Neural networks and Backpropagation

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Neural Network for classification

Vector function with tunable parameters θ

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Sample s in dataset S:

- input: $\mathbf{x}^s \in \mathrm{R}^N$
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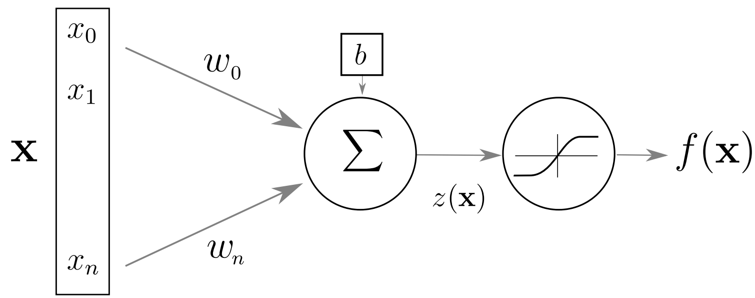
Output is a conditional probability distribution:

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

Artificial Neuron



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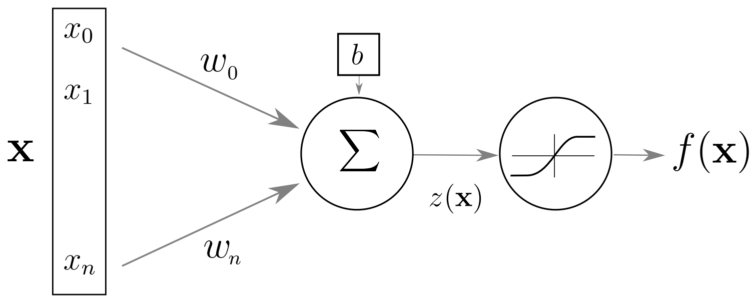
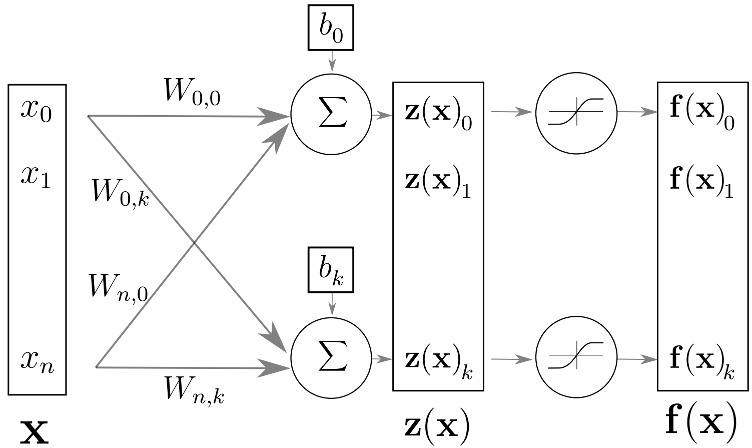


$$z(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

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

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

Layer of Neurons



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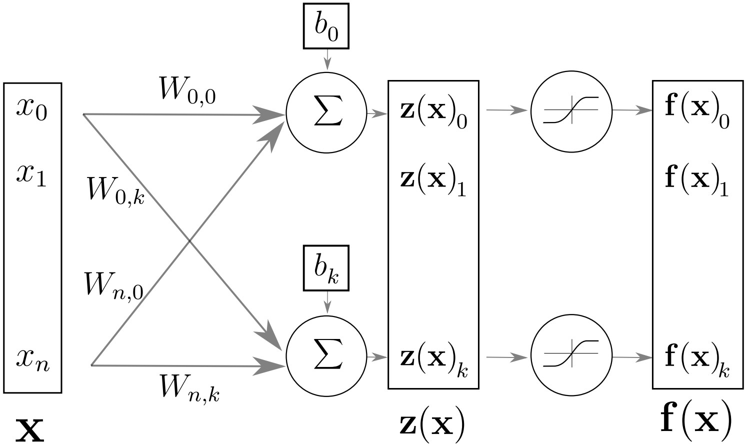
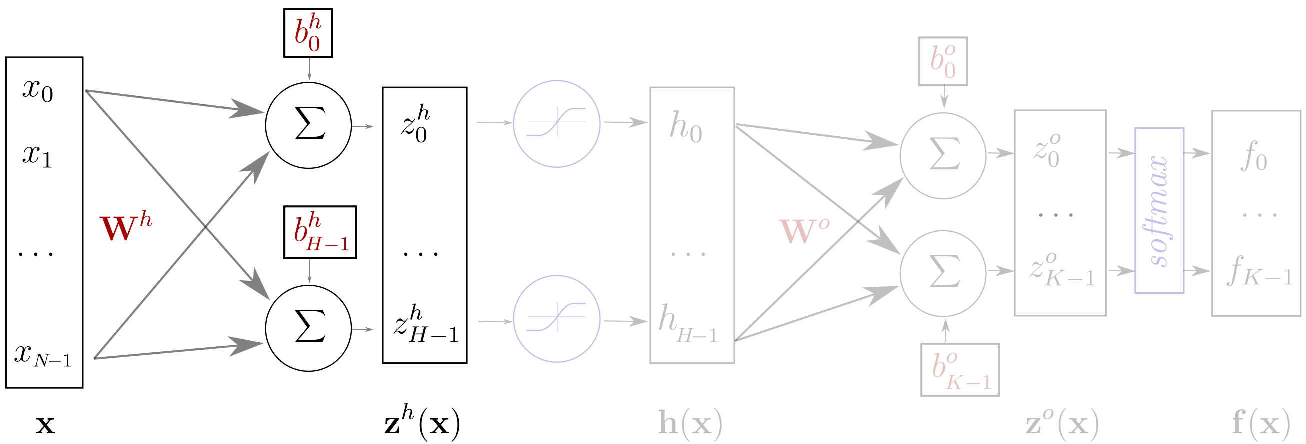


$$\mathbf{f}(\mathbf{x}) = g(\mathbf{z}(\mathbf{x})) = g(\mathbf{W}\mathbf{x} + \mathbf{b})$$

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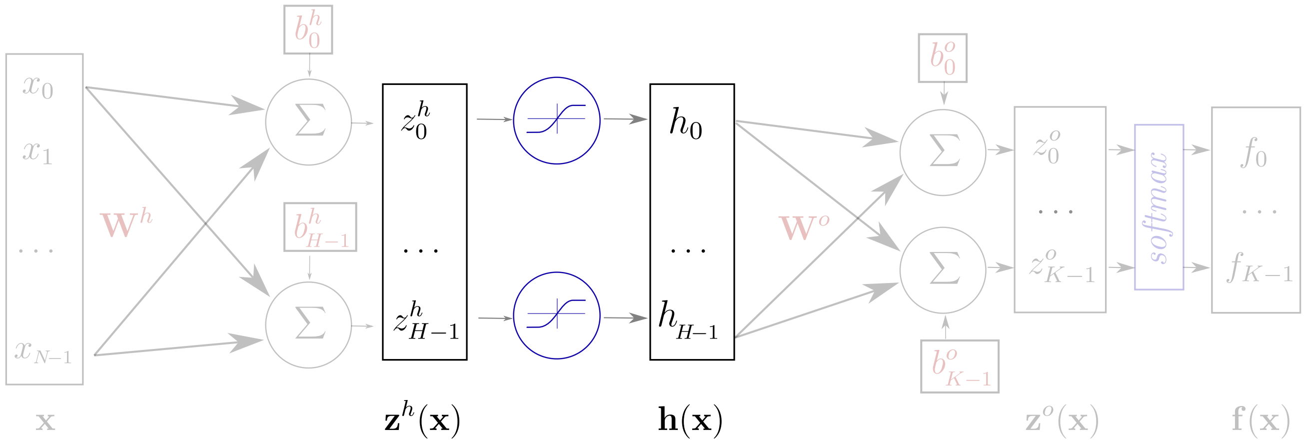

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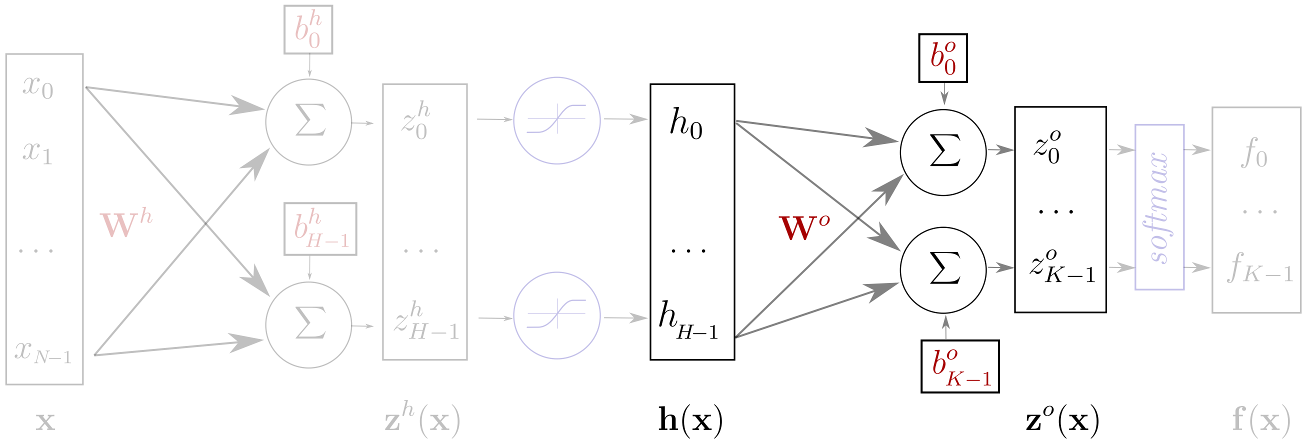

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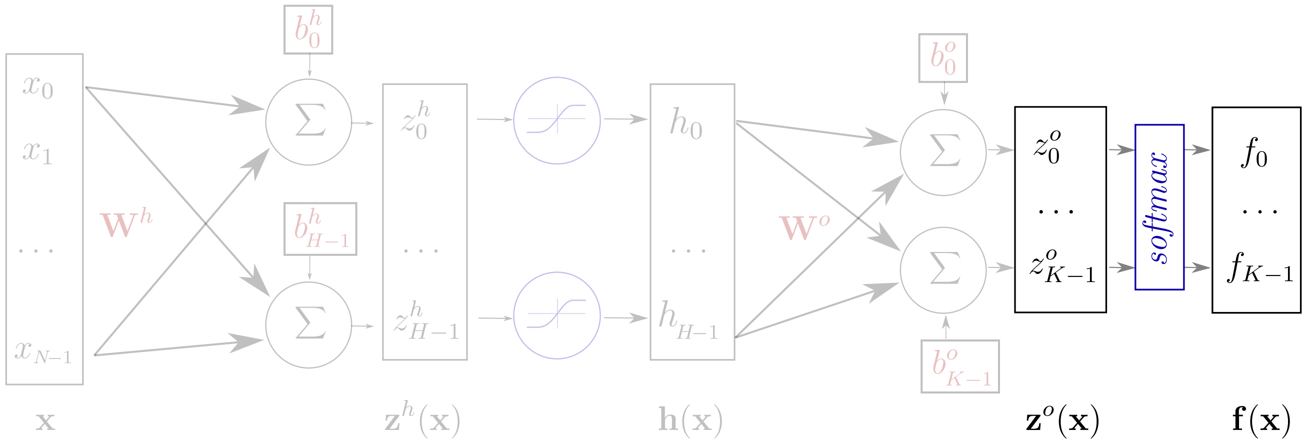

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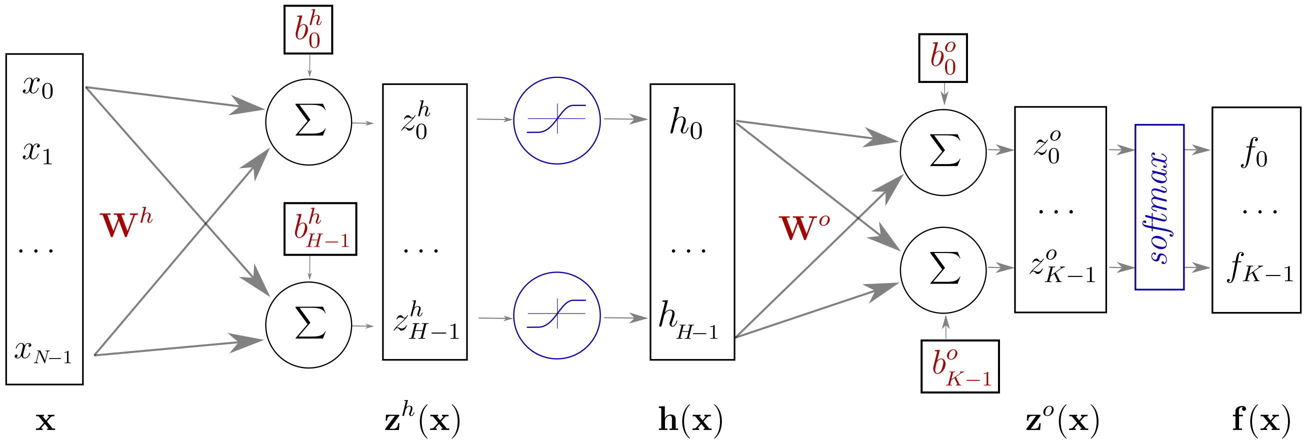
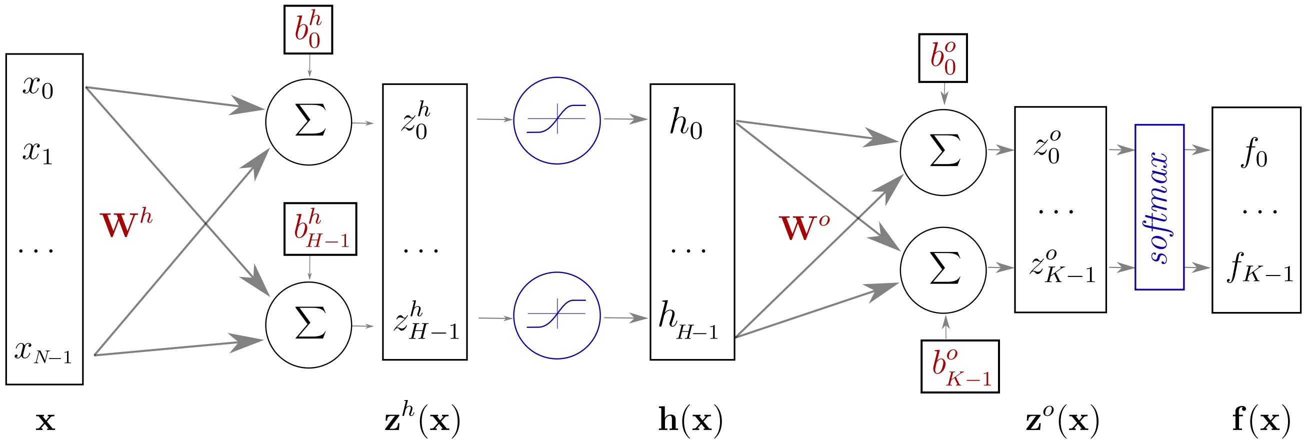


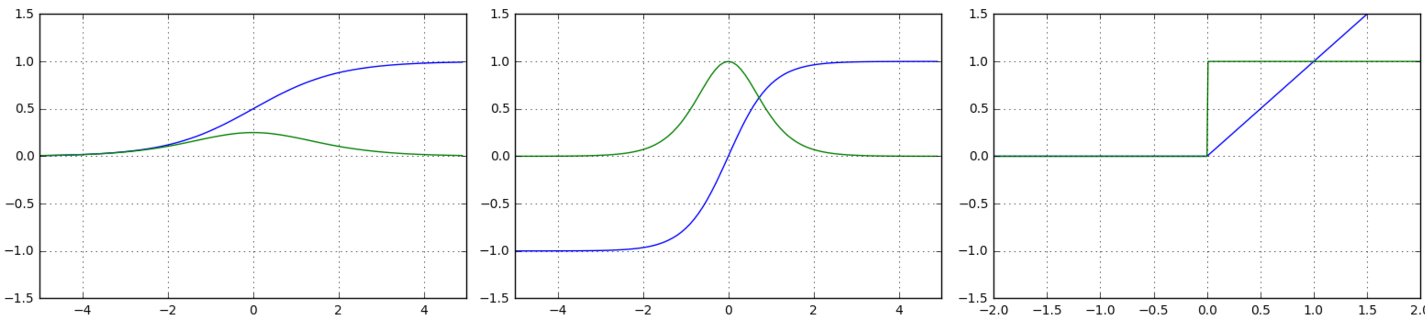
Alternate representation

One Hidden Layer Network



Keras implementation

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

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
- $p(Y = c \,|\, X = \mathbf{x}) = \mathrm{softmax}(\mathbf{z}(\mathbf{x}))_c$
- the pre-activation vector $\mathbf{z}(\mathbf{x})$ is often called "the logits"

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

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example $\quad y^s = 3$

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

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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):

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$\lambda \Omega(\theta) = \lambda(||W^h||^2 + ||W^o||^2)$ 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: $\dfrac{\partial l(\mathbf{f}(\mathbf{x}), y)}{\partial W^{o}_{i,j}}$

Output bias: $\dfrac{\partial l(\mathbf{f}(\mathbf{x}), y)}{\partial b^{o}_{i}}$

Hidden Weights: $\dfrac{\partial l(\mathbf{f}(\mathbf{x}), y)}{\partial W^{h}_{i,j}}$

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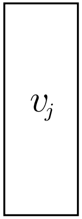
- The network is a composition of differentiable modules
- We can apply the "chain rule"

Chain rule

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

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



$\mathbf{v}$

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

Chain rule

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

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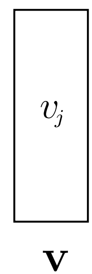

chain-rule

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

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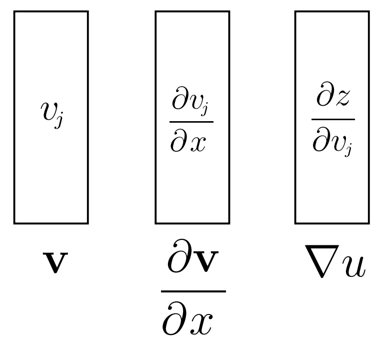
chain-rule

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



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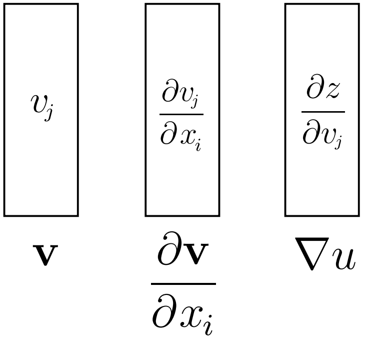
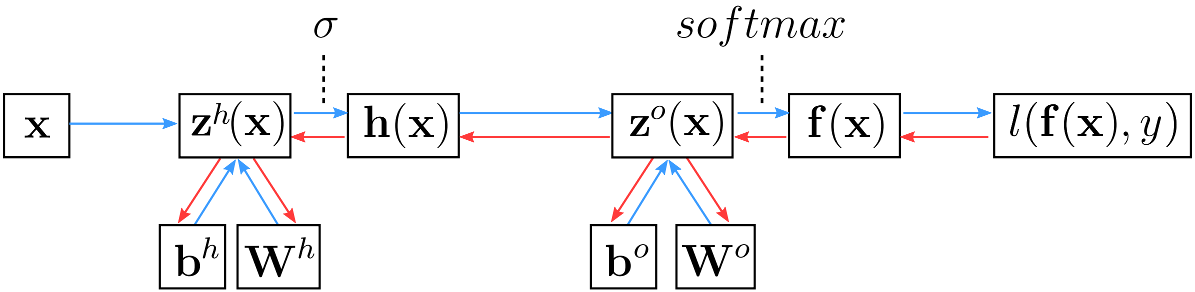


Backpropagation



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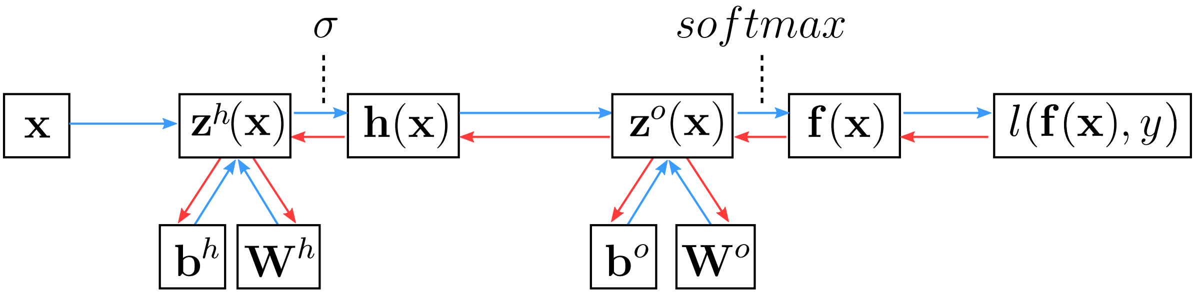
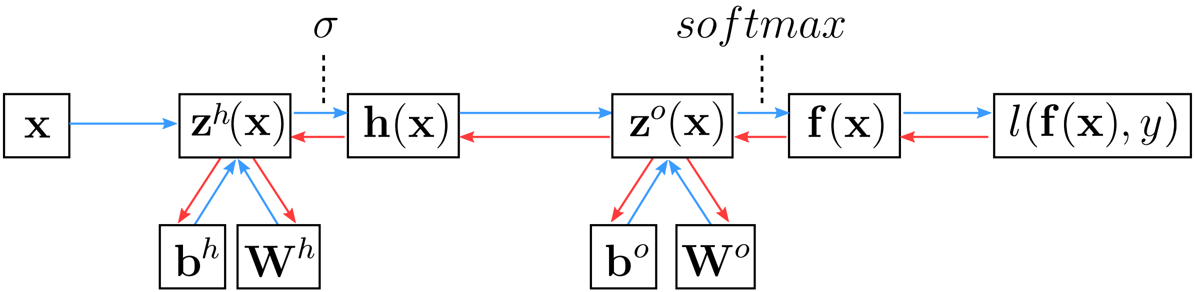


Compute partial derivatives of the loss

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

Backpropagation



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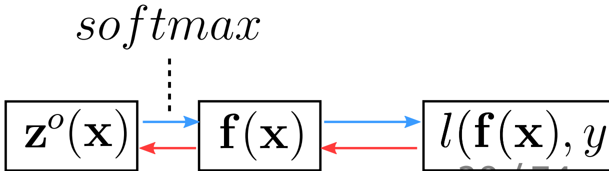
- $\dfrac{\partial \boldsymbol{l}}{\partial \mathbf{z}^o(\mathbf{x})_i} = \ ?$

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

Chain rule!



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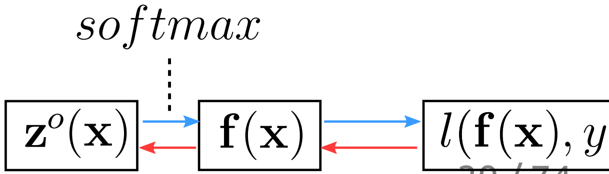
$$= \sum_j \frac{-1_{y=j}}{\mathbf{f}(\mathbf{x})_y} \frac{\partial softmax(\mathbf{z}^o(\mathbf{x}))_j}{\partial \mathbf{z}^o(\mathbf{x})_i}$$

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

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



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\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} \\
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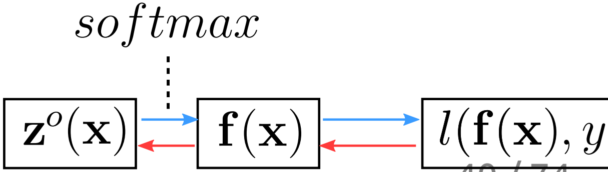
\end{aligned}
$$



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&= \begin{cases} -\frac{1}{\mathbf{f}(\mathbf{x})_y} softmax(\mathbf{z}^o(\mathbf{x}))_y (1 - softmax(\mathbf{z}^o(\mathbf{x}))_y) & \textbf{if } i = \\ \frac{1}{\mathbf{f}(\mathbf{x})_y} softmax(\mathbf{z}^o(\mathbf{x}))_y softmax(\mathbf{z}^o(\mathbf{x}))_i & \textbf{if } i \neq \end{cases} \\
&= \begin{cases} -1 + \mathbf{f}(\mathbf{x})_y & \textbf{if } i = y \\ \mathbf{f}(\mathbf{x})_i & \textbf{if } i \neq y \end{cases}
\end{aligned}
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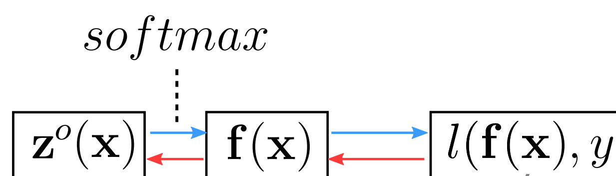

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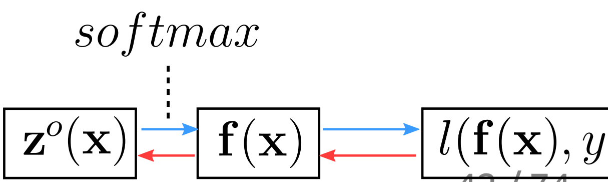
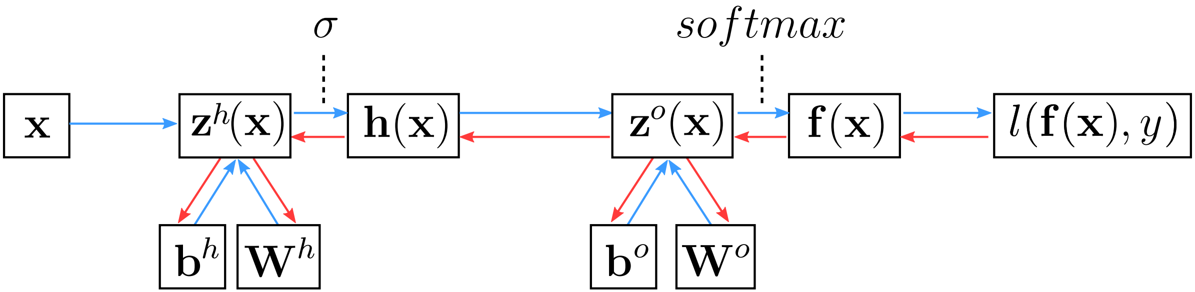
\end{aligned}
$$

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

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



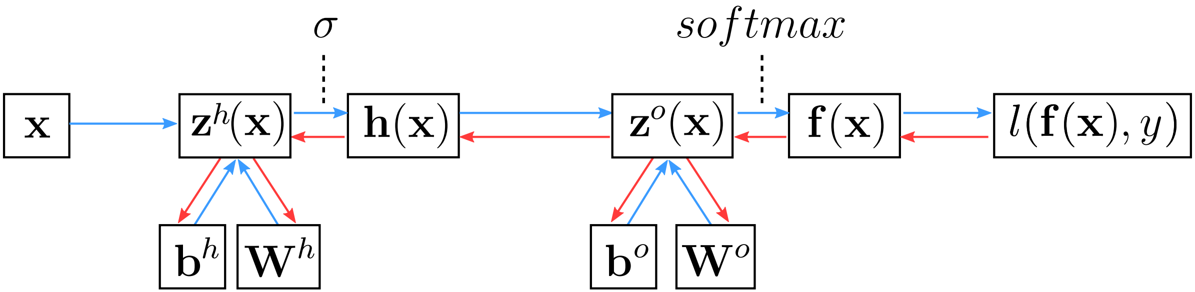
Backpropagation



Gradients

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

Backpropagation



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

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

Backprop gradients

Compute activation gradients

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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: $\mathbf{y} \in \mathrm{R}^n$
  - $Y | X = \mathbf{x} \sim \mathrm{N}(\mu = \mathbf{f}(\mathbf{x}; \theta), \sigma^2 \mathbf{I})$
  - 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)
  - $Y | X = \mathbf{x} \sim GMM_{\mathbf{x}}$

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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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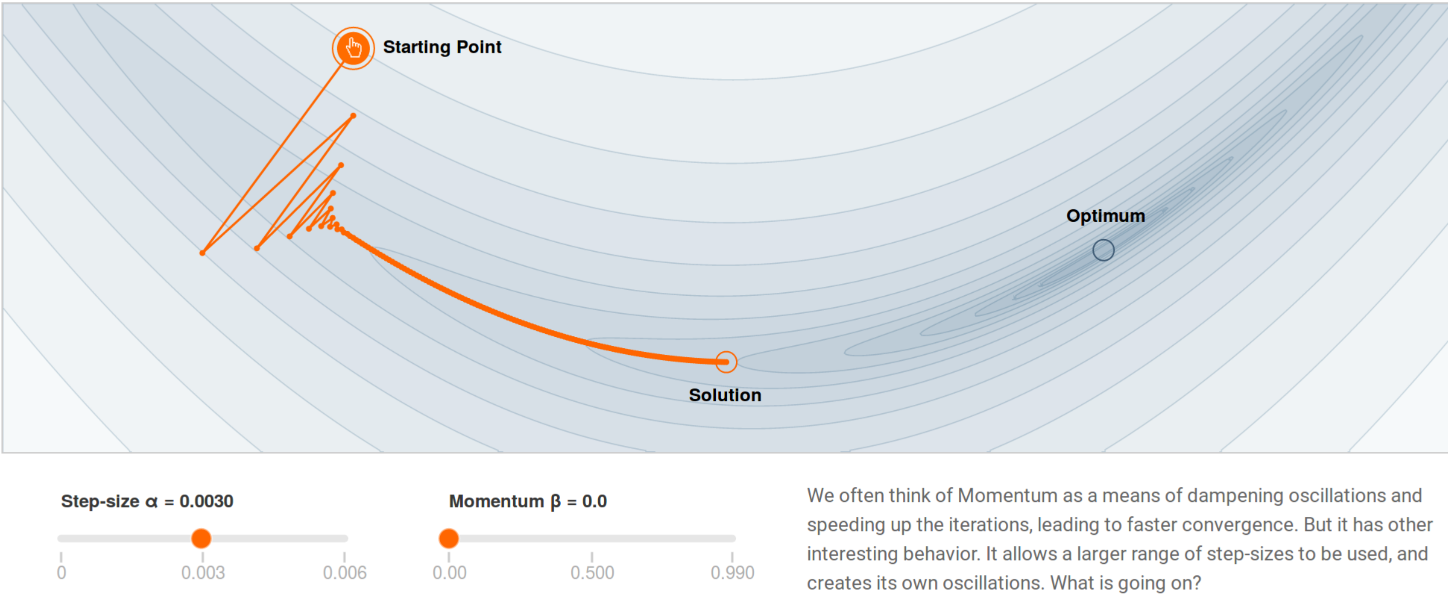
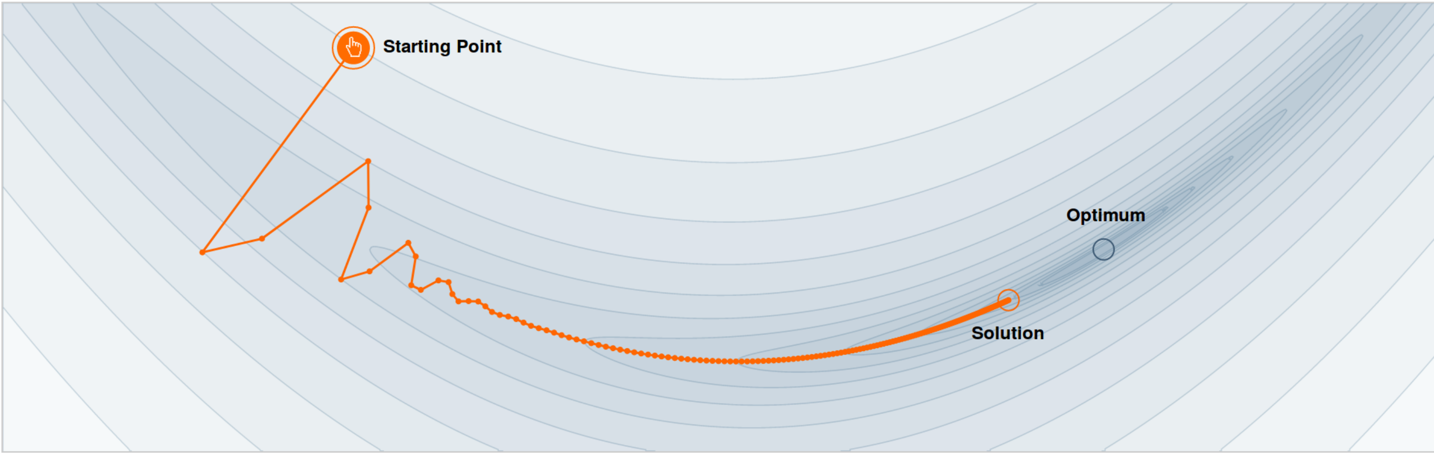
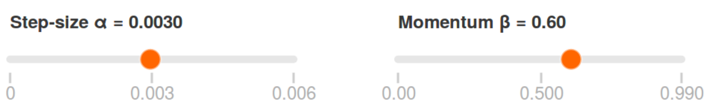


[Why Momentum Really Works]





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?

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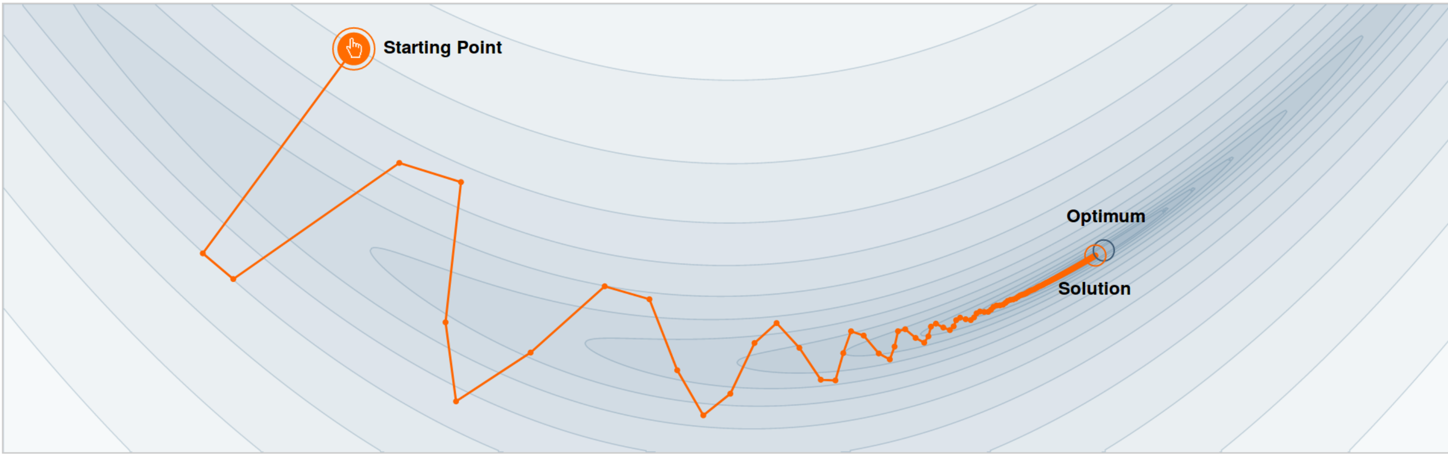

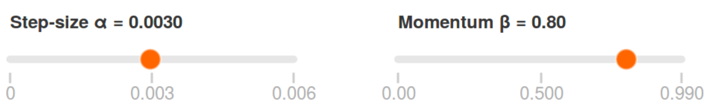

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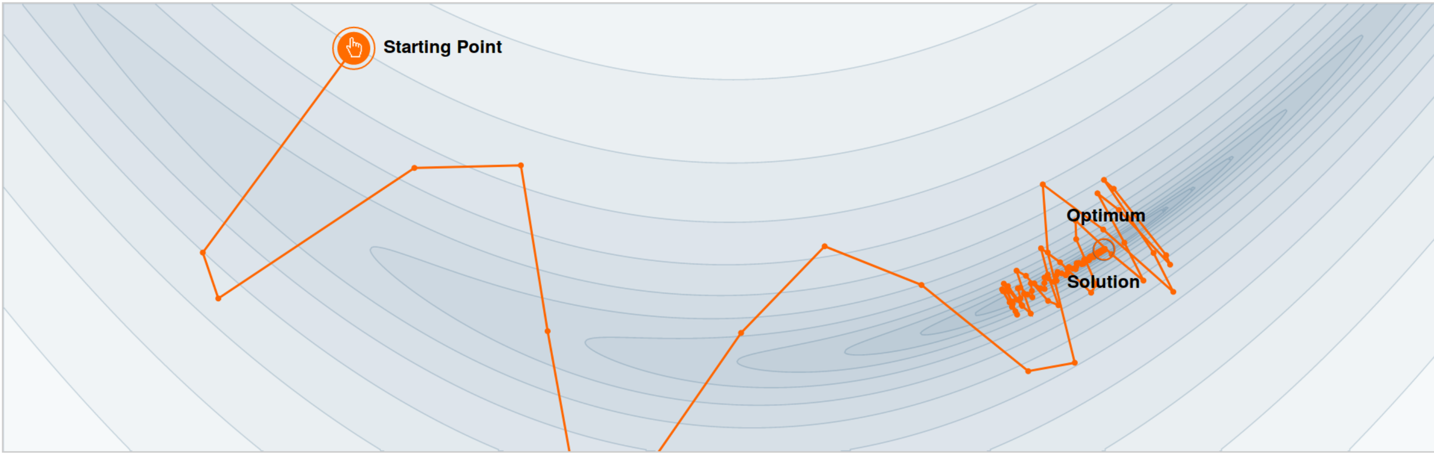

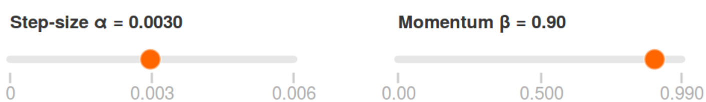

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- But well-tuned SGD with LR scheduling can generalize better than Adam (with naive l2 reg)...
- Active area of research: K-FAC stochastic second-order method based on an invertible approximation of the Fisher information matrix of the network.

The Karpathy Constant for Adam

Andrej Karpathy
@karpathy

Following

3e-4 is the best learning rate for Adam, hands down.

4:01 AM - 24 Nov 2016

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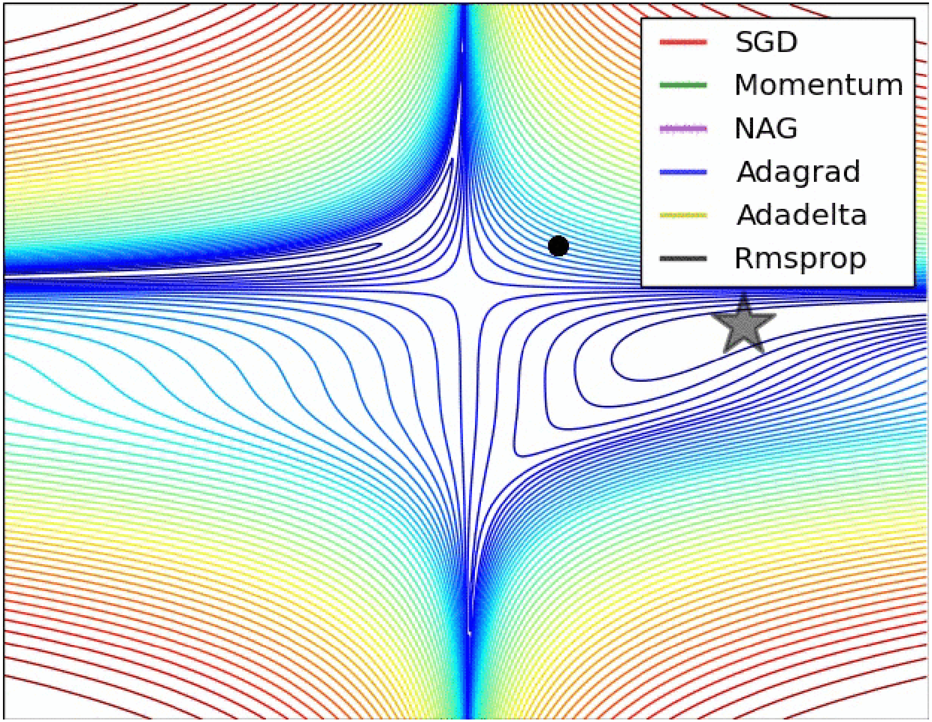
Optimizers around a saddle point



Credits: Alec Radford

Lab 2: back in 15min!