Lecture 3
Feedforward Networks and Backpropagation

CMSC 35246: Deep Learning

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  - Recap of Logistic Regression

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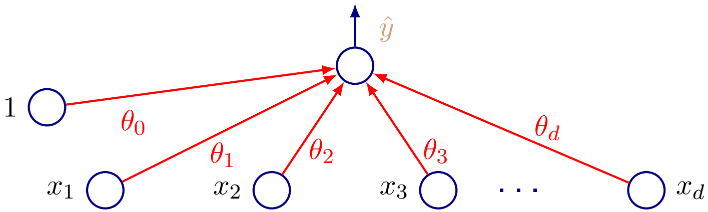
  - Backpropagation

Recap: The Logistic Function (Single Neuron)



$$p(y = 1|\mathbf{x}) = \frac{1}{1 + \exp(-\theta_0 - \theta^T \mathbf{x})}$$

Likelihood under the Logistic Model

$$p(y_i|\mathbf{x};\theta) = \begin{cases} \sigma(\theta_0 + \theta^T\mathbf{x}_i) \text{ if } y_i = 1 \\ 1 - \sigma(\theta_0 + \theta^T\mathbf{x}_i) \text{ if } y_i = 0 \end{cases}$$

- We can rewrite this as:

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- The log-likelihood of θ (cross-entropy!):

$$\log p(Y|X;\theta) = \sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i;\theta)$$

$$= \sum_{i=1}^{N} y_i \log \sigma(\theta_0 + \theta^T \mathbf{x}_i) + (1 - y_i) \log(1 - \sigma(\theta_0 + \theta^T \mathbf{x}_i))$$

The Maximum Likelihood Solution

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- Setting derivatives to zero:

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$$\frac{\partial \log p(Y|X;\theta)}{\partial \theta_0} = \sum_{i=1}^{N} (y_i - \sigma(\theta_0 + \theta^T \mathbf{x}_i)) = 0$$

$$\frac{\partial \log p(Y|X;\theta)}{\partial \theta_j} = \sum_{i=1}^{N} (y_i - \sigma(\theta_0 + \theta^T \mathbf{x}_i)) \mathbf{x}_{i,j} = 0$$

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- Can treat $y_i - p(y_i|\mathbf{x}_i) = y_i - \sigma(\theta_0 + \theta^T \mathbf{x}_i)$ as the prediction error

Finding Maxima

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- Gradient Descent/ascent (descent on $-\log p(y|\mathbf{x};\theta)$, log loss)

Gradient Descent Solution

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$$\theta^{(t+1)} := \theta^t + \frac{\eta_t}{N}\frac{\partial}{\partial\theta}\sum_i \log p(y_i|\mathbf{x}_i;\theta^{(t)})$$

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- Gradient on one example:

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- Above is batch gradient descent

Feedforward Networks

Introduction

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- No feedback connections (Recurrent Networks!)

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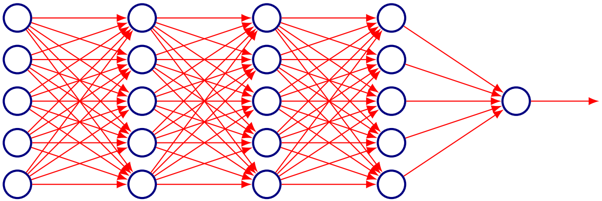

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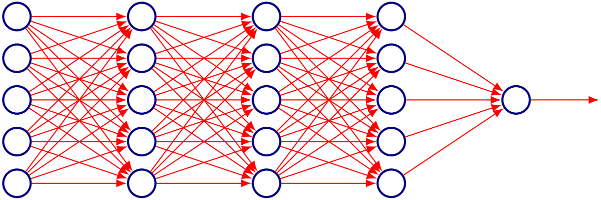

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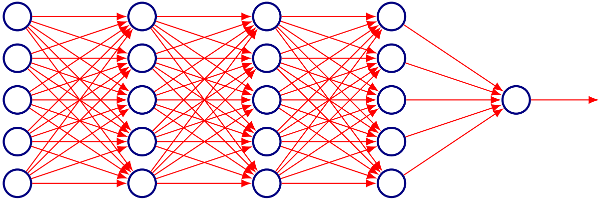

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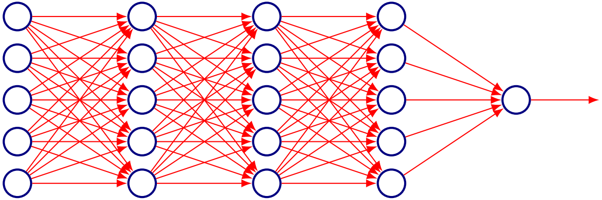

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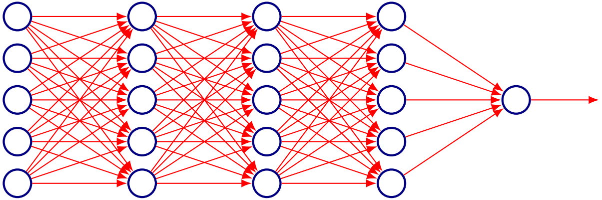

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- Final layer is called the *output* layer

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- **Neural**: Choices of $f^{(i)}$'s and layered organization, loosely inspired by neuroscience (first lecture)

Back to Linear Models

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- How do we choose ϕ?

Choosing ϕ

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- **Positive**: Enough capacity to fit training data
- **Negative**: Poor generalization for highly varying f^*
- Prior used: Function is locally smooth.

Choosing ϕ

- **Option 2**: Engineer ϕ for problem

Choosing ϕ

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- Still convex!

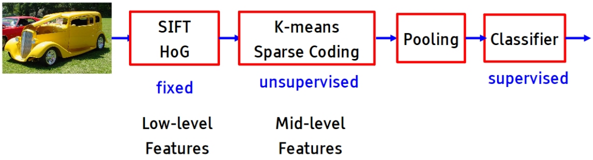

Illustration: Yann LeCun

Choosing ϕ

- **Option 3**: Learn ϕ from data
- Gives up on convexity
- Combines good points of first two approaches: ϕ can be highly generic and the engineering effort can go into architecture

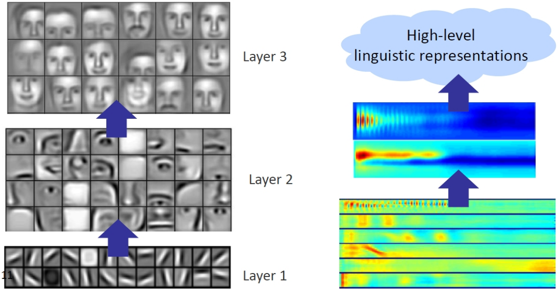

Figure: Honglak Lee

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- Architecture design (number of layers etc)

Back to XOR

XOR

Exclusive-OR gate

A	B	Output
0	0	0
0	1	1
1	0	1
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  $(X, Y) = \{([0,0]^T, 0), ([0,1]^T, 1), ([1,0]^T, 1), ([1,1]^T, 0)\}$

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- Our model $f(\mathbf{x}; \mathbf{w}, b) = \mathbf{x}^T \mathbf{w} + b$

Linear Model

- Recall previous lecture: Normal equations give $\mathbf{w} = 0$ and $b = \frac{1}{2}$

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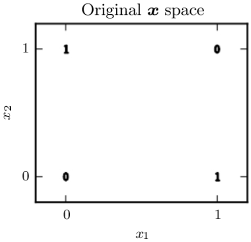

Figure: Goodfellow *et al.*

Solving XOR

- How can we solve the XOR problem?

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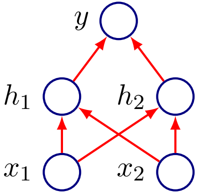
- Idea: Learn a different feature space in which a linear model will work

Solving XOR



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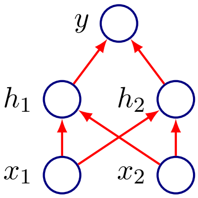
Solving XOR



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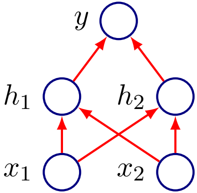

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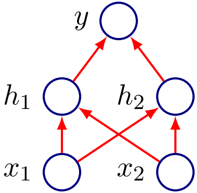

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- What should be $f^{(1)}$? Can it be linear?

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- Note: The activation above is applied element-wise

A Solution

- Let

$$W = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \mathbf{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \mathbf{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}, b = 0$$

A Solution

- Let
$$W = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \mathbf{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \mathbf{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}, b = 0$$
- Our design matrix is:
$$X = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix}$$

A Solution

- Compute the first layer output, by first calculating XW

$$XW = \begin{bmatrix} 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 2 & 2 \end{bmatrix}$$

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- Note: Ignore the type mismatch

A Solution

- Next step: Rectify output

$$\max\{0, XW + \mathbf{c}\} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$$

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- Finally compute $\mathbf{w}^T \max\{0, XW + \mathbf{c}\} + b$

A Solution

- Next step: Rectify output

$$\max\{0, XW + \mathbf{c}\} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$$

- Finally compute $\mathbf{w}^T \max\{0, XW + \mathbf{c}\} + b$

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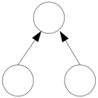
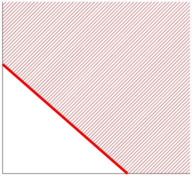
- For more complicated functions, we will proceed by using gradient based learning

An Aside:

1 layer of trainable weights





separating hyperplane

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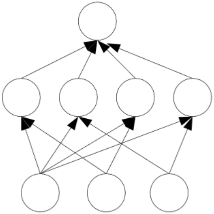

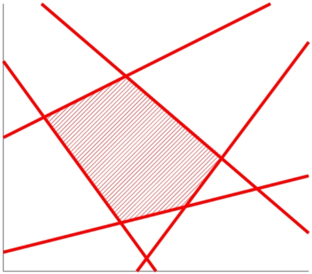

convex polygon region

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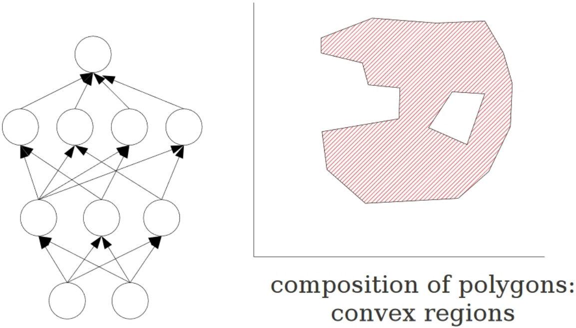

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- To apply gradient descent: Need to specify cost function, and output representation

Cost Functions

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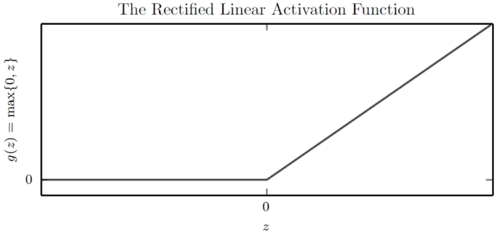
- Design of Hidden units is an active area of research

Rectified Linear Units



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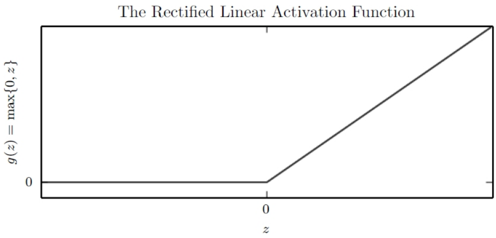

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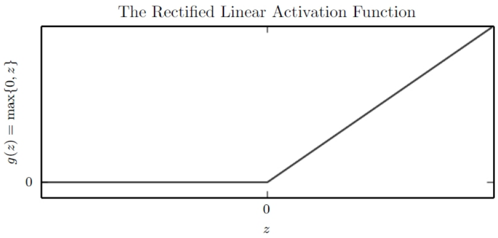

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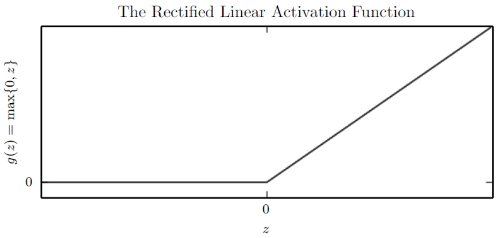

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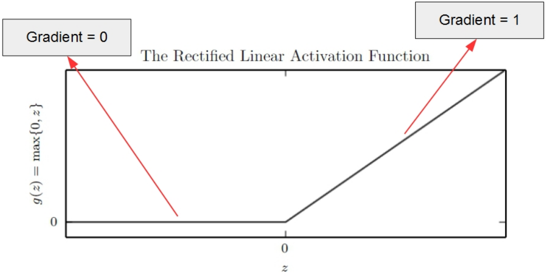

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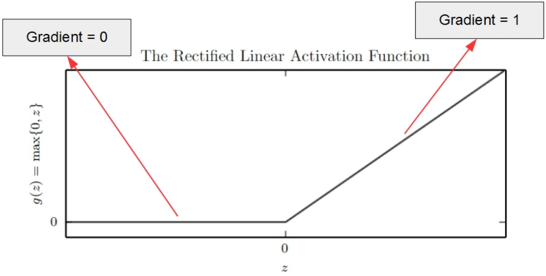

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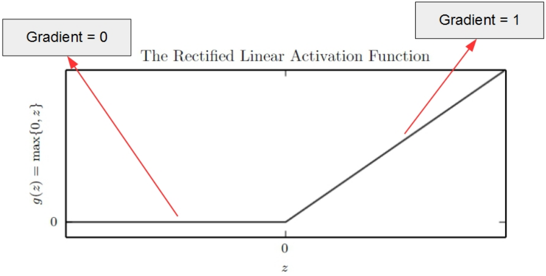

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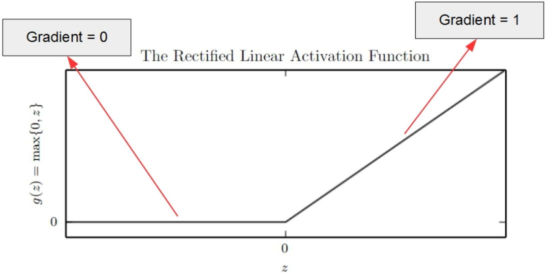

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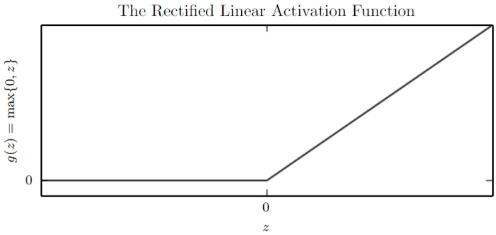

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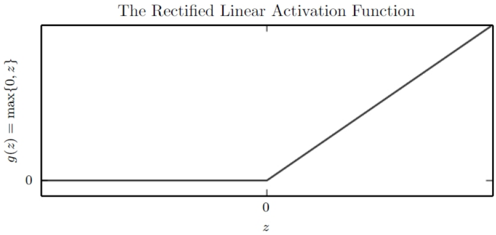

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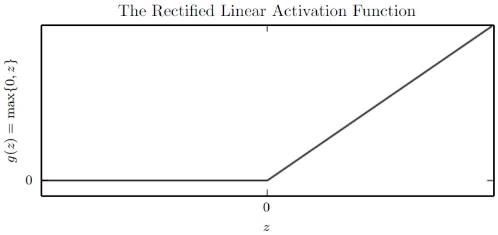

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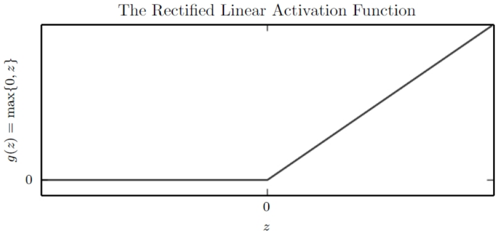

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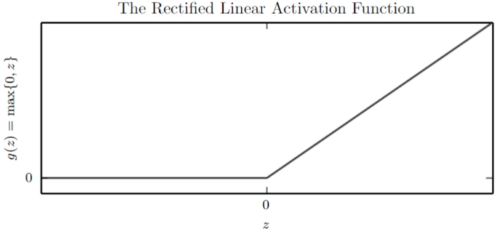

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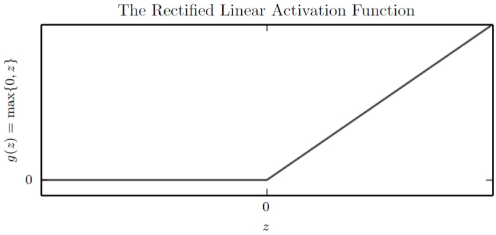

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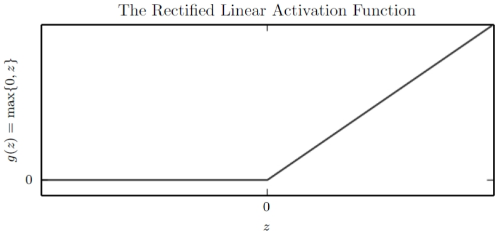

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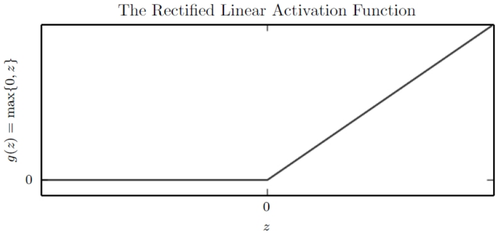

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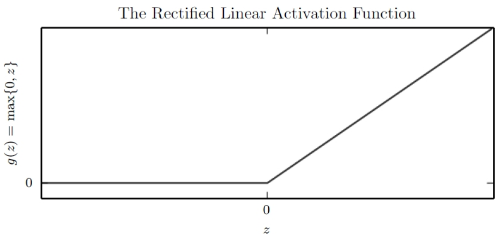

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  - Units "die" i.e. when inactive they will never update

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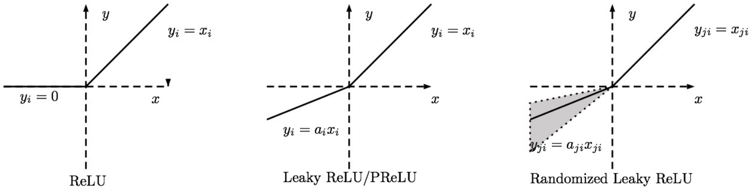

Figure: Xu *et al.* "Empirical Evaluation of Rectified Activations in Convolutional Network"

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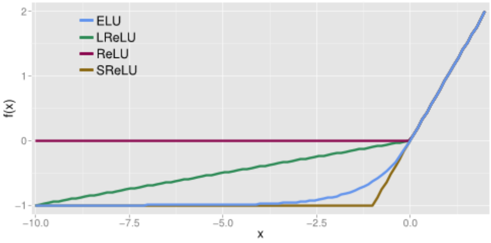

Figure: Clevert *et al.* "Fast and Accurate Deep Network Learning by Exponential Linear Units (ELUs)", 2016

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- Each unit parameterized by k weight vectors instead of 1, needs stronger regularization

Sigmoid Units

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

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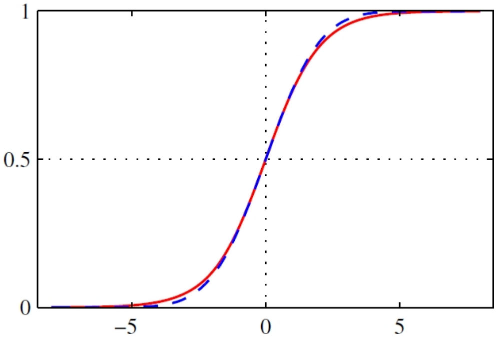
- Squashing type non-linearity: pushes outputs to range $[0, 1]$



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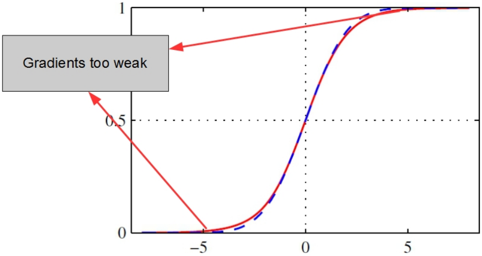

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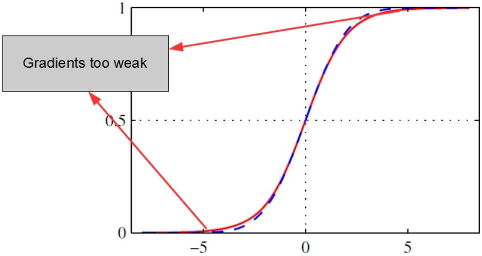

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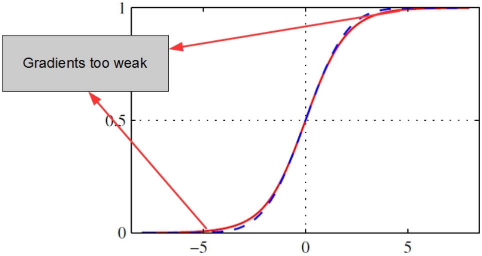

- Problem: Saturate across most of their domain, strongly sensitive only when z is closer to zero
- Saturation makes gradient based learning difficult

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- Positives: Squashes output to range $[-1, 1]$, outputs are zero-centered
- Negative: Also saturates
- Still better than sigmoid as $\hat{y} = \mathbf{w}^T \tanh(U^T \tanh(V^T \mathbf{x}))$ resembles $\hat{y} = \mathbf{w}^T U^T V^T \mathbf{x}$ when activations are small

Other Units

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- **Softplus:** $g(z) = \log(1 + e^z)$. Smooth version of rectifier (Dugas *et al.*, 2001), although differentiable everywhere, empirically performs worse than rectifiers
- **Hard Tanh:** $g(z) = \max(-1, \min(1, z))$, like the rectifier, but bounded (Collobert, 2004)

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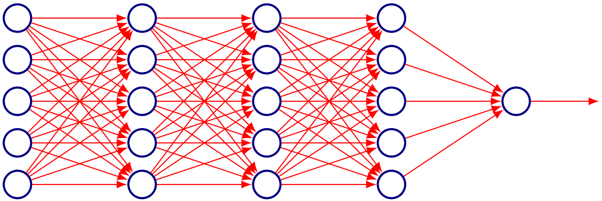
- Try other generalized ReLUs and Maxout for possible improvement

Universality and Depth

Architecture Design



- First layer: $\mathbf{h}^{(1)} = g^{(1)}\left(W^{(1)^T}\mathbf{x} + \mathbf{b}^{(1)}\right)$
- Second layer: $\mathbf{h}^{(2)} = g^{(2)}\left(W^{(2)^T}\mathbf{h}^{(1)} + \mathbf{b}^{(2)}\right)$
- How do we decide *depth*, *width*?
- In theory how many layers *suffice*?

Universality

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- Talked of some suggestive results earlier:

One more result:

- (Montufar *et al.*, 2014) Number of linear regions carved out by a deep rectifier network with d inputs, depth l and n units per hidden layer is:

$$O\left(\binom{n}{d}^{d(l-1)} n^d \right)$$

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- Exponential in depth!
- They showed functions representable with a deep rectifier network can require an exponential number of hidden units with a shallow network

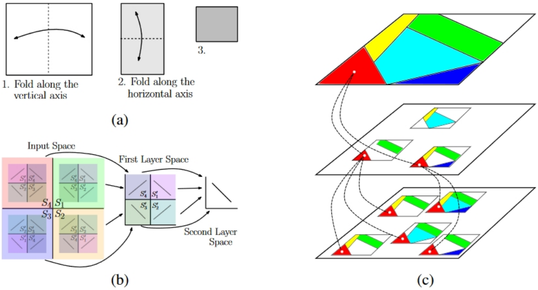

Figure 2: (a) Space folding of 2-D Euclidean space along the two axes. (b) An illustration of how the top-level partitioning (on the right) is replicated to the original input space (left). (c) Identification of regions across the layers of a deep model.

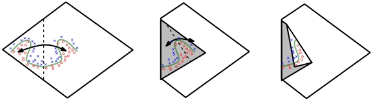

Figure 3: Space folding of 2-D space in a non-trivial way. Note how the folding can potentially identify symmetries in the boundary that it needs to learn.

Figure: Montufar *et al.*, 2014

Advantages of Depth

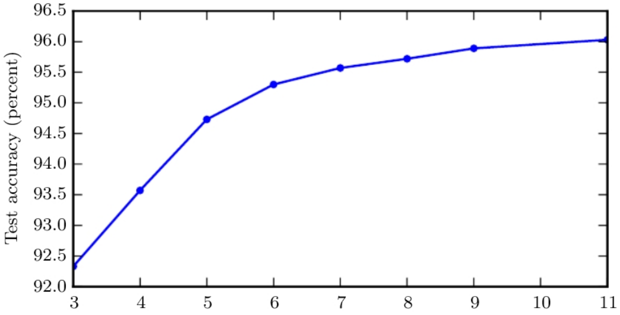

Figure: Goodfellow *et al.*, 2014

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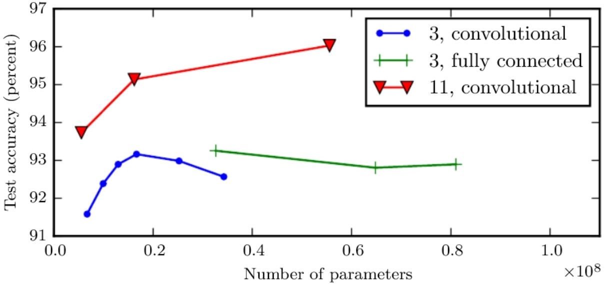
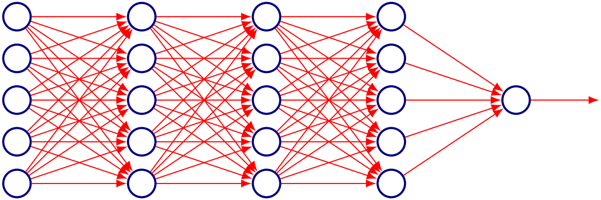


- Control experiments show that other increases to model size don't yield the same effect

Figure: Goodfellow *et al.*, 2014

Backpropagation: Introduction

How do we learn weights?



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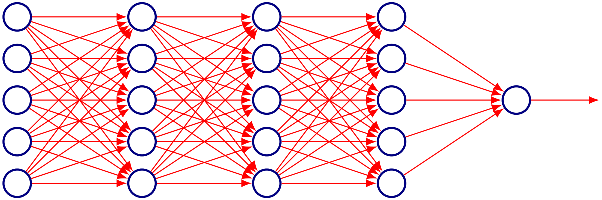

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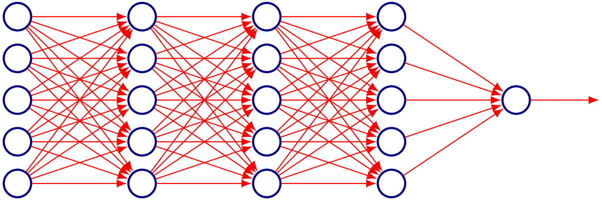

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- What does this remind you of?

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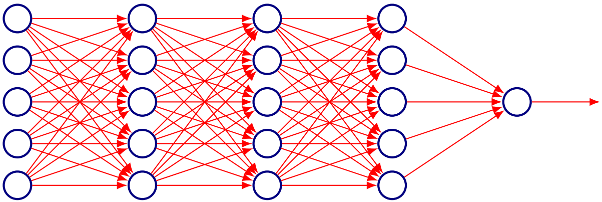

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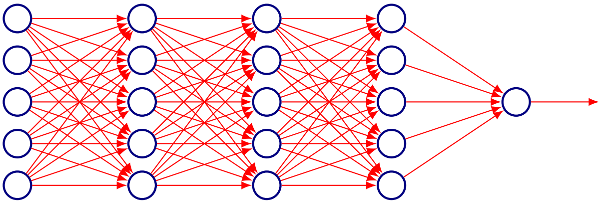

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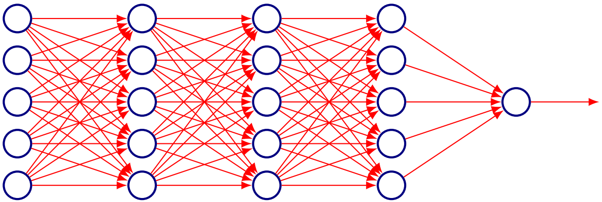
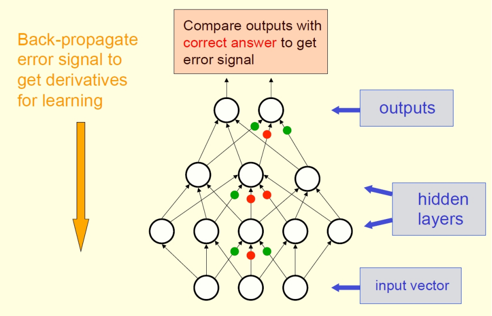


- Another Idea: Perturb all the weights in parallel, and correlate the performance gain with weight changes
- Very hard to implement
- Yet another idea: Only perturb activations (since they are fewer). Still very inefficient.

Backpropagation



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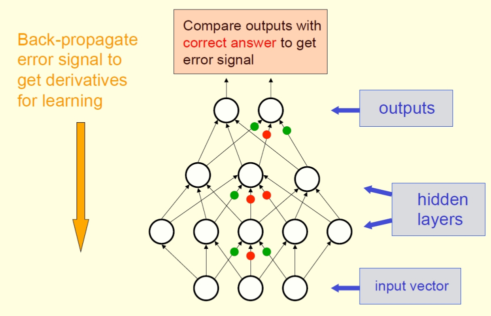
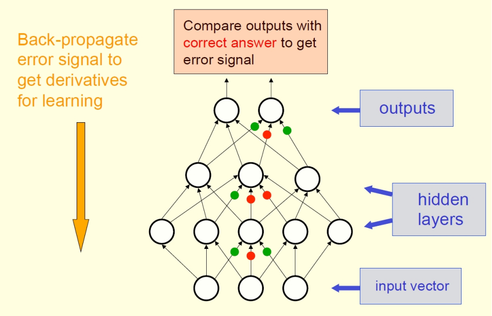


- **Feedforward Propagation**: Accept input x, pass through intermediate stages and obtain output $\hat{y}$

Backpropagation



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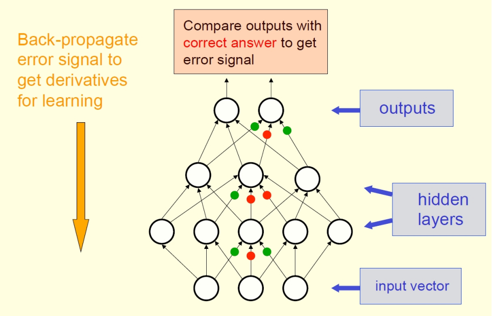

- **Feedforward Propagation**: Accept input x, pass through intermediate stages and obtain output $\hat{y}$
- **During Training**: Use $\hat{y}$ to compute a scalar cost $J(\theta)$
- Backpropagation allows information to flow backwards from cost to compute the gradient

Figure: G. E. Hinton

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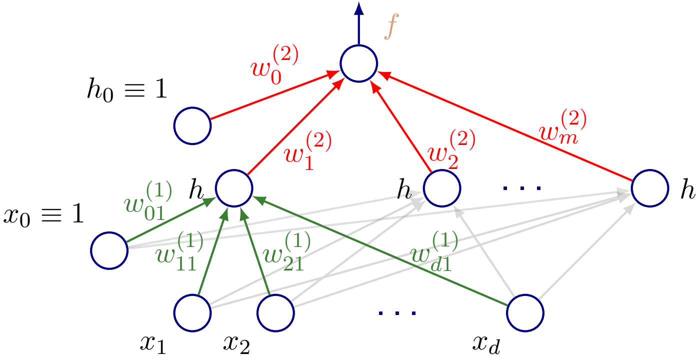
- Can compute error derivatives for hidden units efficiently (and once we have error derivatives for hidden activities, easy to get error derivatives for weights going in)

Slide: G. E. Hinton

Review: neural networks



- Feedforward operation, from input $\mathbf{x}$ to output $\hat{y}$:

$$\hat{y}(\mathbf{x};\mathbf{w}) = f\left(\sum_{j=1}^{m} w_j^{(2)} h\left(\sum_{i=1}^{d} w_{ij}^{(1)} x_i + w_{0j}^{(1)}\right) + w_0^{(2)}\right)$$

Slide adapted from TTIC 31020, Gregory Shakhnarovich

Training the network

- Error of the network on a training set:

$$L(X;\mathbf{w}) \; = \; \sum_{i=1}^{N} \frac{1}{2} \left(y_i - \hat{y}(\mathbf{x}_i;\mathbf{w})\right)^2$$

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- Generally, no closed-form solution;
  resort to gradient descent
- Need to evaluate derivative of L on a single example
- Let's start with a simple linear model $\hat{y} = \sum_j w_j x_{ij}$:

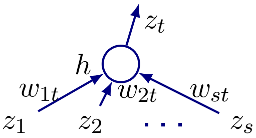
$$\frac{\partial L(\mathbf{x}_i)}{\partial w_j} \;=\; \underbrace{(\hat{y}_i - y_i)}_{\text{error}} x_{ij}.$$

Slide adapted from TTIC 31020, Gregory Shakhnarovich

Backpropagation

- General unit activation in a multilayer network:

$$z_t = h\left(\sum_j w_{jt} z_j\right)$$



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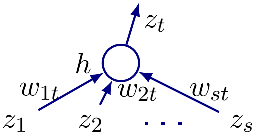

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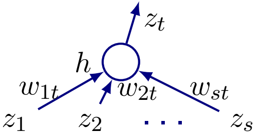

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Slide adapted from TTIC 31020, Gregory Shakhnarovich

Backpropagation

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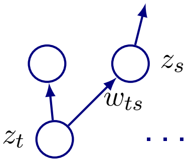
$$\delta_t = \sum_{s \in S} \frac{\partial L}{\partial a_s} \frac{\partial a_s}{\partial a_t}$$
$$= h'(a_t) \sum_{s \in S} w_{ts} \delta_s$$



$$a_s = \sum_{j : j \to s} w_{js} h(a_j)$$

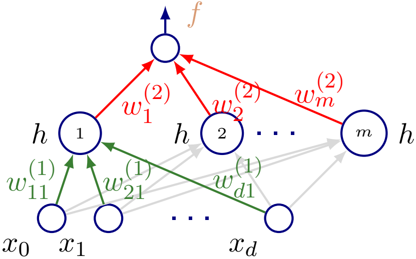
Slide adapted from TTIC 31020, Gregory Shakhnarovich

Backpropagation: example

- Output: $f(a) = a$
- Hidden:

$$h(a) = \tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}},$$

$$h'(a) = 1 - h(a)^2.$$



- Given example $\mathbf{x}$, feed-forward inputs:

$$\text{input to hidden: } a_j = \sum_{i=0}^{d} w_{ij}^{(1)} x_i,$$

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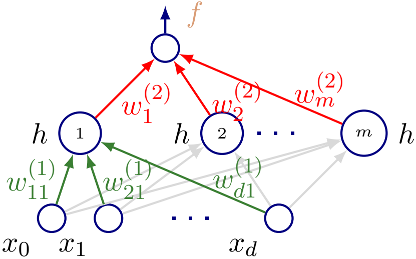

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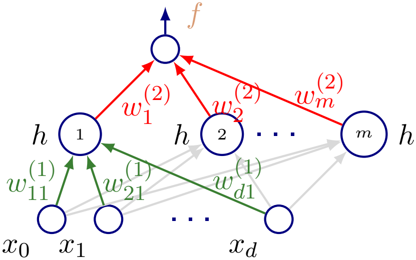
$$h(a) = \tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}},$$

$$h'(a) = 1 - h(a)^2.$$



- Given example $\mathbf{x}$, feed-forward inputs:

$$\text{input to hidden: } a_j = \sum_{i=0}^{d} w_{ij}^{(1)} x_i,$$

$$\text{hidden output: } z_j = \tanh(a_j),$$

$$\text{net output: } \hat{y} = a = \sum_{j=0}^{m} w_j^{(2)} z_j.$$

Backpropagation: example

$$a_j = \sum_{i=0}^{d} w_{ij}^{(1)} x_i, \quad z_j = \tanh(a_j), \quad \hat{y} = a = \sum_{j=0}^{m} w_j^{(2)} z_j.$$

- Error on example $\mathbf{x}$: $L = \frac{1}{2}(y - \hat{y})^2$.

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- Next, compute δs for the hidden units:

$$\delta_j = (1 - z_j)^2 w_j^{(2)} \delta$$

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- Derivatives w.r.t. weights:

$$\frac{\partial L}{\partial w_{ij}^{(1)}} = \delta_j x_i, \qquad \frac{\partial L}{\partial w_j^{(2)}} = \delta z_j.$$

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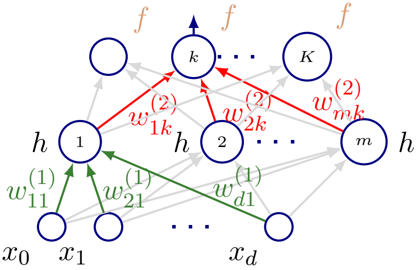
- Update weights: $w_j \leftarrow w_j - \eta \delta z_j$ and $w_{ij}^{(1)} \leftarrow w_{ij}^{(1)} - \eta \delta_j x_i$. η is called the weight decay

Multidimensional output

- Loss on example $(\mathbf{x}, \mathbf{y})$:

$$\frac{1}{2}\sum_{k=1}^{K}(y_k - \hat{y}_k)^2$$



- Now, for each output unit $\delta_k = y_k - \hat{y}_k$;
- For hidden unit j,

$$\delta_j = (1 - z_j)^2 \sum_{k=1}^{K} w_{jk}^{(2)} \delta_k.$$

Next time

- More Backpropagation

Next time

- More Backpropagation
- Start with Regularization in Neural Networks

Next time

- More Backpropagation
- Start with Regularization in Neural Networks
- Quiz