Neural networks and Backpropagation

Charles Ollion - Olivier Grisel

Neural Network for classification

Vector function with tunable parameters θ

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Sample s in dataset S:

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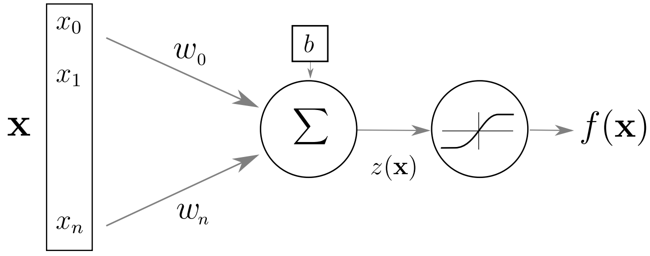
- expected output: $y^s \in [0, K-1]$

Output is a conditional probability distribution:

$$\mathbf{f}(\mathbf{x}^s;\theta)_c = P(Y = c | X = \mathbf{x}^s)$$

Artificial Neuron



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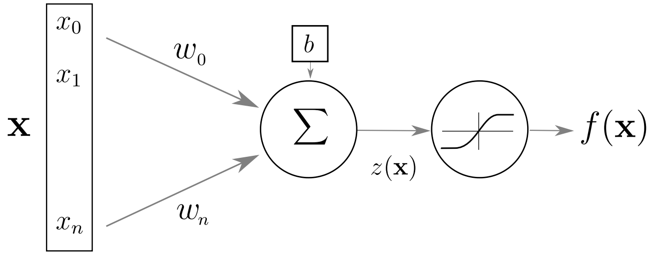
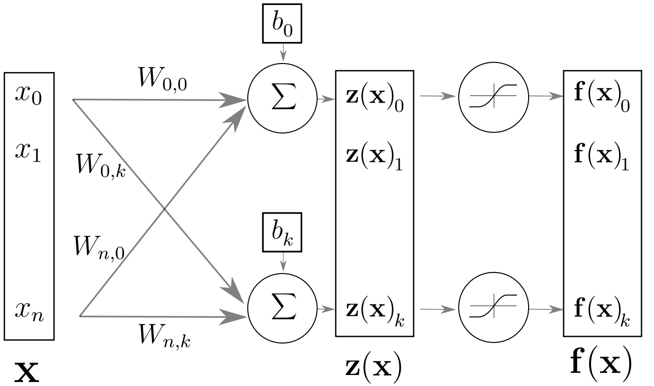


$$z(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

$$f(\mathbf{x}) = g(\mathbf{w}^T\mathbf{x} + b)$$

- $\mathbf{x}, f(\mathbf{x})$ input and output
- $z(\mathbf{x})$ pre-activation
- $\mathbf{w}, b$ weights and bias
- g activation function

Layer of Neurons



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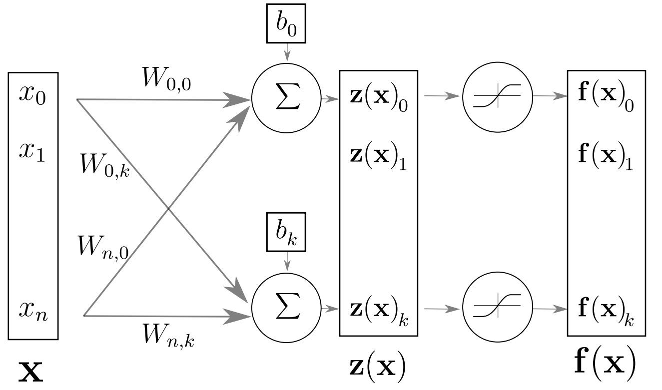
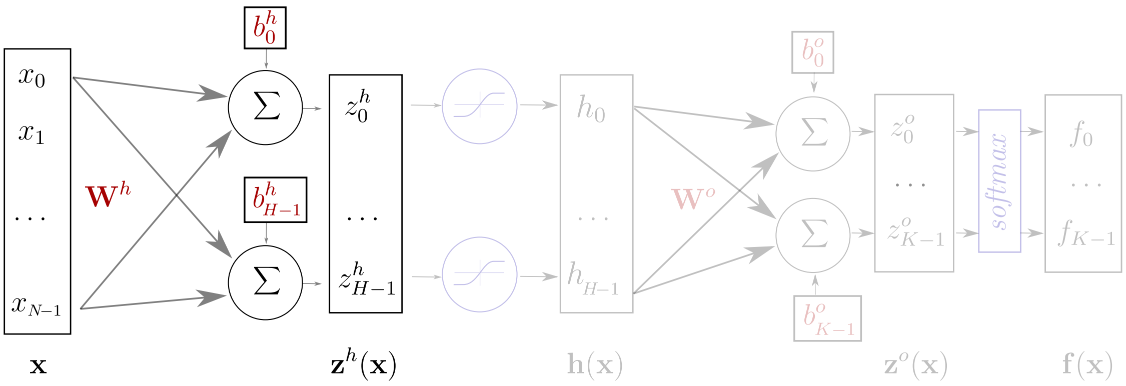


$$\mathbf{f}(\mathbf{x}) = g(\mathbf{z}(\mathbf{x})) = g(\mathbf{W}\mathbf{x} + \mathbf{b})$$

- $\mathbf{W}, \mathbf{b}$ now matrix and vector

One Hidden Layer Network



- $\mathbf{z}^h(\mathbf{x}) = \mathbf{W}^h\mathbf{x} + \mathbf{b}^h$
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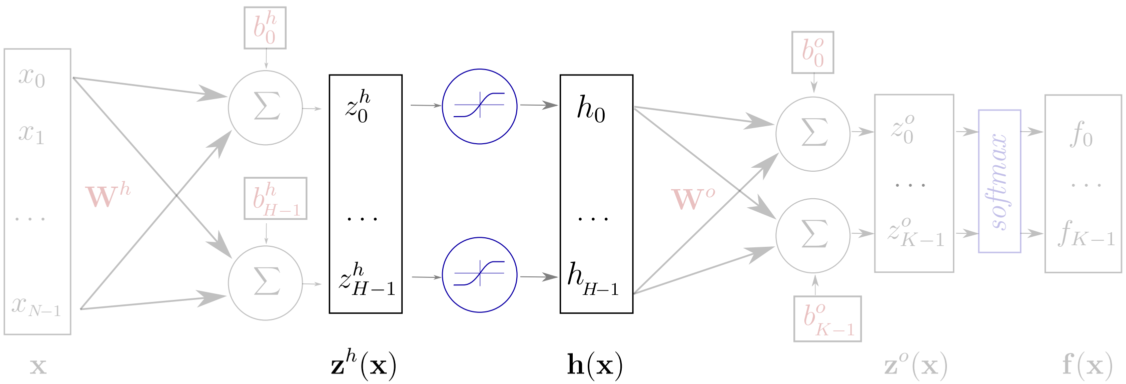

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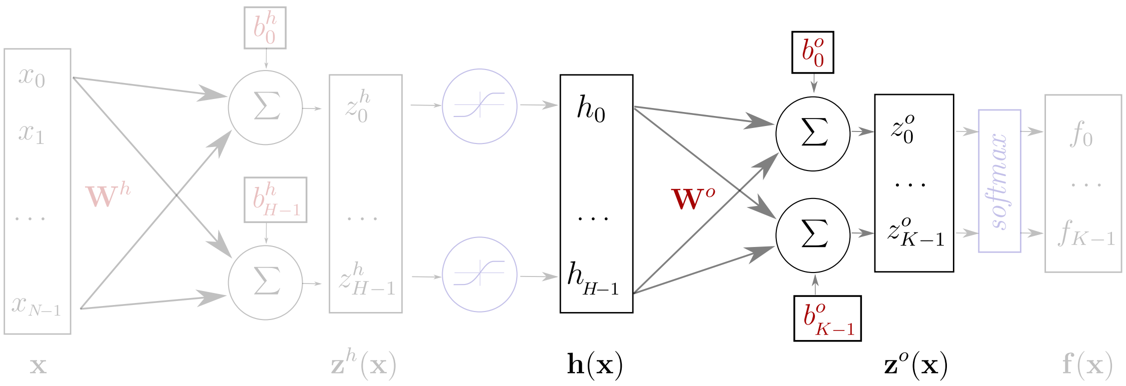

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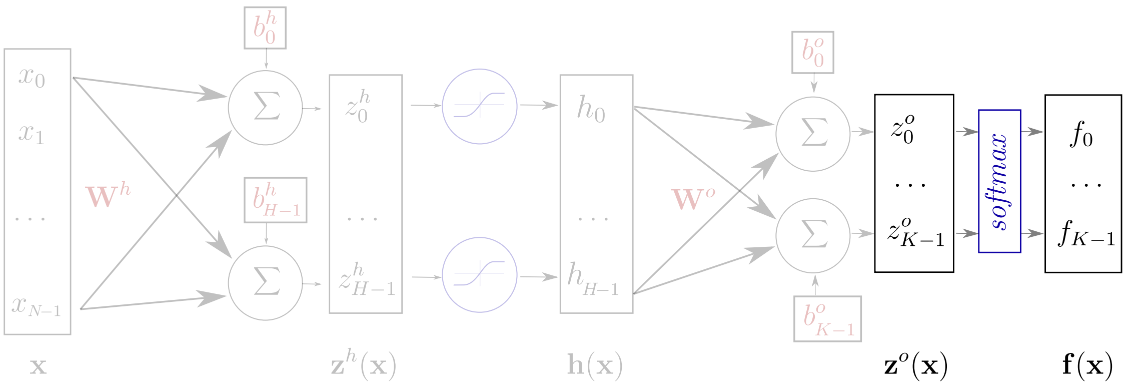

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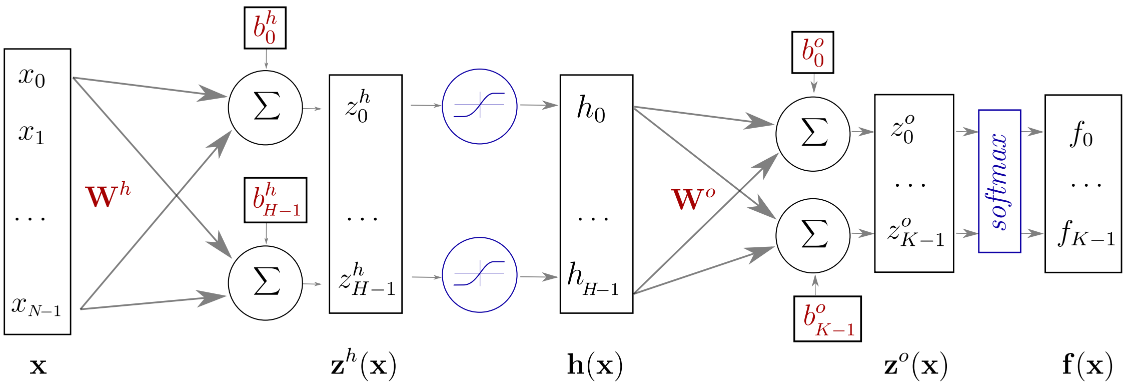
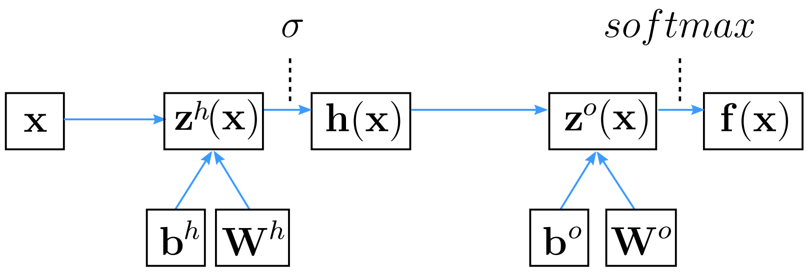
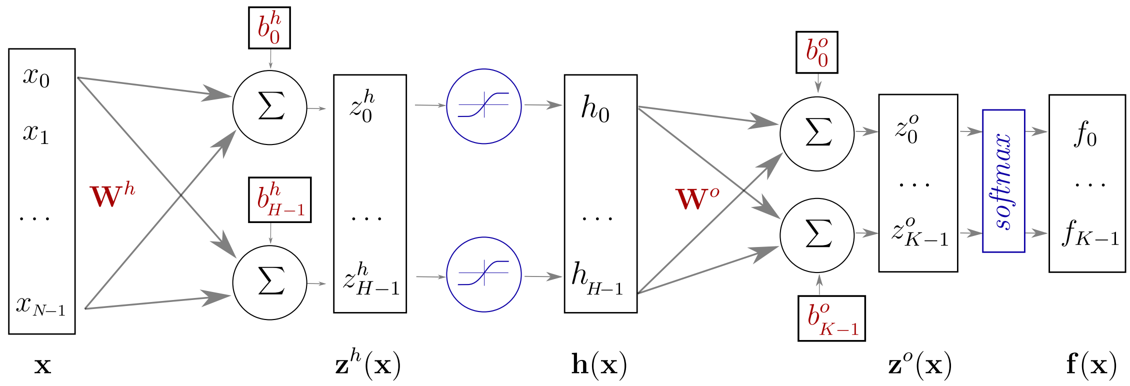


Alternate representation



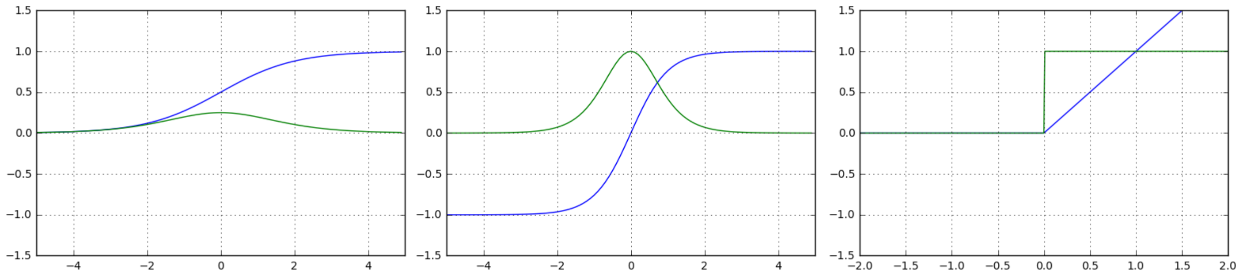
One Hidden Layer Network



Keras implementation

```
model = Sequential()
model.add(Dense(H, input_dim=N))  # weight matrix dim [N * H]
model.add(Activation("tanh"))
model.add(Dense(K))               # weight matrix dim [H x K]
model.add(Activation("softmax"))
```

Element-wise activation functions



$$\mathrm{sigm}(x) = \frac{1}{1+e^{-x}}$$

$$\mathrm{sigm}'(x) = \mathrm{sigm}(x)(1-\mathrm{sigm}(x))$$

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

$$\tanh'(x) = 1 - \tanh(x)^2$$

$$\mathrm{relu}(x) = \max(0, x)$$

$$\mathrm{relu}'(x) = 1_{x>0}$$

- blue: activation function
- green: derivative

Softmax function

$$softmax(\mathbf{x}) = \frac{1}{\sum_{i=1}^{n} e^{x_i}} \cdot \begin{bmatrix} e^{x_1} \\ e^{x_2} \\ \vdots \\ e^{x_n} \end{bmatrix}$$

$$\frac{\partial softmax(\mathbf{x})_i}{\partial x_j} = \begin{cases} softmax(\mathbf{x})_i \cdot (1 - softmax(\mathbf{x})_i) & i = j \\ -softmax(\mathbf{x})_i \cdot softmax(\mathbf{x})_j & i \neq j \end{cases}$$

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- vector of values in (0, 1) that add up to 1
- $p(Y = c|X = \mathbf{x}) = \text{softmax}(\mathbf{z}(\mathbf{x}))_c$
- the pre-activation vector $\mathbf{z}(\mathbf{x})$ is often called "the logits"

Training the network

Find parameters $\theta = (\mathbf{W}^h; \mathbf{b}^h; \mathbf{W}^o; \mathbf{b}^o)$ that minimize the **negative log likelihood** (or cross entropy)

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The loss function for a given sample $s \in S$:

$$l(\mathbf{f}(\mathbf{x}^s;\theta), y^s) = nll(\mathbf{x}^s, y^s; \theta) = -\log \mathbf{f}(\mathbf{x}^s;\theta)_{y^s}$$

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example $y^s = 3$

$$l(\mathbf{f}(\mathbf{x}^s;\theta), y^s) = l\left(\begin{bmatrix} f_0 \\ \cdots \\ f_3 \\ \cdots \\ f_{K-1} \end{bmatrix}, \begin{bmatrix} 0 \\ \cdots \\ 1 \\ \cdots \\ 0 \end{bmatrix} \right) = -\log\ f_3$$

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The cost function is the negative likelihood of the model computed on the full training set (for i.i.d. samples):

$$L_S(\theta) = -\frac{1}{|S|} \sum_{s \in S} \log \mathbf{f}(\mathbf{x}^s;\theta)_{y^s}$$

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$$L_S(\theta) = -\frac{1}{|S|} \sum_{s \in S} \log \mathbf{f}(\mathbf{x}^s;\theta)_{y^s} + \lambda \Omega(\theta)$$

$\lambda \Omega(\theta) = \lambda(||W^h||^2 + ||W^o||^2)$ is an optional regularization term.

Stochastic Gradient Descent

Initialize θ randomly

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Stop when reaching criterion:

- nll stops decreasing when computed on validation set

Computing Gradients

Output Weights: $\frac{\partial l(\mathbf{f}(\mathbf{x}),y)}{\partial W^o_{i,j}}$ Output bias: $\frac{\partial l(\mathbf{f}(\mathbf{x}),y)}{\partial b^o_i}$

Hidden Weights: $\frac{\partial l(\mathbf{f}(\mathbf{x}),y)}{\partial W^h_{i,j}}$ Hidden bias: $\frac{\partial l(\mathbf{f}(\mathbf{x}),y)}{\partial b^h_i}$

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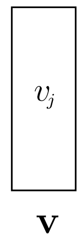
- The network is a composition of differentiable modules
- We can apply the "chain rule"

Chain rule

$$x \longrightarrow \mathbf{v} \longrightarrow z$$

$$z = u(\mathbf{v}(x))$$

$$\frac{\partial z}{\partial x} = ?$$



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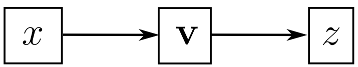

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chain-rule

$$\frac{\partial z}{\partial x} = \sum_j \frac{\partial z}{\partial v_j} \frac{\partial v_j}{\partial x}$$

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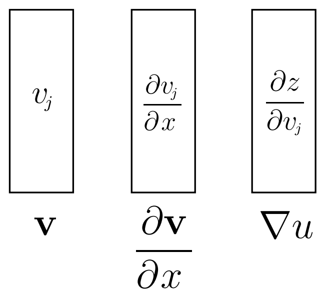
$$\frac{\partial z}{\partial x} = \sum_j \frac{\partial z}{\partial v_j}\frac{\partial v_j}{\partial x} = \nabla u . \frac{\partial \mathbf{v}}{\partial x}$$



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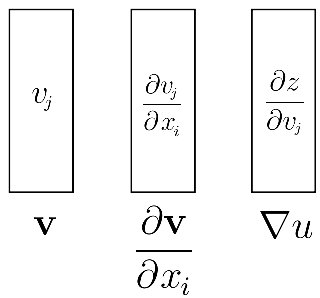
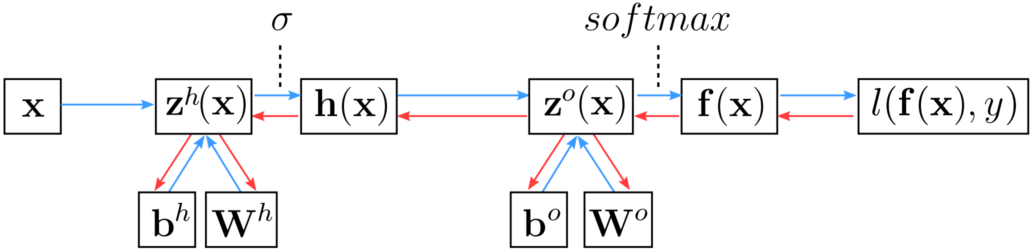


Backpropagation



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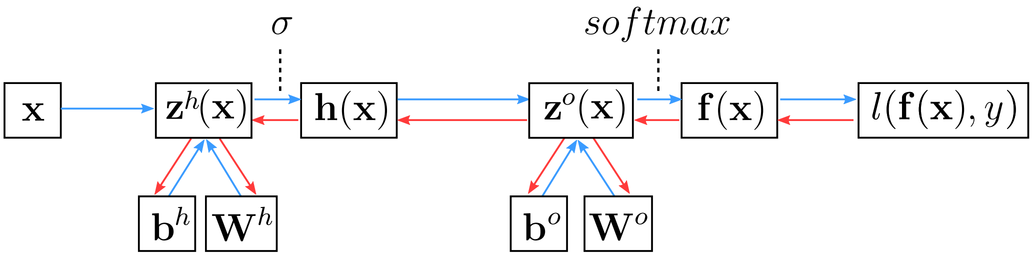
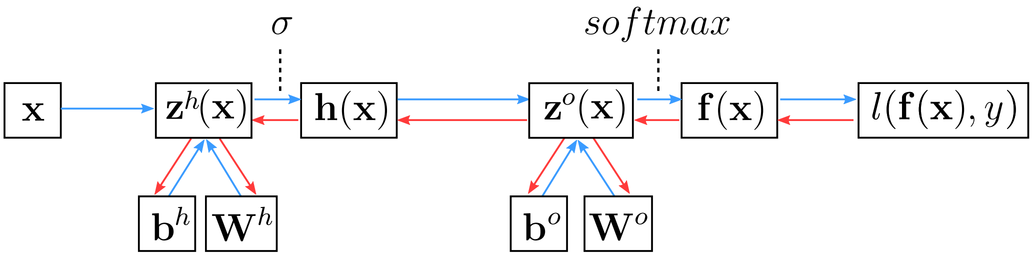


Compute partial derivatives of the loss

- $\frac{\partial l(\mathbf{f}(\mathbf{x}),y)}{\partial \mathbf{f}(\mathbf{x})_i} = \frac{\partial -\log \mathbf{f}(\mathbf{x})_y}{\partial \mathbf{f}(\mathbf{x})_i} = \frac{-1_{y=i}}{\mathbf{f}(\mathbf{x})_y} = \frac{\partial \boldsymbol{l}}{\partial \mathbf{f}(\mathbf{x})_i}$

Backpropagation



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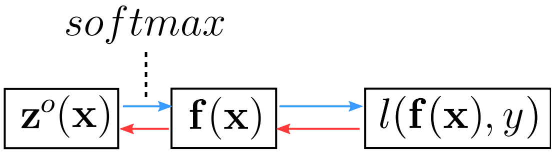
- $\frac{\partial \boldsymbol{l}}{\partial \mathbf{z}^o(\mathbf{x})_i} = ?$

$$\frac{\partial l}{\partial \mathbf{z}^o(\mathbf{x})_i} = \sum_j \frac{\partial l}{\partial \mathbf{f}(\mathbf{x})_j} \frac{\partial \mathbf{f}(\mathbf{x})_j}{\partial \mathbf{z}^o(\mathbf{x})_i}$$

Chain rule!



$$
\begin{aligned}
\frac{\partial l}{\partial \mathbf{z}^{o}(\mathbf{x})_i} &= \sum_j \frac{\partial l}{\partial \mathbf{f}(\mathbf{x})_j} \frac{\partial \mathbf{f}(\mathbf{x})_j}{\partial \mathbf{z}^{o}(\mathbf{x})_i} \\
&= \sum_j \frac{-1_{y=j}}{\mathbf{f}(\mathbf{x})_y} \frac{\partial softmax(\,\mathbf{z}^{o}(\mathbf{x}))_j}{\partial \mathbf{z}^{o}(\mathbf{x})_i}
\end{aligned}
$$

$$\frac{\partial l}{\partial \mathbf{f}(\mathbf{x})_i} = \frac{-1_{y=i}}{\mathbf{f}(\mathbf{x})_y}$$

$$\mathbf{f}(\mathbf{x}) = softmax(\,\mathbf{z}^{o}(\mathbf{x}))$$

$$
\begin{tikzcd}
\boxed{\mathbf{z}^{o}(\mathbf{x})} \arrow[r, shift left, "softmax"] & \boxed{\mathbf{f}(\mathbf{x})} \arrow[l, shift left] \arrow[r, shift left] & \boxed{l(\mathbf{f}(\mathbf{x}), y)} \arrow[l, shift left]
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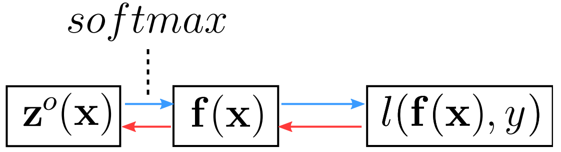

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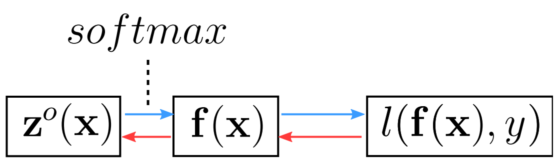

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$$

$$\nabla_{\mathbf{z}^o(\mathbf{x})} l(\mathbf{f}(\mathbf{x}), y) = \mathbf{f}(\mathbf{x}) - \mathbf{e}(y)$$

$\mathrm{e}(y)$: one-hot encoding of y

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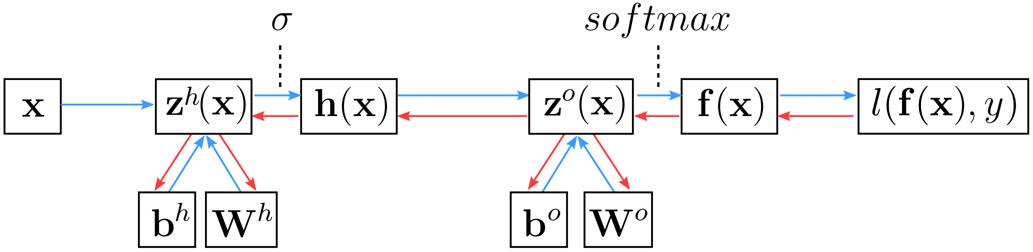
Backpropagation

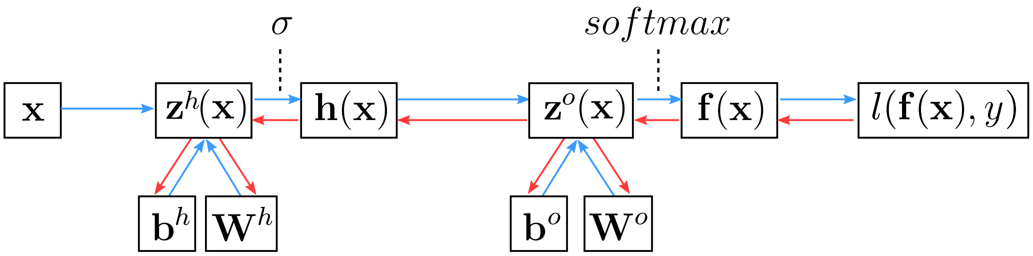


Gradients

- $\nabla_{\mathbf{z}^o(\mathbf{x})} \boldsymbol{l} = \mathbf{f}(\mathbf{x}) - \mathbf{e}(y)$
- $\nabla_{\mathbf{b}^o} \boldsymbol{l} = \mathbf{f}(\mathbf{x}) - \mathbf{e}(y)$

because $\mathbf{z}^o(\mathbf{x}) = \mathbf{W}^o \mathbf{h}(\mathbf{x}) + \mathbf{b}^o$ and then $\frac{\partial \mathbf{z}^o(\mathbf{x})_i}{\partial \mathbf{b}^o_j} = 1_{i=j}$

Backpropagation



Partial derivatives related to $\mathbf{W}^o$

- $\frac{\partial \boldsymbol{l}}{\partial W^o_{i,j}} = \sum_k \frac{\partial \boldsymbol{l}}{\partial \mathbf{z}^o(\mathbf{x})_k} \frac{\partial \mathbf{z}^o(\mathbf{x})_k}{\partial W^o_{i,j}}$
- $\nabla_{\mathbf{W}^o} \boldsymbol{l} = (\mathbf{f}(\mathbf{x}) - \mathbf{e}(y)) . \mathbf{h}(\mathbf{x})^\top$

Backprop gradients

Compute activation gradients

- $\nabla_{\mathbf{z}^{o}(\mathbf{x})} \boldsymbol{l} = \mathbf{f}(\mathbf{x}) - \mathbf{e}(y)$

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Compute prev layer activation gradients

- $\nabla_{\mathbf{h}(\mathbf{x})} \boldsymbol{l} = \mathbf{W}^{o\top} \nabla_{\mathbf{z}^o(\mathbf{x})} \boldsymbol{l}$
- $\nabla_{\mathbf{z}^h(\mathbf{x})} \boldsymbol{l} = \nabla_{\mathbf{h}(\mathbf{x})} \boldsymbol{l} \odot \sigma'(\mathbf{z}^{\mathbf{h}}(\mathbf{x}))$

Loss, Initialization and Learning Tricks

Discrete output (classification)

- Binary classification: $y \in [0, 1]$
  - $Y|X = \mathbf{x} \sim Bernoulli(b = f(\mathbf{x}; \theta))$
  - output function: $logistic(x) = \frac{1}{1+e^{-x}}$
  - loss function: binary cross-entropy
- Multiclass classification: $y \in [0, K-1]$
  - $Y|X = \mathbf{x} \sim Multinoulli(\mathbf{p} = \mathbf{f}(\mathbf{x}; \theta))$
  - output function: $softmax$
  - loss function: categorical cross-entropy

Continuous output (regression)

- Continuous output: $\mathbf{y} \in \mathbb{R}^n$
  - $Y|X = \mathbf{x} \sim \mathcal{N}(\mu = \mathbf{f}(\mathbf{x};\theta), \sigma^2\mathbf{I})$
  - output function: Identity
  - loss function: square loss
- Heteroschedastic if $\mathbf{f}(\mathbf{x};\theta)$ predicts both μ and σ^2
- Mixture Density Network (multimodal output)
  - $Y|X = \mathbf{x} \sim GMM_{\mathbf{x}}$
  - $\mathbf{f}(\mathbf{x};\theta)$ predicts all the parameters: the means, covariance matrices and mixture weights

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- Biases can (should) be initialized to zero

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  - or monitor validation loss and divide η_t by 2 or 10 when no progress
  - See ReduceLROnPlateau in Keras

Momentum

Accumulate gradients across successive updates:

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\begin{aligned}
m_t &= \gamma m_{t-1} + \eta \nabla_\theta L_{B_t}(\theta_{t-1}) \\
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Nesterov accelerated gradient

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m_t &= \gamma m_{t-1} + \eta \nabla_\theta L_{B_t}(\theta_{t-1} - \gamma m_{t-1}) \\
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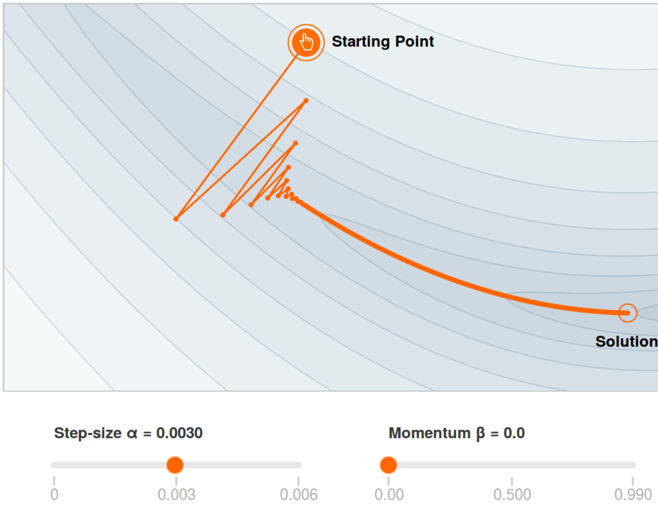
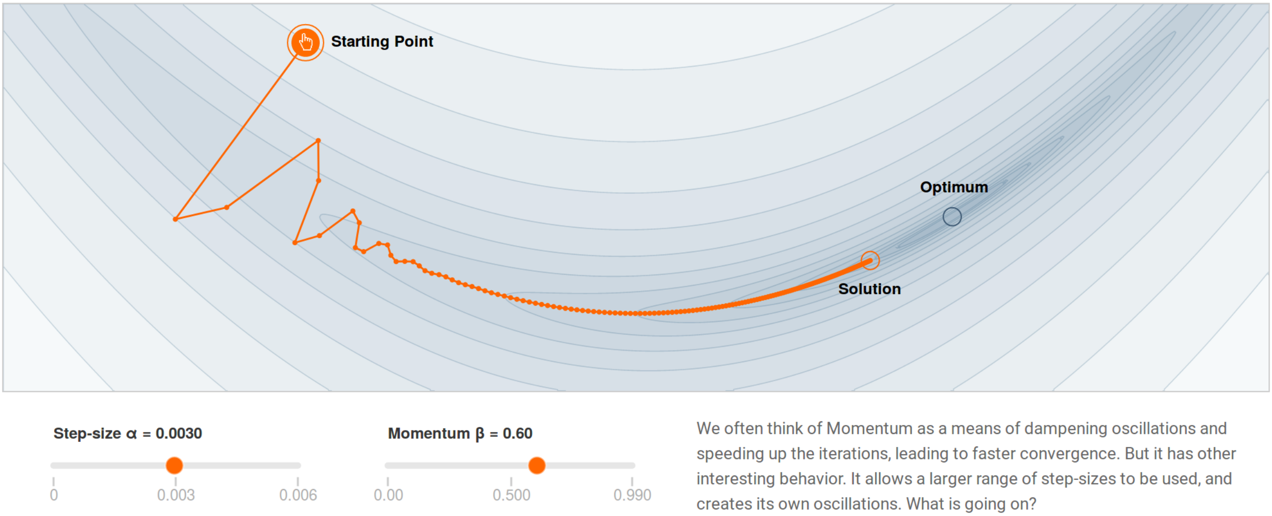
Better at handling changes in gradient direction.



We often think of Momentum as a means of dampening oscillations and speeding up the iterations, leading to faster convergence. But it has other interesting behavior. It allows a larger range of step-sizes to be used, and creates its own oscillations. What is going on?

[Why Momentum Really Works]



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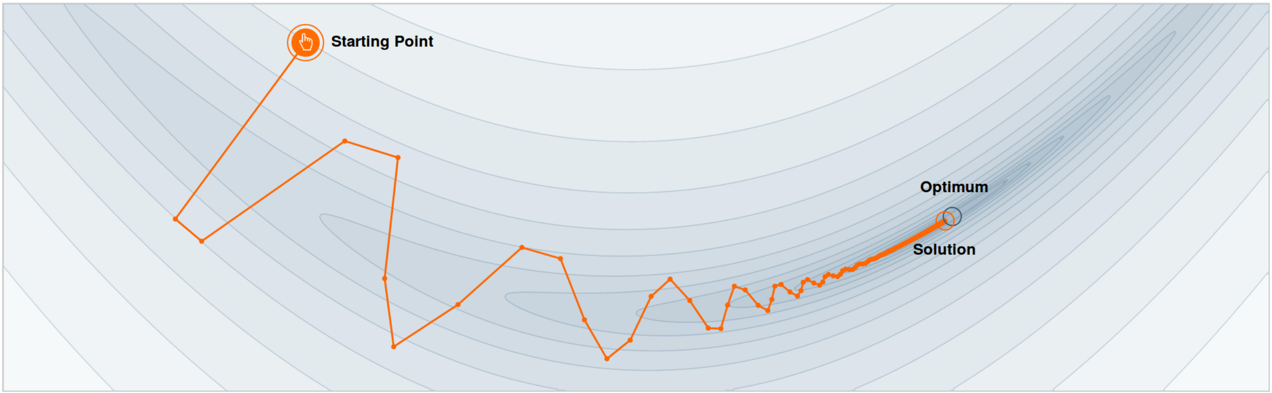

Step-size α = 0.0030

0 0.003 0.006

Momentum β = 0.80

0.00 0.500 0.990

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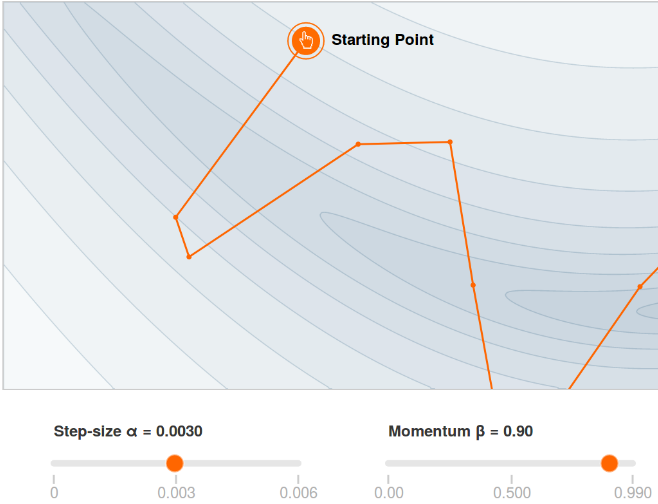

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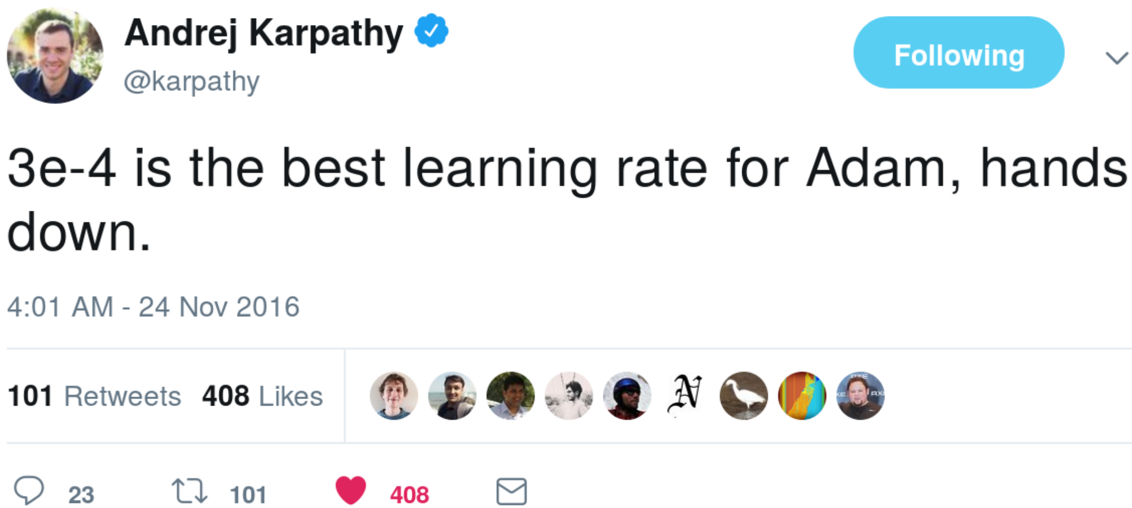
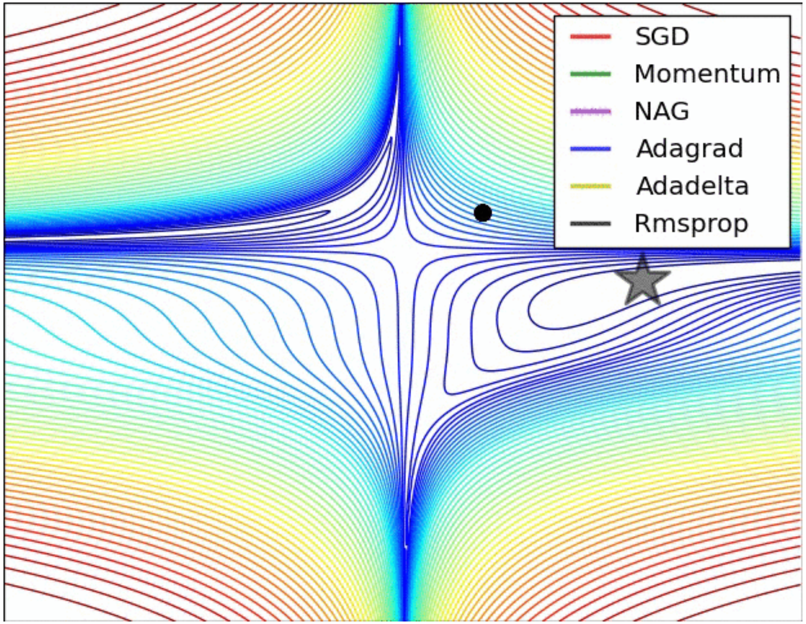
- But well-tuned SGD with LR scheduling can generalize better than Adam (with naive l2 reg)...
- Promising stochastic second order methods: K-FAC and Shampoo can be used to accelerate training of very large models.

The Karpathy Constant for Adam



Optimizers around a saddle point



Credits: Alec Radford