodes on output layer (L2)

784*10 weights + 10 biases for L1
10*10 weights + 10 biases for L2

A total of 7,960 parameters

Each node represents a function, based on a linear combination of inputs + bias

Activation function "repositions" output value.

Sigmoid, sign, ReLU are common…

How Do We Determine the Weights?

First layer of perceptrons

- **784** (28^2) inputs, **1024** outputs, **fully connected**
- **[1024 × 784]** weight matrix ***W***
- **[1024 x 1]** bias vector ***b***

Use labeled training data to pick weights.

Idea:

- given enough labeled input data,
- we can **approximate the input-output function**.

Forward and Backward Propagation

Forward (**inference**):

- given input $\boldsymbol{x}$ (for example, an image),
- **use parameters $\boldsymbol{\theta}$** ($\boldsymbol{W}$ and b for each layer)
- **to compute probabilities *k[i]*** (ex: for each digit *i*).

Backward (**training**):

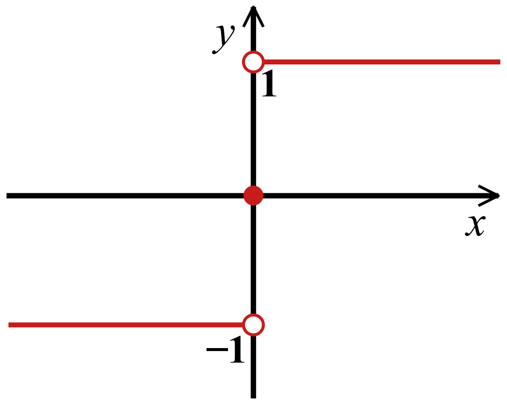
- given input $\boldsymbol{x}$, parameters $\boldsymbol{\theta}$, and outputs ***k[i]***,
- **compute error $\boldsymbol{E}$** based on target label $\boldsymbol{t}$,
- then **adjust $\boldsymbol{\theta}$** proportional to $\boldsymbol{E}$ to reduce error.

Neural Functions Impact Training

Recall perceptron function: **y = sign (W·x + b)**

To propagate error backwards,

- **use chain rule** from calculus.
- **Smooth functions are useful.**



Sign is not a smooth function.

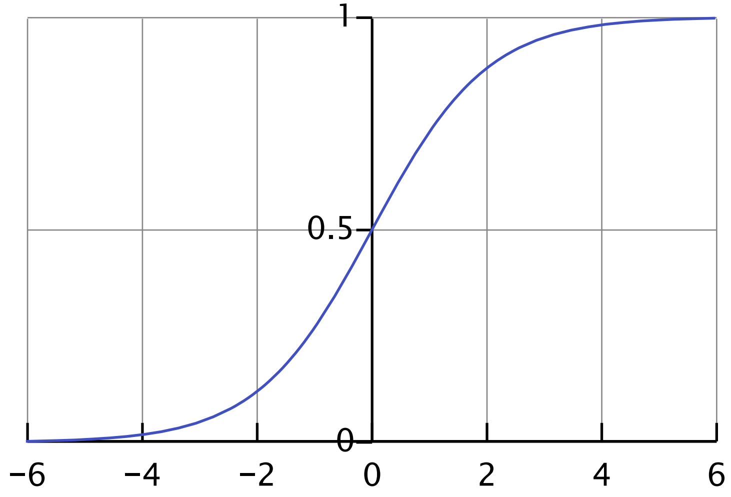
One Choice: Sigmoid/Logistic Function

Until about 2017,

- **sigmoid / logistic function** most popular

$$f(x) = \frac{1}{1+e^{-x}} \qquad (f\colon \mathbb{R} \rightarrow (0,1)\,)$$

  for replacing sign.



- Once we have *f(x)*, finding *df/dx* is easy:

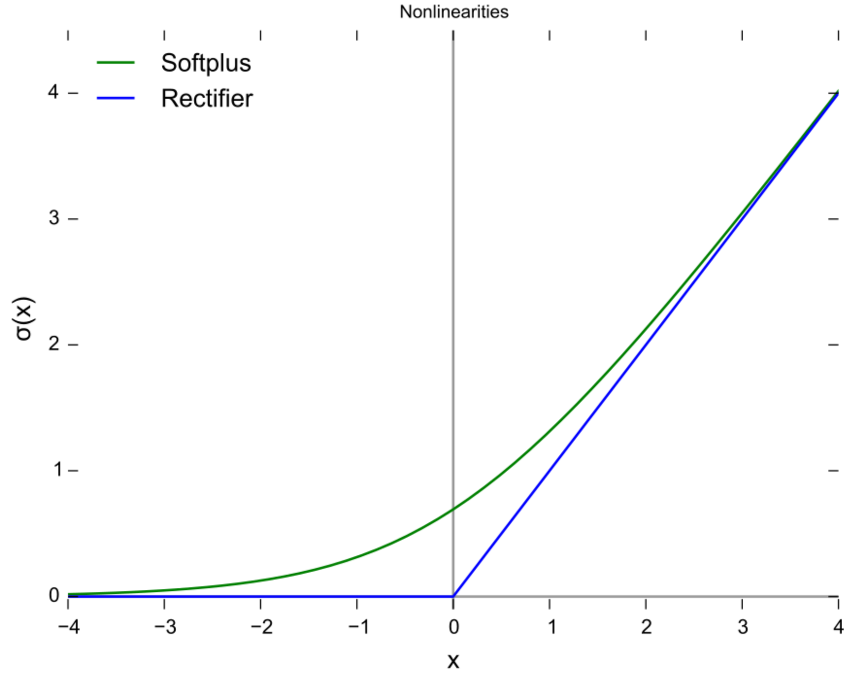
$$\frac{df(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = f(x)\frac{e^{-x}}{(1+e^{-x})} = f(x)(1 - f(x))$$

(Our example used this function.)

Today's Choice: ReLU

In 2017, most common choice became

- **rectified linear unit / ReLU / ramp function**
  $$\boldsymbol{f(x) = \max(0, x)} \quad (\text{f: } \mathbb{R} \rightarrow \mathbb{R}^{+})$$
  which is much faster (no exponent required).
- A smooth approximation is **softplus/SmoothReLU**
  $$\boldsymbol{f(x) = \ln(1 + e^{x})} \quad (\text{f: } \mathbb{R} \rightarrow \mathbb{R}^{+})$$
  which is the integral of the logistic function.
- Lots of variations exist. See Wikipedia for an overview and discussion of tradeoffs.



Use Softmax to Produce Probabilities

How can sigmoid / ReLU produce probabilities?

They can't.

- Instead, given output vector **Z = (z[0], …, z[C-1])***,
- we produce a second vector **K = (k[0], …, k[C-1])**
- using the **softmax function**

$$\boldsymbol{k[i]} = \frac{\boldsymbol{e^{z[i]}}}{\boldsymbol{\sum_{j=0}^{C-1} e^{z[j]}}}$$

Notice that **the k[i] sum to 1.**

*Remember that we classify into one of C categories.

Softmax Derivatives Needed to Train

We also need the **derivatives of softmax**,

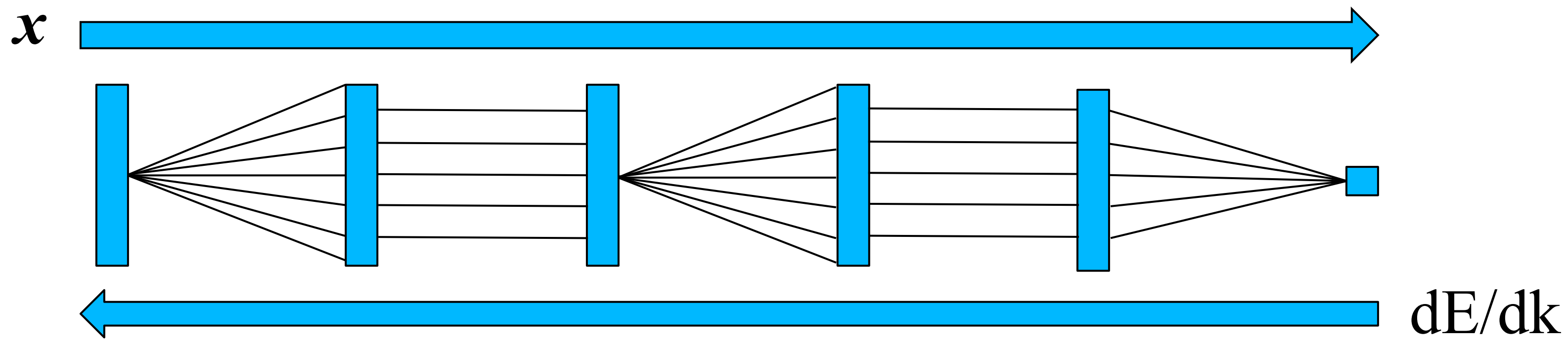
$$\frac{dk[i]}{dz[m]} = k[i](\delta_{i,m} - k[m]),$$

where $\delta_{i,m}$ is the Kronecker delta
(1 if i = m, and 0 otherwise).

Forward and Backward Propagation

Forward:

$fc_1 = W_1 \bullet x + b_1$ $\quad y = sigmoid(fc_1)$ $\quad fc_2 = W_2 \bullet y + b_2$ $\quad z = sigmoid(fc_2)$ $\quad k = softmax(z)$



Backward:

$$\frac{dE}{dfc_1} = \frac{dE}{dy}\frac{dy}{dfc_1} \qquad \frac{dE}{dy} = \frac{dE}{dfc_2}\frac{dfc_2}{dy} \qquad \frac{dE}{dfc_2} = \frac{dE}{dz}\frac{dz}{dfc_2} \qquad \frac{dE}{dz} = \frac{dE}{dk}\frac{dk}{dz}$$

Choosing an Error Function

Many error functions are possible.

For example, **given label *T*** (digit ***T***),

- ***E = 1 – k[T]***, the **probability of not classifying as *t***.

Alternatively, since our categories are numeric,
we can **penalize quadratically**:

$$\boldsymbol{E = \sum_{j=0}^{C-1} k[j](j - T)^2}$$

Let's **go with the latter**.

Stochastic Gradient Descent

How do we calculate the weights?

One common answer: **stochastic gradient descent**.

1. **Calculate**
   - **derivative** of sum **of error *E***
   - **over all** training **inputs**
   - **for** all network parameters ***θ***.
2. **Change *θ* slightly** in the opposite direction (to decrease error).
3. **Repeat**.

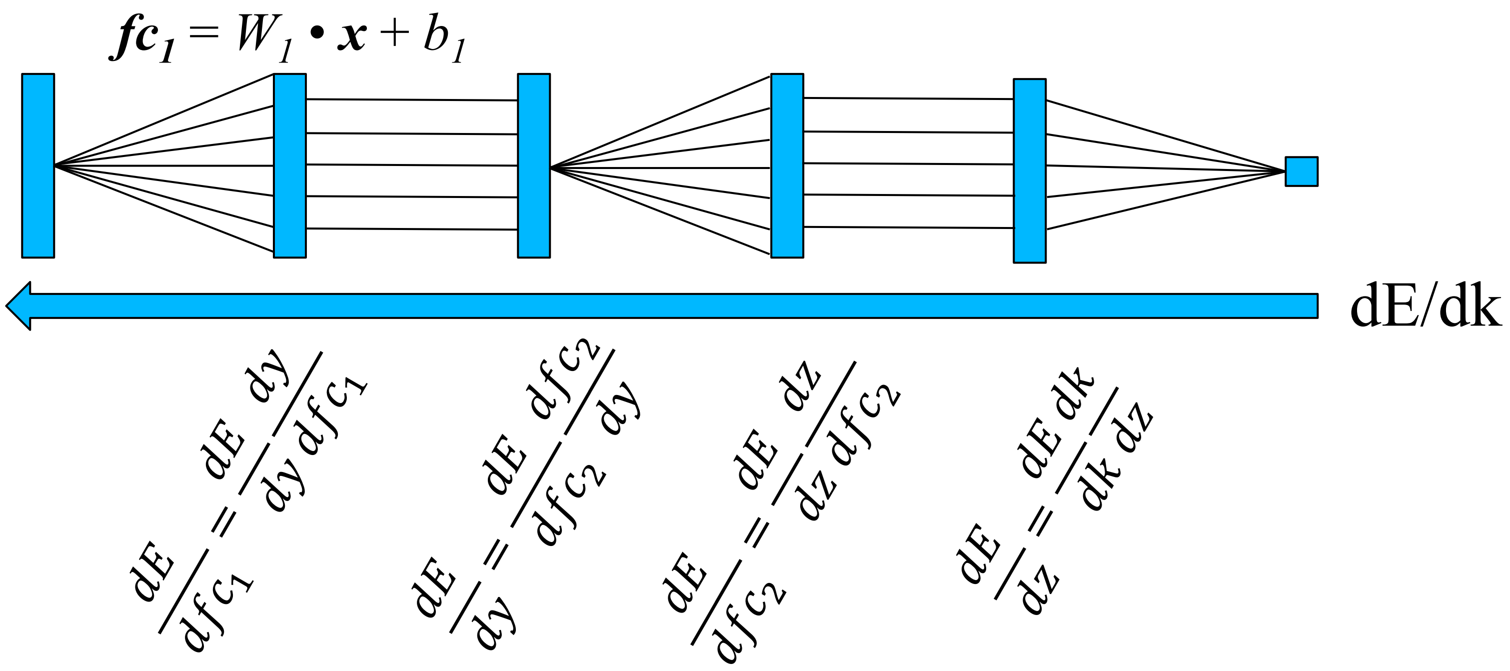
Stochastic Gradient Descent

More precisely,

1. **For every input *X***,
2. evaluate network to **compute *k[i]*** (forward),
3. then **use *k[i]* and label *T*** (target digit) **to compute error *E***.
4. Backpropagate error derivative to **find derivatives for each parameter**.
5. **Adjust θ to reduce total *E*: $\theta_{i+1} = \theta_i - \varepsilon\Delta\theta$**

(Update ε uses most accurate minima estimation.)

Parameter Updates and Propagation



Need propagated error gradient (from backward pass)

Weight update

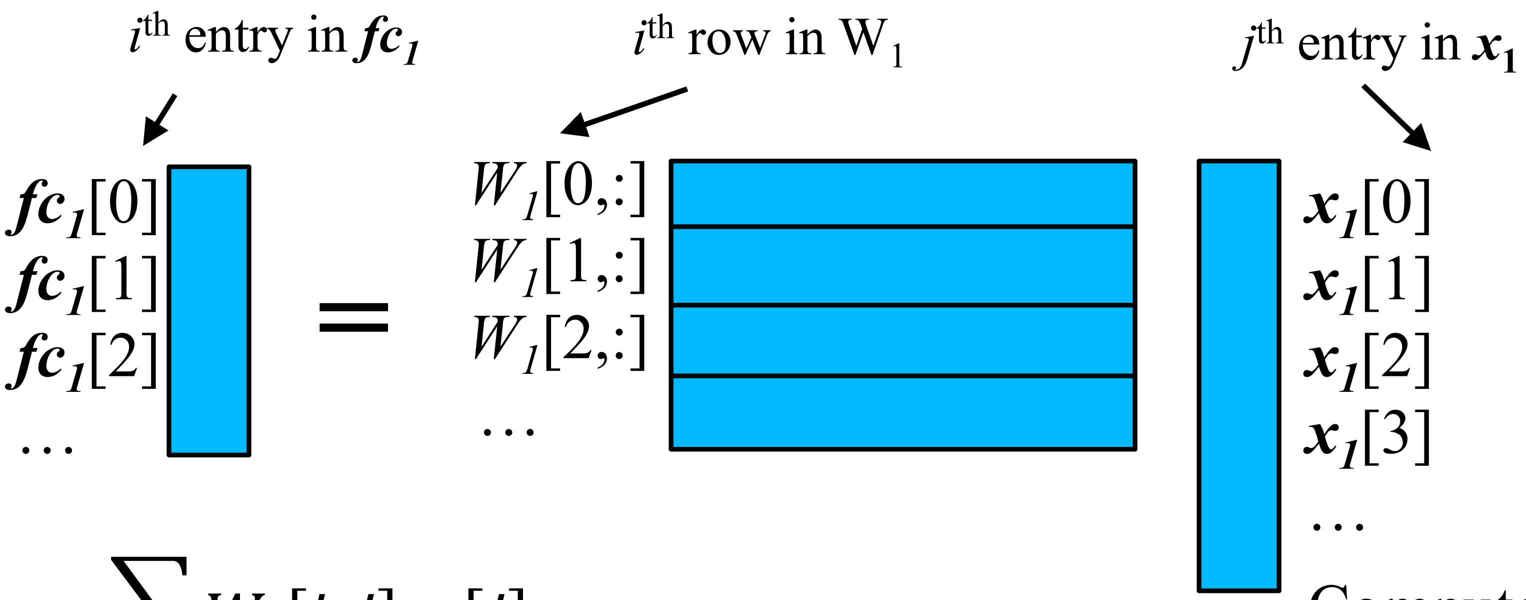
$$\frac{dE}{dW_1} = \frac{dE}{dfc_1}\frac{dfc_1}{dW_1} = \frac{dE}{dfc_1}x$$

Need input (from forward pass)

Example: Gradient Update with One Layer

$\Theta_{i+1} = \Theta_i - \varepsilon\Delta\Theta \quad W_{i+1} = W_i - \varepsilon\Delta W$	Parameter Update
$y = W \bullet \boldsymbol{x} + b$	Network function
$\frac{dy}{dW} = x$	Network weight gradient
$E = \frac{1}{2}(y - t)^2$	Error function
$\frac{dE}{dy} = y - t = Wx + b - t$	Error function gradient
$\Delta W = \frac{dE}{dW} = \frac{dE}{dy}\frac{dy}{dW}$	Full weight update expression
$W_{i+1} = W_i - \varepsilon(W\boldsymbol{x}+b-t)x$	Full weight update term

Fully-Connected Gradient Detail



$$fc_1 = \sum_j W_1[i,j]\,x_1[j]$$

Computed from previous layer

$$\frac{dE}{dW_1[i,j]} = \frac{dE}{dfc_1[i]}\frac{dfc_1[i]}{dW_1[i,j]} = \frac{dE}{dfc_1[i]}x_1[j]$$

Need input to this layer

Batched Stochastic Gradient Descent

- A training *epoch* (a pass through whole training set)
  – *Set* $\Delta\Theta = 0$
  – For each labeled image:
    - Read data to initialize input layer
    - Evaluate network to get y (forward)
    - Compare with target label t to get error E
    - Backpropagate error derivative to get parameter updates
    - Accumulate parameter updates into $\Delta\Theta$
  – $\Theta_{i+1} = \Theta_i - \varepsilon\Delta\Theta$

Aggregate gradient update most accurately reflects true gradient

Mini-batch Stochastic Gradient

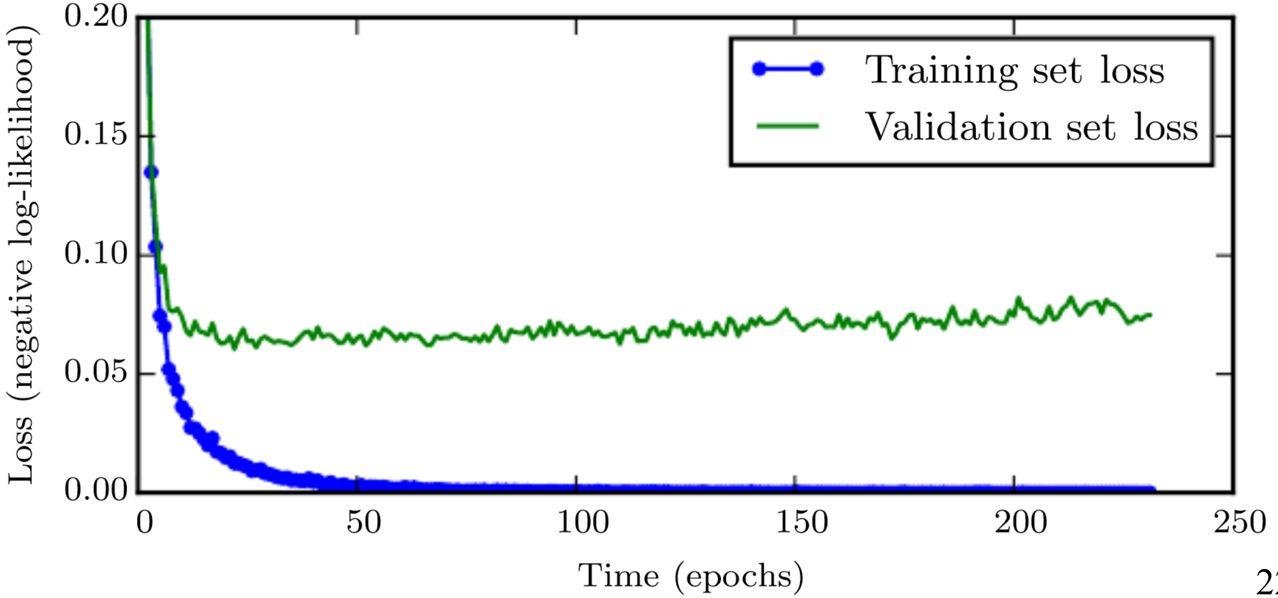
- For each batch in training set
  - For each labeled image in batch:
    - Read data to initialize input layer
    - Evaluate network to get y (forward)
    - Compare with target label t to get error E
    - Backpropagate error derivative to get parameter updates
    - Accumulate parameter updates into $\Delta\Theta$
  - $\Theta_{i+1} = \Theta_i - \varepsilon\Delta\Theta$

Balance between accuracy of gradient estimation and parallelism

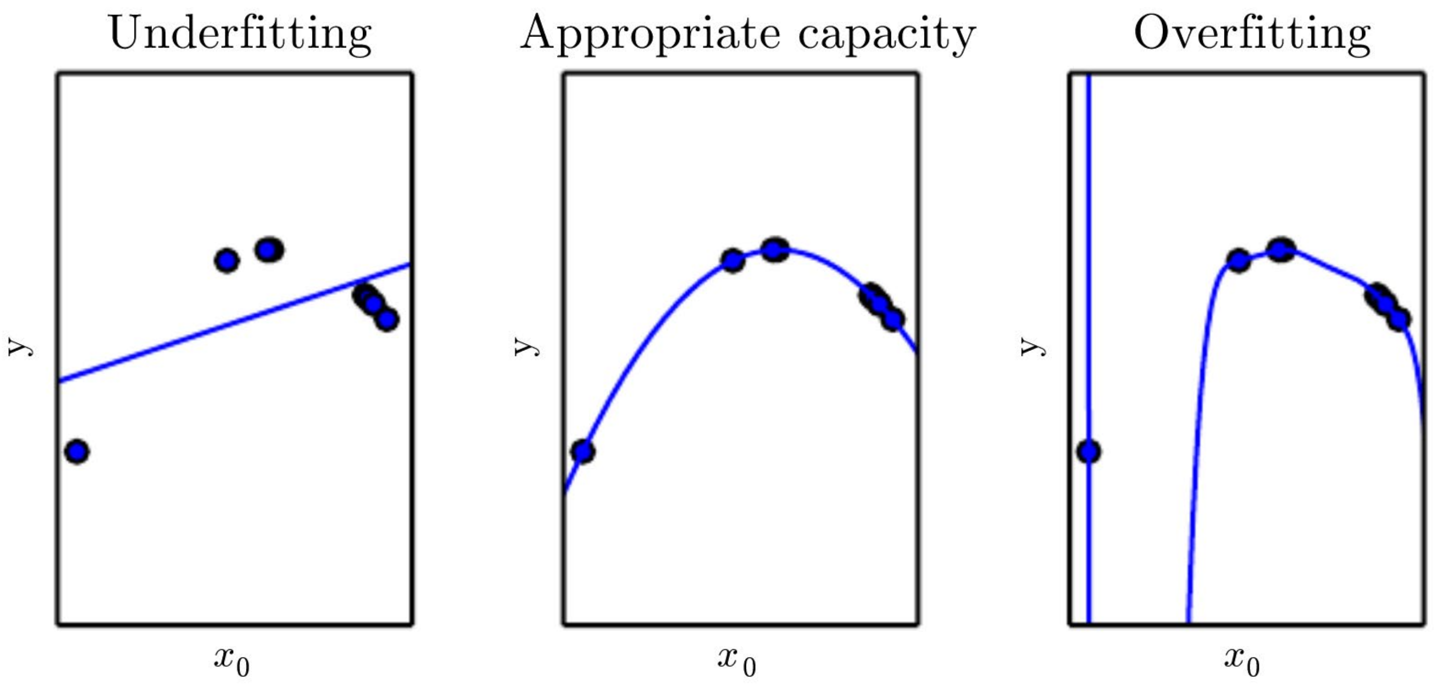
When is Training Done?

Split labeled data into *training* and *test* sets.

- Training data to compute parameter updates.
- Test data to check how model generalizes to new inputs (the ultimate goal!)
- The network can become *too good* at classifying training inputs!

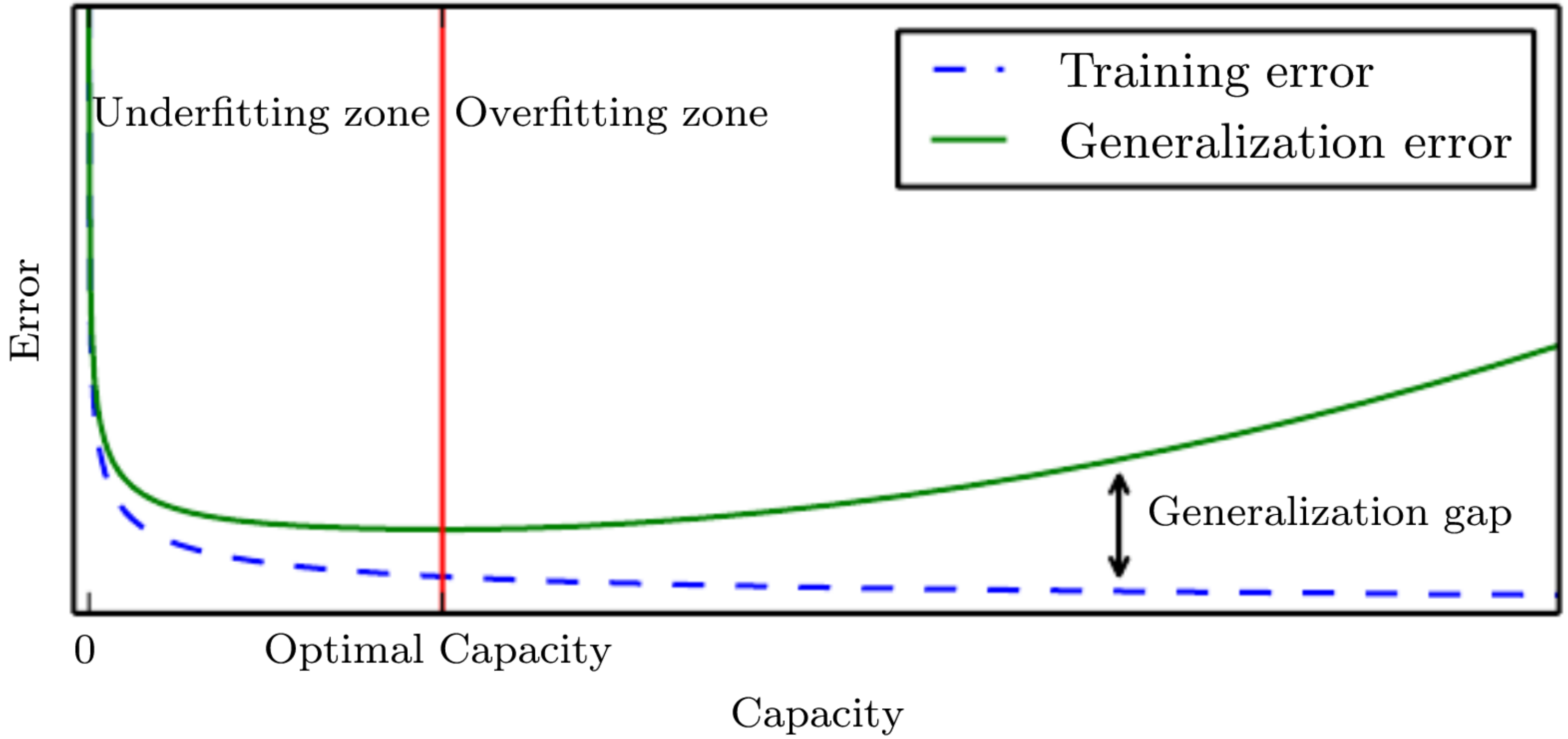


How Complicated Should a Network Be?



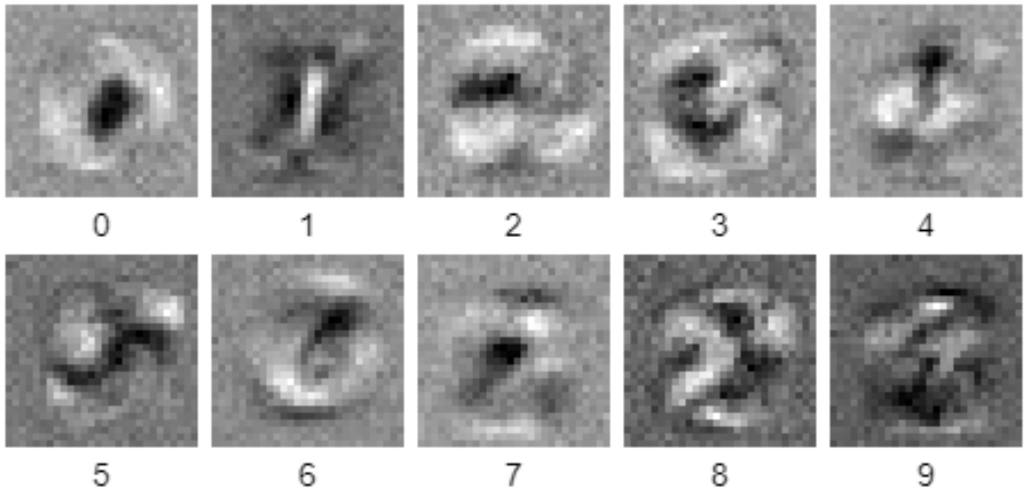
Intuition: like a polynomial fit. High-order terms improve fit, but add unpredictable swings for inputs outside the training set.

Overtraining Decreases Accuracy

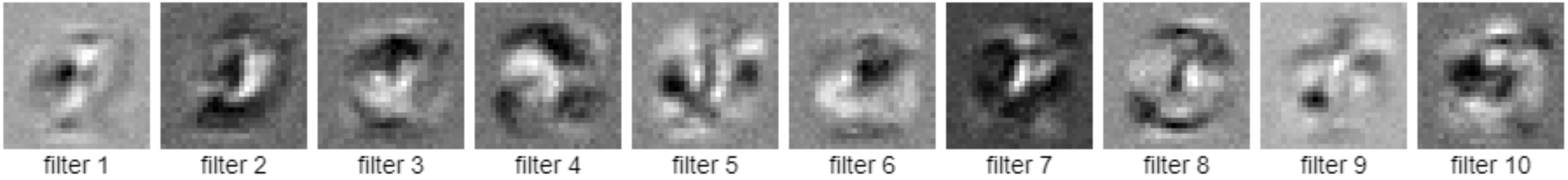


If network works too well for training data,
new inputs cause big unpredictable output changes.

Visualizing Neural Network Weights



MNIST 1st layer



MNIST 2nd layer

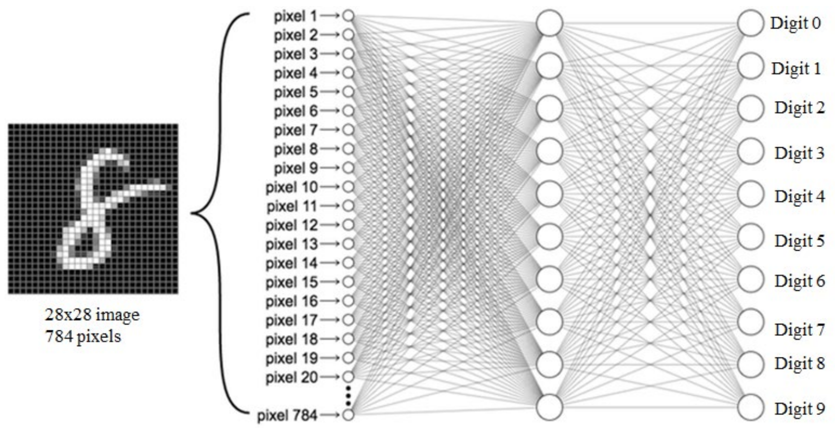
From https://ml4a.github.io/ml4a/looking_inside_neural_nets/

No Free Lunch Theorem

- Every classification algorithm has the same error rate when classifying previously unobserved inputs when averaged over all possible input-generating distributions.

- Neural networks must be tuned for specific tasks

Multi-Layer Perceptron (MLP) for an Image



Consider a 250 x 250 image…

- input: 2D image treated as 1D vector
- Fully connected layer is huge:
  – 62,500 (250^2) weights per node!
  – Comparable number of nodes gives ~4B weights total!
- Need >1 hidden layer? Bigger images?
- Too much computation, and too much memory.

Traditional feature detection in image processing uses

- Filters → Convolution kernels
- Can we use them in neural networks?

2-D Convolution

X

1	2	3	4	5	6	7
2	3	4	5	6	7	8
3	4	5	6	7	8	9
4	5	6	7	8	5	6
5	6	7	8	5	6	7
6	7	8	9	0	1	2
7	8	9	0	1	2	3

W

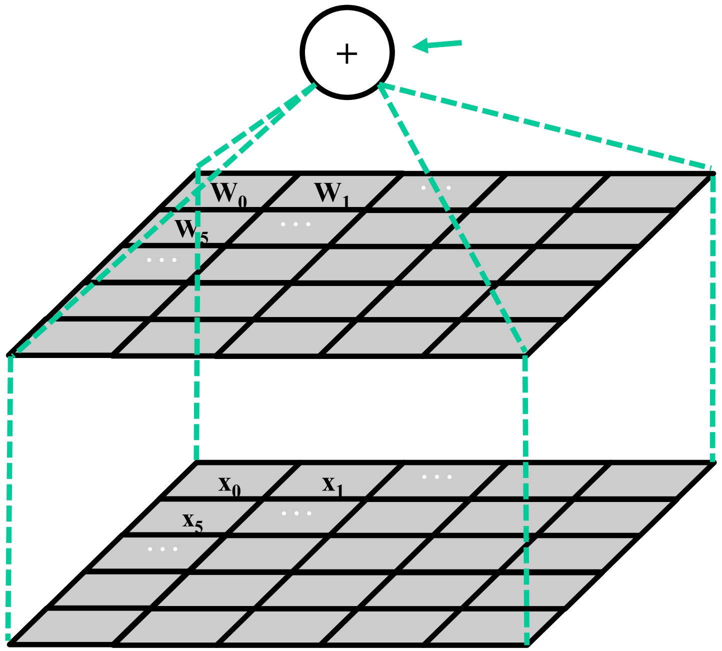
1	2	3	2	1
2	3	4	3	2
3	4	5	4	3
2	3	4	3	2
1	2	3	2	1

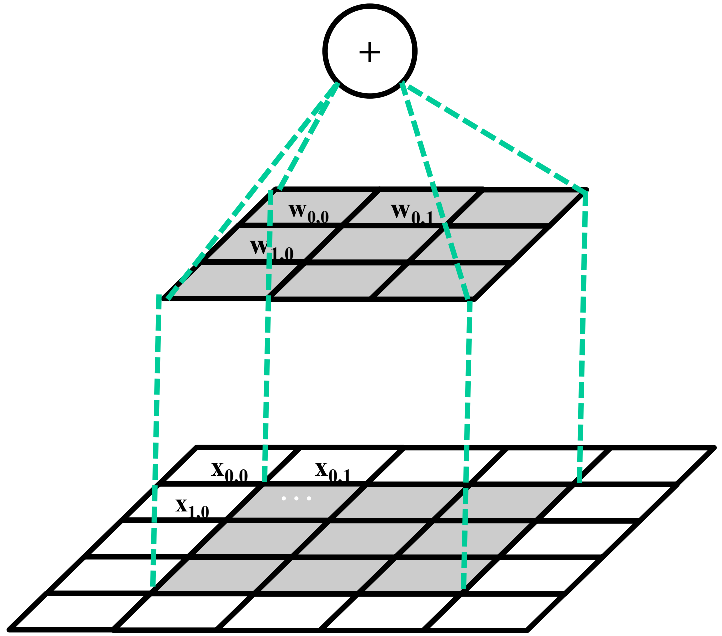
1	4	9	8	5
4	9	16	15	12
9	16	25	24	21
8	15	24	21	16
5	12	21	16	5

Y

		321				

Convolution vs Fully-Connected (Weight Sharing)





Convolution Naturally Supports Varying Input Sizes

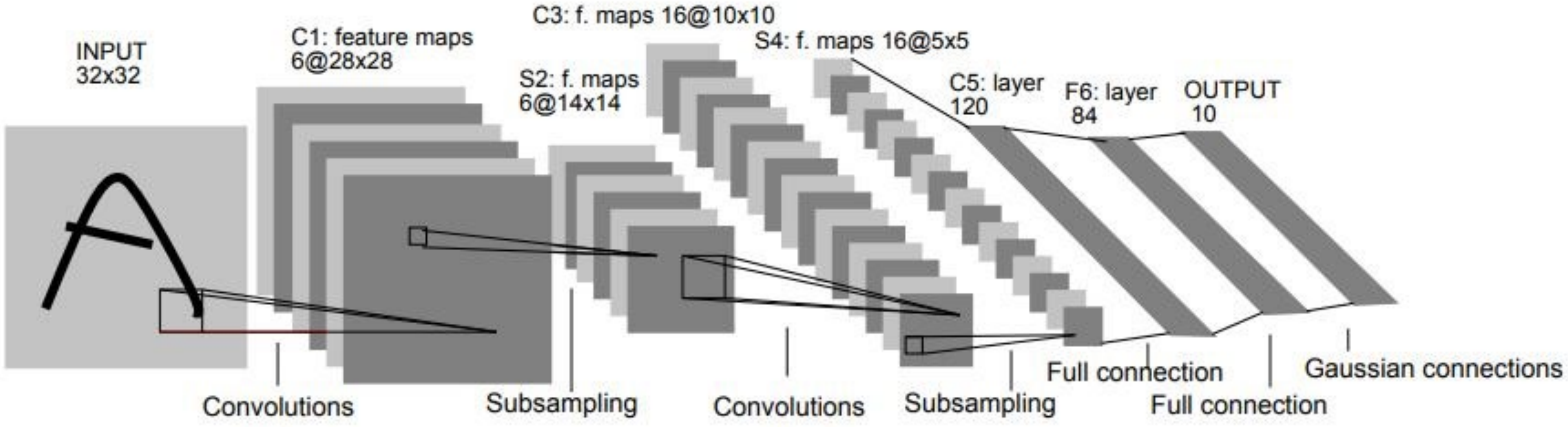
- As discussed so far,
  – perceptron layers have fixed structure, so
  – number of inputs / outputs is fixed.

- Convolution enables variably-sized inputs (observations of the same kind of thing)
  – Audio recording of different lengths
  – Image with more/fewer pixels

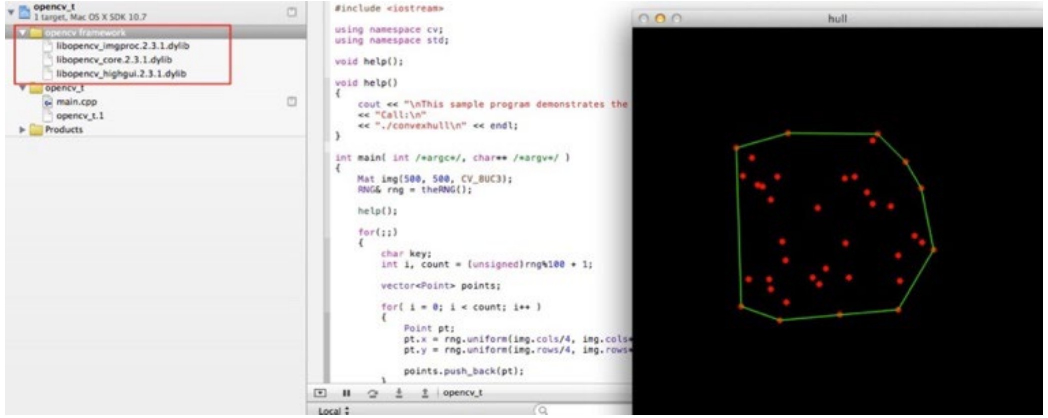
Example Convolution Inputs

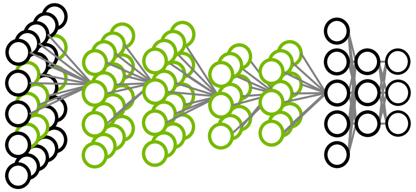
	Single-channel	Multi-channel
1D	audio waveform	Skeleton animation data: 1-D joint angles for each joint
2D	Fourier-transformed audio data Convolve over frequency axis: invariant to frequency shifts Convolve over time axis: invariant to shifts in time	Color image data: 2D data for R,G,B channels
3D	Volumetric data (example: medical imaging)	Color video: 2D data across 1D time for R,G,B channels

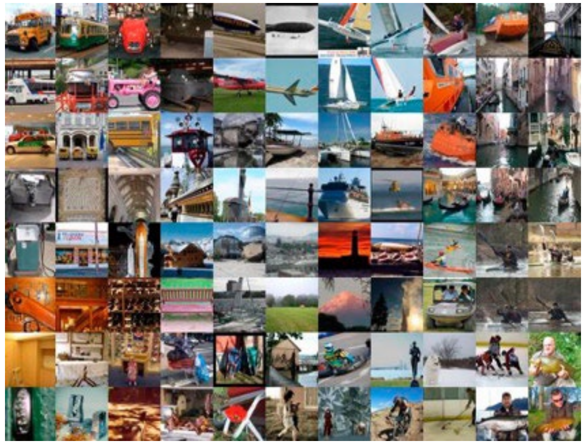
LeNet-5:CNN for hand-written digit recognition



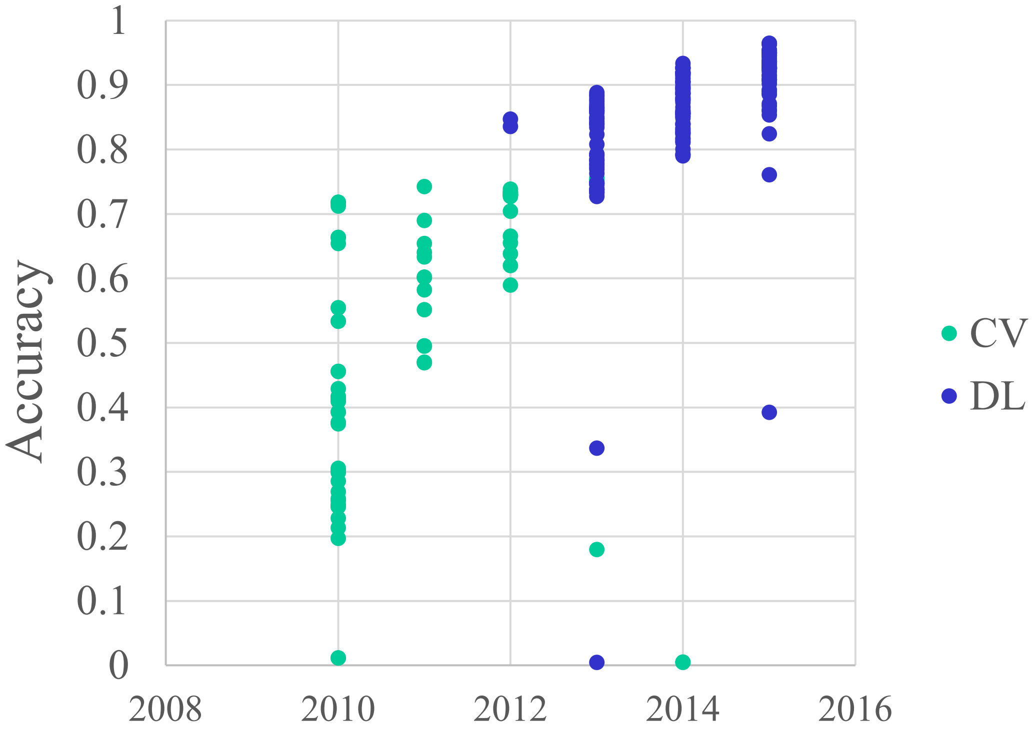
Deep Learning Impact in Computer Vision





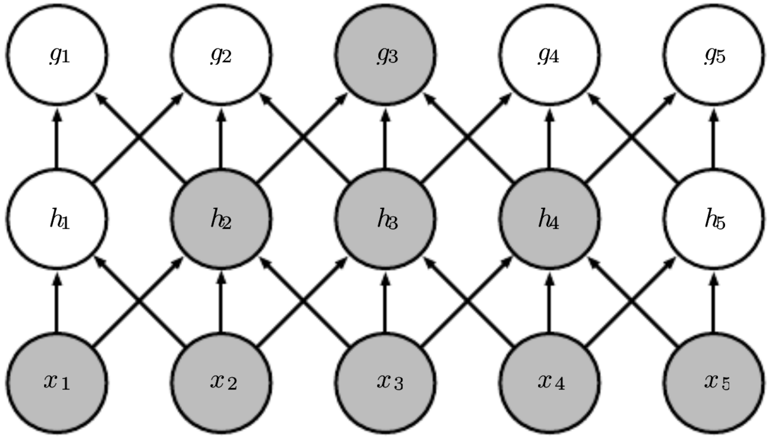


The Toronto team used GPUs and trained on 1.2M images in their 2012 winning entry at the Large Scale Visual Recognition Challenge



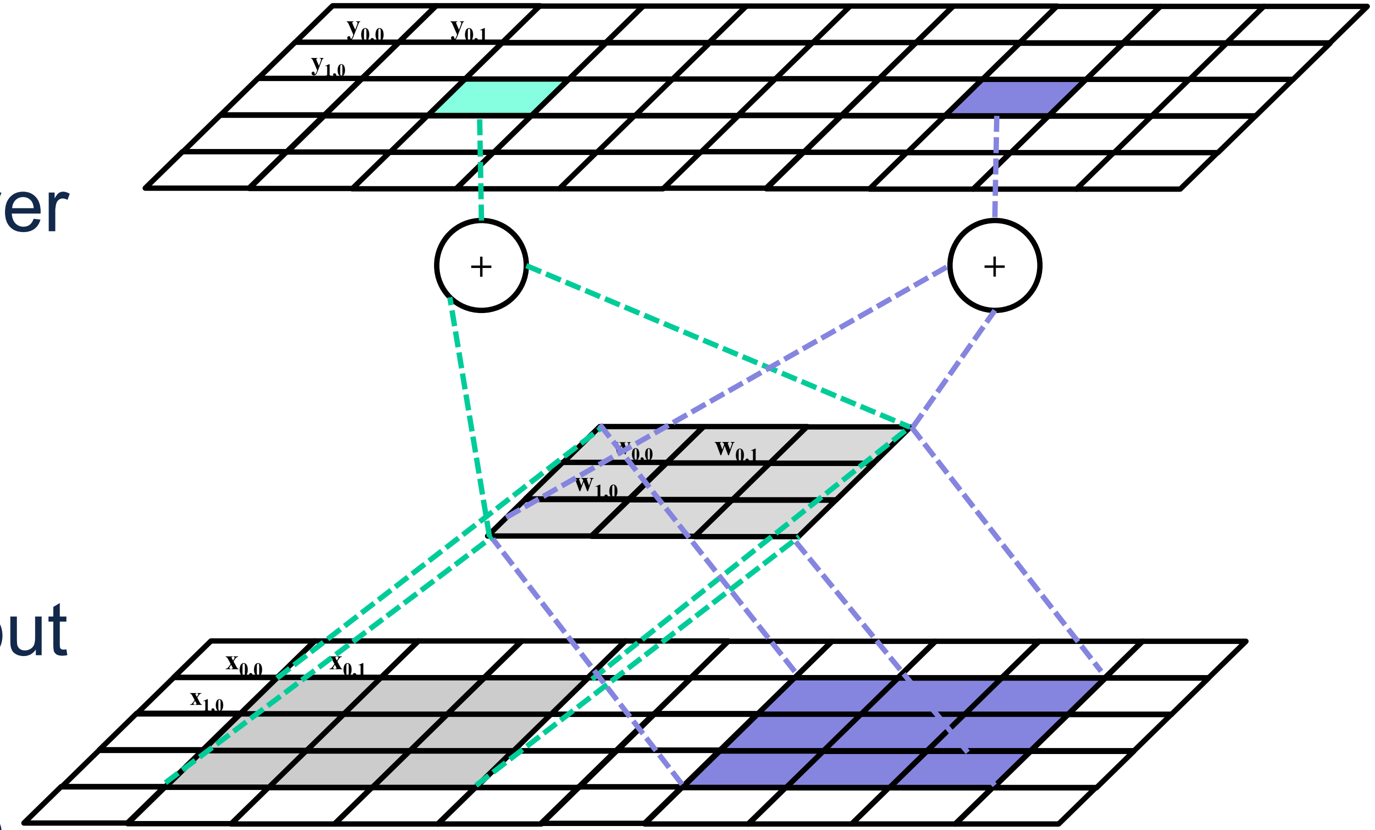
Why Convolution

- Sparse interactions
  - Meaningful features in small spatial regions
  - Need fewer parameters (less storage, better statistical characteristics, faster training)
  - Need multiple layers for wide receptive field



Why Convolution

- Parameter sharing
  - Kernel mask is applied repeatedly computing layer output
- Equivariant Representations
  - If input is translated, output is similarly translated
  - Output is a map of where features appear in input



Convolution

- 2-D Matrix
- $Y = W \otimes X$
- Kernel smaller than input: smaller receptive field
- Fewer Weights

MLP

- Vector
- $Y = w\,x + b$
- Maximum receptive field
- More weights

ANY MORE QUESTIONS?