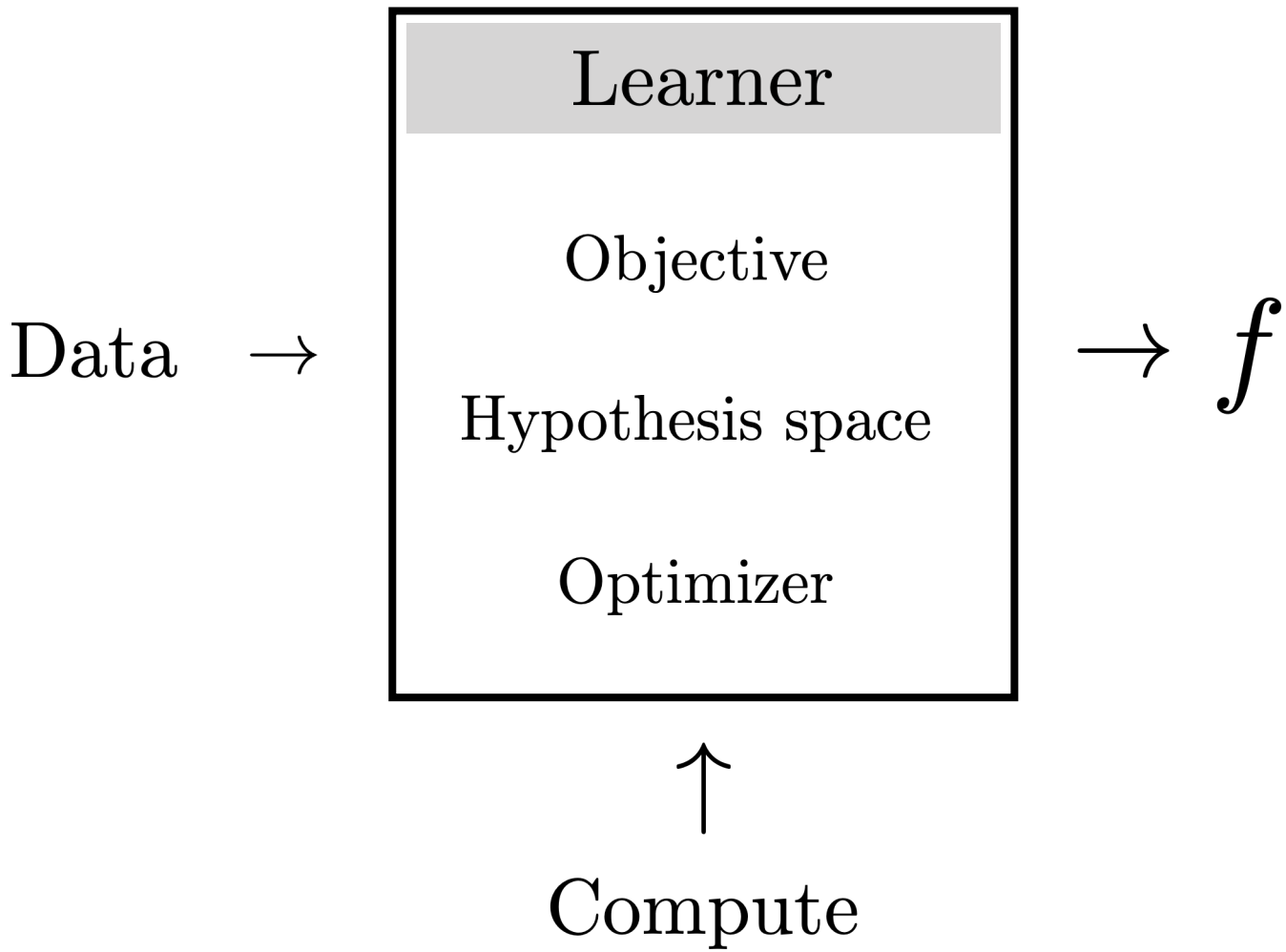
CMSC 472/672

Lecture 9

Neural Network Optimization

CMSC 472/672

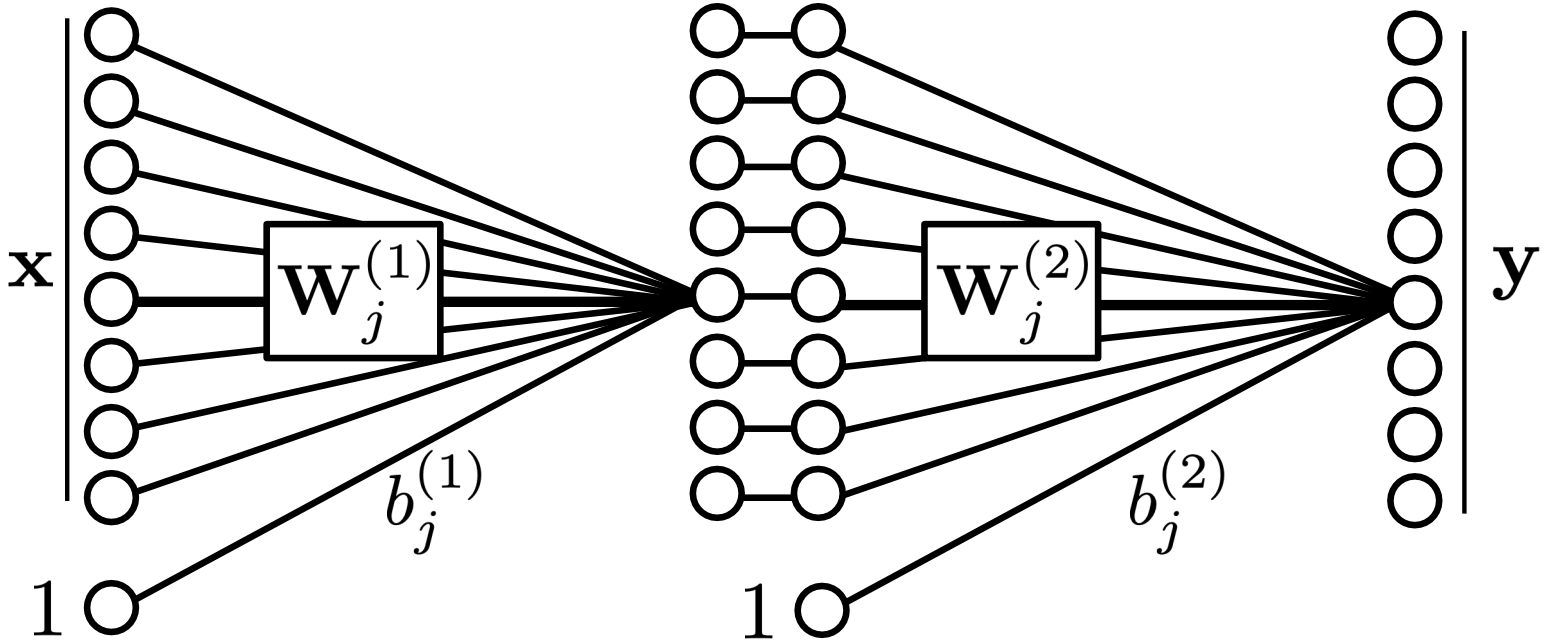

Learner
Objective
Hypothesis space
Optimizer
Data
$\rightarrow$
$\rightarrow f$
Compute

Stacking layers

Input representation

Intermediate representation

Output representation



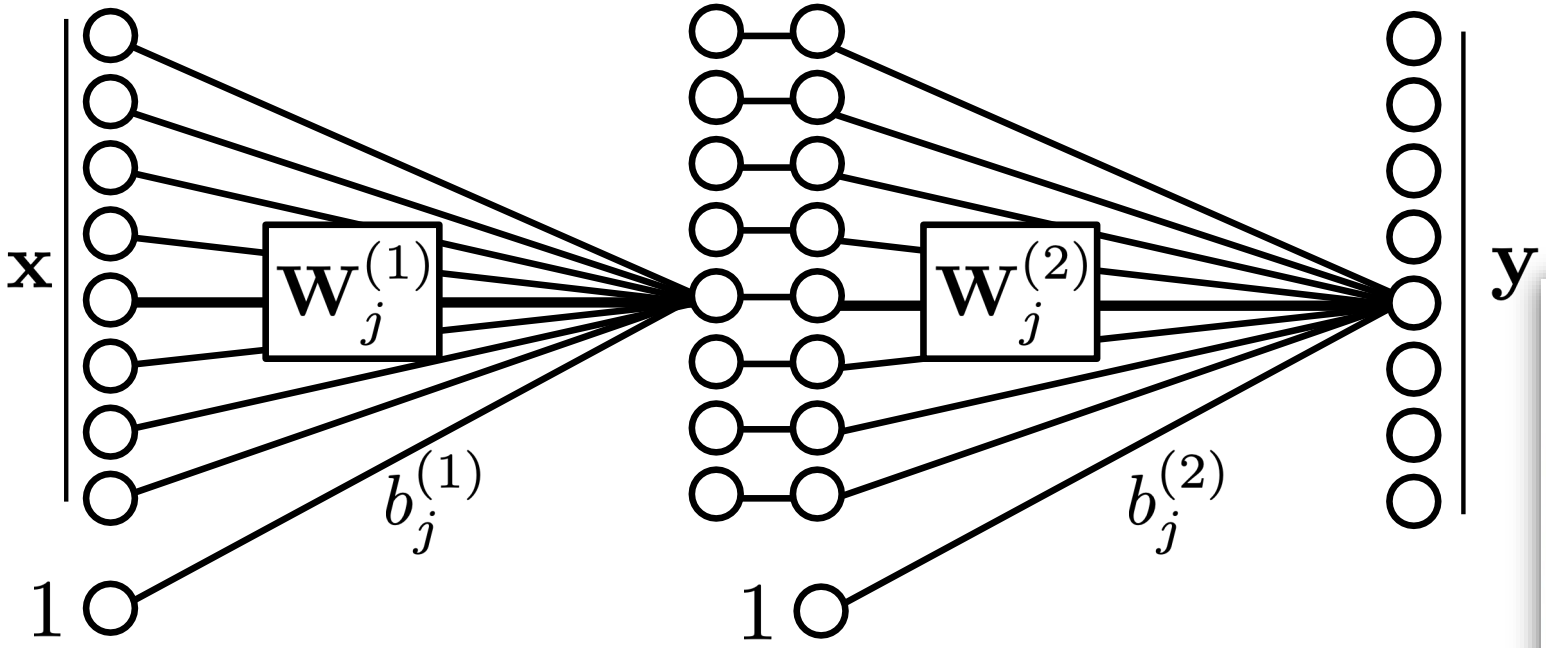
$\mathbf{h}$ = “hidden units”

Stacking layers

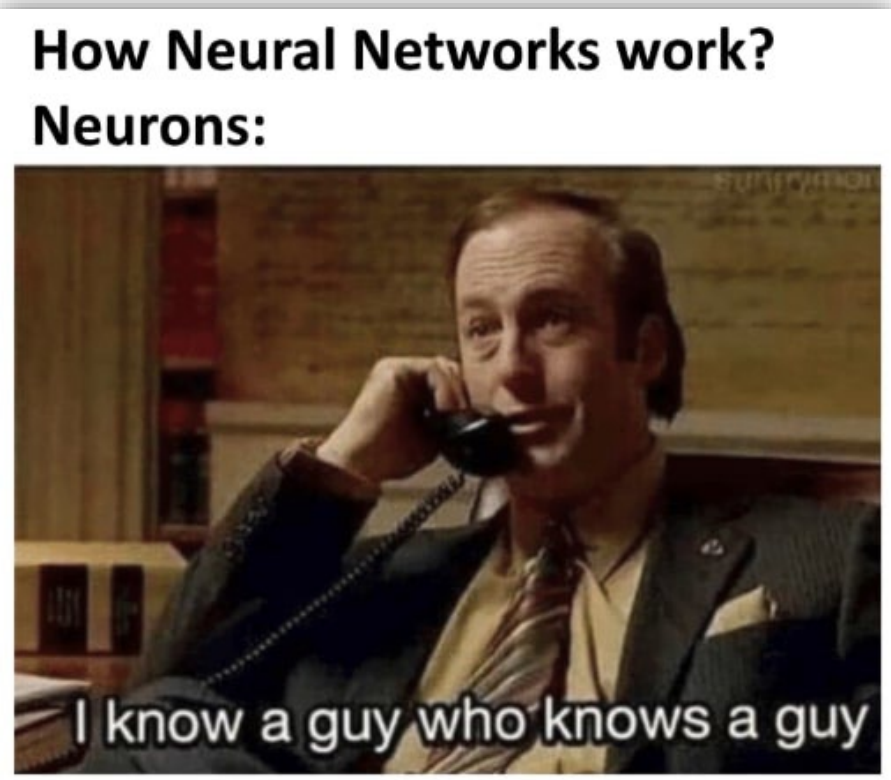
Input representation

Intermediate representation

Output representation



h = “hidden units”



An Incremental Learning Strategy

(gradient descent)

Given several examples

$$\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$$

and a perceptron

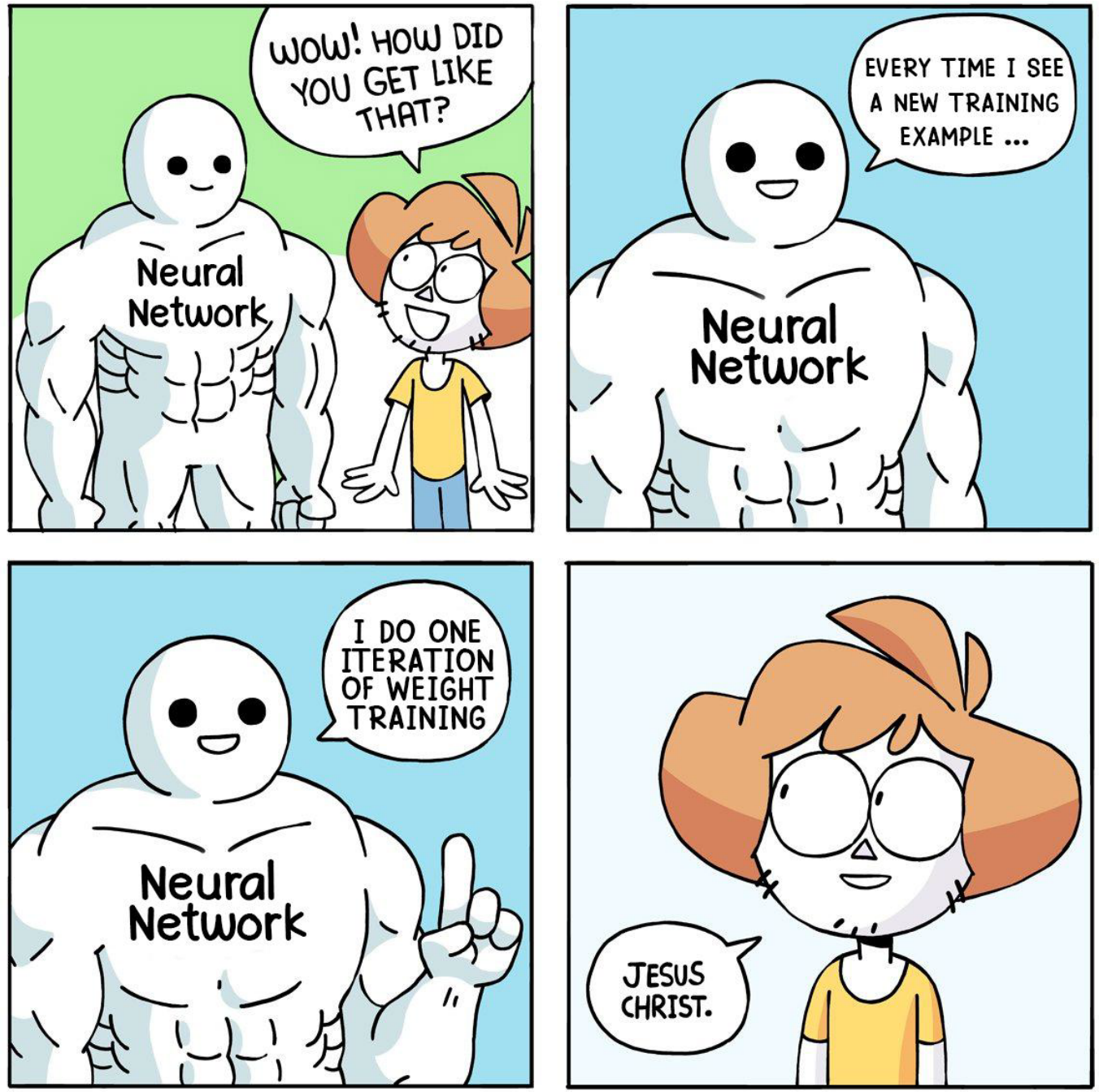
$$\hat{y} = wx$$

Modify weight w such that $\hat{y}$ gets **'closer'** to y

perceptron parameter

perceptron output

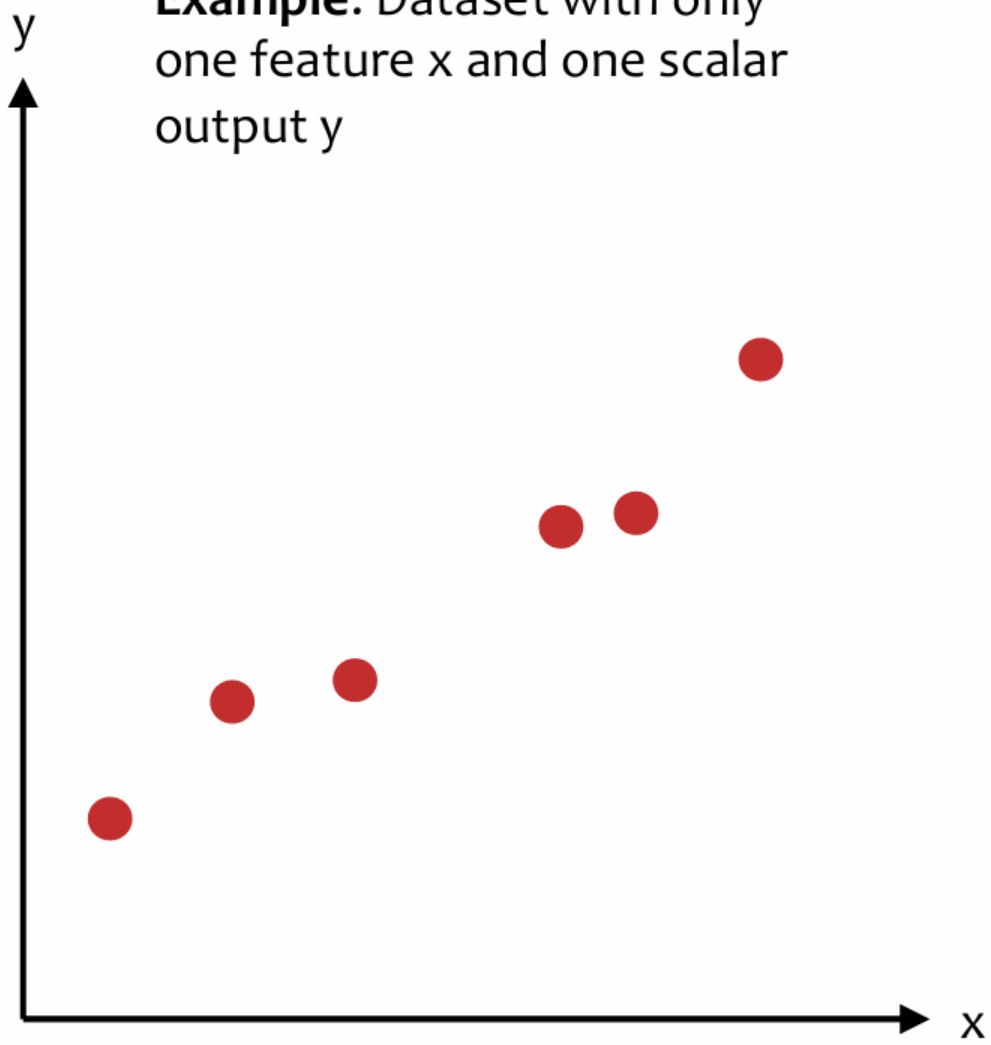
true label


WOW! HOW DID YOU GET LIKE THAT?
Neural Network
EVERY TIME I SEE A NEW TRAINING EXAMPLE ...
Neural Network
I DO ONE ITERATION OF WEIGHT TRAINING
Neural Network
JESUS CHRIST.

SHEN COMIX

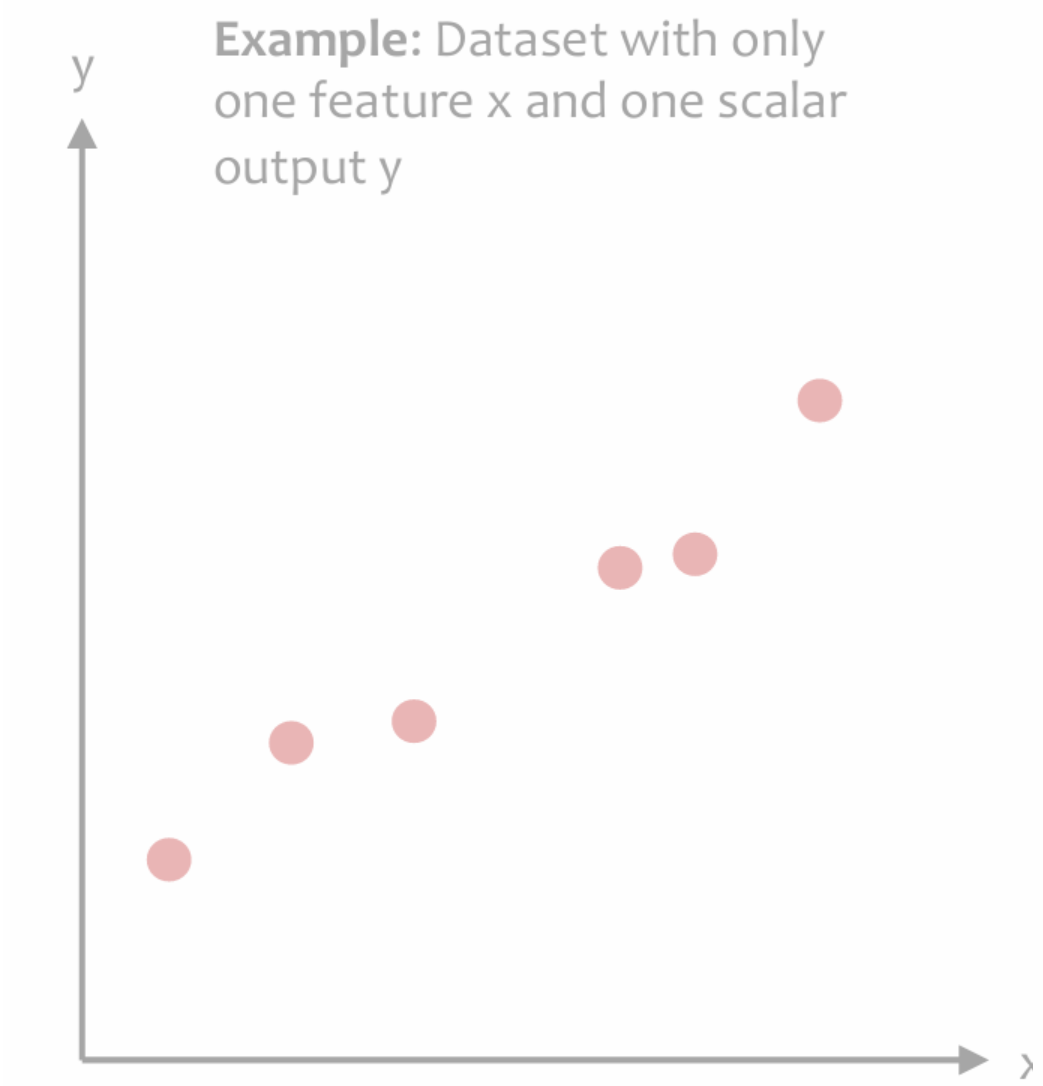
Recap: Linear Regression

Example: Dataset with only one feature x and one scalar output y



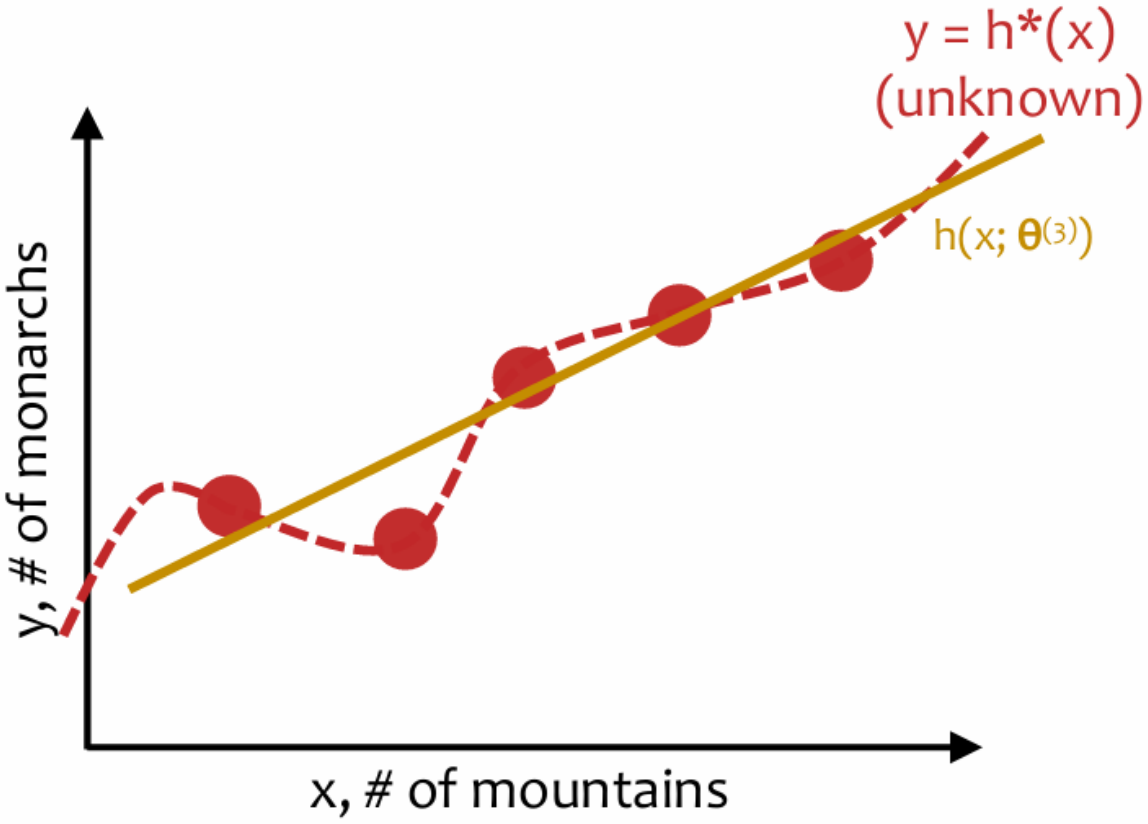
Q: What is the function that best fits these points?

Recap: Linear Regression



Example: Dataset with only one feature x and one scalar output y

Q: What is the function that best fits these points?



Naïve Idea:

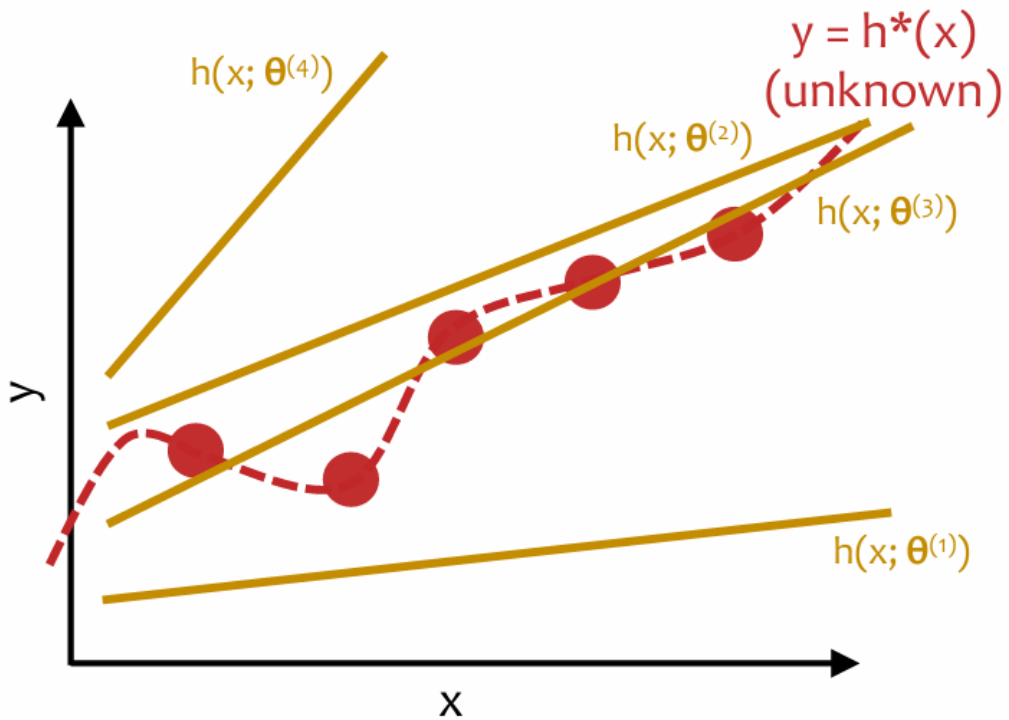
Linear Regression by Random Guessing

!!!

Linear Regression by Rand. Guessing

Optimization Method #0: Random Guessing

1. Pick a random $\boldsymbol{\theta}$
2. Evaluate $J(\boldsymbol{\theta})$
3. Repeat steps 1 and 2 many times
4. Return $\boldsymbol{\theta}$ that gives smallest $J(\boldsymbol{\theta})$



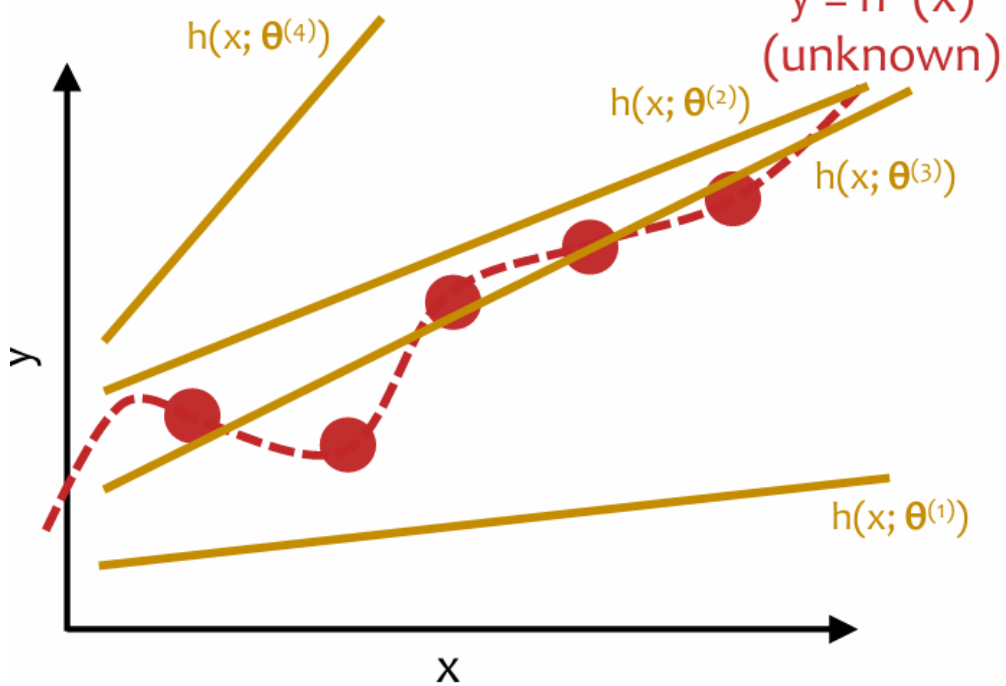
For Linear Regression:

- target function h*(x) is **unknown**
- only have access to h*(x) through **training examples** $(x^{(i)},y^{(i)})$
- want $h(x; \boldsymbol{\theta}^{(t)})$ that **best approximates** h*(x)
- **enable generalization** w/inductive bias that restricts hypothesis class to **linear functions**

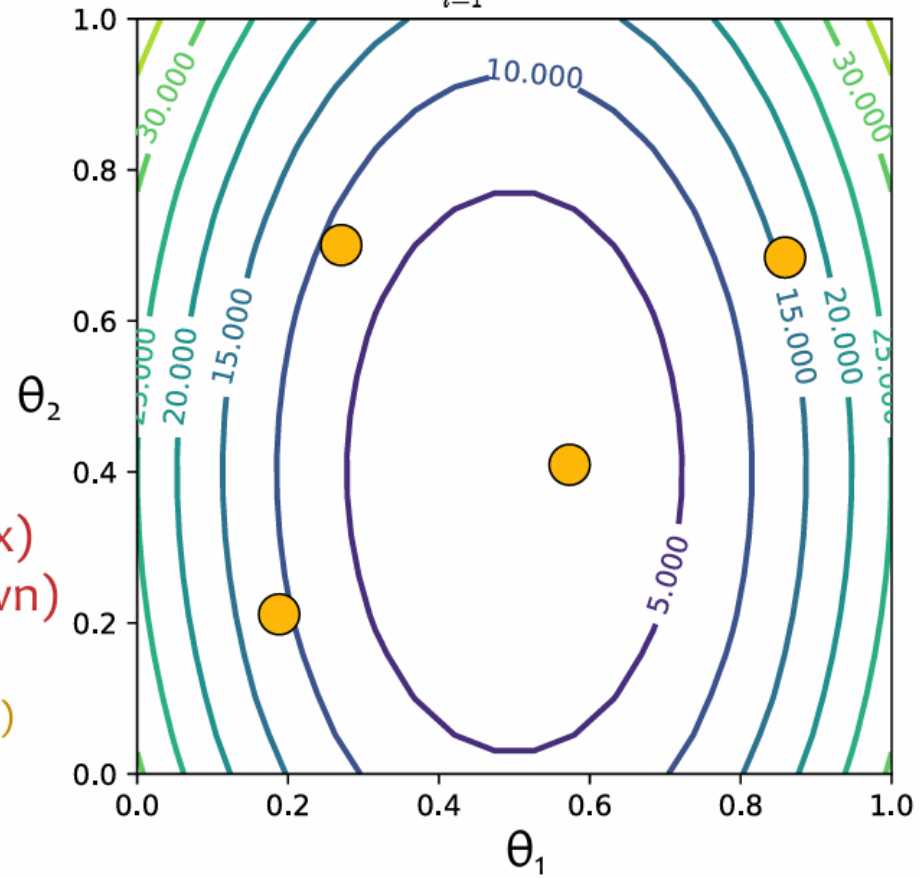
Linear Regression by Rand. Guessing

Optimization Method #0: Random Guessing

1. Pick a random **θ**
2. Evaluate J(**θ**)
3. Repeat steps 1 and 2 many times
4. Return **θ** that gives smallest J(**θ**)



$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)}\right)^2$$



t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.2	0.2	10.4
2	0.3	0.7	7.2
3	0.6	0.4	1.0
4	0.9	0.7	16.2

Better Idea:

An optimization algorithm called

“Gradient Descent”

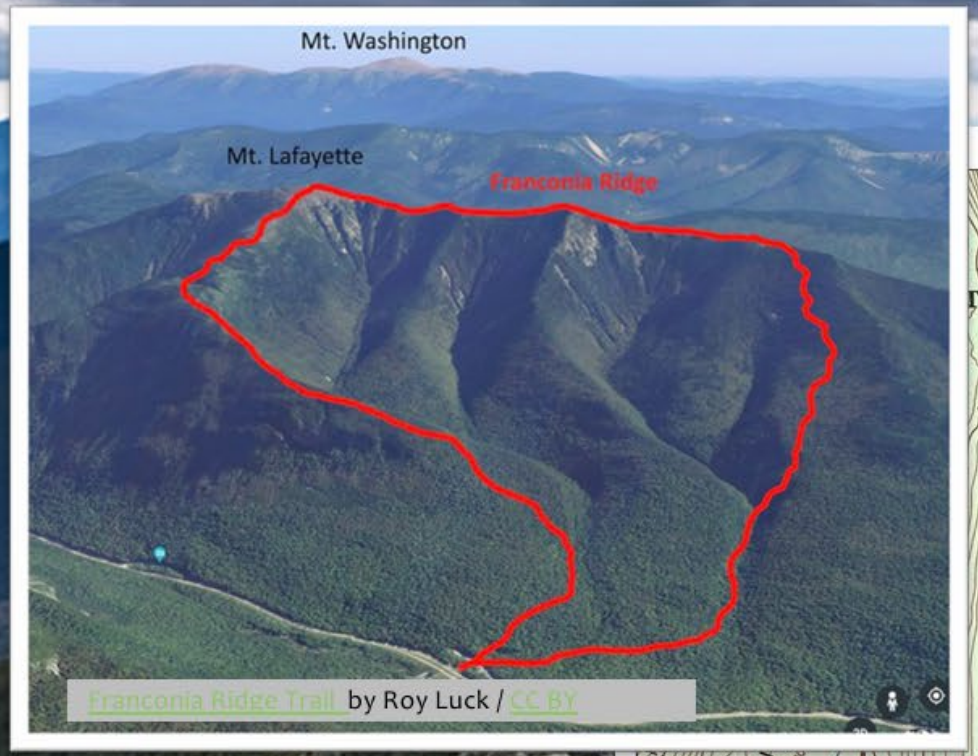
Recall: Gradient of a vector

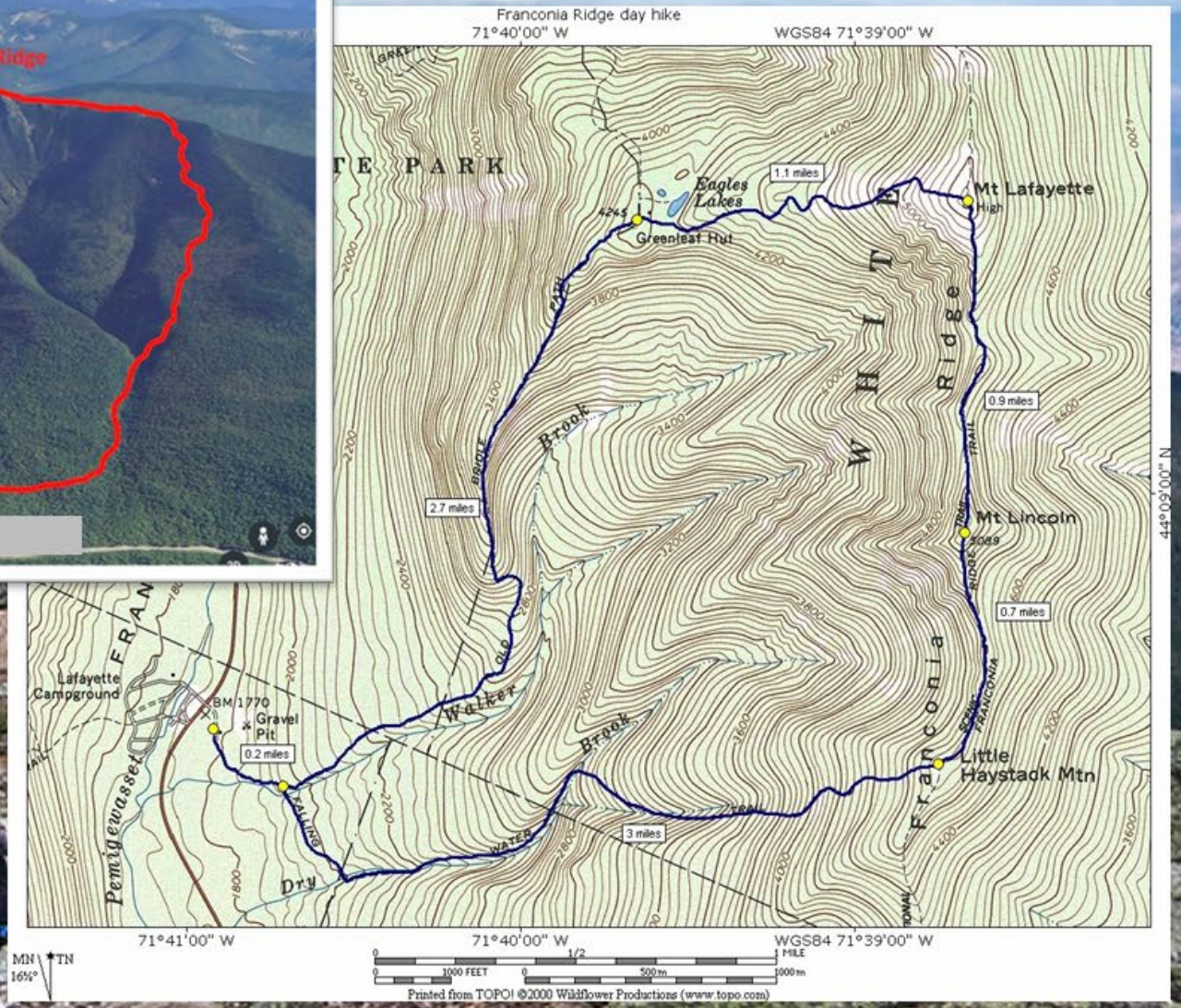
Def: The gradient of $J : \mathbb{R}^M \to \mathbb{R}$ is

$$\nabla J(\boldsymbol{\theta}) = \begin{bmatrix} \frac{\partial J(\boldsymbol{\theta})}{\partial \theta_1} \\ \frac{\partial J(\boldsymbol{\theta})}{\partial \theta_2} \\ \vdots \\ \frac{\partial J(\boldsymbol{\theta})}{\partial \theta_M} \end{bmatrix}$$

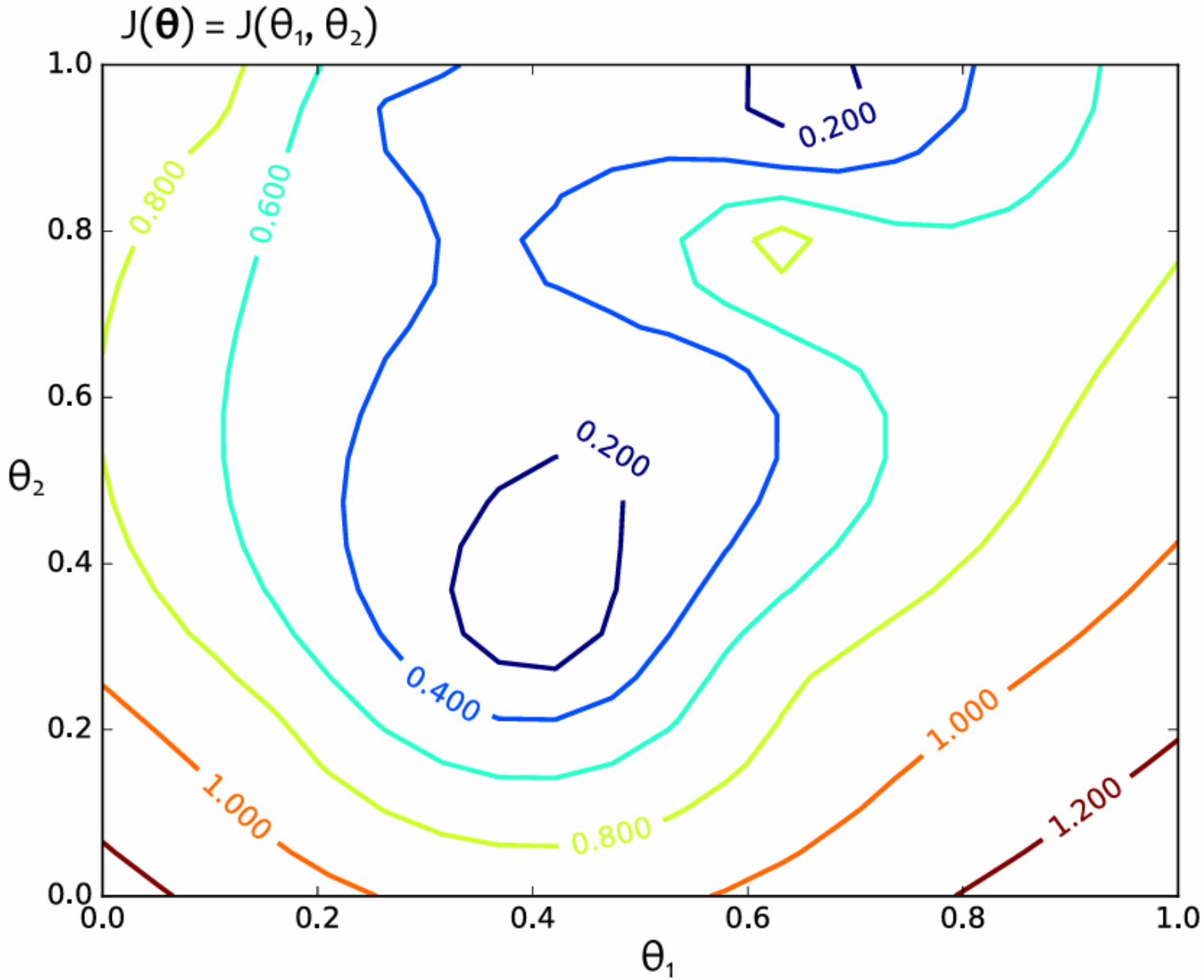
Each entry is a first-order partial derivative

Topographical Maps

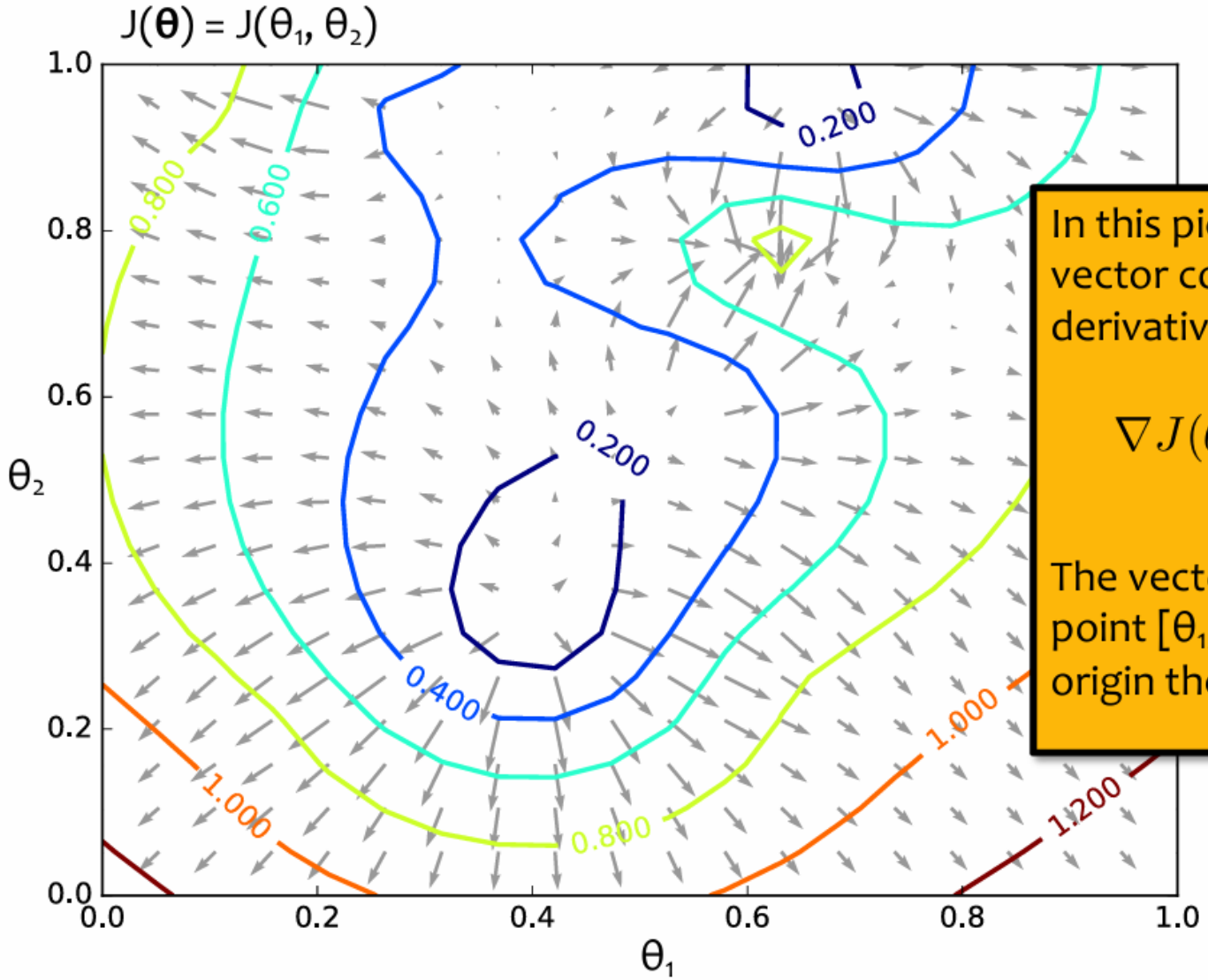




Gradients


J(θ) = J(θ1, θ2)
1.0
0.8
0.6
0.4
0.2
0.0
θ2
0.0
0.2
0.4
0.6
0.8
1.0
θ1
0.200
0.800
0.600
0.200
0.400
1.000
0.800
1.000
1.200

Gradients



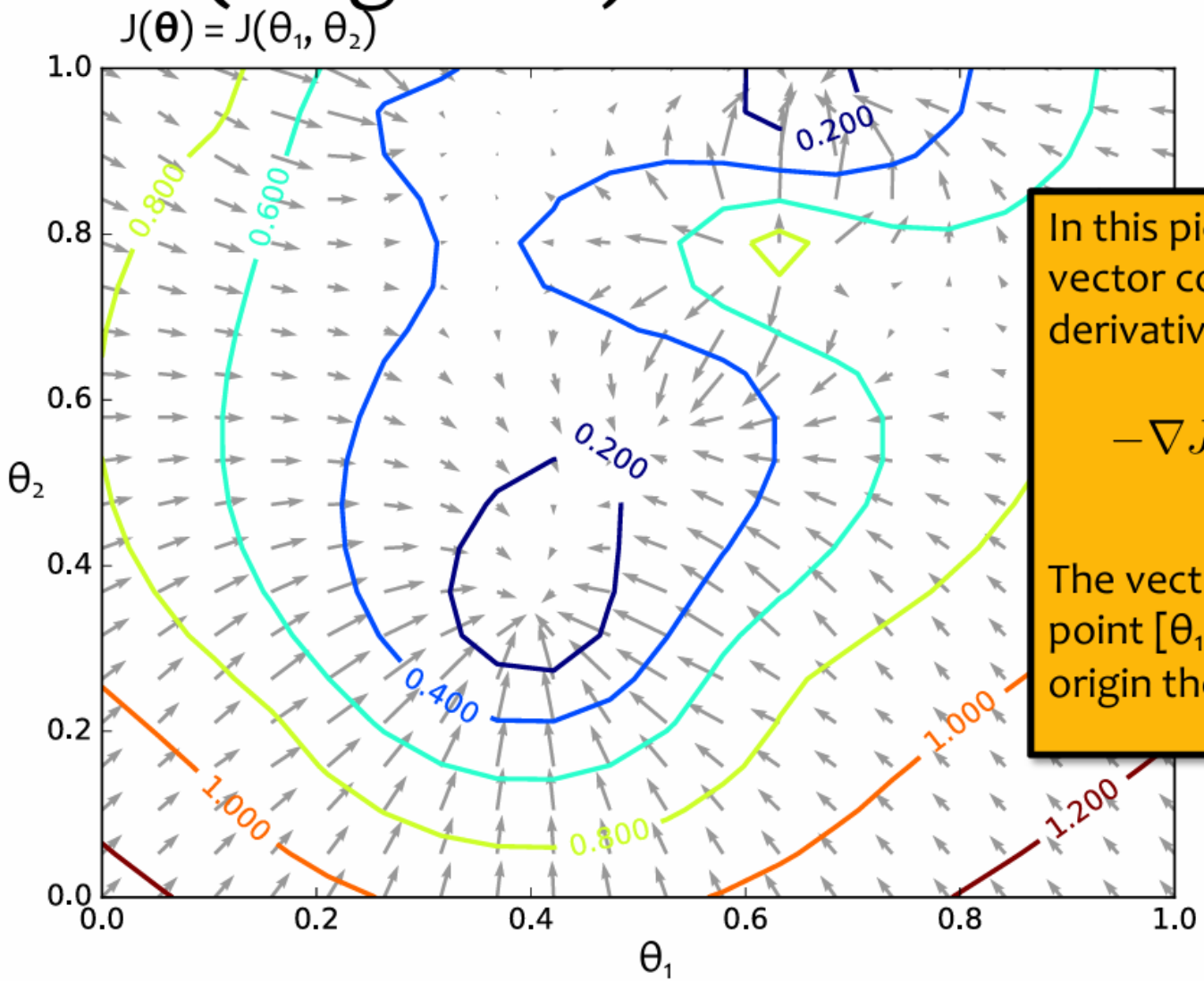
In this picture, each arrow is a 2D vector consisting of two partial derivatives.

$$\nabla J(\theta_1, \theta_2) = \begin{bmatrix} \frac{\partial J}{\partial \theta_1} \\ \\ \frac{\partial J}{\partial \theta_2} \end{bmatrix}$$

The vector is evaluated at the point $[\theta_1, \theta_2]^T$ and plotted with its origin there as well.

These are the **gradients** that Gradient **Ascent** would follow.

(Negative) Gradients



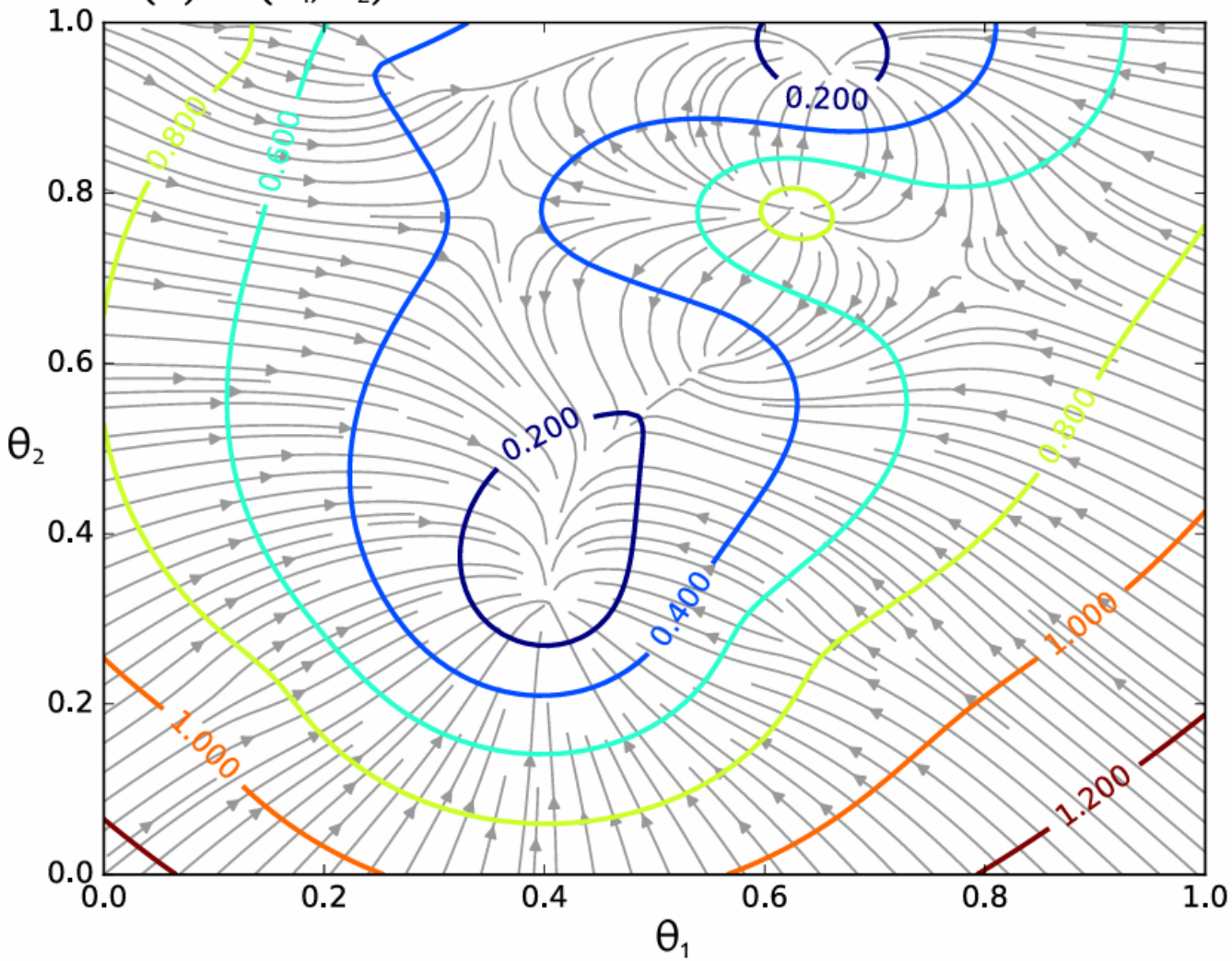
In this picture, each arrow is a 2D vector consisting of two partial derivatives.

$$-\nabla J(\theta_1, \theta_2) = \begin{bmatrix} -\frac{\partial J}{\partial \theta_1} \\ \\ -\frac{\partial J}{\partial \theta_2} \end{bmatrix}$$

The vector is evaluated at the point $[\theta_1, \theta_2]^T$ and plotted with its origin there as well.

These are the **negative** gradients that Gradient **Descent** would follow.

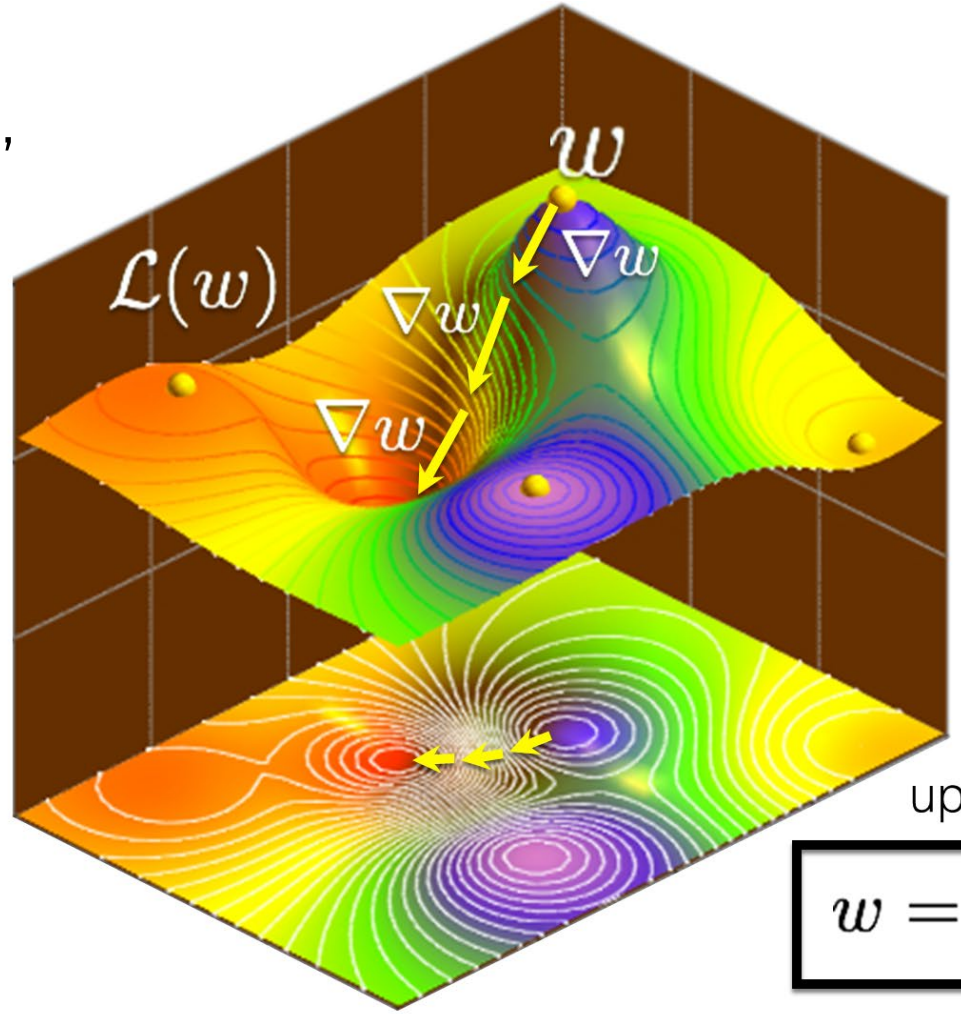
(Negative) Gradient *Paths*



Shown are the **paths** that Gradient Descent would follow if it were making **infinitesimally small steps.**

Gradient Descent

- Go down the path of "steepest descent"



update rule:

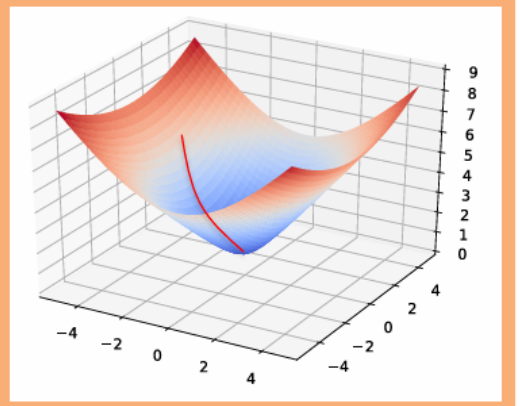
$$w = w - \nabla w$$

Gradient Descent

- Go down the path of steepest descent

Algorithm 1 Gradient Descent

1: **procedure** GD($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
2: $\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
3: $\quad$**while** not converged **do**
4: $\quad\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
5: $\quad$**return** $\boldsymbol{\theta}$



In order to apply GD to Linear Regression all we need is the **gradient** of the objective function (i.e. vector of partial derivatives).

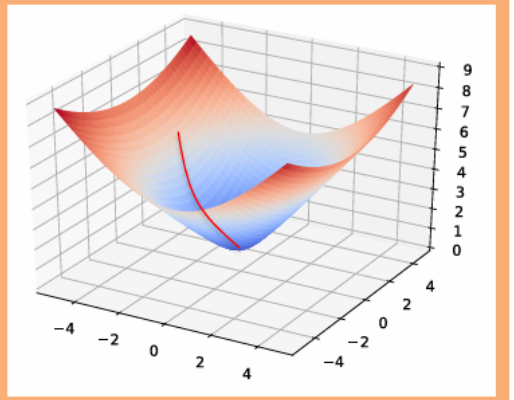
$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \begin{bmatrix} \frac{d}{d\theta_1} J(\boldsymbol{\theta}) \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \\ \vdots \\ \frac{d}{d\theta_M} J(\boldsymbol{\theta}) \end{bmatrix}$$

Gradient Descent

- Go down the path of steepest descent

Algorithm 1 Gradient Descent

procedure GD($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
  while not converged **do**
    $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
  return $\boldsymbol{\theta}$



There are many possible ways to detect **convergence**. For example, we could check whether the L2 norm of the gradient is below some small tolerance.

$$||\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})||_2 \leq \epsilon$$

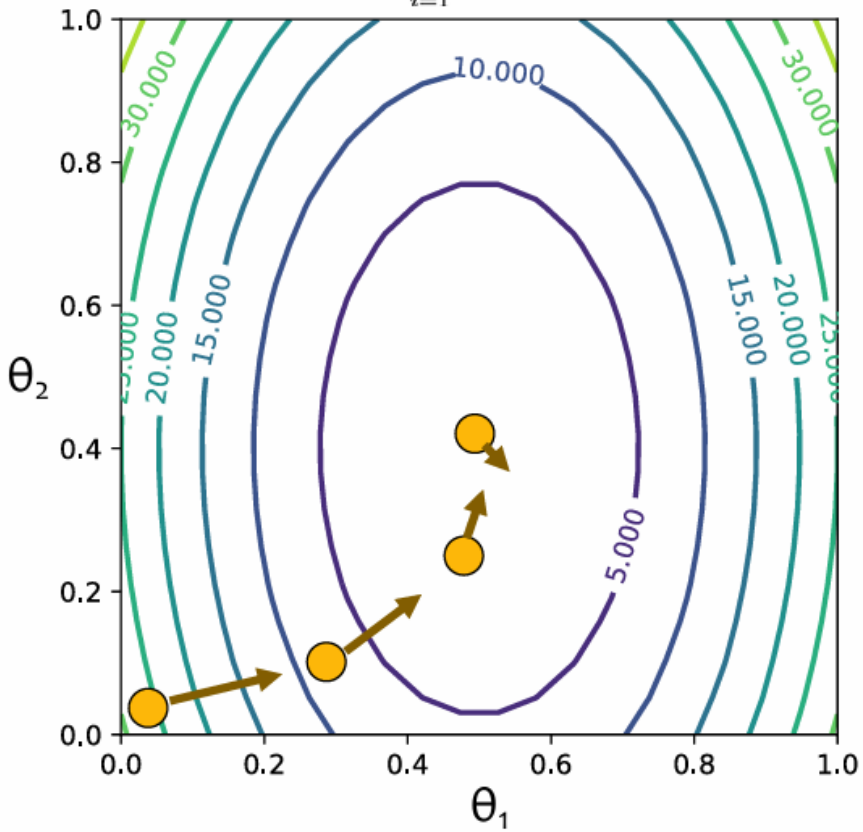
Alternatively we could check that the reduction in the objective function from one iteration to the next is small.

Linear Regression by Gradient Desc.

Optimization Method #1: Gradient Descent

1. Pick a random **θ**
2. Repeat:
   a. Evaluate gradient ∇J(**θ**)
   b. Step opposite gradient
3. Return **θ** that gives smallest J(**θ**)

$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)^2$$



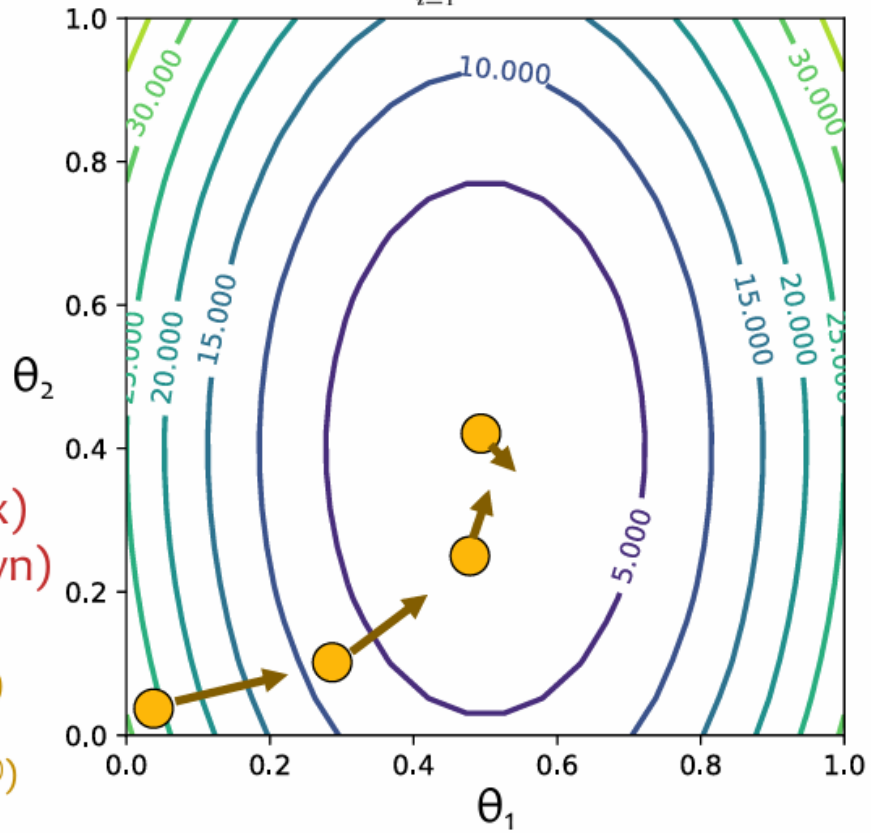
t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
3	0.51	0.30	1.5
4	0.59	0.43	0.2

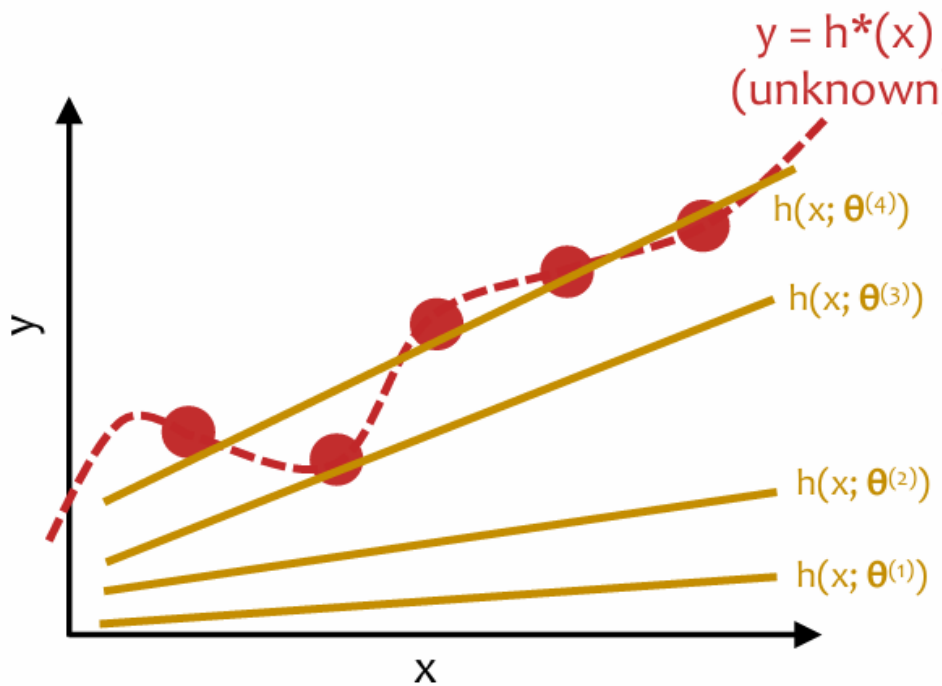
Linear Regression by Gradient Desc.

Optimization Method #1: Gradient Descent

1. Pick a random **θ**
2. Repeat:
   a. Evaluate gradient ∇J(**θ**)
   b. Step opposite gradient
3. Return **θ** that gives smallest J(**θ**)

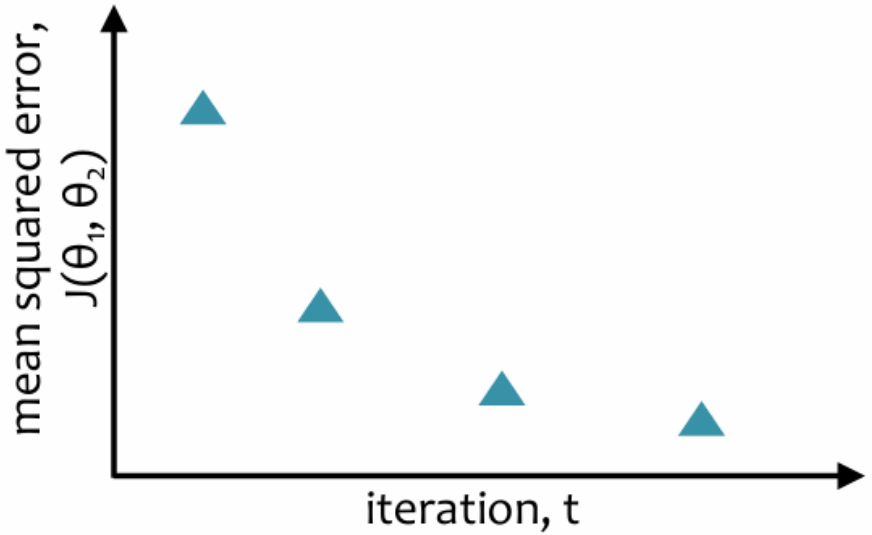
$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)}\right)^2$$



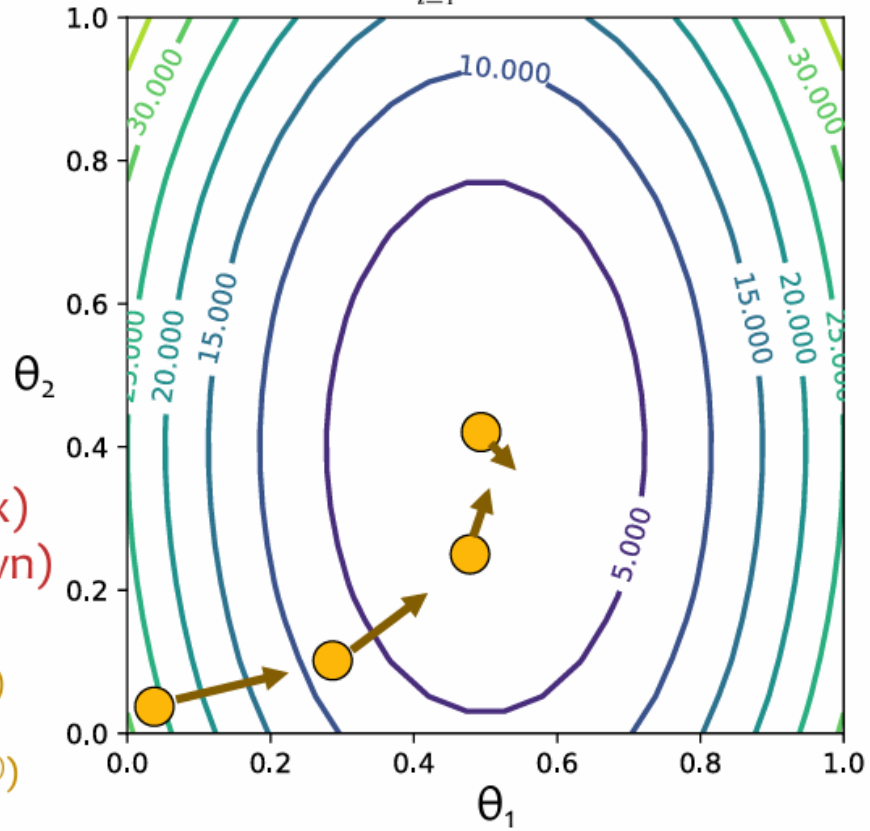


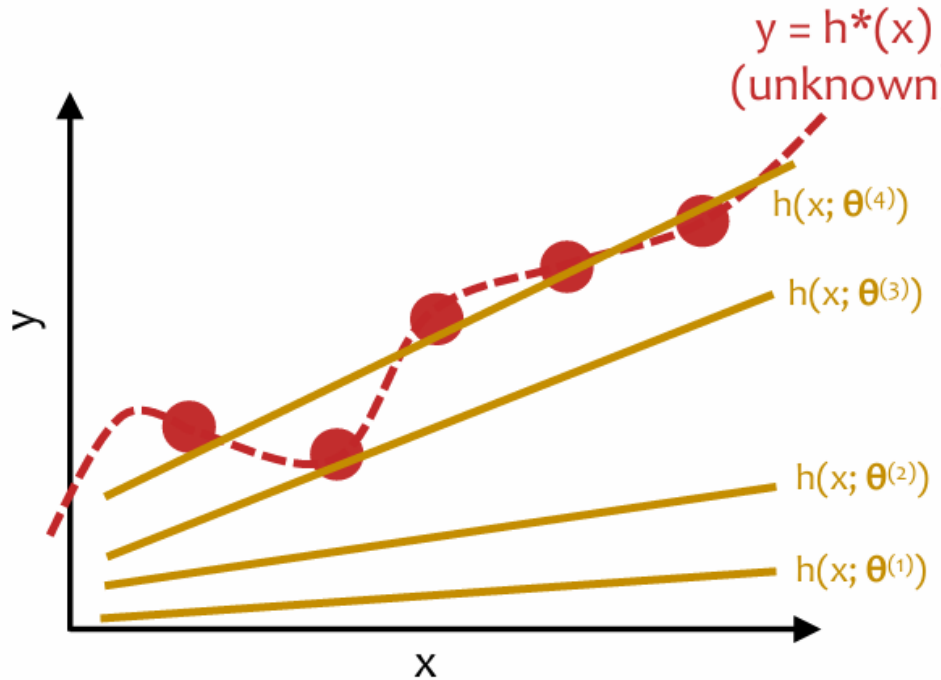
t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
3	0.51	0.30	1.5
4	0.59	0.43	0.2

Linear Regression by Gradient Desc.



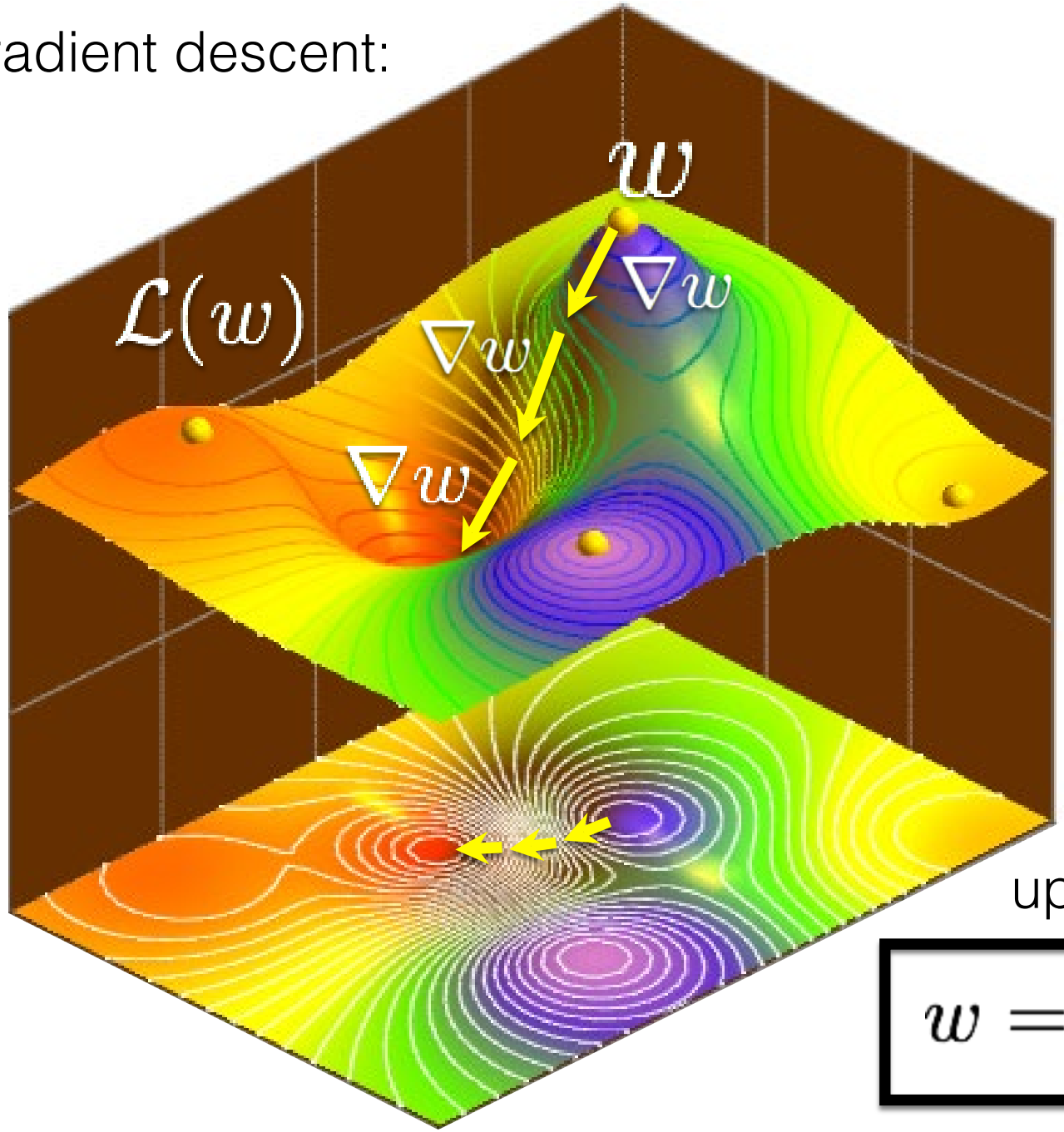
$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)^2$$





t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
3	0.51	0.30	1.5
4	0.59	0.43	0.2

Gradient descent:



update rule:

$$w = w - \nabla w$$

Gradient Descent

For each example sample $\{x_i, y_i\}$

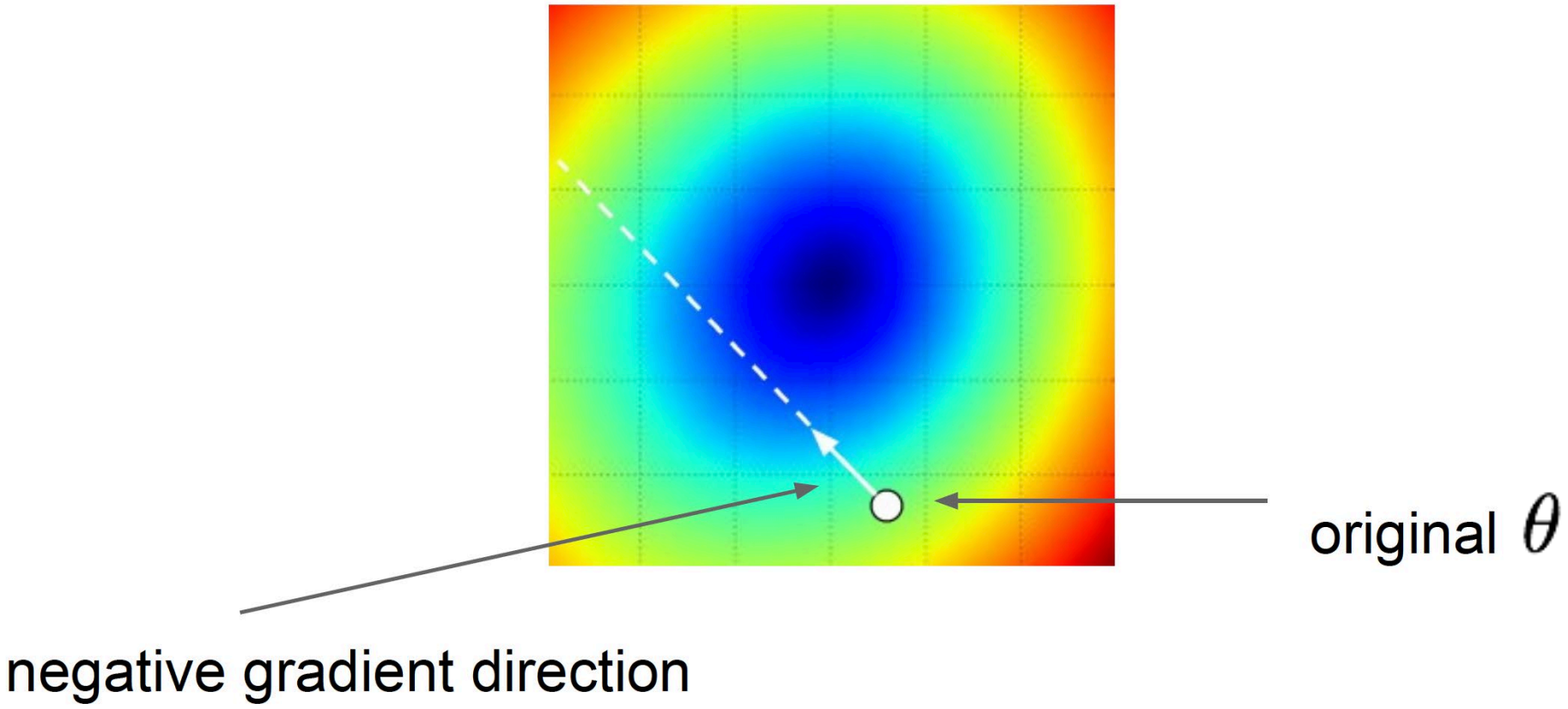
1. Predict
   a. Forward pass $\hat{y} = f_{\text{MLP}}(x_i; \theta)$
   b. Compute Loss $\mathcal{L}_i$
2. Update
   a. Back Propagation $\frac{\partial \mathcal{L}}{\partial \theta}$

vector of parameter partial derivatives

   b. Gradient update $\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$

vector of parameter update equations

Learning rates



$$\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$$

Step size: learning rate
Too big: will miss the minimum
Too small: slow convergence

Gradient Descent

$$\nabla C = \begin{bmatrix} \frac{\partial C}{\partial v_1} \\ \frac{\partial C}{\partial v_2} \end{bmatrix} \qquad \Delta v = \begin{bmatrix} \Delta v_1 \\ \Delta v_2 \end{bmatrix}$$

$$\Delta C \approx \nabla C \cdot \Delta v$$

Let $\Delta v = -\eta \nabla C$

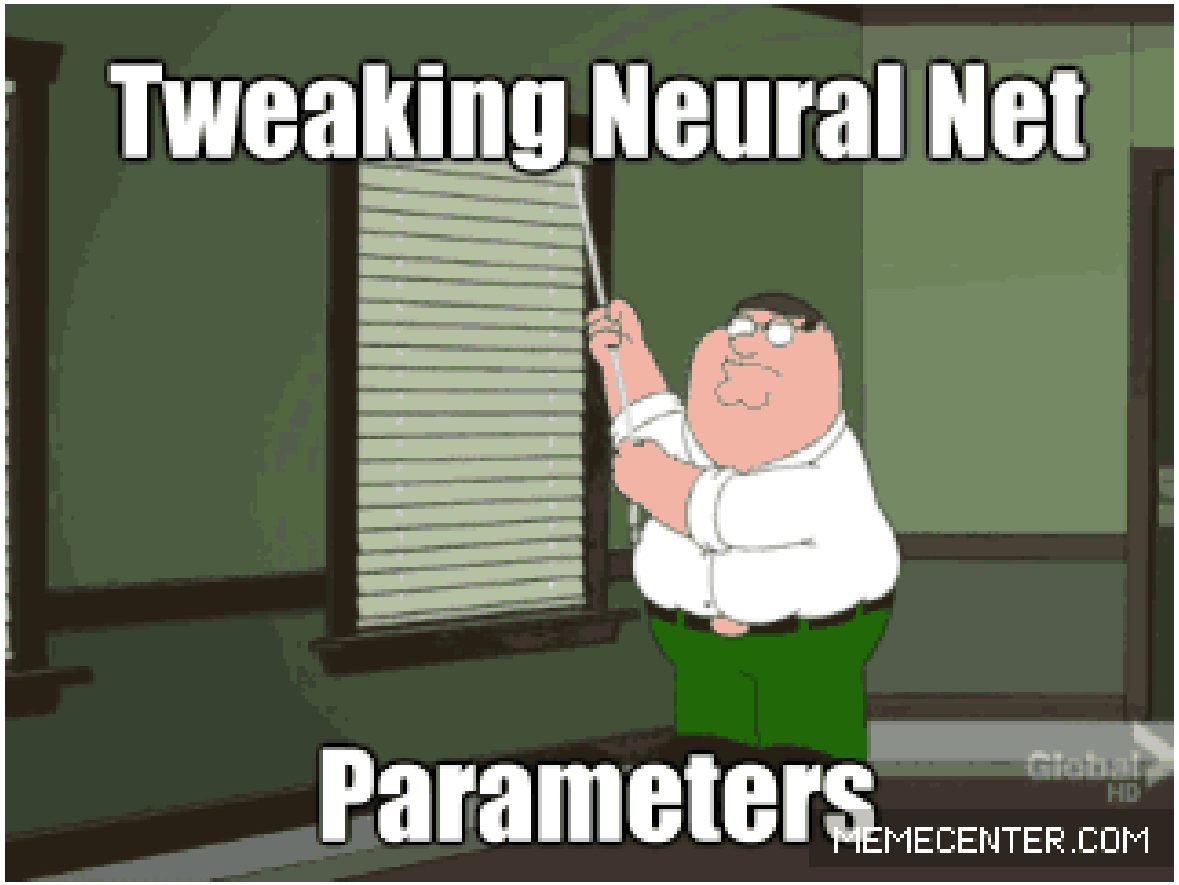
$$\Delta C \approx -\eta \nabla C \cdot \nabla C$$


LEFT
EXIT 12
global minima
local minima
*gradient descent

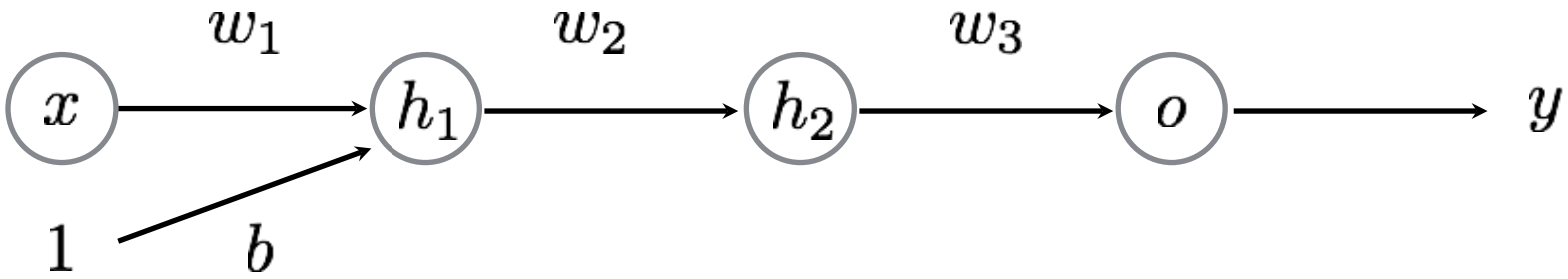
GD for LR: Python Step-by-Step Example

- https://colab.research.google.com/drive/17dK6cynECzk2ObyCqDk5gKcUyN1kMjSR?usp=sharing

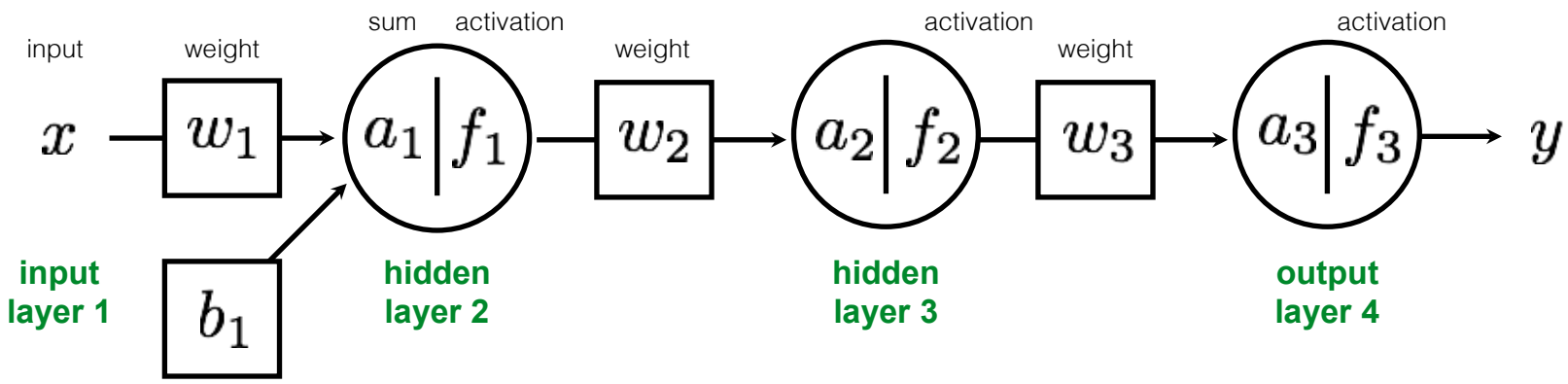
Backpropagation

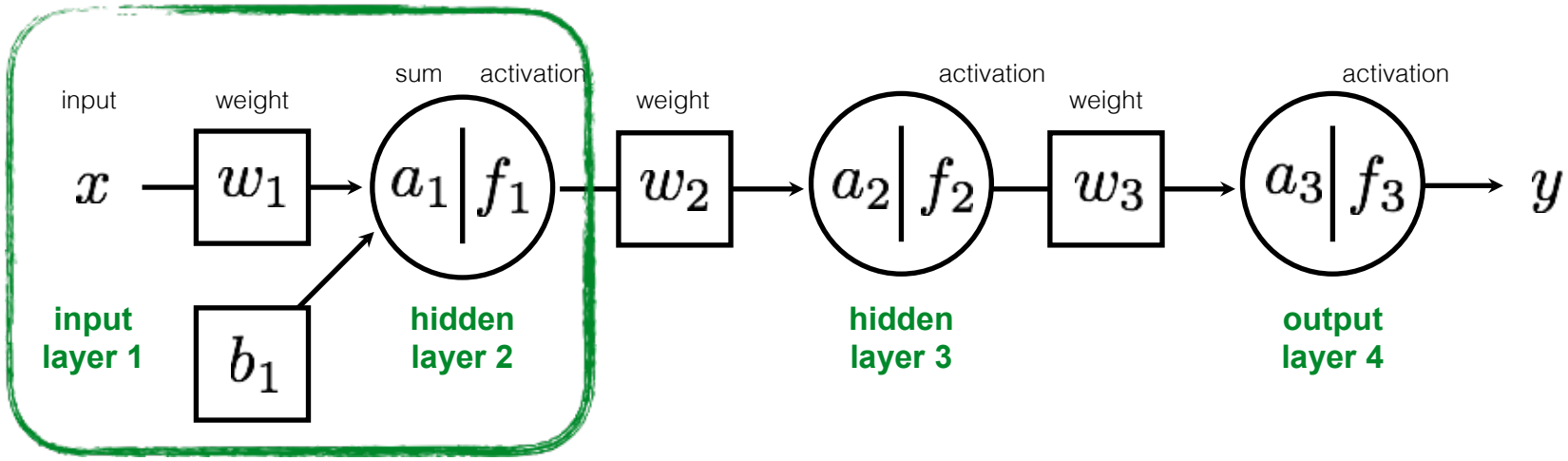


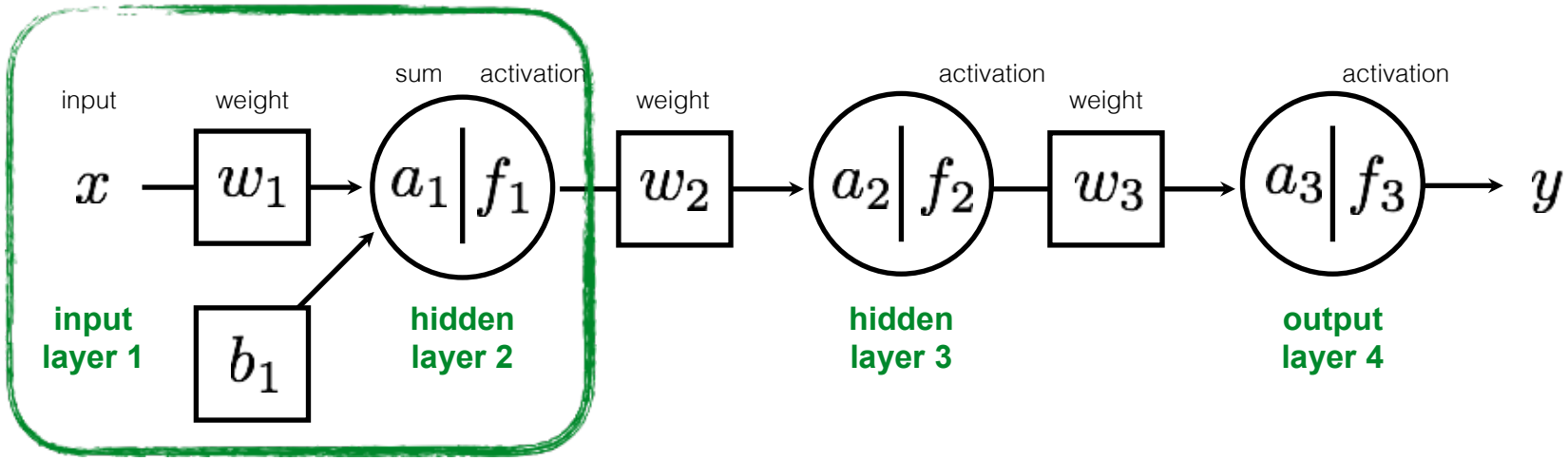
Example of a multi-layer perceptron



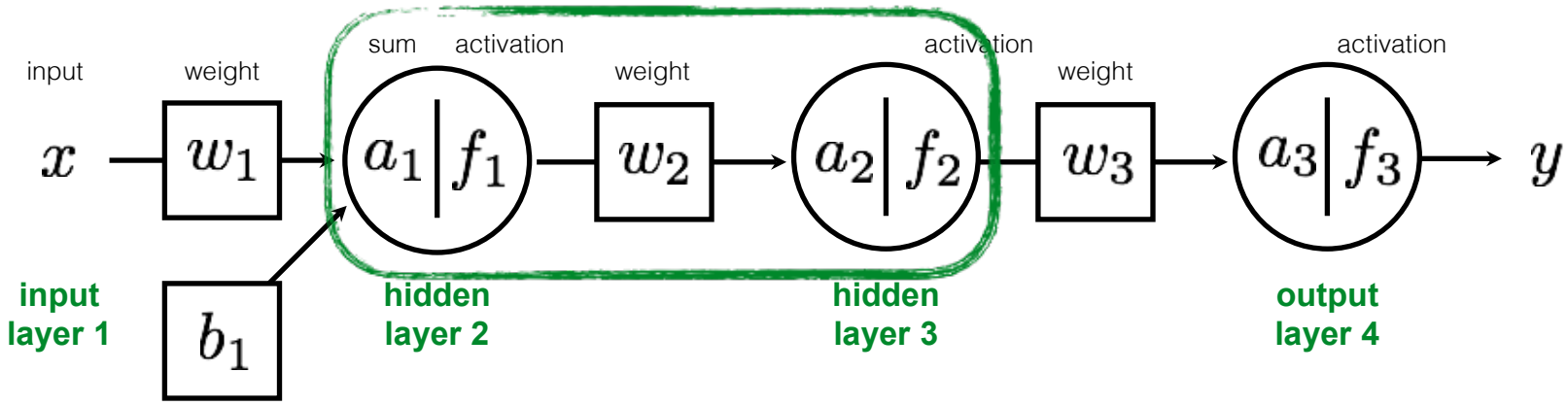
function of **FOUR** parameters and **FOUR** layers!


input
weight
sum
activation
weight
activation
weight
activation
x
w_1
a_1 f_1
w_2
a_2 f_2
w_3
a_3 f_3
y
b_1
input layer 1
hidden layer 2
hidden layer 3
output layer 4

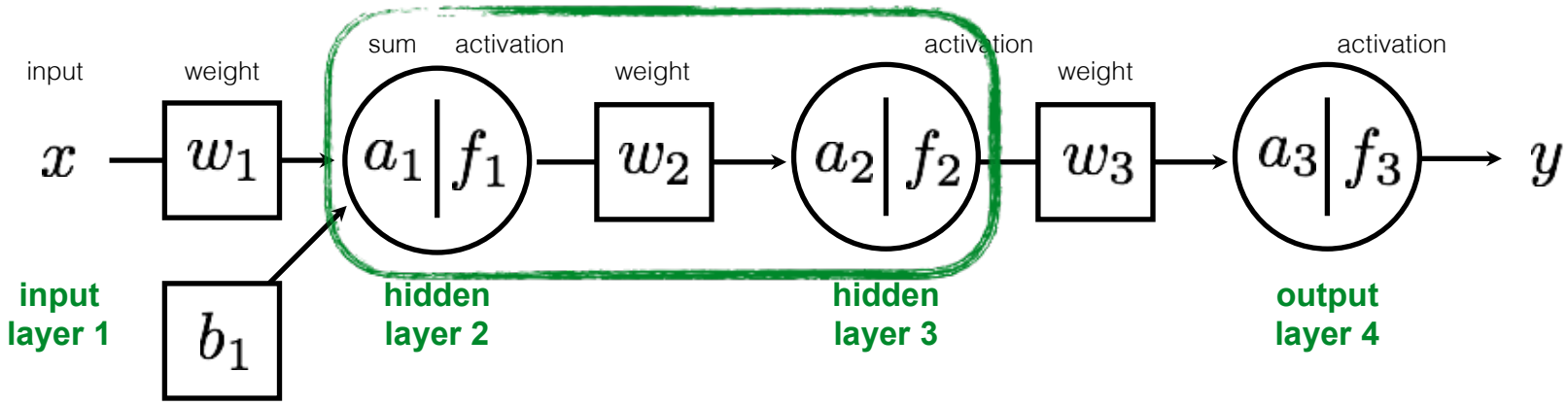

input
weight
sum
activation
weight
activation
weight
activation
x
w_1
a_1 f_1
w_2
a_2 f_2
w_3
a_3 f_3
y
b_1
input layer 1
hidden layer 2
hidden layer 3
output layer 4



$$a_1 = w_1 \cdot x + b_1$$

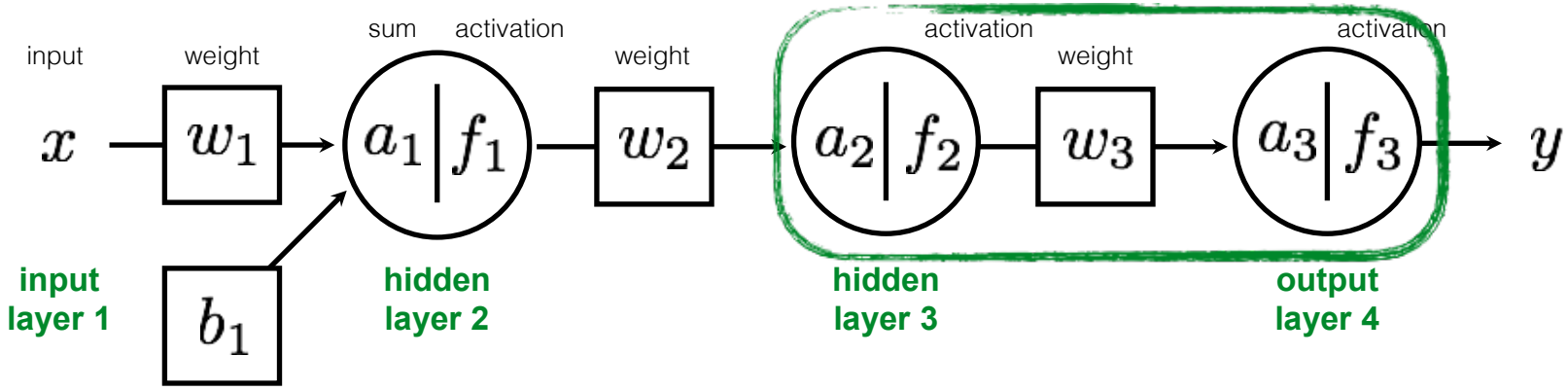


$$a_1 = w_1 \cdot x + b_1$$



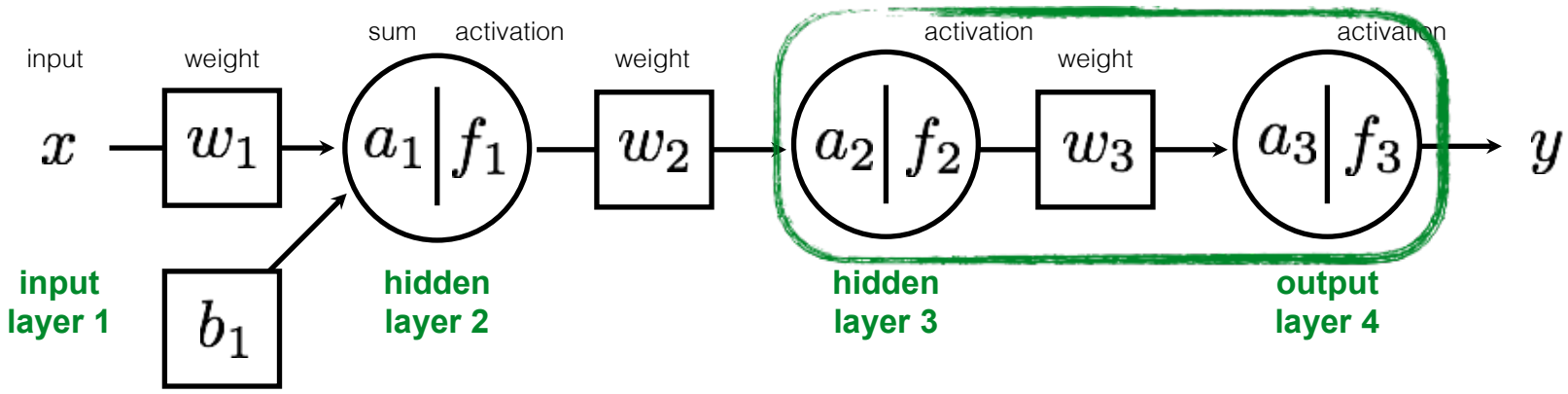
$$a_1 = w_1 \cdot x + b_1$$

$$a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$$



$$a_1 = w_1 \cdot x + b_1$$

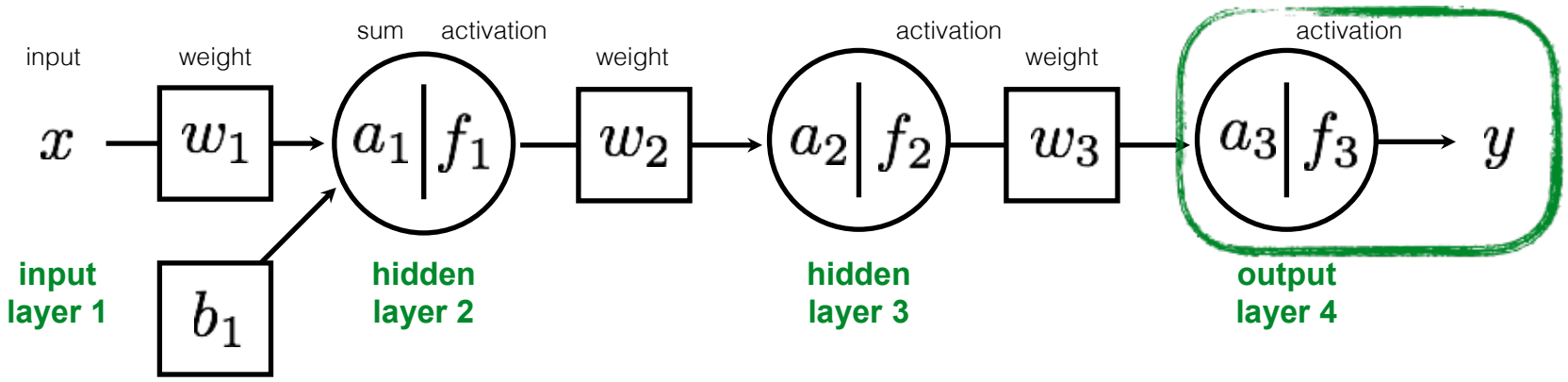
$$a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$$



$$a_1 = w_1 \cdot x + b_1$$

$$a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$$

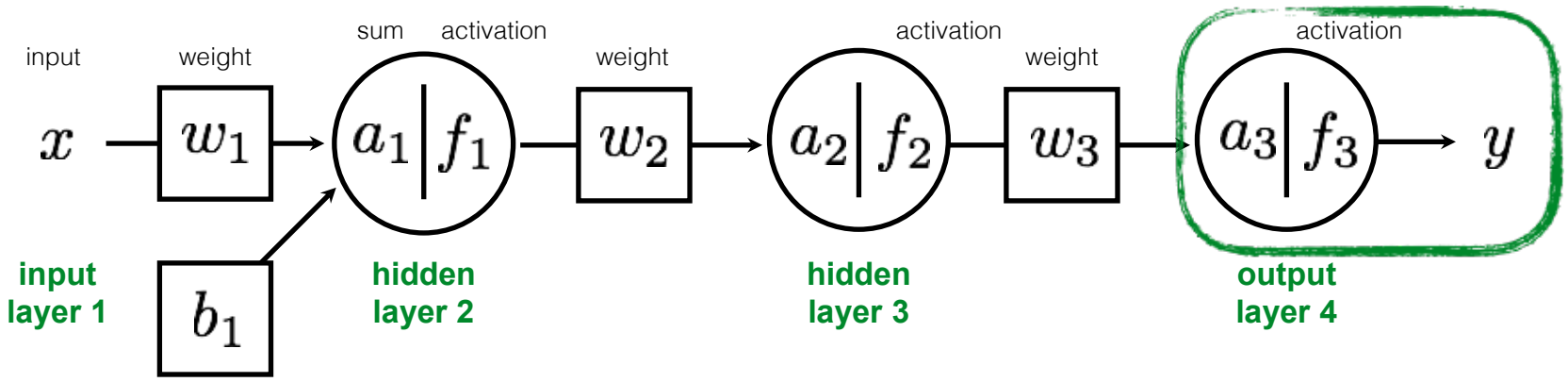
$$a_3 = w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1))$$



$$a_1 = w_1 \cdot x + b_1$$

$$a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$$

$$a_3 = w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1))$$



$$a_1 = w_1 \cdot x + b_1$$

$$a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$$

$$a_3 = w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1))$$

$$y = f_3(w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1)))$$

Entire network can be written out as one long equation

$$y = f_3(w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1)))$$

We need to train the network:

What is known? What is unknown?

Entire network can be written out as one long equation

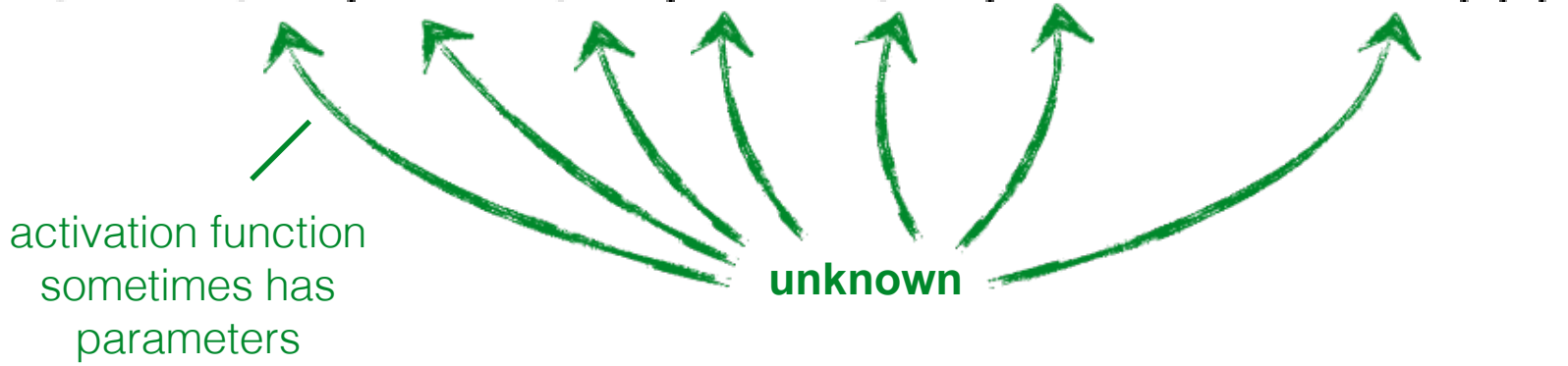
$$y = f_3(w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1)))$$

We need to train the network:

What is known? What is unknown?

Entire network can be written out as one long equation

$$y = f_3(w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1)))$$



We need to train the network:

What is known? What is unknown?

Learning an MLP

Given a set of samples and a MLP

$$\{x_i, y_i\}$$

$$y = f_{\text{MLP}}(x; \theta)$$

Estimate the parameters of the MLP

$$\theta = \{f, w, b\}$$

Gradient Descent

For each **random** sample $\{x_i, y_i\}$

1. Predict
   a. Forward pass $\hat{y} = f_{\text{MLP}}(x_i; \theta)$
   b. Compute Loss
2. Update
   a. Back Propagation $\frac{\partial \mathcal{L}}{\partial \theta}$ vector of parameter partial derivatives
   b. Gradient update $\theta \leftarrow \theta - \eta \nabla \theta$

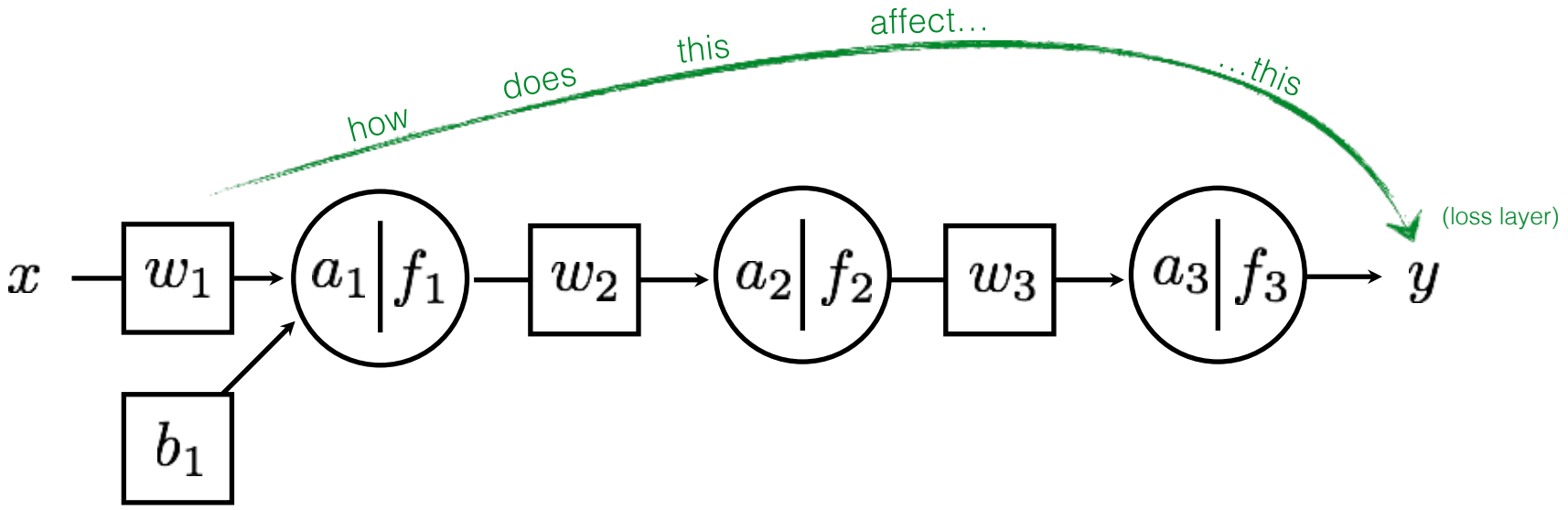
vector of parameter update equations

So we need to compute the partial derivatives

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} = \left[\frac{\partial \mathcal{L}}{\partial w_3} \frac{\partial \mathcal{L}}{\partial w_2} \frac{\partial \mathcal{L}}{\partial w_1} \frac{\partial \mathcal{L}}{\partial b} \right]$$

Remember,

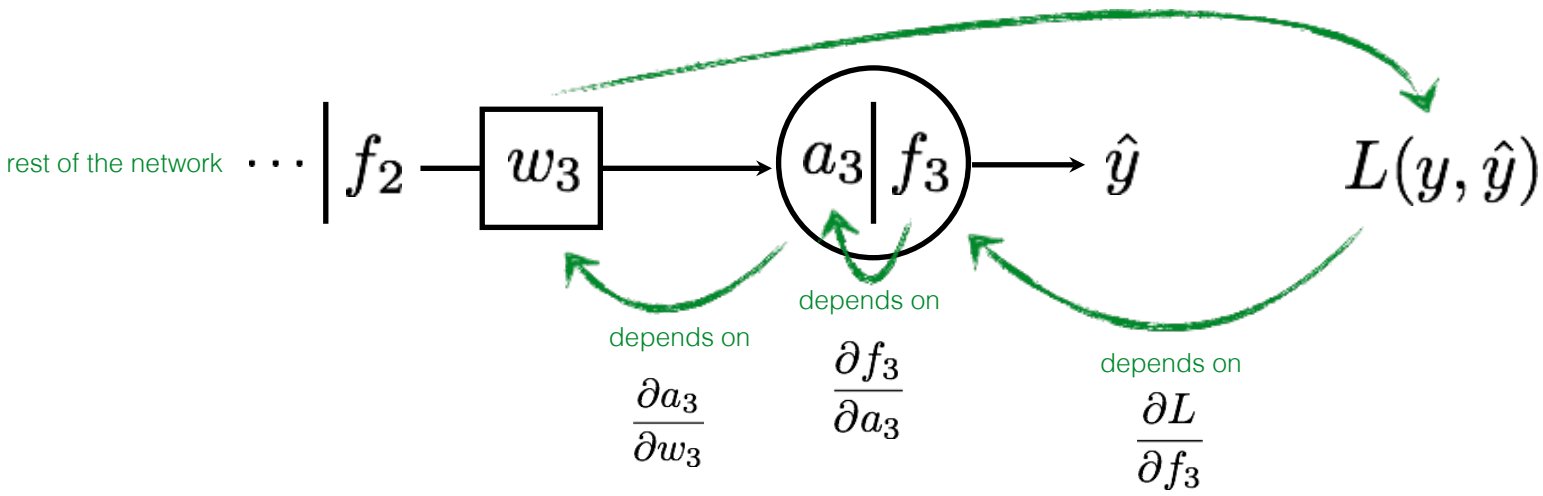
Partial derivative $\frac{\partial L}{\partial w_1}$ describes…

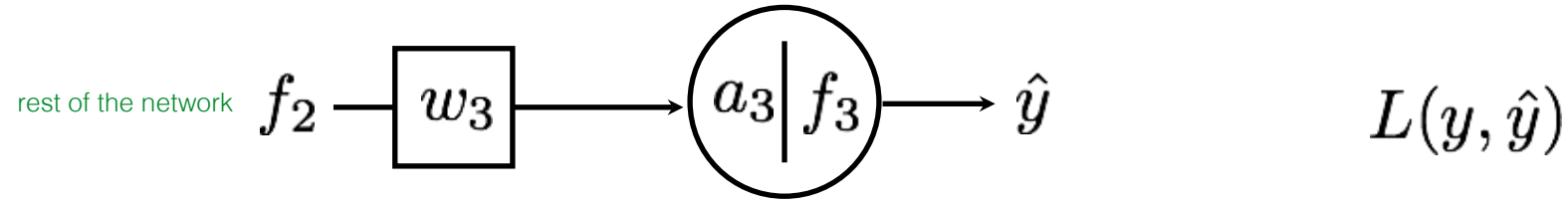


According to the chain rule…

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

Intuitively, the effect of weight on loss function : $\frac{\partial L}{\partial w_3}$

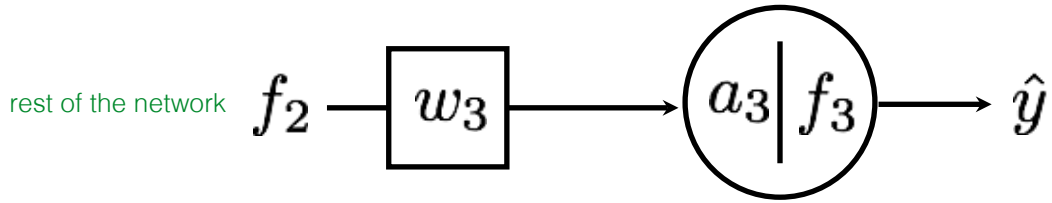




$$L(y, \hat{y})$$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial w_3}$$

Chain Rule!

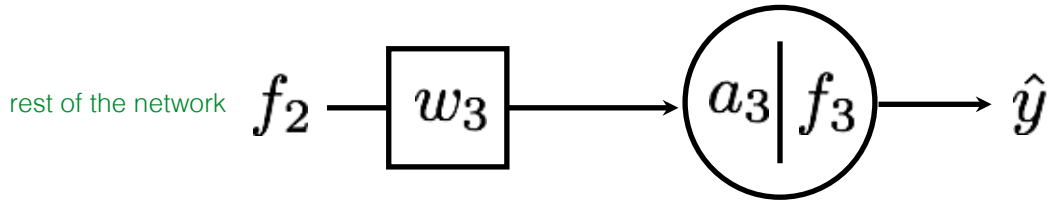


$$L(y, \hat{y})$$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

$$= -\eta(y - \hat{y})\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

Just the partial derivative of L2 loss



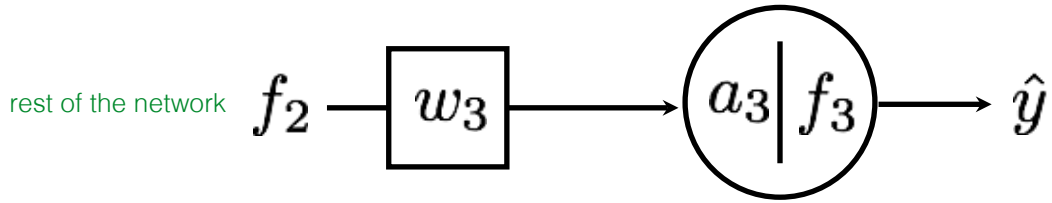
$$L(y, \hat{y})$$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

$$= -\eta(y - \hat{y})\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

Let's use a Sigmoid function

$$\frac{ds(x)}{dx} = s(x)(1 - s(x))$$



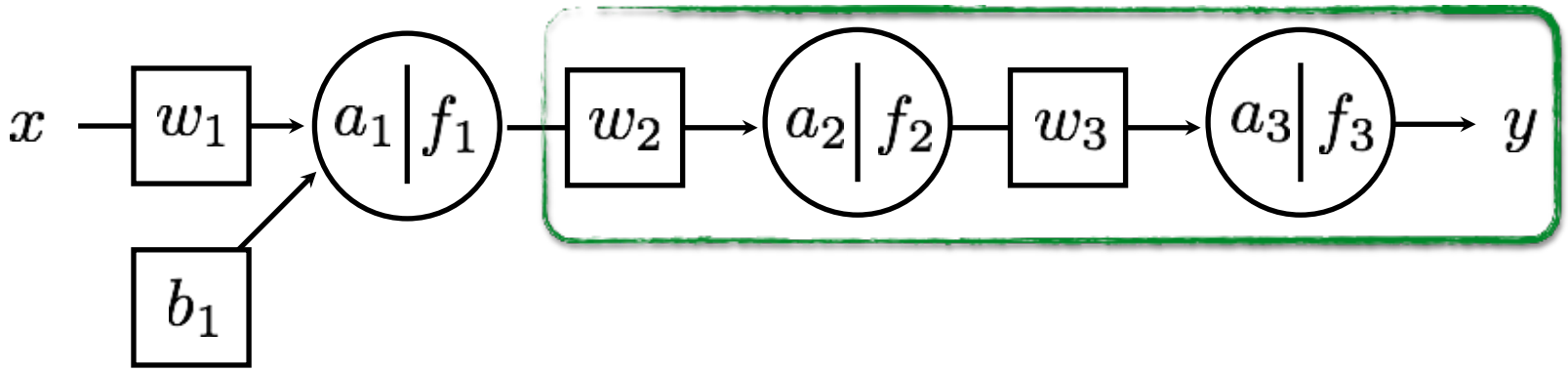
$L(y, \hat{y})$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

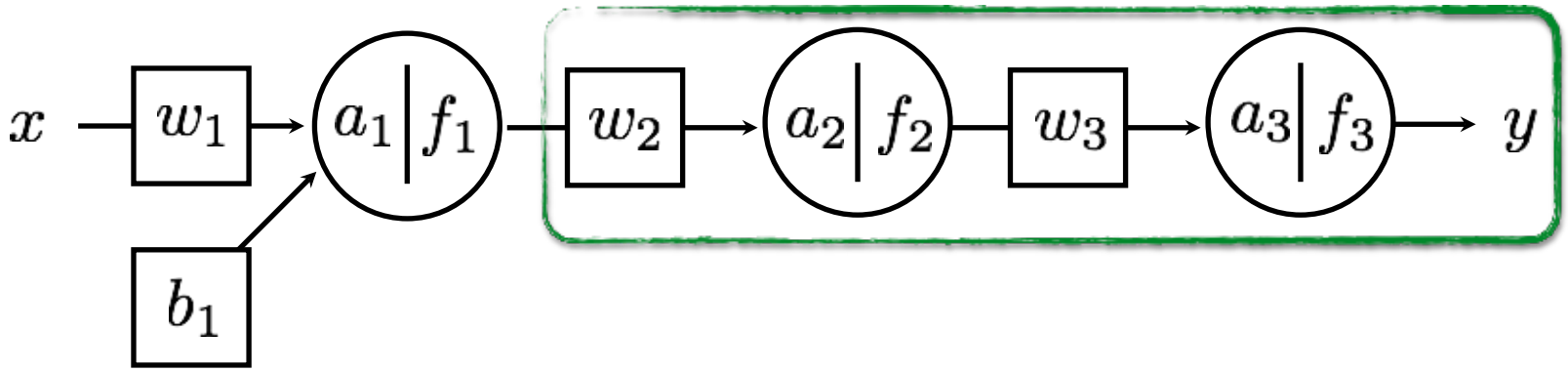
$$= -\eta(y - \hat{y})\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

$$= -\eta(y - \hat{y}) f_3(1 - f_3)\frac{\partial a_3}{\partial w_3}$$

$$= -\eta(y - \hat{y}) f_3(1 - f_3) f_2$$



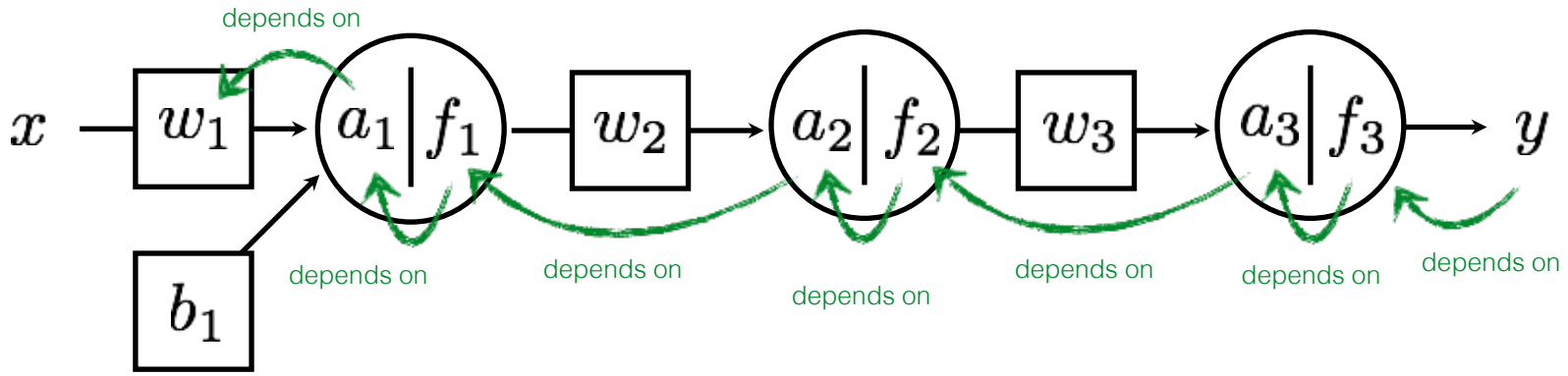
$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$



$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$

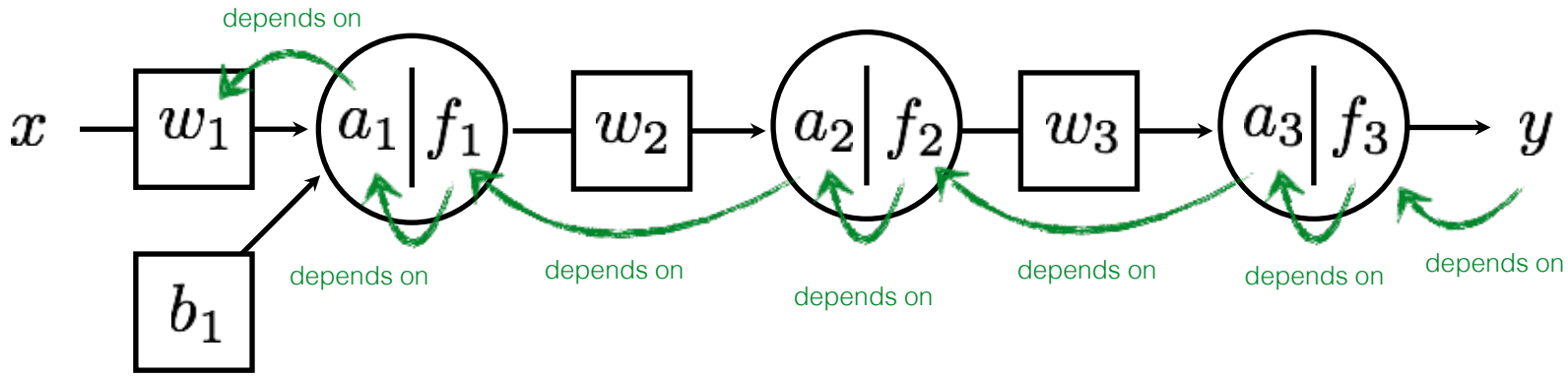
already computed.
re-use (propagate)!

The chain rule says…



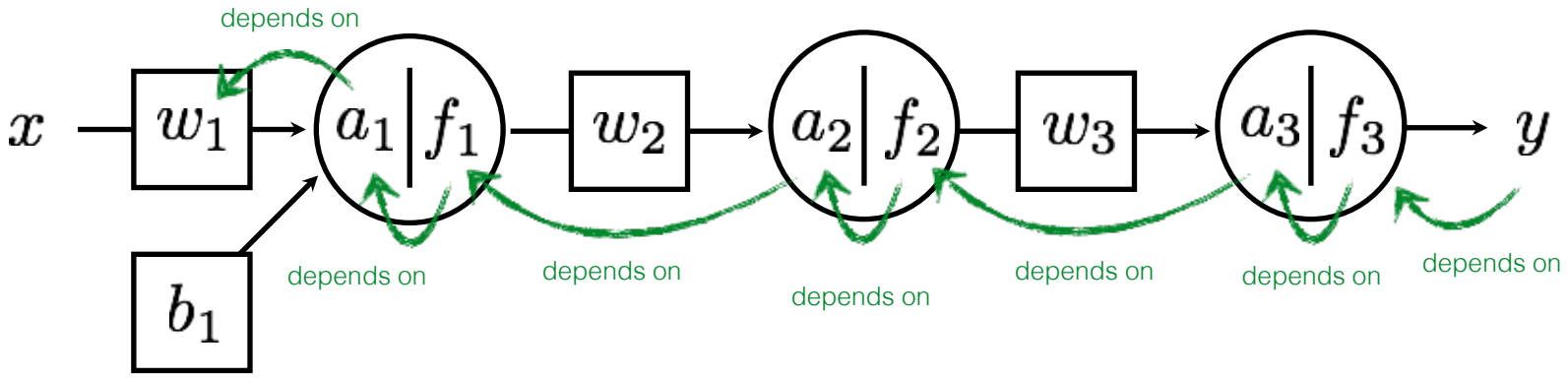
$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$

The chain rule says…



$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$

already computed.
re-use (propagate)!

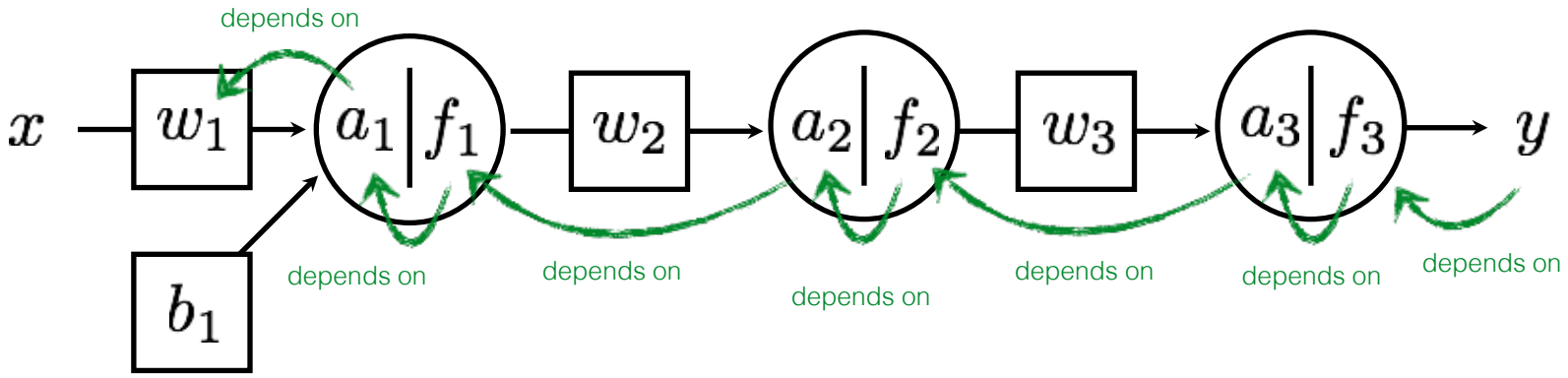


$$\frac{\partial \mathcal{L}}{\partial w_3} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial b}$$

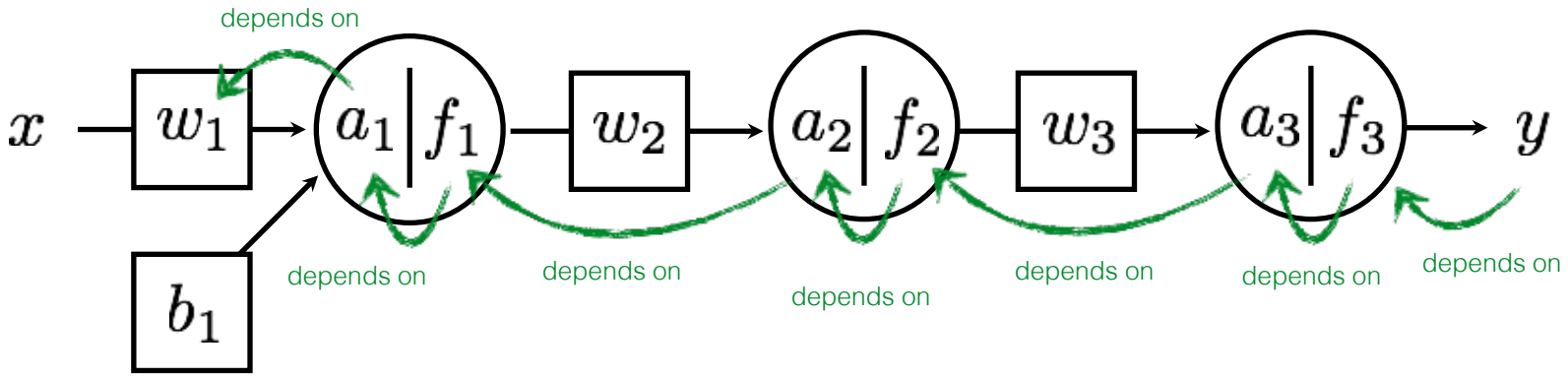


$$\frac{\partial \mathcal{L}}{\partial w_3} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial b}$$



$$\frac{\partial \mathcal{L}}{\partial w_3} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial b}$$

Gradient Descent

For each example sample $\{x_i, y_i\}$

1. Predict
   a. Forward pass $\hat{y} = f_{\text{MLP}}(x_i; \theta)$
   b. Compute Loss $\mathcal{L}_i$
2. Update
   a. Back Propagation

$$\frac{\partial \mathcal{L}}{\partial w_3} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$
$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$
$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$
$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial b}$$

   b. Gradient update

$$w_3 = w_3 - \eta\nabla w_3$$
$$w_2 = w_2 - \eta\nabla w_2$$
$$w_1 = w_1 - \eta\nabla w_1$$
$$b = b - \eta\nabla b$$

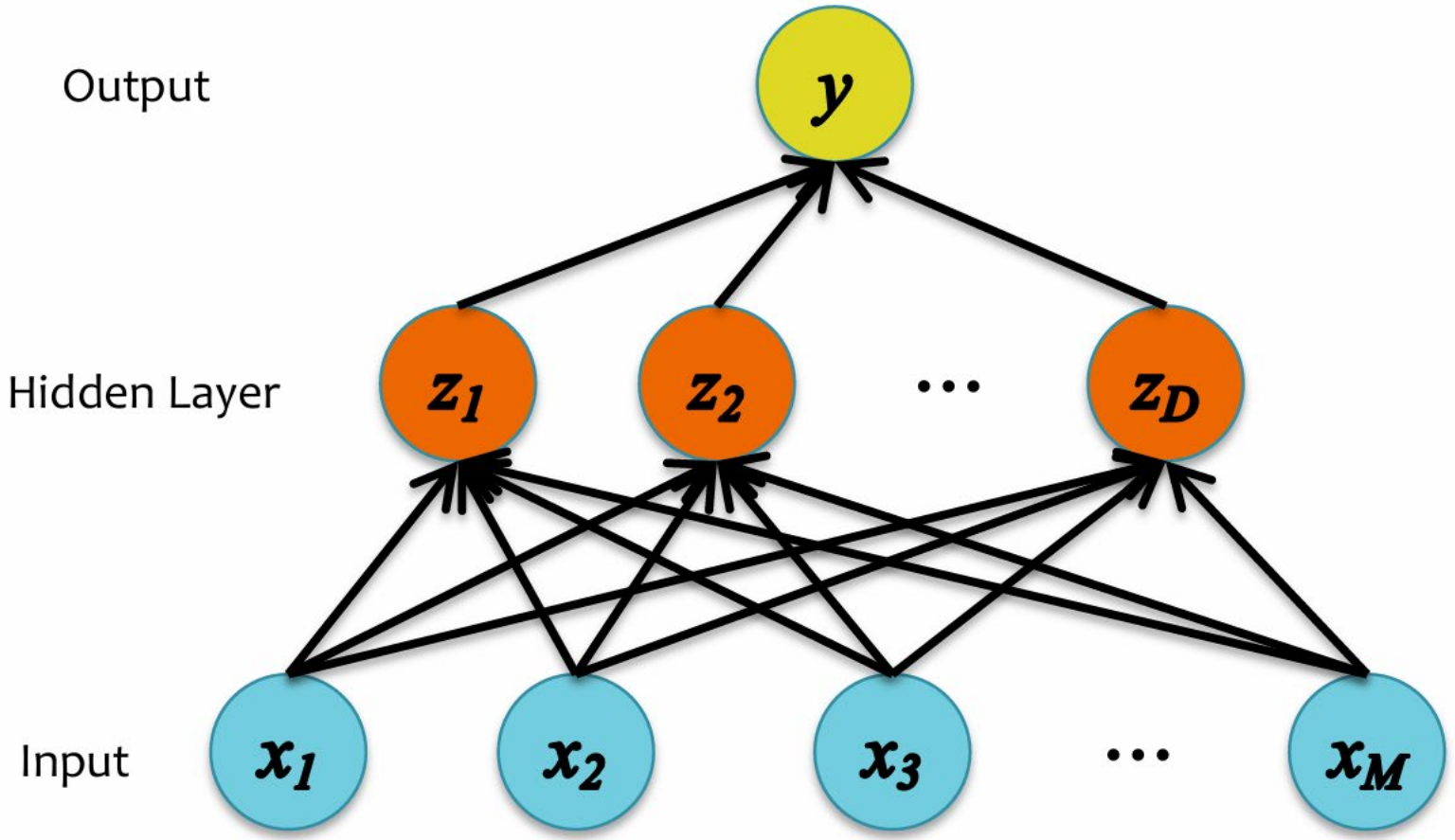
Gradient Descent

For each example sample $\{x_i, y_i\}$

1. Predict
   a. Forward pass $\hat{y} = f_{\text{MLP}}(x_i; \theta)$
   b. Compute Loss $\mathcal{L}_i$
2. Update
   a. Back Propagation $\frac{\partial \mathcal{L}}{\partial \theta}$ vector of partial derivatives
   b. Gradient update $\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$ vector of update equations

Single Output Neural Networl

Let's write the equation



Objective Functions for NNs

1. Quadratic Loss:
   - the same objective as Linear Regression
   - i.e. mean squared error

$$J = \ell_Q(y, y^{(i)}) = \frac{1}{2}(y - y^{(i)})^2$$
$$\frac{dJ}{dy} = y - y^{(i)}$$

2. Binary Cross-Entropy:
   - the same objective as Binary Logistic Regression
   - i.e. negative log likelihood
   - This requires our output y to be a probability in [0,1]

$$J = \ell_{CE}(y, y^{(i)}) = -(y^{(i)} \log(y) + (1 - y^{(i)}) \log(1 - y))$$
$$\frac{dJ}{dy} = -\left(y^{(i)} \frac{1}{y} + (1 - y^{(i)}) \frac{1}{y - 1}\right)$$

Objective Functions for NNs

Cross-entropy vs. Quadratic loss

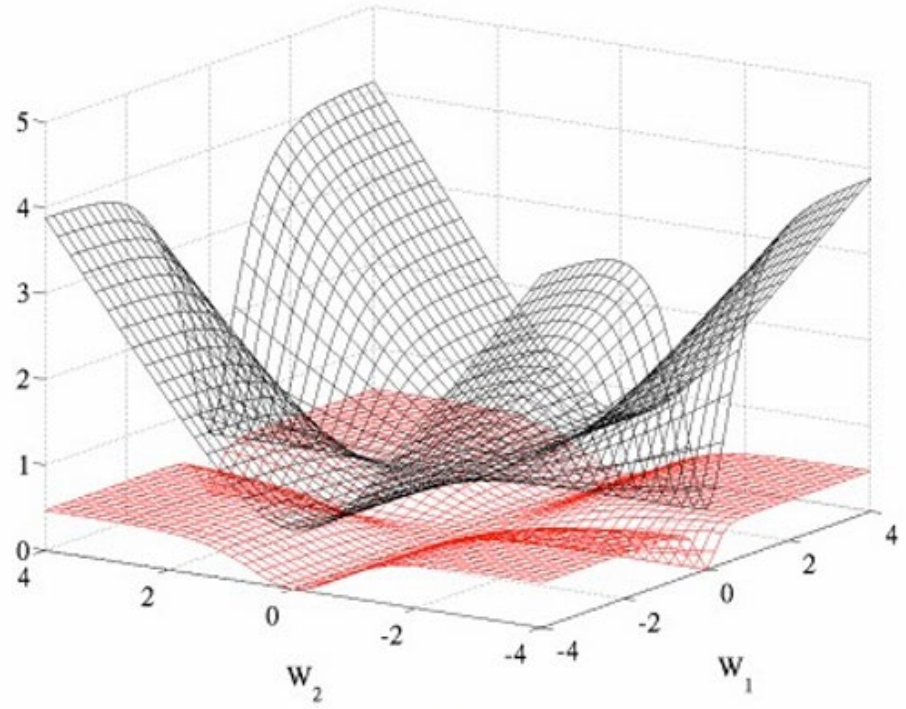
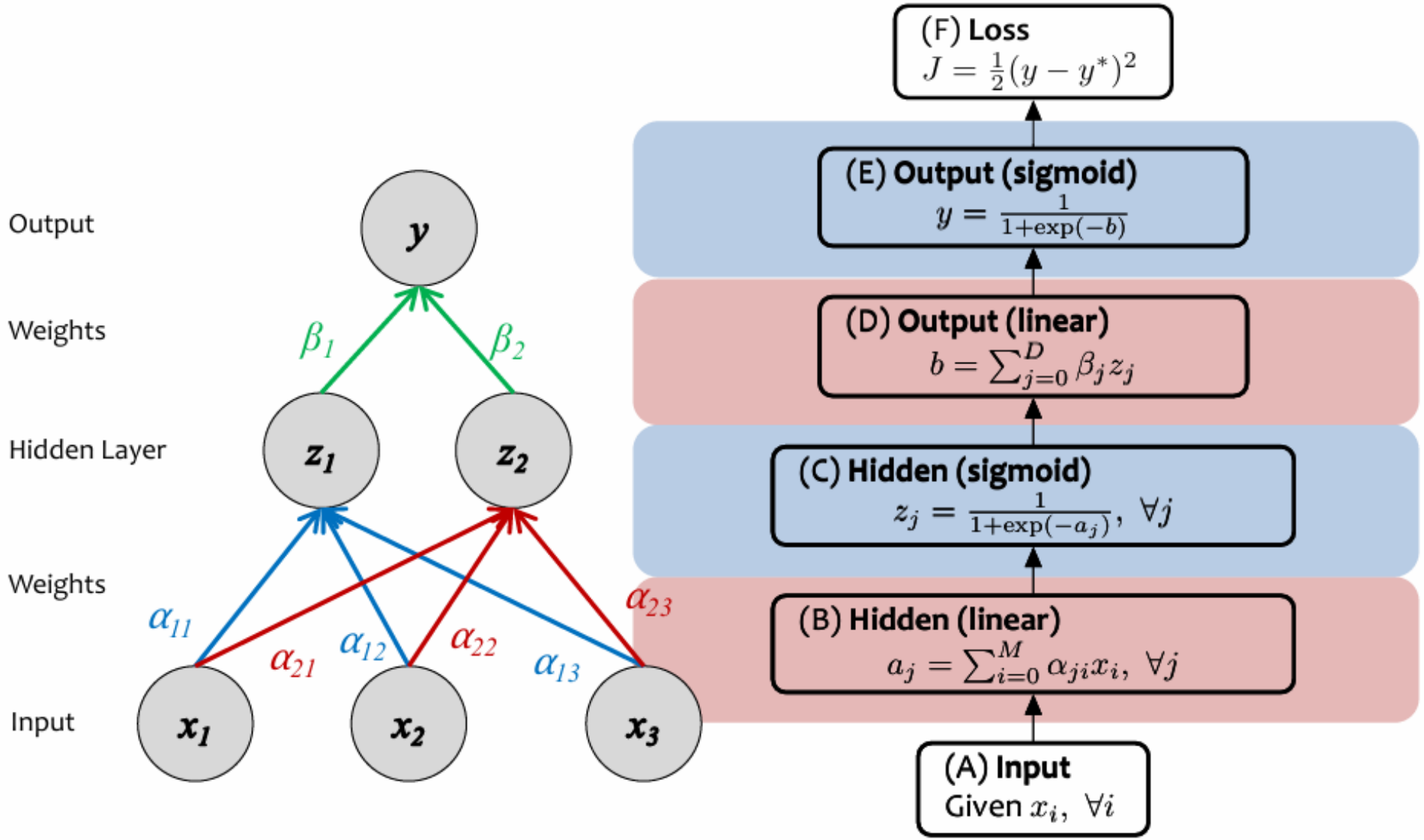


Figure 5: *Cross entropy (black, surface on top) and quadratic (red, bottom surface) cost as a function of two weights (one at each layer) of a network with two layers, W_1 respectively on the first layer and W_2 on the second, output layer.*

Figure from Glorot & Bentio (2010)

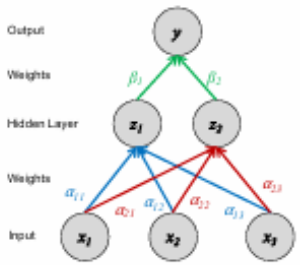
Training

Forward-Computation



Case 2: Neural Network

Backpropagation

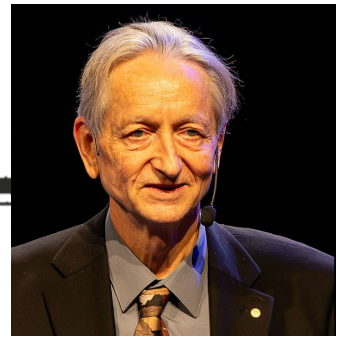


	Forward	Backward
Loss	$J = y^* \log y + (1 - y^*) \log(1 - y)$	$g_y = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$
Sigmoid	$y = \frac{1}{1 + \exp(-b)}$	$g_b = g_y \frac{\partial y}{\partial b}, \frac{\partial y}{\partial b} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$
Linear	$b = \sum_{j=0}^{D} \beta_j z_j$	$g_{\beta_j} = g_b \frac{\partial b}{\partial \beta_j}, \frac{\partial b}{\partial \beta_j} = z_j$ $g_{z_j} = g_b \frac{\partial b}{\partial z_j}, \frac{\partial b}{\partial z_j} = \beta_j$
Sigmoid	$z_j = \frac{1}{1 + \exp(-a_j)}$	$g_{a_j} = g_{z_j} \frac{\partial z_j}{\partial a_j}, \frac{\partial z_j}{\partial a_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$
Linear	$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$	$g_{\alpha_{ji}} = g_{a_j} \frac{\partial a_j}{\partial \alpha_{ji}}, \frac{\partial a_j}{\partial \alpha_{ji}} = x_i$ $g_{x_i} = \sum_{j=0}^{D} g_{a_j} \frac{\partial a_j}{\partial x_i}, \frac{\partial a_j}{\partial x_i} = \alpha_{ji}$

some history / controversy …

Nature **volume 323**, pages533–536 (1986)

Nobel Prize in Physics 2024



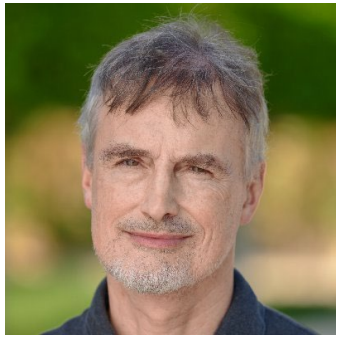
Learning representations by back-propagating errors

David E. Rumelhart*, Geoffrey E. Hinton† & Ronald J. Williams*

* Institute for Cognitive Science, C-015, University of California, San Diego, La Jolla, California 92093, USA
† Department of Computer Science, Carnegie-Mellon University, Pittsburgh, Philadelphia 15213, USA

- An efficient application of the chain rule (first written down by Leibniz, 1676)
- Precursors to backpropagation appeared in optimal control theory since 1950s.
  - LeCun et al 1985 credits 1950s work by Pontryagin.
- Modern backpropagation was first published by Seppo Linnainmaa as "reverse mode of automatic differentiation" (1970) for discrete connected networks of nested differentiable functions.
- Rumelhart “independently developed” backpropagation. He did not cite previous work as he was “unaware” of them.

https://people.idsia.ch/~juergen/who-invented-backpropagation.html



Why are NNs such good function approximators?

Universal Approximation Theorem:

"A neural network $\hat{f}(x)$ with a single hidden-layer
can approximate any continuous real function $f(x)$
to within any arbitrary degree of accuracy ϵ
given a sufficient number of neurons in the hidden layer"

Nice Explanation:
https://www.deep-mind.org/2023/03/26/the-universal-approximation-theorem/

Why are NNs such good function approximators?

Universal Approximation Theorem (UAT) limitations:

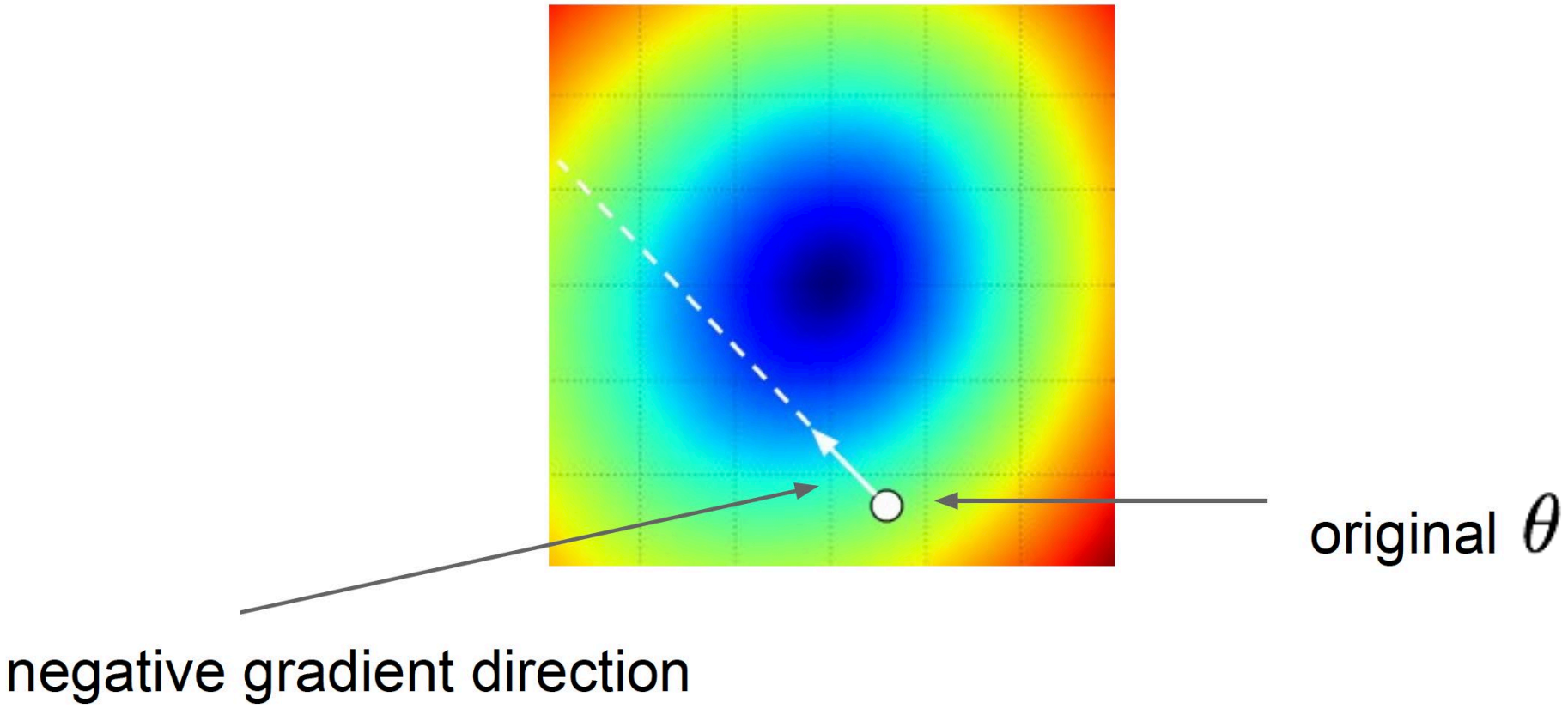
1. Does not specify what the network size should be

2. Only guarantees *function approximation* on the given training data*;* does not guarantee generalization on new test data

3. Only assures that approximation exists; does not provide insights on how to train the network to achieve that optimal function

"A neural network $\hat{f}(x)$ with a single hidden-layer
can approximate any continuous real function $f(x)$
to within any arbitrary degree of accuracy ϵ
given a sufficient number of neurons in the hidden layer"

Learning rates



$$\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$$

Step size: learning rate
Too big: will miss the minimum
Too small: slow convergence

Learning rate scheduling

- Use different learning rate at each iteration.
- Most common choice:

$$\eta_t = \frac{\eta_0}{\sqrt{t}}$$

Need to select initial learning rate η_0

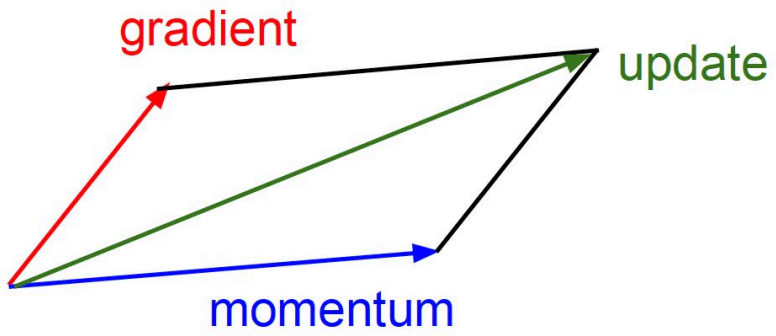
More modern choice: Adaptive learning rates.

$$\eta_t = G\left(\left\{\frac{\partial L}{\partial \theta}\right\}_{i=0}^{t}\right)$$

Many choices for G (Adam, Adagrad, Adadelta).

Momentum Update

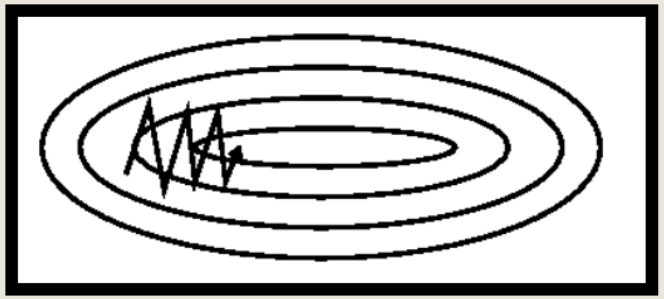
$$\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$$



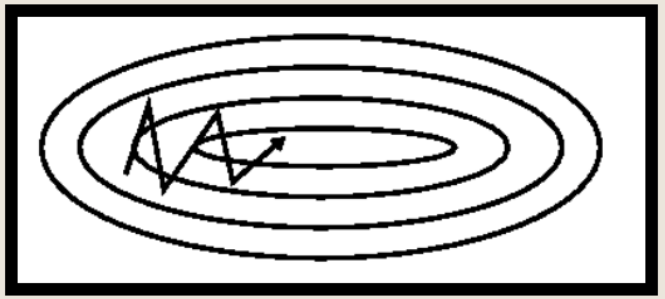
$$\Delta\theta \leftarrow w \frac{\partial L}{\partial \theta} + (1 - w)\Delta\theta$$

Take direction history into account!

```
weights_grad = evaluate_gradient(loss_fun, data, weights)
vel = vel * 0.9 - step_size * weights_grad
weights += vel
```



(Fig. 2a)



(Fig. 2b)

Many other ways to perform optimization…

- Second order methods that use the Hessian (or its approximation): BFGS, **LBFGS**, etc.

- Currently, the lesson from the trenches is that well-tuned SGD+Momentum is very hard to beat for CNNs.

- No consensus on Adam etc.: Seem to give faster performance to worse local minima.