Neural networks and Backpropagation

Yesterday

- Overview
- Computation graph view of neural networks
- Linear operation followed by non-linear activation

  ...But what is the linear operation, really?

Today

- A closer look at what's going on in a "neuron"
- Backpropagation: how do we train a neural network?

Neural Network for classification

Vector function with tunable parameters θ

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

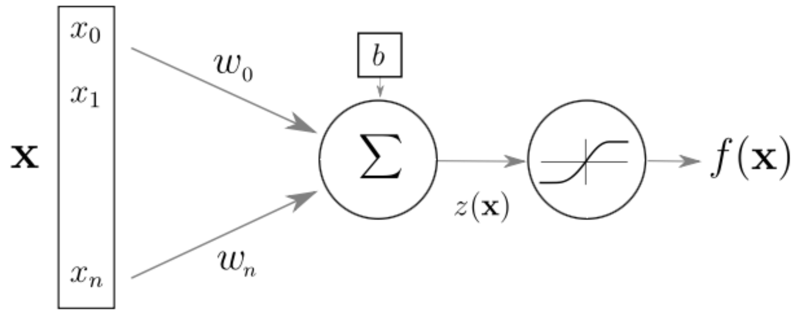
Sample s in dataset S:

- 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



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

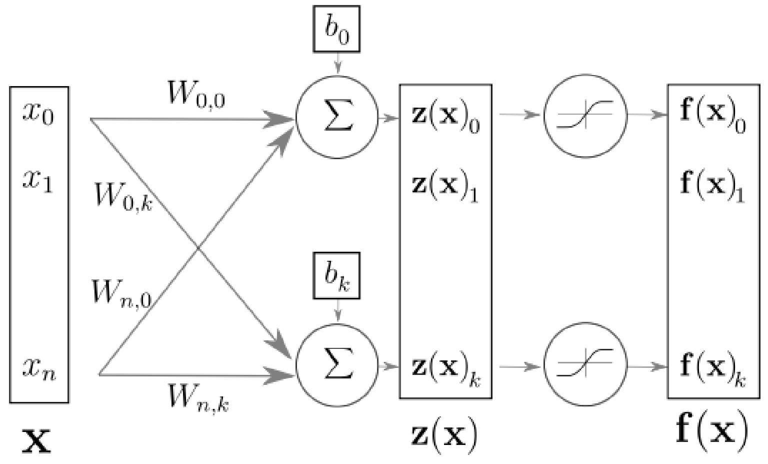
$$f(\mathbf{x}) = g(\mathbf{w}^T\mathbf{x} + b)$$

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

Concrete Example

- Say we have two input dimensions x_1 and x_2 and one output dimension f(x) (sometimes, $\hat{y}$ - the predicted value of y - is used instead of $f(x)$)
- Our weights and biases could be $W = [3, -2]$ and $b = 1$
- Our non-linearity could be ReLU: $g(z) = max(0, z)$
- Now $z(x) = 3x1 - 2x_2 + 1$ and $f(x) = max(0, 3x_1 - 2x_2 + 1)$
- Every neuron in a neural network is a function like this!

Layer of Neurons (Vectorization)

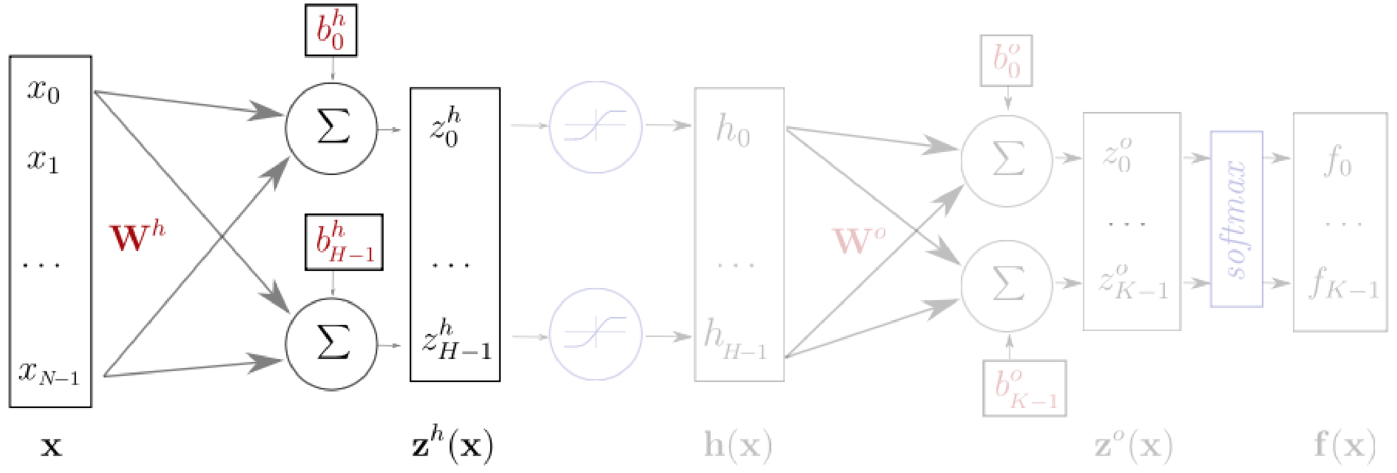


b_0
b_k
x_0
x_1
x_n
$W_{0,0}$
$W_{0,k}$
$W_{n,0}$
$W_{n,k}$
Σ
$\mathbf{z}(\mathbf{x})_0$
$\mathbf{z}(\mathbf{x})_1$
$\mathbf{z}(\mathbf{x})_k$
$\mathbf{f}(\mathbf{x})_0$
$\mathbf{f}(\mathbf{x})_1$
$\mathbf{f}(\mathbf{x})_k$
$\mathbf{x}$
$\mathbf{z}(\mathbf{x})$
$\mathbf{f}(\mathbf{x})$

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

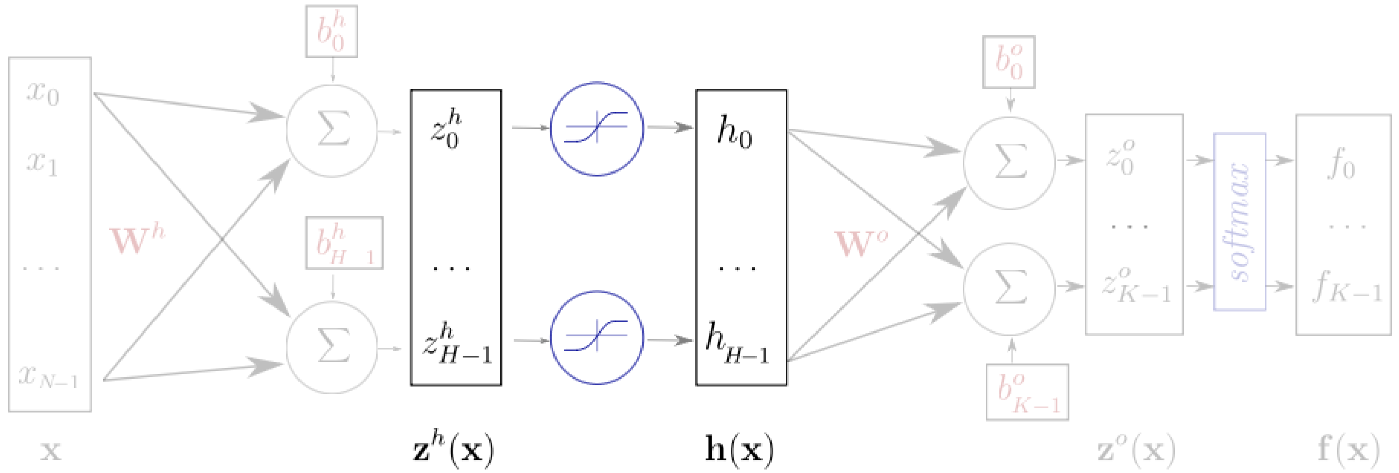
- $\mathbf{W}, \mathbf{b}$ now matrix and vector

One Hidden Layer Network



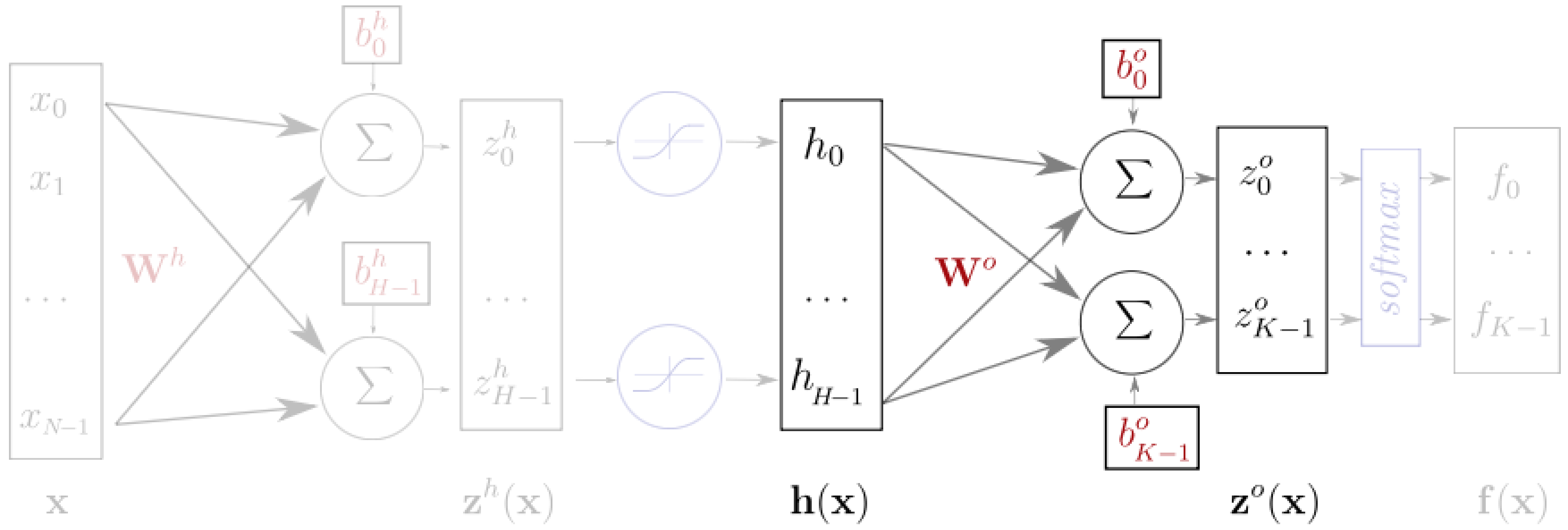
- $\mathbf{z}^h(\mathbf{x}) = \mathbf{W}^h\mathbf{x} + \mathbf{b}^h$

One Hidden Layer Network



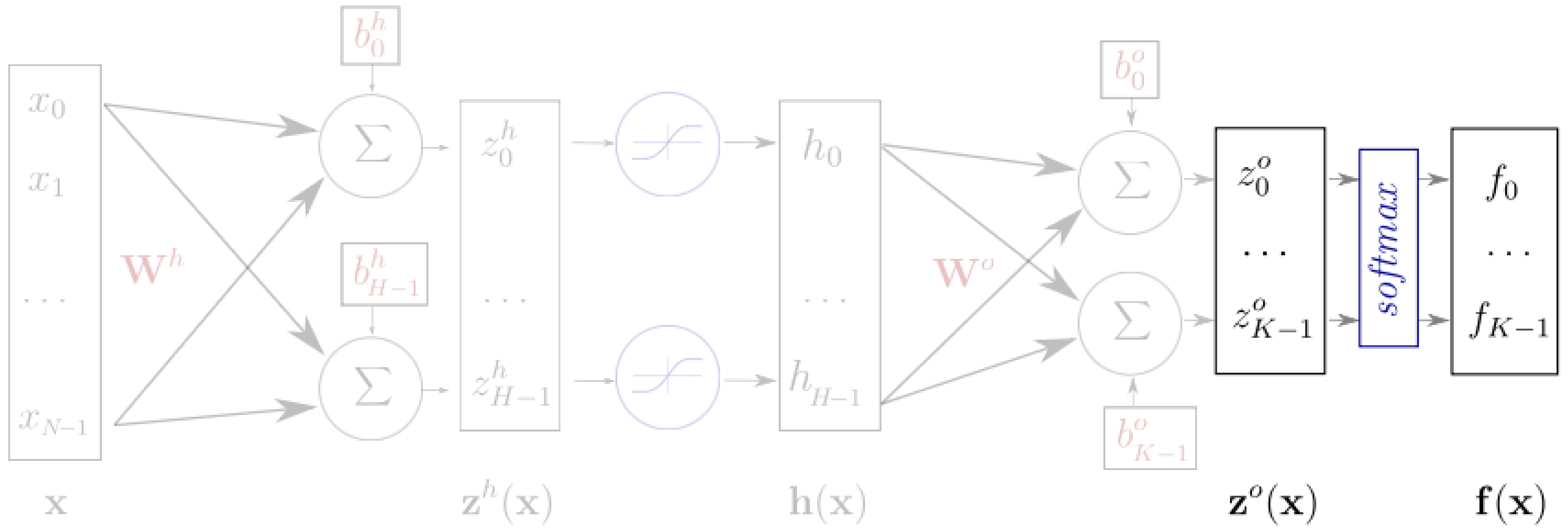
- $\mathbf{h}(\mathbf{x}) = g(\mathbf{z}^h(\mathbf{x})) = g(\mathbf{W}^h\mathbf{x}$

One Hidden Layer Network



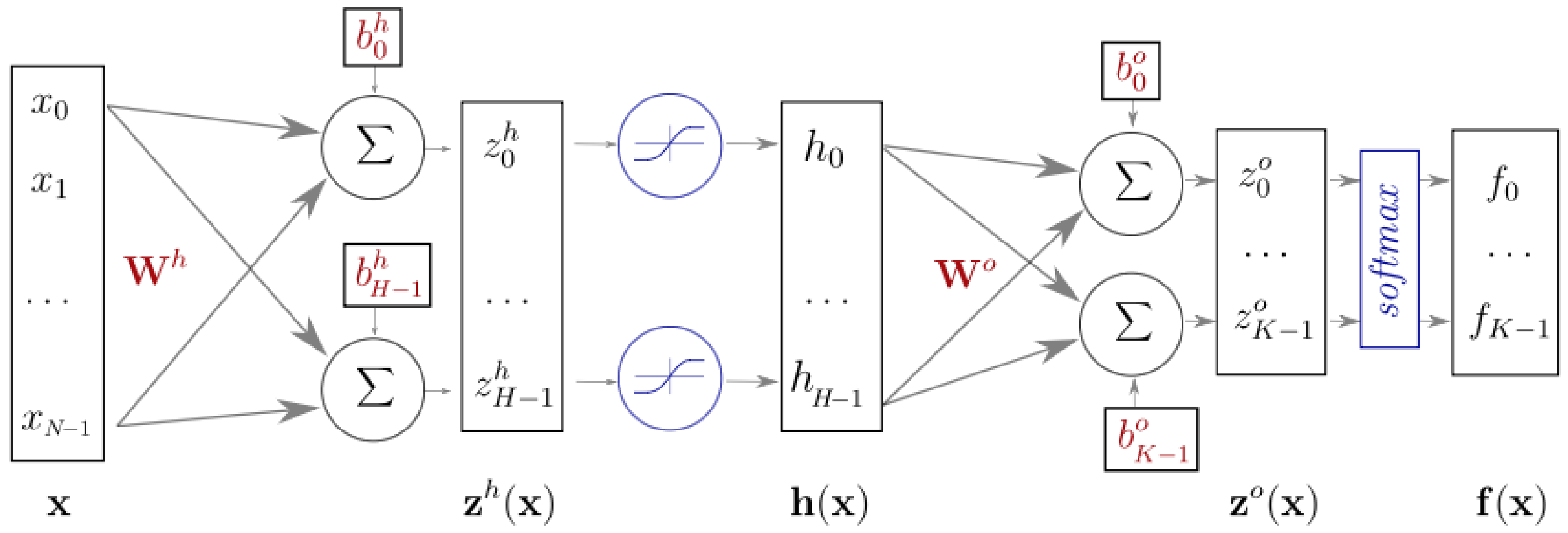
- $\mathbf{z}^o(\mathbf{x}) = \mathbf{W}^o\mathbf{h}(\mathbf{x}) + \mathbf{b}^o$

One Hidden Layer Network

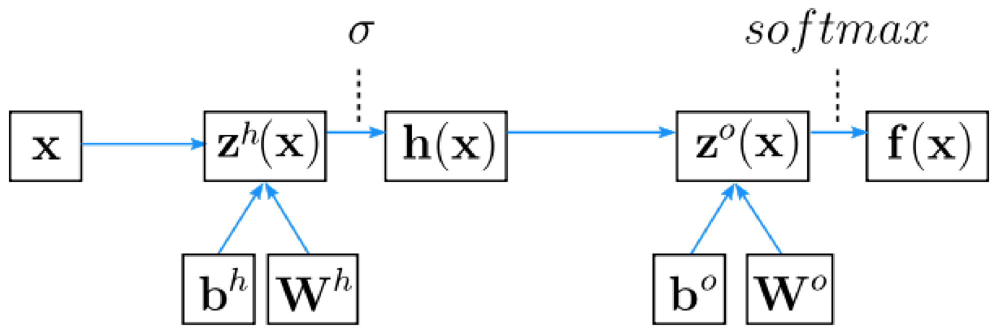


- $\mathbf{f}(\mathbf{x}) = softmax(\mathbf{z}^o) = softmax(\mathbf{W}^o\mathbf{h}(\mathbf{x}) + \mathbf{b}^o)$

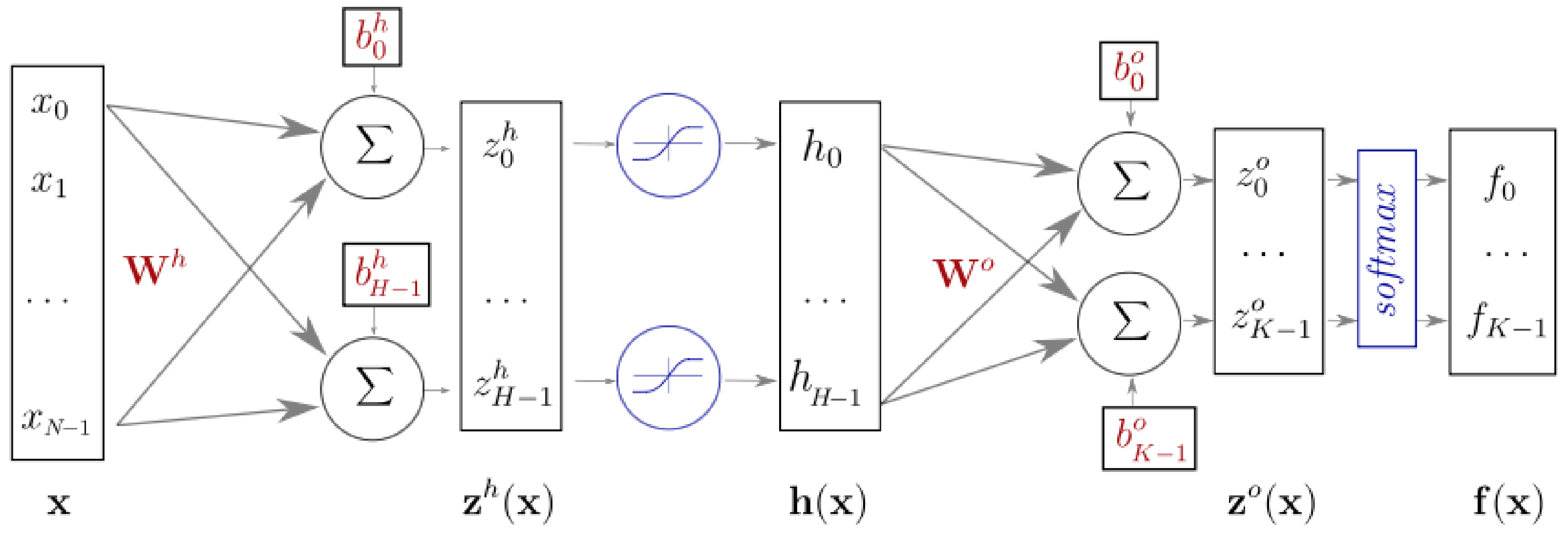
One Hidden Layer Network



Alternate representation


$$\begin{tikzcd}
\boxed{\mathbf{x}} \arrow[r] & \boxed{\mathbf{z}^h(\mathbf{x})} \arrow[r, "\sigma"] & \boxed{\mathbf{h}(\mathbf{x})} \arrow[r] & \boxed{\mathbf{z}^o(\mathbf{x})} \arrow[r, "softmax"] & \boxed{\mathbf{f}(\mathbf{x})} \\
 & \boxed{\mathbf{b}^h}\ \boxed{\mathbf{W}^h} \arrow[u] & & \boxed{\mathbf{b}^o}\ \boxed{\mathbf{W}^o} \arrow[u] &
\end{tikzcd}$$

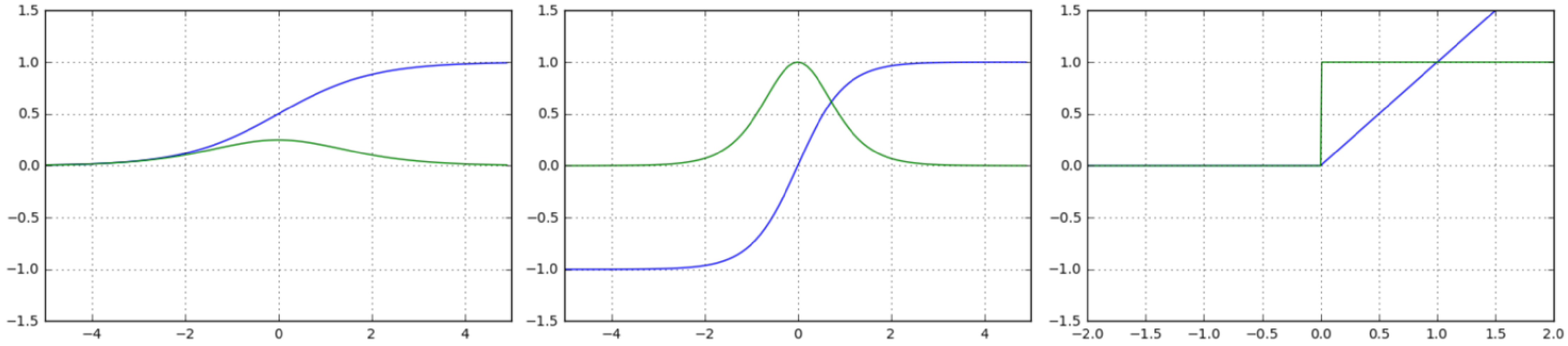
One Hidden Layer Network



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

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

- vector of values in (0, 1) that add up to 1
- for example, $\mathbf{x} = [1, 2, 3]$ becomes $\frac{1}{e^1+e^2+e^3} \cdot [e^1, e^2, e^3]^T = [0.09, 0.24, 0.67]$
- $p(Y = c|X = \mathbf{x}) = \text{softmax}(\mathbf{z}(\mathbf{x}))_c$
- the pre-activation vector $\mathbf{z}(\mathbf{x})$ is often called "the logits"

Training the network

Find parameters 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 $y^s = 3$

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

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 $s \in S$:

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

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

- Now we have a mathematical function representing the network
- And we have a way of measuring how good it is
- How do we find the parameters that minimize the loss?

Gradient Descent

- Let's imagine we only have one parameter θ
- We can compute the derivative of the loss with respect to θ
- The derivative, $\frac{dL}{d\theta}$, tells us the slope of the loss function at a given point
- If $\frac{dL}{d\theta} > 0$, increasing θ will increase the loss, and vice versa
- To minimize loss, we adjust θ in the opposite direction of $\frac{dL}{d\theta}$
- This is done using the update rule: $\theta = \theta_{old} - \eta \frac{dL}{d\theta}$

Gradient Descent

- We can use gradient descent to play "guess what number I'm thinking of"
- If your guess is too high, you decrease it
- If your guess is too low, you increase it
- The error function is a parabola
- By finding the lowest point on the parabola, you find the best guess

Implementing Gradient Descent

- Start with an initial guess for θ
- Calculate $\frac{dL}{d\theta}$ using the current value of θ
- Update θ using the update rule
- Repeat the process until the change in loss is below a threshold or a set number of iterations is reached
- The choice of learning rate η is crucial: too high, and we may overshoot the minimum; too low, and convergence will be slow

Stochastic Gradient Descent

- Traditional Gradient Descent uses the entire dataset to compute the gradient, which can be computationally expensive
- Stochastic Gradient Descent (SGD) updates the parameters using only a single data point (or a small batch)
- In SGD, for each iteration, a data point (or batch) is randomly selected to compute the gradient
- Since only a subset of data is used, the gradient estimation can be noisy, leading to a less smooth path towards the minimum
- However, SGD is much faster than traditional gradient descent

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: $\theta \leftarrow \theta - \eta\Delta$
- 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: $\frac{\partial l(\mathbf{f(x)},y)}{\partial W^o_{i,j}}$

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

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

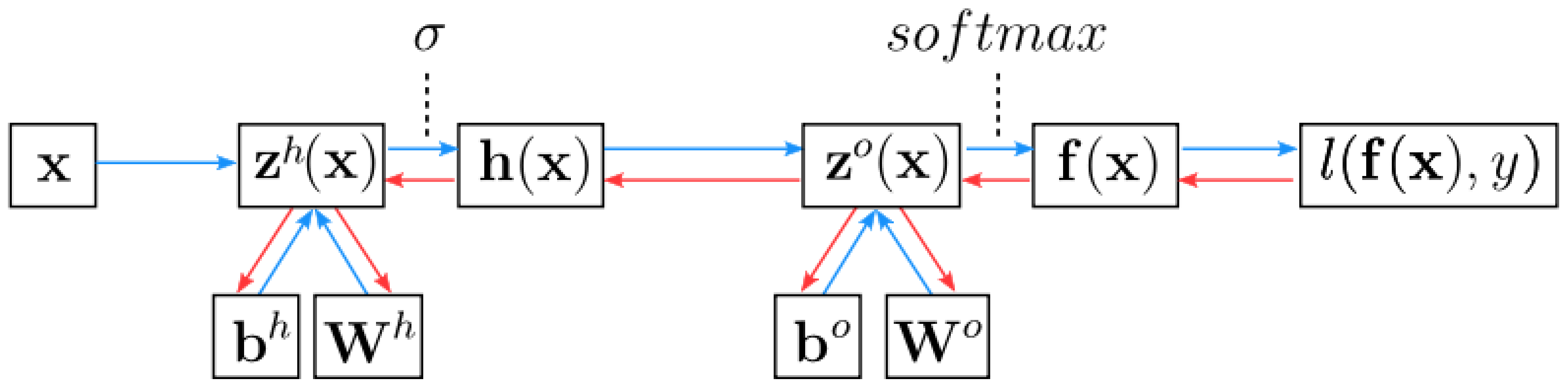
Hidden bias: $\frac{\partial l(\mathbf{f(x)},y)}{\partial b^h_i}$

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

Chain rule

- Mathematical theorem that lets us compute derivatives when functions are inside other functions
- Remember, our neural network is a composition of functions: $f(x) = g(h(x))$
- The chain rule tells us how to compute $\frac{df}{dx}$
- $\frac{df}{dx} = \frac{df}{dg}\frac{dg}{dh}\frac{dh}{dx}$
- In English: The derivative of the overall network with respect to its input is the product of derivatives of each function in the network

Backpropagation



- Compute partial derivatives of the loss
- For any given function in the network, we can compute how changing its parameters will affect the loss
- In other words, we can find how much each parameter's value contributes to the loss

Initialization and Learning Tricks

Initialization and normalization

- Input data should be normalized to have approx. same range:
  - standardization or quantile normalization
- Initializing weights:
  - Zero is a saddle point: no gradient, no learning
  - Constant init: all neurons compute the same function
  - Solution: random init, ex: $w \sim \mathcal{N}(0, 0.1)$
  - 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

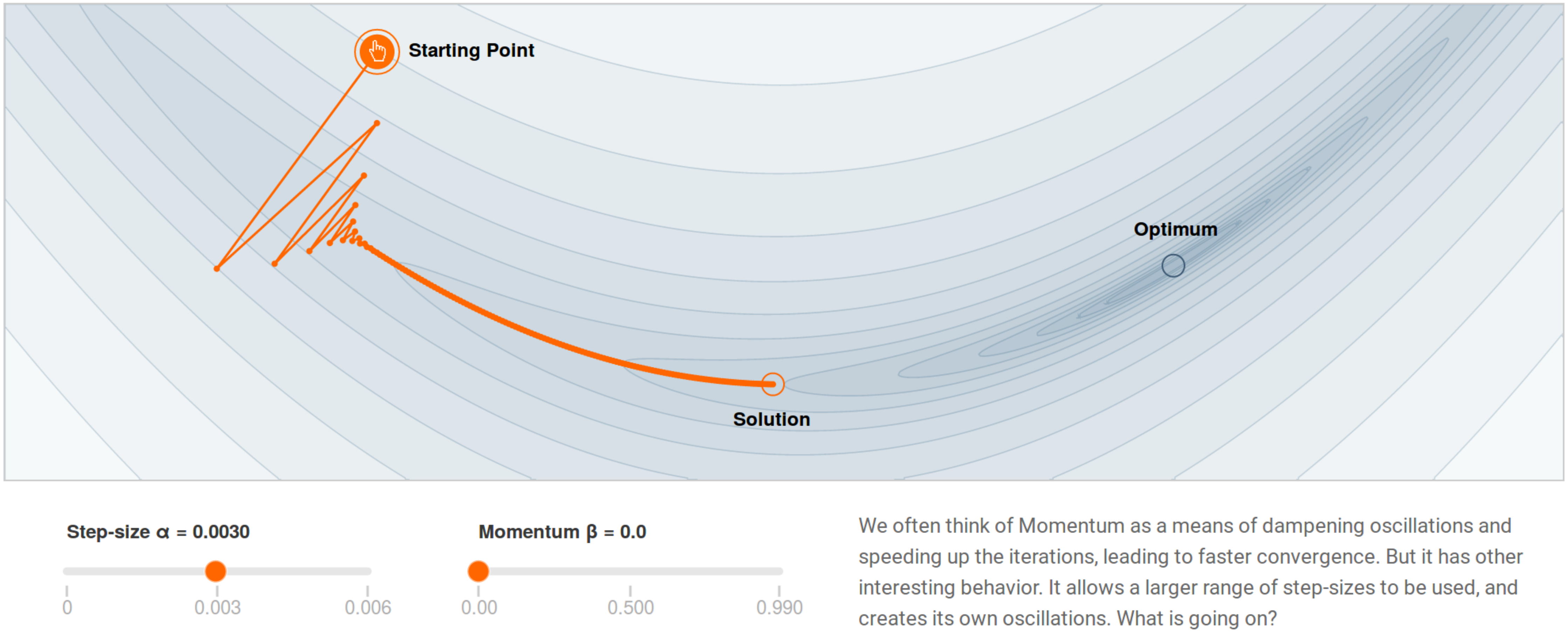
Accumulate gradients across successive updates:

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

$$\theta_t = \theta_{t-1} - m_t$$

γ is typically set to 0.9

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

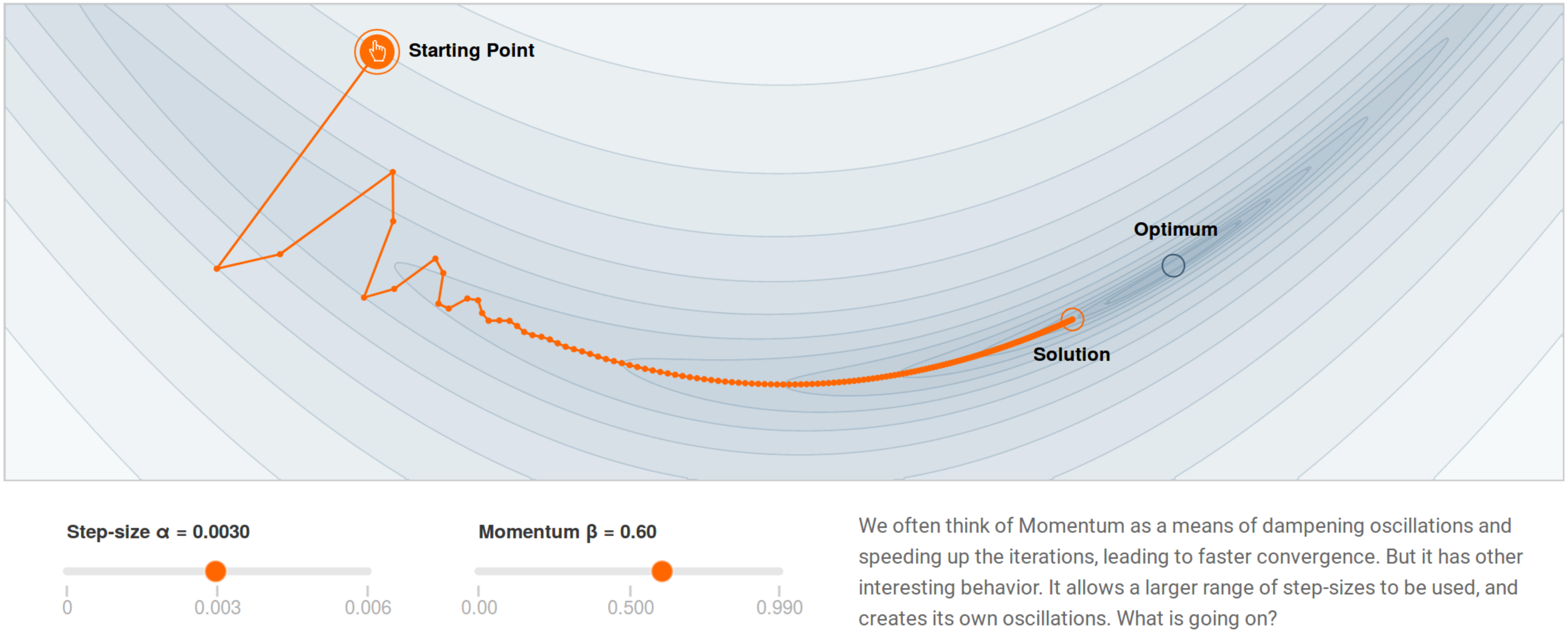


Step-size α = 0.0030

Momentum β = 0.0

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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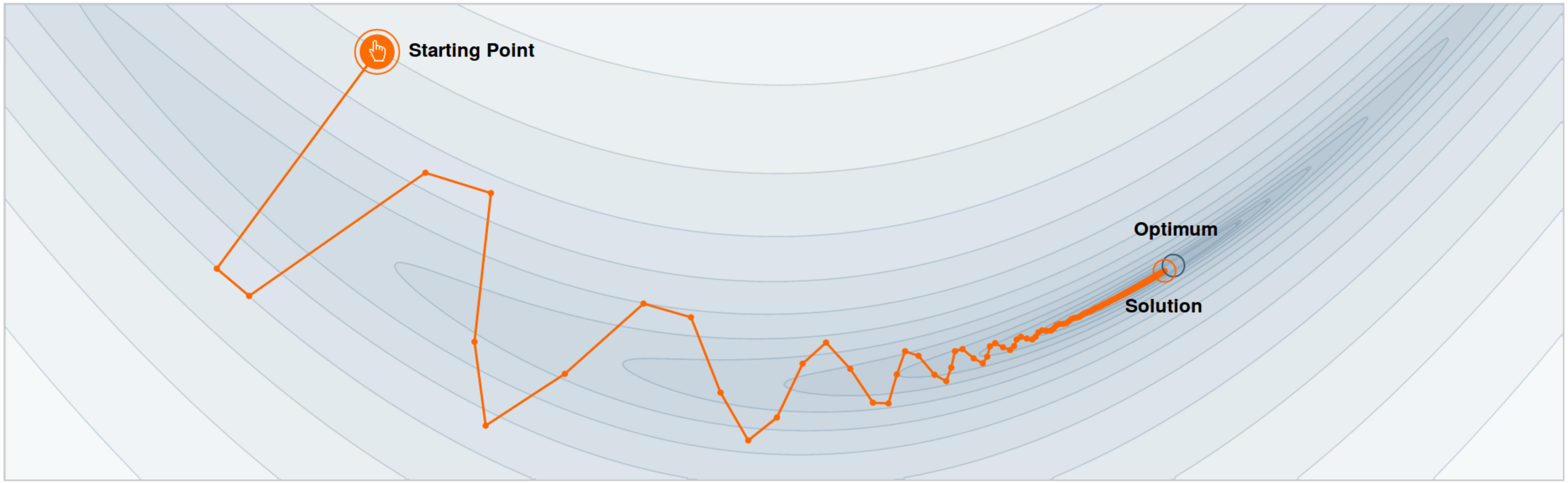

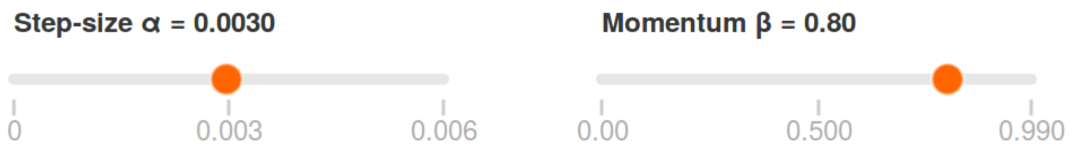

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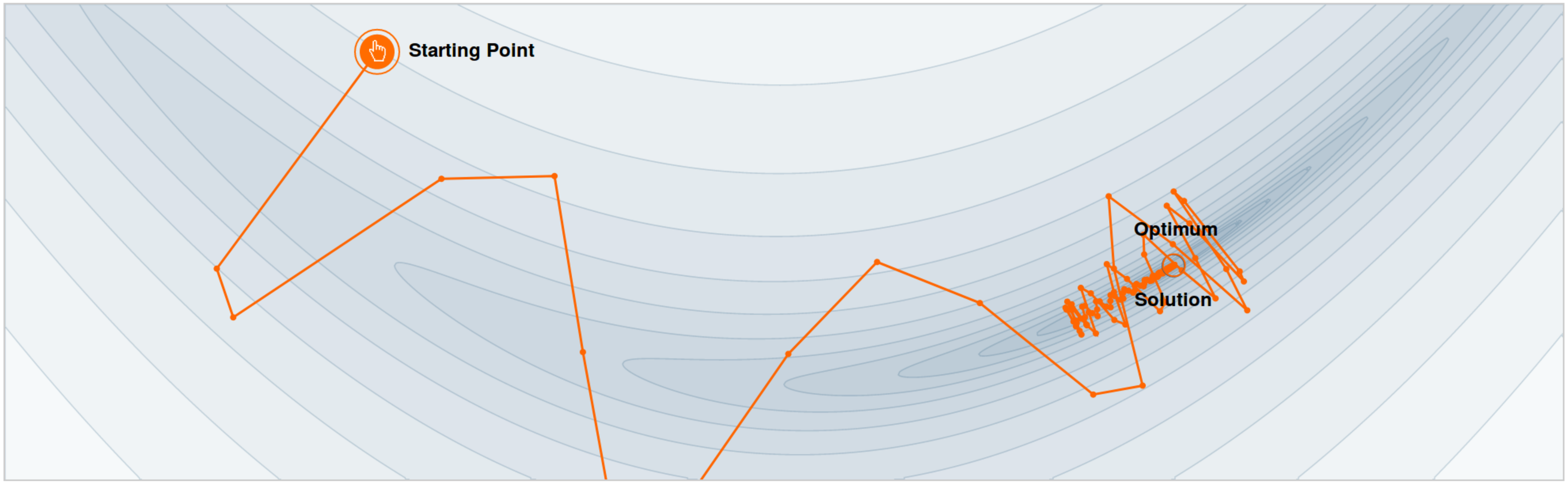


Step-size α = 0.0030

Momentum β = 0.90

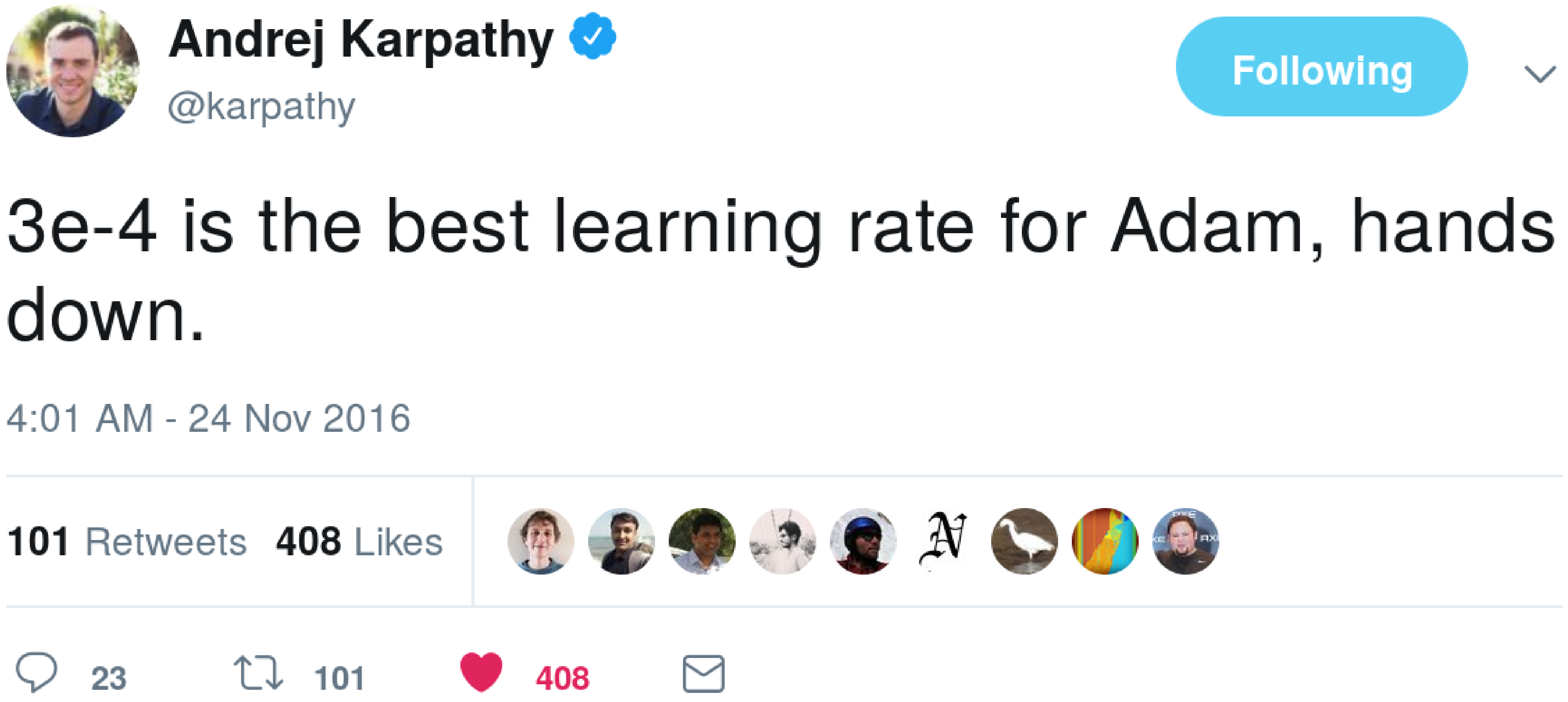
We often think of Momentum as a means of dampening oscillations and speeding up the iterations, leading to faster convergence. But it has other interesting behavior. It allows a larger range of step-sizes to be used, and creates its own oscillations. What is going on?

Why Momentum Really Works

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)
- Many other promising methods:
  - RMSProp, Adagrad, Adadelta, Nadam, ...
  - Often takes some experimentation to find the best one

The Karpathy Constant for Adam



Andrej Karpathy
@karpathy

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

4:01 AM - 24 Nov 2016

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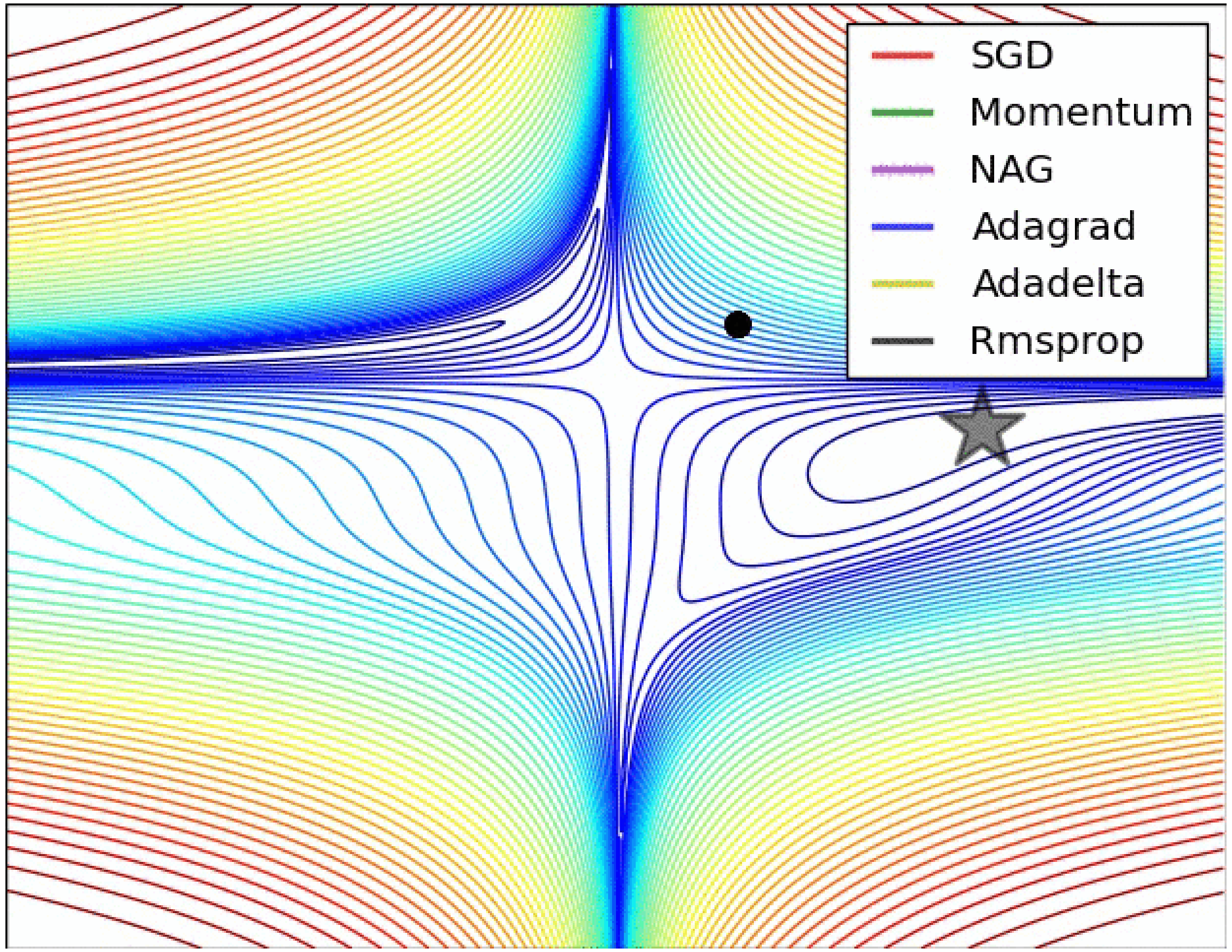
Optimizers around a saddle point



Credits: Alec Radford

Next: Lab 2!