Neural networks and Backpropagation

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https://github.com/m2dsupsdlclass/lectures-labs

Neural Network for classification

Vector function with tunable parameters θ

$$\mathbf{f}(\cdot;\theta) : \mathbb{R}^N \rightarrow (0,1)^K$$

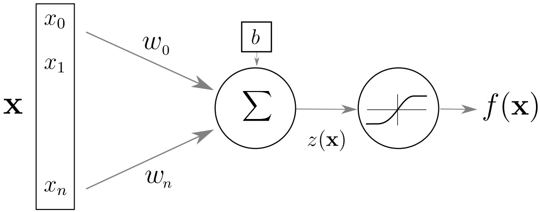
Sample s in dataset S:

- input: $\mathbf{x}^s \in \mathbb{R}^N$
- 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

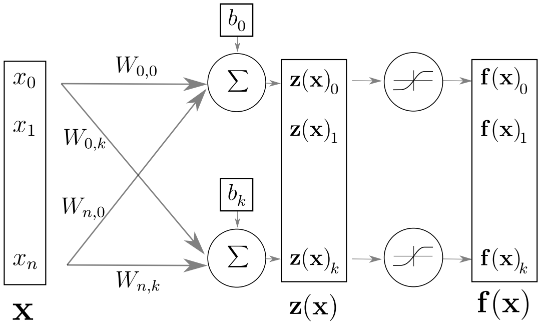


$$z(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

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

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

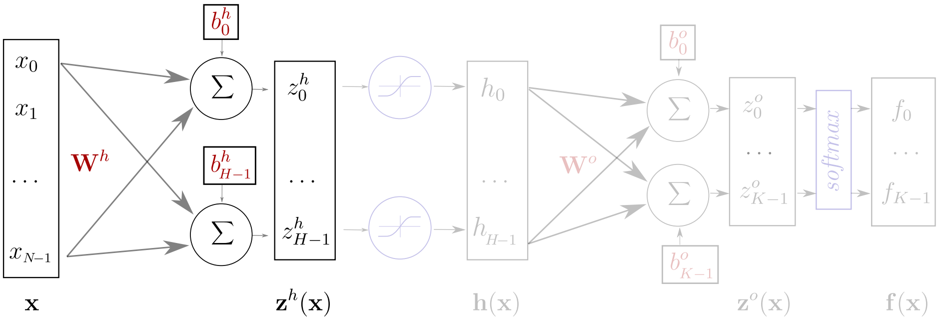
Layer of Neurons



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

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

One Hidden Layer Network



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

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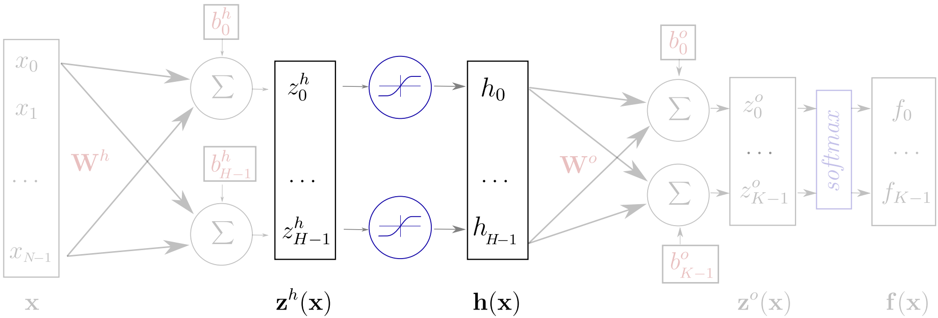

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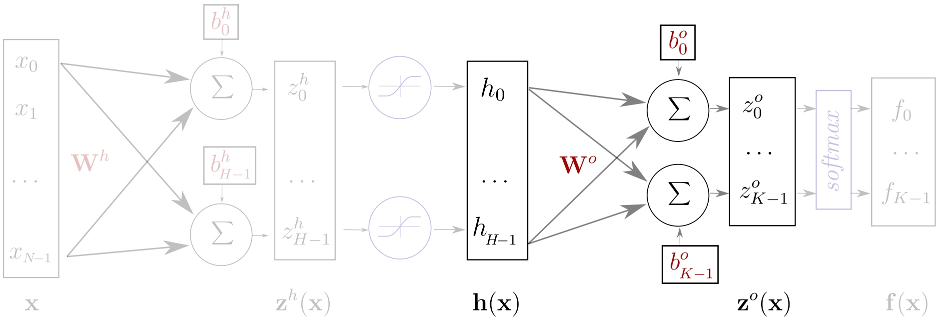

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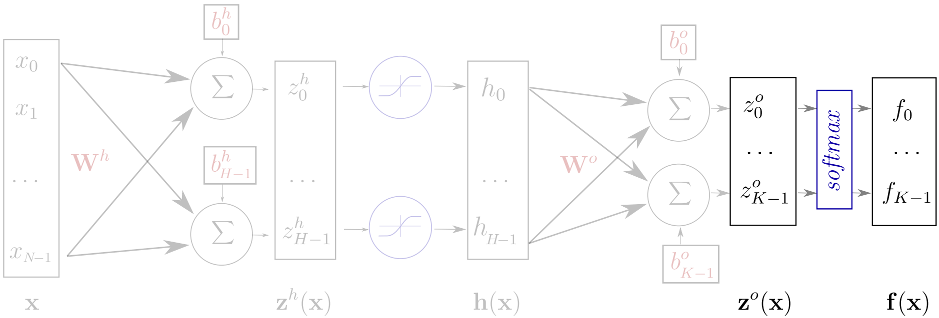

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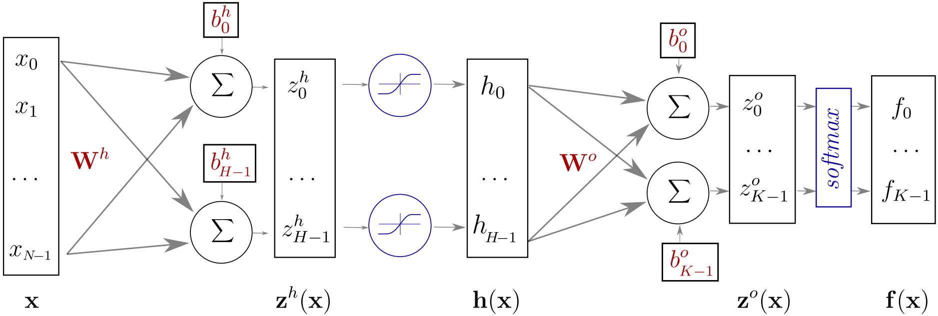
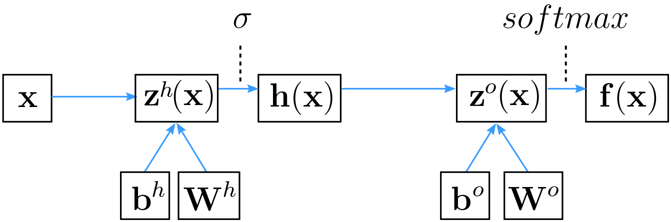
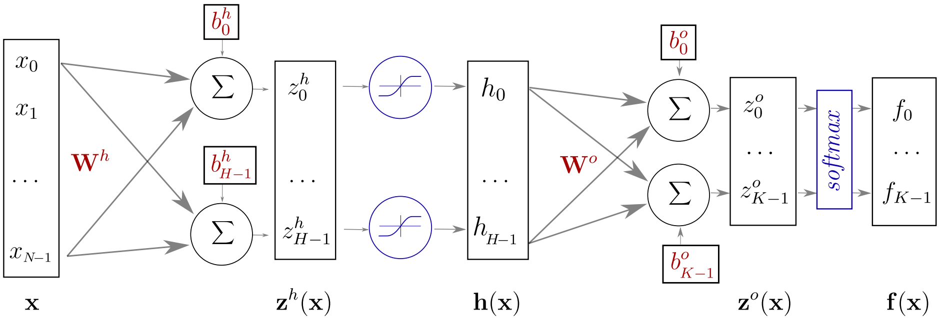


Alternate representation



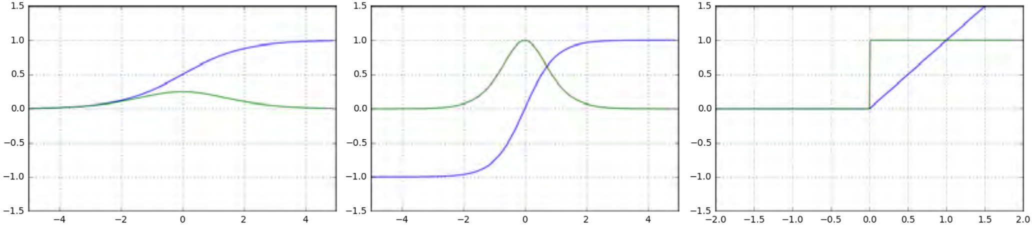
One Hidden Layer Network



Keras implementation

```
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



$$\mathrm{sigm}(x) = \frac{1}{1+e^{-x}} \qquad \tanh(x) = \frac{e^{2x}-1}{e^{2x}+1} \qquad \mathrm{relu}(x) = \max(0, x)$$

$$\mathrm{sigm}'(x) = \mathrm{sigm}(x)(1-\mathrm{sigm}(x)) \qquad \tanh'(x) = 1 - \tanh(x)^2 \qquad \mathrm{relu}'(x) = 1_{x>0}$$

- blue: activation function
- green: derivative

Softmax function

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

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

- 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"

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)

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

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

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):

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

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

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

Stochastic Gradient Descent

Initialize θ randomly

For E epochs perform:

- Randomly select a small batch of samples $(B \subset S)$
  - Compute gradients: $\Delta = \nabla_\theta L_B(\theta)$
  - Update parameters: $\theta \leftarrow \theta - \eta\Delta$
  - $\eta > 0$ is called the learning rate
- Repeat until the epoch is completed (all of S is covered)

Stop when reaching criterion:

- nll stops decreasing when computed on validation set

Computing Gradients

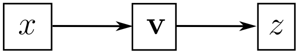
Output Weights: $\frac{\partial l(\mathbf{f(x)},y)}{\partial W^{o}_{i,j}}$

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

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

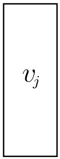
Hidden bias: $\frac{\partial l(\mathbf{f(x)},y)}{\partial b^{h}_{i}}$

Chain rule



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

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



$\mathbf{v}$

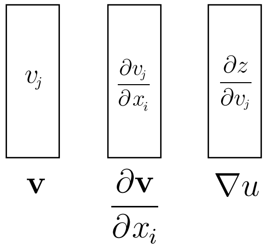
Chain rule

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

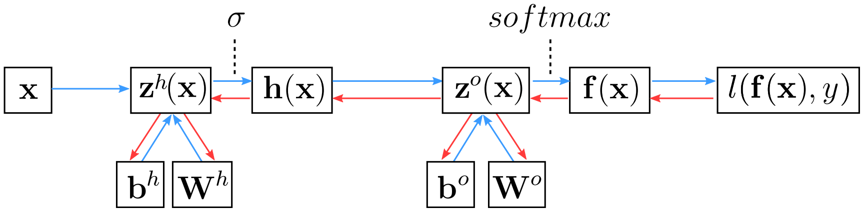
$$z = u(\mathbf{v}(\mathbf{x}))$$

chain-rule

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



Backpropagation



Compute partial derivatives of the loss

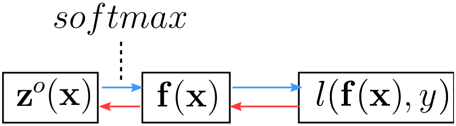
- $\frac{\partial l(\mathbf{f}(\mathbf{x}),y)}{\partial \mathbf{f}(\mathbf{x})_i} = \frac{\partial - \log \mathbf{f}(\mathbf{x})_y}{\partial \mathbf{f}(\mathbf{x})_i} = \frac{-1_{y=i}}{\mathbf{f}(\mathbf{x})_y} = \frac{\partial \boldsymbol{l}}{\partial \mathbf{f}(\mathbf{x})_i}$
- $\frac{\partial \boldsymbol{l}}{\partial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

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

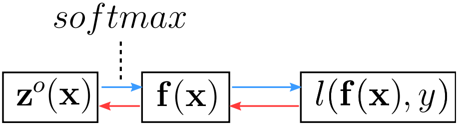
$$= \sum_j \frac{-1_{y=j}}{\mathbf{f}(\mathbf{x})_y} \frac{\partial softmax(\mathbf{z}^o(\mathbf{x}))_j}{\partial \mathbf{z}^o(\mathbf{x})_i}$$

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

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



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



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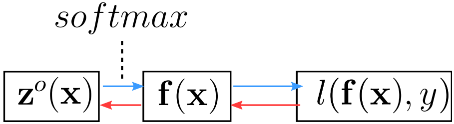
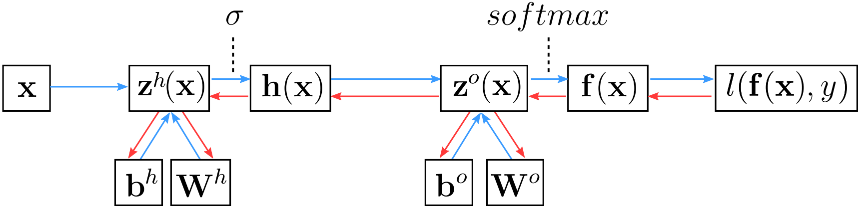
\end{aligned}
$$

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

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



Backpropagation

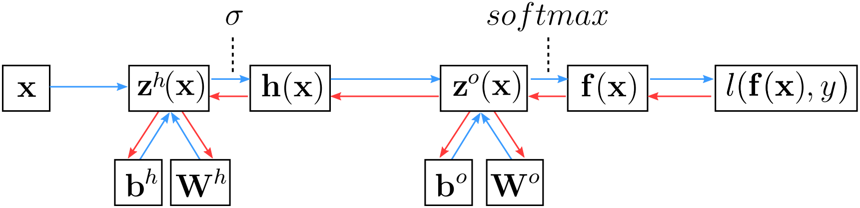


Gradients

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

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

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

Compute layer params gradients

- $\nabla_{\mathbf{W}^o} \boldsymbol{l} = \nabla_{\mathbf{z}^o(\mathbf{x})} \boldsymbol{l} \cdot \mathbf{h}(\mathbf{x})^\top$
- $\nabla_{\mathbf{b}^o} \boldsymbol{l} = \nabla_{\mathbf{z}^o(\mathbf{x})} \boldsymbol{l}$

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

Initialization and normalization

- Input data should be normalized to have approx. same range:
  - standardization or quantile normalization
- Initializing W^h and W^o:
  - Zero is a saddle point: no gradient, no learning
  - Constant init: hidden units collapse by symmetry
  - Solution: random init, ex: $w \sim \mathcal{N}(0, 0.01)$
  - Better inits: Xavier Glorot and Kaming He & orthogonal
- Biases can (should) be initialized to zero

SGD learning rate

- Very sensitive:
  - Too high $\rightarrow$ early plateau or even divergence
  - Too low $\rightarrow$ slow convergence
  - Try a large value first: $\eta = 0.1$ or even $\eta = 1$
  - Divide by 10 and retry in case of divergence
- Large constant LR prevents final convergence
  - multiply η_t by $\beta < 1$ after each update
  - 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:

$$
\begin{aligned}
m_t &= \gamma m_{t-1} + \eta \nabla_\theta L_{B_t}(\theta_{t-1}) \\
\theta_t &= \theta_{t-1} - m_t
\end{aligned}
$$

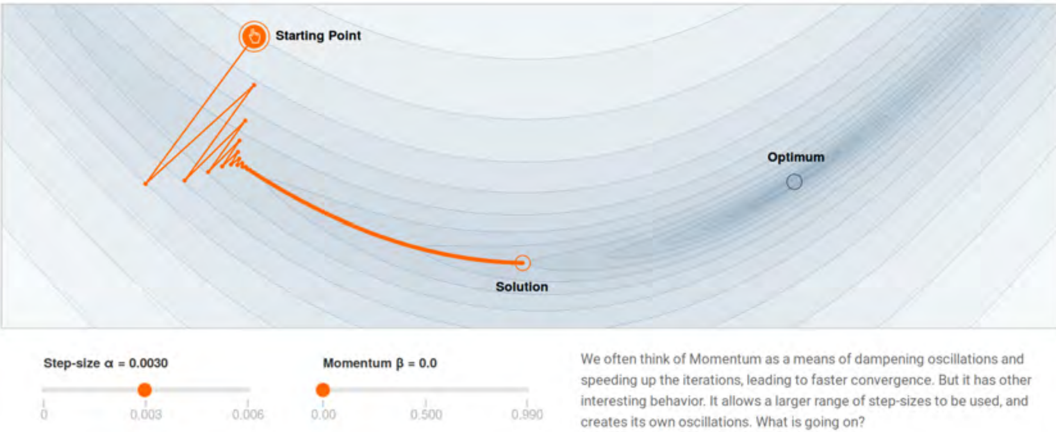
γ is typically set to 0.9

Larger updates in directions where the gradient sign is constant to accelerate in low curvature areas

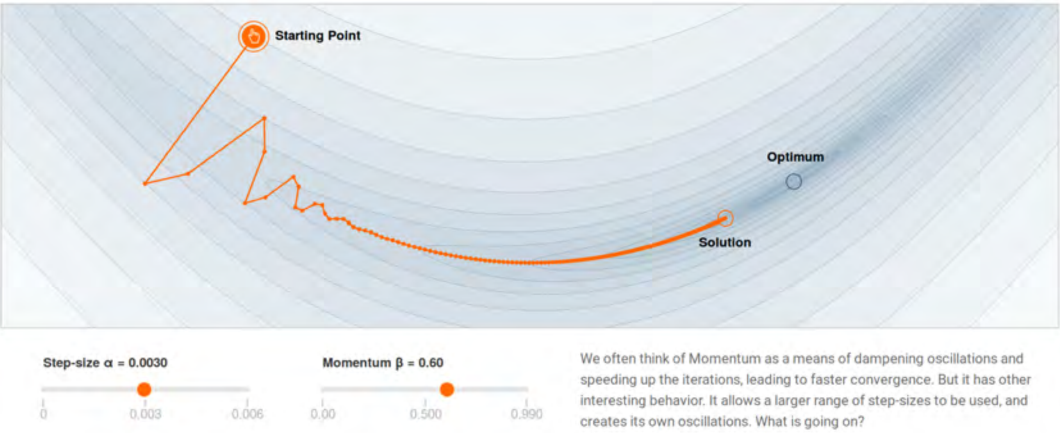
Nesterov accelerated gradient

$$
\begin{aligned}
m_t &= \gamma m_{t-1} + \eta \nabla_\theta L_{B_t}(\theta_{t-1} - \gamma m_{t-1}) \\
\theta_t &= \theta_{t-1} - m_t
\end{aligned}
$$

Better at handling changes in gradient direction.



[Why Momentum Really Works]



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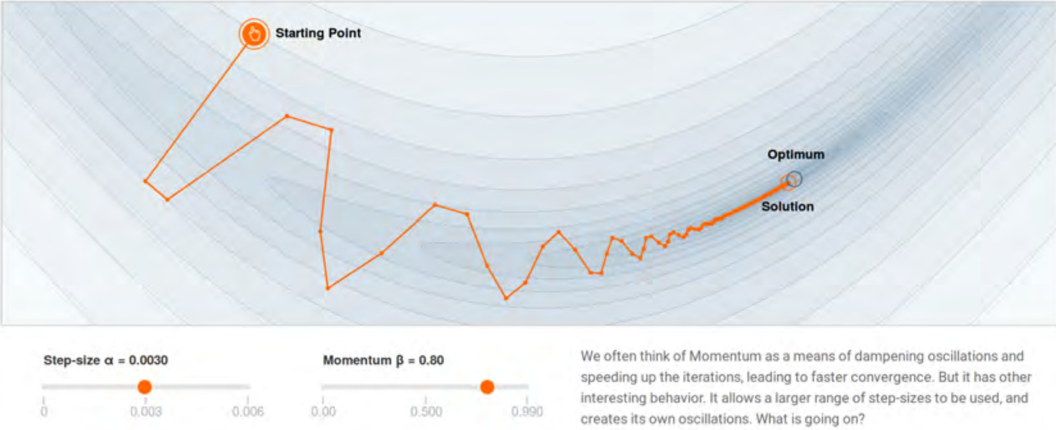

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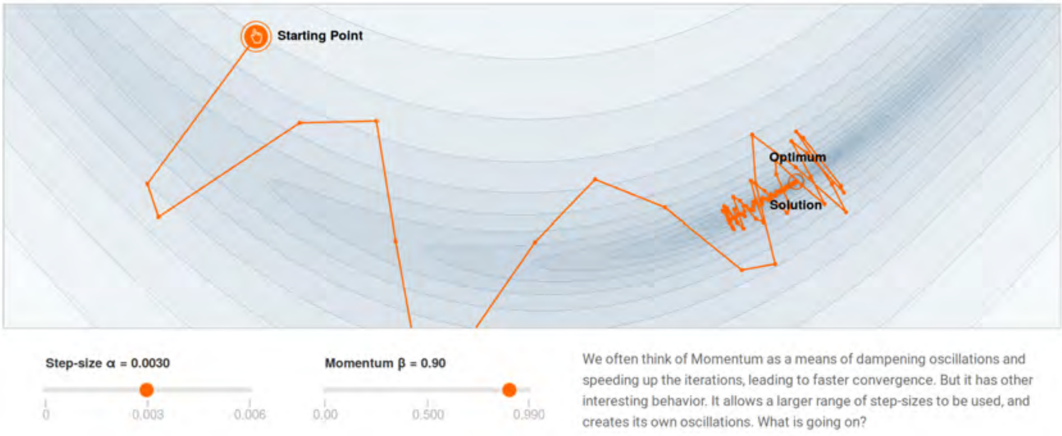


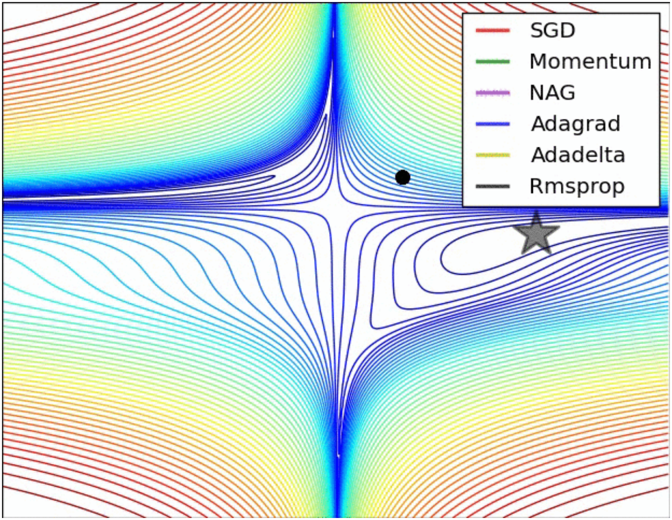
[Why Momentum Really Works]

Alternative optimizers

- SGD (with Nesterov momentum)
    - Simple to implement
    - Very sensitive to initial value of η
    - Need learning rate scheduling
- Adam: adaptive learning rate scale for each param
    - Global η set to 3e-4 often works well enough
    - Good default choice of optimizer (often)
- 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