Lecture 12-13: Basic Neural Nets
Deep Feedforward Networks

CS 109B, STAT 121B, AC 209B, CSE 109B

Mark Glickman and Pavlos Protopapas

- http://video.arstechnica.com/watch/sunspring-sci-fi-short-film

Today’s news

An AI just beat top lawyers at their own game

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IMAGE: BOB AL-GREEN/MASHABLE

BY MONICA CHIN

FEB 2018

The nation's top lawyers recently battled artificial intelligence in a competition to interpret contracts — and they lost.

A new study, conducted by legal AI platform [LawGeex] in consultati Share Quote ssors from Stanford University, Duke University School of Law, and University of Southern California, pitted twenty experienced lawyers against an AI trained to evaluate legal contracts.

Competitors were given four hours to review five non-disclosure agreements (NDAs) and identify 30 legal issues, including arbitration, confidentiality of relationship, and indemnification. They were scored by how accurately they identified each issue.

SEE ALSO: Google's new AI can predict heart disease by simply scanning your eyes

Google's new AI can predict heart disease by simply scanning your eyes

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IMAGE: BEN BRAIN/DIGITAL CAMERA MAGAZINE VIA GETTY IMAGES

BY MONICA CHIN

FEB 2018

The secret to identifying certain health conditions may be hidden in our eyes.

Researchers from Google and its health-tech subsidiary Verily announced on Monday that they have successfully created algorithms to predict whether someone has high blood pressure or is at risk of a heart attack or stroke simply by scanning a person's eyes, the *Washington Post* reports.

SEE ALSO: This fork helps you stay healthy

Google's researchers trained the algorithm with images of scanned retinas from more than 280,000 patients. By reviewing this massive database, Google's algorithm trained itself to recognize the patterns that designated people as at-risk.

This algorithm's success is a sign of exciting developments in healthcare on the horizon. As Google fine-tunes the technology, it could one day

AlphaZero (2017)

DeepMind

AlphaZero AI beats champion chess program after teaching itself in four hours

Google's artificial intelligence sibling DeepMind repurposes Go-playing AI to conquer chess and shogi without aid of human knowledge

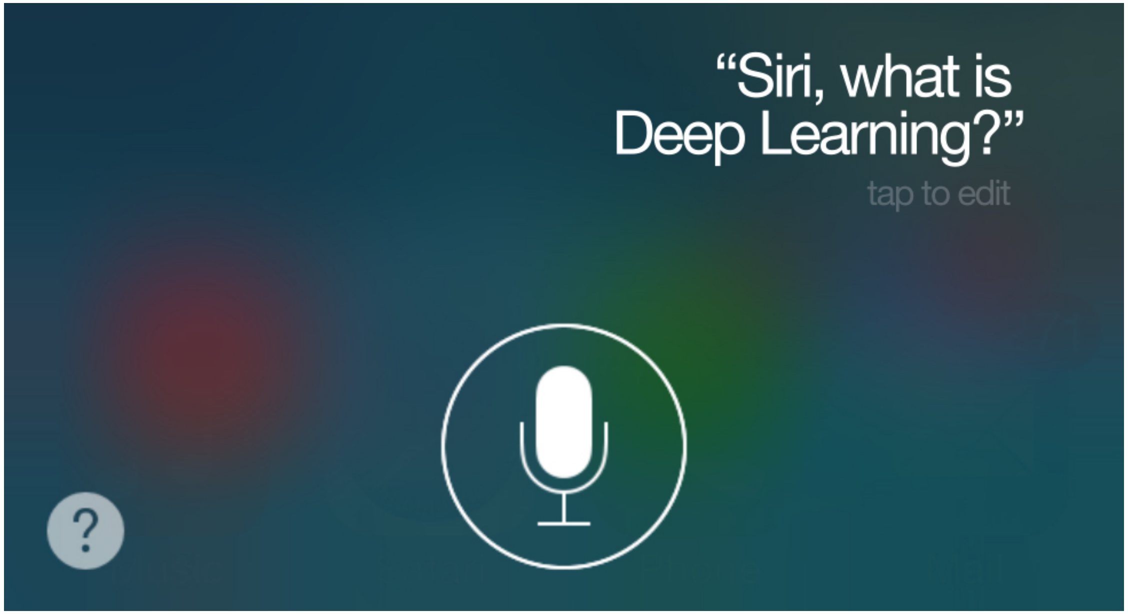
theguardian.com

AlphaGo (2015)

First program to beat a professional Go player

iOS Speech Synthesis (2016-)

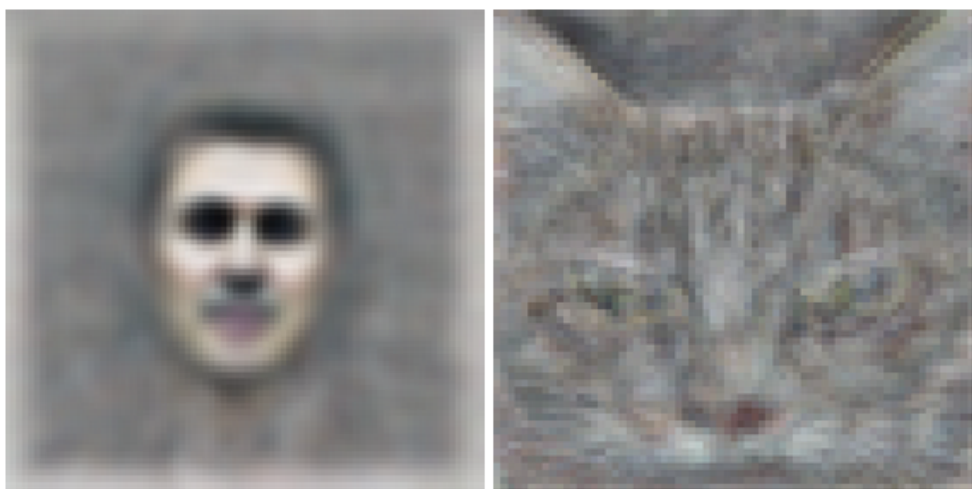
Trained from 20 hours of high quality speech



machinelearning.apple.com

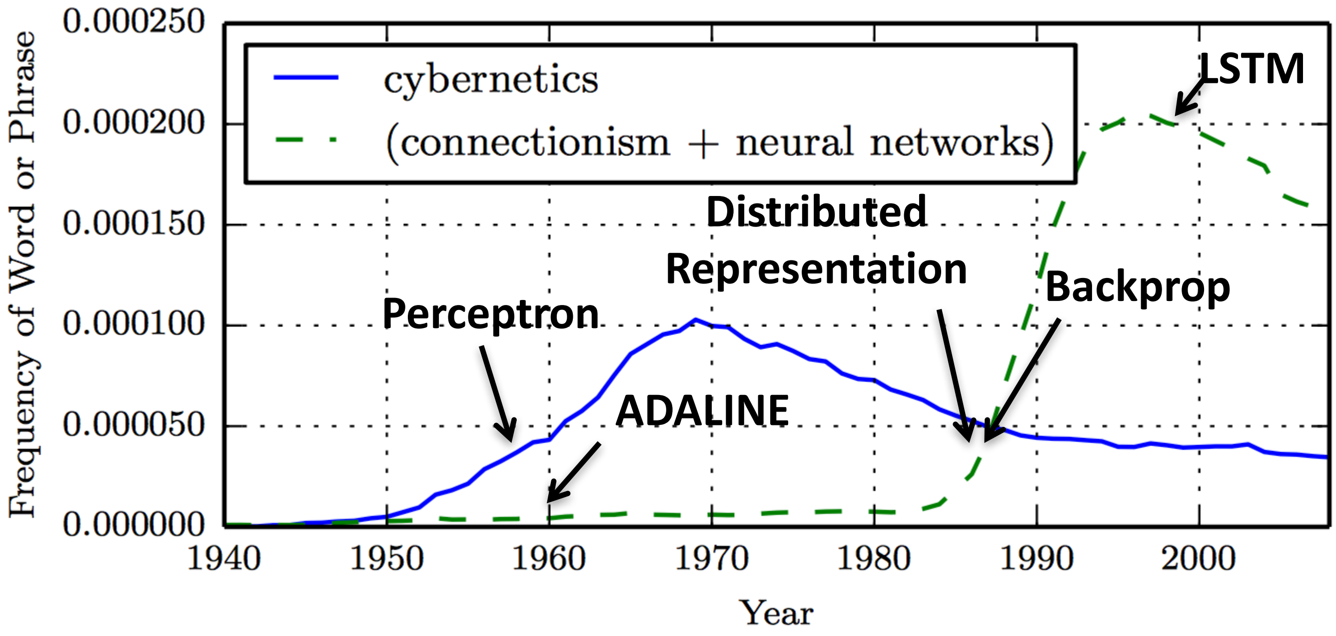
Google Brain (2012)

- Differentiate between human face and cat
  - Neural network with 1 billion connections
  - 10 million 200x200 pixel images from YouTube



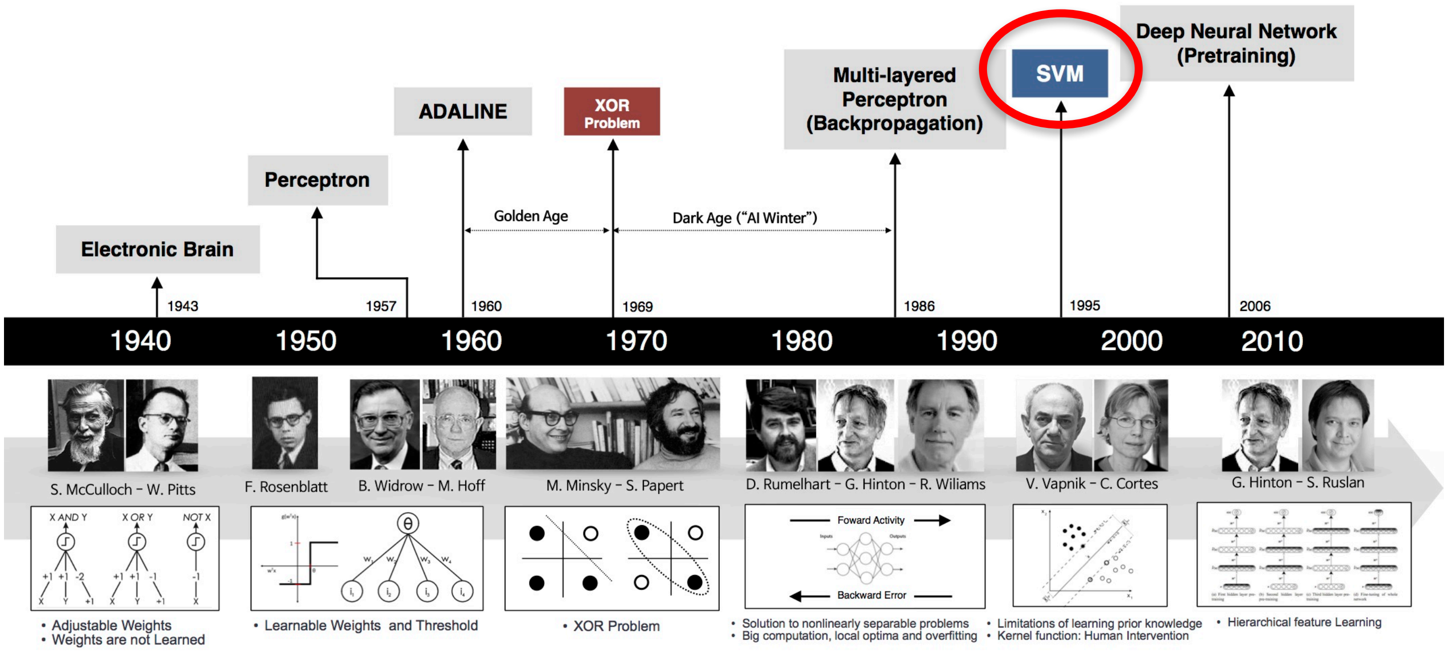
Le et al., ICML 2012

Historical Trends



(Goodfellow 2016)

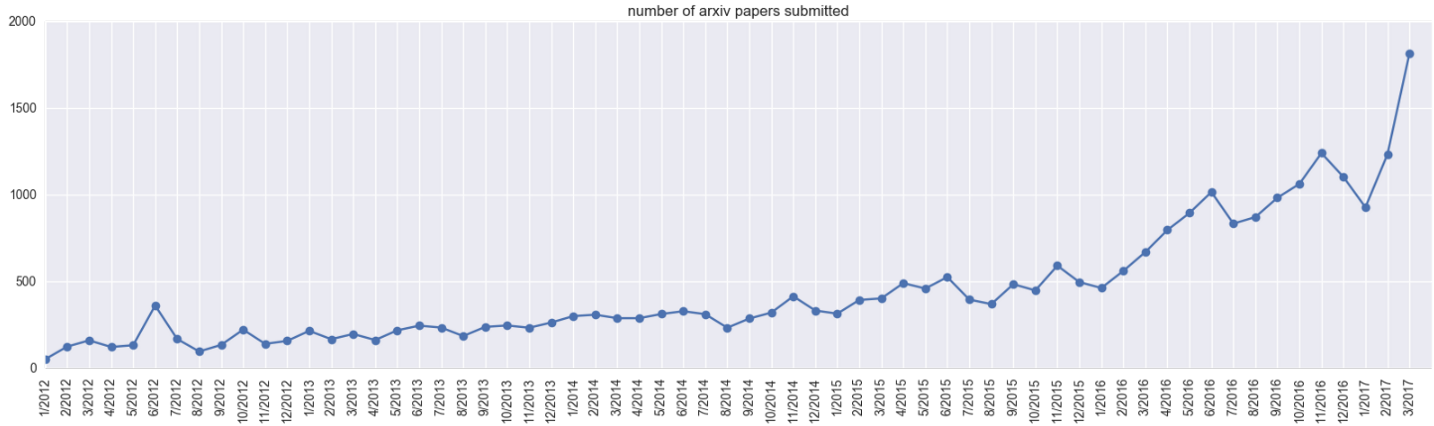
Historical Trends



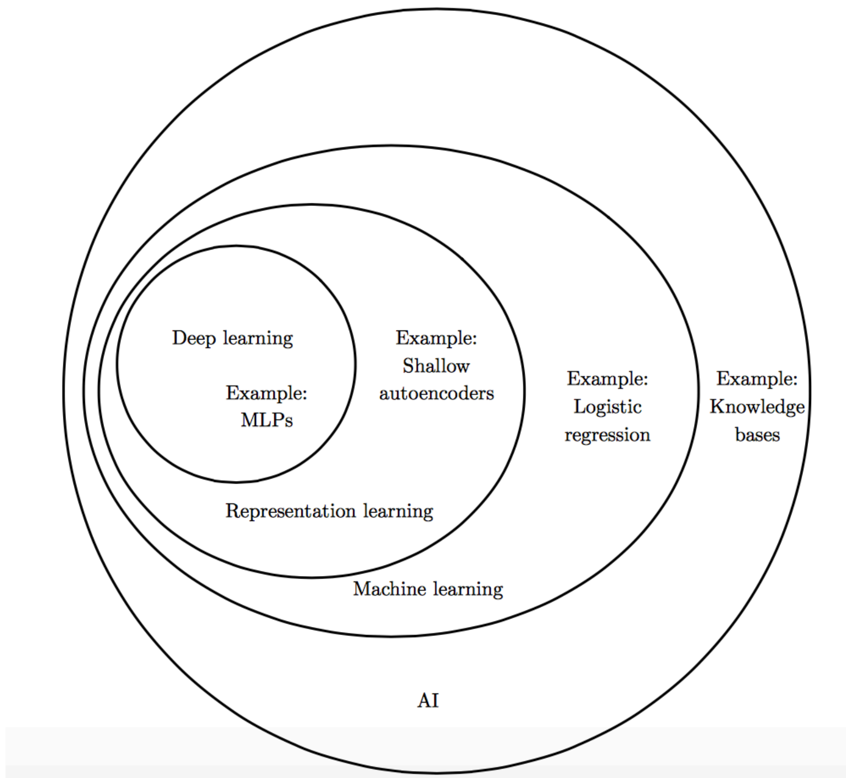
beamandrew.github.io/

Historical Trends

ArXiv papers on deep learning: 2012-2017

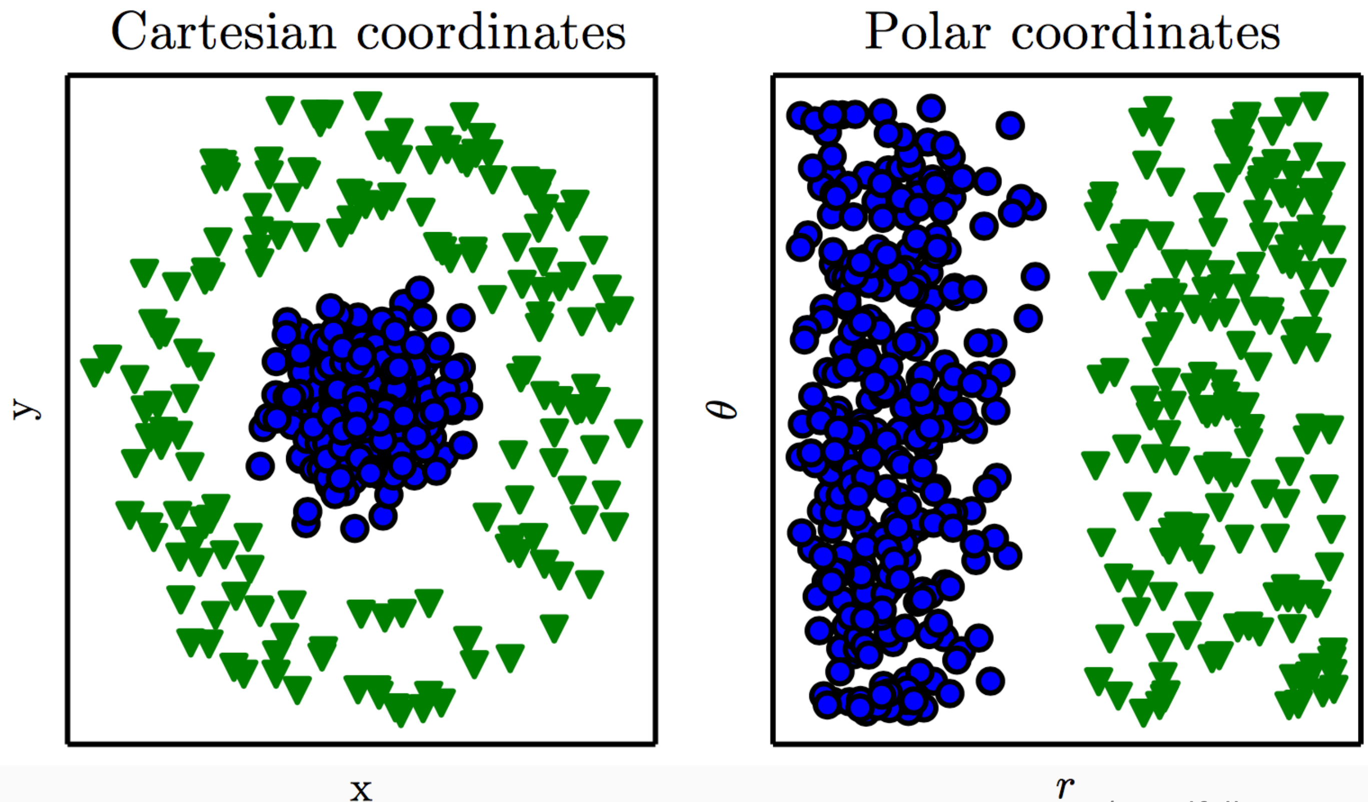


Deep Learning vs Classical ML



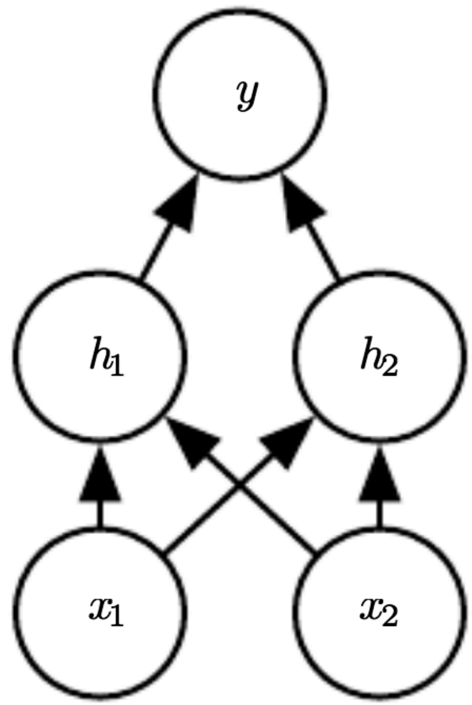
(Goodfellow 2016)

Representation Matters

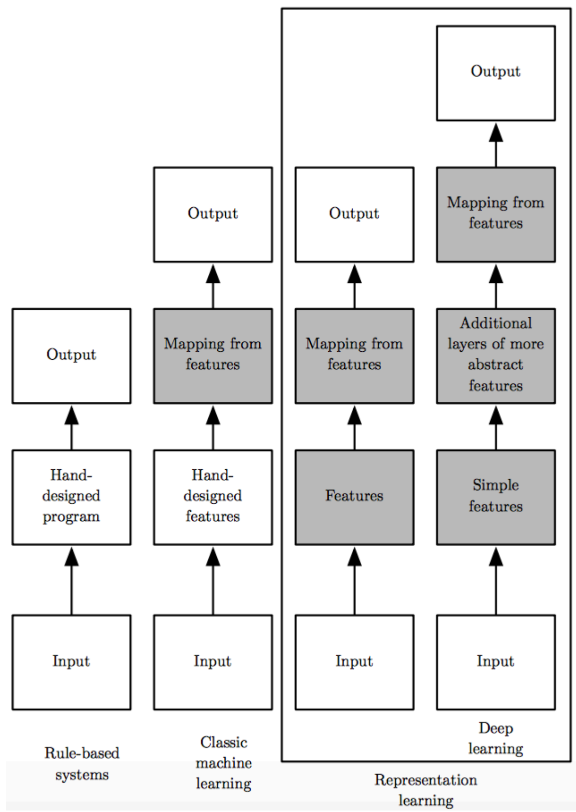


(Goodfellow 2016)

Neural Network

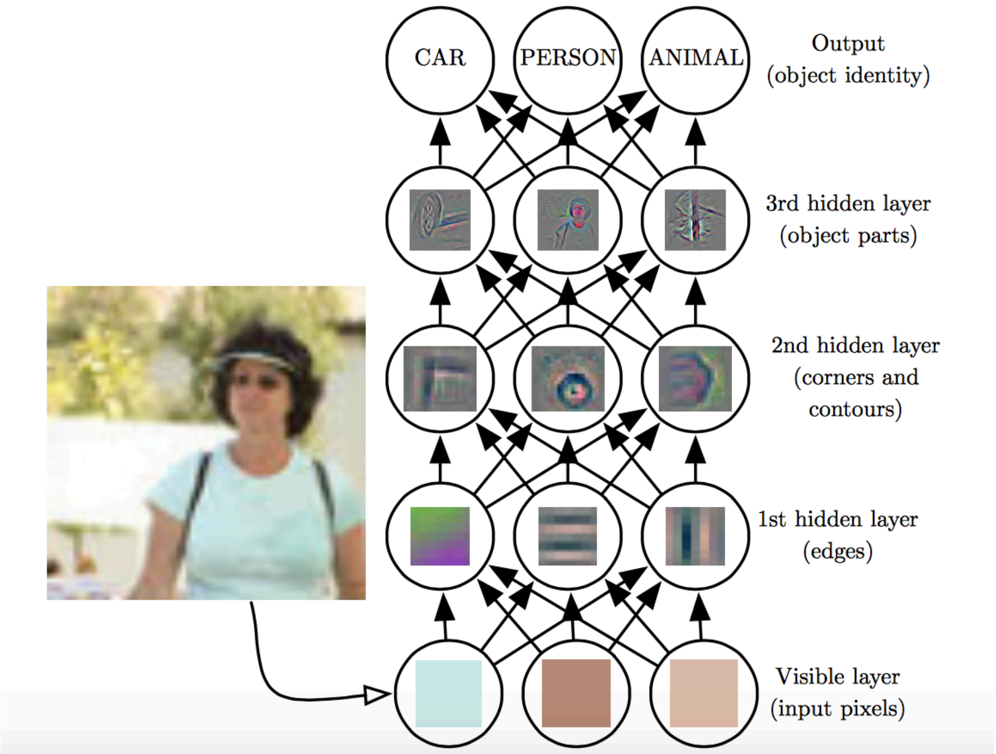


Learning Multiple Components



(Goodfellow 2016)

Depth = Repeated Compositions



(Goodfellow 2016)

Beyond Linear Models

- Linear models
  - Can be fit efficiently (via convex optimization)
  - Limited model capacity
- Alternative:

$$f(x) = w^T \phi(x)$$

where ϕ is a *non-linear transform*

Traditional ML

- Manually engineer ϕ
  - Domain specific, enormous human effort
- Generic transform
  - Maps to a higher-dimensional space
  - Kernel methods: e.g. RBF kernels
  - Over fitting: does not generalize well to test set
  - Cannot encode enough prior information

Deep Learning

- Directly learn ϕ

$$f(x;\theta) = w^T \phi(x;\theta)$$

  where θ are parameters of the transform

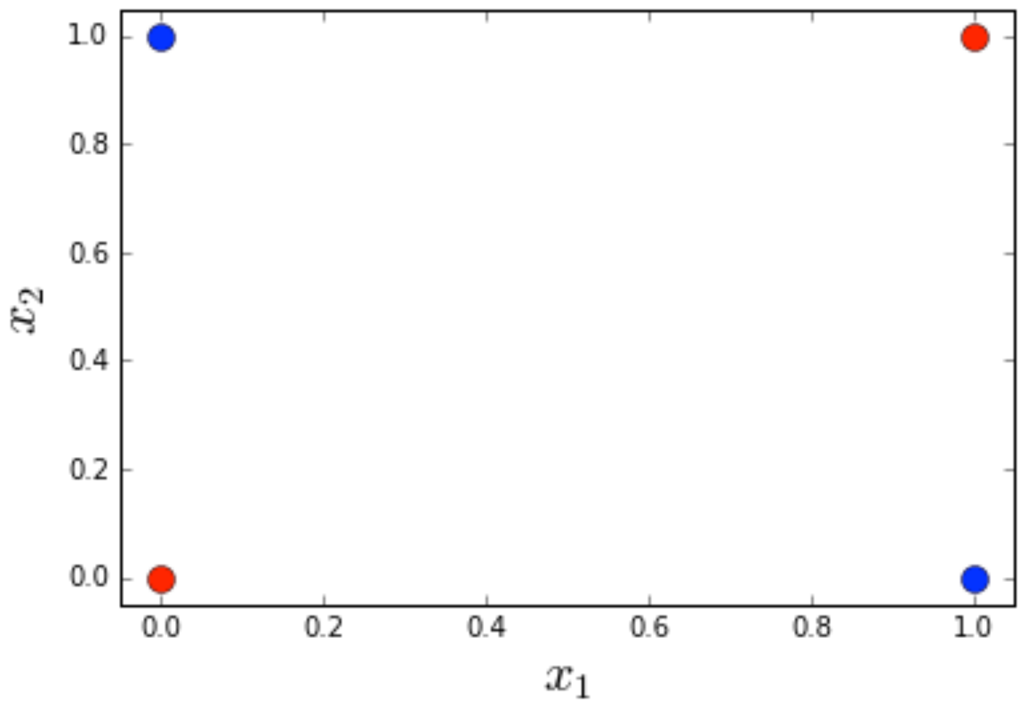
- ϕ defines hidden layers
- Non-convex optimization
- Can encode prior beliefs, generalizes well

SVM vs Neural Networks

- Hand-written digit recognition: MNIST data

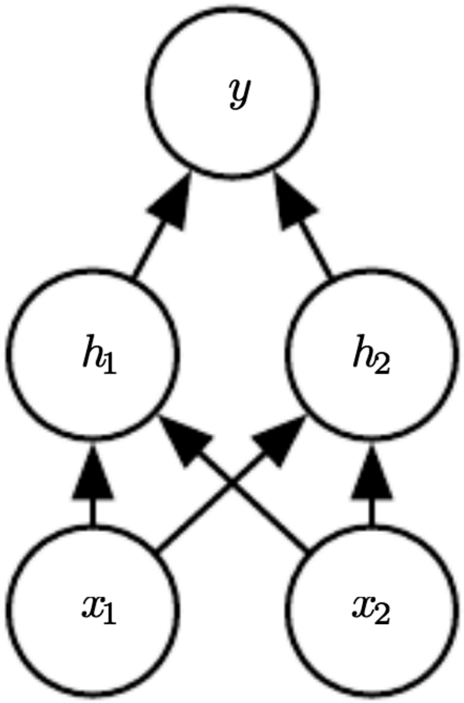
See illustration in notebook

Example: Learning XOR



- Optimal linear model (sq. loss)
  - Predicts 0.5 on all points

Example: Learning XOR



$$h_1 = \sigma(w_1^T x + c_1)$$

$$h_2 = \sigma(w_2^T x + c_2)$$

$$y = \quad (w^T h + b)$$

where,

$$\sigma(z) = \max\{0, z\}$$

See illustration in notebook

Design Choices

- Cost function
- Output units
- Hidden units
- Architecture
- Optimizer

Cost Function

- Cross-entropy between training data and model distribution (i.e. negative log-likelihood)

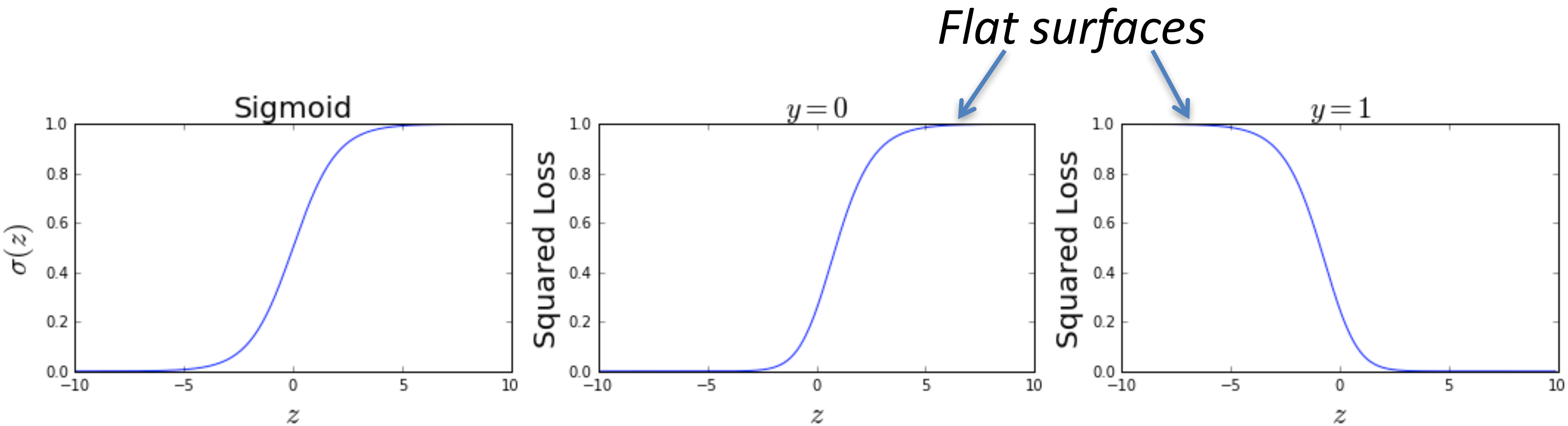
$$J(\boldsymbol{\theta}) = -\mathbb{E}_{\mathbf{x},\mathbf{y}\sim\hat{p}_{\text{data}}} \log p_{\text{model}}(\boldsymbol{y} \mid \boldsymbol{x})$$

- Do not need to design separate cost functions
- Gradient of cost function must be large enough

Cost Function

- Example: sigmoid output + squared loss

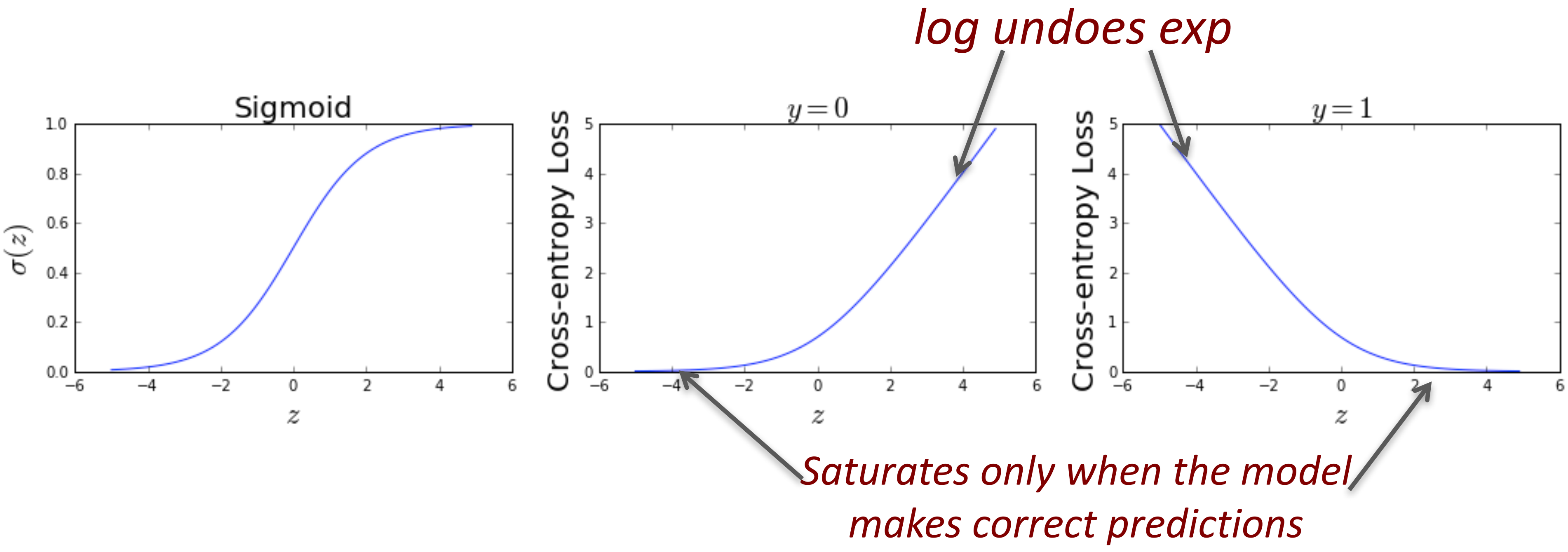
$$\sigma(z) = \frac{1}{1+e^{-z}} \qquad L_{sq}(y,z) = (y - \sigma(z))^2$$



Cost Function

- Example: sigmoid output + cross-entropy loss

$$L_{ce}(y,z) = -(y\log(z) + (1-y)\log(1-z))$$



Design Choices

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Output Units

Output Type	Output Distribution	Output Layer	Cost Function
Binary	Bernoulli	Sigmoid	Binary cross-entropy
Discrete	Multinoulli	Softmax	Discrete cross-entropy
Continuous	Gaussian	Linear	Gaussian cross-entropy (MSE)
Continuous	Mixture of Gaussian	Mixture Density	Cross-entropy
Continuous	Arbitrary	See part III: GAN, VAE, FVBN	Various

(Goodfellow 2017)

Softmax Output

- Discrete / Multinoulli output distribution
- For output scores $z_1, \ldots, z_n$

$$\text{softmax}(z)_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

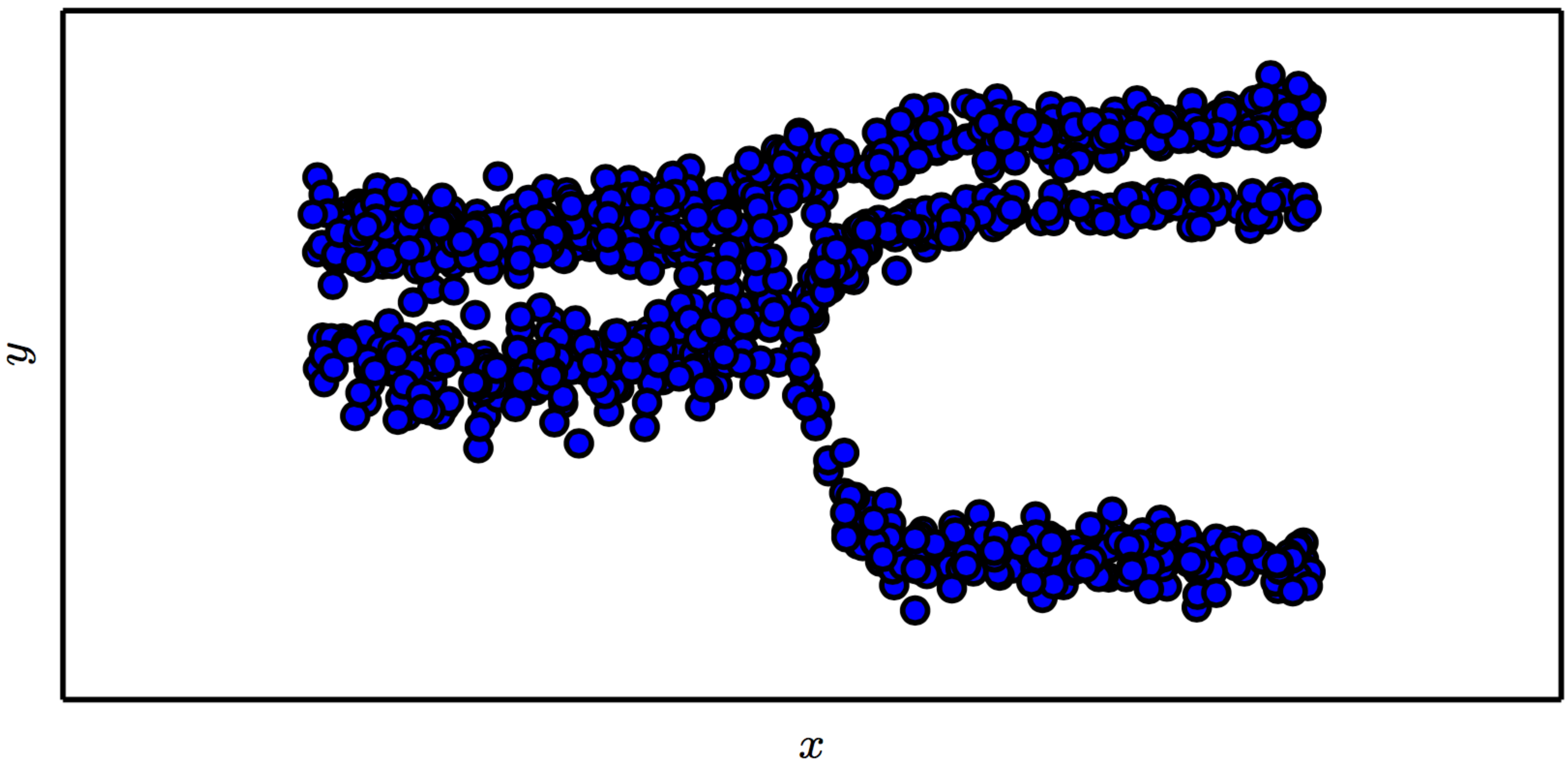
- Log-likelihood undoes exp

$$\log \text{softmax}(z)_i = z_i - \log \sum_j \exp(z_j)$$

$$\approx z_i - \max_j z_j$$

(Score to target label – Maximum score)

Mixture Density Output



(Goodfellow 2017)

Design Choices

- Cost function
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- Hidden units
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Hidden Units

$$\mathbf{h} = g(\mathbf{W}^T x + \mathbf{b})$$

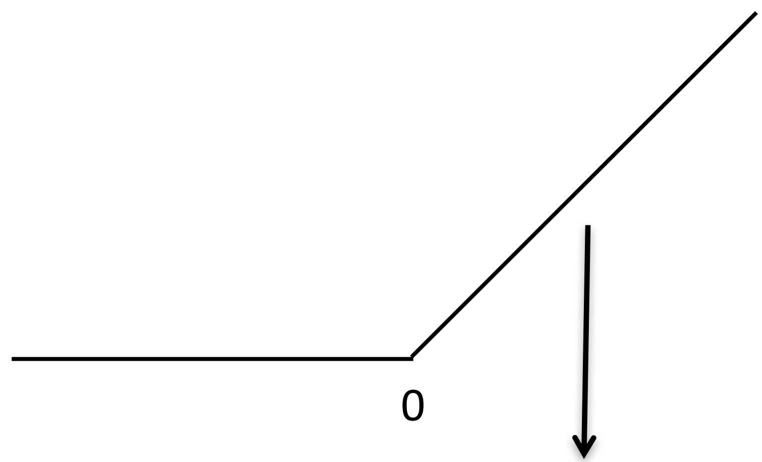
with activation function g

- Ensure gradients remain large through hidden unit
- Preferred: piece-wise linear activation
- Avoid sigmoid/tanh activation
  - Do not provide useful gradient info when they saturate

ReLU

- Rectified Linear Units

$$g(z) = \max\{0, z\}$$



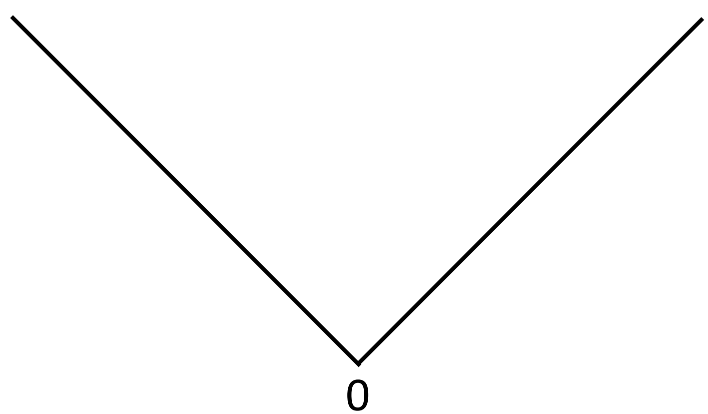
- Gradient is 1 whenever unit is active
  - More useful for learning compared to sigmoid
  - No useful gradient information when z<0

Generalized ReLU

- Generalization: For $\alpha_i > 0$,

$$g(z;\alpha)_i = \max\{0, z_i\} + \alpha_i \min\{0, z_i\}$$

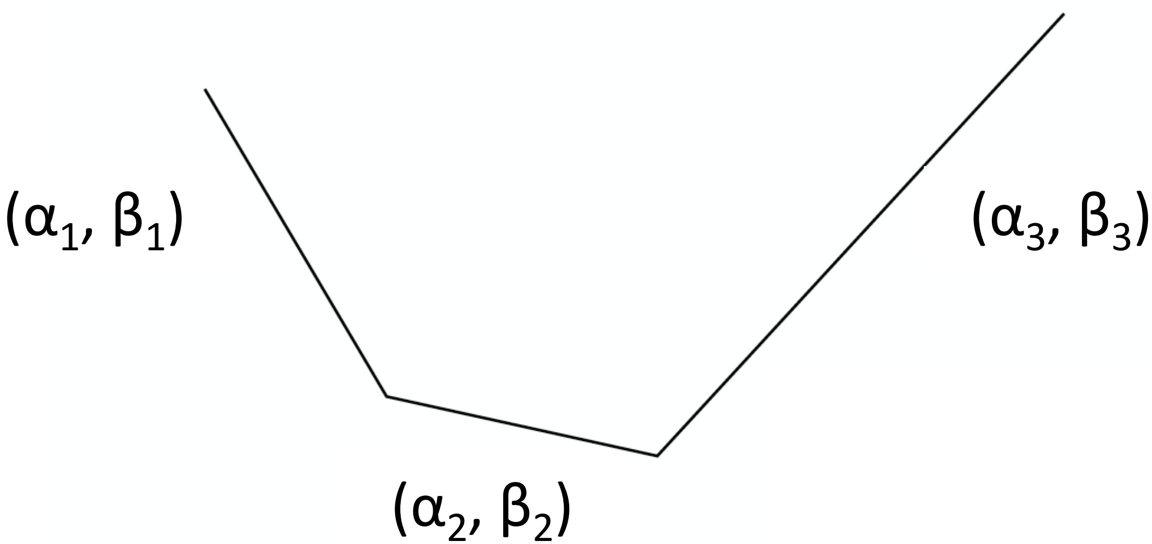
- E.g. Absolute value ReLU: $\alpha_i = -1 \Rightarrow g(z) = |z|$



Maxout

- Directly learn the activation function
  - Max of k linear functions

$$g(z) = \max_{i \in \{1,\ldots,k\}} \alpha_i z_i + \beta_i$$



Design Choices

- Cost function
- Output units
- Hidden units
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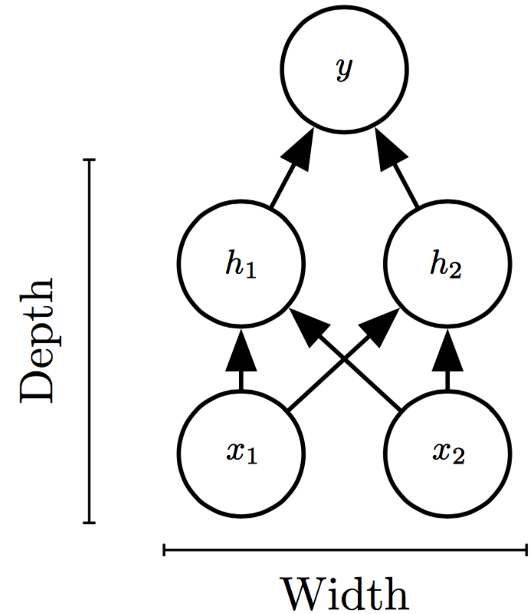
Universal Approximation Theorem

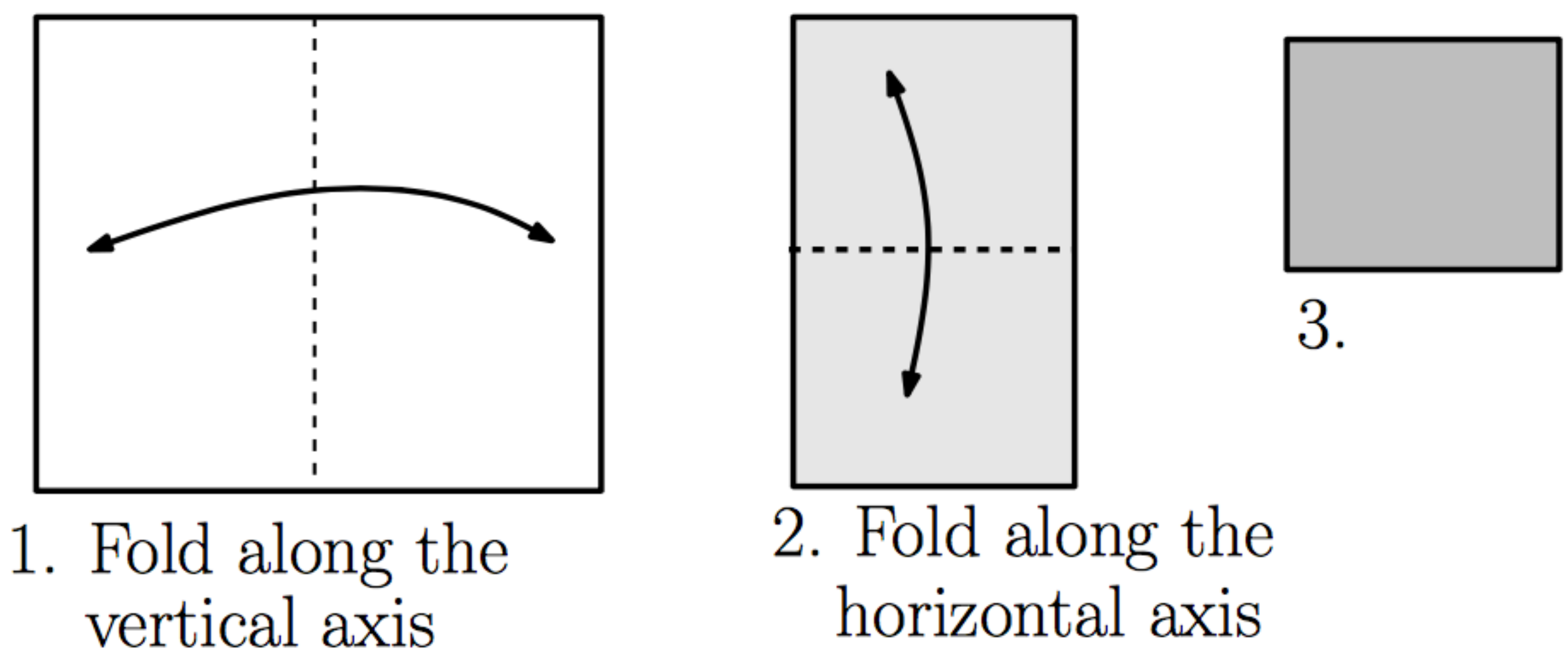
- One hidden layer is enough to *represent* an approximation of any function to an arbitrary degree of accuracy
- So why deeper?
  - Shallow net may need (exponentially) more width
  - Shallow net may overfit more



Exponential Gain with Depth

- Each hidden layer folds the space of activations of the previous layer. E.g. abs activation $g(z) = |z|$

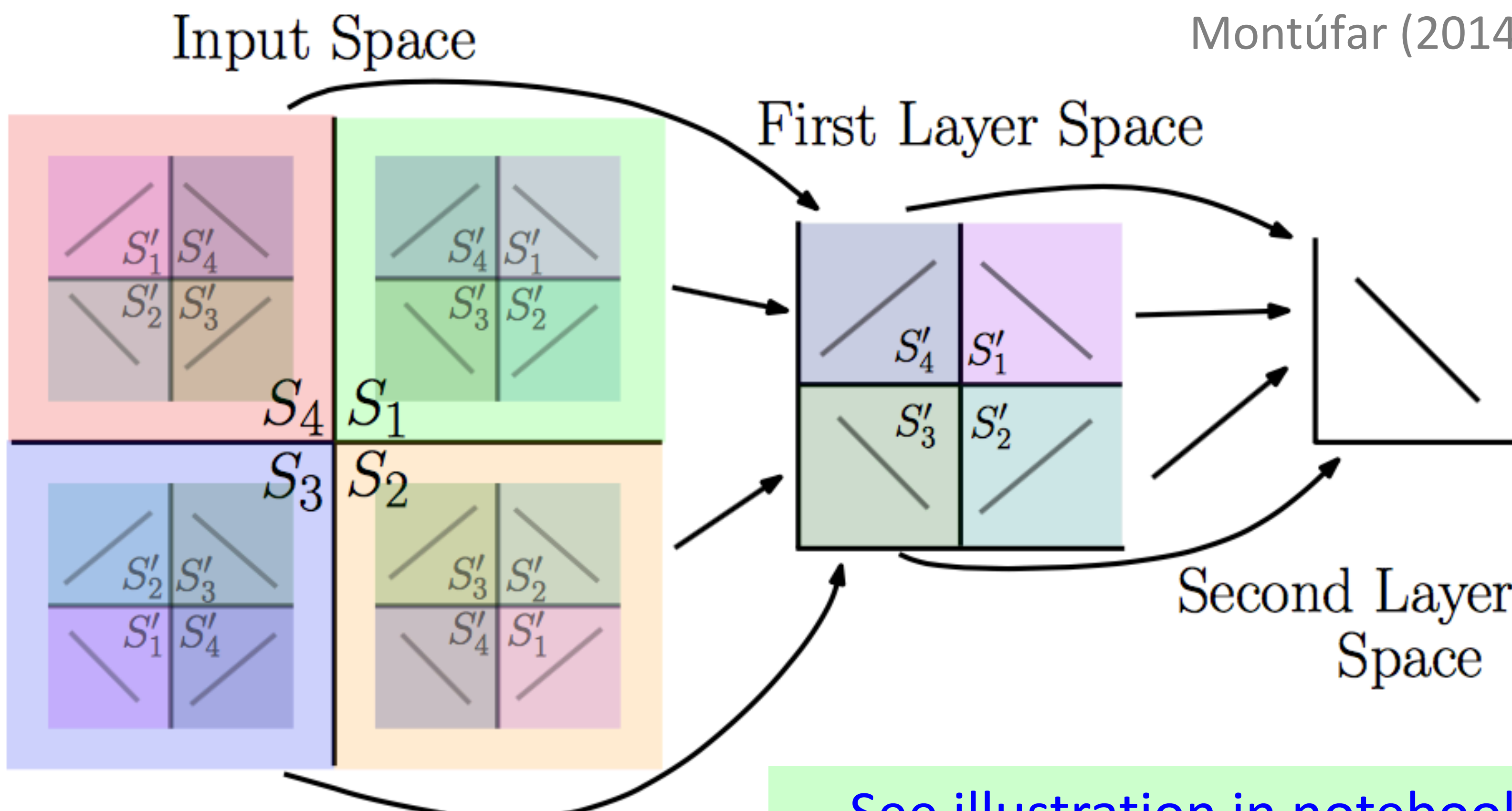
Montúfar (2014)



Exponential Gain with Depth

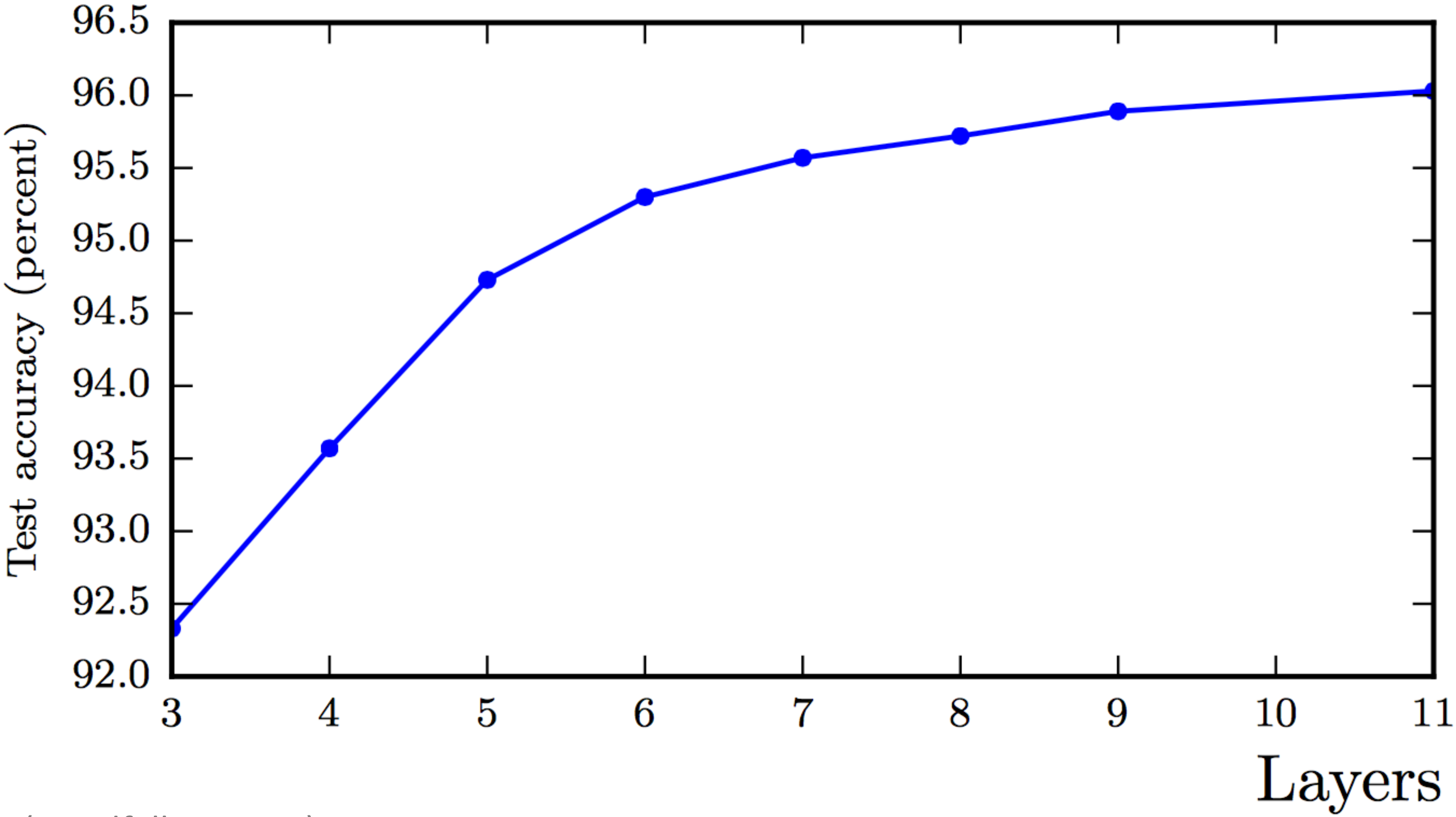
- With *N* hidden layers, there are $O(4^N)$ piecewise linear regions

Montúfar (2014)



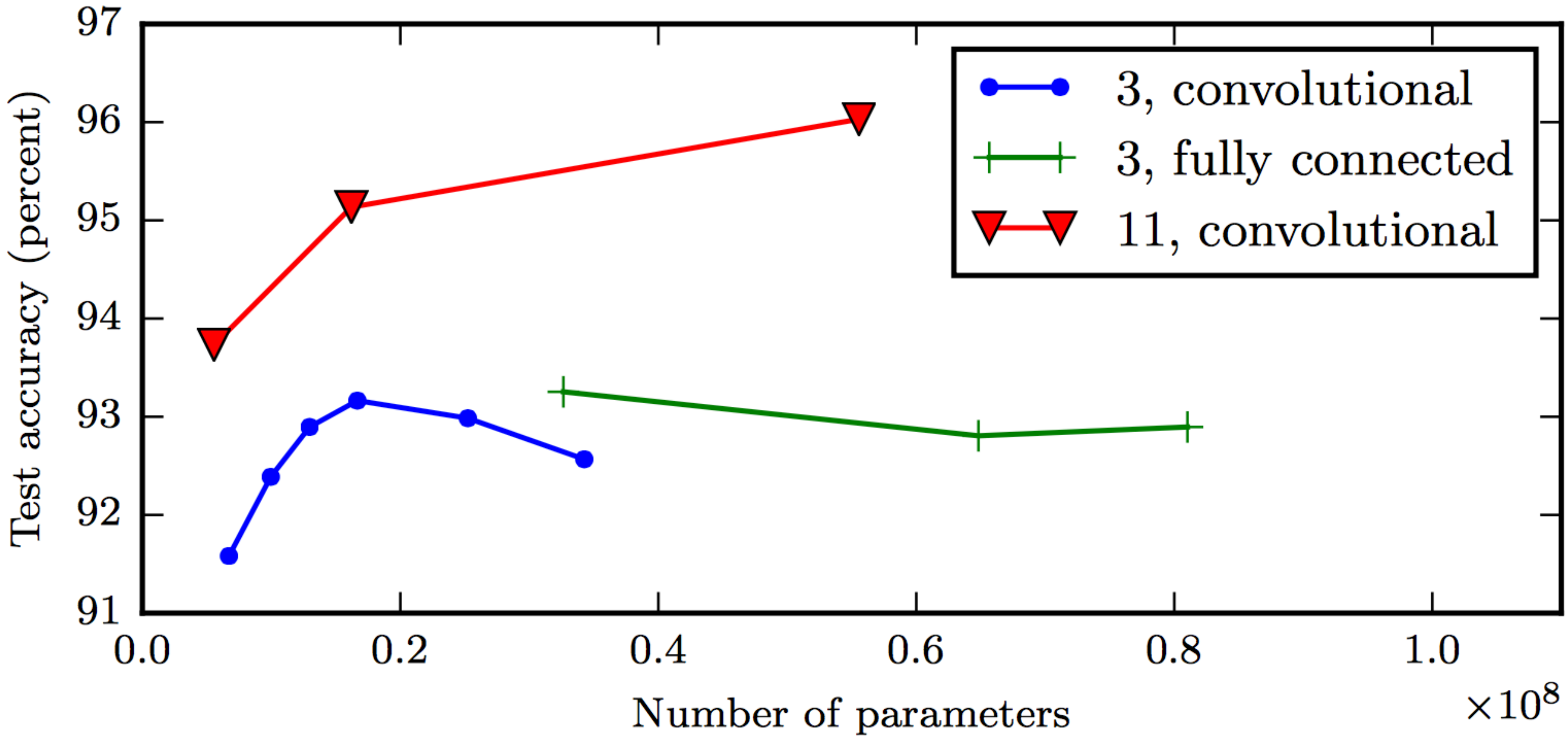
See illustration in notebook

Better Generalization with Depth



(Goodfellow 2017)

Large, Shallow Nets Overfit More



(Goodfellow 2017)

Design Choices

- Cost function
- Output units
- Hidden units
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- Optimizer

Gradient-based Optimizer

(e.g. stochastic gradient descent)

- "Chain rule" for computing gradients:

$$\mathbf{y} = g(\mathbf{x}) \qquad z = f(\mathbf{y})$$

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$$

- For deeper networks

Naïve computation takes exponential time

$$\frac{\partial z}{\partial x_i} = \sum_{j_1} \cdots \sum_{j_m} \frac{\partial z}{\partial y_{j_1}} \cdots \frac{\partial y_{j_m}}{\partial x_i}$$

Backpropagation

- Avoids repeated sub-expressions
- Uses dynamic programming (table filling)
- Trades-off memory for speed

Backprop: Arithmetic

- Jacobian-gradient products

$$\mathbf{z} = g(\mathbf{x})$$

$$y = f(\mathbf{z})$$

$$\begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \vdots \\ \frac{\partial y}{\partial x_m} \end{bmatrix} = \begin{bmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_m}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial z_1}{\partial x_n} & \cdots & \frac{\partial z_m}{\partial x_n} \end{bmatrix} \times \begin{bmatrix} \frac{\partial y}{\partial z_1} \\ \vdots \\ \frac{\partial y}{\partial z_m} \end{bmatrix}$$

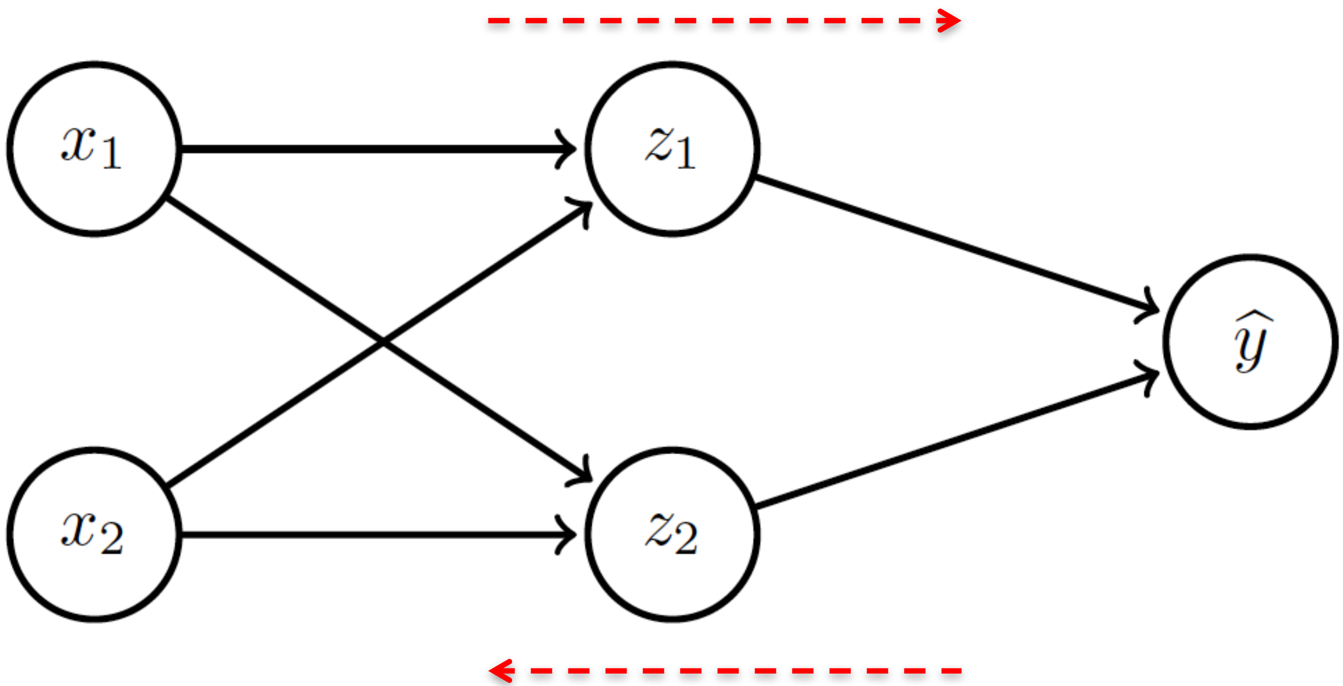
grad w.r.t. **x** | Jacobian of 'g' | grad w.r.t. **z**

$$\nabla_{\mathbf{x}} y = \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right)^T \nabla_{\mathbf{z}} y$$

Apply recursively!

Backprop: Overview

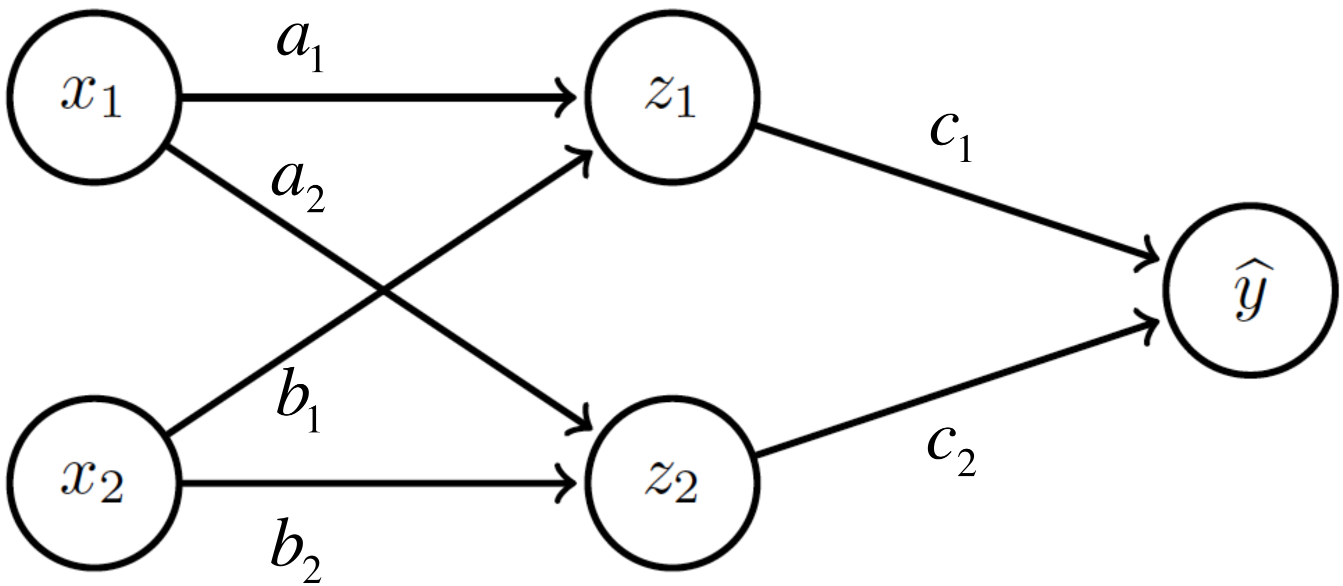
Forward prop: compute activations



Compute loss

Back-prop: compute derivatives

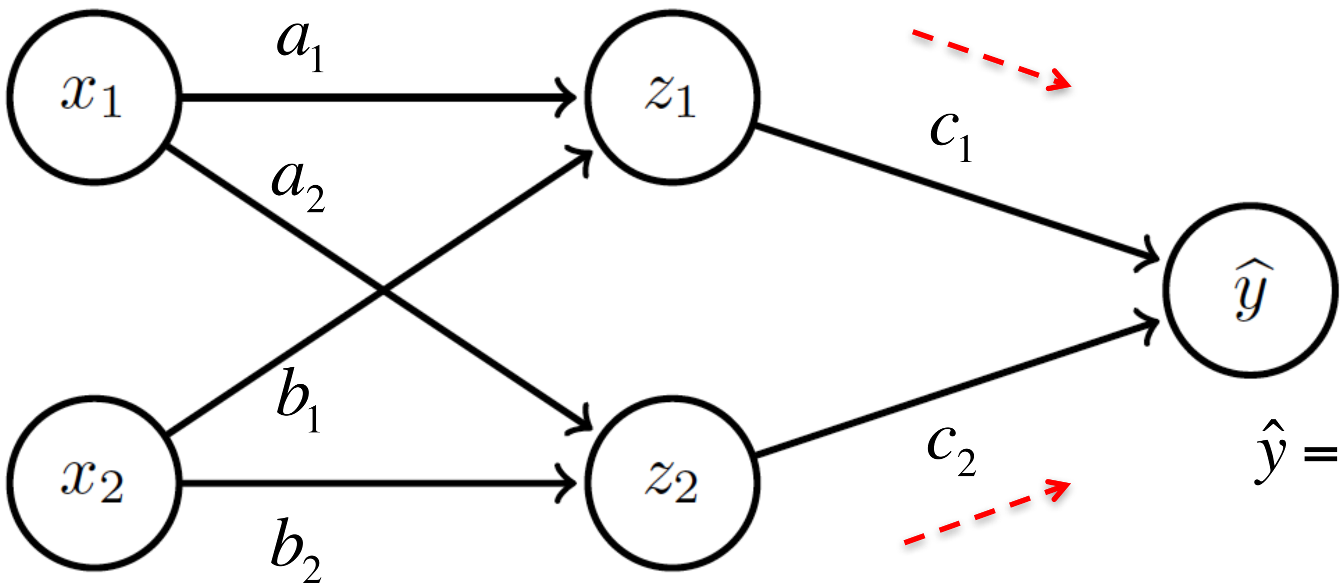
Backprop: Example



Linear activation functions
No bias
Squared loss

Backprop: Example

$$z_1 = a_1 x_1 + a_2 x_2$$

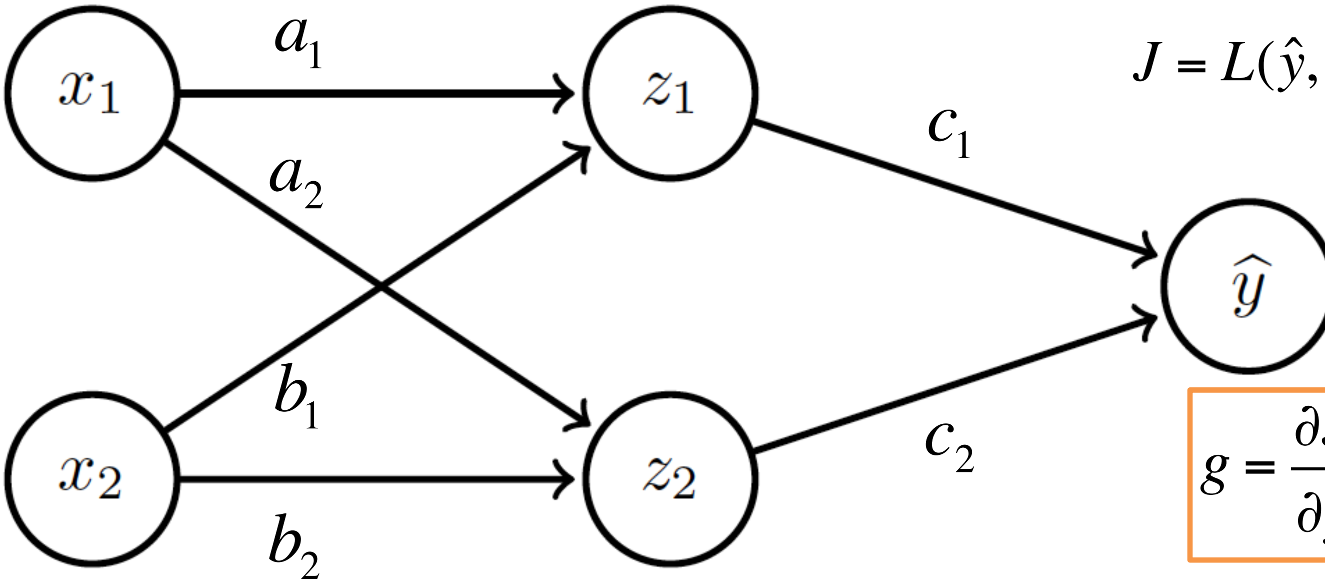


$$\hat{y} = c_1 z_1 + c_2 z_2$$

$$z_2 = b_1 x_1 + b_2 x_2$$

Forward prop: Propagate activations to output layer

Backprop: Example



$J = L(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$

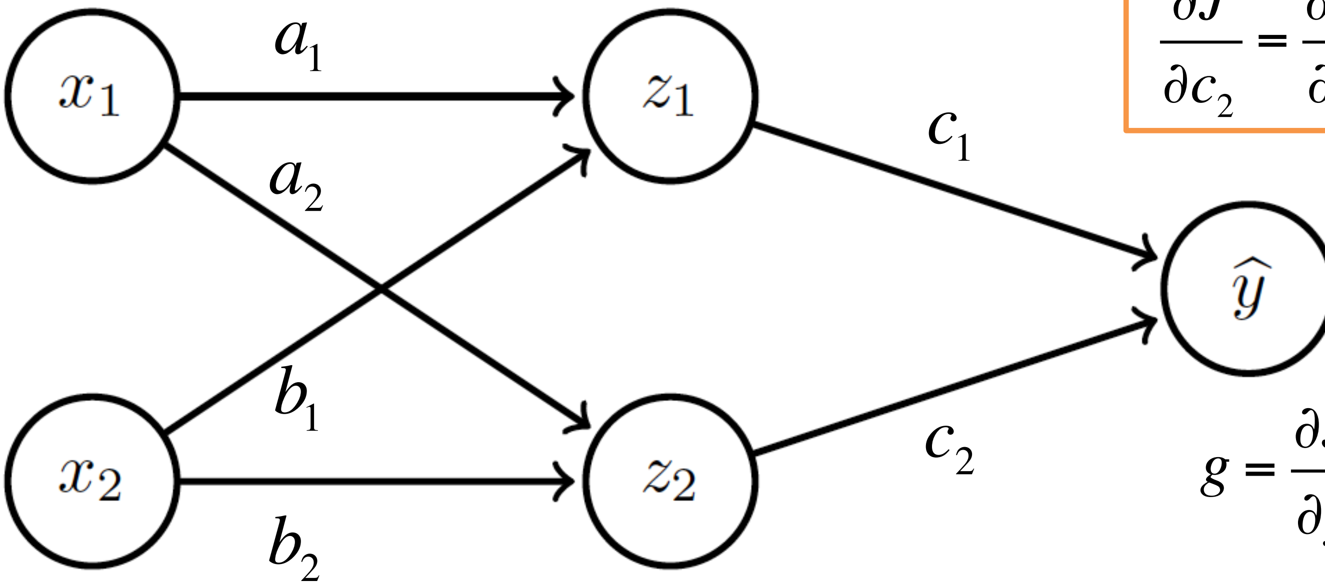
$$g = \frac{\partial J}{\partial \hat{y}} = \hat{y} - y$$

Backward prop: Compute loss and its derivative

Backprop: Example

$$\frac{\partial J}{\partial c_1} = \frac{\partial J}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial c_1}$$

$$\frac{\partial J}{\partial c_2} = \frac{\partial J}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial c_2}$$



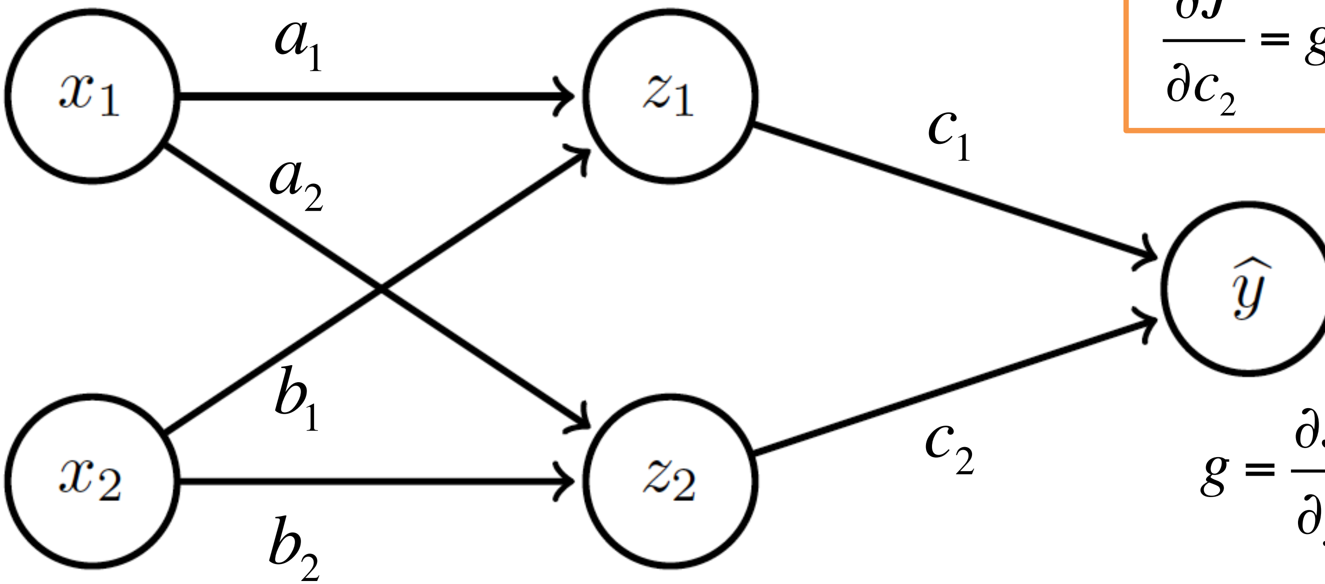
$$g = \frac{\partial J}{\partial \hat{y}} = \hat{y} - y$$

Backward prop: Compute derivatives w.r.t. weights c_1 and c_2

Backprop: Example

$$\frac{\partial J}{\partial c_1} = g \cdot z_1$$

$$\frac{\partial J}{\partial c_2} = g \cdot z_2$$

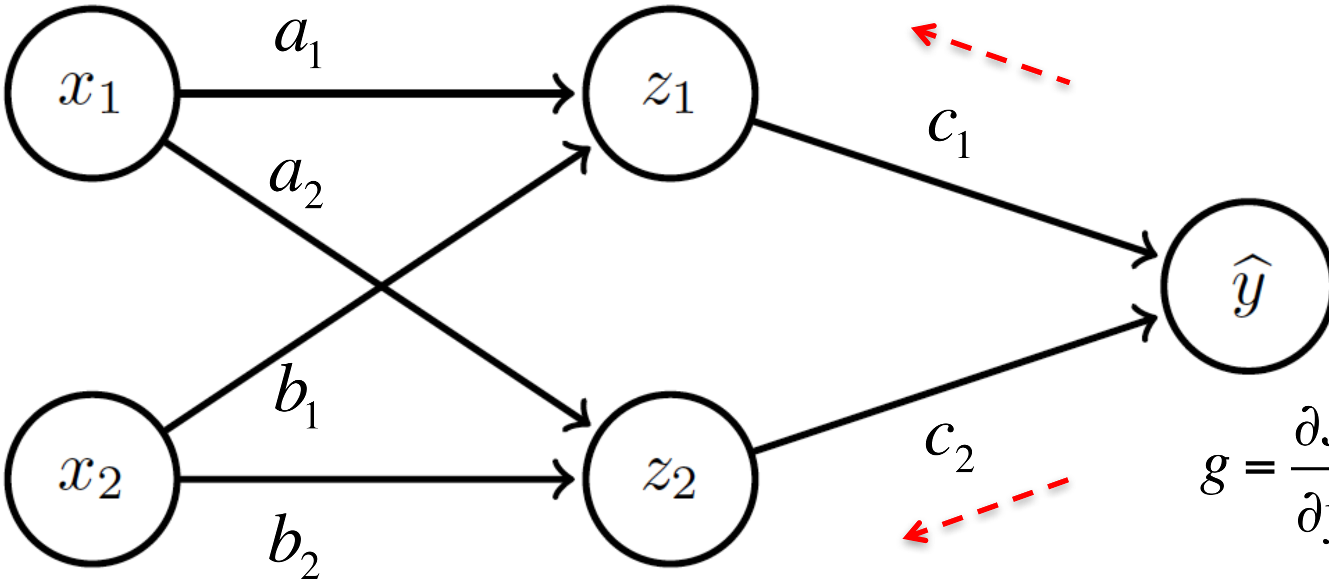


$$g = \frac{\partial J}{\partial \hat{y}} = \hat{y} - y$$

Backward prop: Compute derivatives w.r.t. weights c_1 and c_2

Backprop: Example

$$g_1' = \frac{\partial J}{\partial z_1} = g c_1$$



$$g = \frac{\partial J}{\partial \hat{y}} = \hat{y} - y$$

$$g_2' = \frac{\partial J}{\partial z_2} = g c_2$$

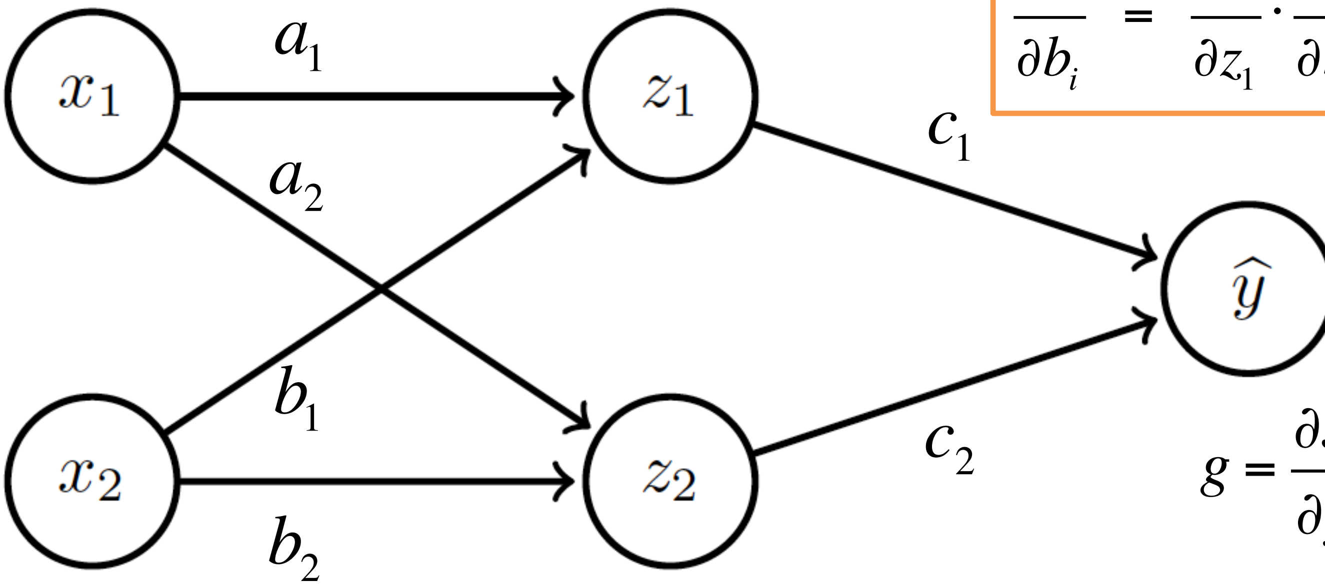
Backward prop: Propagate derivative to hidden layer

Backprop: Example

$$\frac{\partial J}{\partial a_i} = \frac{\partial J}{\partial z_1} \cdot \frac{\partial z_1}{\partial a_i} + \frac{\partial J}{\partial z_2} \cdot \frac{\partial z_2}{\partial a_i}$$

$$\frac{\partial J}{\partial b_i} = \frac{\partial J}{\partial z_1} \cdot \frac{\partial z_1}{\partial b_i} + \frac{\partial J}{\partial z_2} \cdot \frac{\partial z_2}{\partial b_i}$$

$$g_1' = \frac{\partial J}{\partial z_1} = g c_1$$



$$g = \frac{\partial J}{\partial \hat{y}} = \hat{y} - y$$

$$g_2' = \frac{\partial J}{\partial z_2} = g c_2$$

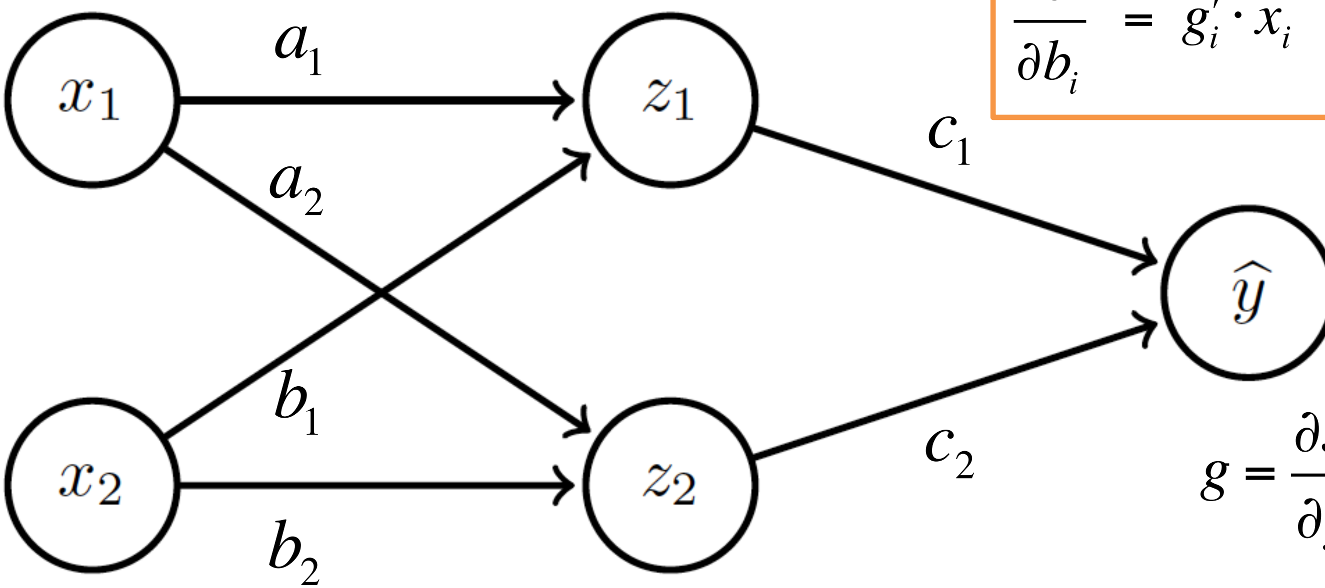
Backward prop: Compute derivatives w.r.t. weights a_1, a_2, b_1 and b_2

Backprop: Example

$$\frac{\partial J}{\partial a_i} = g_i' \cdot x_i$$

$$\frac{\partial J}{\partial b_i} = g_i' \cdot x_i$$

$$g_1' = \frac{\partial J}{\partial z_1} = g c_1$$



$$g = \frac{\partial J}{\partial \hat{y}} = \hat{y} - y$$

$$g_2' = \frac{\partial J}{\partial z_2} = g c_2$$

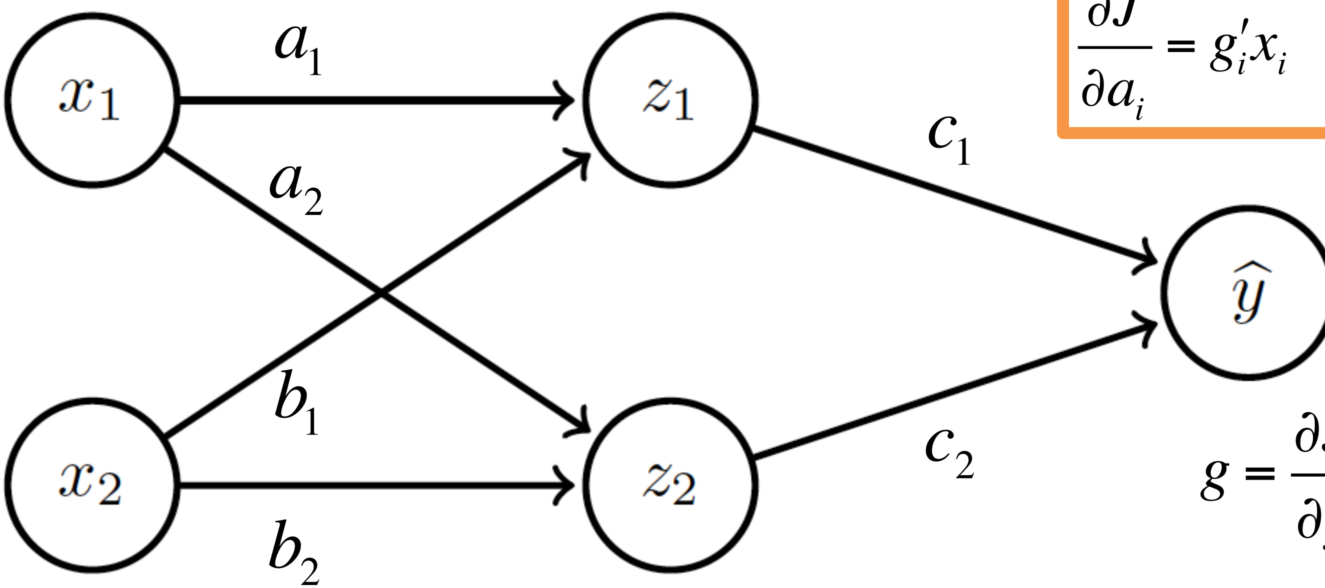
Backward prop: Compute derivatives w.r.t. weights a_1, a_2, b_1 and b_2

Backprop: Example

$$\frac{\partial J}{\partial c_1} = g z_1 \qquad \frac{\partial J}{\partial c_2} = g z_2$$

$$\frac{\partial J}{\partial a_i} = g_i' x_i \qquad \frac{\partial J}{\partial b_i} = g_i' x_i$$

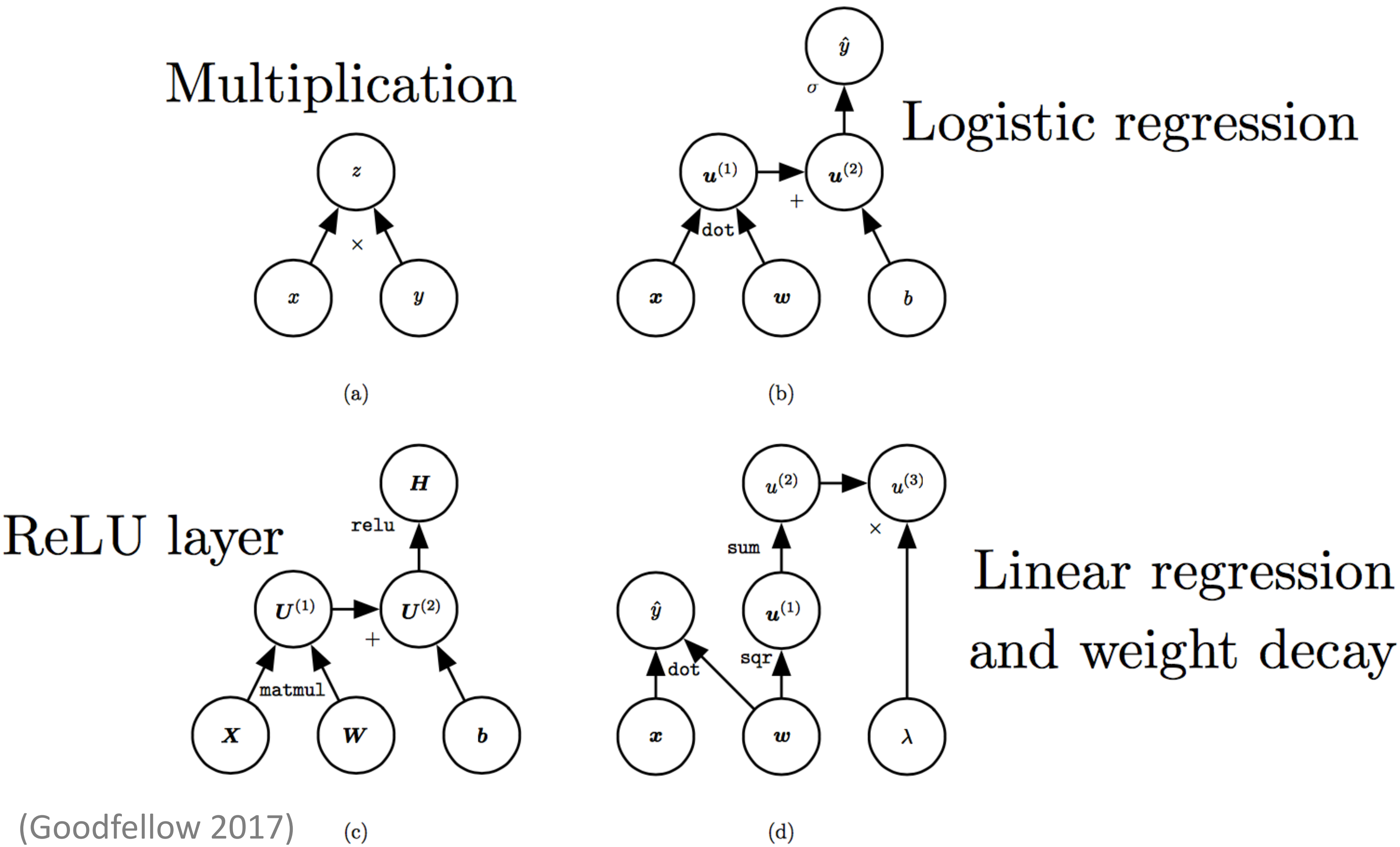
$$g_1' = \frac{\partial J}{\partial z_1} = g c_1$$



$$g = \frac{\partial J}{\partial \hat{y}} = \hat{y} - y$$

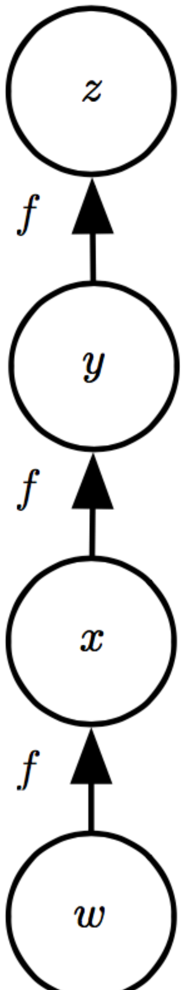
$$g_2' = \frac{\partial J}{\partial z_2} = g c_2$$

Computation Graphs



(Goodfellow 2017)

Repeated Sub-expressions



$$
\begin{aligned}
& \frac{\partial z}{\partial w} \\
= & \frac{\partial z}{\partial y} \frac{\partial y}{\partial x} \frac{\partial x}{\partial w} \\
= & f'(y) f'(x) f'(w) \\
= & f'(f(f(w))) f'(f(w)) f'(w)
\end{aligned}
$$

Back-prop avoids computing this twice

(Goodfellow 2017)

Backprop on Computation Graph

Maintain grad table

1: Initialize $\mathbf{g} \in R^n$ where g_i denotes $\dfrac{\partial u^n}{\partial u^i}$

2: for $j = n-1$ to 1 do:

3: $$g_j = \sum_{i:j \in Pa(u^i)} g_i \frac{\partial u^i}{\partial u^j}$$

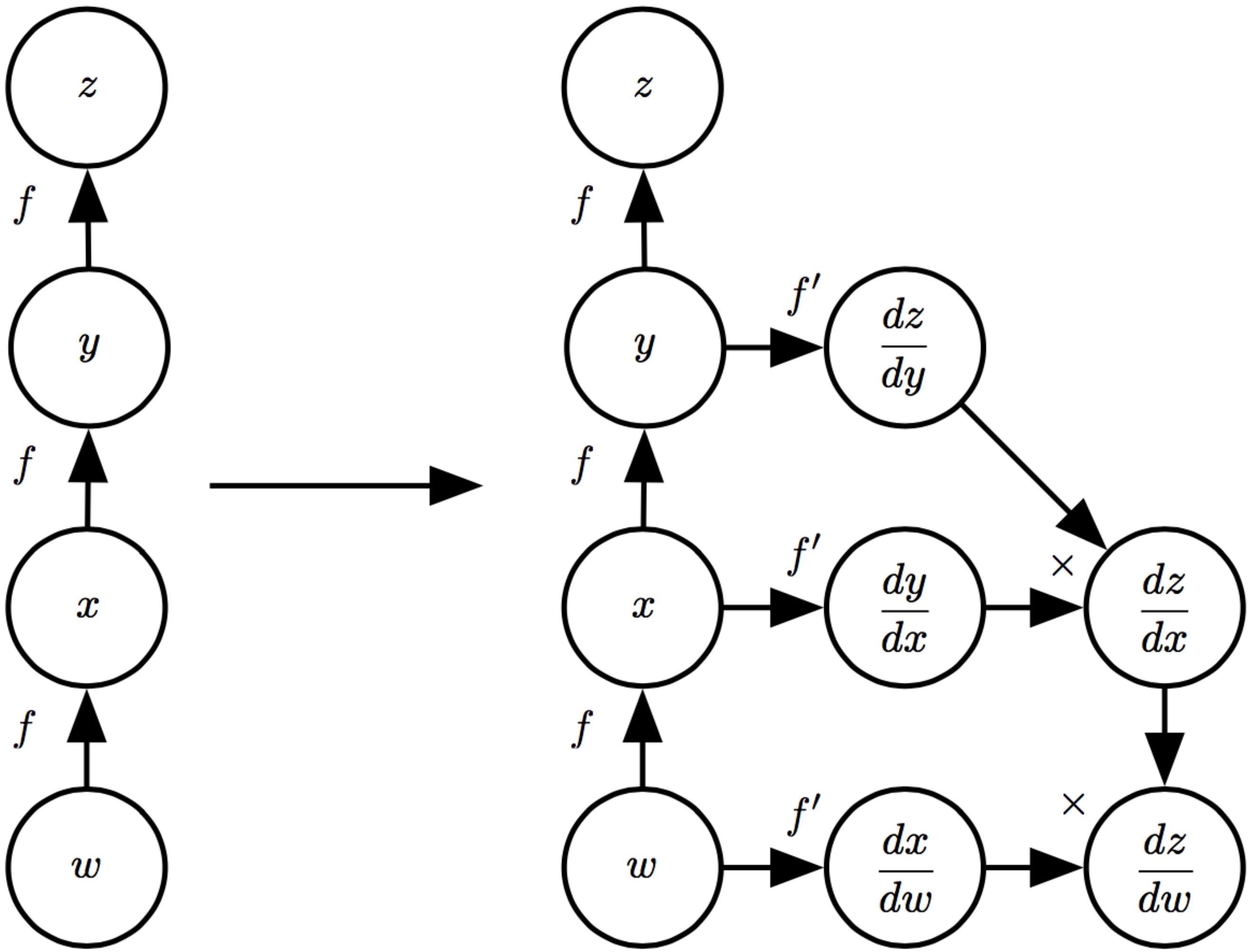
4: return $\mathbf{g}$

Parents of u^i

Symbol-to-symbol Differentiation

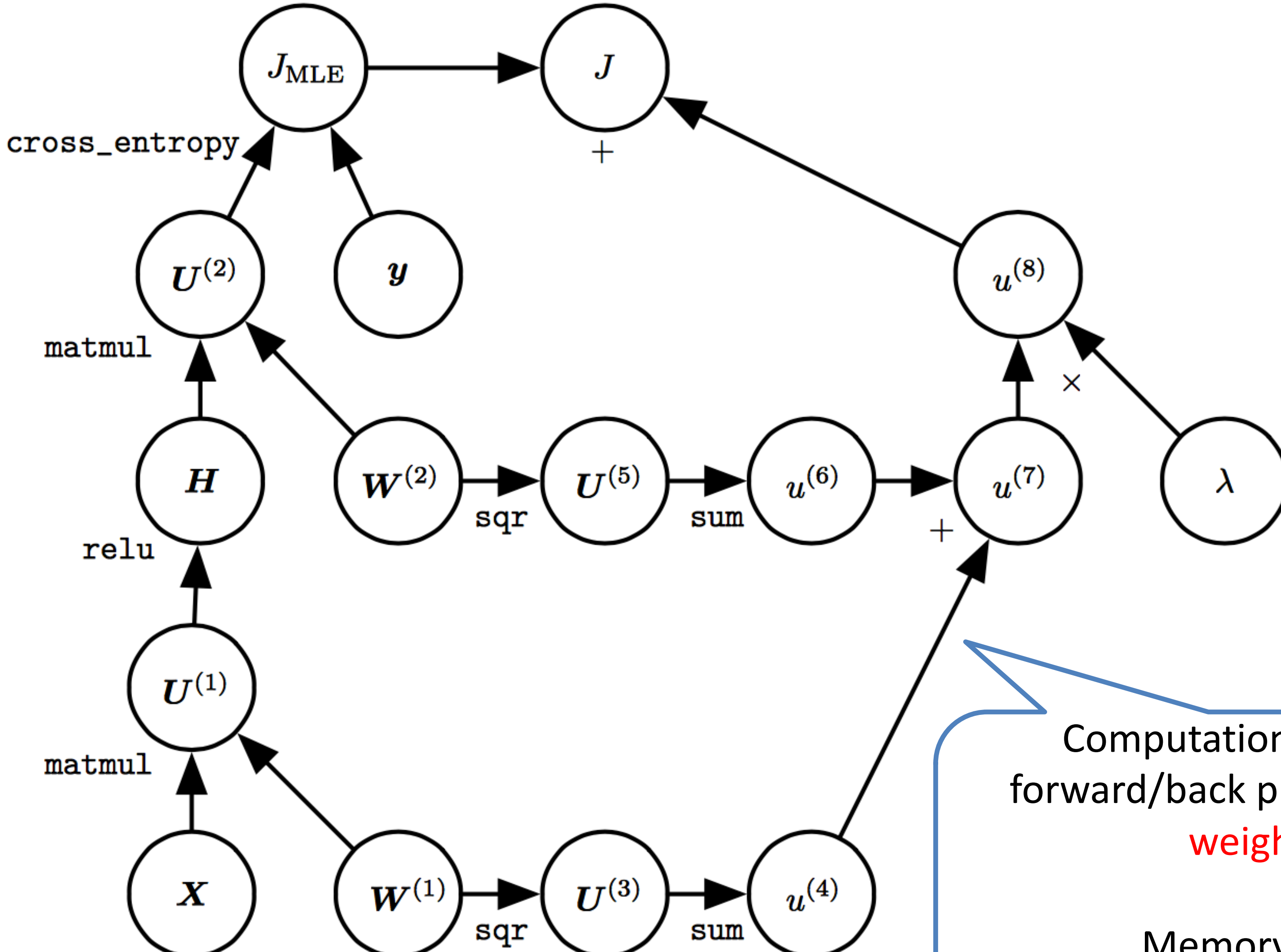
- Derivatives as computation graphs
  - Same language for both forward and back-propagation
- During execution, replace symbolic inputs with numeric value
- Used by Theano and TensorFlow
- Symbol-to-number differentiation: e.g. Torch and Caffe

Symbol-to-symbol Differentiation



(Goodfellow et al. 2017)

Training Feed-forward Nets



Computational cost for forward/back prop: O(#num-weights)

Memory cost: O(#num-layers x minibatch-size)

(Goodfellow et al. 2017)