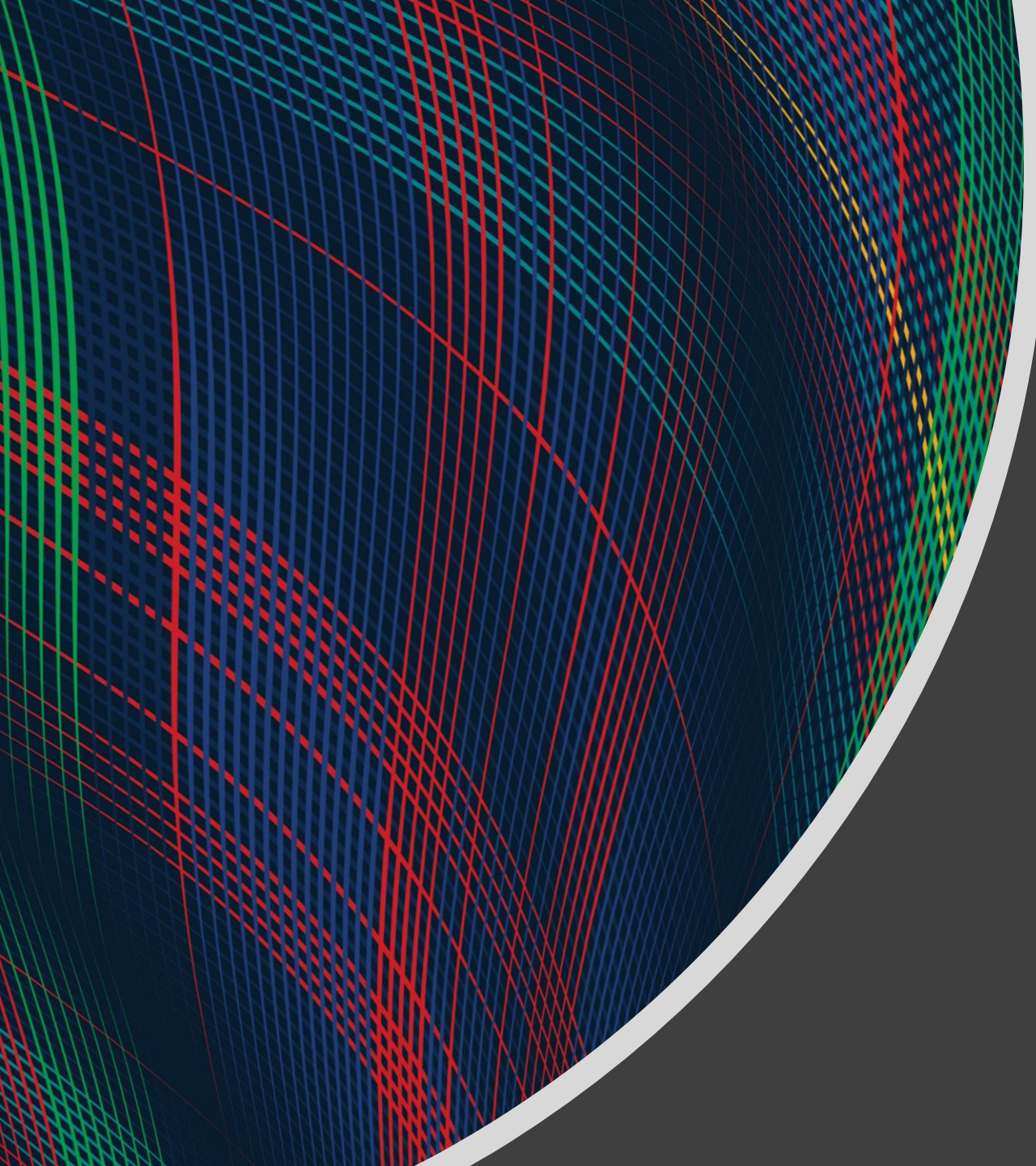


An abstract graphic on the left side of the slide, featuring a sphere-like shape composed of a dense grid of intersecting red, green, and blue lines. The lines are curved and follow the contour of the sphere, creating a complex, woven pattern. The sphere is set against a dark gray background.

10-315
Introduction to ML

Neural Networks

Instructor: Pat Virtue

Outline

Last time: Neural Networks

- Three-neuron network + optimization
- Neural network structure (adding more neurons)
- Forward pass and Backpropagation (scalar version)

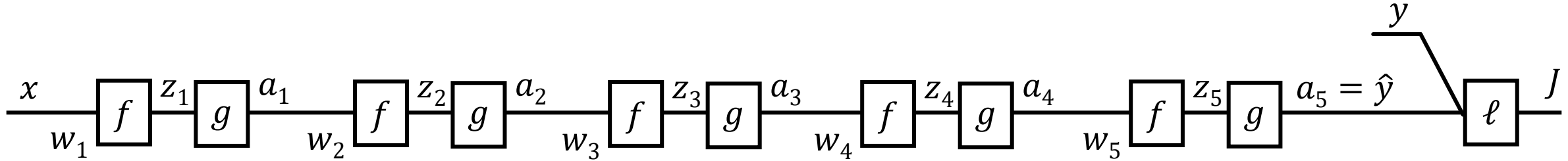
Today: Neural Networks

- Calculus: multi-variate chain rule
- Backpropagation (vector version)
- Optimization intuition (sliders)
- Neural Network Properties and Intuition

Forward Pass

$$\hat{y} = h_{\theta}(\mathbf{x}) = g \left(w_5 \cdot g \left(w_4 \cdot g \left(w_3 \cdot g \left(w_2 \cdot g(w_1 \cdot x) \right) \right) \right) \right)$$

Width 1 deep network (no bias) (dumb but will help with calculus)



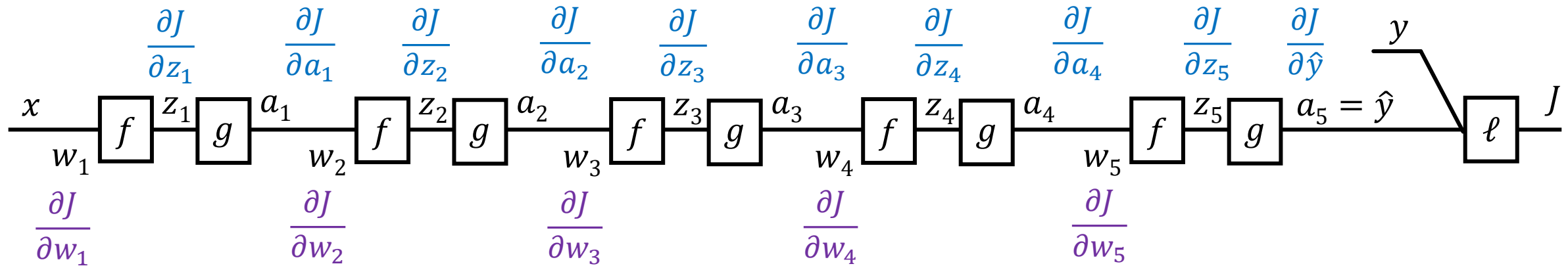
With a new data point (x, y) , we have our current weight values but we don't have $\hat{y}$ (or any of the intermediate values z_ℓ and a_ℓ) or the value of our object function J

The forward pass propagates x (forward) through the network to give us these values

Backpropagation

$$\hat{y} = h_{\theta}(\mathbf{x}) = g \left(w_5 \cdot g \left(w_4 \cdot g \left(w_3 \cdot g \left(w_2 \cdot g \left(w_1 \cdot x \right) \right) \right) \right) \right)$$

Width 1 deep network (no bias) (dumb but will help with calculus)



To do gradient descent we need the partial derivative of the objective with respect to each parameter, $w_{\ell} \leftarrow w_{\ell} - \alpha \frac{\partial J}{\partial w_{\ell}}$

The backward pass propagates the change in the objective with respect to intermediate values ($\frac{\partial J}{\partial z_{\ell}}$ and $\frac{\partial J}{\partial a_{\ell}}$) back through the network to produce each $\frac{\partial J}{\partial w_{\ell}}$

Generic Layer Implementation (so-far)

Compute derivatives per layer, utilizing previous derivatives

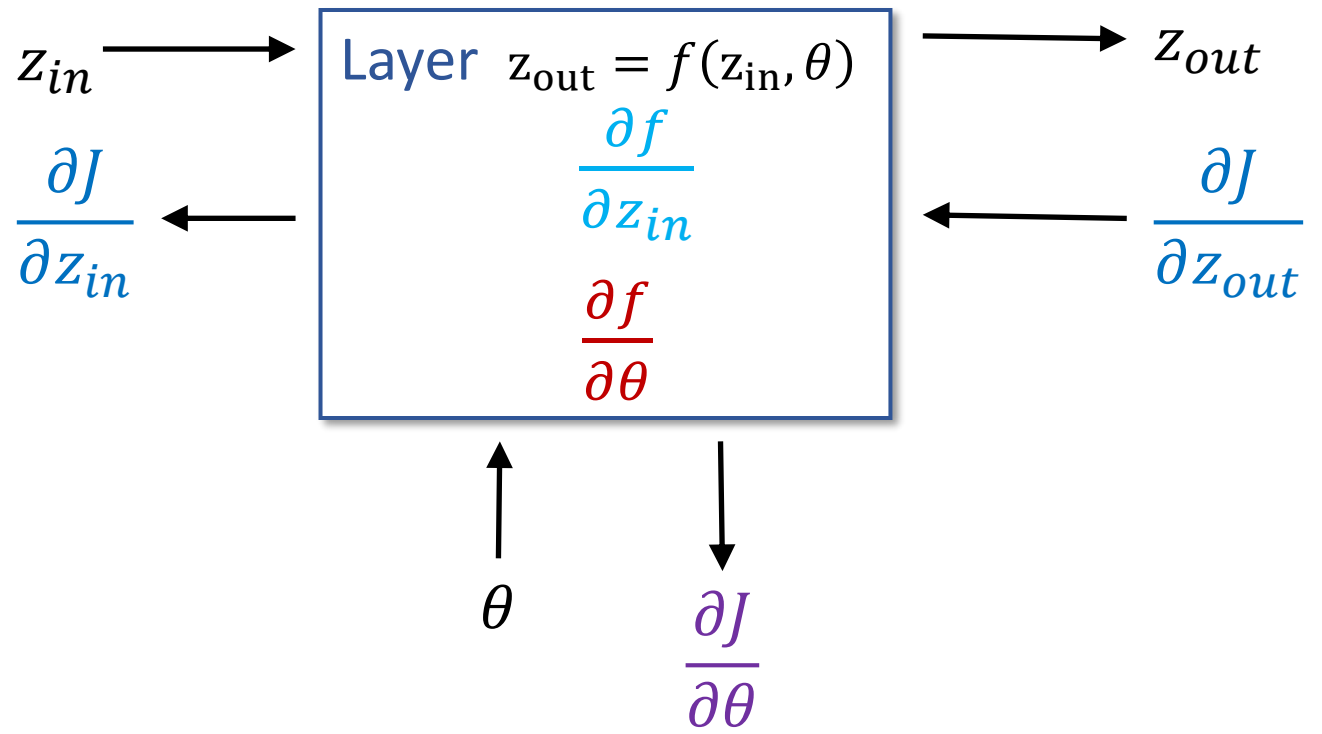
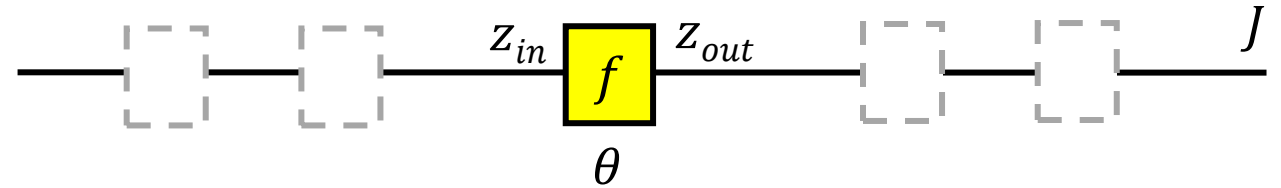
Objective: $J(\theta)$

Arbitrary layer: $z_{out} = f(z_{in}, \theta)$

Need:

- $\frac{\partial J}{\partial z_{in}} = \frac{\partial J}{\partial z_{out}} \frac{\partial f}{\partial z_{in}}$

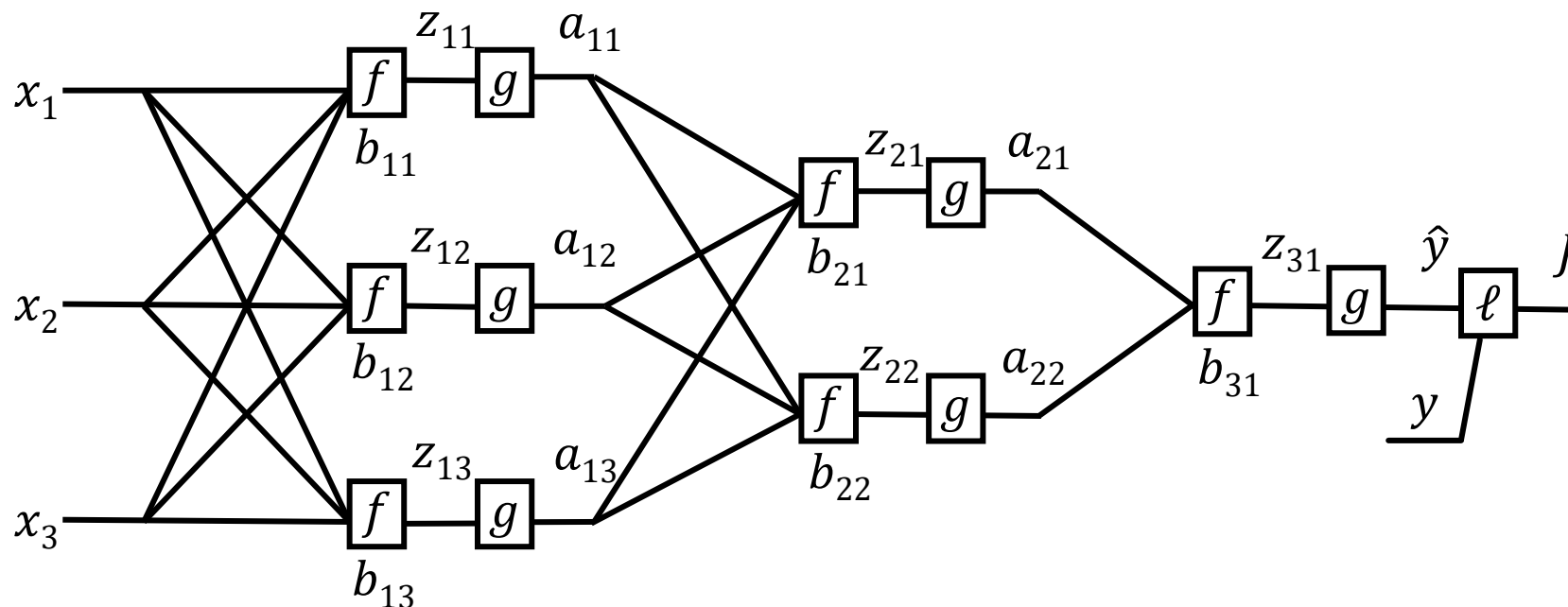
- $\frac{\partial J}{\partial \theta} = \frac{\partial J}{\partial z_{out}} \frac{\partial f}{\partial \theta}$



Optimization

$$\hat{y} = h_{\theta}(\mathbf{x}) = g \left(b_{3,1} + \sum_k w_{3,1,k} g \left(b_{2,k} + \sum_i w_{2,k,i} g \left(b_{1,i} + \sum_j w_{1,i,j} x_j \right) \right) \right)$$

Tons of repeated partial derivatives



$$\frac{\partial J}{\partial b_{3,1}} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial a_{3,1}}{\partial z_{3,1}} \frac{\partial z_{3,1}}{\partial b_{3,1}}$$

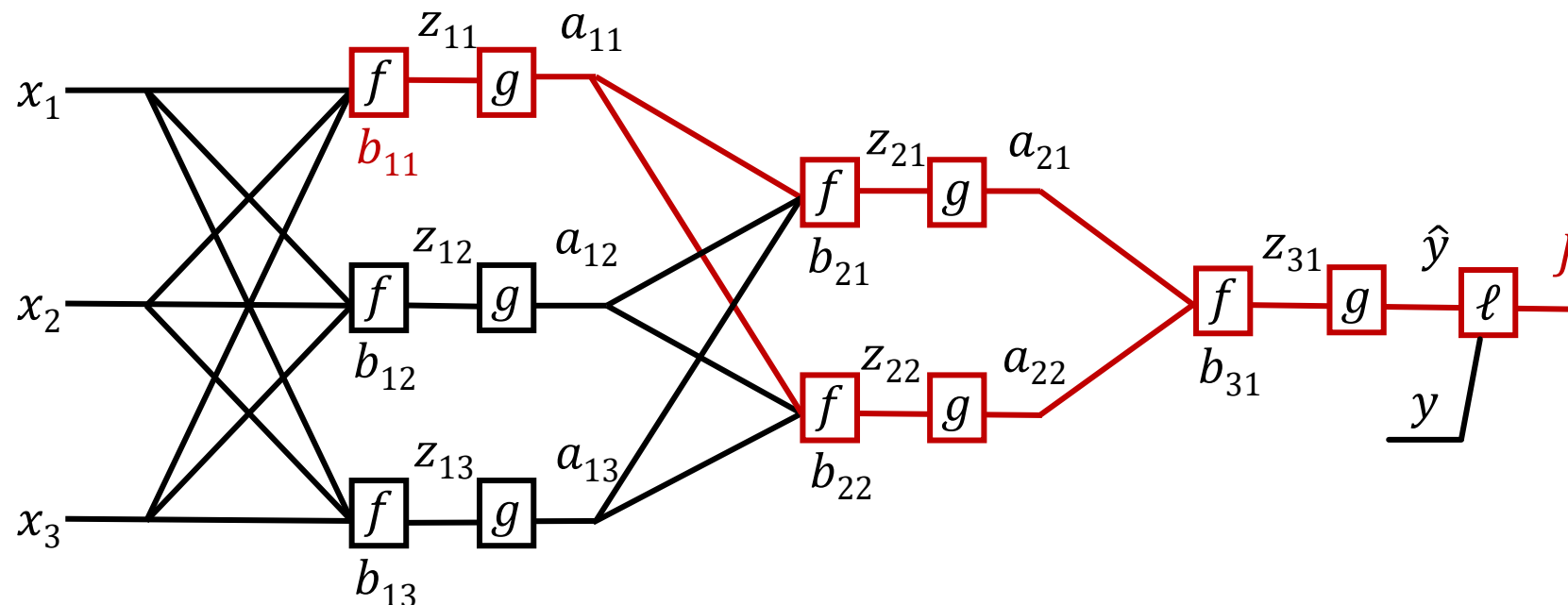
$$\frac{\partial J}{\partial b_{2,i}} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial a_{3,1}}{\partial z_{3,1}} \frac{\partial z_{3,1}}{\partial a_{2,i}} \frac{\partial a_{2,i}}{\partial z_{2,i}} \frac{\partial z_{2,i}}{\partial b_{2,i}}$$

$$\frac{\partial J}{\partial b_{1,i}} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial a_{3,1}}{\partial z_{3,1}} \frac{\partial z_{3,1}}{\partial \mathbf{a}_2} \frac{\partial \mathbf{a}_2}{\partial \mathbf{z}_2} \frac{\partial \mathbf{z}_2}{\partial a_{1,i}} \frac{\partial a_{1,i}}{\partial z_{1,i}} \frac{\partial z_{1,i}}{\partial b_{1,i}}$$

Optimization

$$\hat{y} = h_{\theta}(\mathbf{x}) = g \left(b_{3,1} + \sum_k w_{3,1,k} g \left(b_{2,k} + \sum_i w_{2,k,i} g \left(b_{1,i} + \sum_j w_{1,i,j} x_j \right) \right) \right)$$

Tons of repeated partial derivatives



$$\frac{\partial J}{\partial b_{3,1}} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial a_{3,1}}{\partial z_{3,1}} \frac{\partial z_{3,1}}{\partial b_{3,1}}$$

$$\frac{\partial J}{\partial b_{2,i}} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial a_{3,1}}{\partial z_{3,1}} \frac{\partial z_{3,1}}{\partial a_{2,i}} \frac{\partial a_{2,i}}{\partial z_{2,i}} \frac{\partial z_{2,i}}{\partial b_{2,i}}$$

$$\frac{\partial J}{\partial b_{1,i}} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial a_{3,1}}{\partial z_{3,1}} \frac{\partial z_{3,1}}{\partial \mathbf{a}_2} \frac{\partial \mathbf{a}_2}{\partial \mathbf{z}_2} \frac{\partial \mathbf{z}_2}{\partial a_{1,i}} \frac{\partial a_{1,i}}{\partial z_{1,i}} \frac{\partial z_{1,i}}{\partial b_{1,i}}$$

Calculus Time-out

Multivariate-chain rule

Multivariable Chain Rule

$$g_1(x) = 3x$$

$$g_2(x) = 5x$$

$$f(z_1, z_2) = 2z_1 + 7z_2$$

$$y = f(g_1(x), g_2(x))$$

Multivariable Chain Rule

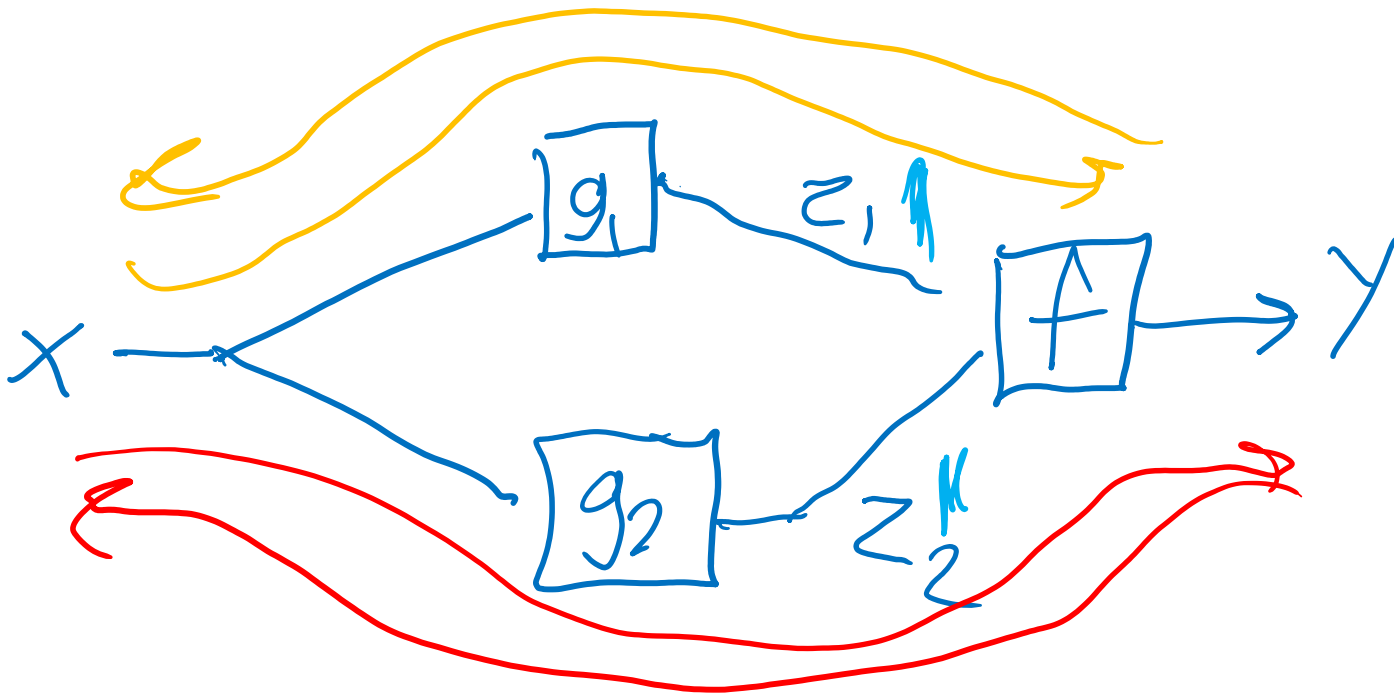
$$g_1(x) = 3x$$

$$g_2(x) = 5x$$

$$f(z_1, z_2) = 2z_1 + 7z_2$$

$$y = f(g_1(x), g_2(x))$$

$$\begin{aligned}\frac{\partial y}{\partial x} &= \frac{\partial y}{\partial z_1} \frac{dz_1}{dx} + \frac{\partial y}{\partial z_2} \frac{dz_2}{dx} \\ &= (2)(3) + (7)(5) \\ &= 41\end{aligned}$$



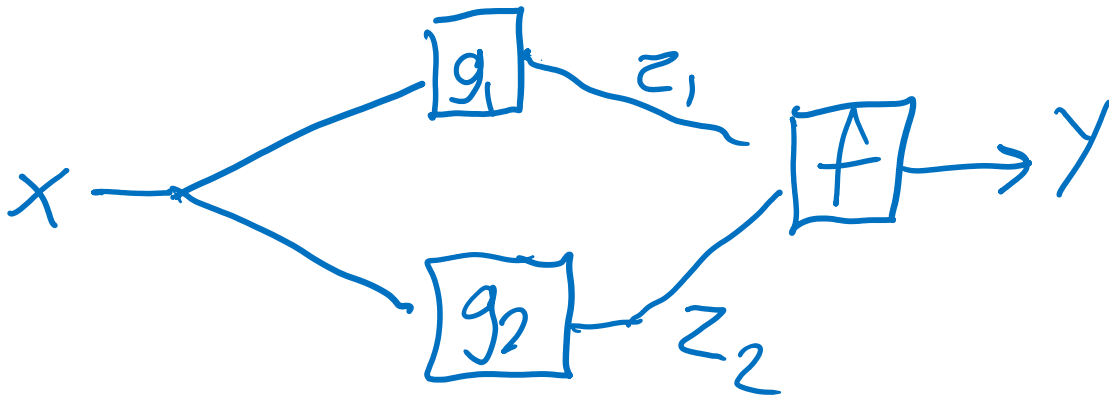
Exercise: Multivariable Chain Rule

$$\frac{df}{dx} = \frac{\partial f}{\partial g_1} \frac{\partial g_1}{\partial x} + \frac{\partial f}{\partial g_2} \frac{\partial g_2}{\partial x}$$

$$z_1 = g_1(x) = \sin(x)$$

$$z_2 = g_2(x) = x^3$$

$$y = f(z_1, z_2) = z_1^4 e^{z_2} + 5z_1 + 7z_2$$



Multivariable Chain Rule

$$z_1 = g_1(x) = \sin(x)$$

$$z_2 = g_2(x) = x^3$$

$$y = f(z_1, z_2) = z_1 z_2$$

$$\partial g_1 / \partial x = \cos x$$

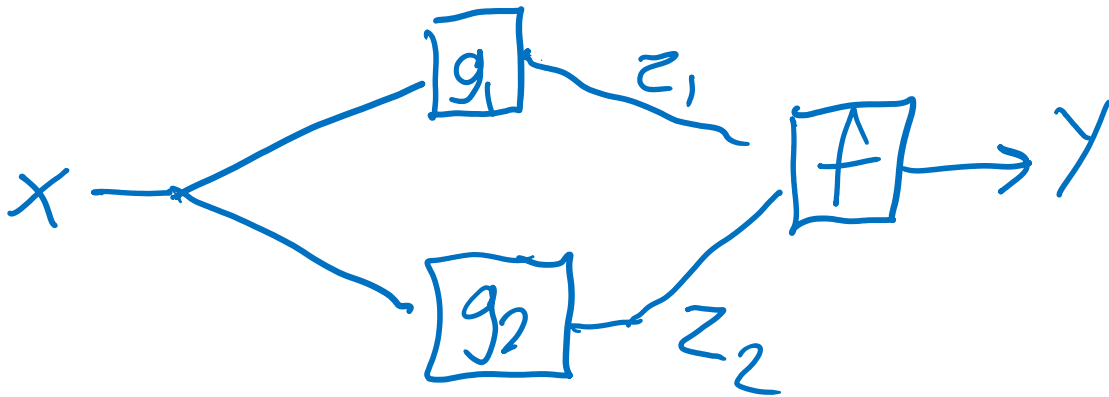
$$\partial g_2 / \partial x = 3x^2$$

$$\frac{\partial f}{\partial z_1} =$$

$$\frac{\partial f}{\partial z_2} =$$

$$\frac{\partial f}{\partial x} =$$

$$\frac{df}{dx} = \frac{\partial f}{\partial g_1} \frac{\partial g_1}{\partial x} + \frac{\partial f}{\partial g_2} \frac{\partial g_2}{\partial x}$$



Calculus Chain Rule

Scalar:

$$y = f(z)$$

$$z = g(x)$$

$$\frac{dy}{dx} = \frac{dy}{dz} \frac{dz}{dx}$$

Multivariate:

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

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

$$\frac{dy}{dx} = \sum_j \frac{\partial y}{\partial z_j} \frac{\partial z_j}{\partial x}$$

Multivariate:

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

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

$$\frac{dy_i}{dx_k} = \sum_j \frac{\partial y_i}{\partial z_j} \frac{\partial z_j}{\partial x_k}$$

Multivariable Chain Rule

	Numerator layout	Denominator layout	Notes
$\frac{d}{dt} f(g(t), h(t))$	$\frac{df}{dg} \frac{dg}{dt} + \frac{df}{dh} \frac{dh}{dt}$	Same	$f : (\mathbb{R} \times \mathbb{R}) \rightarrow \mathbb{R}, t \in \mathbb{R}$ $g : \mathbb{R} \rightarrow \mathbb{R}, h : \mathbb{R} \rightarrow \mathbb{R}$
$\frac{d}{dt} f(g_1(t), \dots, g_N(t))$	$\sum_{i=1}^N \frac{df}{dg_i} \frac{dg_i}{dt}$	Same	$h : (\mathbb{R} \times \dots \times \mathbb{R}) \rightarrow \mathbb{R}, t \in \mathbb{R}$ $f_i : \mathbb{R} \rightarrow \mathbb{R} \quad \forall i \in \{1, \dots, N\}$
$\frac{d}{dt} f(\mathbf{g}(t))$	$\frac{\partial f}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial t}$	$\frac{\partial \mathbf{g}}{\partial t} \frac{\partial f}{\partial \mathbf{g}}$	$f : \mathbb{R}^N \rightarrow \mathbb{R}, \mathbf{g} : \mathbb{R} \rightarrow \mathbb{R}^N$ $t \in \mathbb{R}$
$\frac{\partial}{\partial \mathbf{v}} f(\mathbf{g}(\mathbf{v}))$	$\frac{\partial f}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{v}}$	$\frac{\partial \mathbf{g}}{\partial \mathbf{v}} \frac{\partial f}{\partial \mathbf{g}}$	$f : \mathbb{R}^N \rightarrow \mathbb{R}, \mathbf{g} : \mathbb{R}^M \rightarrow \mathbb{R}^N$ $\mathbf{v} \in \mathbb{R}^M$
$\frac{\partial}{\partial \mathbf{v}} f(\mathbf{g}(\mathbf{v}), \mathbf{h}(\mathbf{v}))$	$\frac{\partial f}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{v}} + \frac{\partial f}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{v}}$	$\frac{\partial \mathbf{g}}{\partial \mathbf{v}} \frac{\partial f}{\partial \mathbf{g}} + \frac{\partial \mathbf{h}}{\partial \mathbf{v}} \frac{\partial f}{\partial \mathbf{h}}$	$h : \mathbb{R}^K \times \mathbb{R}^N \rightarrow \mathbb{R}, \mathbf{v} \in \mathbb{R}^M$ $f : \mathbb{R}^M \rightarrow \mathbb{R}^K, \mathbf{g} : \mathbb{R}^M \rightarrow \mathbb{R}^N$

Backpropagation (vector version)

Network Optimization

$$J(\mathbf{w}) = z_4$$

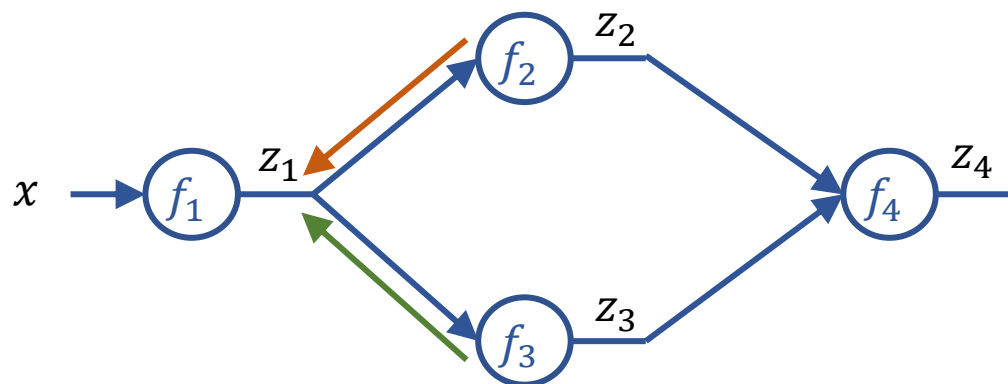
$$z_4 = f_4(w_D, w_E, z_2, z_3)$$

$$z_3 = f_3(w_C, z_1)$$

$$z_2 = f_2(w_B, z_1)$$

$$z_1 = f_1(w_A, x)$$

Need multivariate chain rule!



$$\frac{\partial J}{\partial w_E} = \frac{\partial J}{\partial z_4} \frac{\partial z_4}{\partial w_E}$$

$$\frac{\partial J}{\partial w_D} = \frac{\partial J}{\partial z_4} \frac{\partial z_4}{\partial w_D}$$

$$\frac{\partial J}{\partial z_3} = \frac{\partial J}{\partial z_4} \frac{\partial z_4}{\partial z_3}$$

$$\frac{\partial J}{\partial z_2} = \frac{\partial J}{\partial z_4} \frac{\partial z_4}{\partial z_2}$$

$$\frac{\partial J}{\partial w_C} = \frac{\partial J}{\partial z_3} \frac{\partial z_3}{\partial w_C}$$

$$\frac{\partial J}{\partial w_B} = \frac{\partial J}{\partial z_2} \frac{\partial z_2}{\partial w_B}$$

$$\frac{\partial J}{\partial z_1} = \frac{\partial J}{\partial z_2} \frac{\partial z_2}{\partial z_1} + \frac{\partial J}{\partial z_3} \frac{\partial z_3}{\partial z_1}$$

$$\frac{\partial J}{\partial w_A} = \frac{\partial J}{\partial z_1} \frac{\partial z_1}{\partial w_A}$$

Generic Layer Implementation (updated)

Compute derivatives per layer, utilizing previous derivatives

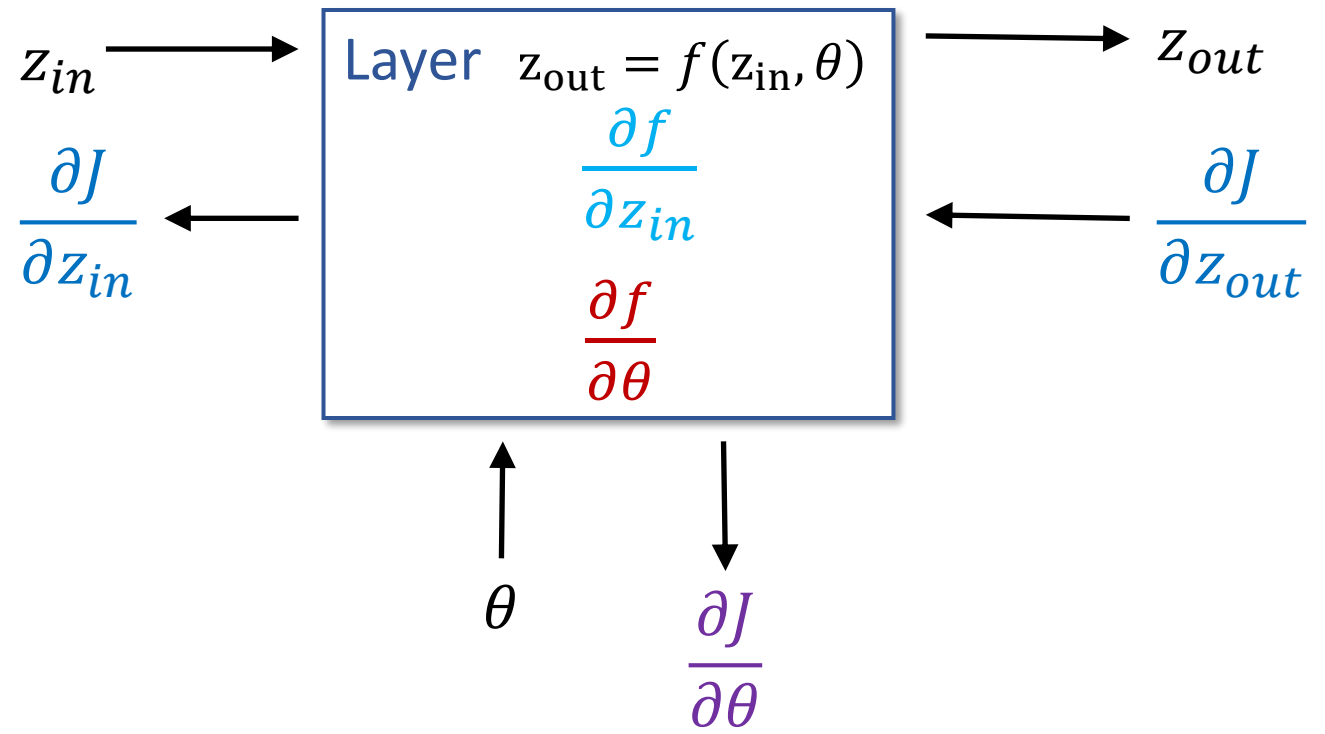
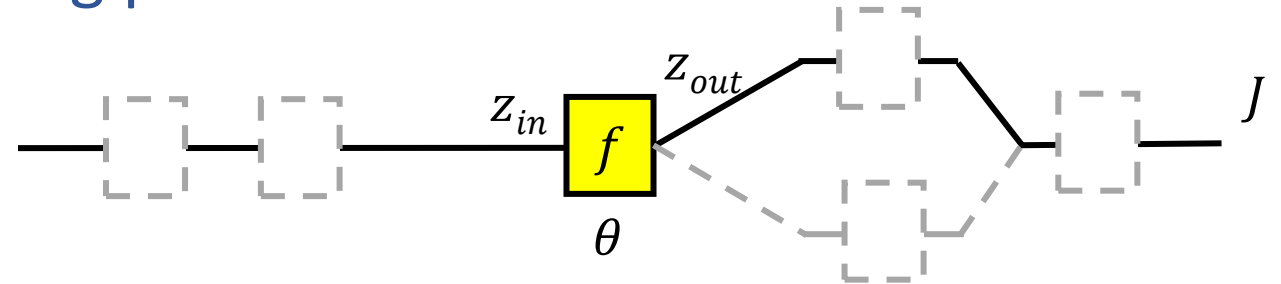
Objective: $J(\theta)$

Arbitrary layer: $z_{out} = f(z_{in}, \theta)$

Need:

- $\frac{\partial J}{\partial z_{in}} + = \frac{\partial J}{\partial z_{out}} \frac{\partial f}{\partial z_{in}}$

- $\frac{\partial J}{\partial \theta} + = \frac{\partial J}{\partial z_{out}} \frac{\partial f}{\partial \theta}$



Generic Layer Implementation (vector output version)

Compute derivatives per layer, utilizing previous derivatives

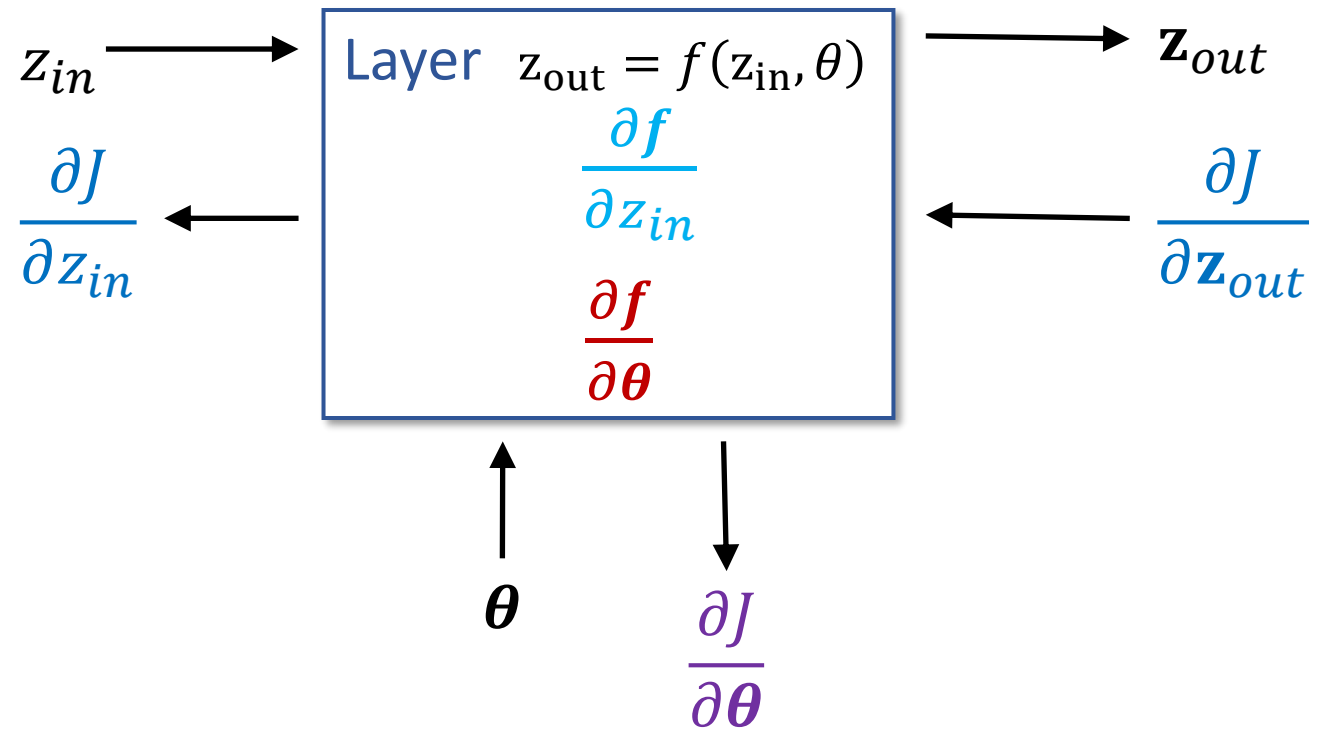
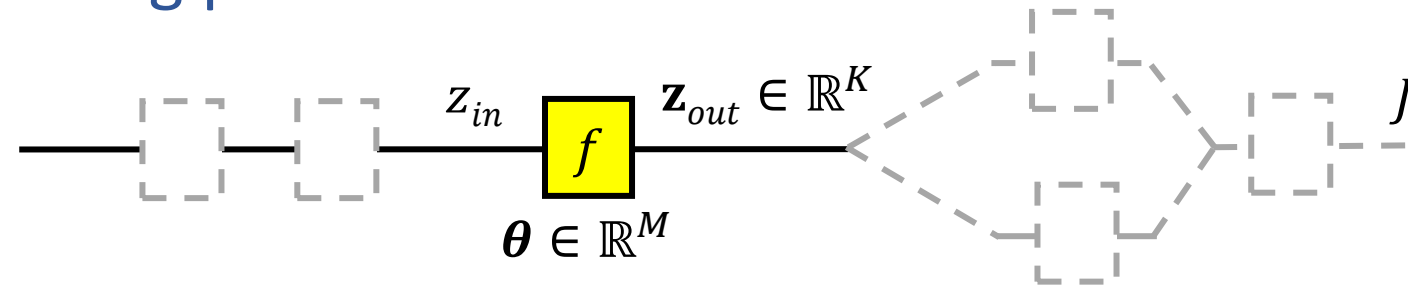
Objective: $J(\theta)$

Arbitrary layer: $\mathbf{z}_{\text{out}} = f(\mathbf{z}_{\text{in}}, \theta)$

Need:

- $\frac{\partial J}{\partial \mathbf{z}_{\text{in}}} =$

- $\frac{\partial J}{\partial \theta_j} =$



Generic Layer Implementation (vector output version)

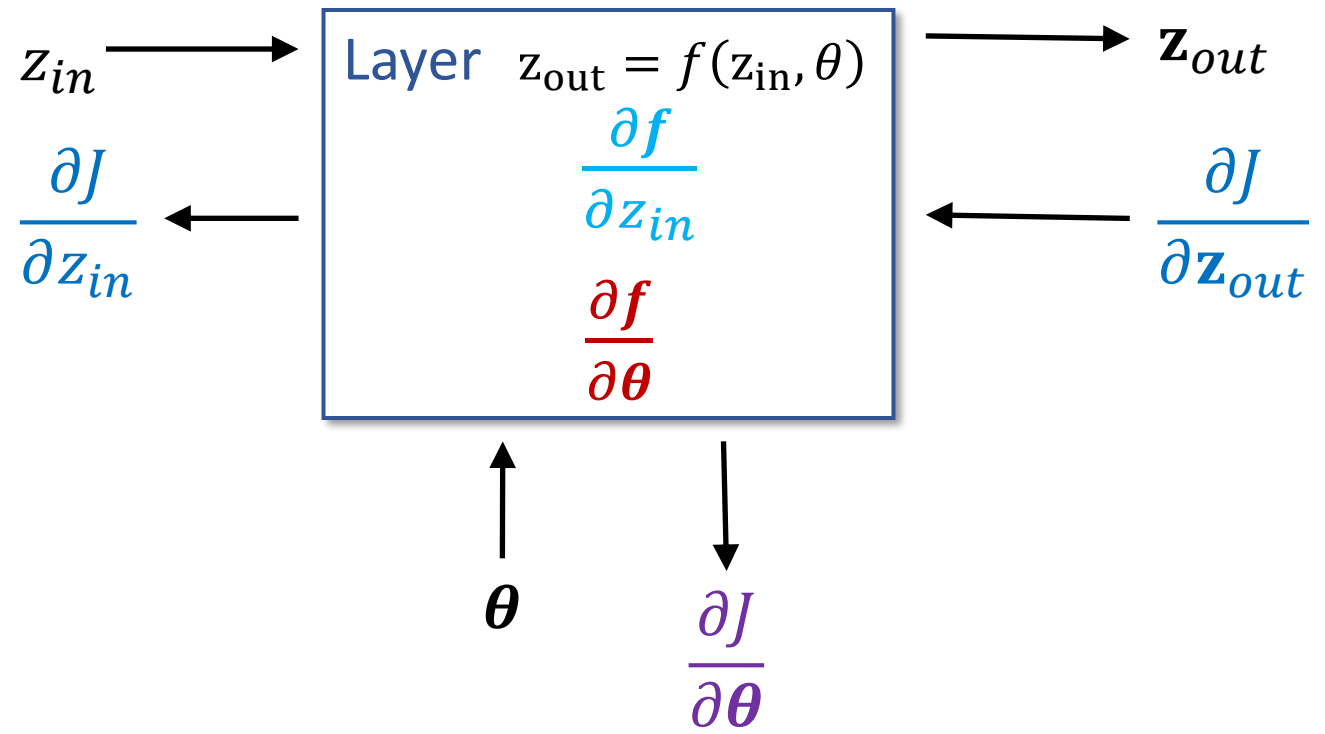
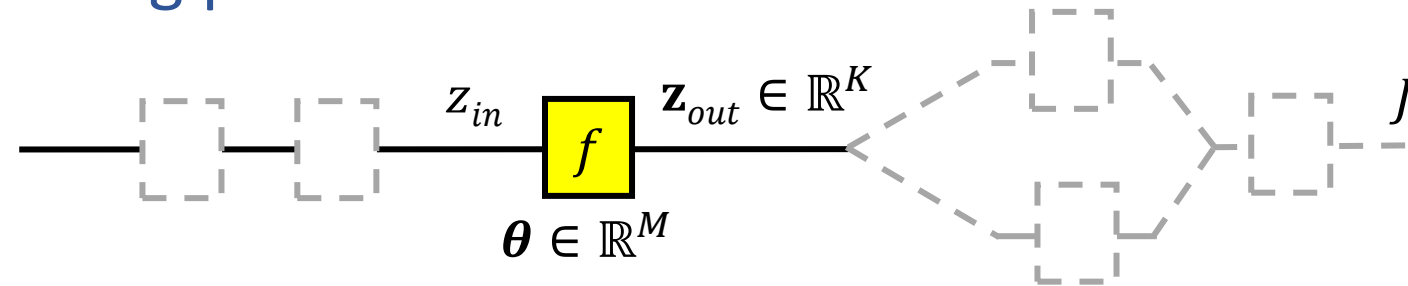
Compute derivatives per layer, utilizing previous derivatives

Objective: $J(\theta)$

Arbitrary layer: $\mathbf{z}_{out} = f(\mathbf{z}_{in}, \theta)$

Need:

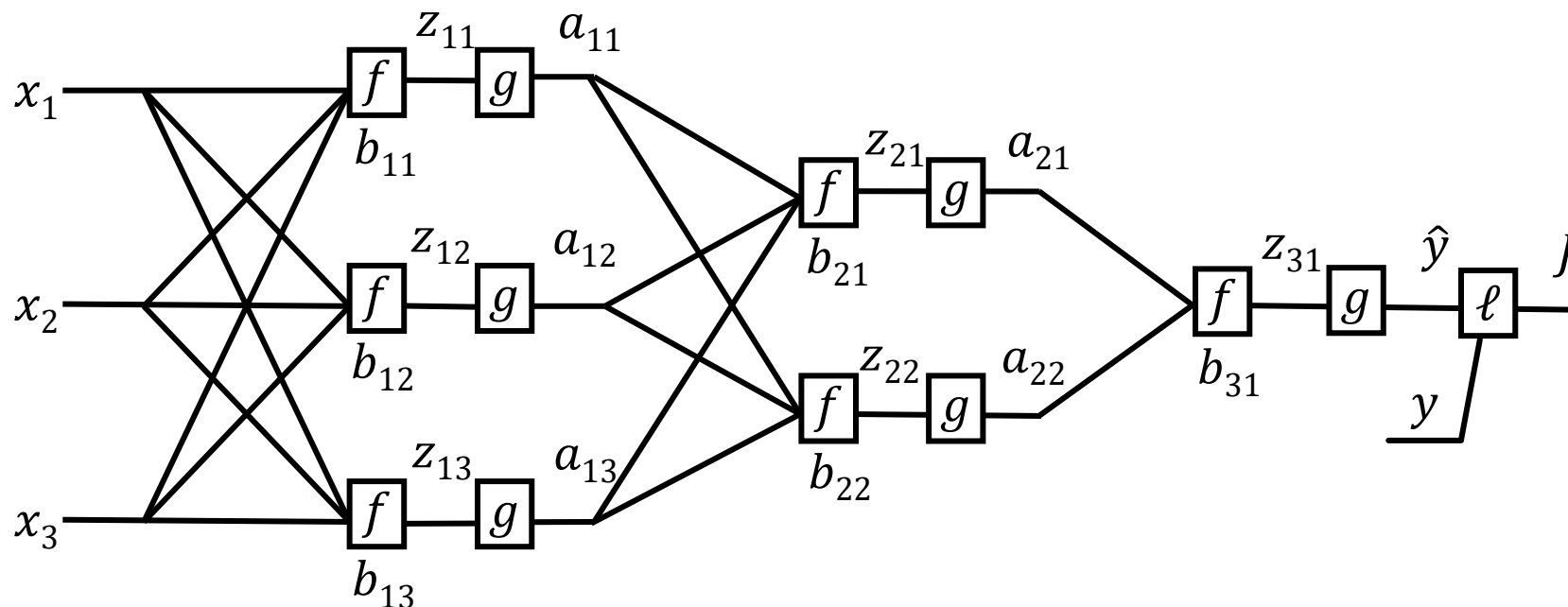
- $\frac{\partial J}{\partial \mathbf{z}_{in}} = \sum_k \frac{\partial J}{\partial \mathbf{z}_{out,k}} \frac{\partial \mathbf{z}_{out,k}}{\partial \mathbf{z}_{in}}$
- $\frac{\partial J}{\partial \theta_j} = \sum_k \frac{\partial J}{\partial \mathbf{z}_{out,k}} \frac{\partial f}{\partial \theta_j}$



Optimization

$$\hat{y} = h_{\theta}(\mathbf{x}) = g \left(b_{3,1} + \sum_k w_{3,1,k} g \left(b_{2,k} + \sum_i w_{2,k,i} g \left(b_{1,i} + \sum_j w_{1,i,j} x_j \right) \right) \right)$$

Where do we need chain rule?



$$\frac{\partial J}{\partial b_{3,1}} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial a_{3,1}}{\partial z_{3,1}} \frac{\partial z_{3,1}}{\partial b_{3,1}}$$

$$\frac{\partial J}{\partial b_{2,i}} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial a_{3,1}}{\partial z_{3,1}} \frac{\partial z_{3,1}}{\partial a_{2,i}} \frac{\partial a_{2,i}}{\partial z_{2,i}} \frac{\partial z_{2,i}}{\partial b_{2,i}}$$

$$\frac{\partial J}{\partial b_{1,i}} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial a_{3,1}}{\partial z_{3,1}} \frac{\partial z_{3,1}}{\partial \mathbf{a}_2} \frac{\partial \mathbf{a}_2}{\partial \mathbf{z}_2} \frac{\partial \mathbf{z}_2}{\partial a_{1,i}} \frac{\partial a_{1,i}}{\partial z_{1,i}} \frac{\partial z_{1,i}}{\partial b_{1,i}}$$

Linear Layer Implementation

Compute derivatives per layer

Objective: $J(\theta)$

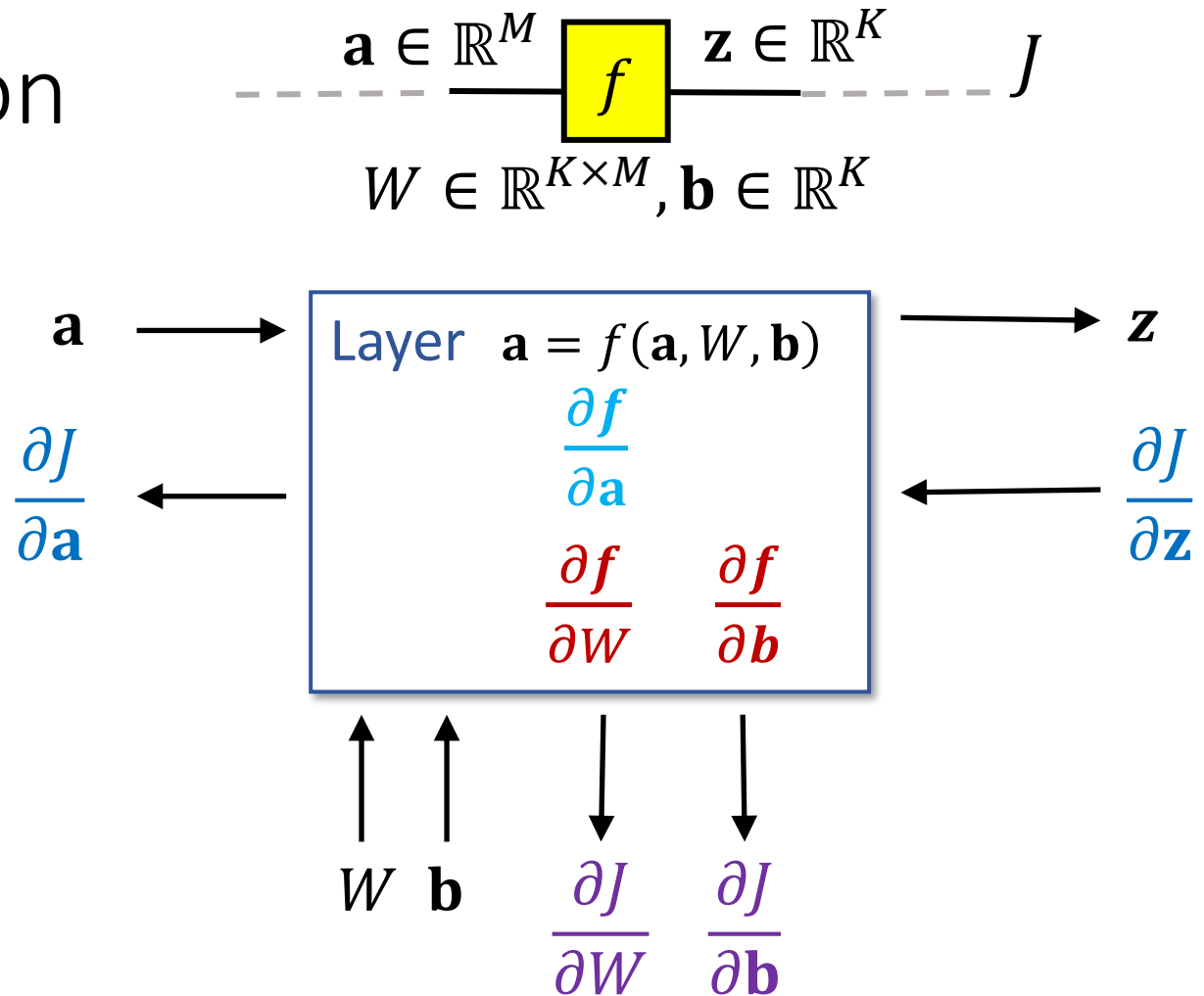
Layer: $\mathbf{z} = f(\mathbf{a}, W, \mathbf{b}) = W\mathbf{a} + \mathbf{b}$

Scalar version (no formatting)

$$\blacksquare \frac{\partial J}{\partial a_j} =$$

$$\blacksquare \frac{\partial J}{\partial W_{i,j}} =$$

$$\blacksquare \frac{\partial J}{\partial b_i} =$$



$$\mathbf{z} = W\mathbf{a} + \mathbf{b}$$

$$z_k = b_k + \sum_j W_{k,j} a_j$$

Linear Layer Implementation

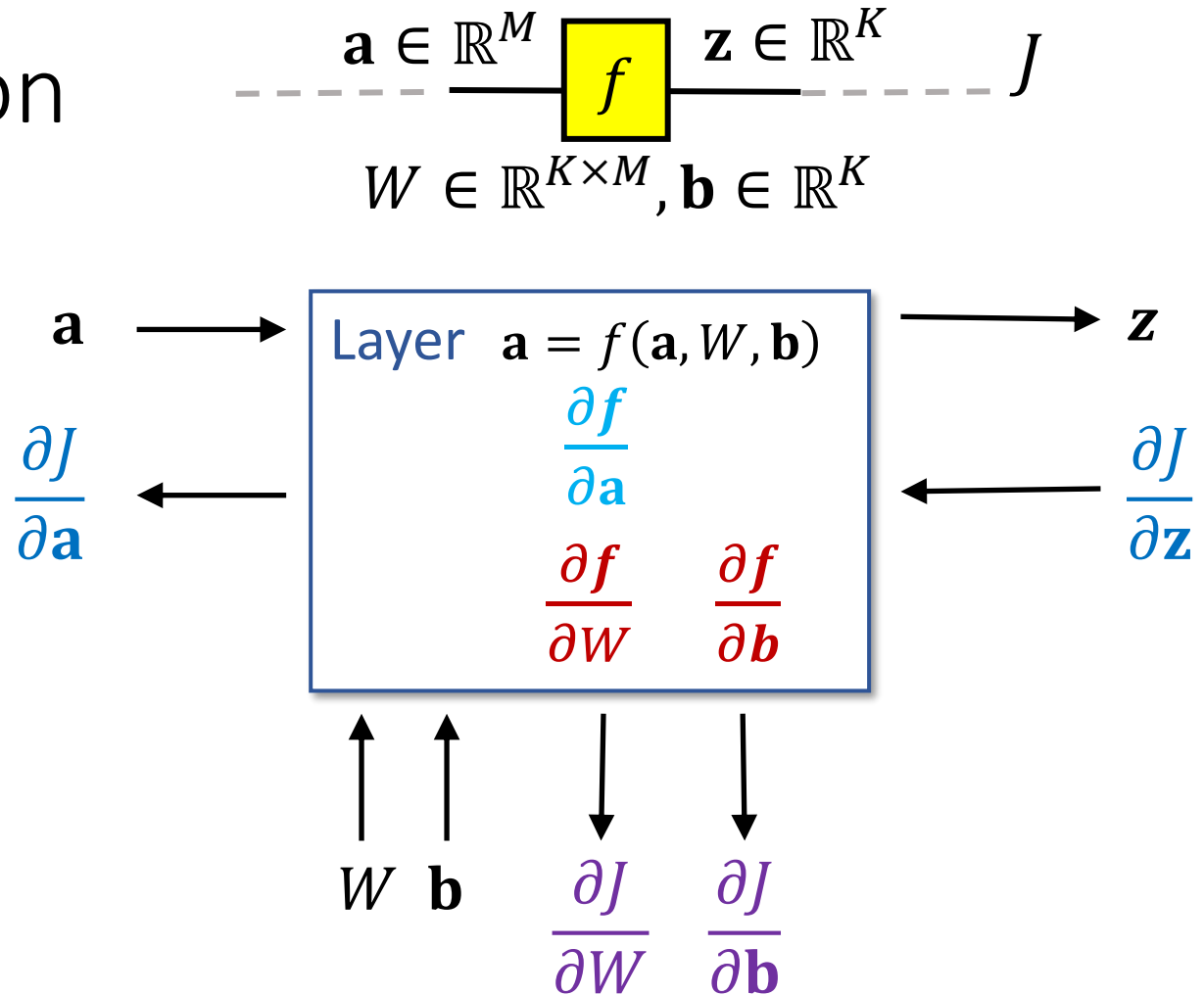
Compute derivatives per layer

Objective: $J(\theta)$

Layer: $\mathbf{z} = f(\mathbf{a}, W, \mathbf{b}) = W\mathbf{a} + \mathbf{b}$

Scalar version (no formatting)

- $\frac{\partial J}{\partial a_j} = \sum_k \frac{\partial J}{\partial z_k} \frac{\partial z_k}{\partial a_j}$
- $\frac{\partial J}{\partial W_{i,j}} = \sum_k \frac{\partial J}{\partial z_k} \frac{\partial z_k}{\partial W_{i,j}}$
- $\frac{\partial J}{\partial b_i} = \sum_k \frac{\partial J}{\partial z_k} \frac{\partial z_k}{\partial b_i}$



$$\mathbf{z} = W\mathbf{a} + \mathbf{b}$$

$$z_k = b_k + \sum_j W_{k,j} a_j$$

Linear Layer Implementation

Compute derivatives per layer

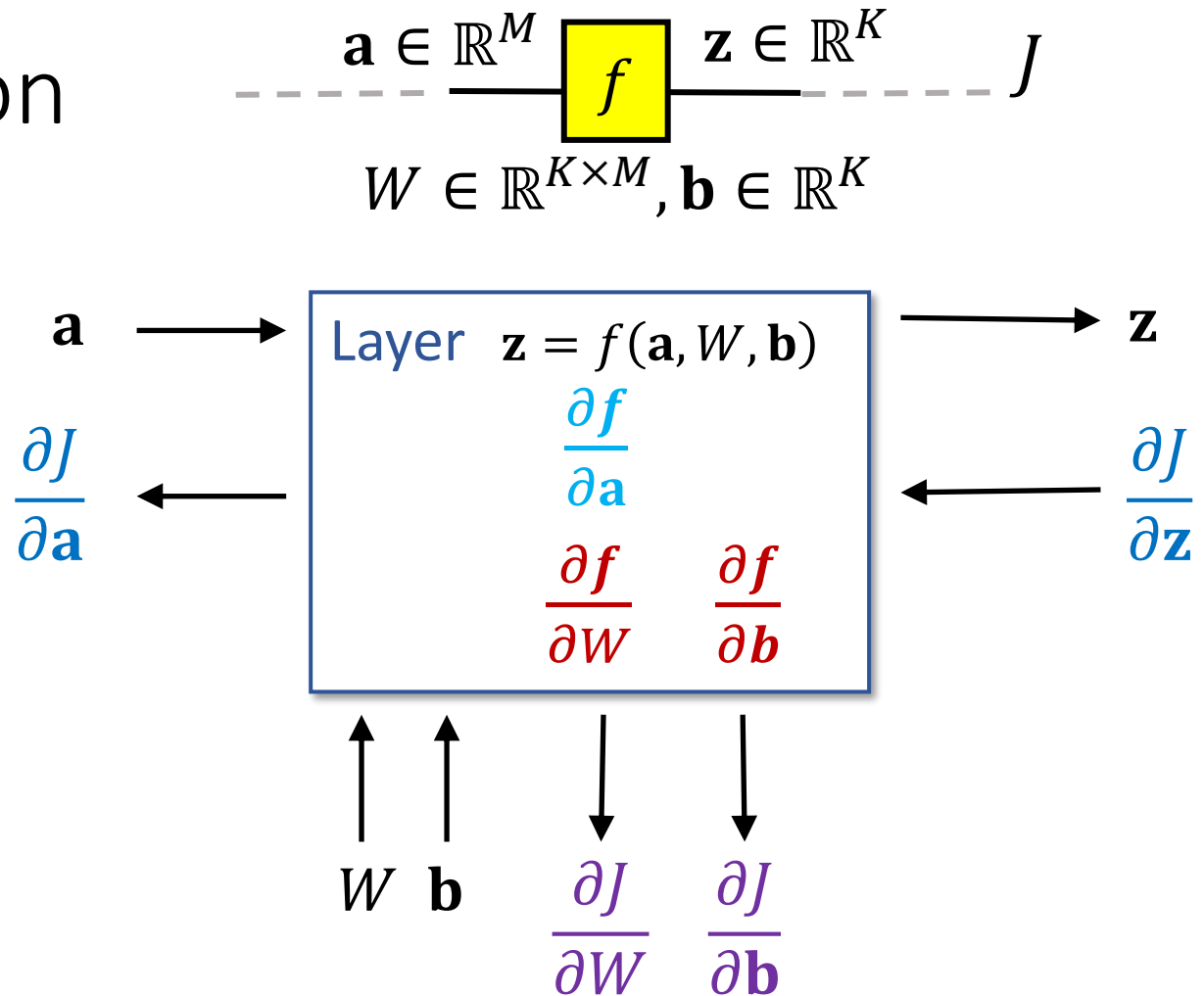
Objective: $J(\theta)$

Layer: $\mathbf{z} = f(\mathbf{a}, W, \mathbf{b}) = W\mathbf{a} + \mathbf{b}$
(Numerator format)

■ $\frac{\partial J}{\partial \mathbf{a}}$

■ $\frac{\partial J}{\partial W}$

■ $\frac{\partial J}{\partial \mathbf{b}}$



Linear Layer Implementation

Compute derivatives per layer

Objective: $J(\theta)$

Layer: $\mathbf{z} = f(\mathbf{a}, W, \mathbf{b}) = W\mathbf{a} + \mathbf{b}$

(Numerator format)

$$\begin{matrix} [1 \times M] & [1 \times K][K \times M] & [1 \times K][K \times M] \\ \blacksquare \frac{\partial J}{\partial \mathbf{a}} & = \frac{\partial J}{\partial \mathbf{z}} \frac{\partial f}{\partial \mathbf{a}} & = \frac{\partial J}{\partial \mathbf{z}} W \end{matrix}$$

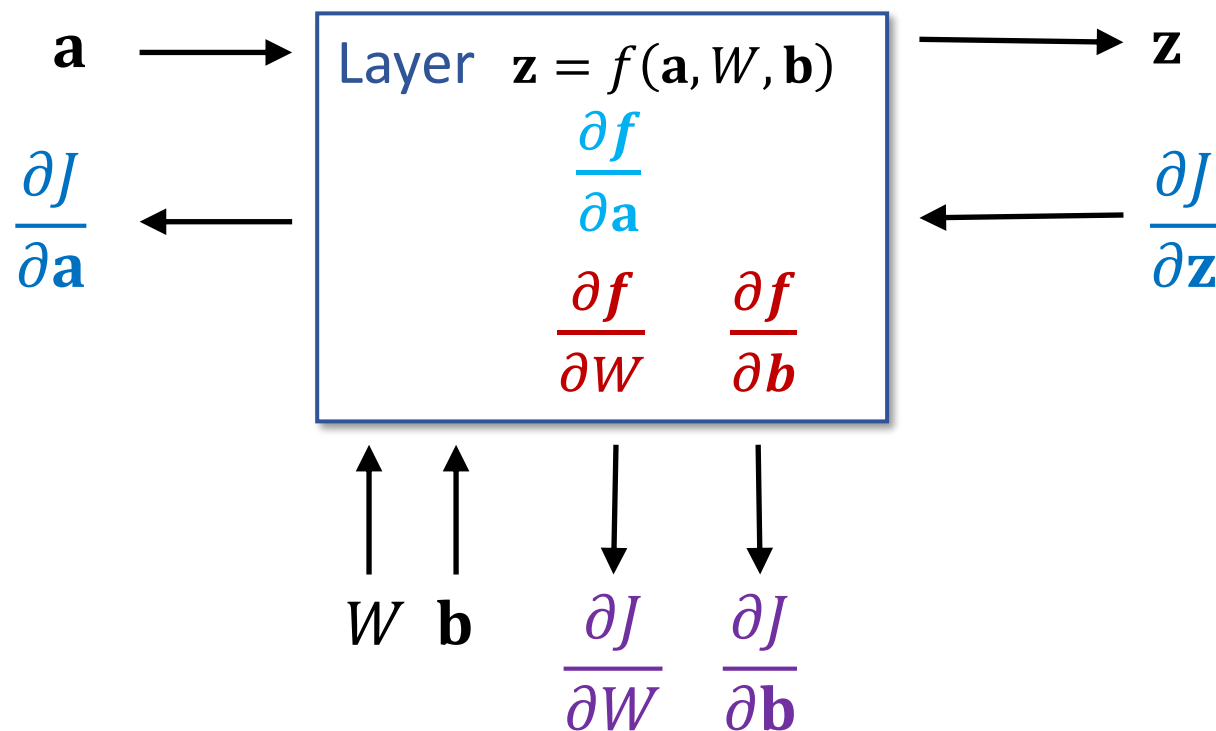
Fixed dimensions to
be outer product

$$\begin{matrix} [M \times K] & [1 \times K][? \times ?] & [1 \times K][M \times 1] & [M \times 1][1 \times K] \\ \blacksquare \frac{\partial J}{\partial W} & = \frac{\partial J}{\partial \mathbf{z}} \frac{\partial f}{\partial W} & = \frac{\partial J}{\partial \mathbf{z}} \mathbf{a} & = \mathbf{a} \frac{\partial J}{\partial \mathbf{z}} \end{matrix}$$

Broken!

$$\begin{matrix} [1 \times M] & [1 \times K][K \times K] & [1 \times K][K \times K] \\ \blacksquare \frac{\partial J}{\partial \mathbf{b}} & = \frac{\partial J}{\partial \mathbf{z}} \frac{\partial f}{\partial \mathbf{b}} & = \frac{\partial J}{\partial \mathbf{z}} I_K \end{matrix}$$

$$\begin{array}{c} \text{---} \mathbf{a} \in \mathbb{R}^M \text{---} \boxed{f} \text{---} \mathbf{z} \in \mathbb{R}^K \text{---} J \\ W \in \mathbb{R}^{K \times M}, \mathbf{b} \in \mathbb{R}^K \end{array}$$



Linear Layer Implementation

Compute derivatives per layer

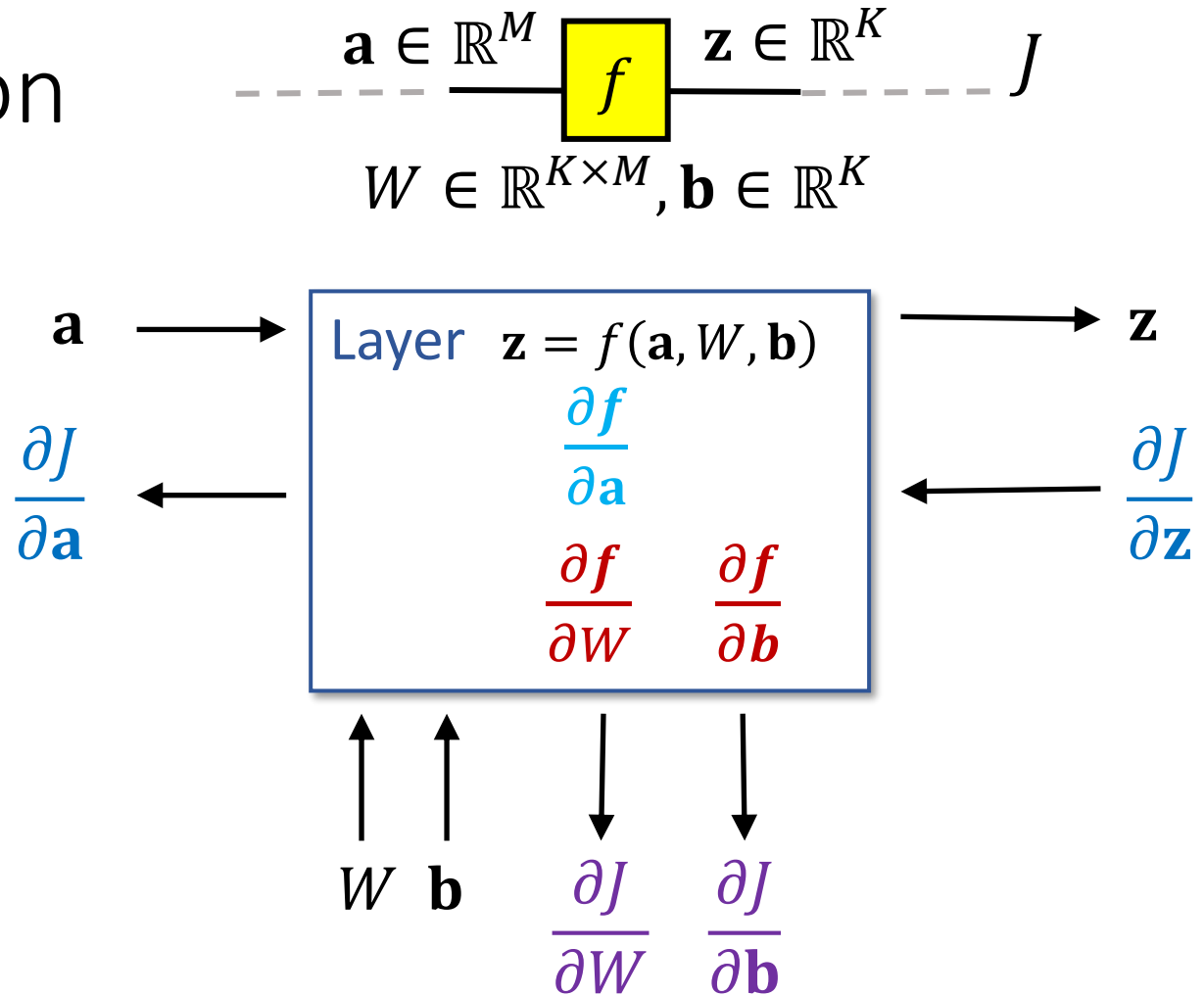
Objective: $J(\theta)$

Layer: $\mathbf{z} = f(\mathbf{a}, W, \mathbf{b}) = W\mathbf{a} + \mathbf{b}$
(Denominator format)

- $\frac{\partial J}{\partial \mathbf{a}}$

- $\frac{\partial J}{\partial W}$

- $\frac{\partial J}{\partial \mathbf{b}}$



Linear Layer Implementation

Compute derivatives per layer

Objective: $J(\theta)$

Layer: $\mathbf{z} = f(\mathbf{a}, W, \mathbf{b}) = W\mathbf{a} + \mathbf{b}$

(Denominator format)

$$\frac{\partial J}{\partial \mathbf{a}} = \frac{\partial f}{\partial \mathbf{a}} \frac{\partial J}{\partial \mathbf{z}} = W^\top \frac{\partial J}{\partial \mathbf{z}}$$

Fixed dimensions to be outer product

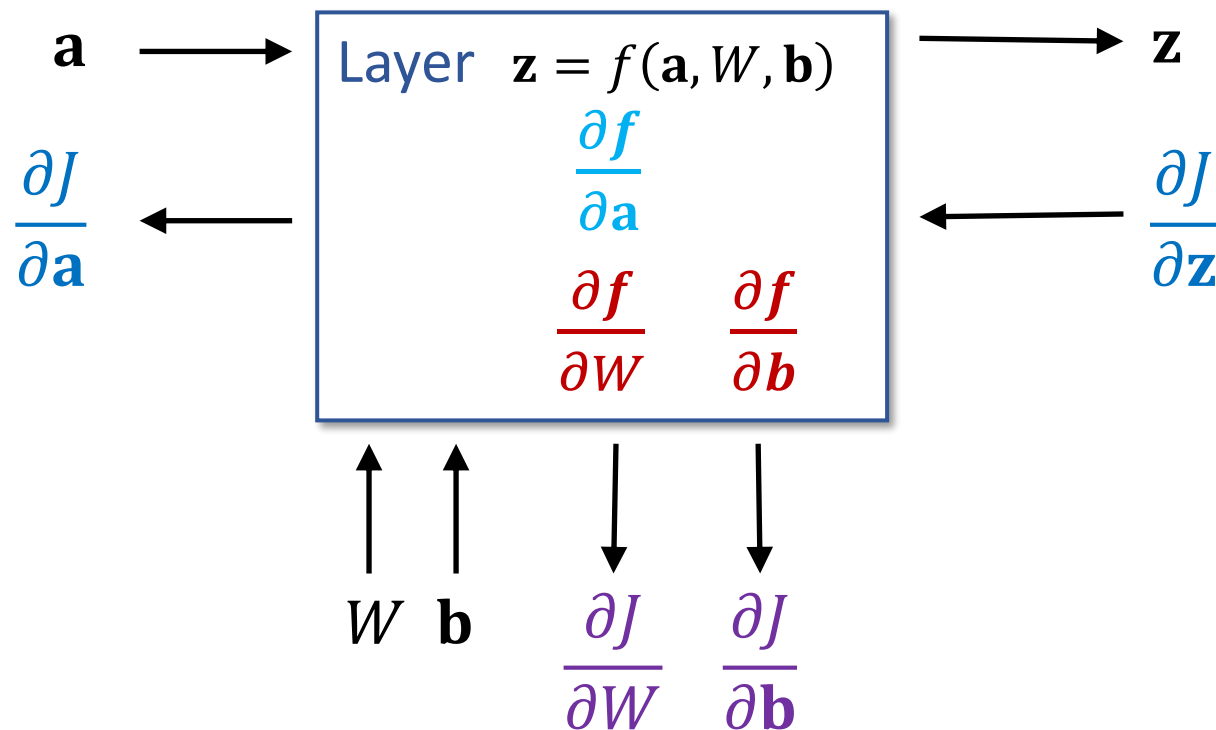
$$\frac{\partial J}{\partial W} = \frac{\partial f}{\partial W} \frac{\partial J}{\partial \mathbf{z}} = \mathbf{a} \frac{\partial J}{\partial \mathbf{z}} = \frac{\partial J}{\partial \mathbf{z}} \mathbf{a}^\top$$

Broken!

$$\frac{\partial J}{\partial \mathbf{b}} = \frac{\partial f}{\partial \mathbf{b}} \frac{\partial J}{\partial \mathbf{z}} = I_K \frac{\partial J}{\partial \mathbf{z}}$$

$$\mathbf{a} \in \mathbb{R}^M \xrightarrow{f} \mathbf{z} \in \mathbb{R}^K \xrightarrow{J}$$

$$W \in \mathbb{R}^{K \times M}, \mathbf{b} \in \mathbb{R}^K$$



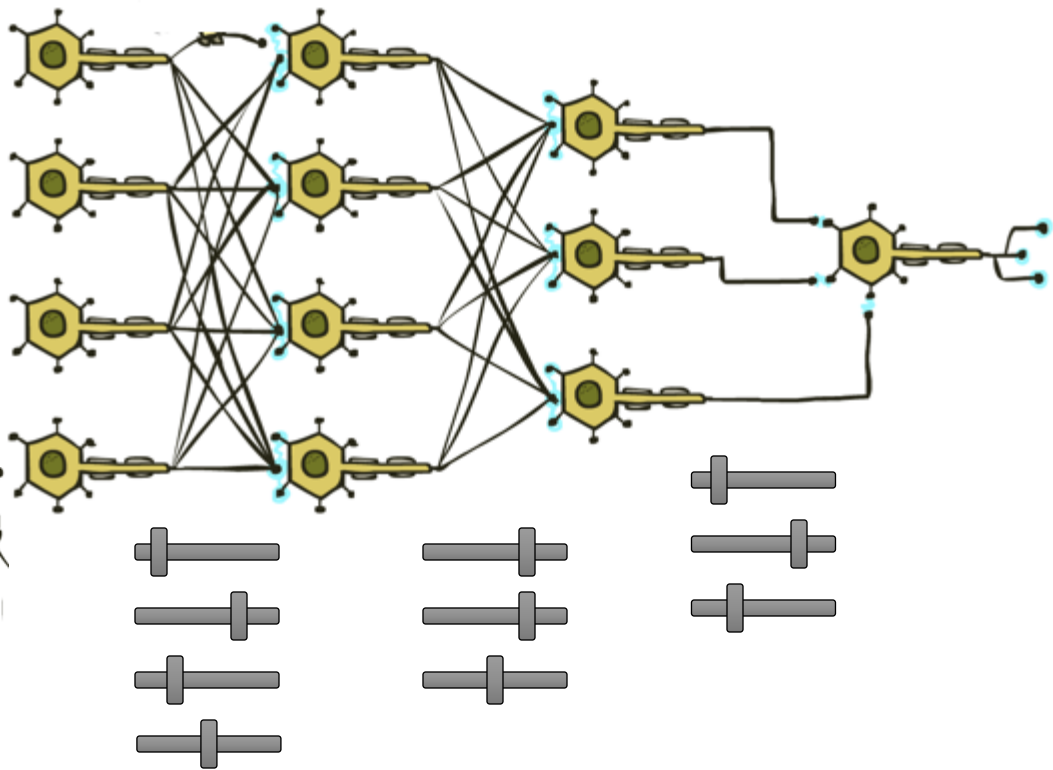
Optimization Intuition

Neural Networks

Many layers of neurons, millions of parameters

Output
Signal

Input
Signal



$\hat{y}$



DOG



CAT



TREE



CAR

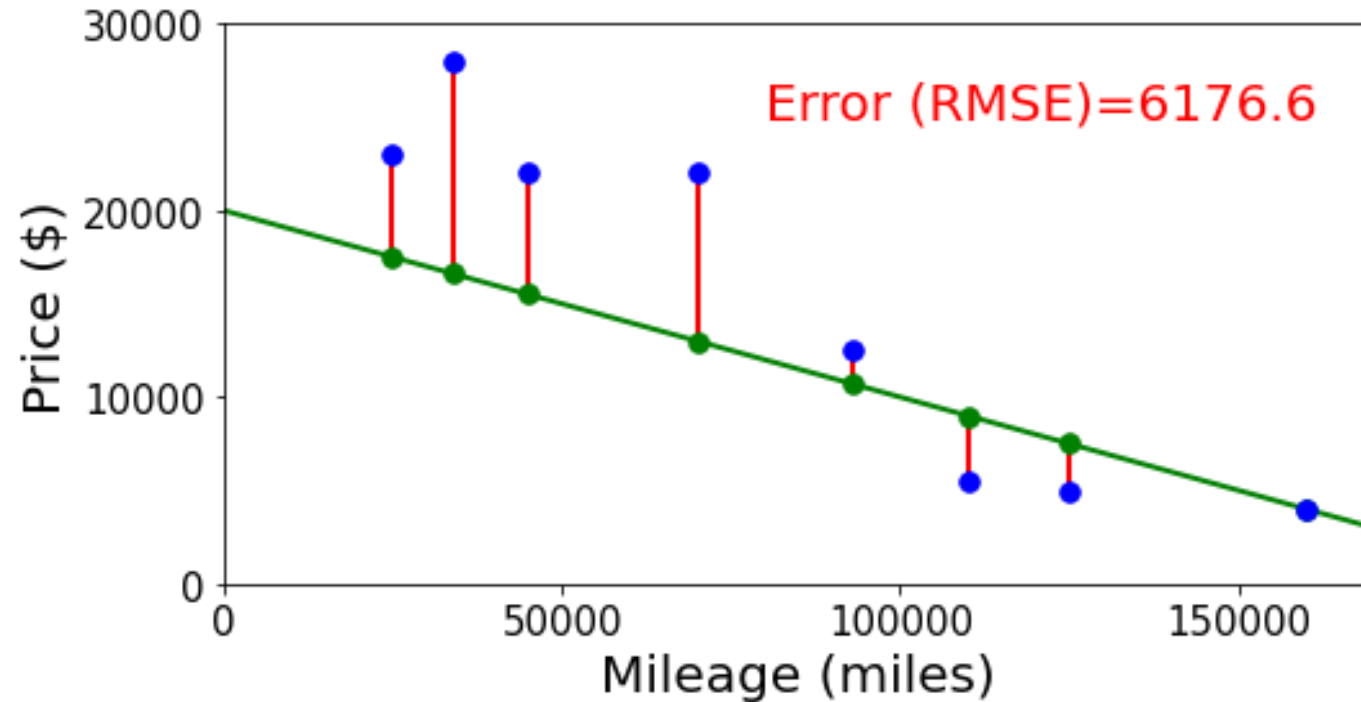
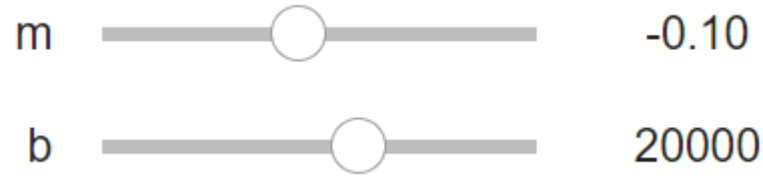


SKY

Neural Networks

Building on optimization for linear and logistic regression

- Selling my car

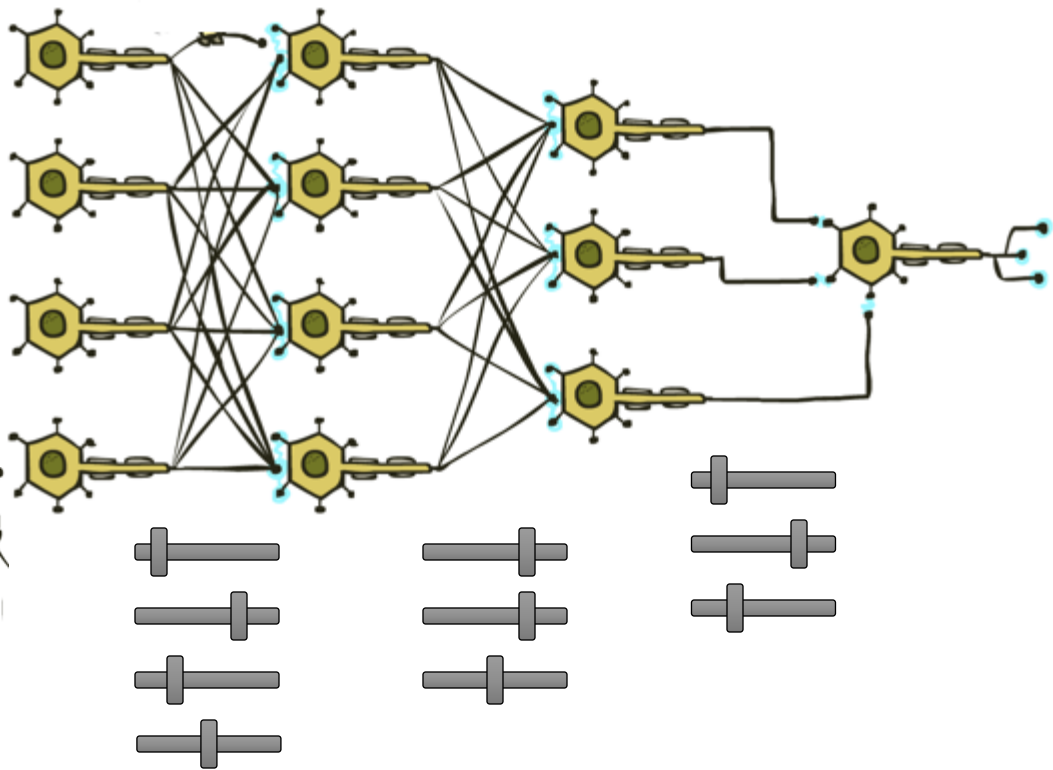


Neural Networks

Many layers of neurons, millions of parameters

Output
Signal

Input
Signal



$\hat{y}$



DOG



CAT



TREE



CAR



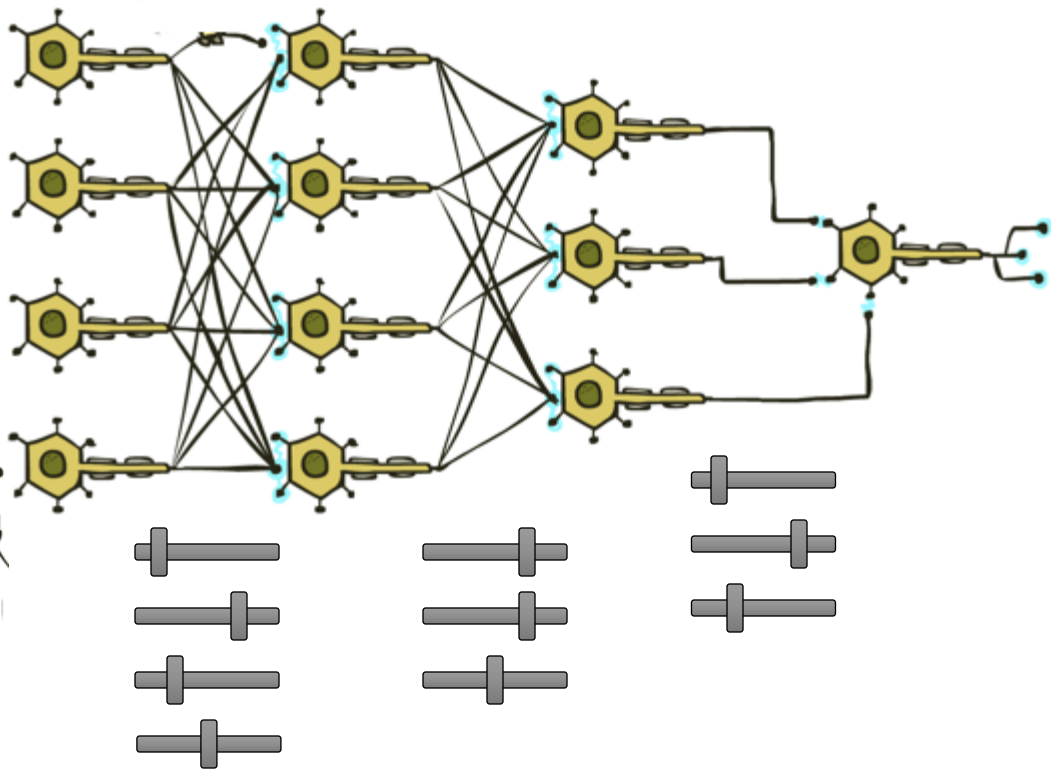
SKY

Neural Networks

Many layers of neurons, millions of parameters

Output
Signal

Input
Signal



$\hat{y}$

y



0

DOG



1

CAT



0

TREE



0

CAR



0

SKY

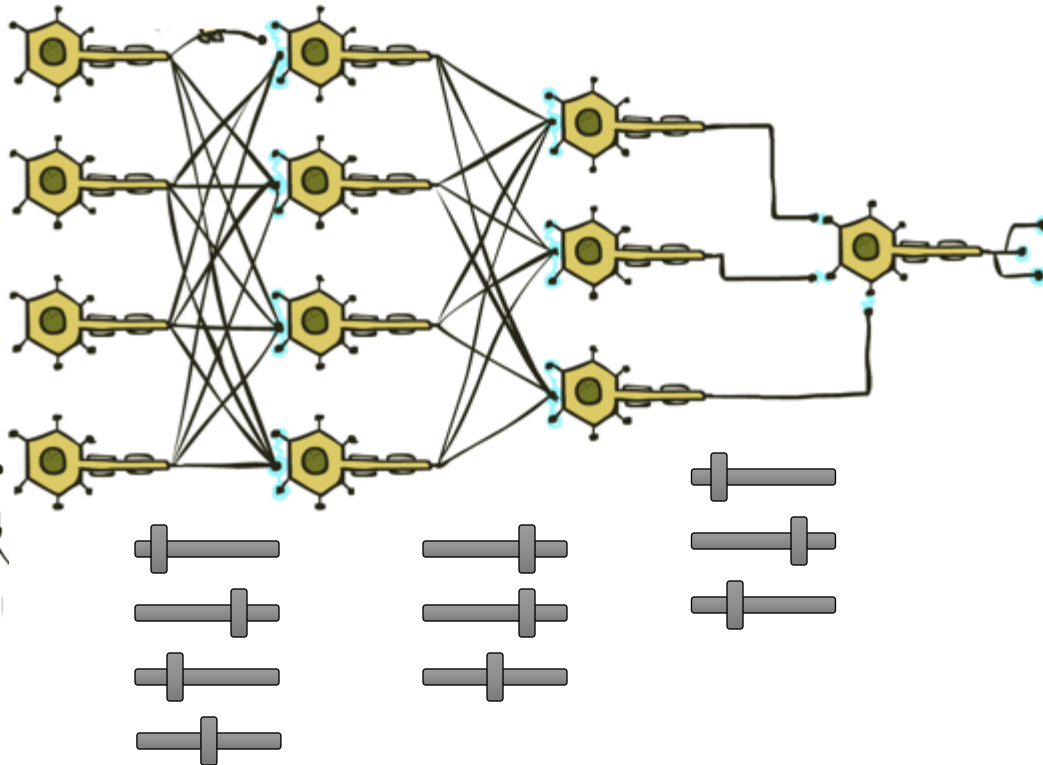
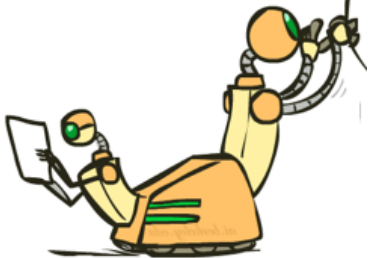
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Many layers of neurons, millions of parameters

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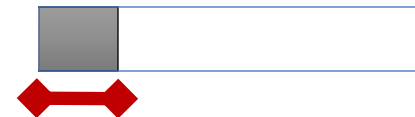
Input
Signal



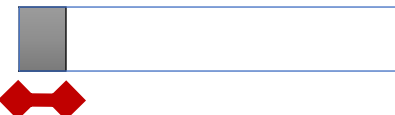
LEFT



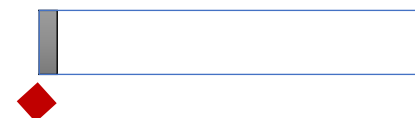
RIGHT



UP



DOWN



BUTTON

Outline

Last time: Neural Networks

- Three-neuron network + optimization
- Neural network structure (adding more neurons)
- Forward pass and Backpropagation (scalar version)

Today: Neural Networks

- Calculus: multi-variate chain rule
- Backpropagation (vector version)
- Optimization intuition (sliders)
- Neural Network Properties and Intuition

Neural Network Properties

Neural Networks Properties

Practical considerations

- Large number of neurons
 - Danger for overfitting
- Modeling assumptions vs data assumptions trade-off
- Gradient descent can easily get stuck local optima

What if there are no non-linear activations?

- A deep neural network with only linear layers can be reduced to an exactly equivalent single linear layer

Universal Approximation Theorem:

- A two-layer neural network with a sufficient number of neurons can approximate any continuous function to any desired accuracy.

Neural Networks Properties

Non-linearity

Fitting complex functions

Fitting any! function (universal approximation theorem)

Overfitting

Neural Network Properties

Non-linearity

Non-linearity

Neural network prediction function, $\hat{y} = h(x)$, is definitely not linear. The non-linear activation functions provide this non-linearity

What if there are no non-linear activations?

- A deep neural network with only linear layers can be reduced to an exactly equivalent single linear layer

Example

What happens with you add to linear functions together?

- Adding two lines? $h(x) = f_1(x, w_1, b_1) + f_2(x, w_2, b_2)$
- Adding two planes?

Objective Function is Not Convex

Objective function for...	Convex?	Closed-form solution?
Linear regression		
Logistic regression		
Neural networks		

Optimization

Convex function

If $f(\mathbf{x})$ is convex, then:

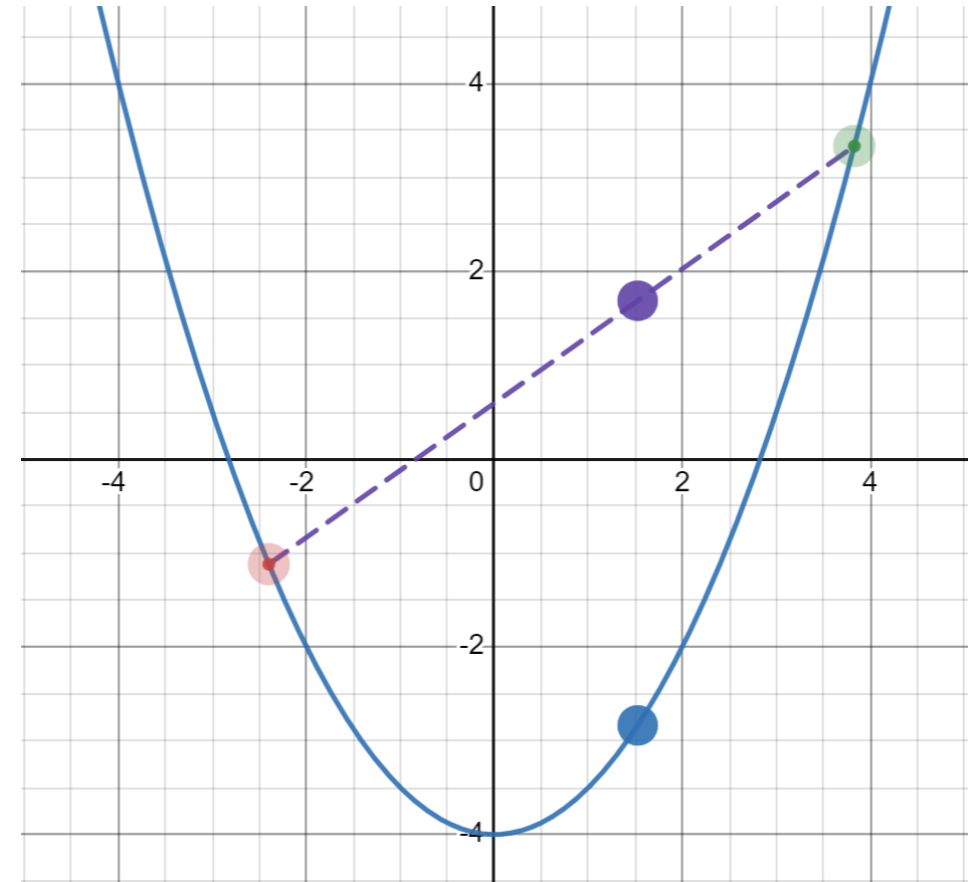
- $f(\alpha \mathbf{x} + (1 - \alpha) \mathbf{z}) \leq \alpha f(\mathbf{x}) + (1 - \alpha) f(\mathbf{z})$
 $\forall 0 \leq \alpha \leq 1$

Convex optimization

If second derivative is ≥ 0
everywhere then function is
convex

If $f(\mathbf{x})$ is convex, then:

- Every local minimum is also a
global minimum 😊



Non-linearity

Prediction function

Neural network prediction function, $\hat{y} = h(x)$, is definitely not linear. The non-linear activation functions provide this non-linearity

Objective function

Neural network prediction function, $\hat{y} = h(x)$, is definitely not linear. The non-linear activation functions provide this non-linearity

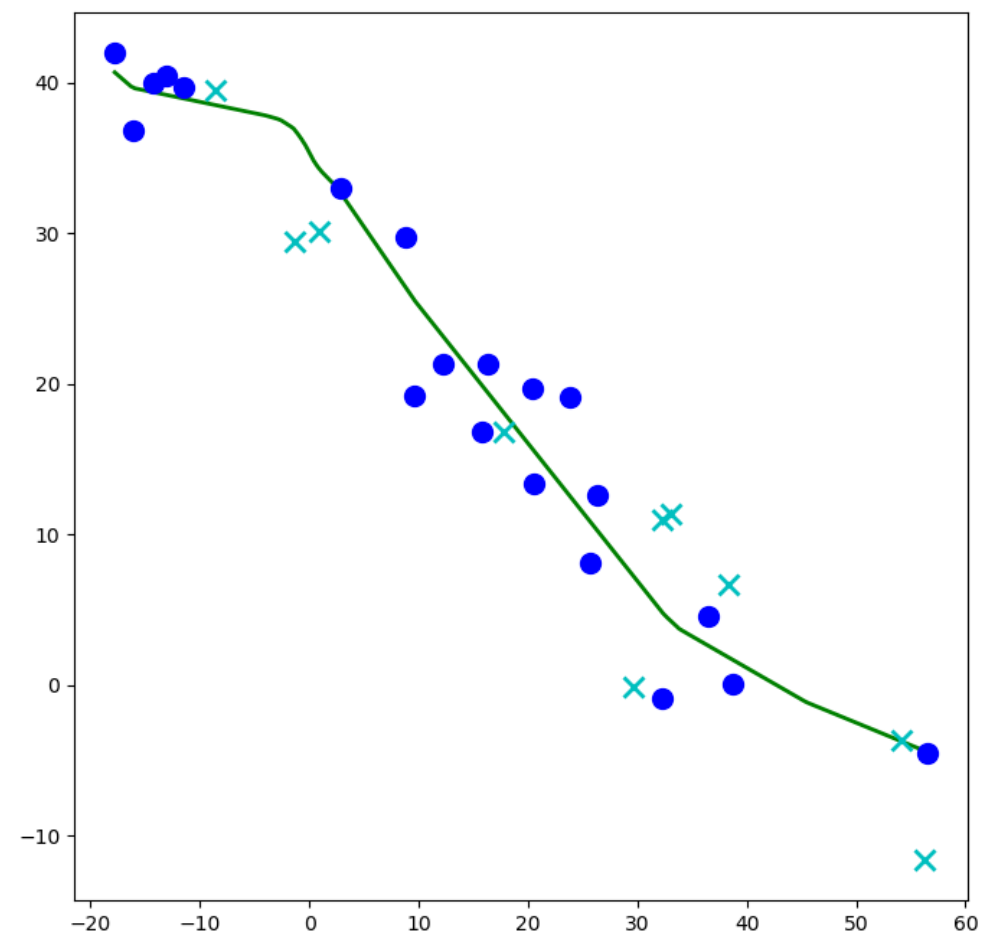
Just because it can fit any function will it?

- Objective function is non-convex
 - it will get stuck in local minima
- *Stochastic* gradient decent take pseudorandom steps
 - Helps pop out of local minima
- Is getting stuck at a local minima necessarily a bad thing??

Neural Network Properties

Fitting complex functions (with 1-D input)

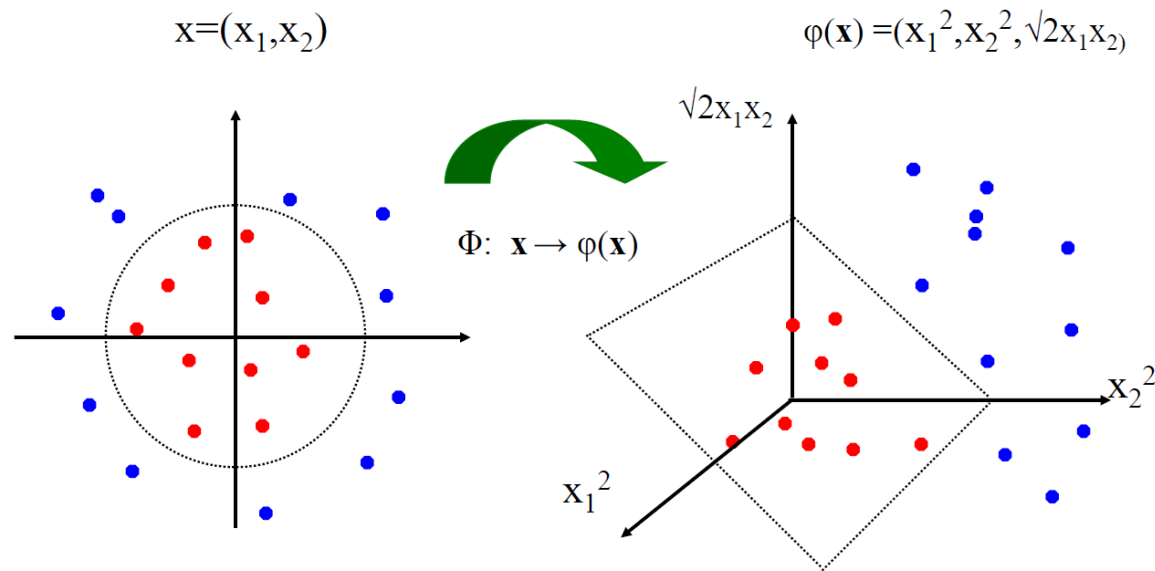
Network to Approximate a 1-D Function



Linear Classifiers for Nonlinear Data

Linear classifiers have linear decision boundaries

Feature mapping can convert nonlinear data to higher dimensions

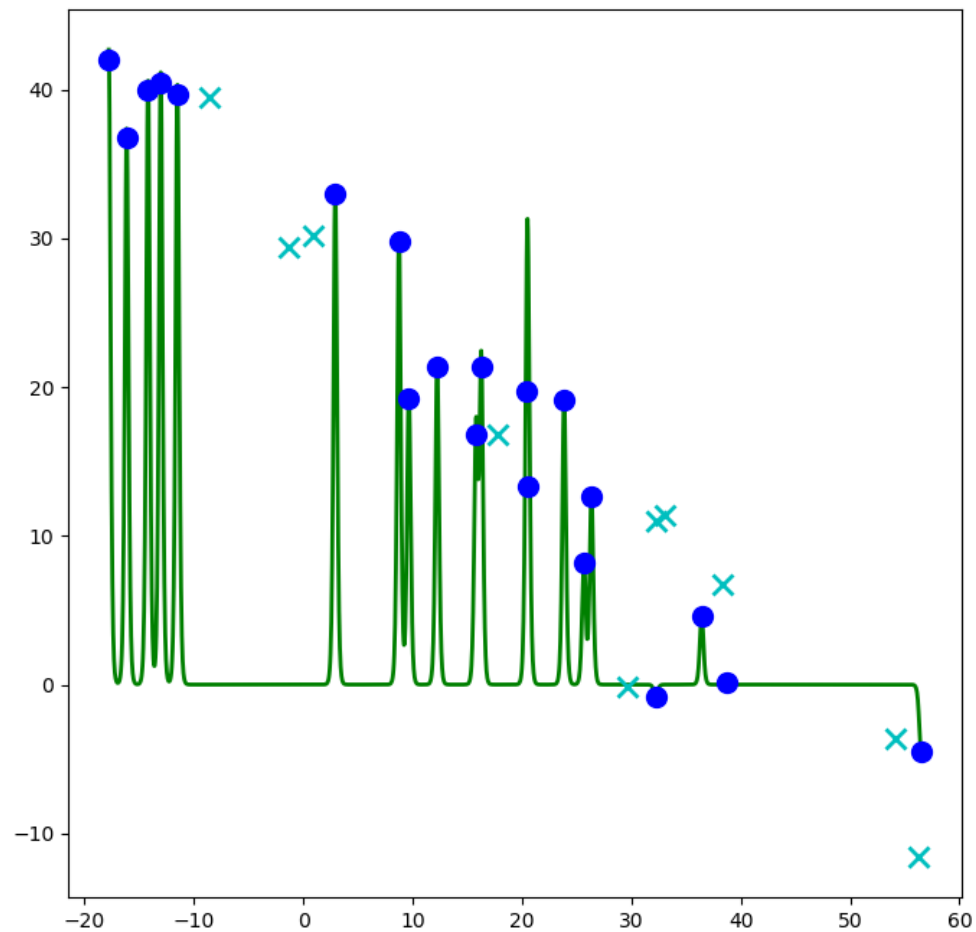
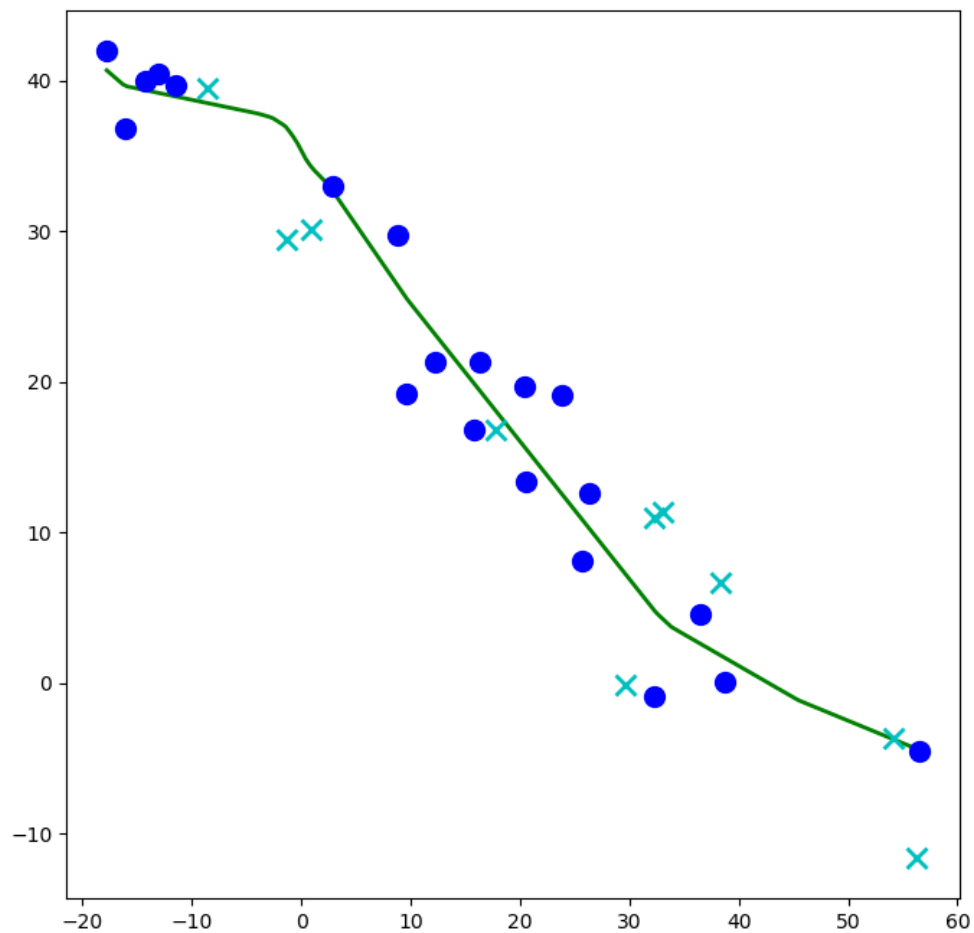


This slide is courtesy of www.iro.umontreal.ca/~pift6080/documents/papers/svm_tutorial.ppt

Today, instead of choosing a feature mapping function, we'll use neural networks to learn nonlinear decision boundaries.

- We'll quickly shift this to doing nonlinear regression too!

Network to Approximate a 1-D Function

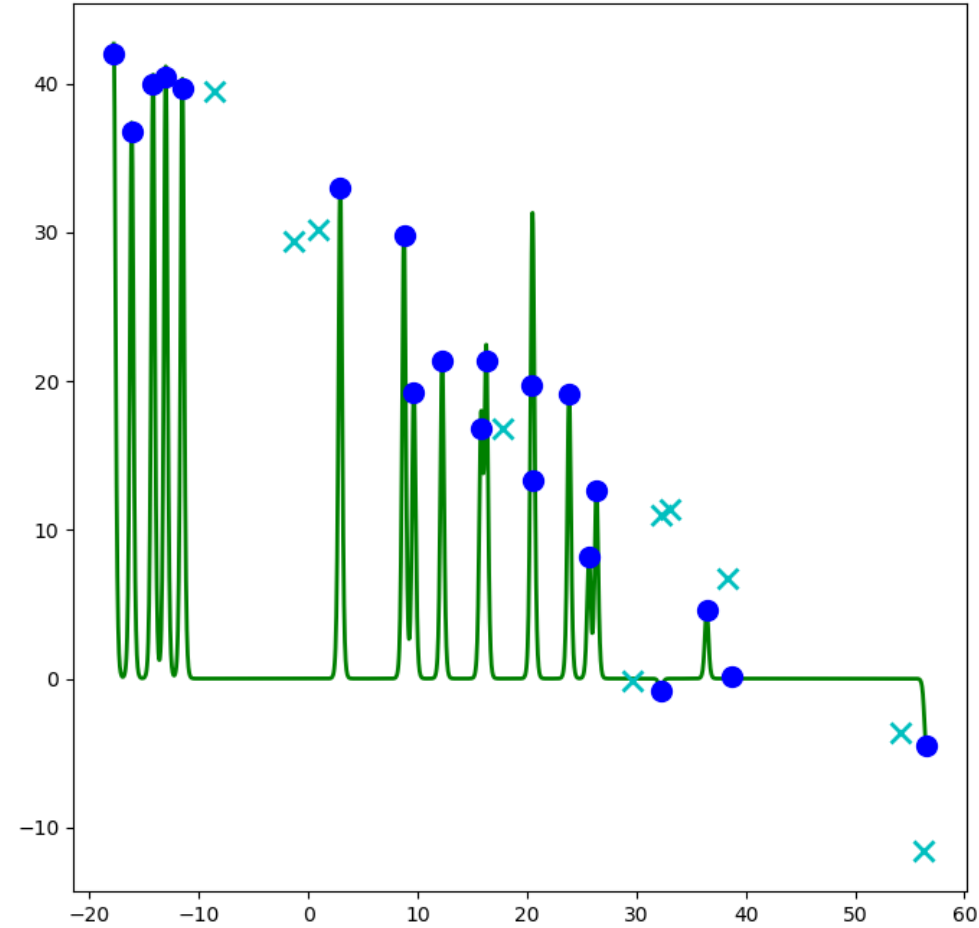


Network to Approximate a 1-D Function

Design a network to approximate this function using:

Linear, Sigmoid, Step, or ReLU

Network to Approximate a 1-D Function



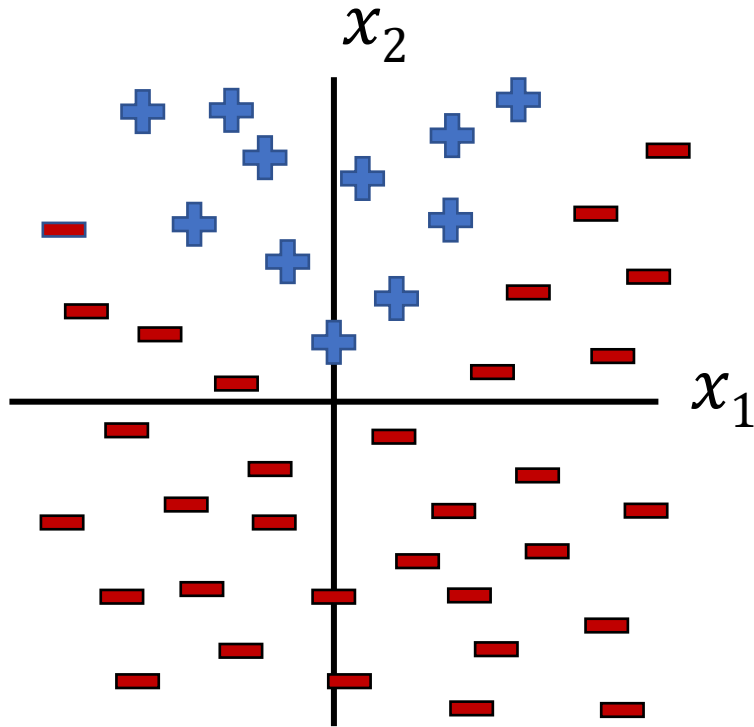
Neural Network Properties

Fitting complex functions (with 2-D input)

Classification Design Challenge

How could you configure three specific perceptrons to classify this data?

$$h_A(\mathbf{x}) = \text{sign}(\mathbf{w}_A^T \mathbf{x} + b_A)$$
$$h_B(\mathbf{x}) = \text{sign}(\mathbf{w}_B^T \mathbf{x} + b_B)$$
$$h_C(\mathbf{x}) = \text{sign}(\mathbf{w}_C^T \mathbf{x} + b_C)$$

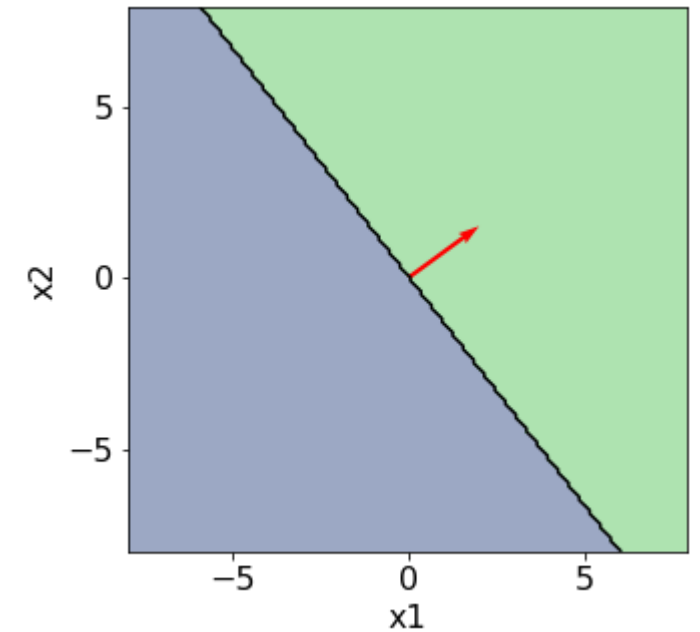
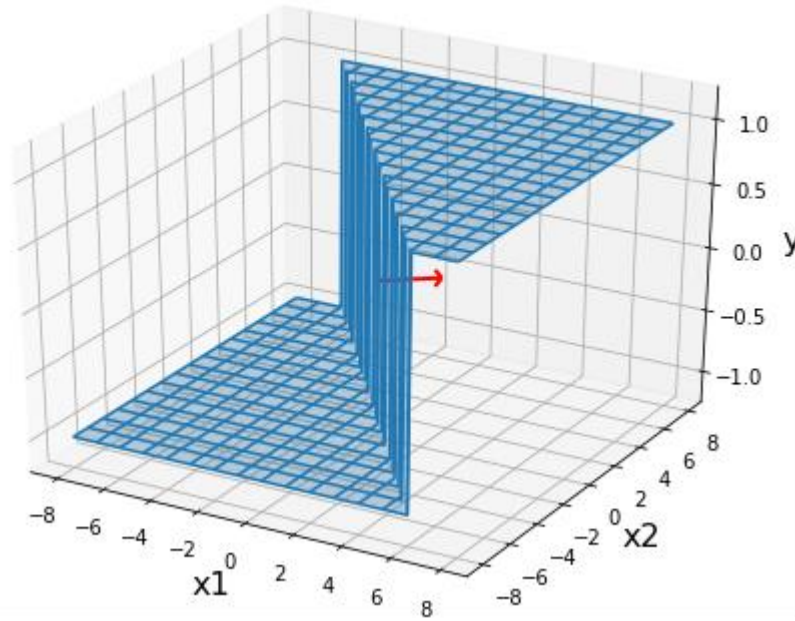
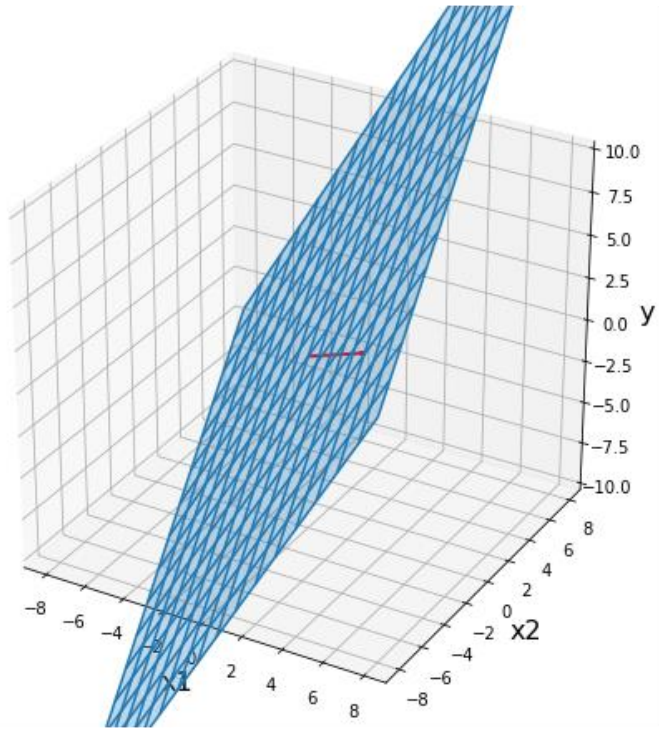


Perceptron

Classification: Hard threshold on linear model

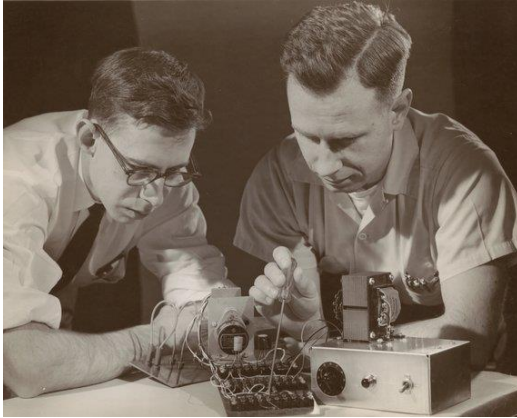
$$h(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$$

$$\text{sign}(z) = \begin{cases} 1, & \text{if } z \geq 0 \\ -1, & \text{if } z < 0 \end{cases}$$



Perceptron History

Frank Rosenblatt, 1957



The New Yorker, December 6, 1958 P. 44

Talk story about the perceptron, a new electronic brain which hasn't been built, but which has been successfully simulated on the I.B.M. 704. Talk with Dr. Frank Rosenblatt, of the Cornell Aeronautical Laboratory, who is one of the two men who developed the prodigy; the other man is Dr. Marshall C. Yovits, of the Office of Naval Research, in Washington. Dr. Rosenblatt defined the perceptron as the first non-biological object which will achieve an organization o its external environment in a meaningful way. It interacts with its environment, forming concepts that have not been made ready for it by a human agent. If a triangle is held up, the perceptron's eye picks up the image & conveys it along a random succession of lines to the response units, where the image is registered. It can tell the difference betw. a cat and a dog, although it wouldn't be able to tell whether the dog was to theleft or right of the cat. Right now it is of no practical use, Dr. Rosenblatt conceded, but he said that one day it might be useful to send one into outer space to take in impressions for us.



Exercise

Which of the following perceptron parameters will perfectly classify this data?

$$h(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$$

$$\text{sign}(z) = \begin{cases} 1, & \text{if } z \geq 0 \\ -1, & \text{if } z < 0 \end{cases}$$

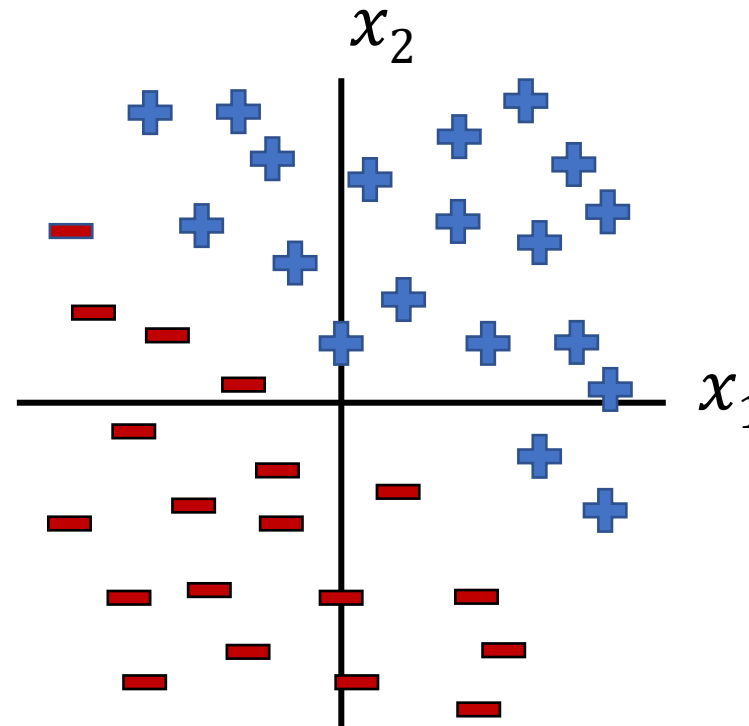
A. $\mathbf{w} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, b = 0$

B. $\mathbf{w} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}, b = 0$

C. $\mathbf{w} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, b = 0$

D. $\mathbf{w} = \begin{bmatrix} -1 \\ -1 \end{bmatrix}, b = 0$

E. None of the above



Poll

Which of the following perceptron parameters will perfectly classify this data?

$$h(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$$

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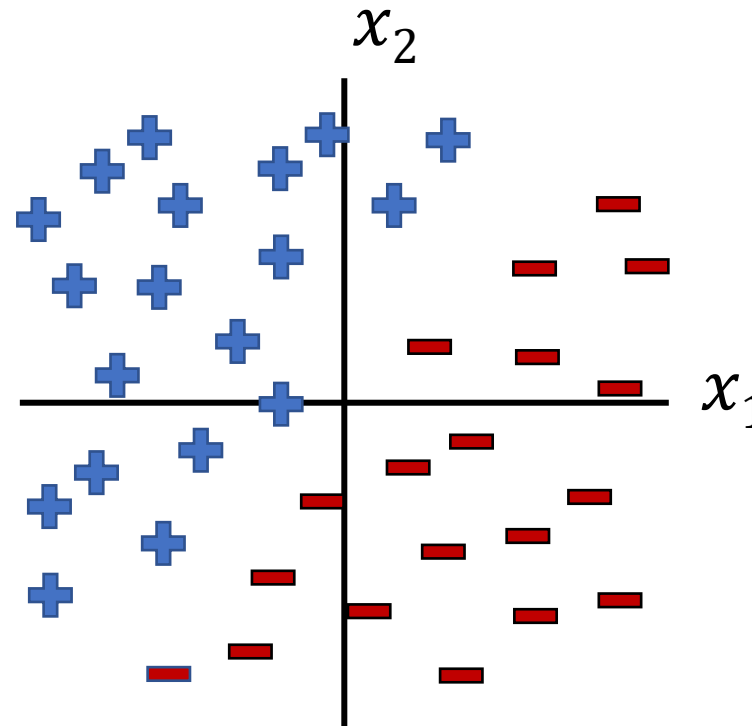
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D. $\mathbf{w} = \begin{bmatrix} -1 \\ -1 \end{bmatrix}, b = 0$

E. None of the above



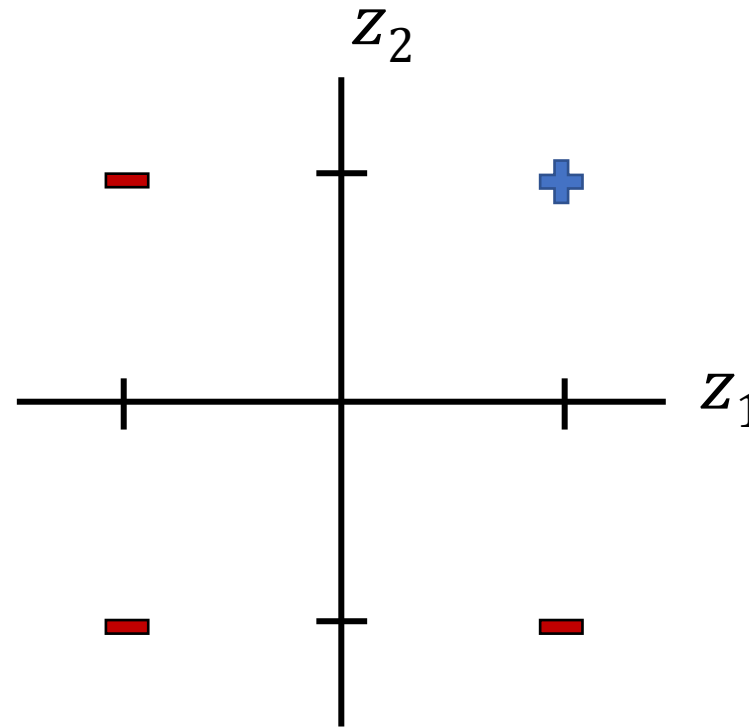
Poll

Which of the following parameters of $h_c(\mathbf{z})$ will perfectly classify this data?

$$h_c(\mathbf{z}) = \text{sign}(\mathbf{w}_c^T \mathbf{z} + b_c)$$

$$\text{sign}(x) = \begin{cases} 1, & \text{if } x \geq 0 \\ -1, & \text{if } x < 0 \end{cases}$$

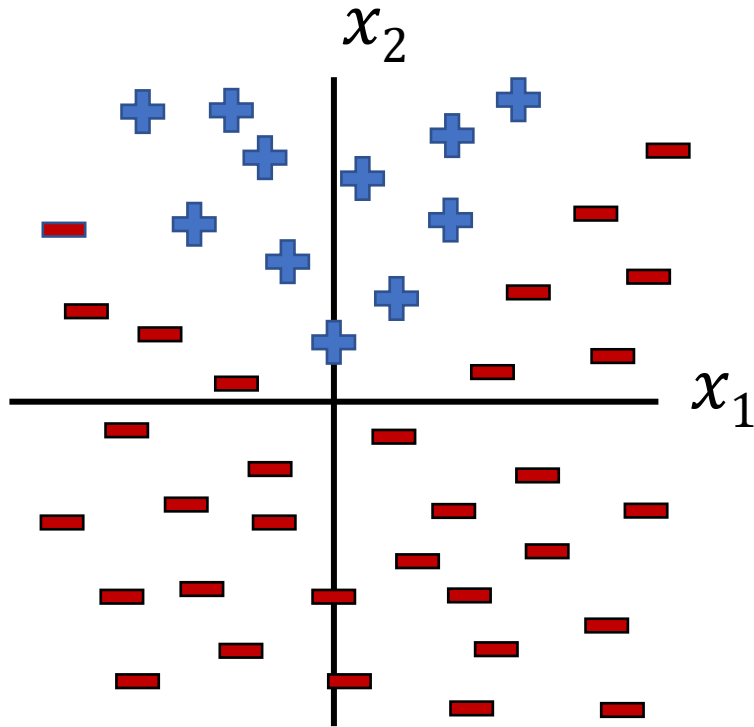
- A. $\mathbf{w}_c = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, b_c = 0$
- B. $\mathbf{w}_c = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, b_c = 1$
- C. $\mathbf{w}_c = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, b_c = -1$
- D. None of the above



Classification Design Challenge

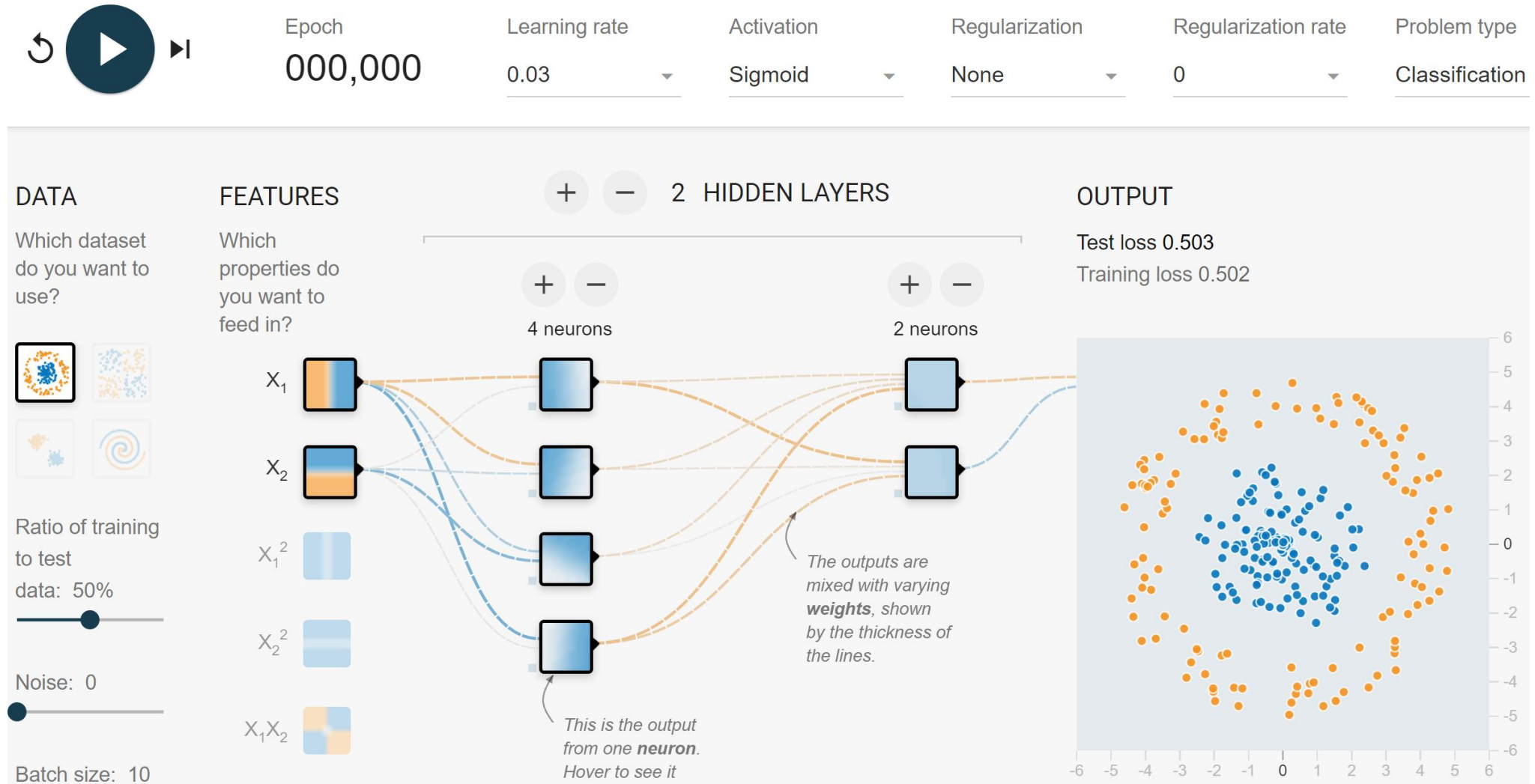
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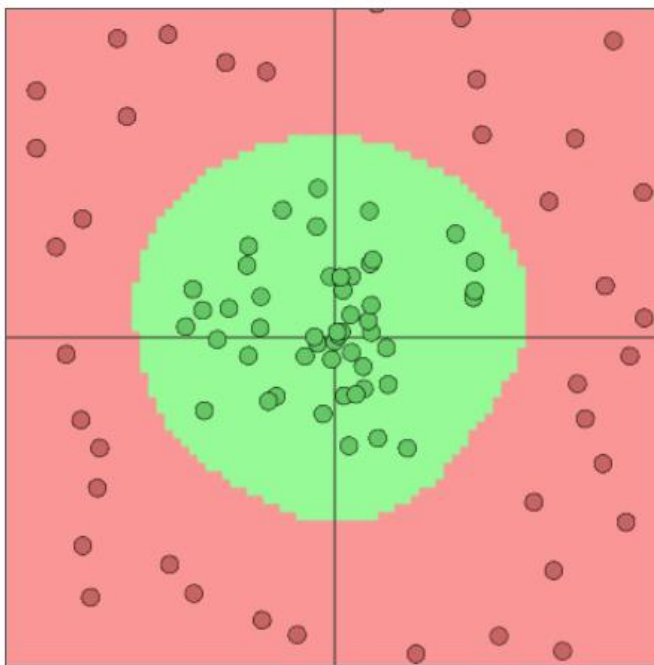
Network to Approximate Binary Classification

<https://playground.tensorflow.org/#activation=sigmoid>



Network to Approximate Binary Classification

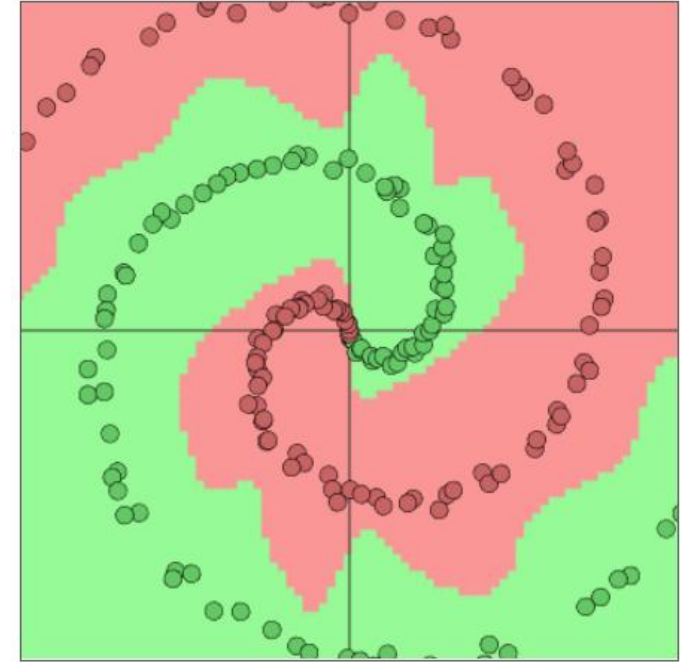
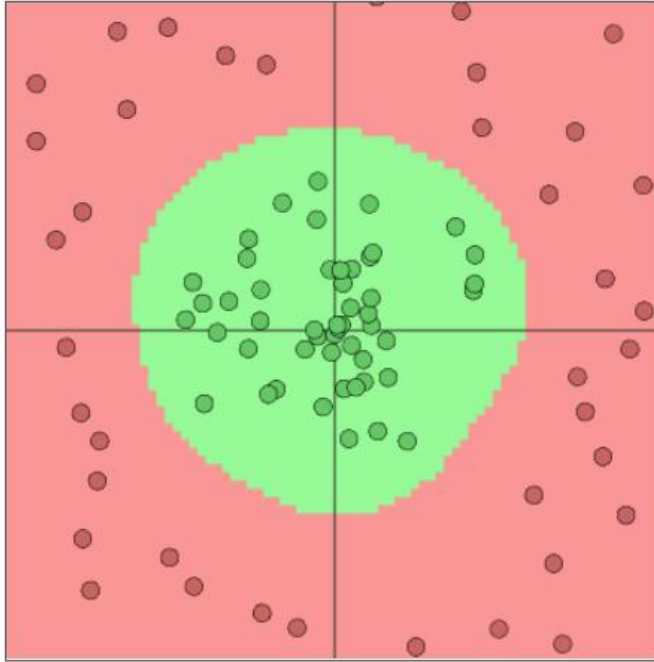
Approximate arbitrary decision boundary



<https://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html>

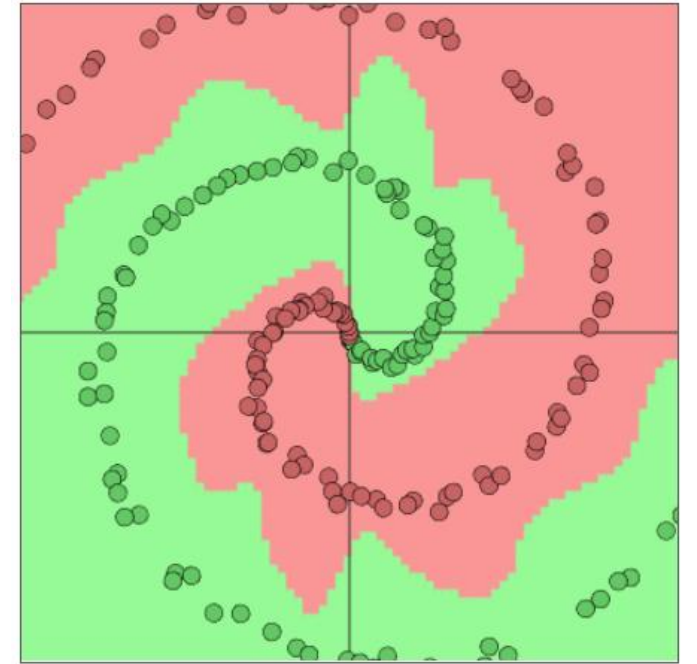
Network to Approximate Binary Classification

Approximate arbitrary decision boundary



Network to Approximate Binary Classification

Approximate arbitrary decision boundary



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Neural Network Properties

(Over?) Fitting any function

Neural Networks Properties

Universal Approximation Theorem

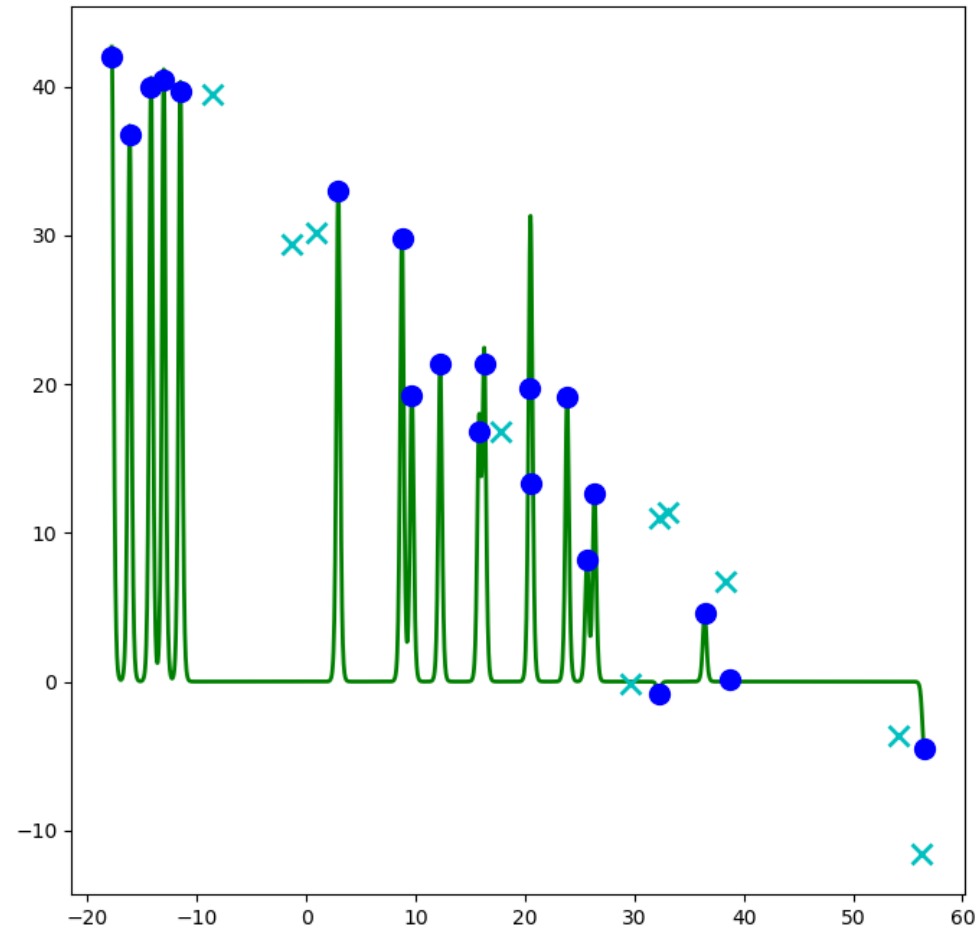
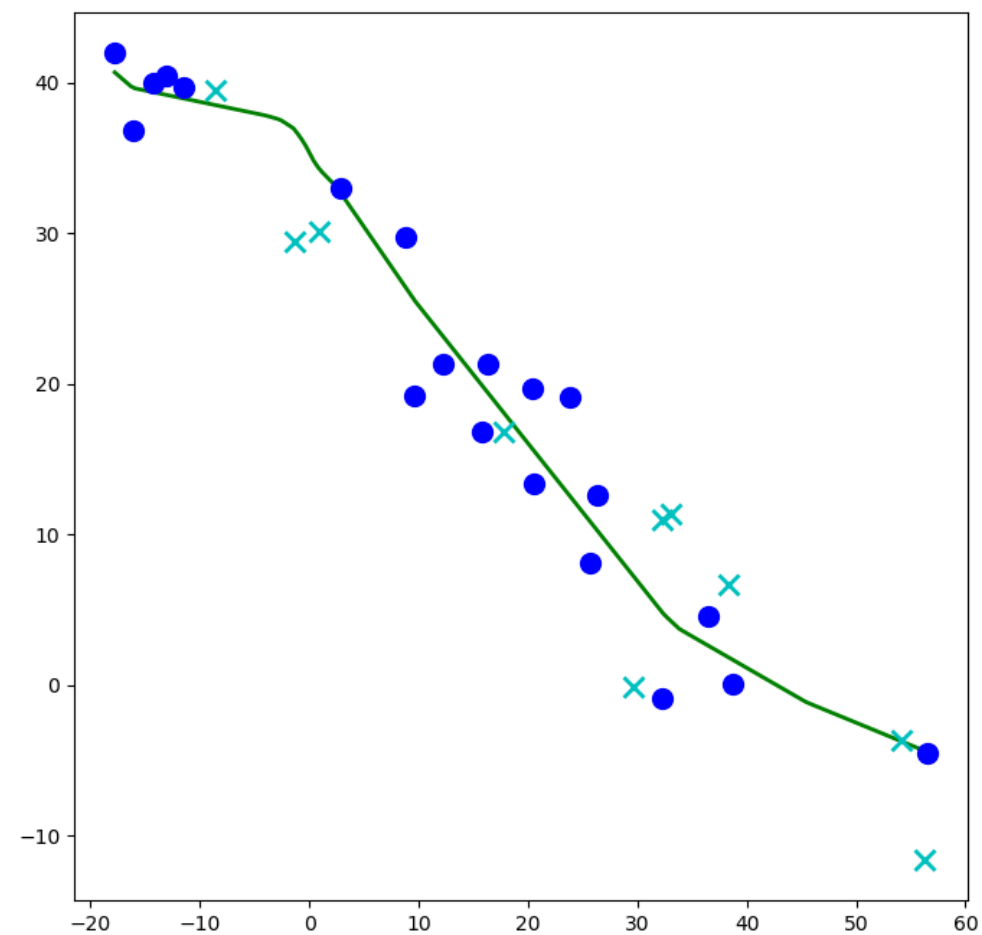
- A two-layer neural network with a sufficient number of neurons can approximate any continuous function to any desired accuracy

Reminder

Just because it can fit any function will it?

- Objective function is non-convex
 - it will get stuck in local minima
- *Stochastic* gradient decent take pseudorandom steps
 - Helps pop out of local minima
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Network to Approximate a 1-D Function



Debugging Overfitting and Underfitting

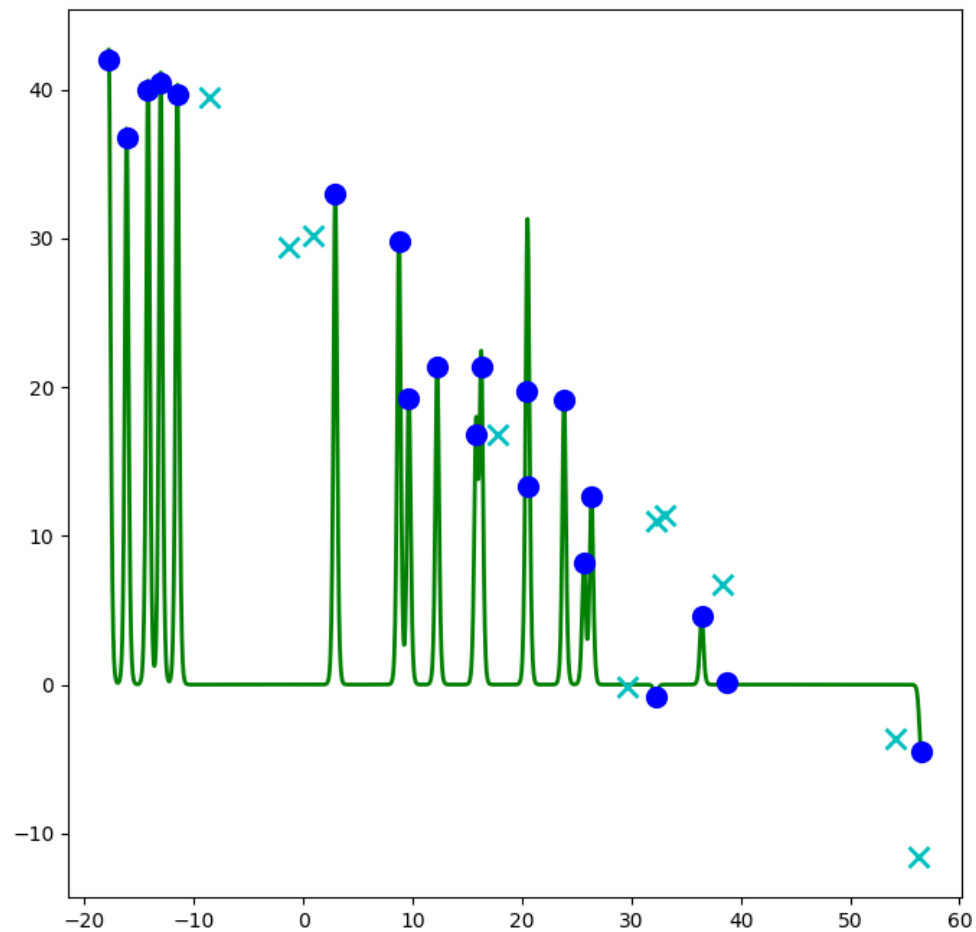
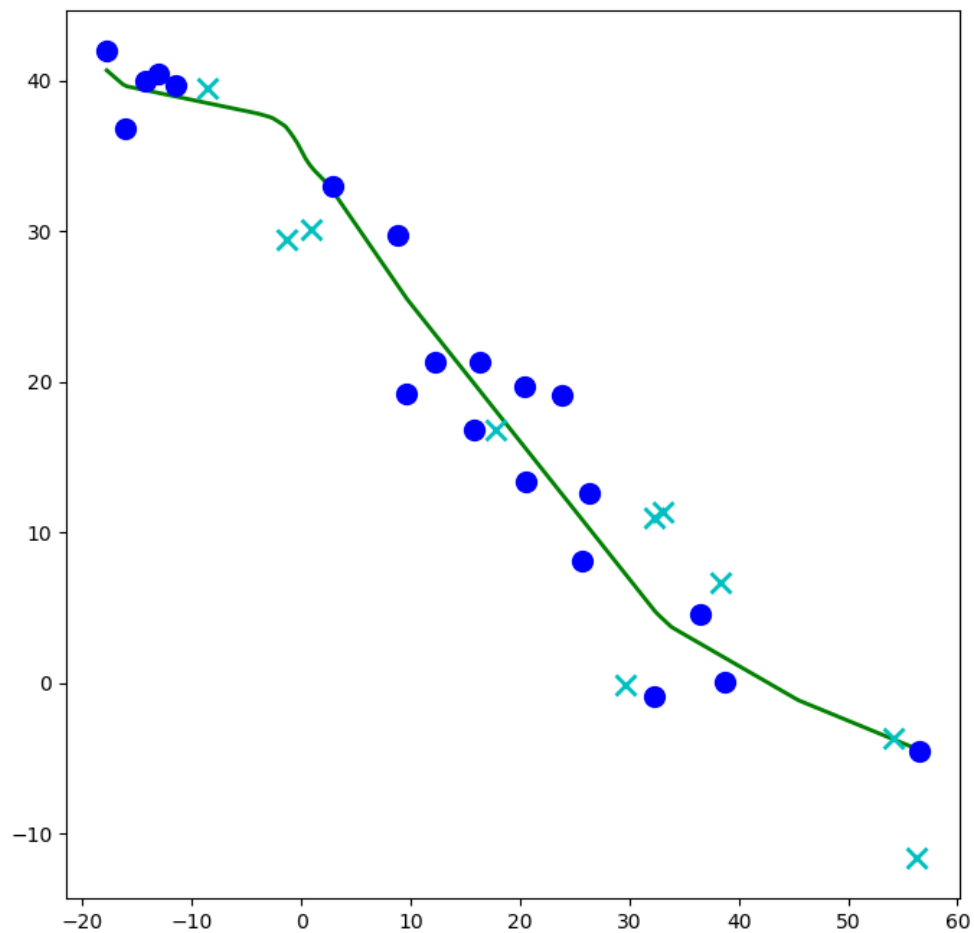
Underfitting (check this first!)

- Evidence: poor training loss (and poor validation loss)
 - Note: Compare with human performance as a baseline, i.e., make sure the task isn't impossible for a human (with unlimited resources)
- Try: Adding more capacity to network (wider or deeper)
 - But how do we choose a new network structure?

Overfitting

- Evidence: good training loss, but poor validation loss
- Evidence: really large parameter values
- Try: Regularization (we'll learn about this soon!)
- Try: Adding more data

Network to Approximate a 1-D Function



Summary: Neural Networks Properties

Practical considerations

- Large number of neurons
 - Danger for overfitting
- Modeling assumptions vs data assumptions trade-off
- Gradient descent can easily get stuck local optima

What if there are no non-linear activations?

- A deep neural network with only linear layers can be reduced to an exactly equivalent single linear layer

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