Neural Networks

Chapter 18.6.3, 18.6.4, 18.7
and "Deep Learning" paper

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Introduction

- Known as
  - **Neural Networks** (NNs)
  - **Artificial Neural Networks** (ANNs)
  - **Connectionist Models**
  - **Parallel Distributed Processing** (PDP) Models
- Neural Networks are a fine-grained, parallel, distributed, computing model

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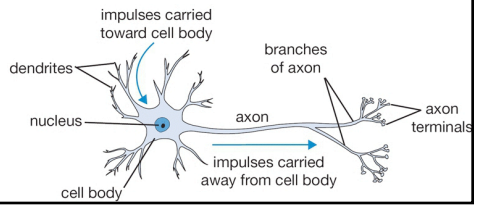
- NNs are inspired by the brain:
  - knowledge is acquired experientially (learning)
  - knowledge stored in connections (weights)
- Brain composed of neurons:
  - dendrites collect input from ~10^4 other neurons
  - axon sends output to other neurons
  - connected at synapses that have varying strength
  - this model is greatly simplified



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Introduction

Characteristics of human information processing

- number of neurons: ~10^{11}
- number of connections: ~10^4 per neuron
- Processing speed: ~100 Hz

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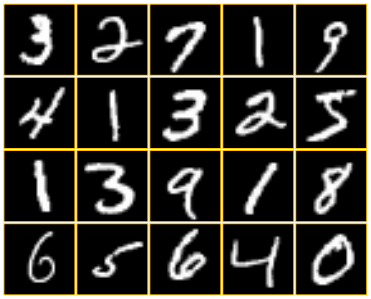
Recognizing Digits using a Neural Net



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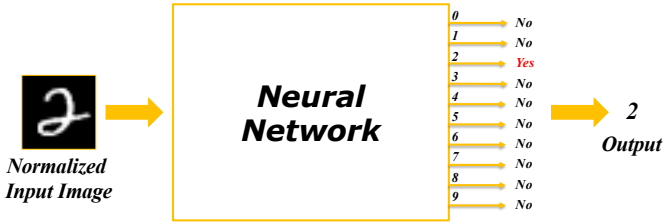
Recognizing Digits using a Neural Network as a Classifier



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Strengths of NN Approach

- Massively parallel
  - from a large collection of simple processing elements emerges complex, global behavior
- Can do complex tasks
  - pattern recognition (handwriting, facial expressions)
  - forecasting (stock prices, power grid demand)
  - adaptive control (autonomous vehicle control, robot control)
- Robust computation
  - can handle noisy and incomplete data due to fine-grained, distributed and continuous knowledge representation

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Strengths of NN Approach

- Fault tolerant
  - ok to have faulty elements and bad connections
  - isn't dependent on a fixed set of elements and connections
- Degrades gracefully
  - continues to function, possibly at a lower level of performance, when portions of the network are faulty
- Uses inductive learning
  - useful for a wide variety of applications

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Neural Network Architecture

- large number of **units**
  - simple neuron-like processing elements
- connected by a large number of **links**
  - directed from one unit to another
- a **weight** associated with each link
  - positive or negative real values
  - means of long term storage
  - adjusted by learning
- an **activation** function associated with each unit
  - result of the unit's processing
  - unit's output

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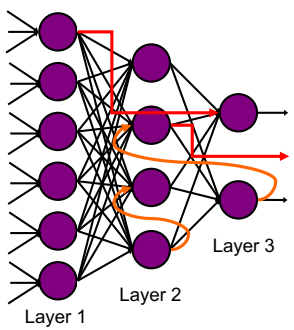
Neural Network Architecture

- represent as a **graph**
  - **Nodes: units**
  - **Arcs: links**
- single layer
- multi-layer
- Feedback (cycles)?
- layer skipping?
- fully connected?



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Basics of NN

Structure of a "Unit":

- set of **input links**
  - *from* other units or features from the environment
- set of **output links**
  - *to* other units or effectors of the environment
- an **activation function**
  - computes an output scalar value using a simple non-linear function of the linear combination of its inputs

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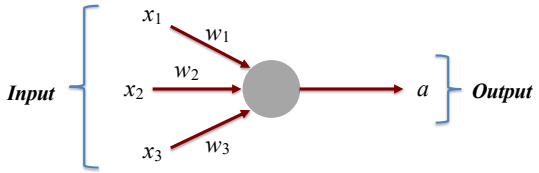
Computation by a Unit

Takes several inputs and computes a single scalar output value



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Basics of NN

Given n inputs, the unit's **activation** (i.e., output) is defined by:

$$a = g(w_1 x_1 + w_2 x_2 + ... + w_n x_n) = g(\sum_{i=1}^{n} w_i x_i) = g(in)$$

where

- w_i are the real-valued weights
- x_i are the scalar input values (in general, real values)
- $g(\,)$ is a simple, non-linear function, commonly:
  - **Step (LTU)**: activation *flips* from 0 to 1 when $in \geq$ threshold
  - **tanh**: $g(in) = \tanh(in)$
  - **Sigmoid / Logistic**: $g(in) = 1 / (1 + \exp(-in))$
  - **Rectified Linear (ReLU)**: $g(in) = \max(0, in)$

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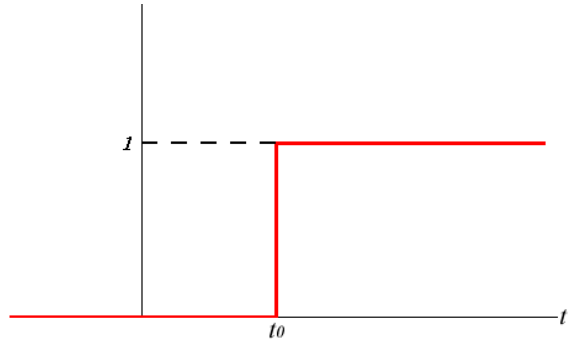
Step Function (aka Linear Threshold Unit) (LTU)



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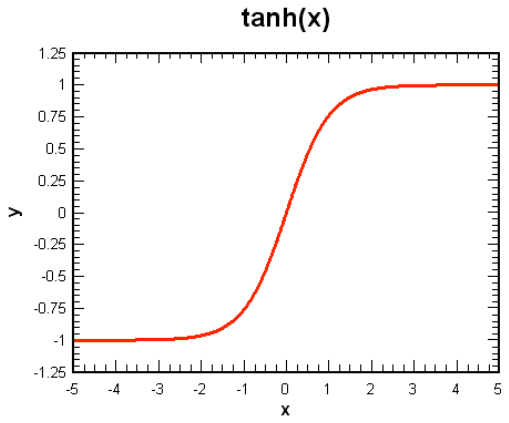
Hyperbolic Tangent Function



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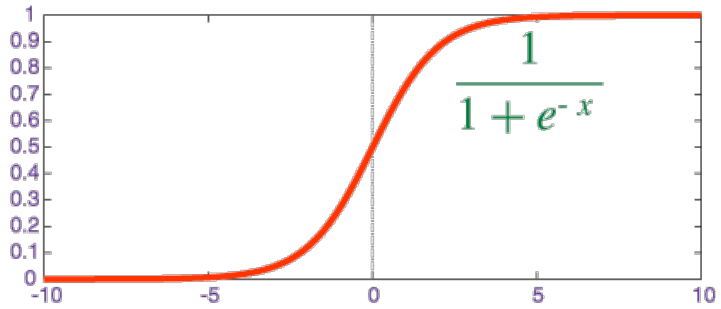
Sigmoid Function (aka Logistic function)



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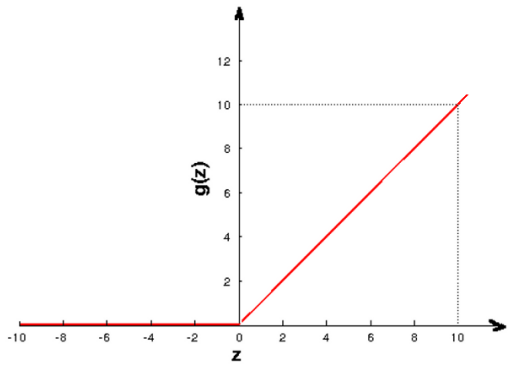
Rectified Linear Function (ReLU)



The rectified linear activation function

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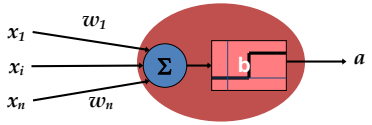
Perceptrons

- Studied in the 1950s and 1960s as simple networks for which there was an effective learning algorithm
- "**1-layer network**": one or more *output units*
- "Input units" don't count as a layer because they don't compute anything
- Output units are all **linear threshold units** (**LTU**s)
  - a unit's inputs, x_i, are weighted, w_i, and **linearly combined**
  - **Step** function computes binary output activation value, a



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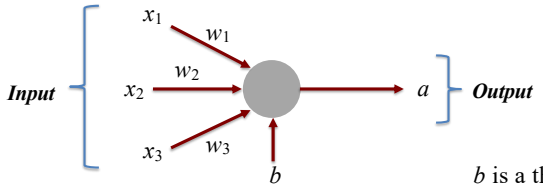
Computation by an LTU

Takes several inputs and computes a single scalar output value



b is a threshold

$$a = \begin{cases} 0 & \text{if } \sum_i w_i x_i < b \\ 1 & \text{if } \sum_i w_i x_i \geq b \end{cases}$$

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Linear Threshold Units (LTU)

Threshold is just another weight (called the **bias**):

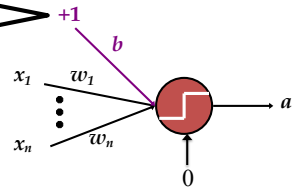
$(w_1\, x_1) + (w_2\, x_2) + \ldots + (w_n\, x_n) \geq b$

which is equivalent to

$(w_1\, x_1) + (w_2\, x_2) + \ldots + (w_n\, x_n) + (b\ (-1)) \geq 0$

Use +1 instead of -1, however

Every unit uses a fixed threshold = 0



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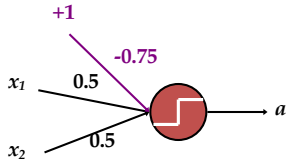
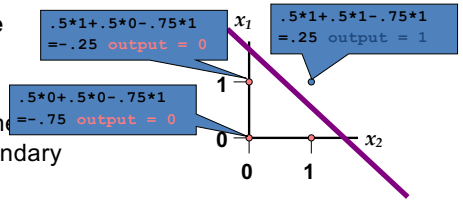
Perceptron Examples

- "AND" Perceptron:
  - inputs are 0 or 1
  - output is 1 when both x_1 and x_2 are 1



- **2D input space**
  - 4 possible data points
  - weights define decision boundary



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Perceptron is a Linear Classifier

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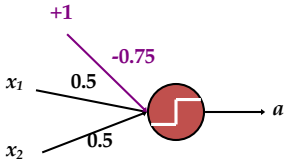

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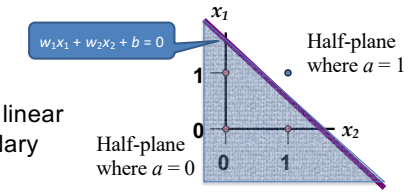

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Perceptron Examples

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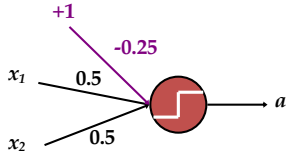

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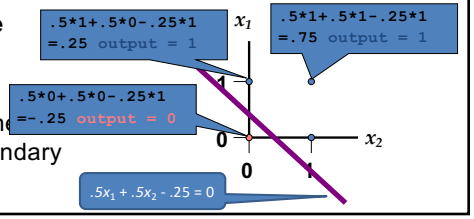

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Perceptron Learning

How are the weights learned by a Perceptron?

- Programmer specifies:
  - numbers of units in each layer
  - connectivity between units
- Only unknown is the set of weights
- Learning of weights is *supervised*
  - for each training example
    - a list of values for the input units of the network
  - the correct output is given
    - a list of desired output values for all output units

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Perceptron Learning Algorithm

1. Initialize the weights in the network
   (usually with random values)
2. Repeat until all examples correctly classified or some other stopping criterion is met

   foreach example, ***e***, in the training set **do**

   O = neural_net_output(network, e);

   T = desired output; // **T**arget or **T**eacher output

   update_weights(***e***, O, T);

- Each pass through *all* of the training examples is called an **epoch**
- Step 2 takes *many epochs* in general!

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Perceptron Learning Rule

How should the weights be updated?

- Determining how to update the weights is an instance of the **credit assignment problem**

Perceptron Learning Rule:

$$w_i = w_i + \Delta w_i$$

where $\Delta w_i = \alpha\, x_i\, (T - O)$

x_i is the input associated with i^{th} input unit

α is a real-valued constant between 0.0 and 1.0 called the **learning rate**

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Perceptron Learning Rule Properties

- $\Delta w_i = \alpha\, x_i\, (T - O)$ doesn't depend on w_i
- No change in weight (i.e., $\Delta w_i = 0$) if:
  - **correct output**, i.e., $T = O$ gives $\alpha \times x_i \times 0 = 0$
  - **0 input**, i.e., $x_i = 0$ gives $\alpha \times 0 \times (T - O) = 0$
- If T=1 and O=0, *increase* the weight

  so that maybe next time the result will exceed the output unit's threshold, causing it to be 1
- If T=0 and O=1, *decrease* the weight

  so that maybe next time the result won't exceed the output unit's threshold, causing it to be 0
- So, when error occurs, update the weight so that it changes the activation *towards* the desired output/activation value

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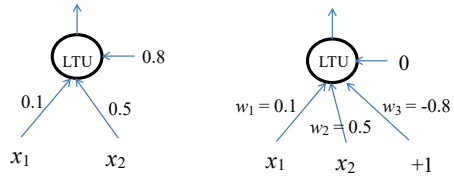
Example: Learning OR

- $\Delta w_i = \alpha(T - O)x_i = 0.2(T - O)x_i$
- Initial network:



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Example: Learning OR

bias

x1	x2	T	O	Δw1	w1	Δw2	w2	Δw3	w3
					0.1		0.5		-0.8
0	0	0	0	0	0.1	0	0.5	0	-0.8
0	1	1	0	0	0.1	0.2	0.7	0.2	-0.6
1	0	1	0	0.2	0.3	0	0.7	0.2	-0.4
1	1	1	1	0	0.3	0	0.7	0	-0.4
0	0	0	0	0	0.3	0	0.7	0	-0.4
0	1	1	1	0	0.3	0	0.7	0	-0.4
1	0	1	0	0.2	0.5	0	0.7	0.2	-0.2
1	1	1	1	0	0.5	0	0.7	0	-0.2
0	0	0	0	0	0.5	0	0.7	0	-0.2
0	1	1	1	0	0.5	0	0.7	0	-0.2
1	0	1	1	0	0.5	0	0.7	0	-0.2
1	1	1	1	0	0.5	0	0.7	0	-0.2

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Perceptron Learning Rule (PLR)

Perceptron Convergence Theorem:

- ***If a set of examples is learnable, then PLR will find an appropriate set of weights***
  - in a finite number of steps
  - independent of the initial weights
  - Using a sufficiently small value for α
- This theorem says that if a solution exists, PLR's gradient descent is guaranteed to find an optimal solution (i.e., 100% correct classification) for any 1-layer neural network

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Perceptron Learning Rule (PLR)

- PLR is a "local" learning rule in that only local information in the network is needed to update a weight
- **PLR performs gradient descent (hill-climbing) in "weight space"**
- Iteratively adjusts all weights so that for each training example the error decreases (more correctly, error is monotonically non-increasing)

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Limits of Perceptron Learning

What Can be Learned by a Perceptron?

- Perceptron's output is determined by the separating hyperplane (linear decision boundary) defined by

$$(w_1\ x_1) + (w_2\ x_2) + \ldots + (w_n\ x_n)\ =\ b$$

- So, Perceptrons can *only* learn functions that are **linearly separable** (in **input space**)

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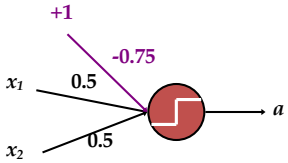
Separating Hyperplane Example

- "AND" Perceptron:
  - inputs are 0 or 1
  - output is 1 when both x_1 and x_2 are 1

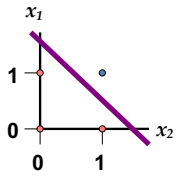


- **2D "input space"**

  decision line equation:

  $0.5x_1 + 0.5x_2 - 0.75 = 0$

  or, in slope-intercept form: **$x_1 = -x_2 + 1.5$**



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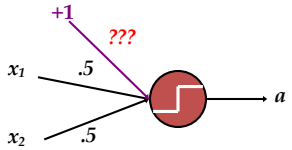
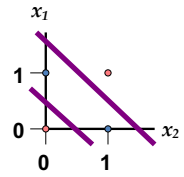
Limits of Perceptron Learning

- "XOR" Perceptron?
  - inputs are 0 or 1
  - output is 1 when x_1 is 1 and x_2 is 0 or x_1 is 0 and x_2 is 1



- **2D input space with 4 possible data points**



Can't separate + from – using a single straight line, so XOR is not linearly-separable and can't be learned by a Perceptron

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Perceptron Learning Summary

In general, the goal of learning in a 1-output-unit Perceptron is to adjust the **separating hyperplane** (i.e., linear decision boundary) that divides an *n*-dimensional "input space," where *n* is the number of input units, by modifying the weights (including the bias) until all the examples with target value 1 are on one side of the hyperplane, and all the examples with target value 0 are on the other side of the hyperplane

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Recognizing Digits using a Neural Network as a Classifier

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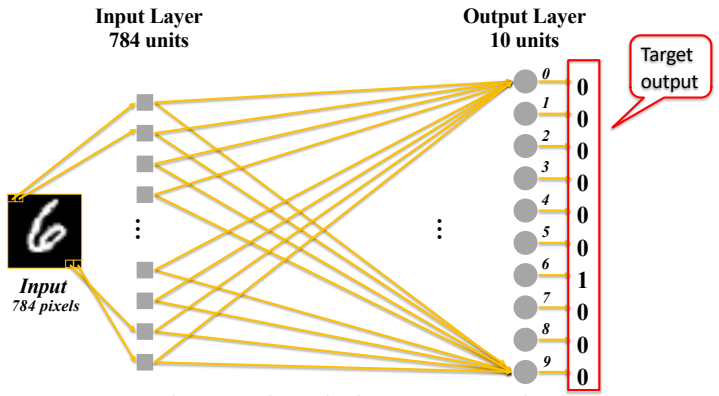
Digit Recognition using a Perceptron



Note: Figure does not show the bias input to each output unit

Classification accuracy ≈ 90% (random guessing = 10%)

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Perceptron Summary

- 1-layer network
- 1 or more units in a single "output" layer, with each unit using an LTU activation function
- "Input" layer defines inputs from 1 example
- Complete connectivity: All inputs are connected to each output unit
- Uses the Perceptron Learning Rule to update all weights
- Can only learn linearly-separable functions

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Perceptron Learning Summary

In general, the goal of learning in a 1-output-unit Perceptron is to adjust the **separating hyperplane** (i.e., linear decision boundary) that divides an *n*-dimensional "input space," where *n* is the number of input units, by modifying the weights (including the bias) until all the examples with target value 1 are on one side of the hyperplane, and all the examples with target value 0 are on the other side of the hyperplane

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Beyond Perceptrons

- Perceptrons are weak computing models because they **can only learn linearly-separable functions**
- General NN's can have multiple "layers" of units, which enhance their computational power; the challenge is to find a learning rule that works for multi-layered networks

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Beyond Perceptrons

- A ***Multi-Layer, Feed-Forward Network*** computes a function of the inputs and the weights
- Input "units"
  - Input values are given; no activation function
- Output units
  - activation value is the output result
- **Hidden units** (between input and output units)
  - cannot observe directly
- Perceptrons have input units followed by one layer of output units, i.e., no hidden units

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Beyond Perceptrons

- NN's with one hidden layer of a sufficient number of units, can compute functions associated with convex classification regions in input space
  - And can *approximate* any continuous function
- NN's with two hidden layers are universal computing devices, although the complexity of the function is limited by the number of units
  - **If too few**, the network will be unable to represent the function
  - **If too many**, the network can memorize examples and is subject to "overfitting"

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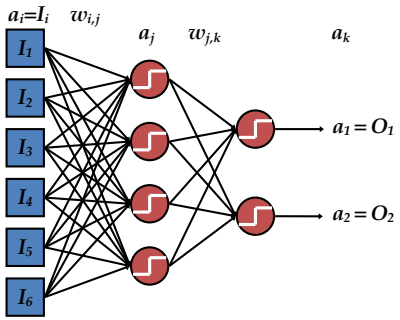
Two-Layer, Feed-Forward Neural Network

Input Units
Hidden Units
Output Units

Weights on links from input to hidden

Weights on links from hidden to output

Network Activations



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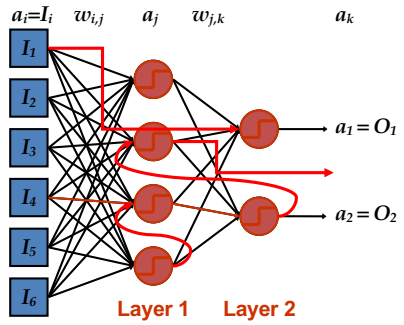
Two-Layer, Feed-Forward Neural Network

Two Layers: count layers with units computing an activation

Feed-Forward: each unit in a layer connects to ***all*** units in the next layer

no cycles
- links within the same layer
- links to prior layers

no skipping layers



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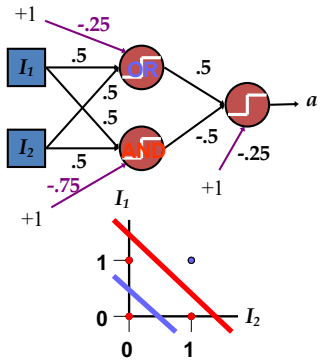
XOR Example

XOR 2-Layer Feed-Forward Network

- inputs are 0 or 1
- output is 1 when
  I_1 is 1 and I_2 is 0, or
  I_1 is 0 and I_2 is 1

Each unit in hidden layer acts like a Perceptron learning a decision line

- top hidden unit acts like an OR Perceptron
- bottom hidden unit acts like an AND Perceptron



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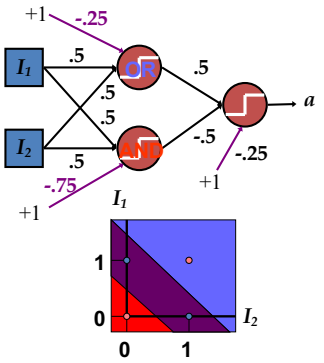
XOR Example

XOR 2-Layer Feed-Forward Network

- inputs are 0 or 1
- output is 1 when
  I_1 is 1 and I_2 is 0 or
  I_1 is 0 and I_2 is 1

To classify an example each unit in the output layer combines these decision lines by intersecting their "half-planes":

when OR is 1 and AND is 0
then output, a, is 1



55

Learning in Multi-Layer, Feed-Forward Neural Nets

- PLR doesn't work in multi-layered feed-forward nets because the desired target values for the hidden units are *not known*
- Must again solve the **Credit Assignment Problem**
  - determine which weights to credit/blame for the output error in the network, and how to update them

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Learning in Multi-Layer, Feed-Forward Neural Nets

Back-Propogation

- Method for learning weights in these networks
- Generalizes PLR
- Rumelhart, Hinton and Williams, 1986

Approach

- **Gradient-descent algorithm** to minimize the total error on the training set
- Errors are propagated through the network starting at the output units and working *backwards* towards the input units

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Back-Propagation Algorithm

Initialize the weights in the network (usually random values)
Repeat until stopping criterion is met **{**
  forall p,q in network, $\Delta \boldsymbol{W}_{p,q} = 0$
  foreach example ***e*** in training set **do {**
    O = neural_net_output(***network***, ***e***) // forward pass
    Calculate error (***T*** - ***O***) at the output units // ***T*** = teacher output
    Compute $\Delta w_{j,k}$ for all weights from hidden unit j to output unit k
    Compute $\Delta w_{i,j}$ for all weights from input unit i to hidden unit j
    forall p,q in network $\Delta \boldsymbol{W}_{p,q} = \Delta \boldsymbol{W}_{p,q} + \Delta w_{\boldsymbol{p,q}}$
    }
  for all p,q in network $\Delta \boldsymbol{W}_{p,q} = \Delta \boldsymbol{W}_{p,q}$ / num_training_examples
  network = update_weights(***network***, $\Delta \boldsymbol{W}_{p,q}$)
}

backward pass

Note: Uses average gradient for *all* training examples when updating weights

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Back-Prop using Stochastic Gradient Descent (SGD)

- Most practitioners use SGD to update weights using the *average gradient computed using a small batch of examples*, and repeating this process for many small batches from the training set
- In extreme case, update after *each* example
- Called *stochastic* because each small set of examples gives a noisy estimate of the average gradient over *all* training examples

60

Updating the Weights

- Back-Propagation performs a ***gradient descent search*** in "weight space" to learn the network weights
- Given a network with n weights:
  - each configuration of weights is a vector, $\boldsymbol{W}$, of length n that defines an instance of the network
  - $\boldsymbol{W}$ can be considered a point in an n-dimensional **weight space**, where each dimension is associated with one of the connections in the network

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Updating the Weights

- Given a training set of m examples:
  - Each network defined by the vector $\boldsymbol{W}$ has an associated total error, $\boldsymbol{E}$, on ***all*** the training data
  - $\boldsymbol{E}$ is the sum squared error (SSE) defined by
    $$E = E_1 + E_2 + \ldots + E_m$$
    where E_i is the squared error of the network on the i^{th} training example
- Given t output units in the network:
  $$E_i = (T_{i1} - O_{i1})^2 + (T_{i2} - O_{i2})^2 + \ldots + (T_{it} - O_{it})^2$$
  - T_{ij} is the target value for the i^{th} example's j^{th} output unit
  - O_{ij} is the network output value for the i^{th} example's j^{th} output unit

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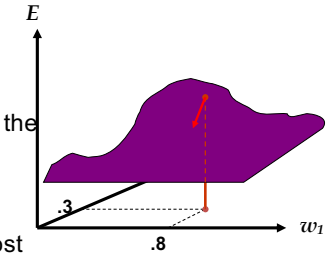
Updating the Weights

Visualized as an error surface in "weight space"

- For example, when a network has 2 weights, each point in $w_1 w_2$ plane is a weight configuration, ***W***
- Each point has a total error E
- 2D surface represents errors for all weight configurations
- Goal is to find a lower point on the error surface (local minimum)
- Gradient descent follows the direction of steepest descent, i.e., where E decreases the most



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Updating the Weights

- The **gradient** is defined as

$$\nabla E = [\partial E / \partial w_1, \partial E / \partial w_2, \ldots, \partial E / \partial w_n]$$

- Update the ith weight using

$$\Delta w_i = -\alpha \, \partial E / \partial w_i$$

- Can't use the Step function (LTU) because it's derivative is 0 almost everywhere and undefined at the step
- Instead, let's use (for now) the **Sigmoid function**

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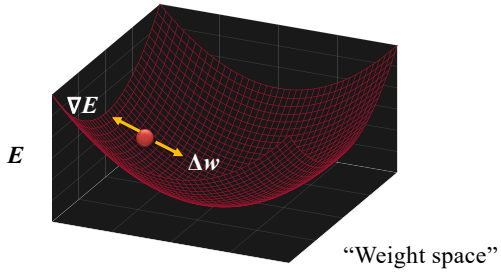
Back-Propagation Algorithm

1. Make prediction (Forward Pass)
2. Calculate the total Error (Loss), E
3. Calculate gradient of the loss function w.r.t. each weight, $\partial E/\partial w_i$
4. Update all weights by taking a step in the opposite direction: $\Delta w_i = -\alpha \, \partial E / \partial w_i$
5. Iterate

66

Gradient Descent

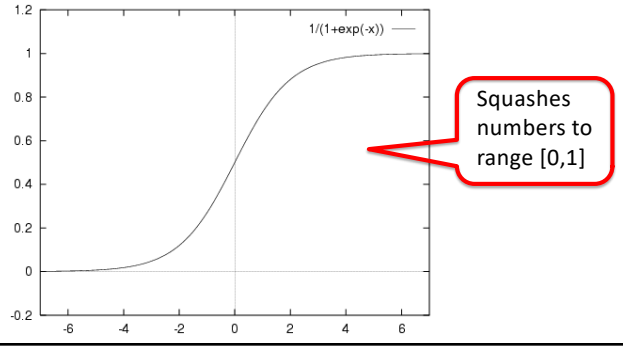


67

Sigmoid Activation Function

Use a smooth, "soft threshold" function such as **Sigmoid function** (aka **Logistic Sigmoid function**):

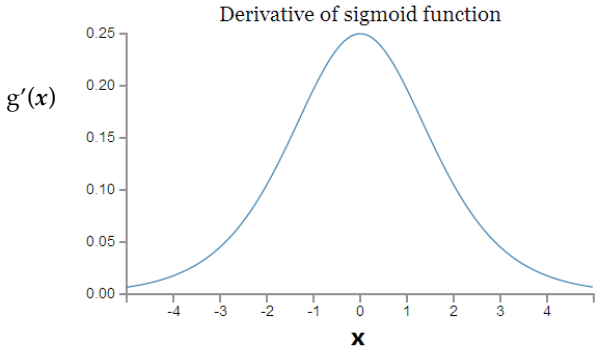
$g_w(x) = 1 \,/\, (1 + e^{-wx})$



68

First Derivative of Sigmoid Function

$g'(x) = g(x)\,(1 - g(x))$



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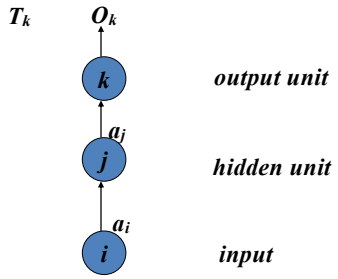
Updating the Weights



70

Perceptron Learning Rule

$w_i = w_i + \Delta w_i$

where $\Delta w_i = \alpha\, x_i\, (T - O)$

x_i is the input associated with i^{th} input "unit"

$T - O$ is the error at the output unit

α is a real-valued constant between 0.0 and 1.0 called the **learning rate**

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Updating Weights in a 2-Layer Neural Network

For **weights between hidden and output units**, generalized PLR for ***Sigmoid activation function*** is

$$\Delta w_{j,k} = -\alpha\, \partial E / \partial w_{j,k}$$
$$= -\alpha\, -a_j\, (T_k - O_k)\, g'(in_k)$$
$$= \alpha\, a_j\, (T_k - O_k)\, O_k\, (1 - O_k)$$
$$= \alpha\, a_j\, \Delta_k$$

$\Delta_k = Err_k \times g'(in_k)$

- $w_{j,k}$ weight on link **from hidden unit *j* to output unit *k***
- α learning rate parameter
- a_j activation (i.e., output) of hidden unit j
- T_k teacher output for output unit k
- O_k actual output of output unit k
- g' derivative of the sigmoid activation function, which is $g' = g(1 - g)$
- Δ_k modified error

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Updating Weights in a 2-Layer Neural Network

For **weights between input and hidden units**:

- We don't have teacher-supplied correct activation values for the hidden units
- Must infer the error at these units by "back-propagating"
- Error at an output unit is "distributed" back to each of the hidden units in proportion to the weight of the connection between them
- Each hidden unit accumulates some error from *each* of the output units to which it is connected

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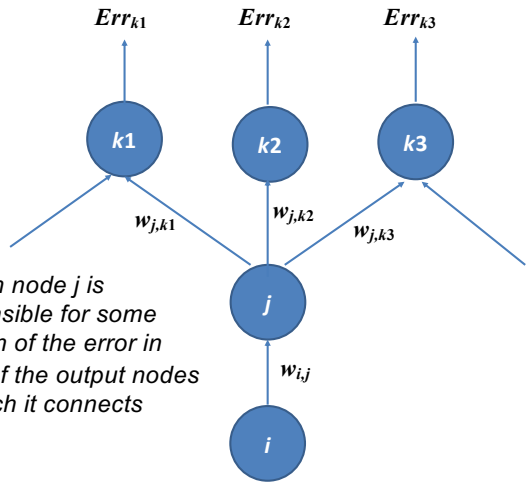

Hidden node j is responsible for some fraction of the error in each of the output nodes to which it connects

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Updating Weights in a 2-Layer Neural Network

For **weights between inputs and hidden units**:

$$\Delta w_{i,j} = -\alpha\, \partial E / \partial w_{i,j}$$
$$= -\alpha(-a_i) g'(in_j) \sum_k w_{j,k} (T_k - O_k) g'(in_k)$$
$$= \alpha\; a_i\; a_j (1 - a_j) \sum_k w_{j,k} (T_k - O_k)\; O_k (1 - O_k)$$
$$= \alpha\; a_i\; \Delta_j \quad \text{where} \quad \Delta_j = g'(in_j) \sum_k w_{j,k} \Delta_k$$

$\Delta_k = Err_k \times g'(in_k)$

- $w_{i,j}$ weight on link **from input *i* to hidden unit *j***
- $w_{j,k}$ weight on link from hidden unit j to output unit k
- α learning rate parameter
- a_j activation (i.e., output) of hidden unit j
- T_k teacher output for output unit k
- O_k actual output of output unit k
- a_i input value i
- g' derivative of sigmoid activation function, which is $g' = g(1\text{-}g)$

75

Back-Propagation Algorithm

Initialize the weights in the network (usually random values)
Repeat until stopping criterion is met
  foreach example, *e,* in training set **do**
    { O = neural_net_output(network, *e*) ← forward pass
    T = desired output, i.e., Target or Teacher's output
    calculate error (T_k - O_k) at each output unit *k*
    foreach hidden unit *j* and output unit *k* compute
      $\Delta w_{j,k} = \alpha\ a_j\ \Delta_k\ =\ \alpha\ a_j\ (T_k - O_k)\ g'(in_k)$
    foreach input unit *i* and hidden unit *j* compute
      $\Delta w_{i,j} = \alpha\ a_i\ \Delta_j = \alpha\ a_i\ g'(in_j) \sum_k w_{j,k} (T_k - O_k) g'(in_k)$
    forall *p*, *q* in network $w_{p,q} = w_{p,q} + \Delta w_{p,q}$ ← Simplistic SGD: update all weights after *each* example
  }

backward pass

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Notes for HW #4, Problem 3

- At each **hidden unit**, use the **ReLU activation function**
- In forward pass use the ReLU activation function: $g(x) = \max(0, x)$
- In backward pass use the derivative of the ReLU function:

$$g'(x) = \begin{cases} 0, & \text{if } x \le 0 \\ 1, & \text{otherwise} \end{cases}$$

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Multi-Class Classification with Neural Networks

- Use a number of output units equal to the number of classes
- Represent each class with 1 at a particular output unit and 0 at all other output units

$$\begin{bmatrix}1\\0\\0\end{bmatrix} \quad \begin{bmatrix}0\\1\\0\end{bmatrix} \quad \begin{bmatrix}0\\0\\1\end{bmatrix}$$

Cat *Dog* *Toaster*

Teacher output

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Notes for HW #4, Problem 3

- At all **output units**, use the **Softmax activation function** and define the Error (Loss) function using **Cross-Entropy**

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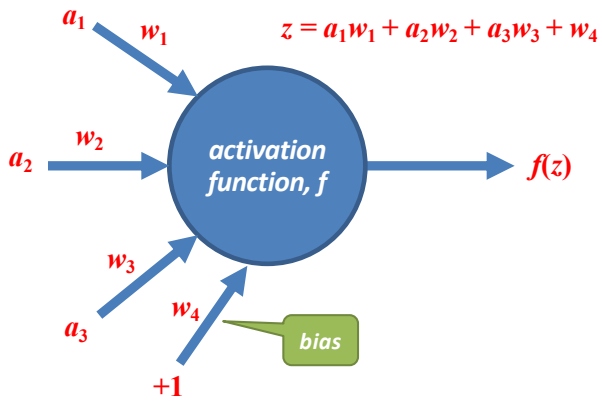
Multi-Class Classification with Neural Networks

- At each **output unit** use the **Softmax activation function**:

$$\text{Softmax}(z_i) = \frac{e^{z_i}}{\sum_{k=1}^{K} e^{z_k}}$$

  where z_i is the weighted sum of the inputs to the i^{th} output unit, and there are K output units
- Means output units all have values between 0 and 1, and sum to 1; can be interpreted as probabilities
- Note: [3,1,1] does *not* become [.6, .2, .2] but rather [.78, .11, .11] since we are exponentiating before normalizing

80



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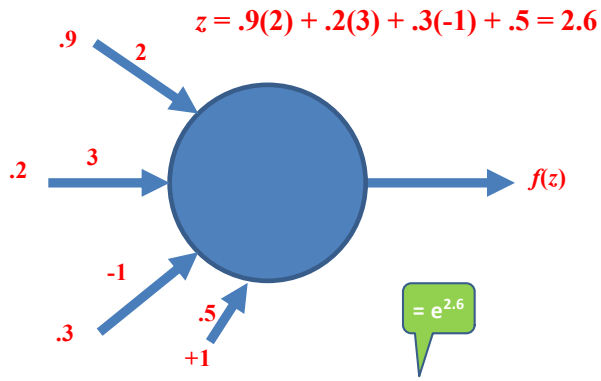
Example Output Unit Computation



$f(2.6) = \text{Softmax}(2.6) = 13.46 / \sum e^{zk}$

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Multi-class Classification with Neural Networks

- For the error function, instead of SSE, use "Cross-Entropy" loss, which for a *single* training example is:

$$C.E. = -\sum_{i=1}^{K} T_i \log(O_i)$$

Measures distance between target distribution and output distribution

  where O_i is the computed output at output unit i and T_i is the target output at unit I, and K is the number of output units
- Derivative has a nice property when used with Softmax:

$$\frac{\partial C.E.}{\partial softmax} \cdot \frac{\partial softmax}{\partial z_i} = O_i - T_i$$

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- Also must compute the **total Cross-Entropy loss** over the *entire* training set at end of each epoch, which is defined as the average Cross-Entropy loss:

$$Total\ Loss = \frac{1}{N}\sum_{i=1}^{N} CE(example_i)$$

- Note: The entire training set is "shuffled" at the end of each epoch to aid convergence

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Updating Weights in a 2-Layer Neural Network

For **weights between input and hidden units with ReLU at hidden units**:

$$\Delta w_{i,j} = -\alpha\, \partial E / \partial w_{i,j}$$
$$= \alpha\, a_i\, g'(in_j) \sum_{k=1}^{K} w_{j,k} \Delta_k$$

$w_{i,j}$ weight on link **from input i to hidden unit j**
$w_{j,k}$ weight on link from hidden unit j to output unit k
K number of output units
α learning rate parameter
T_k teacher output for output unit k
O_k Softmax output of output unit k
a_i input value i
$g'(in_j)$ derivative of ReLU activation function
$\Delta_k = (T_k - O_k)$

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Updating Weights in a 2-Layer Neural Network

For **weights between hidden and output units**, using the **Softmax activation function** and **Cross-Entropy error function**:

$$\Delta w_{j,k} = -\alpha\, \partial E / \partial w_{j,k}$$
$$= \alpha\, a_j\, (T_k - O_k)$$
$$= \alpha\, a_j\, \Delta_k$$

where

$w_{j,k}$ weight on link **from hidden unit j to output unit k**
α learning rate parameter
a_j activation (i.e., output) of hidden unit j
T_k teacher output for output unit k
O_k Softmax output of output unit k

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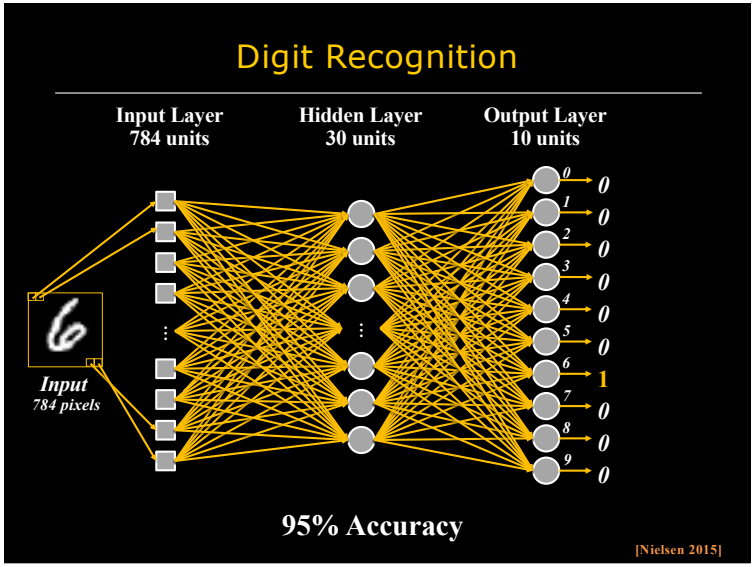

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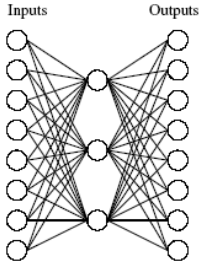
Learning Hidden Layer Representation



Input		Output
10000000	→	10000000
01000000	→	01000000
00100000	→	00100000
00010000	→	00010000
00001000	→	00001000
00000100	→	00000100
00000010	→	00000010
00000001	→	00000001

Training set size = 8

Can this be learned?

Slide by Guoping Qiu

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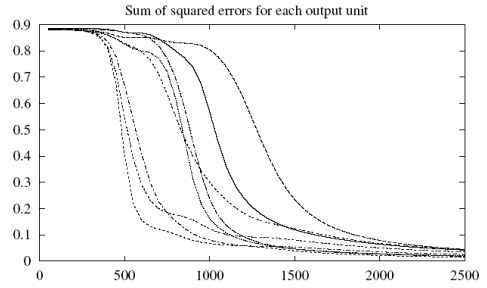
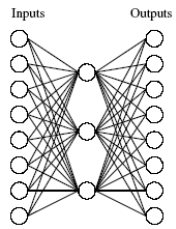
Learning Hidden Layer Representation

Training





The evolving sum of squared errors for each of the eight output units

Slide by Guoping Qiu

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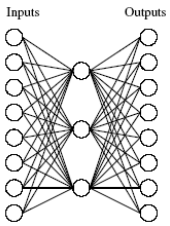
Learning Hidden Layer Representation



Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

Learned hidden layer representation (encoder)

Slide by Guoping Qiu

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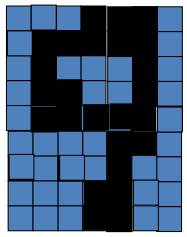
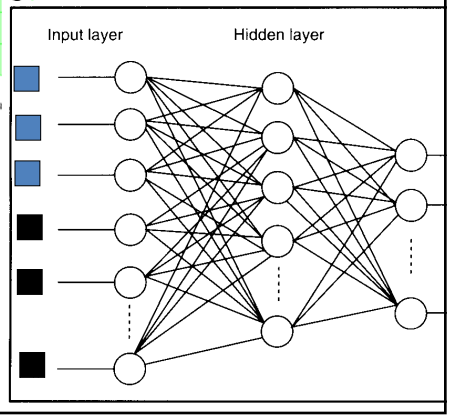
Figure 1.2: *Examples of handwritten digits from postal envelopes.*



Feature Detectors



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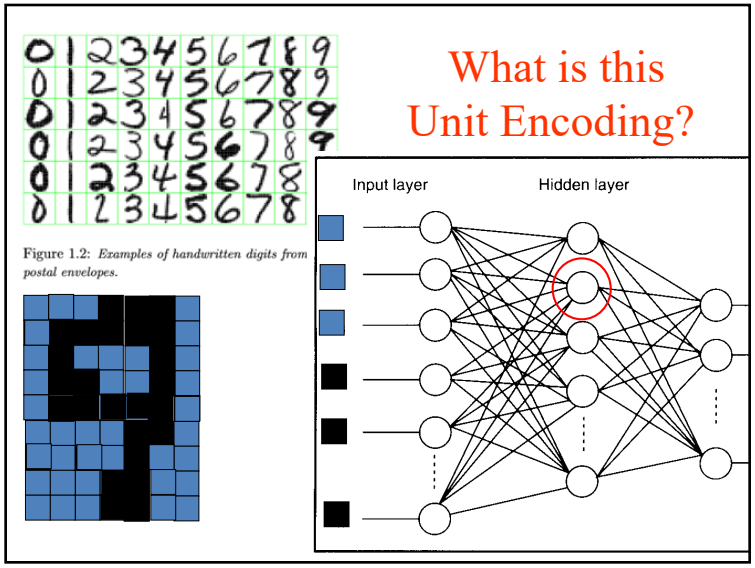
What is this Unit Encoding?
Figure 1.2: Examples of handwritten digits from postal envelopes.
Input layer
Hidden layer

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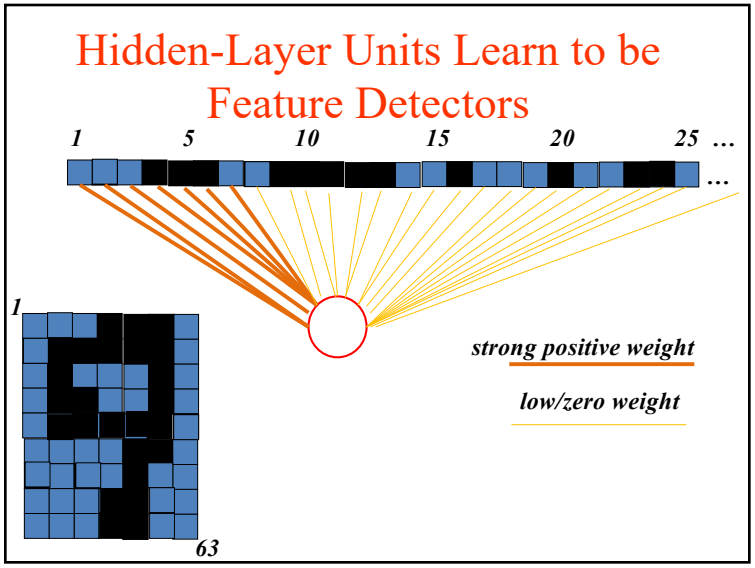
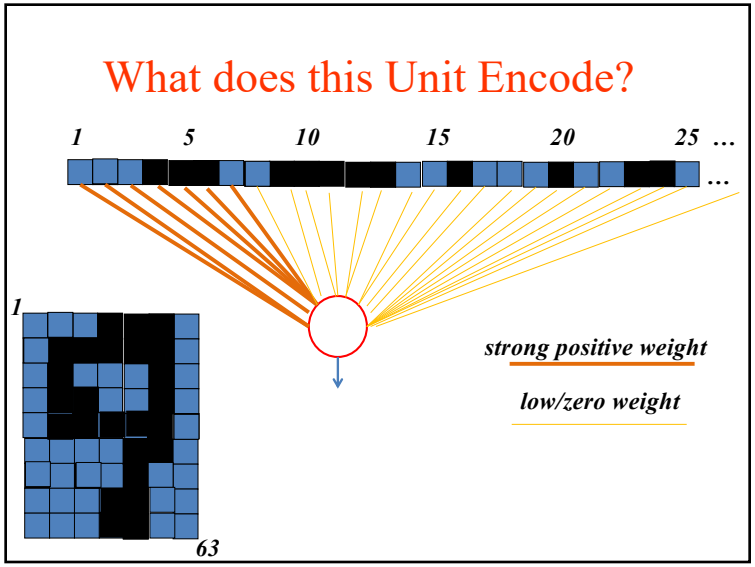
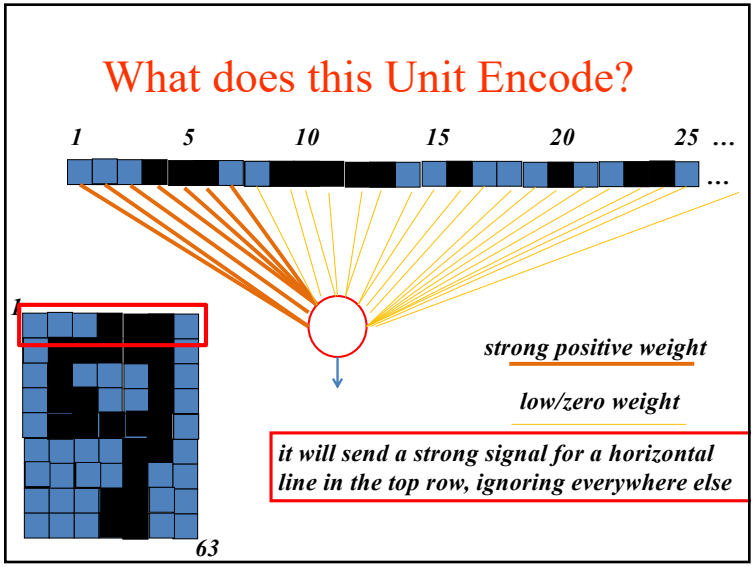

Hidden-Layer Units Learn to be Feature Detectors
1
5
10
15
20
25 …
…
1
63
strong positive weight
low/zero weight

95


What does this Unit Encode?
1
5
10
15
20
25 …
…
1
63
strong positive weight
low/zero weight

96


What does this Unit Encode?
1
5
10
15
20
25 …
…
1
63
strong positive weight
low/zero weight
it will send a strong signal for a horizontal line in the top row, ignoring everywhere else

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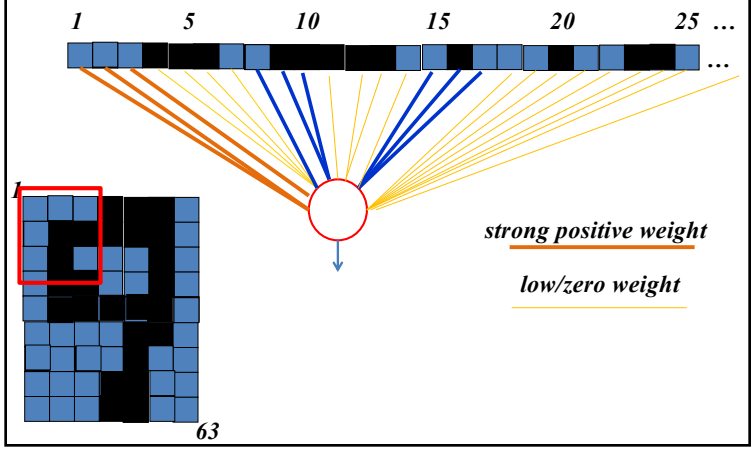
What does this Unit Encode?



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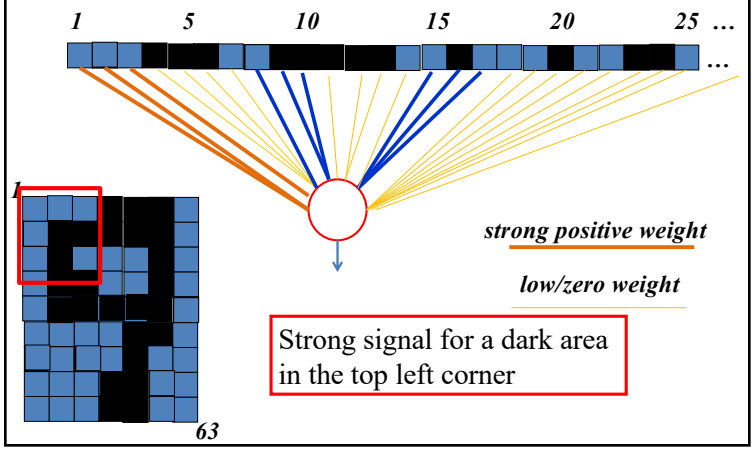
What does this Unit Encode?



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Multi-layer Feed-forward Networks

- Back-propagation algorithm performs gradient descent in the "weight space" of the network
- Include a bias input at *every* (non-input) unit
- In practice, use ReLU, not Sigmoid, for the activation function in order to speed up training
- Will, in general, find a **local, not global, error minimum**
- Training can take thousands of epochs, but can be computed efficiently using matrix vector operations and GPU implementation

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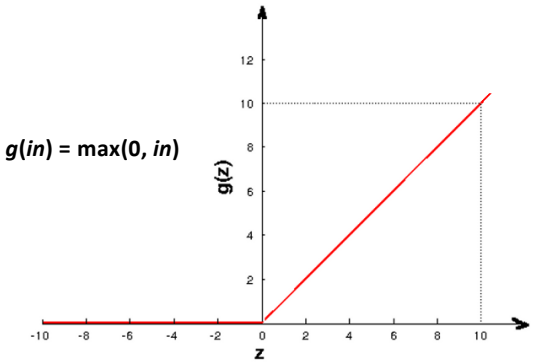
Rectified Linear Function (ReLU)



The rectified linear activation function

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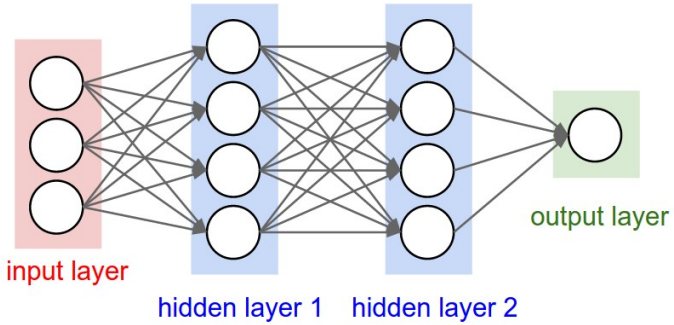
How Many Weights?



3 layers, 9 units with activation function,
((3x4)+4) + ((4x4)+4) + ((4x1)+1) = 41 weights incl. biases

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Other Issues

How should the learning rate parameter, α, be set?

Use a **tuning set** (aka **validation set**) to train using several candidate values for α, and then select the value that gives the lowest error

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Using Data

- **Training set** is used to *learn a "model"* (i.e., the neural network's weights)
- **Tuning set** is used to judge and *select parameters* (e.g., learning rate and the number of hidden units with best accuracy)
- **Testing set** is used to judge in a fair manner the final *model's performance accuracy* (using cross-validation or leave-one-out)
- All 3 datasets must be disjoint!

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Other Issues

- When should training stop?
  - too soon and the concept isn't learned
  - too late:
    - overfitting, poor generalization
    - error rate will go up on the testing set
- Train the network until the error rate on a **tuning set** begins *increasing* rather than training until the error (SSE) on the training set is minimized

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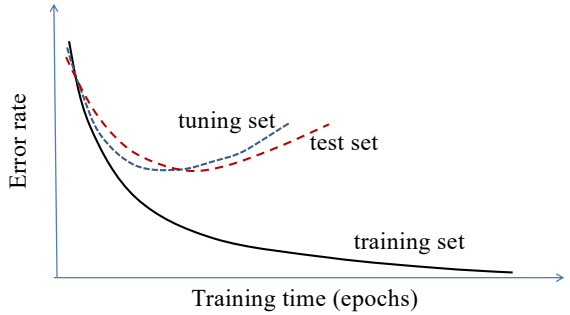
Tuning Sets



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Other Issues

How many examples should be in the training set?

– ***The more the better, but training takes longer***

To obtain $1 - e$ correct classification on testing set, the training set should be of size approximately n/e

- n is the number of weights in the network
- e is test set error fraction between 0 and 1

– train to classify $1 - e/2$ of the training set correctly

e.g., if $n = 80$ and $e = 0.1$ (i.e., 10% error on test set)

– Use training set of size is 800

– train until 95% correct classification on training set

– should produce ~90% correct classification on test set

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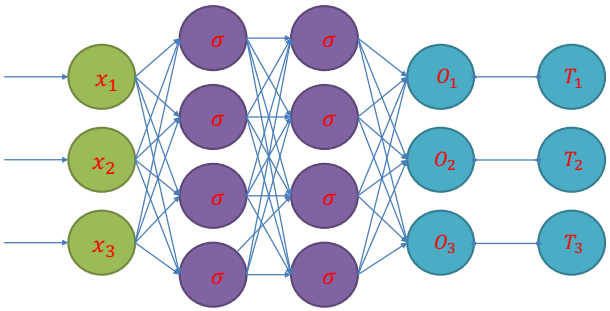
Recap: Multi-Layer, Feed-Forward Neural Networks



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Back-Propagation Recap

- Back-Propagation performs a ***gradient descent search*** in "weight space" to learn the neural network weights that minimize the total error on the training set
- Given a neural network with *n* weights:
  - each configuration of weights is a vector, W, of length *n* that defines an instance of the network
  - W can be considered a point in an *n*-dimensional **weight space**, where each dimension is associated with one of the connections in the network

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Updating the Weights

- Given a training set of m examples:
  - Each network defined by the vector $\boldsymbol{W}$ has an associated total error, E, on ***all*** the training data
  - E is the sum squared error (SSE) defined by
    $$E = E_1 + E_2 + \ldots + E_m$$
    where E_i is the squared error of the network on the i^{th} training example
- Given t output units in the network:
  $$E_i = (T_{i1} - O_{i1})^2 + (T_{i2} - O_{i2})^2 + \ldots + (T_{it} - O_{it})^2$$
  - T_{ij} is the target value for the i^{th} example's j^{th} output unit
  - O_{ij} is the network output value for the i^{th} example's j^{th} output unit

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Back-Propagation using SGD

Initialize the weights in the network (usually random values)
Repeat until stopping criterion is met
  foreach example, *ex,* in training set **do**
    { O = neural_net_output(network, *ex*) **forward pass**
    T = desired output, i.e., **T**arget or **T**eacher's output
    calculate error (T_k - O_k) at each output unit *k*
    foreach hidden unit *j* and output unit *k* compute $\Delta w_{j,k}$
    foreach input unit *i* and hidden unit *j* compute $\Delta w_{i,j}$
    forall *p*, *q* in network $w_{p,q} = w_{p,q} + \Delta w_{p,q}$
    }

backward pass

Simplistic SGD: update all weights after *each* example

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Other Issues

- How many hidden layers should be in the network?
  - often just one hidden layer is used
- How many hidden units should be in a layer?
  - too few: concept *can't* be learned
  - too many:
    - examples just memorized
    - overfitting, poor generalization

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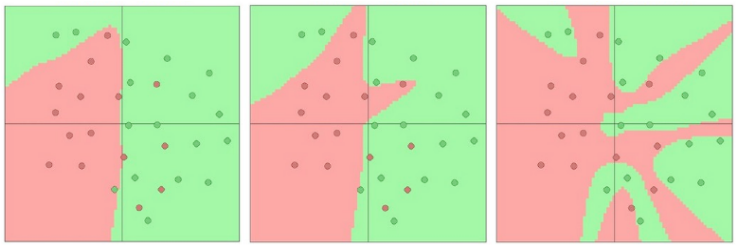
How Many Hidden Units?

Decision regions learned by a 2-layer network:
Larger networks can represent more complicated functions, but make it easier to overfit the training data



3 hidden units 6 hidden units 20 hidden units

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Application: Autonomous Driving

- ALVINN (Pomerleau, 1988)
  learned to control vehicle steering to stay in the middle of its lane
- Topology: 2-layer, feed-forward network using back-propagation learning
  - **Input layer:** 480 × 512 image @ 15 frames per second
    - color image is preprocessed to obtain a 30 × 32 image
    - each pixel is one byte, an integer from 0 to 255 corresponding to the brightness of the image
    - networks has 960 input units (= 30 × 32)

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ALVINN

steering direction

[Pomerleau, 1995]

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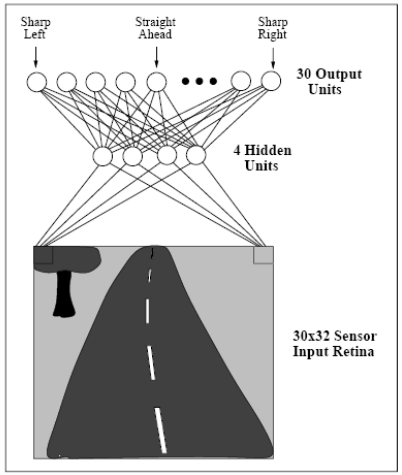
ALVINN's 2-Layer Network



[Pomerleau, 1995]

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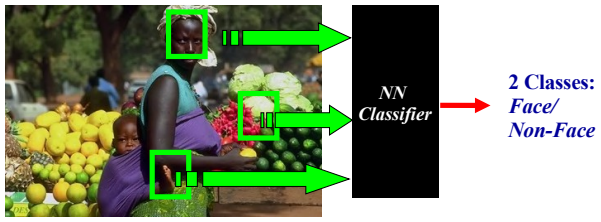
Application: Face Detection



- Input = 20 x 20 pixel window, outputs a value ranging from –1 to +1 signifying the presence or absence of a face in the region
- The window is positioned at every location of the image
- To detect faces larger than 20 x 20 pixel, the image is repeatedly reduced in size

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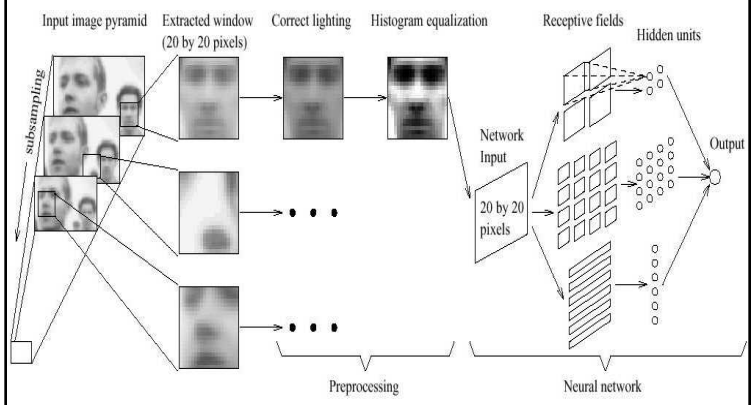
2-Layer Network



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Application: Face Detection

- 2-layer feed-forward neural network
- Three types of hidden units
  - 4 look at 10 x 10 subregions
  - 16 look at 5 x 5 subregions
  - 6 look at 20 x 5 horizontal stripes of pixels
- Training set
  - 1,050 initial face images. More face examples generated from this set by rotation and scaling. Desired output: +1
  - Non-face training samples: 8,000 non-face training samples from 146,212,178 subimage regions! Desired output: -1

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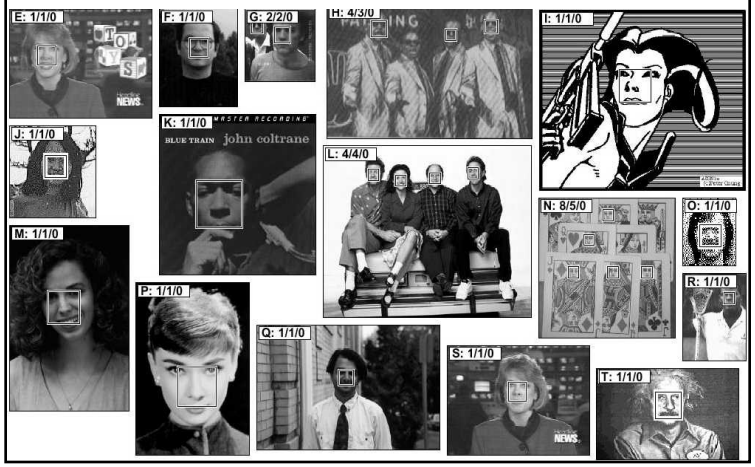
Face Detection Results



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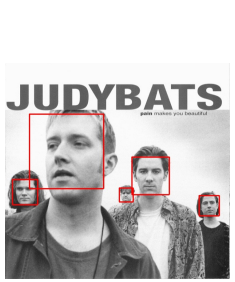
Results

- Notice detection at multiple scales



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What is Wrong with Back-Propagation?

- Requires labeled training data
  - Almost all data is **unlabeled**
- Learning time does not scale well
  - It is very slow to converge in networks with multiple hidden layers
- Might get stuck at a poor local minimum
- Overfitting problem

from G. Hinton

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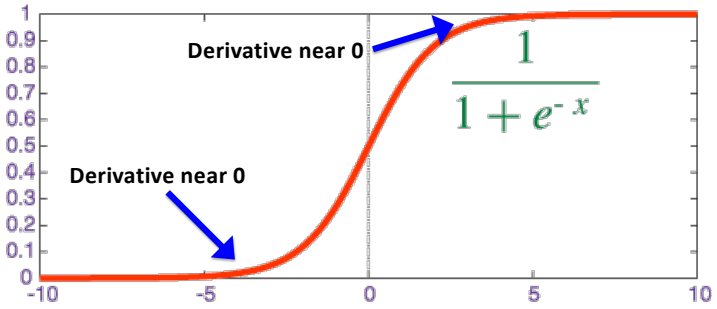
Sigmoid Function

Slow learning because "saturated" units "kill" gradients



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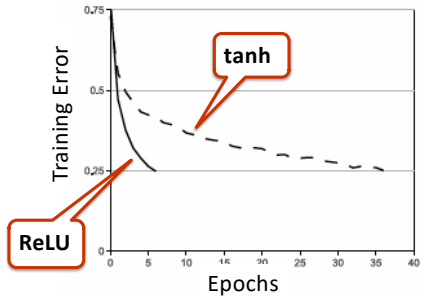
Speeding Up Training

Use ReLU instead of Sigmoid (or Tanh)

- Rectified Linear Unit: $g(x) = \max(0, x)$
- ReLU reaches 25% error rate 6x faster than tanh
- Computationally efficient



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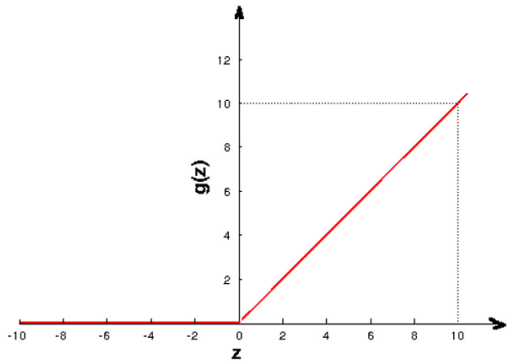
Rectified Linear Function (ReLU)



The rectified linear activation function

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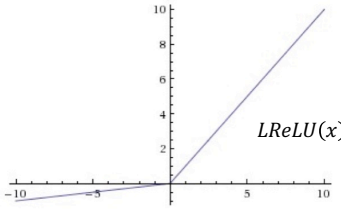
What's the Derivative of the ReLU Function?

$$g'(x) = \begin{cases} 0, & \text{if } x \le 0 \\ 1, & \text{otherwise} \end{cases}$$

But this means when x ≤ 0 the unit will never update because $\Delta_i = 0$

– Fix using a variation such as "**Leaky ReLU**":



$$LReLU(x) = \begin{cases} \alpha \boldsymbol{x}, & \boldsymbol{x} < 0 \\ \boldsymbol{x}, & \boldsymbol{x} \ge 0 \end{cases}$$

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Preventing Overfitting: Dropout

To prevent overfitting the training set, "dropout" is often performed:

- During training: At each hidden layer, "drop out" a random set of units from that layer by setting their outputs to 0 in the forward pass
  - Each unit is retained with probability *p* (= 0.5)
  - Back-propagation is performed only on the thinned network
- During testing: Use the whole network (but weights must all be re-scaled)

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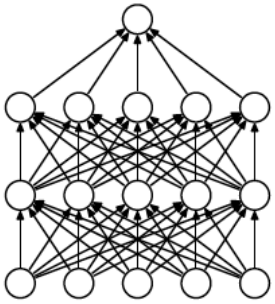
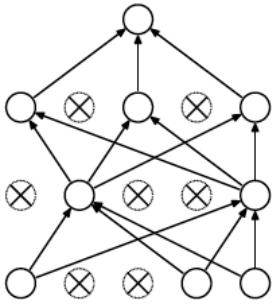
Dropout



Original Neural Net



Neural Net after Dropping Out "X"ed nodes

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Why Dropout?

- If a hidden unit knows which other hidden units are present, it can co-adapt to them on the training data
  - But complex co-adaptations are likely to go wrong on new test data
  - Big, complex conspiracies are not robust
- If a hidden unit has to work well with combinatorially many sets of co-workers, it is more likely to do something that is individually useful
  - But it will also tend to do something that is only marginally useful given what its co-workers achieve

G. Hinton

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- Early NNs used only 1 or 2 hidden layers because training was slow, thought to converge to poor local minima, and overfit

- Recent results suggest that local minima are ***not*** a serious problem – regardless of initial conditions, *bigger NNs contain many more local minima but nearly all are solutions of very similar quality*. And overfitting can be avoided using regularization techniques such as dropout rather than using fewer units

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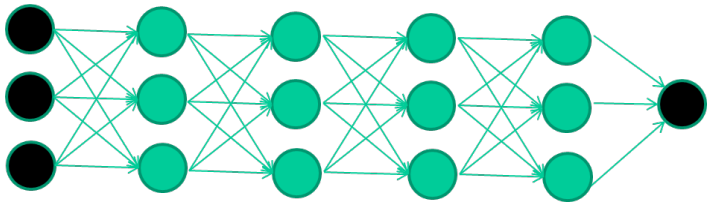
Deep Learning

- Use *many hidden layers* (often 10-20)
- Called **Deep Neural Nets** or **Deep Nets**



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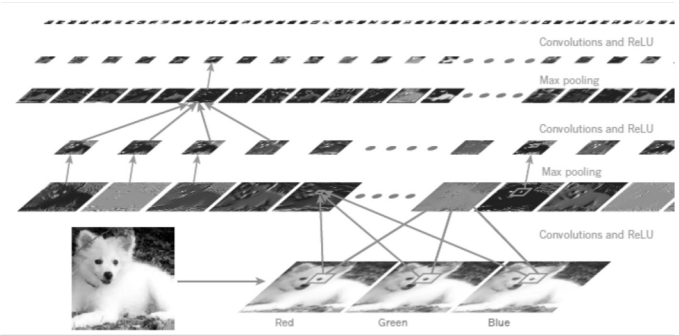
Reading: "Deep learning," Y. LeCun, Y. Bengio and G. Hinton, *Nature*, 2015



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A Lot of Buzz about Deep Learning

Google Scoops Up Neural Networks Startup DNNresearch To Boost Its Voice And Image Search Tech

RIP EMPSON

Tuesday, March 12th, 2013 5 Comments

Similarly, big groups at Facebook, Microsoft, Baidu, Amazon, …

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Why Deep Learning?

- Biological Plausibility – your brain works that way
- Problems that can be represented with a polynomial number of nodes with *k* layers, may require an exponential number of nodes with *k*-1 layers
- Complex functions can be efficiently represented with deep architectures
  - Fewer weights/parameters to update than a less efficient shallow representation
- Features learned in deep architecture can potentially be shared between multiple tasks
  - Type of Transfer/Multi-task learning

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Why Deep Learning?

- Learn better features: **Features matter!**
- Use **context** better

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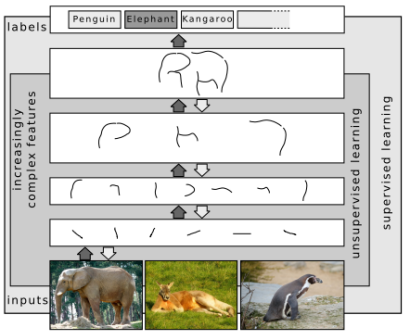
Hierarchical, Representation Learning



- Natural progression from low-level to high-level features as seen in natural complexity
- **Automatically learns features from the raw data**
- Easier to monitor what is being learned and to guide the learner to better subspaces

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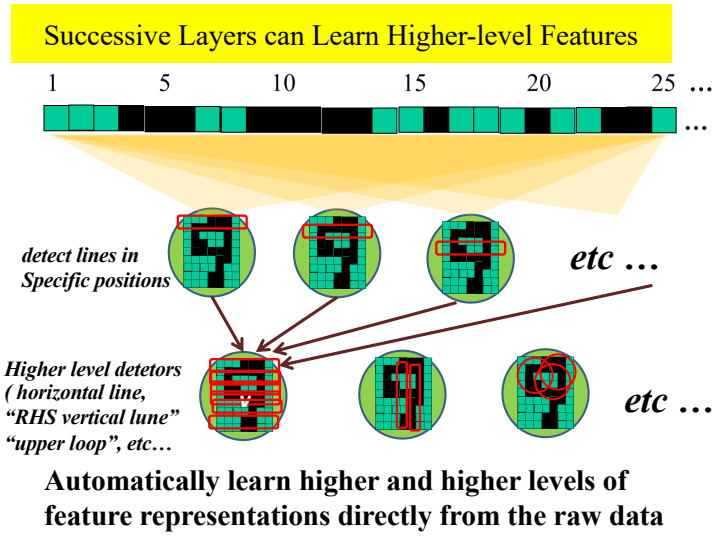

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Difficulties Training Deep Networks

- Bottom layers do not get trained easily
  - **Error attenuates as it propagates to earlier layers**
  - Leads to very slow training
- For small data sets, not enough labeled data available for training
  - Use a pre-processing step to initialize weights
  - Then use traditional back-prop to train the full network

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Convolutional Neural Networks

also called **CNNs** and **ConvNets**

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CNNs

- Many applications process **array data**
  - 1D: time-series, acoustic, text data
  - 2D: images and audio spectrograms
  - 3D: video and volumetric data
- Properties of these types of data
  - Local, shift-invariant processing (i.e., doesn't depend on position in the input array)
  - Hierarchy of feature descriptions
  - Noisy data

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CNNs are an extension of traditional multi-layer, feed-forward networks that incorporate **4 key ideas**:

- Use of **many layers**
  - Learn a hierarchy of features
- **Local "receptive fields"/filters and local connections**
  - Layers are *not* completely connected
  - Want translation-invariant and distortion-invariant local features
- **Shared weights**
- **Pooling**

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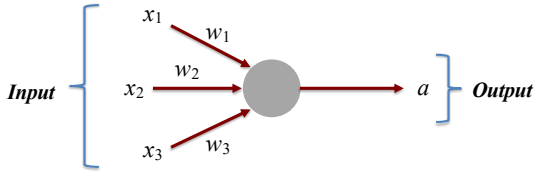
Computation by a Unit

Takes several inputs and computes a single scalar output value



$$a = g(w_1x_1 + w_2x_2 + ... + w_nx_n) = g(\sum_{i=1}^{n} w_ix_i) = g(in)$$

First step is to compute *in*, the linear combination of the inputs

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Image Filtering

Filter

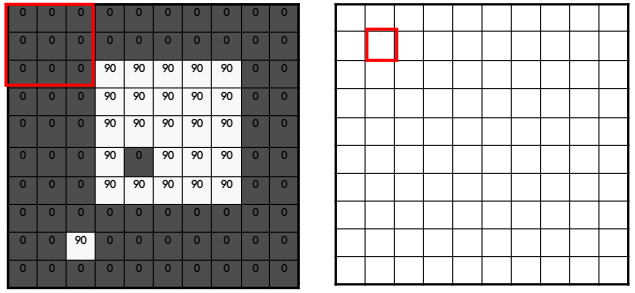
$g[\cdot,\cdot]$ $\frac{1}{9}$ [1 1 1; 1 1 1; 1 1 1]

Input Image

$f[.,.]$

Output Image

$h[.,.]$



$$h[m,n] = \sum_{k,l} g[k,l]\, f[m+k,n+l]$$

Credit: S. Seitz

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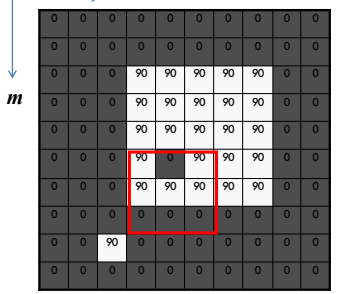
Image Filtering

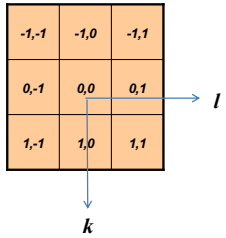
$g[\cdot,\cdot]$

$f[.,.]$



$\frac{1}{9}$

-1,-1	-1,0	-1,1
0,-1	0,0	0,1
1,-1	1,0	1,1



$$h[m,n] = \sum_{k,l=-1}^{+1} g[k,l] f[m+k,n+l]$$

$h[7,5] = g[-1,-1]f[6,4] + g[-1,0]f[6,5] +$
$g[-1,1]f[6,6] + g[0,-1]f[7,4] +$
$g[0,0]f[7,5] + ...$

Credit: S. Seitz

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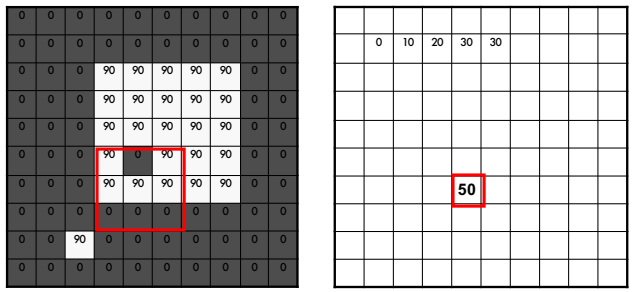
Image Filtering

$g[\cdot,\cdot]$ $\frac{1}{9}$ [1 1 1; 1 1 1; 1 1 1]

$f[.,.]$

$h[.,.]$



$$h[m,n] = \sum_{k,l} g[k,l]\, f[m+k,n+l]$$

Credit: S. Seitz

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Example: Box Filter

$g[\cdot,\cdot]$

$$\frac{1}{9}\begin{bmatrix}1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 1\end{bmatrix} = \begin{bmatrix}1/9 & 1/9 & 1/9\\ 1/9 & 1/9 & 1/9\\ 1/9 & 1/9 & 1/9\end{bmatrix}$$

Credit: David Lowe

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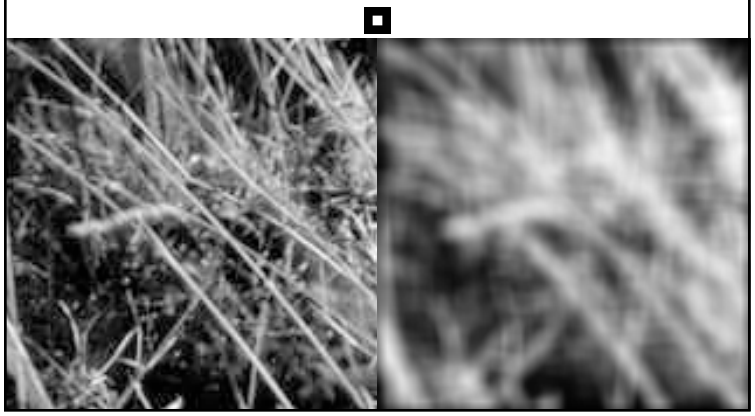
Image Smoothing with Box Filter



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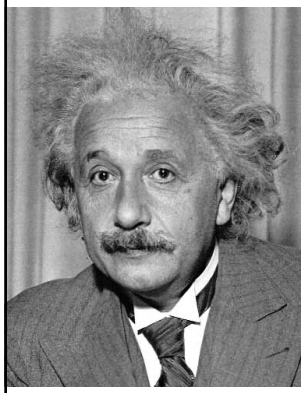
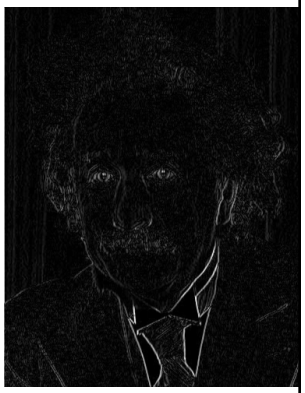
Vertical Edge Detection Filter



1	0	-1
2	0	-2
1	0	-1

Sobel filter



Vertical edges (absolute value)

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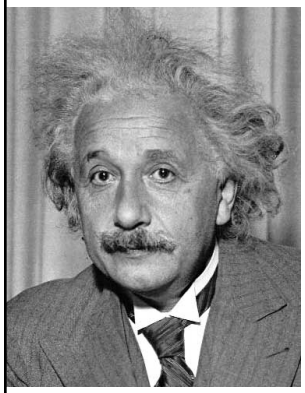
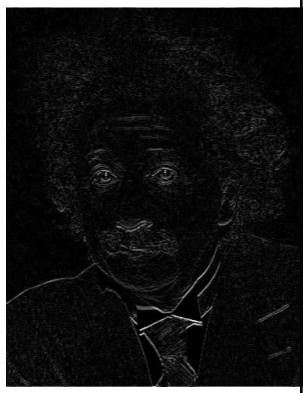
Horizontal Edge Detection Filter



1	2	1
0	0	0
-1	-2	-1

Sobel filter



Horizontal edges (absolute value)

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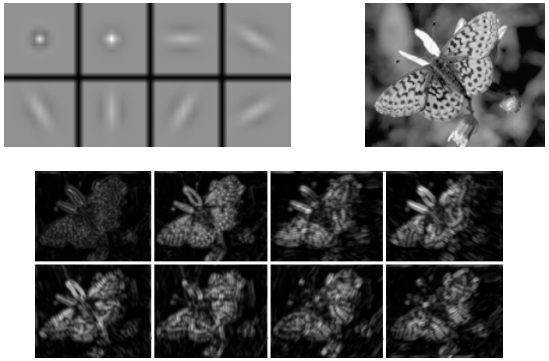
Other Filters



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Why are they called "Convolutional" NNs?

The image filtering operation defined as

$$h[m,n] = \sum_{k,l} g[k,l]\, f[m+k, n+l]$$

is very similar to the **Convolution** operation defined as

$$h[m,n] = \sum_{k,l} g[k,l]\, f[m-k, n-l]$$

- **In CNN's, *f* corresponds to the inputs from the layer below and *g* corresponds to the weights**
- So, CNN's will learn a set of filters!

Credit: K. Grauman

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Convolution Layers

- Learn "filters" (i.e., weights) that process only **small regions** of the layer below it and compute "features" at many spatial positions
- Example: 32 x 32 x 3 input RGB image, and receptive field (filter size): 5 x 5
  - Each unit in the "Conv layer" will have weights connected to a 5 x 5 x 3 region in the input layer, with 5*5*3 = 75 weights
  - Can have multiple units associated with a given receptive field in order to compute multiple features at each position
  - "Stride" parameter defines shift amount

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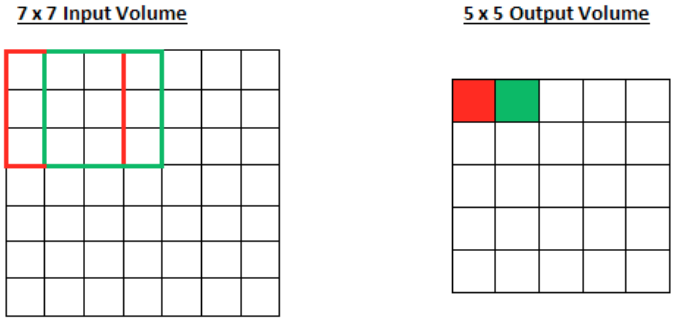
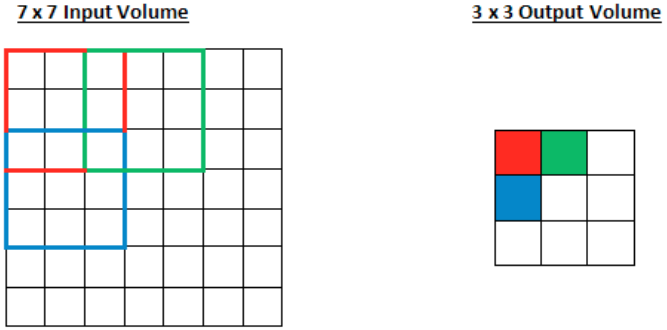
3 x 3 Filter, Stride = 1



246

3 x 3 Filter, Stride = 2



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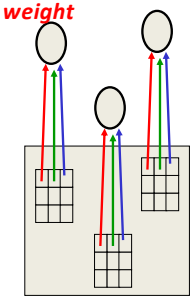
The Replicated Feature Approach: Local Connections and Shared Weights

- Use many different copies of the *same feature detector* at different positions
  - Could also replicate across scale and orientation (but tricky and expensive)
  - Replication greatly reduces the number of weights to be learned
- Use several different feature types, each with its own map of replicated detectors
  - Allows each patch of image to be represented in several ways

The red connections all have the same weight



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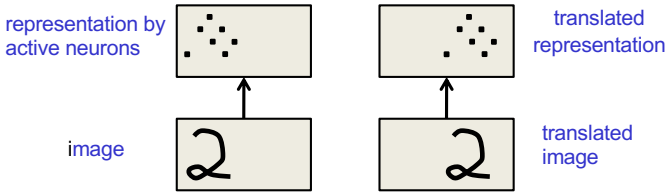
What does Replicating the Feature Detectors Achieve?

- Equivariant activities



- Invariant knowledge: If a feature is useful in some locations during training, detectors for that feature will be available in ***all*** locations during testing

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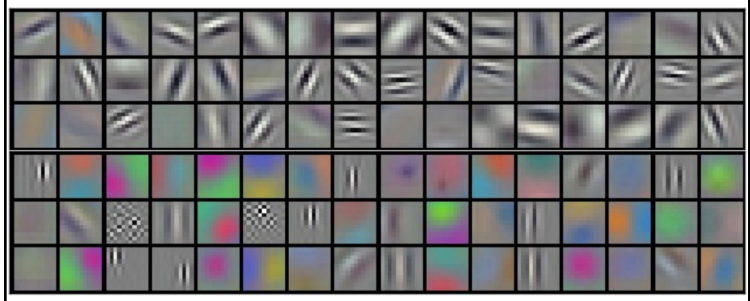
Learned Features

96 learned low-level (1st layer) filters:



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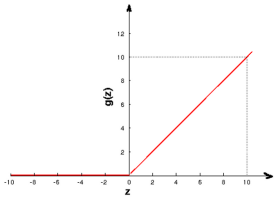
ReLU Layers

- Each Convolution layer often followed by an "**ReLU layer**," which applies the ReLU function to the output of each "**Convolution layer**"
- No weights to be learned
- Layer size equal to size of the layer below it



The rectified linear activation function

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Pooling Layers

- Each ReLU layer usually followed by a "**Pooling layer**"
- Get a small amount of translational invariance and robustness to noise by combining *neighboring values* to give a *single output* at the next layer
- **Max Pooling**: Combine by taking the *maximum*
- **Average Pooling**: Combine by taking the *average*
- **Sub-Sampling**: Reduces the size of the next layer according to the size of the pooling filter
  - For example, a 2 x 2 pooling filter reduces the size by ½ in each dimension

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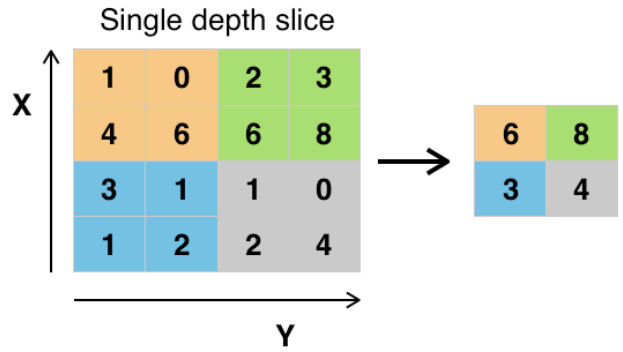
Max Pooling Example



2 x 2 filter with a stride of 2

Adit Deshpande

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Top Layers Fully Connected

- Top few layers are usually fully-connected, feed-forward layers
- Hidden layers and Output layer

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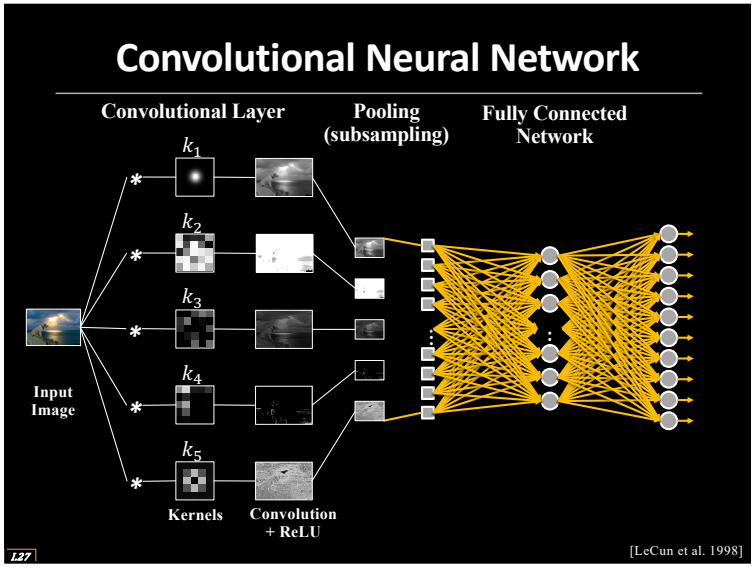
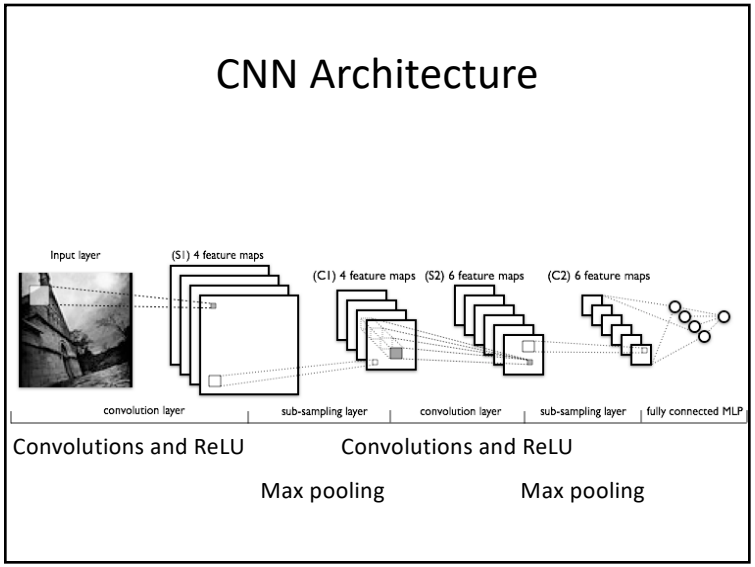
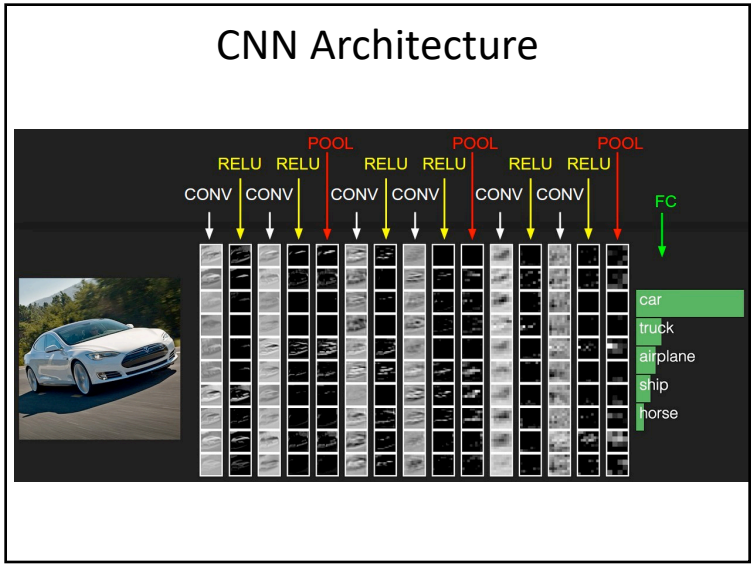


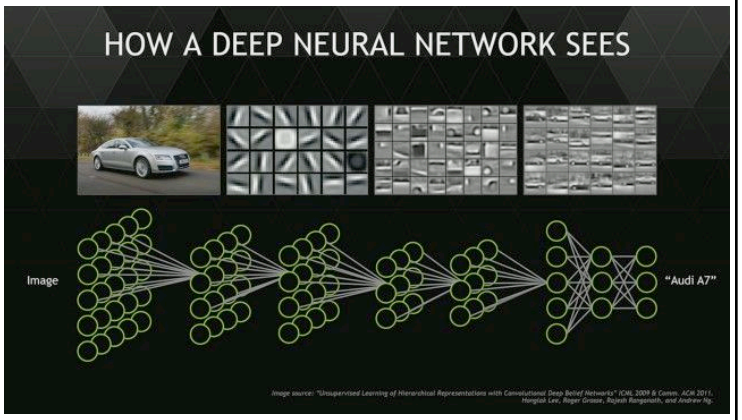
257



258



259



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CNNs are an extension of traditional multi-layer, feed-forward networks that incorporate **4 key ideas**:

- Use of **many layers**
  - Learn a hierarchy of features
- **Local "receptive fields"/filters and local connections**
  - Layers are *not* completely connected
  - Want translation-invariant and distortion-invariant local features
- **Shared weights**
- **Pooling**

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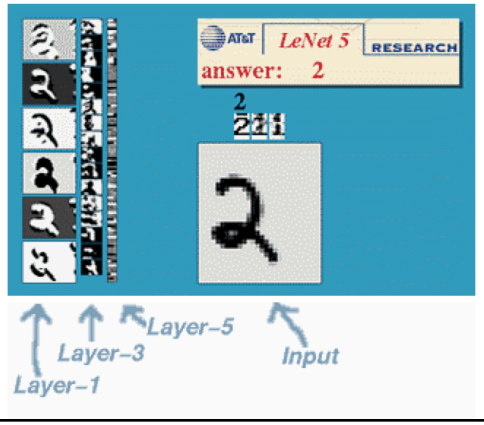
LeCunn's Digit Recognizer: LeNet

http://yann.lecun.com/exdb/lenet/index.html



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LeNet

- Yann LeCun and his collaborators developed a really good recognizer for handwritten digits by using backpropagation in a feed-forward net with:
  - Many hidden layers
  - Many maps of replicated units in each layer
  - Pooling of the outputs of nearby replicated units
  - A wide net that can cope with several characters at once even if they overlap
- This net was used for reading ~10% of the checks in North America

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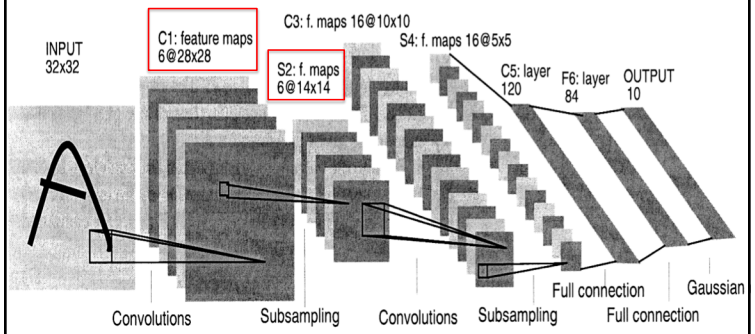
The Architecture of LeNet5



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From Handwritten Digits to 3D Objects

- Recognizing real objects in color photographs downloaded from the web is much more complicated than recognizing handwritten digits:
  - Hundred times as many classes (1,000 vs 10)
  - Hundred times as many pixels (256 x 256 color vs 28 x 28 grayscale images)
  - Cluttered scenes
  - Multiple objects in each image
- Will the same type of CNN work?

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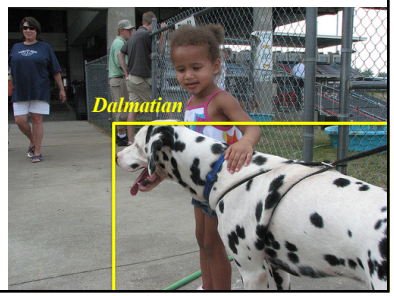
IMAGENET Large Scale Visual Recognition Challenge (ILSVRC 2010)

Training set: 1.2 million 256 x 256 RGB images

- Classification task:
  –Get the "correct" class in your top 5 predictions. There are **1000 classes**
- Localization task:
  –For each prediction, put a box around the object. Your box must have at least 50% overlap with the correct box



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ImageNet

- Over 15M labeled high-resolution images
- About 22K categories
- Collected from the web and manually labeled by Amazon Mechanical Turk

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Variety of Object Classes in ILSVRC

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AlexNet

A. Krizhevsky, I. Sutskever, G. Hinton, *NIPS* 2012

- 7 hidden "weight" layers:
- `data` → `conv1` → `pool1` → `conv2` → `pool2` → `conv3` → `conv4` → `conv5` → `pool3` → `full` → `full` → `output`
- 650K units, 60M weights, 630M connections
- ReLUs, max pooling, dropout trick
- Top feature layer: 4096 units
- Output layer: 1000 units
- Trained with SGD on two GPUs for a week
- Classification: "Top-1" error rate: 37.5%
  "Top-5" error rate: 17%
- Localization: Regression on (x,y,w,h)

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Dropout Observations by G. Hinton

- If your deep neural net is significantly overfitting, dropout will usually reduce the number of errors by a lot
  - Any net that uses "early stopping" can do better by using dropout (at the cost of taking quite a lot longer to train)
- If your deep neural net is not overfitting, you should be using a bigger one!

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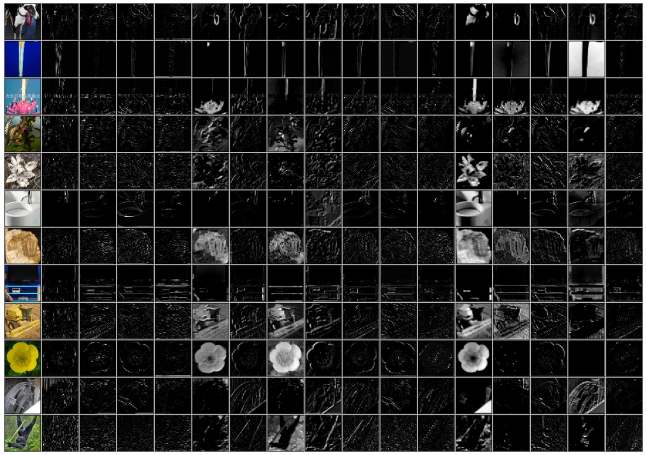
Learned Features at 1st Layer



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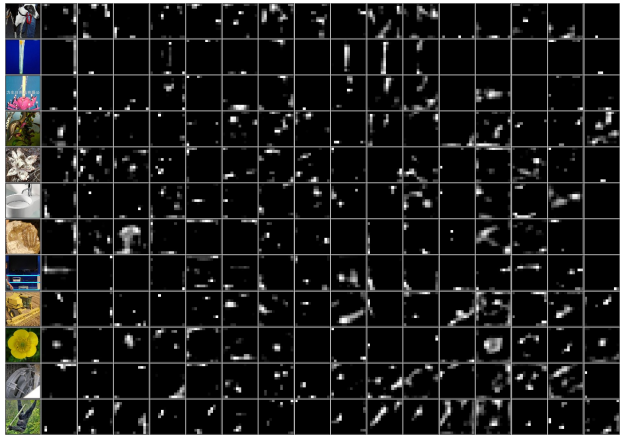
Learned Features at 5th Layer



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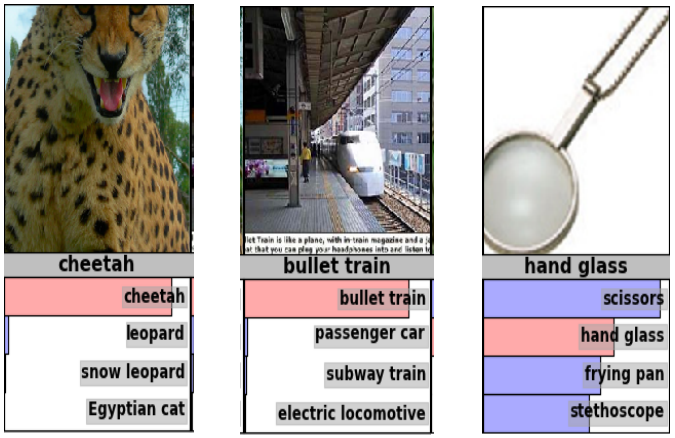
Examples from the Test Set (with the network's predictions)



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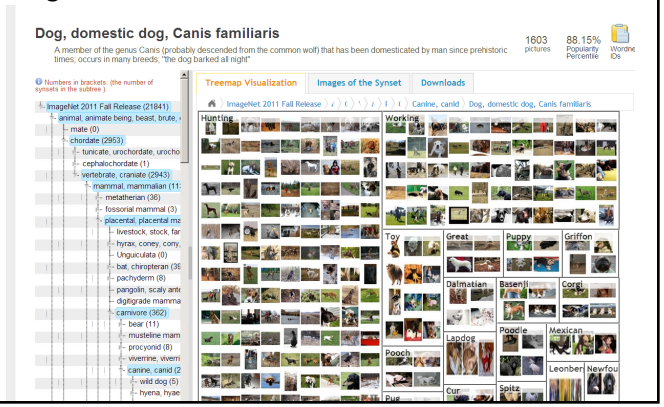
ILSVRC 2012

Training set: 15 million labeled images from ImageNet, 20K categories



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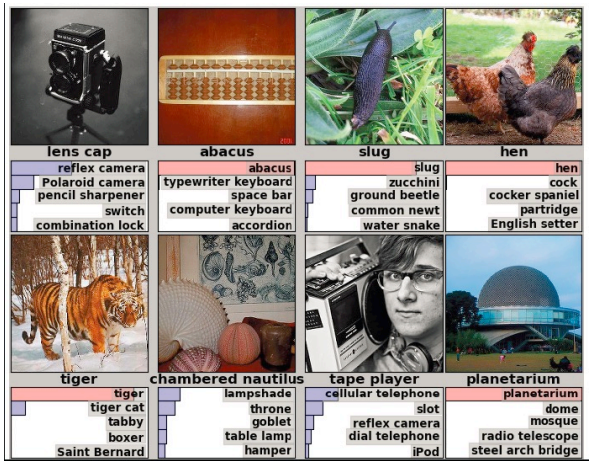
Example Classification Results



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Error Rates on the ILSVRC 2012 Competition

	classification	*classification & localization*
• University of Toronto (CNN)	16.4%	34.1%
• University of Tokyo	26.1%	53.6%
• Oxford University	26.9%	50.0%
• INRIA + Xerox	27.0%	
• University of Amsterdam	29.5%	

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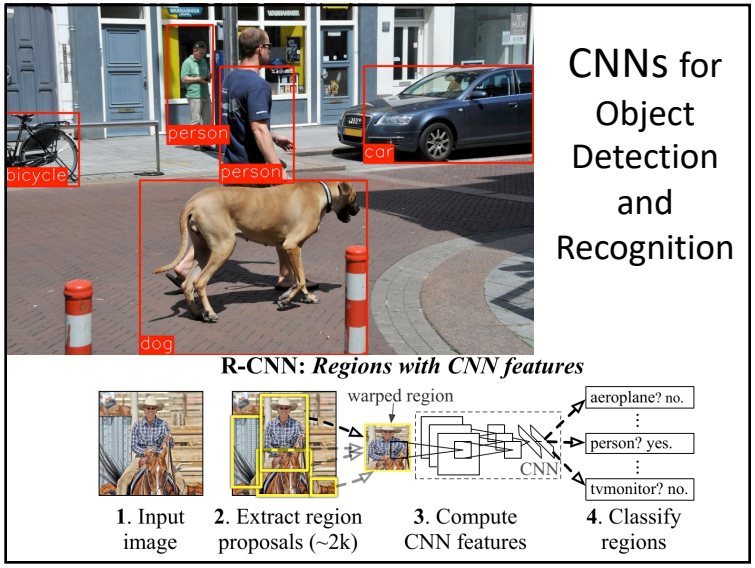
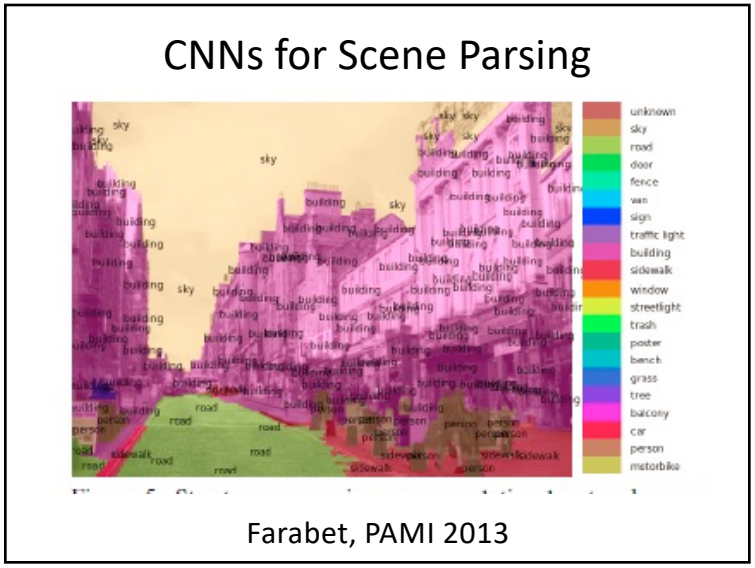


286



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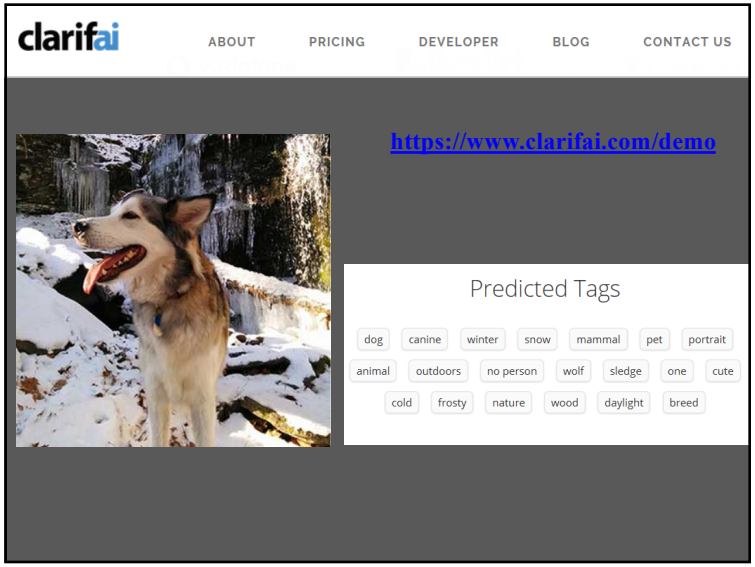

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Deep Learning Demos and Startups

- Clarifai
  - http://www.clarifai.com
- Dextro
  - www.dextro.co
- Microsoft's CaptionBot
  - https://www.captionbot.ai
- Yann LeCun's Digit Recognizer
  - http://yann.lecun.com/exdb/lenet/
- Toronto Deep Learning Demos
  - http://deeplearning.cs.toronto.edu/

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Number Recognition from Google's Street View Images

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Number Recognition from Google's Street View Images

- Training set: 200,000 images of (cropped) house numbers (up to 5 digits long)
- CNN with 11 hidden layers
  - 54 x 54 input image layer
  - 8 convolutional layers
    - 48 x 54 x 54 = 140,000 units at first hidden layer
    - 5 x 5 convolution kernels
  - 1 locally-connected hidden layer
  - 2 densely-connected hidden layers
    - 3,072 units in each

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- Training time: 6 days
- Accuracy: Transcribed ~100 million numbers with ~98% accuracy (meaning *all* numbers in a sequence were recognized correctly) and 95% coverage

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ResNets @ ILSVRC & COCO 2015 Competitions

- **1st places in all five main tracks**
  - ImageNet Classification: "*Ultra-deep*" 152-layer nets
  - ImageNet Detection: 16% better than 2nd
  - ImageNet Localization: 27% better than 2nd
  - COCO Detection: 11% better than 2nd
  - COCO Segmentation: 12% better than 2nd

Also have tried using a 1000-layer network!

Deep residual learning for image recognition, K. He *et al.*, *Proc. CVPR*, 2016 (Best paper award)

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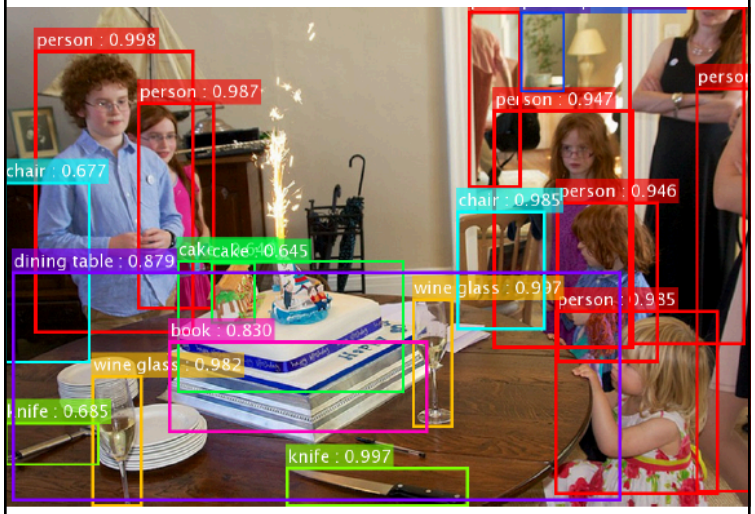

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Results on Real Video (trained on 80 categories)

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CNNs for Video Classification

[Karpathy 2014]

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Image Style Transfer using CNN

"Image style transfer using convolutional neural networks," L. Gatys, *CVPR* 2015

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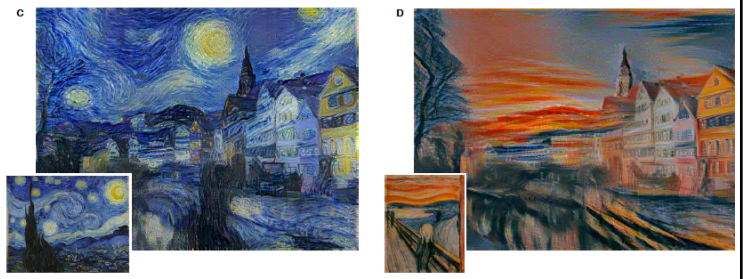

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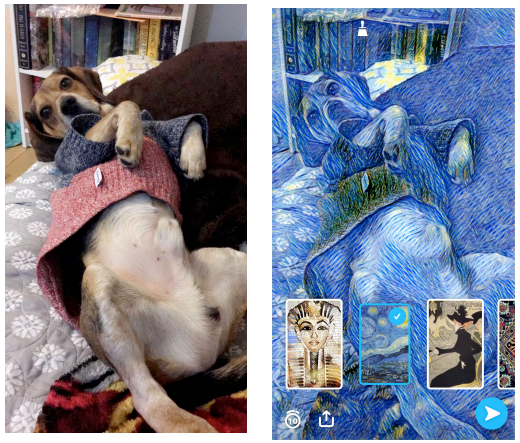
Snapchat's Paintbrush



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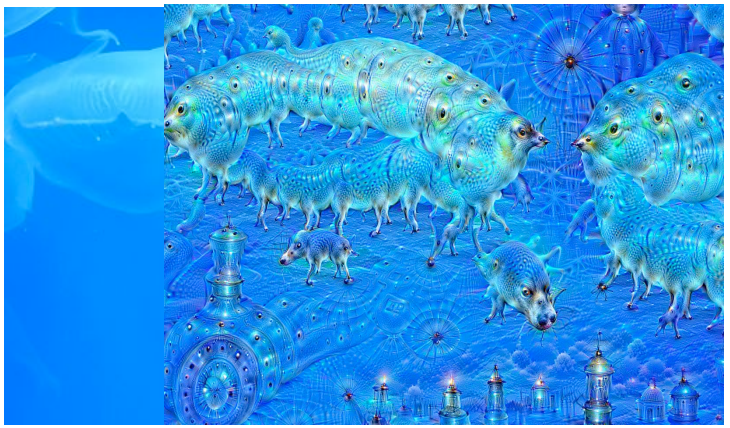
Google's DeepDream



Input image Output image

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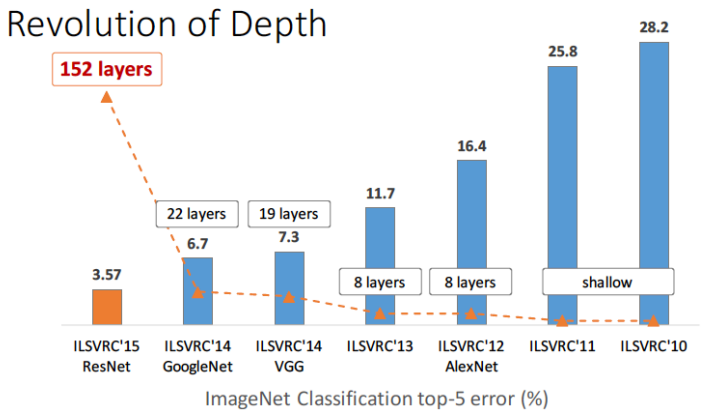
Current Trend: *Very Deep* Networks (using Deep Residual Learning)



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Deep Learning Software

- TensorFlow (Google)
- Caffe (UC Berkeley)
- Torch
- Deeplearning4j
- OpenNN
- Microsoft Cognitive Toolkit
- ConvNetJS
- etc.

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