Lecture 20: Back Propagation

CS109A Introduction to Data Science

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Outline

1. Back Propagation
2. Optimizers

Outline

1. **Back Propagation**
2. Optimizers

Learning the coefficients

Start with Regression or Logistic Regression

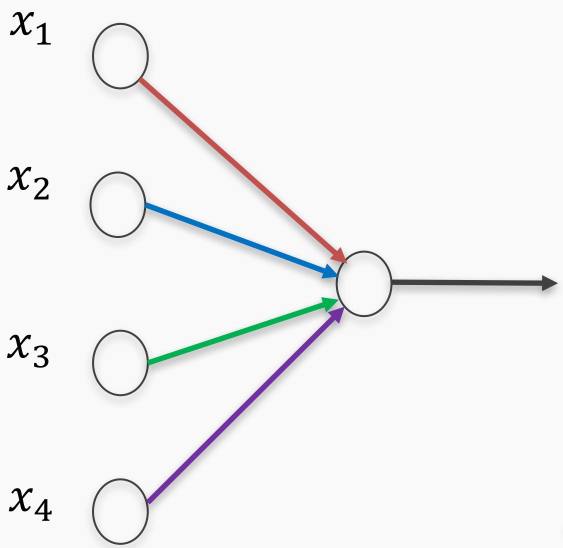
Classification

$$f(X) = \frac{1}{1+e^{-W^T X}}$$

Regression

$$f(X) = W^T X$$

$$W^T = [W_0, W_1, \ldots, W_4] = [\beta_0, \beta_1, \ldots, \beta_4]$$



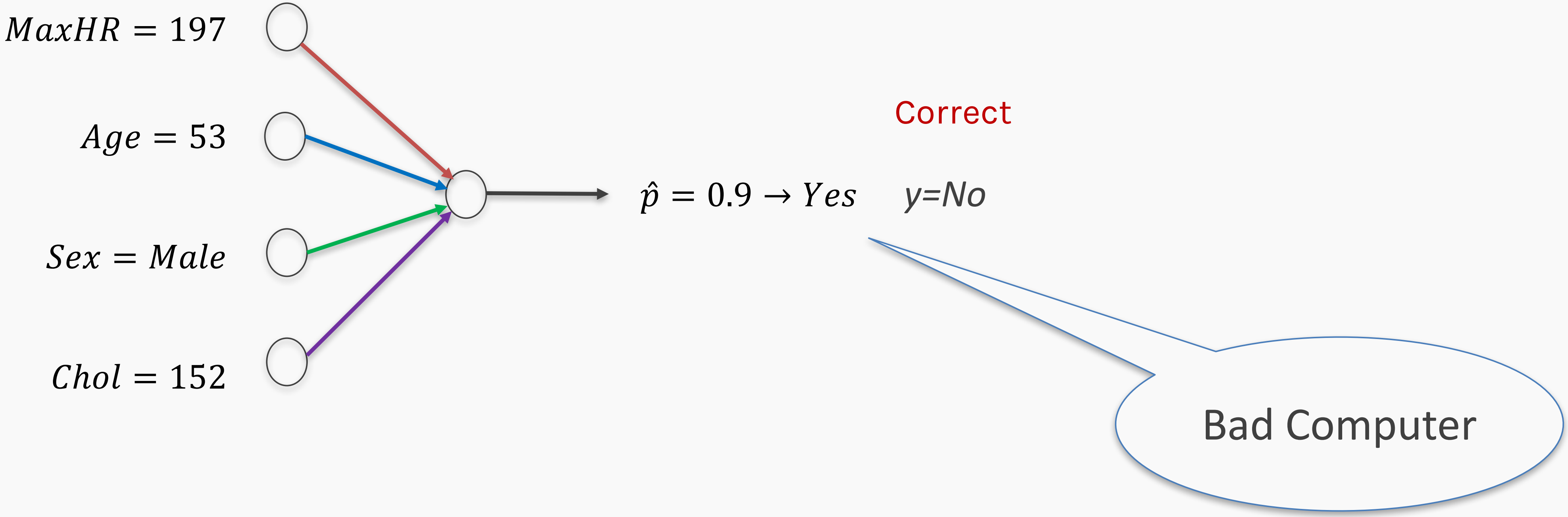
$$Y = f(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4)$$

Intercept or **Bias**

Coefficients or **Weights**

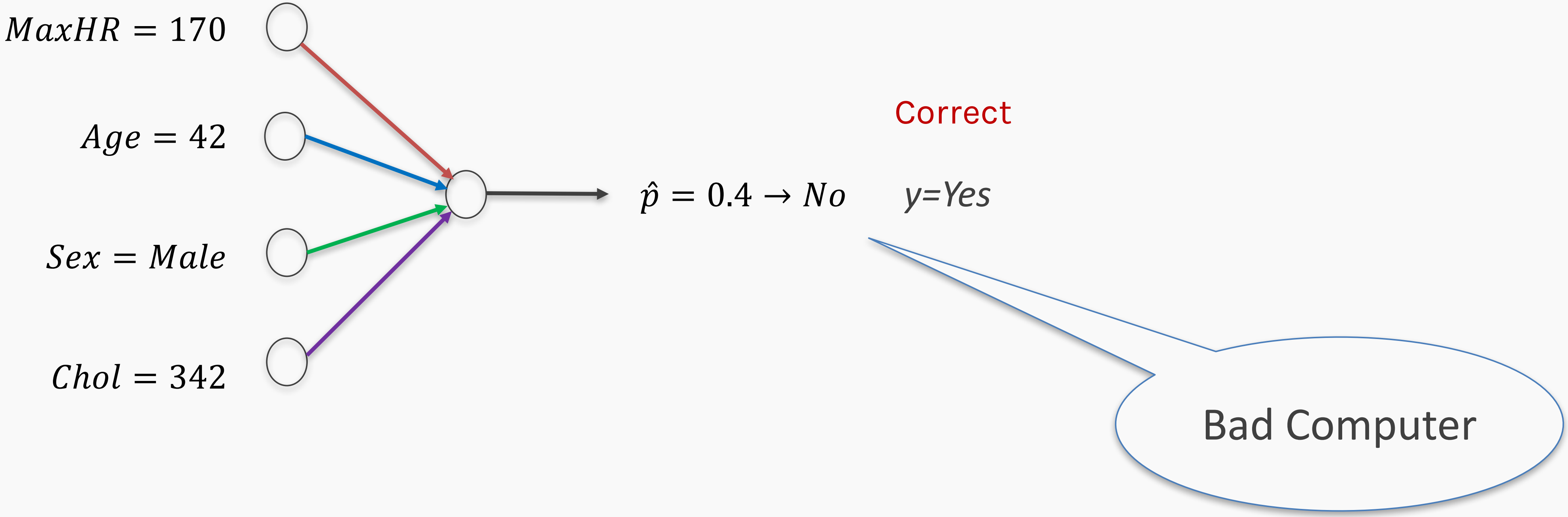
But what is the idea?

Start with all randomly selected weights. Most likely it will perform horribly. For example, in our heart data, the model will be giving us the wrong answer.



But what is the idea?

Start with all randomly selected weights. Most likely it will perform horribly. For example, in our heart data, the model will be giving us the wrong answer.



But what is the idea?

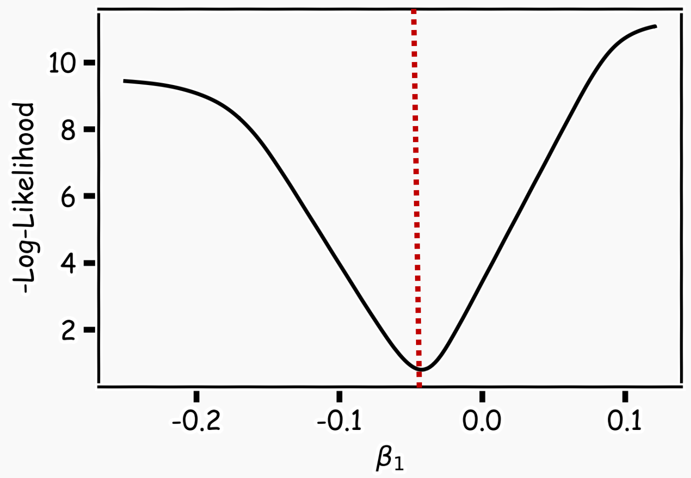
- **Loss Function:** Takes all of these results and averages them and tells us how bad or good the computer or those weights are.
- Telling the computer how **bad** or **good** is, does not help.
- You want to tell it how to change those weights so it gets better.

Loss function: $\mathcal{L}(w_0, w_1, w_2, w_3, w_4)$

For now let's only consider one weight, $\mathcal{L}(w_1)$

Minimizing the Loss function

Ideally we want to know the value of w_1 that gives the minimul $\mathcal{L}(W)$

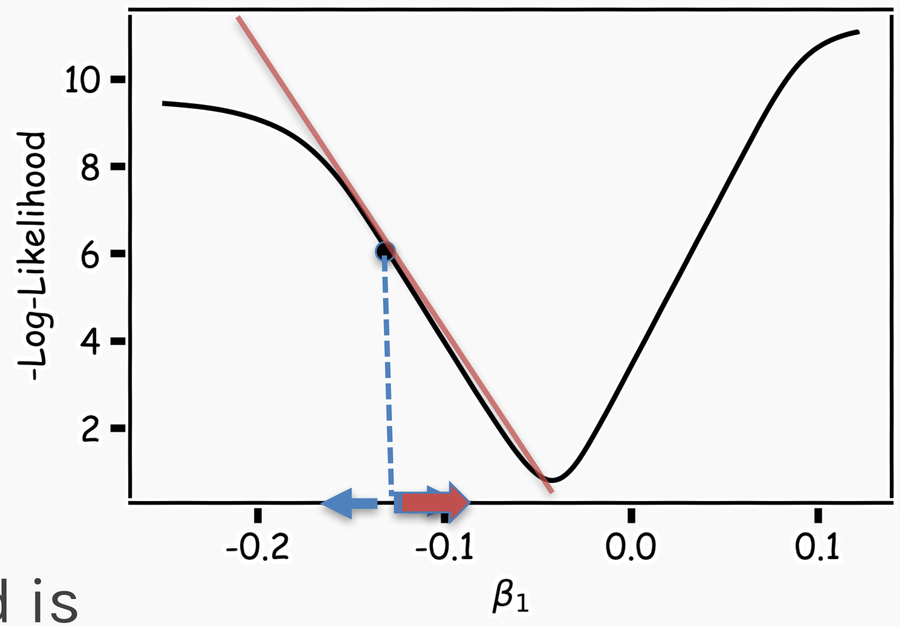


To find the optimal point of a function $\mathcal{L}(W)$

$$\frac{d\mathcal{L}(W)}{dW} = 0$$

And find the W that satisfies that equation. Sometimes there is no explicit solution for that.

Estimate of the regression coefficients: gradient descent

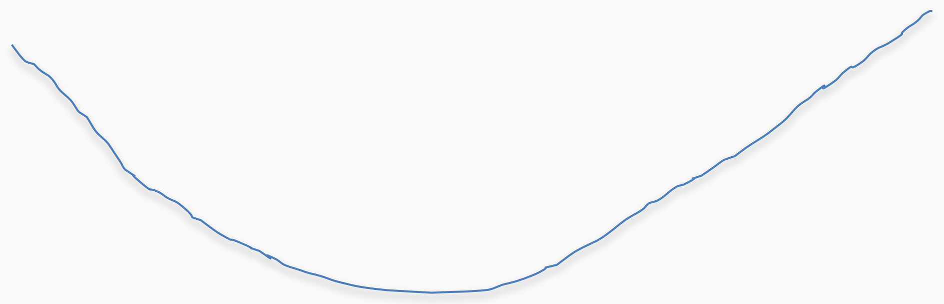


A more flexible method is

- Start from a random point
  1. Determine which direction to go to reduce the loss (left or right)
  2. Compute the slope of the function at this point and step to the right if slope is negative or step to the left if slope is positive
  3. Goto to #1

Gradient Descent (cont.)

If the step is proportional to the slope then you avoid overshooting the minimum. How?



Minimization of the Loss Function

Question: What is the mathematical function that describes the slope?

Derivative

Question: How do we generalize this to more than one predictor?

Take the derivative with respect to each coefficient and do the same sequentially

Question: What do you think it is a good approach for telling the model how to change (what is the step size) to become better?

Let's play the Pavlos game

We know that we want to go in the opposite direction of the derivative and we know we want to be making a step proportionally to the derivative.

Making a step means:

$$w^{new} = w^{old} + step$$

Step size is proportional to derivative

Opposite direction of the derivative means:

$$w^{new} = w^{old} - \lambda \frac{d\mathcal{L}}{dw}$$

Learning Rate

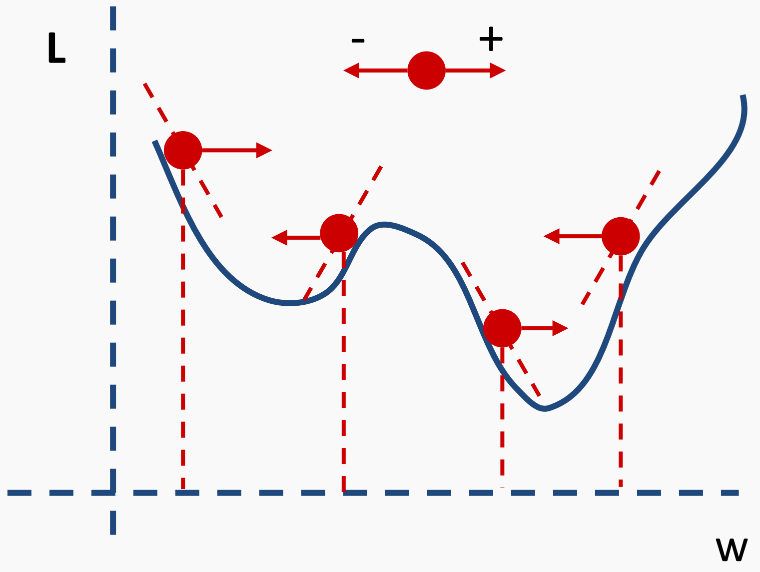
Change to more conventional notation:

$$w^{(i+1)} = w^{(i)} - \lambda \frac{d\mathcal{L}}{dw}$$

Gradient Descent

- Algorithm for optimization of first order to finding a minimum of a function.
- It is an iterative method.
- L is decreasing much faster in the direction of the negative derivative.
- The learning rate is controlled by the magnitude of λ.

$$w^{(i+1)} = w^{(i)} - \lambda \frac{d\mathcal{L}}{dw}$$



Considerations

- We still need to calculate the derivatives.
- We need to know what is the learning rate or how to set it.
- Local vs global minima.
- The full likelihood function includes summing up all individual '*errors*'. Unless you are a statistician, sometimes this includes hundreds of thousands of examples.

Considerations

- **We still need to calculate the derivatives.**
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Calculate the Derivatives

Example: Logistic Regression Derivatives

Can we do it?

Wolfram Alpha can do it for us!

We need a formalism to deal with these derivatives.

Chain Rule

Chain rule for computing gradients:

- $y = g(x) \qquad z = f(y) = f\big(g(x)\big)$ $\qquad\qquad$ $\boldsymbol{y} = g(\boldsymbol{x}) \qquad z = f(\boldsymbol{y}) = f\big(g(\boldsymbol{x})\big)$

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

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j}\frac{\partial y_j}{\partial x_i}$$

- For longer chains $\displaystyle \frac{\partial z}{\partial x_i} = \sum_{j_1} \dots \sum_{j_m} \frac{\partial z}{\partial y_{j_1}} \dots \frac{\partial y_{j_m}}{\partial x_i}$

Logistic Regression derivatives

For logistic regression, the –ve log of the likelihood is:

$$\mathcal{L} = \sum_i \mathcal{L}_i = -\sum_i \log L_i = -\sum_i [y_i \log p_i + (1 - y_i)\log(1 - p_i)]$$

$$\mathcal{L}_i = -y_i \log \frac{1}{1 + e^{-W^T X}} - (1 - y_i)\log(1 - \frac{1}{1 + e^{-W^T X}})$$

To simplify the analysis let us split it into two parts,

$$\mathcal{L}_i = \mathcal{L}_i^A + \mathcal{L}_i^B$$

So the derivative with respect to W is:

$$\frac{\partial \mathcal{L}}{\partial W} = \sum_i \frac{\partial \mathcal{L}_i}{\partial W} = \sum_i (\frac{\partial \mathcal{L}_i^A}{\partial W} + \frac{\partial \mathcal{L}_i^B}{\partial W})$$

$$\mathcal{L}_i^A = -y_i \log \frac{1}{1+e^{-W^TX}}$$

Variables	Partial derivatives	Partial derivatives
$\xi_1 = -W^TX$	$\frac{\partial \xi_1}{\partial W} = -X$	$\frac{\partial \xi_1}{\partial W} = -X$
$\xi_2 = e^{\xi_1} = e^{-W^TX}$	$\frac{\partial \xi_2}{\partial \xi_1} = e^{\xi_1}$	$\frac{\partial \xi_2}{\partial \xi_1} = e^{-W^TX}$
$\xi_3 = 1 + \xi_2 = 1 + e^{-W^TX}$	$\frac{\partial \xi_3}{\partial \xi_2} = 1$	$\frac{\partial \xi_3}{\partial \xi_2} = 1$
$\xi_4 = \frac{1}{\xi_3} = \frac{1}{1+e^{-W^TX}} = p$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\xi_3^2}$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\left(1+e^{-W^TX}\right)^2}$
$\xi_5 = \log \xi_4 = \log p = \log \frac{1}{1+e^{-W^TX}}$	$\frac{\partial \xi_5}{\partial \xi_4} = \frac{1}{\xi_4}$	$\frac{\partial \xi_5}{\partial \xi_4} = 1 + e^{-W^TX}$
$\mathcal{L}_i^A = -y\xi_5$	$\frac{\partial \mathcal{L}}{\partial \xi_5} = -y$	$\frac{\partial \mathcal{L}}{\partial \xi_5} = -y$
$\frac{\partial \mathcal{L}_i^A}{\partial W} = \frac{\partial \mathcal{L}_i}{\partial \xi_5}\frac{\partial \xi_5}{\partial \xi_4}\frac{\partial \xi_4}{\partial \xi_3}\frac{\partial \xi_3}{\partial \xi_2}\frac{\partial \xi_2}{\partial \xi_1}\frac{\partial \xi_1}{\partial W}$		$\frac{\partial \mathcal{L}_i^A}{\partial W} = -yXe^{-W^TX}\frac{1}{\left(1+e^{-W^TX}\right)}$

$$\mathcal{L}_i^B = -(1-y_i)\log[1 - \frac{1}{1+e^{-W^TX}}]$$

Variables	derivatives	Partial derivatives wrt to X,W
$\xi_1 = -W^TX$	$\frac{\partial \xi_1}{\partial W} = -X$	$\frac{\partial \xi_1}{\partial W} = -X$
$\xi_2 = e^{\xi_1} = e^{-W^TX}$	$\frac{\partial \xi_2}{\partial \xi_1} = e^{\xi_1}$	$\frac{\partial \xi_2}{\partial \xi_1} = e^{-W^TX}$
$\xi_3 = 1 + \xi_2 = 1 + e^{-W^TX}$	$\frac{\partial \xi_3}{\partial \xi_2} = 1$	$\frac{\partial \xi_3}{\partial 2}$ =1
$\xi_4 = \frac{1}{\xi_3} = \frac{1}{1+e^{-W^TX}} = p$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\xi_3^2}$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\left(1+e^{-W^TX}\right)^2}$
$\xi_5 = 1 - \xi_4 = 1 - \frac{1}{1+e^{-W^TX}}$	$\frac{\partial \xi_5}{\partial \xi_4} = -1$	$\frac{\partial \xi_5}{\partial \xi_4}$ =-1
$\xi_6 = \log \xi_5 = \log(1-p) \ = \log \frac{1}{1+e^{-W^TX}}$	$\frac{\partial \xi_6}{\partial \xi_5} = \frac{1}{\xi_5}$	$\frac{\partial \xi_6}{\partial \xi_5} = \frac{1+e^{-W^TX}}{e^{-W^TX}}$
$\mathcal{L}_i^B = (1-y)\xi_6$	$\frac{\partial \mathcal{L}}{\partial \xi_6} = 1-y$	$\frac{\partial \mathcal{L}}{\partial \xi_6} = 1-y$
$\frac{\partial \mathcal{L}_i^B}{\partial W} = \frac{\partial \mathcal{L}_i^B}{\partial \xi_6}\frac{\partial \xi_6}{\partial \xi_5}\frac{\partial \xi_5}{\partial \xi_4}\frac{\partial \xi_4}{\partial \xi_3}\frac{\partial \xi_3}{\partial \xi_2}\frac{\partial \xi_2}{\partial \xi_1}\frac{\partial \xi_1}{\partial W}$		$\frac{\partial \mathcal{L}_i^B}{\partial W} = (1-y)X\frac{1}{\left(1+e^{-W^TX}\right)}$

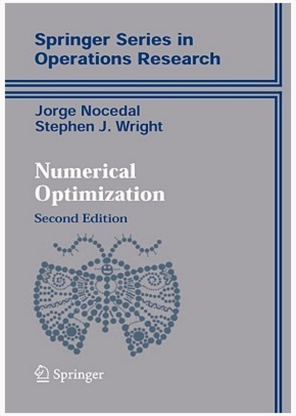
Considerations

- We still need to calculate the derivatives.
- **We need to know what is the learning rate or how to set it.**
- Local vs global minima.
- The full likelihood function includes summing up all individual '*errors*'. Unless you are a statistician, sometimes this includes hundreds of thousands of examples.

Learning Rate

Trial and Error.

There are many alternative methods which address how to set or adjust the learning rate, using the derivative or second derivatives and or the momentum. To be discussed in the next lectures on NN.

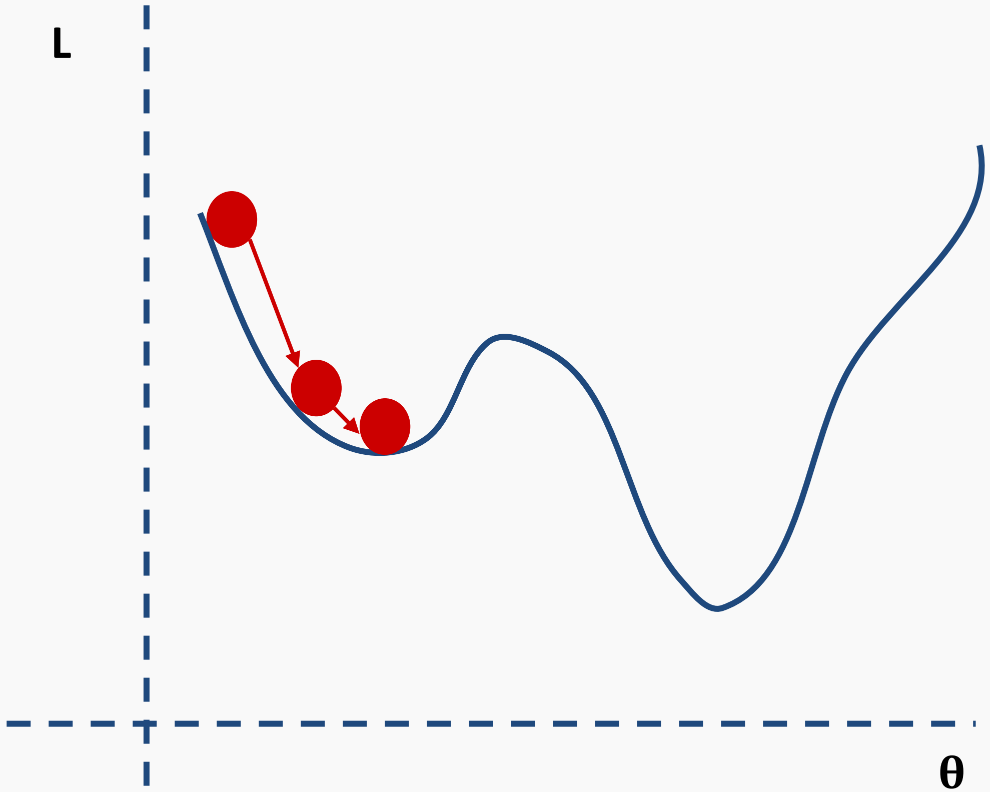


* J. Nocedal y S. Wright, “Numerical optimization”, Springer, 1999 🔗
* *TLDR*: J. Bullinaria, “Learning with Momentum, Conjugate Gradient Learning”, 2015 🔗

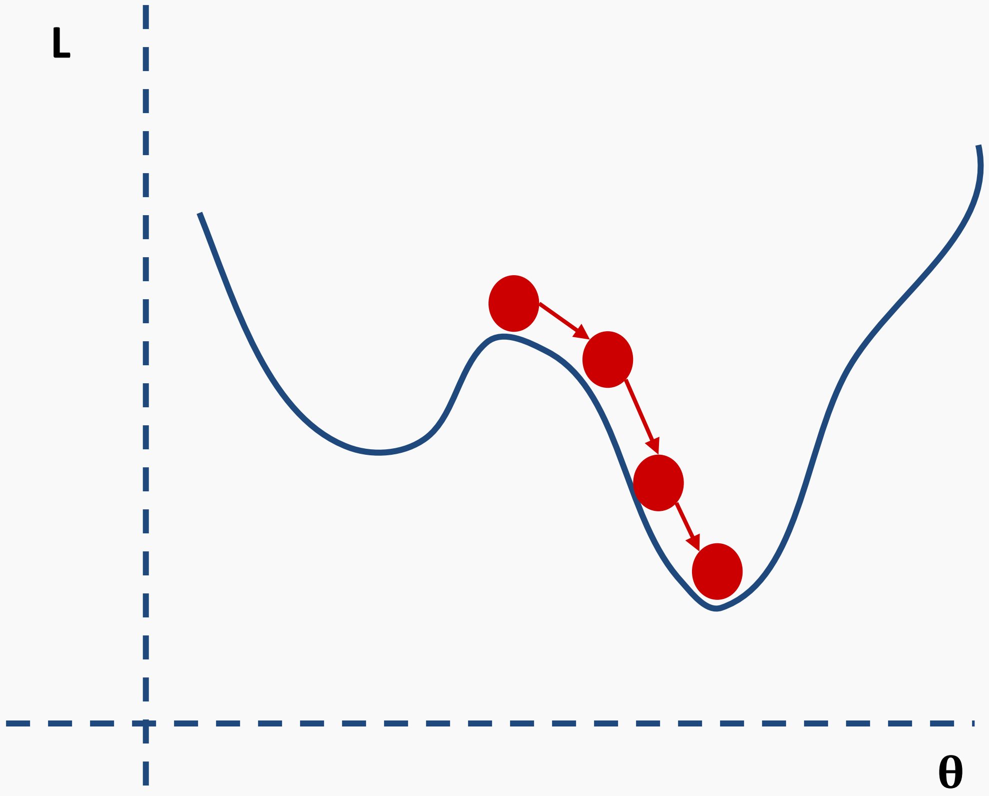
Considerations

- We still need to calculate the derivatives.
- We need to know what is the learning rate or how to set it.
- **Local vs global minima.**
- The full likelihood function includes summing up all individual '*errors*'. Unless you are a statistician, sometimes this includes hundreds of thousands of examples.

Local vs Global Minima



Local vs Global Minima



Local vs Global Minima

No guarantee that we get the global minimum.

Question: What would be a good strategy?

Considerations

- We still need to calculate the derivatives.
- We need to know what is the learning rate or how to set it.
- Local vs global minima.
- **The full likelihood function includes summing up all individual '*errors*'. Unless you are a statistician, sometimes this includes hundreds of thousands of examples.**

Batch and Stochastic Gradient Descent

$$\mathcal{L} = -\sum_{i} [y_i \log p_i + (1 - y_i) \log(1 - p_i)]$$

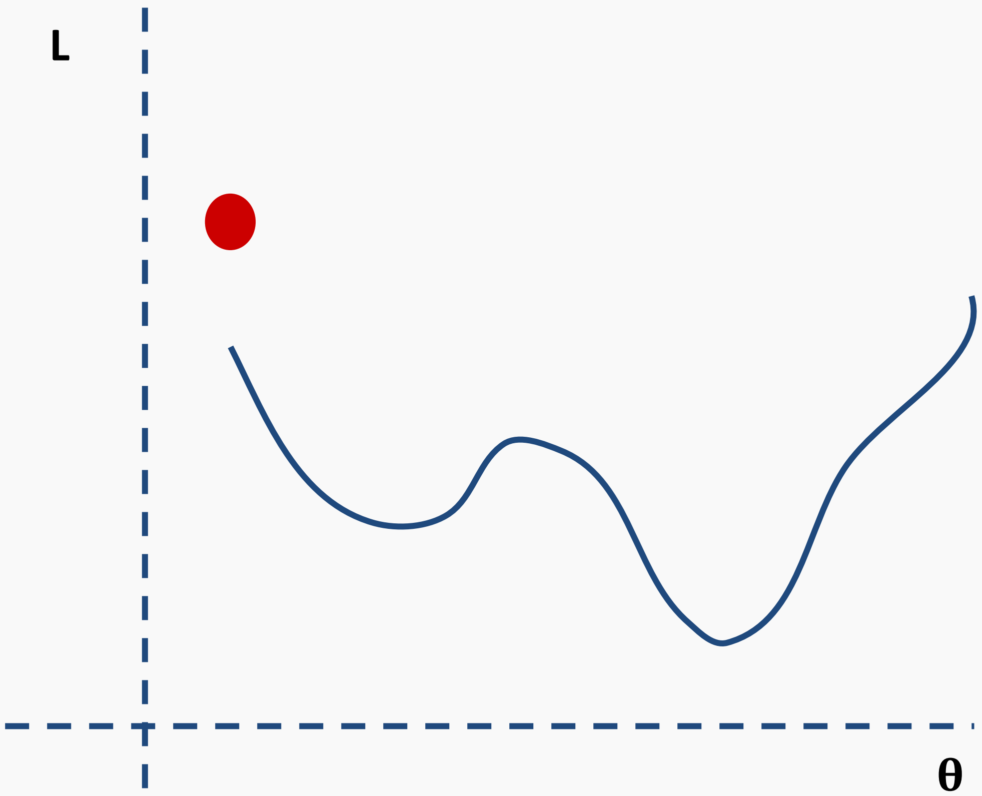
Instead of using all the examples for every step, use a subset of them (batch).

For each iteration *k*, use the following loss function to derive the derivatives:

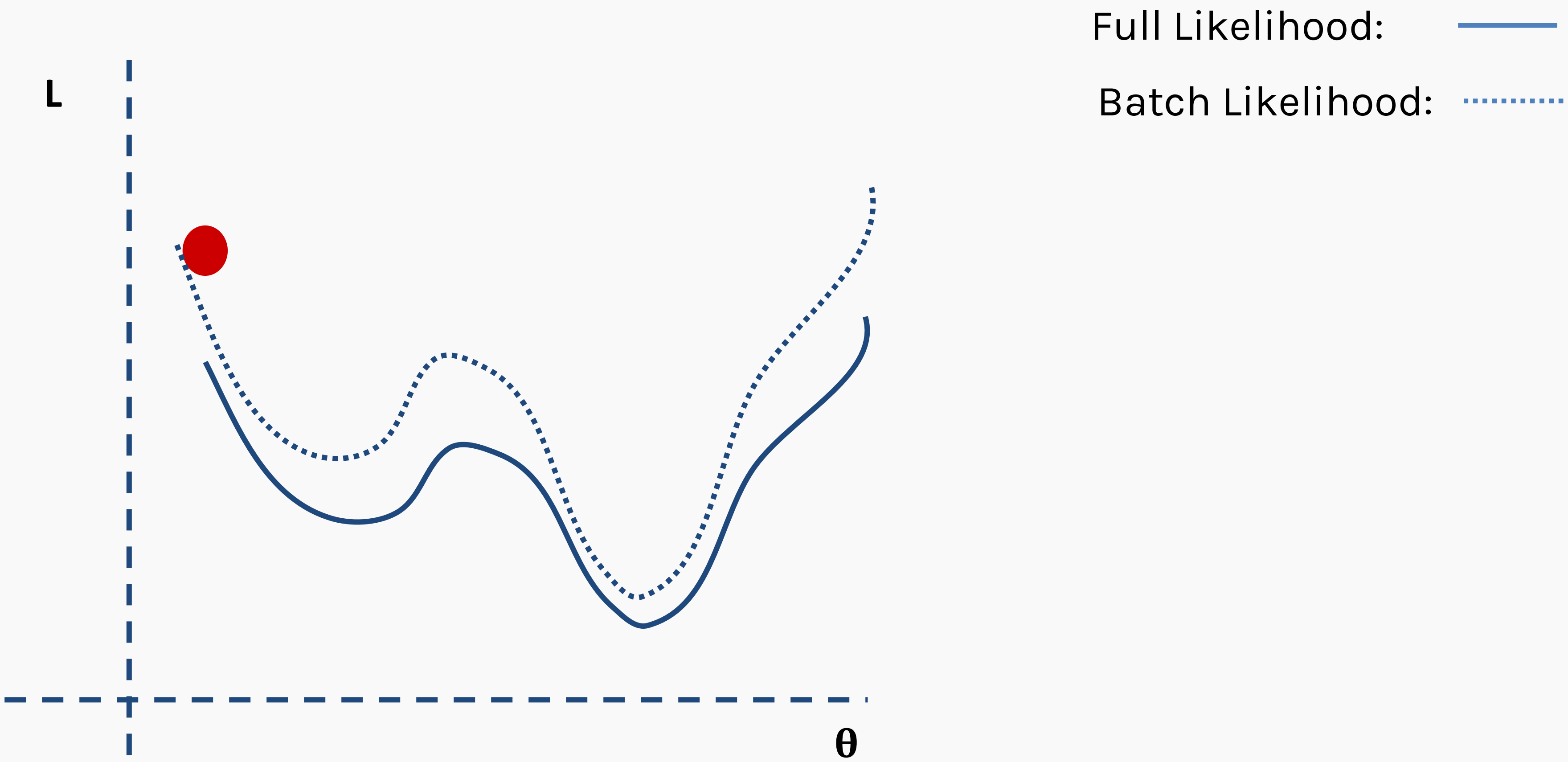
$$\mathcal{L}^k = -\sum_{i \in b^k} [y_i \log p_i + (1 - y_i) \log(1 - p_i)]$$

which is an **approximation** to the full loss function.

Batch and Stochastic Gradient Descent



Batch and Stochastic Gradient Descent



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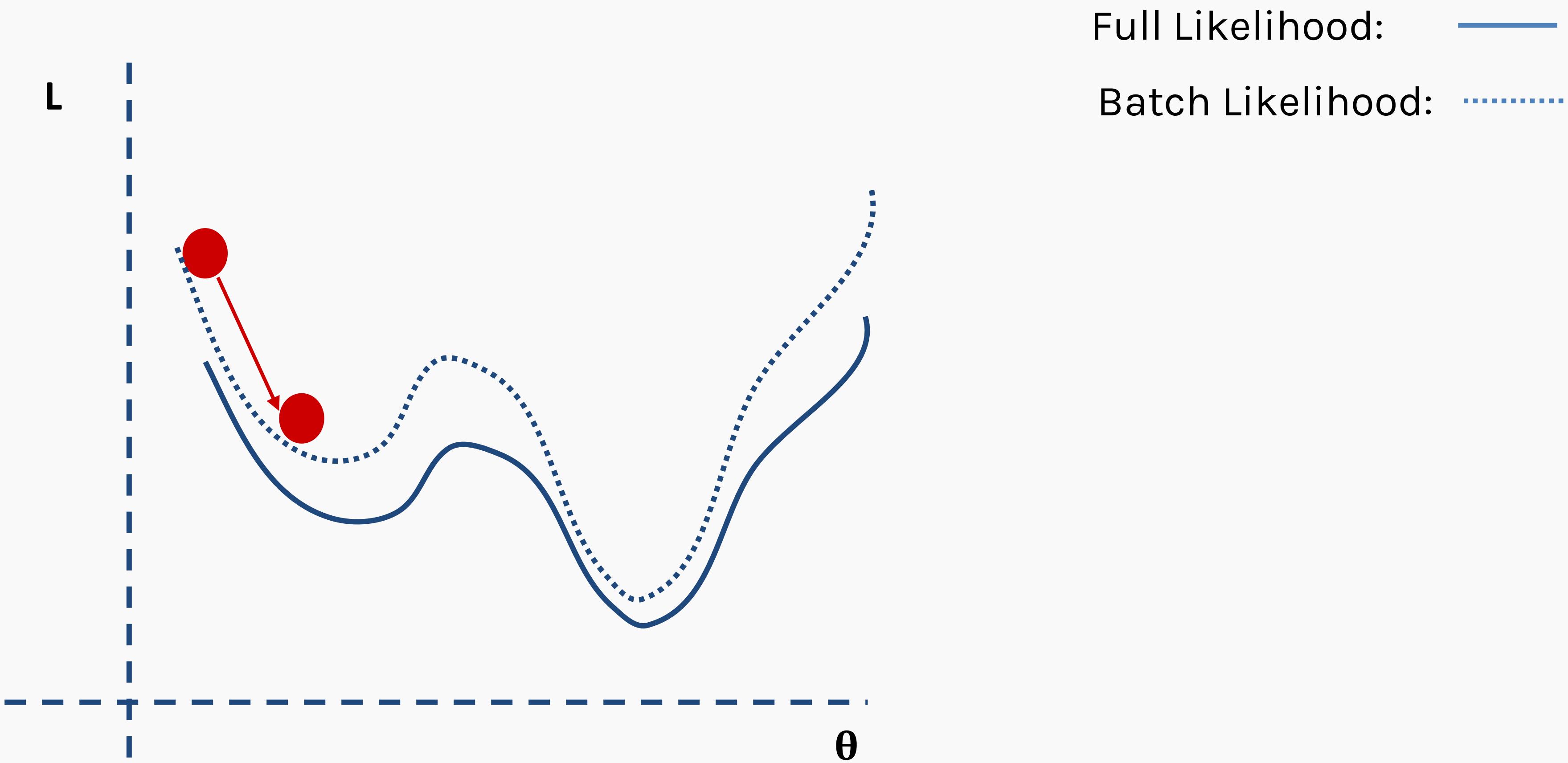

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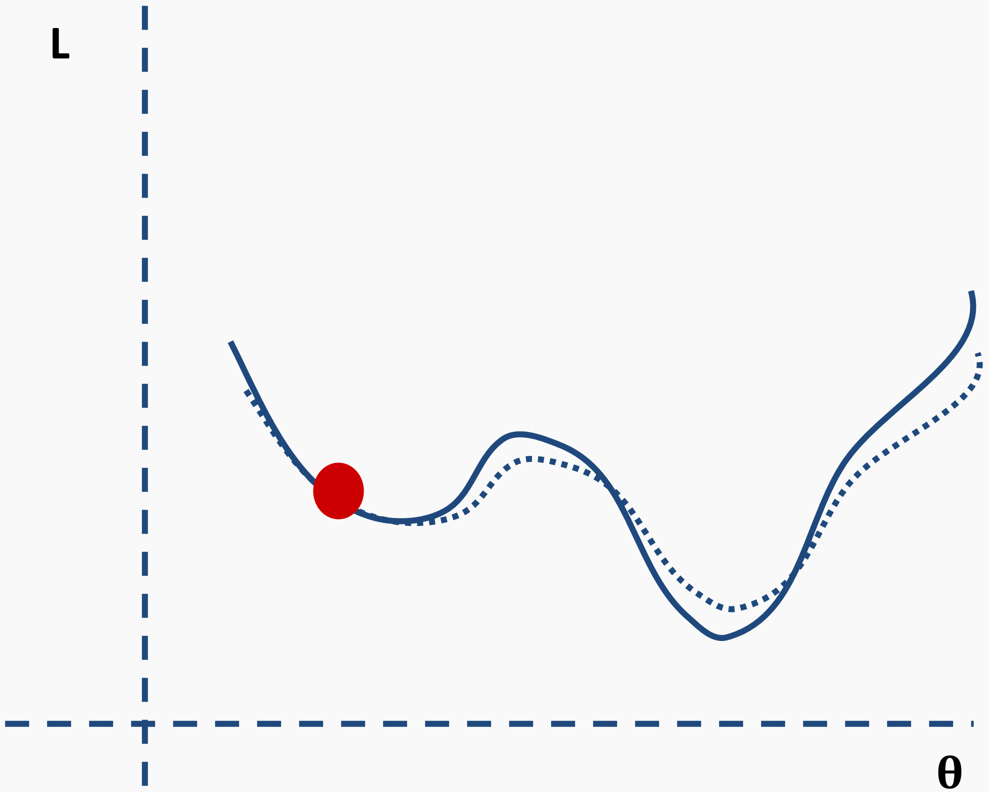

Full Likelihood:

Batch Likelihood:

Batch and Stochastic Gradient Descent

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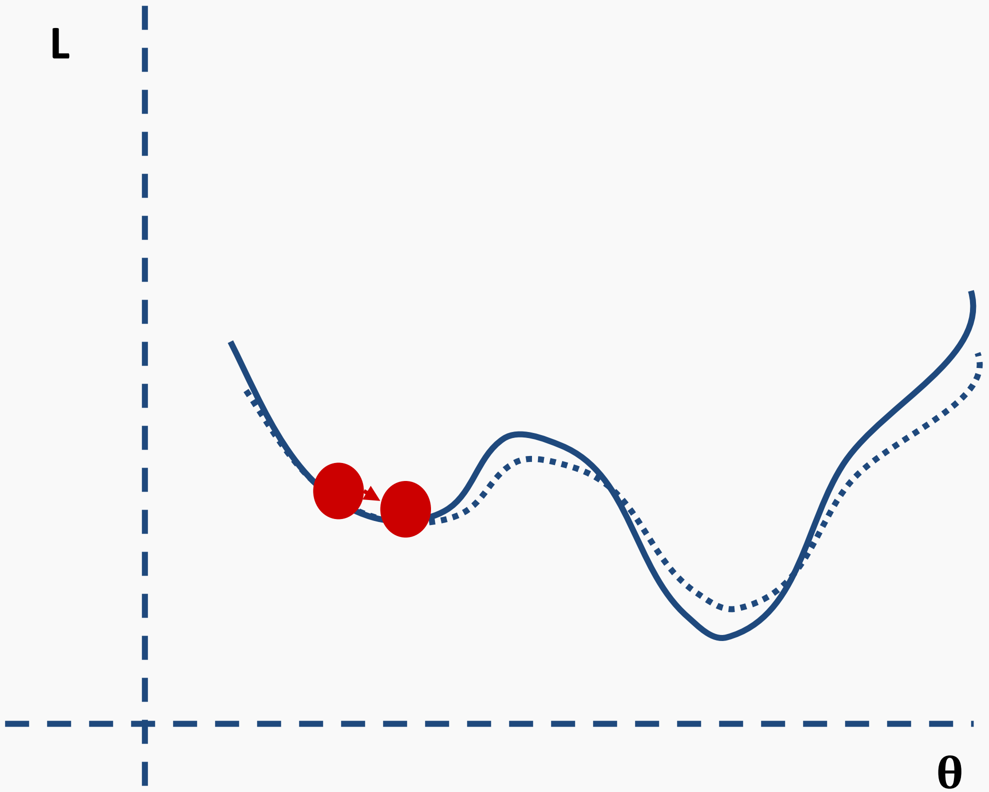

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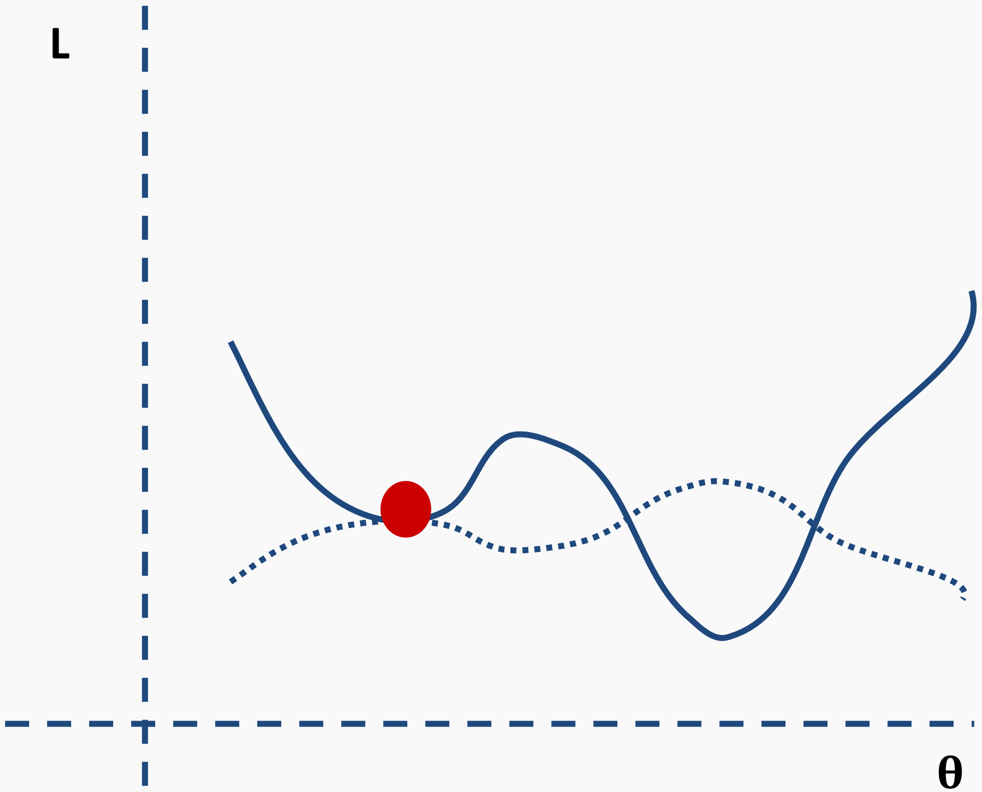

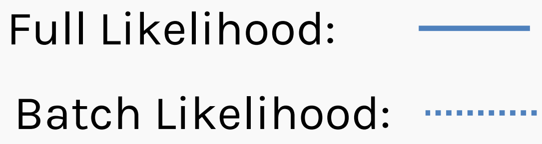

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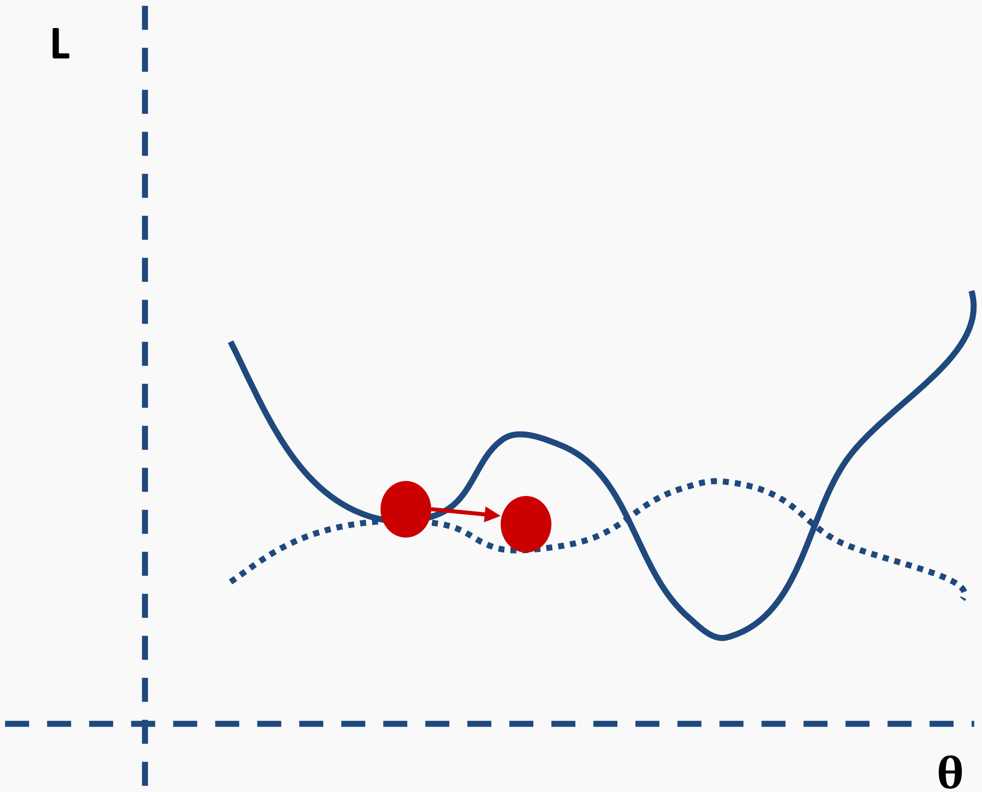

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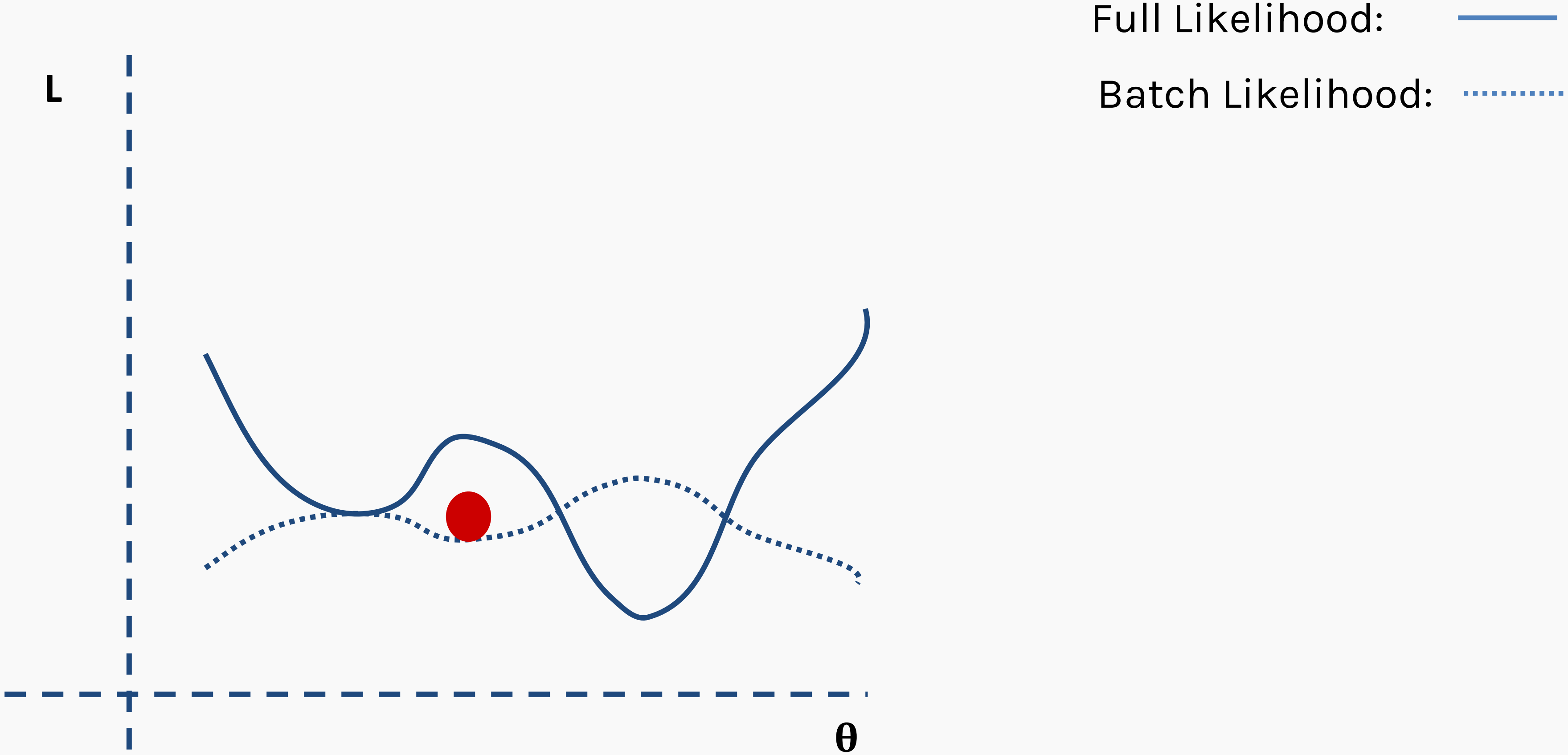
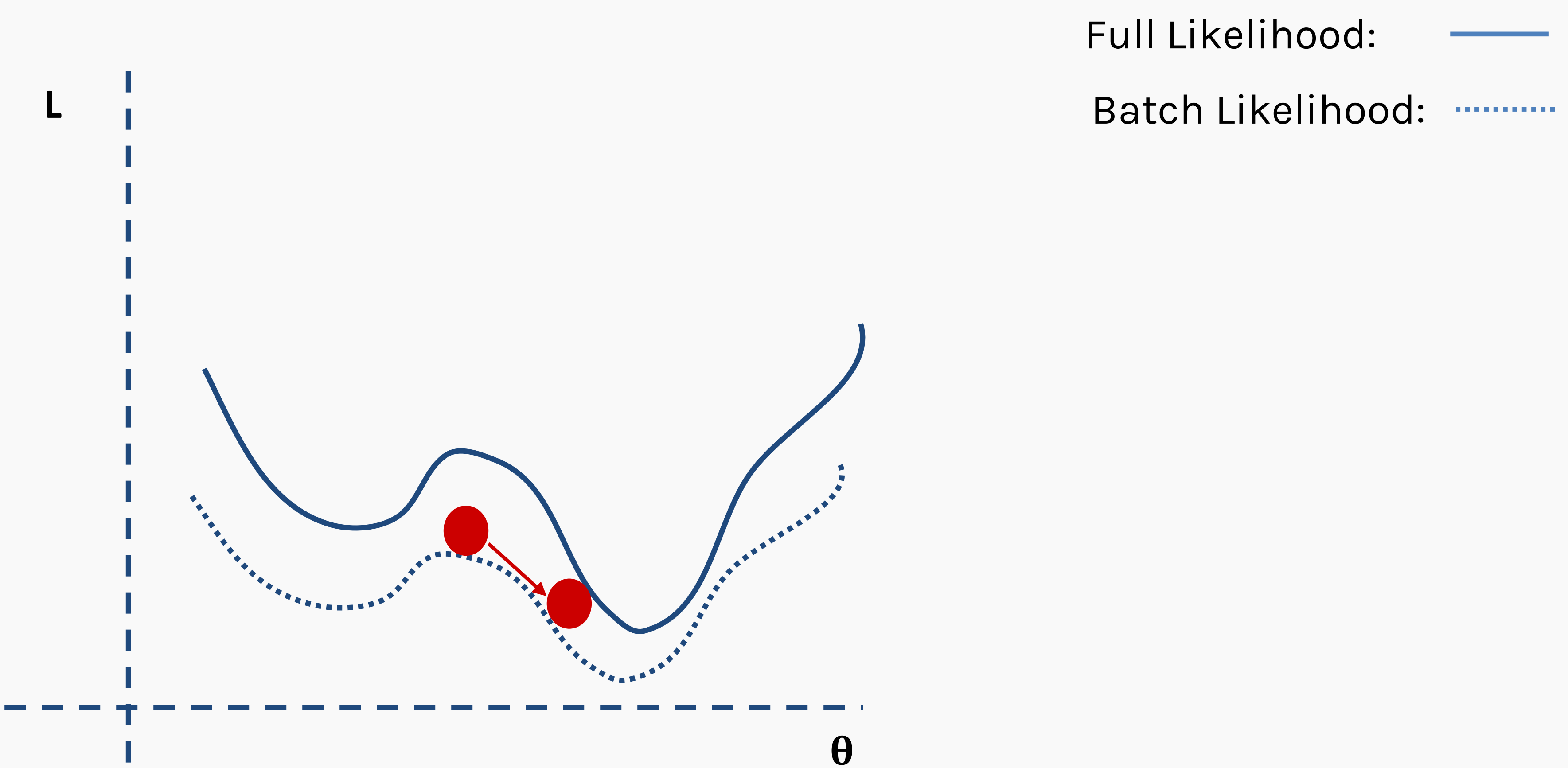


Batch and Stochastic Gradient Descent



Backpropagation

Backpropagation: Logistic Regression Revisited

$$X \longrightarrow \boxed{\text{Affine}} \longrightarrow h = \beta_0 + \beta_1 X \longrightarrow \boxed{\text{Activation}} \longrightarrow p = \frac{1}{1+e^{-h}} \longrightarrow \boxed{\text{Loss Fun}} \longrightarrow \mathcal{L}(\beta) = \sum_i^n \mathcal{L}_i(\beta)$$

$$\frac{\partial \mathcal{L}}{\partial p}\frac{\partial p}{\partial h}\frac{\partial h}{\partial \beta} \longleftarrow \frac{\partial \mathcal{L}}{\partial p}\frac{\partial p}{\partial h} \longleftarrow \frac{\partial \mathcal{L}}{\partial p}$$

$$\frac{\partial h}{\partial \beta_1} = X, \frac{d\mathcal{L}}{d\beta_0} = 1 \qquad \frac{\partial p}{\partial h} = \sigma(h)(1-\sigma(h)) \qquad \frac{\partial \mathcal{L}}{\partial p} = -y\frac{1}{p} - (1-y)\frac{1}{1-p}$$

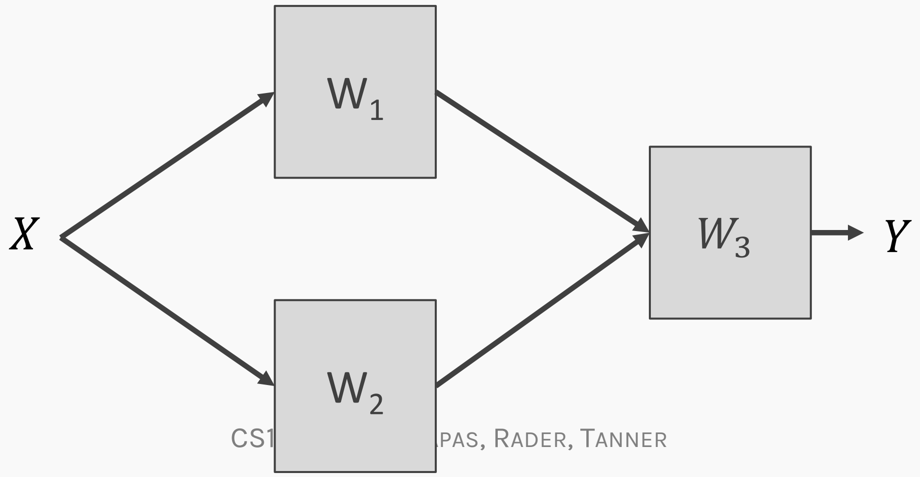
$$\frac{\partial \mathcal{L}}{\partial \beta_1} = -X\sigma(h)\big(1-\sigma(h)\big)[y\frac{1}{p} + (1-y)\frac{1}{1-p}]$$

$$\frac{\partial \mathcal{L}}{\partial \beta_0} = -\sigma(h)\big(1-\sigma(h)\big)[\,y\frac{1}{p} + (1-y)\frac{1}{1-p}]$$

Backpropagation

1. Derivatives need to be evaluated at some values of *X*,*y* and *W*.
2. But since we have an expression, we can build a function that takes as input *X*,*y*,*W* and returns the derivatives and then we can use gradient descent to update.
3. This approach works well but it does not generalize. For example if the network is changed, we need to write a new function to evaluate the derivatives.

For example this network will need a different function for the derivatives



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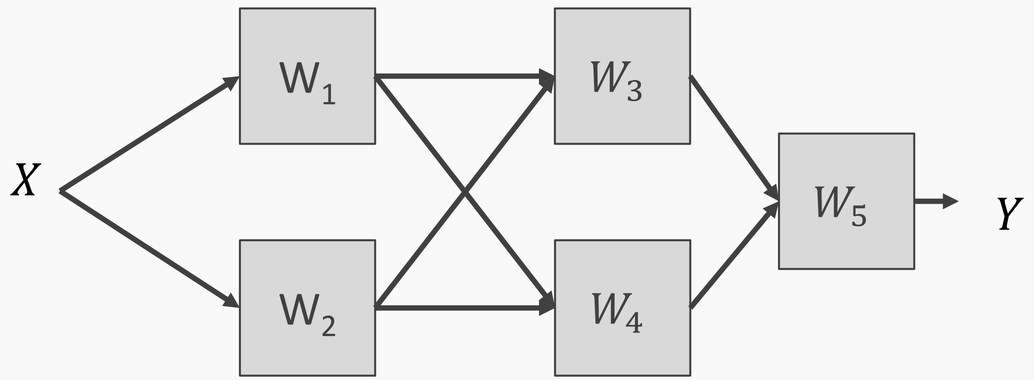


Backpropagation. Pavlos game #456

Need to find a formalism to calculate the derivatives of the loss wrt to weights that is:

1. Flexible enough that adding a node or a layer or changing something in the network won't require to re-derive the functional form from scratch.
2. It is exact.
3. It is computationally efficient.

Hints:

1. Remember we only need to evaluate the derivatives at X_i, y_i and $W^{(k)}$.
2. We should take advantage of the chain rule we learned before

Idea 1: Evaluate the derivative at: $X=\{3\}, y=1, W=3$

Variables	derivatives	Value of the variable	Value of the partial derivative	$\frac{d\xi_n}{dW}$
$\xi_1 = -W^T X$	$\frac{\partial \xi_1}{\partial W} = -X$	-9	-3	-3
$\xi_2 = e^{\xi_1} = e^{-W^T X}$	$\frac{\partial \xi_2}{\partial \xi_1} = e^{\xi_1}$	e^{-9}	e^{-9}	-3e^{-9}
$\xi_3 = 1 + \xi_2 = 1 + e^{-W^T X}$	$\frac{\partial \xi_3}{\partial \xi_2} = 1$	1+e^{-9}	1	-3e^{-9}
$\xi_4 = \frac{1}{\xi_3} = \frac{1}{1 + e^{-W^T X}} = p$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\xi_3^2}$	$\frac{1}{1 + e^{-9}}$	$\left(\frac{1}{1 + e^{-9}}\right)^2$	-3$e^{-9}\left(\frac{1}{1+e^{-9}}\right)^2$
$\xi_5 = \log \xi_4 = \log p = \log \frac{1}{1 + e^{-W^T X}}$	$\frac{\partial \xi_5}{\partial \xi_4} = \frac{1}{\xi_4}$	$\log \frac{1}{1 + e^{-9}}$	$1 + e^{-9}$	-3$e^{-9}\left(\frac{1}{1+e^{-9}}\right)$
$\mathcal{L}_i^A = -y\xi_5$	$\frac{\partial \mathcal{L}}{\partial \xi_5} = -y$	$-\log \frac{1}{1 + e^{-9}}$	-1	$3e^{-9}\left(\frac{1}{1+e^{-9}}\right)$
$\frac{\partial \mathcal{L}_i^A}{\partial W} = \frac{\partial \mathcal{L}_i}{\partial \xi_5}\frac{\partial \xi_5}{\partial \xi_4}\frac{\partial \xi_4}{\partial \xi_3}\frac{\partial \xi_3}{\partial \xi_2}\frac{\partial \xi_2}{\partial \xi_1}\frac{\partial \xi_1}{\partial W}$			-3	0.00037018372

Basic functions

We still need to derive **derivatives** ☹

Variables	derivatives	Value of the variable	Value of the partial derivative	$\frac{d\xi_n}{dW}$
$\xi_1 = -W^T X$	$\frac{\partial \xi_1}{\partial W} = -X$	-9	-3	-3
$\xi_2 = e^{\xi_1} = e^{-W^T X}$	$\frac{\partial \xi_2}{d\partial \xi_1} = e^{\xi_1}$	e^{-9}	e^{-9}	-3e^{-9}
$\xi_3 = 1 + \xi_2 = 1 + e^{-W^T X}$	$\frac{\partial \xi_3}{\partial \xi_2} = 1$	1+e^{-9}	1	-3e^{-9}
$\xi_4 = \frac{1}{\xi_3} = \frac{1}{1 + e^{-W^T X}} = p$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\xi_3^2}$	$\frac{1}{1 + e^{-9}}$	$\left(\frac{1}{1 + e^{-9}}\right)^2$	-3$e^{-9}\left(\frac{1}{1+e^{-9}}\right)^2$
$\xi_5 = \log \xi_4 = \log p = \log \frac{1}{1 + e^{-W^T X}}$	$\frac{\partial \xi_5}{\partial \xi_4} = \frac{1}{\xi_4}$	$\log \frac{1}{1 + e^{-9}}$	$1 + e^{-9}$	-3$e^{-9}\left(\frac{1}{1+e^{-9}}\right)$
$\mathcal{L}_i^A = -y\xi_5$	$\frac{\partial \mathcal{L}}{\partial \xi_5} = -y$	$-\log \frac{1}{1 + e^{-9}}$	-1	3$e^{-9}\left(\frac{1}{1+e^{-9}}\right)$
$\frac{\partial \mathcal{L}_i^A}{\partial W} = \frac{\partial \mathcal{L}_i}{\partial \xi_5}\frac{\partial \xi_5}{\partial \xi_4}\frac{\partial \xi_4}{\partial \xi_3}\frac{\partial \xi_3}{\partial \xi_2}\frac{\partial \xi_2}{\partial \xi_1}\frac{\partial \xi_1}{\partial W}$			-3	0.00037018372

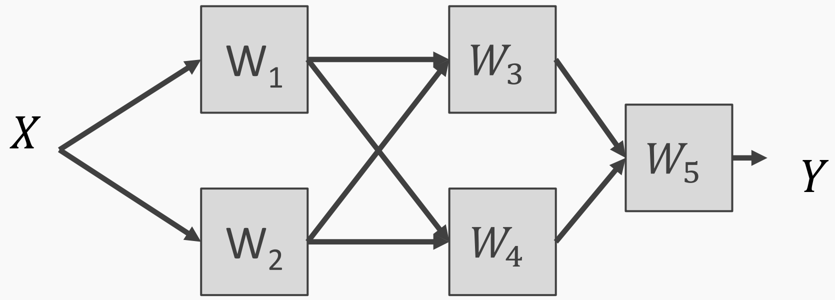
Basic functions

Notice though those are basic functions that my grandparent can do

$\xi_0 = X$	$\frac{\partial \xi_0}{\partial X} = 1$	`def x0(x):` `    return X`	`def derx0():` `    return 1`
$\xi_1 = -W^T \xi_0$	$\frac{\partial \xi_1}{\partial W} = -X$	`def x1(a,x):` `    return -a*X`	`def derx1(a,x):` `    return -a`
$\xi_2 = \mathrm{e}^{\xi_1}$	$\frac{\partial \xi_2}{\partial \xi_1} = e^{\xi_1}$	`def x2(x):` `    return np.exp(x)`	`def derx2(x):` `        return np.exp(x)`
$\xi_3 = 1 + \xi_2$	$\frac{\partial \xi_3}{\partial \xi_2} = 1$	`def x3(x):` `    return 1+x`	`def derx3(x):` `        return 1`
$\xi_4 = \frac{1}{\xi_3}$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\xi_3^2}$	`def der1(x):` `    return 1/(x)`	`def derx4(x):` `        return  -(1/x)**(2)`
$\xi_5 = \log \xi_4$	$\frac{\partial \xi_5}{\partial \xi_4} = \frac{1}{\xi_4}$	`def der1(x):` `    return np.log(x)`	`def derx5(x)` `        return 1/x`
$\mathcal{L}_i^A = -y\xi_5$	$\frac{\partial \mathcal{L}}{\partial \xi_5} = -y$	`def der1(y,x):` `    return -y*x`	`def derL(y):` `    return -y`

Putting it altogether

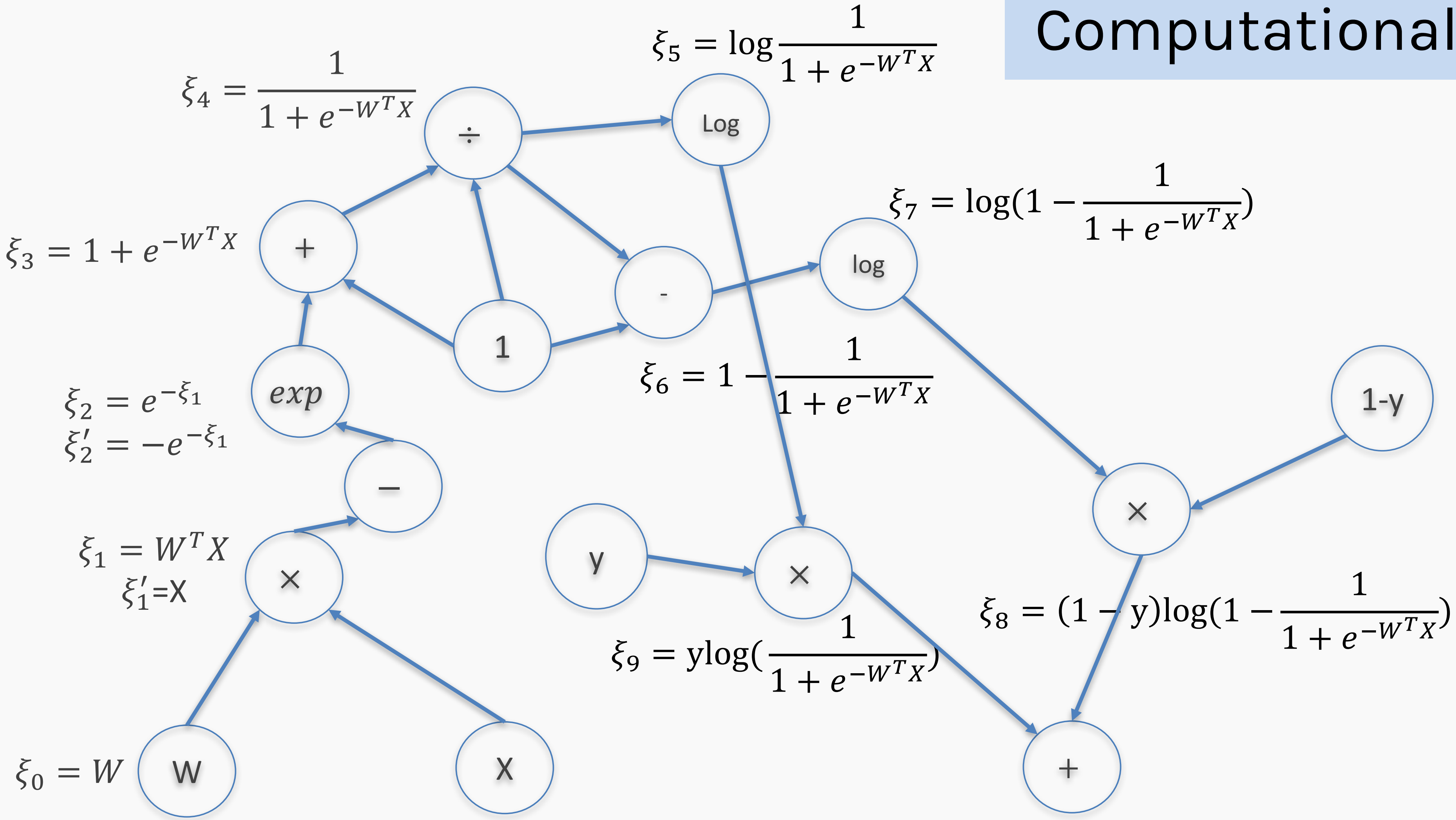
1. We specify the network structure



2. We create the computational graph …

What is computational graph?

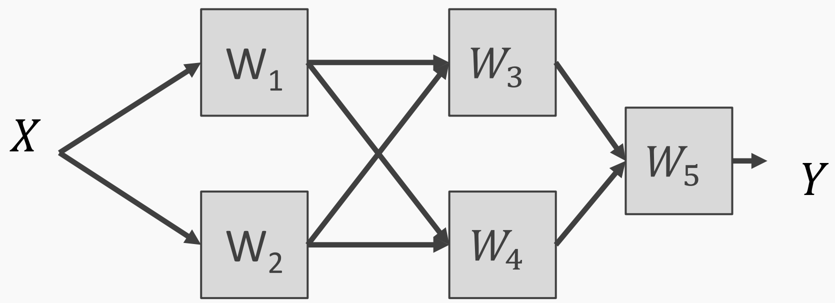
Computational Graph



$$-\mathcal{L} = \xi_9 = \text{y}\log(\frac{1}{1+e^{-W^TX}}) + (1-\text{y})\log(1 - \frac{1}{1+e^{-W^TX}})$$

Putting it altogether

1. We specify the network structure



- We create the computational graph.
- At each node of the graph we build two functions: the evaluation of the variable and its partial derivative with respect to the previous variable (as shown in the table 3 slides back)
- Now we can either go forward or backward depending on the situation. In general, forward is easier to implement and to understand. The difference is clearer when there are multiple nodes per layer.

Forward mode: Evaluate the derivative at: *X={3}, y=1, W=3*

Variables	derivatives	Value of the variable	Value of the partial derivative	$\frac{d\mathcal{L}}{d\xi_n}$
$\xi_1 = -W^T X$	$\frac{\partial \xi_1}{\partial W} = -X$	-9	-3	-3
$\xi_2 = e^{\xi_1} = e^{-W^T X}$	$\frac{\partial \xi_2}{\partial \xi_1} = e^{\xi_1}$	e^{-9}	e^{-9}	-3e^{-9}
$\xi_3 = 1 + \xi_2 = 1 + e^{-W^T X}$	$\frac{\partial \xi_3}{\partial \xi_2} = 1$	1+e^{-9}	1	-3e^{-9}
$\xi_4 = \frac{1}{\xi_3} = \frac{1}{1 + e^{-W^T X}} = p$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\xi_3^2}$	$\frac{1}{1 + e^{-9}}$	$\left(\frac{1}{1 + e^{-9}}\right)^2$	-3$e^{-9}\left(\frac{1}{1+e^{-9}}\right)^2$
$\xi_5 = \log \xi_4 = \log p = \log \frac{1}{1 + e^{-W^T X}}$	$\frac{\partial \xi_5}{\partial \xi_4} = \frac{1}{\xi_4}$	$\log \frac{1}{1 + e^{-9}}$	$1 + e^{-9}$	-3$e^{-9}\left(\frac{1}{1+e^{-9}}\right)$
$\mathcal{L}_i^A = -y\xi_5$	$\frac{\partial \mathcal{L}}{\partial \xi_5} = -y$	$-\log \frac{1}{1 + e^{-9}}$	-1	3$e^{-9}\left(\frac{1}{1+e^{-9}}\right)$
$\frac{\partial \mathcal{L}_i^A}{\partial W} = \frac{\partial \mathcal{L}_i}{\partial \xi_5}\frac{\partial \xi_5}{\partial \xi_4}\frac{\partial \xi_4}{\partial \xi_3}\frac{\partial \xi_3}{\partial \xi_2}\frac{\partial \xi_2}{\partial \xi_1}\frac{\partial \xi_1}{\partial W}$			-3	0.00037018372

Backward mode: Evaluate the derivative at: $X=\{3\}, y=1, W=3$

Variables	derivatives	Value of the variable	Value of the partial derivative
$\xi_1 = -W^T X$	$\frac{\partial \xi_1}{\partial W} = -X$	-9	-3
$\xi_2 = e^{\xi_1} = e^{-W^T X}$	$\frac{\partial \xi_2}{\partial \xi_1} = e^{\xi_1}$	e^{-9}	e^{-9}
$\xi_3 = 1 + \xi_2 = 1 + e^{-W^T X}$	$\frac{\partial \xi_3}{\partial \xi_2} = 1$	1+e^{-9}	1
$\xi_4 = \frac{1}{\xi_3} = \frac{1}{1+e^{-W^T X}} = p$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\xi_3^2}$	$\frac{1}{1+e^{-9}}$	$\left(\frac{1}{1+e^{-9}}\right)^2$
$\xi_5 = \log \xi_4 = \log p \ = \log \frac{1}{1+e^{-W^T X}}$	$\frac{\partial \xi_5}{\partial \xi_4} = \frac{1}{\xi_4}$	$\log \frac{1}{1+e^{-9}}$	$1+e^{-9}$
$\mathcal{L}_i^A = -y\xi_5$	$\frac{\partial \mathcal{L}}{\partial \xi_5} = -y$	$-\log \frac{1}{1+e^{-9}}$	-1
$\frac{\partial \mathcal{L}_i^A}{\partial W} = \frac{\partial \mathcal{L}_i}{\partial \xi_5} \frac{\partial \xi_5}{\partial \xi_4} \frac{\partial \xi_4}{\partial \xi_3} \frac{\partial \xi_3}{\partial \xi_2} \frac{\partial \xi_2}{\partial \xi_1} \frac{\partial \xi_1}{\partial W}$			Type equation here.

Store all these values

Optimizers

Learning vs. Optimization

Goal of learning: minimize generalization error, or the loss function

$$\mathcal{L}(W) = \mathbb{E}_{(x,y)\sim p_{data}}[L(W; x, y)]$$

In practice, empirical risk minimization:

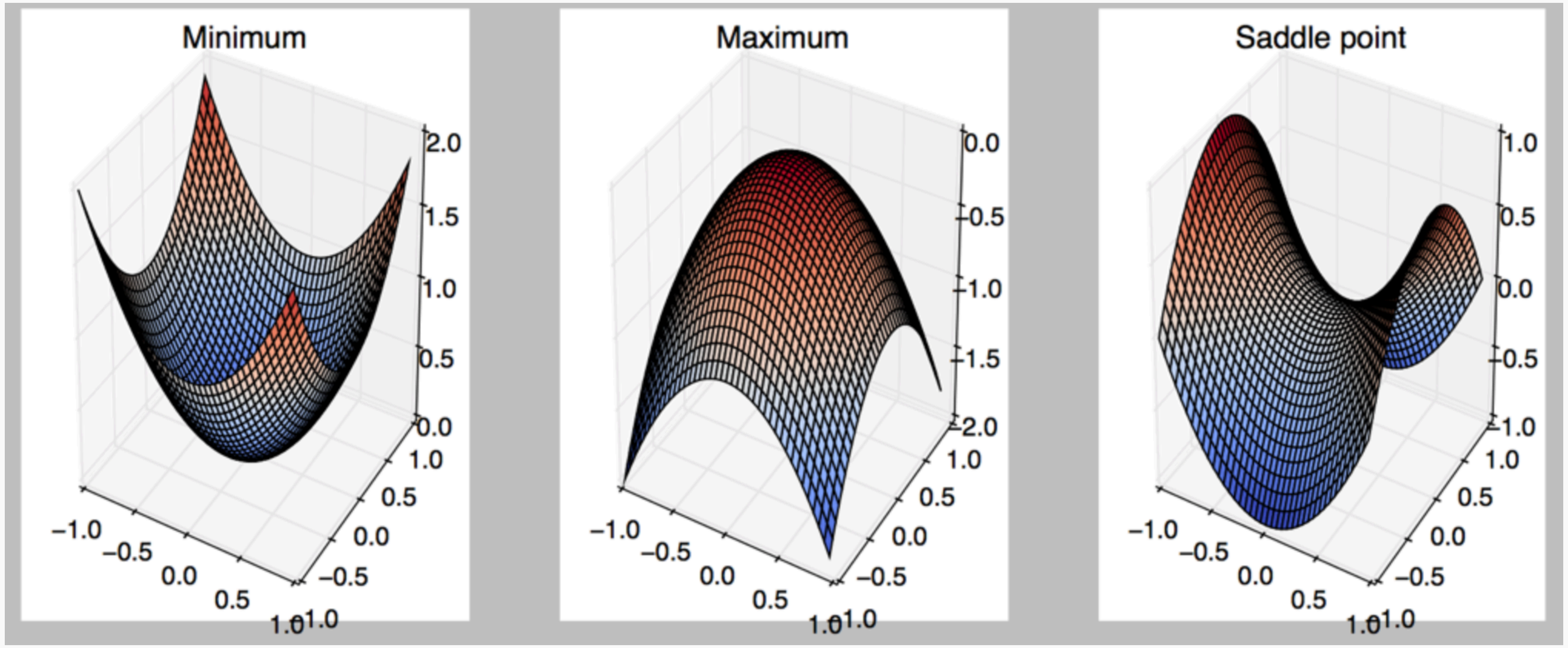
$$\mathcal{L}(W) = \sum_i [L(W; x_i, y_i)]$$

Quantity optimized
different from the quantity
we care about

Critical Points

Points with zero gradient

2nd-derivate (Hessian) determines curvature



Goodfellow et al. (2016)

Outline

Optimization

- **Challenges in Optimization**
- Momentum
- Adaptive Learning Rate
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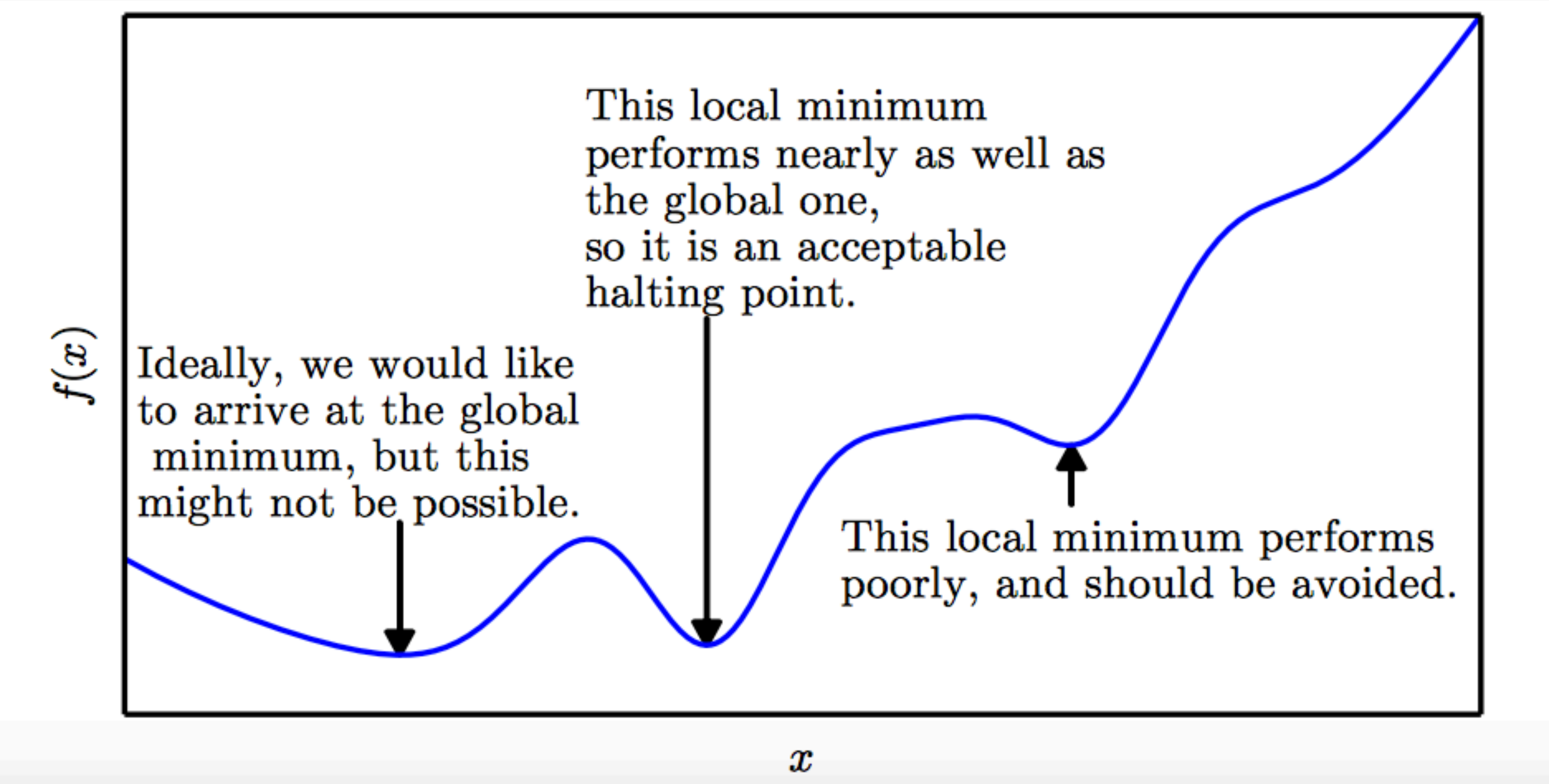
Local Minima



Goodfellow et al. (2016)

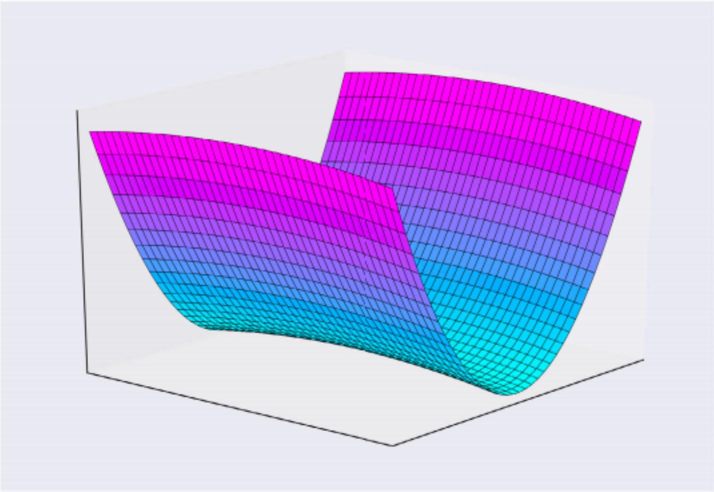
Local Minima

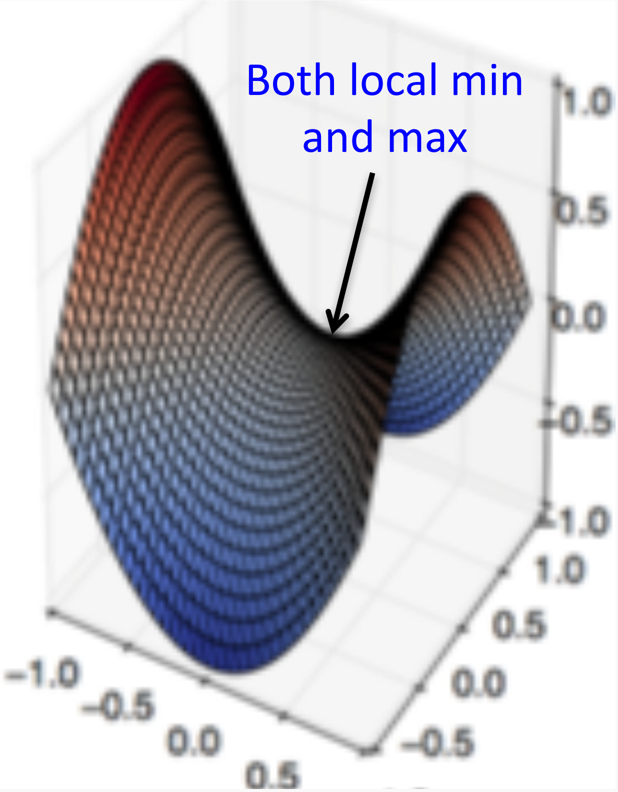
Old view: local minima is major problem in neural network training

Recent view:

- For sufficiently large neural networks, most local minima incur low cost
- Not important to find true global minimum

Saddle Points





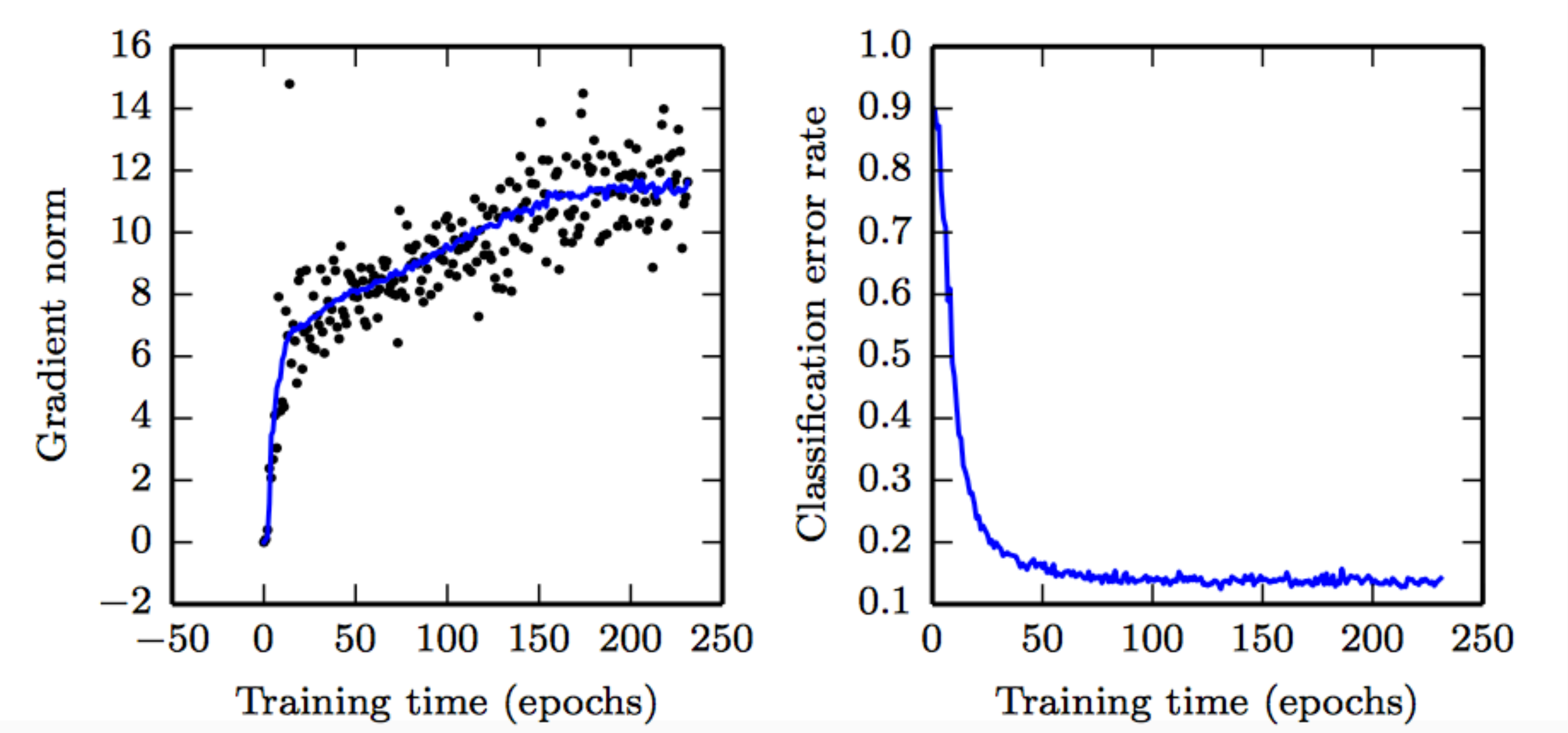
Recent studies indicate that in high dim, saddle points are more likely than local min

Gradient can be very small near saddle points

Goodfellow et al. (2016)

No Critical Points

Gradient norm increases, but validation error decreases



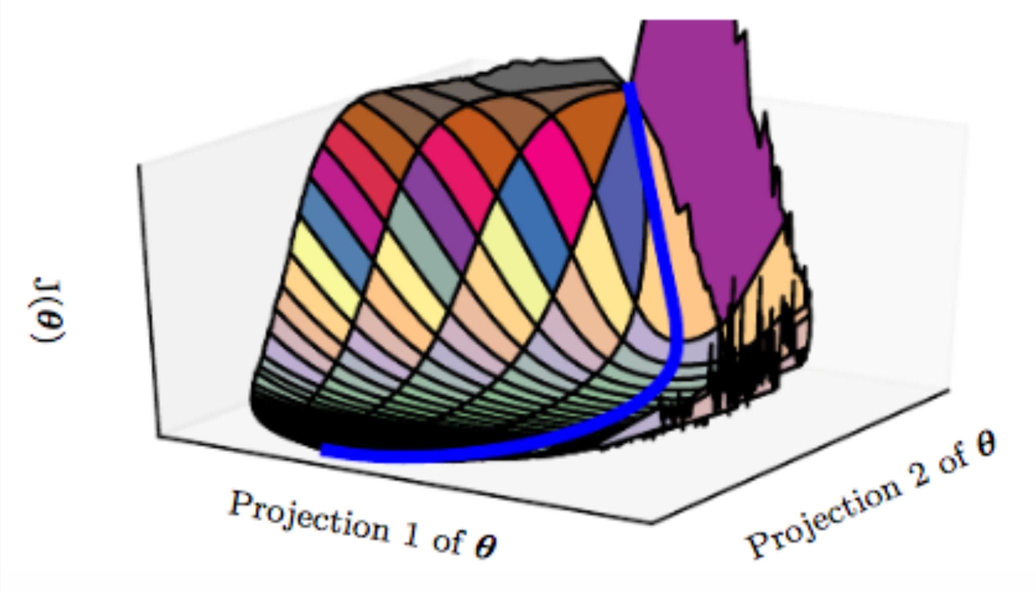
Convolution Nets for Object Detection

Goodfellow et al. (2016)

Saddle Points

SGD is seen to escape saddle points

– Moves down-hill, uses noisy gradients



Second-order methods get stuck

– solves for a point with zero gradient

Goodfellow et al. (2016)

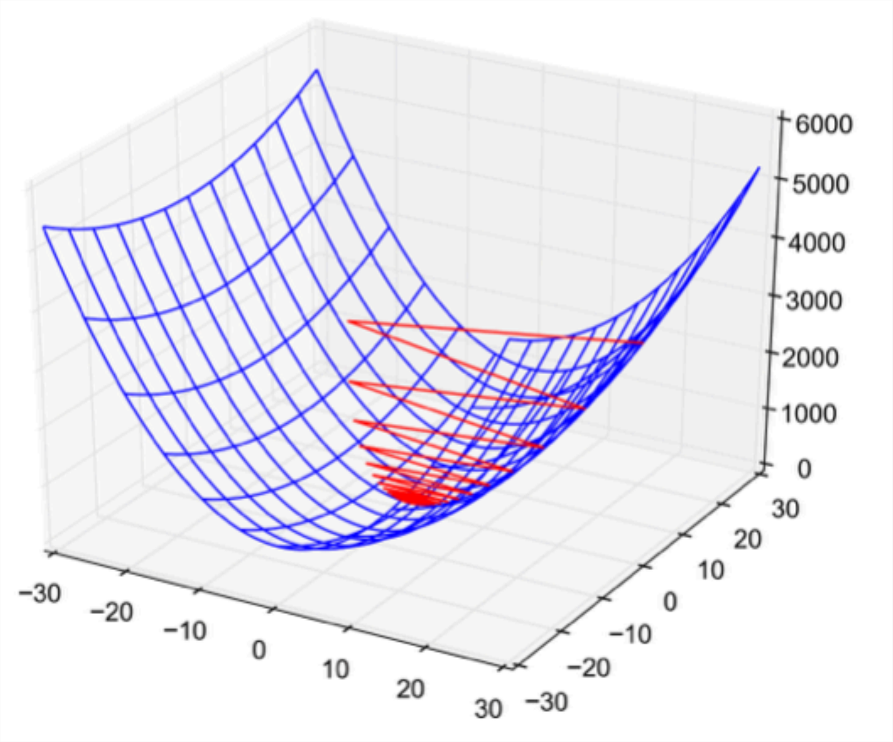
Poor Conditioning

Poorly conditioned Hessian matrix

- High curvature: small steps leads to huge increase

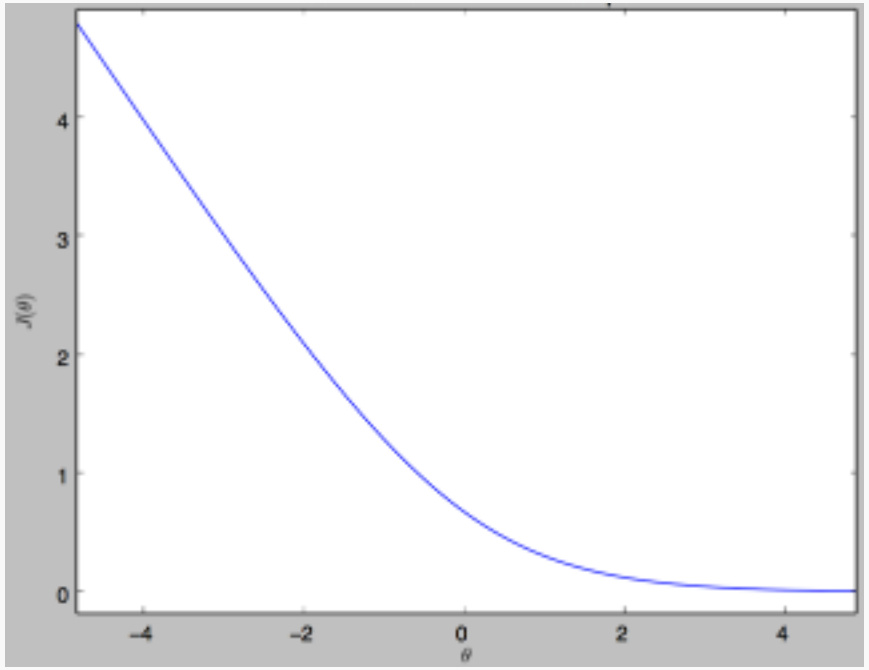
Learning is slow despite strong gradients

Oscillations slow down progress

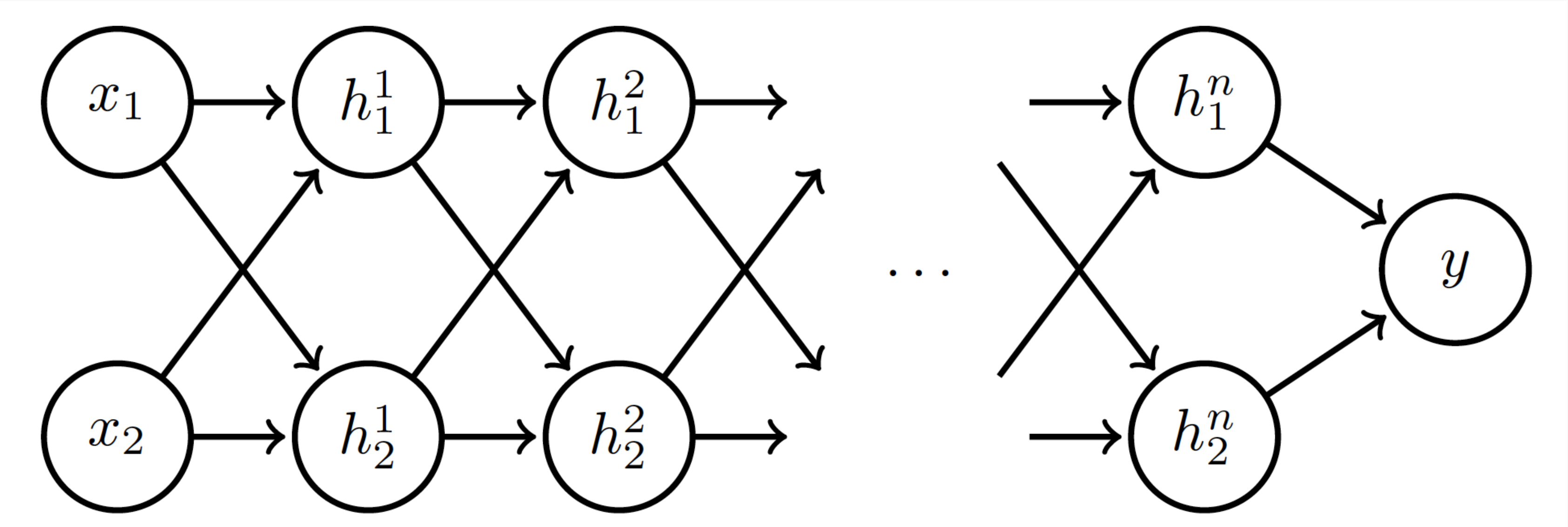


No Critical Points

Some cost functions do not have critical points. In particular classification.



Exploding and Vanishing Gradients



Linear activation

$$h_i = Wx$$

$$h_i = Wh_{i-1}, \qquad i = 2, \ldots, n$$

Exploding and Vanishing Gradients

$$\text{Suppose } \mathbf{W} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}:$$

$$\begin{bmatrix} h_1^1 \\ h_2^1 \end{bmatrix} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \cdots \qquad \begin{bmatrix} h_1^n \\ h_2^n \end{bmatrix} = \begin{bmatrix} a^n & 0 \\ 0 & b^n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Exploding and Vanishing Gradients

$$\text{Suppose } x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\text{Case 1: } a = 1,\ b = 2:$$

$$y \to 1, \quad \nabla y \to \begin{bmatrix} n \\ n2^{n-1} \end{bmatrix}$$

Explodes!

$$\text{Case 2: } a = 0.5,\ b = 0.9:$$

$$y \to 0, \quad \nabla y \to \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Vanishes!

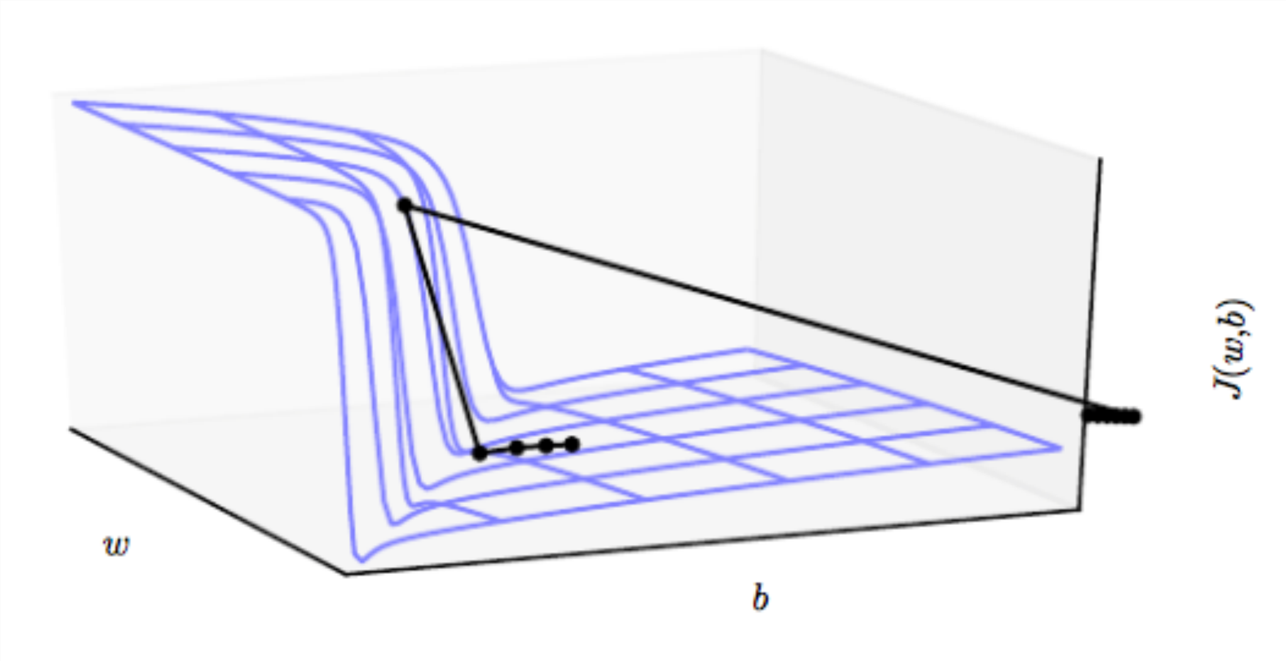
Exploding and Vanishing Gradients

Exploding gradients lead to cliffs

Can be mitigated using gradient clipping

$$\text{if } ||g|| > u$$

$$g \leftarrow \frac{gu}{||g||}$$



Goodfellow et al. (2016)

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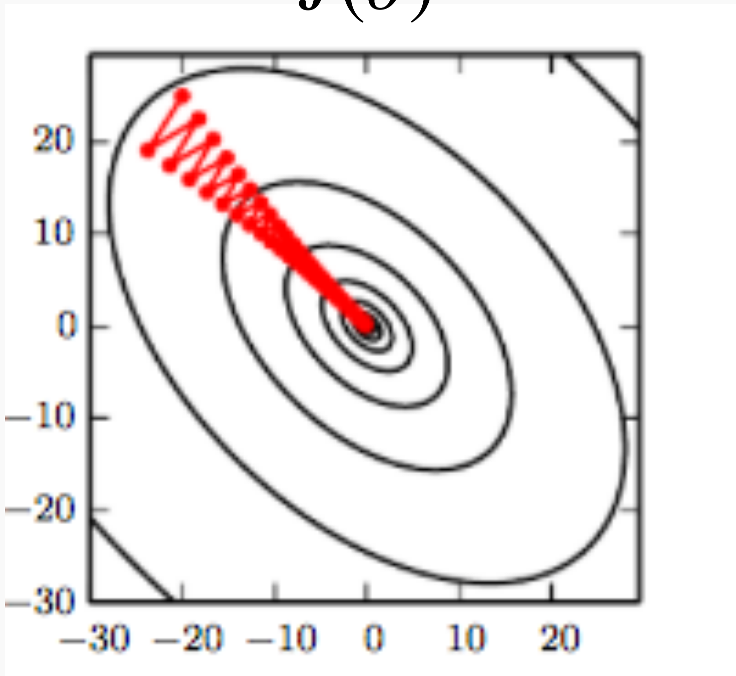
Stochastic Gradient Descent

$J(\theta)$

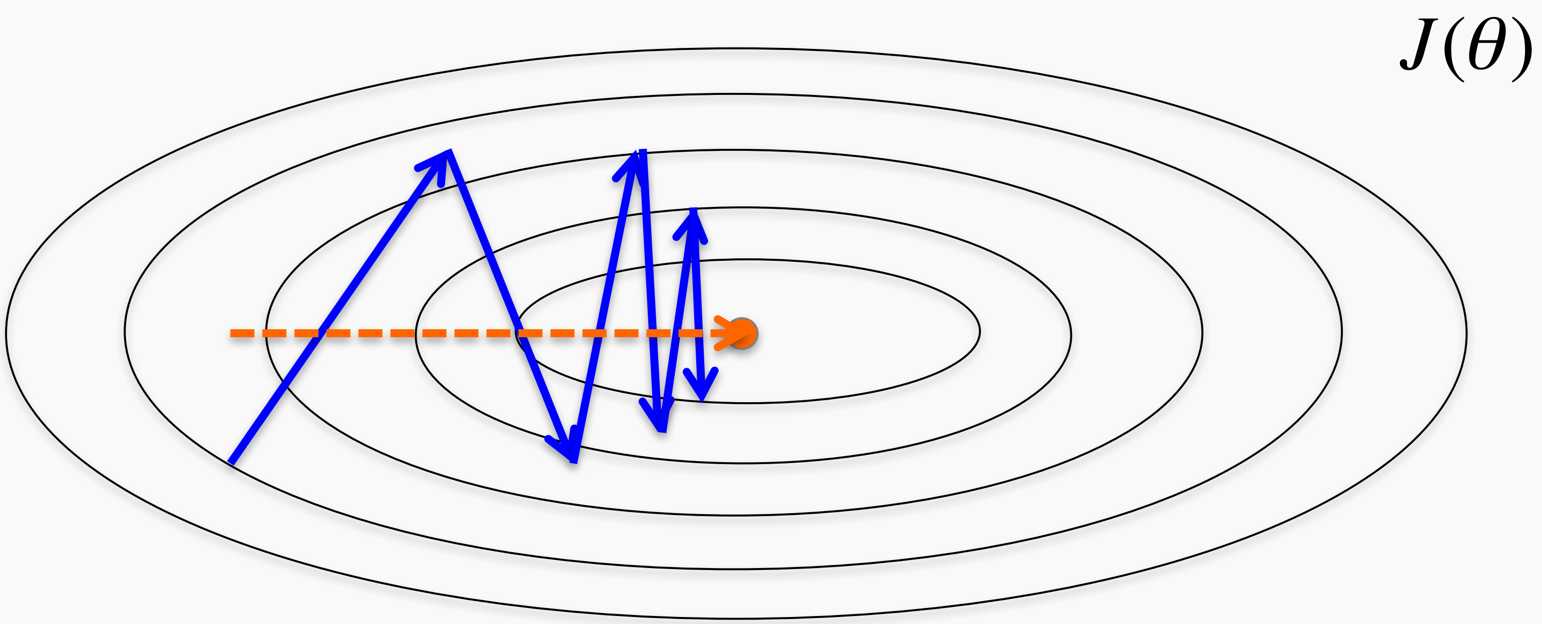


Oscillations because updates do not exploit curvature information

Goodfellow et al. (2016)

Momentum

SGD is slow when there is high curvature



Average gradient presents faster path to opt:

– vertical components cancel out

Momentum

Uses past gradients for update

Maintains a new quantity: ‘velocity’

Exponentially decaying average of gradients:

$$g = \frac{1}{m}\sum_i \nabla_\theta L(f(x^{(i)};\theta), y^{(i)})$$

Current gradient update

$$v = \alpha v + (-\varepsilon g)$$

$\alpha \in [0,1)$ controls how quickly effect of past gradients decay

Momentum

Compute gradient estimate:

$$g = \frac{1}{m}\sum_i \nabla_\theta L(f(x^{(i)};\theta), y^{(i)})$$

Update velocity:

$$v = \alpha v - \varepsilon g$$

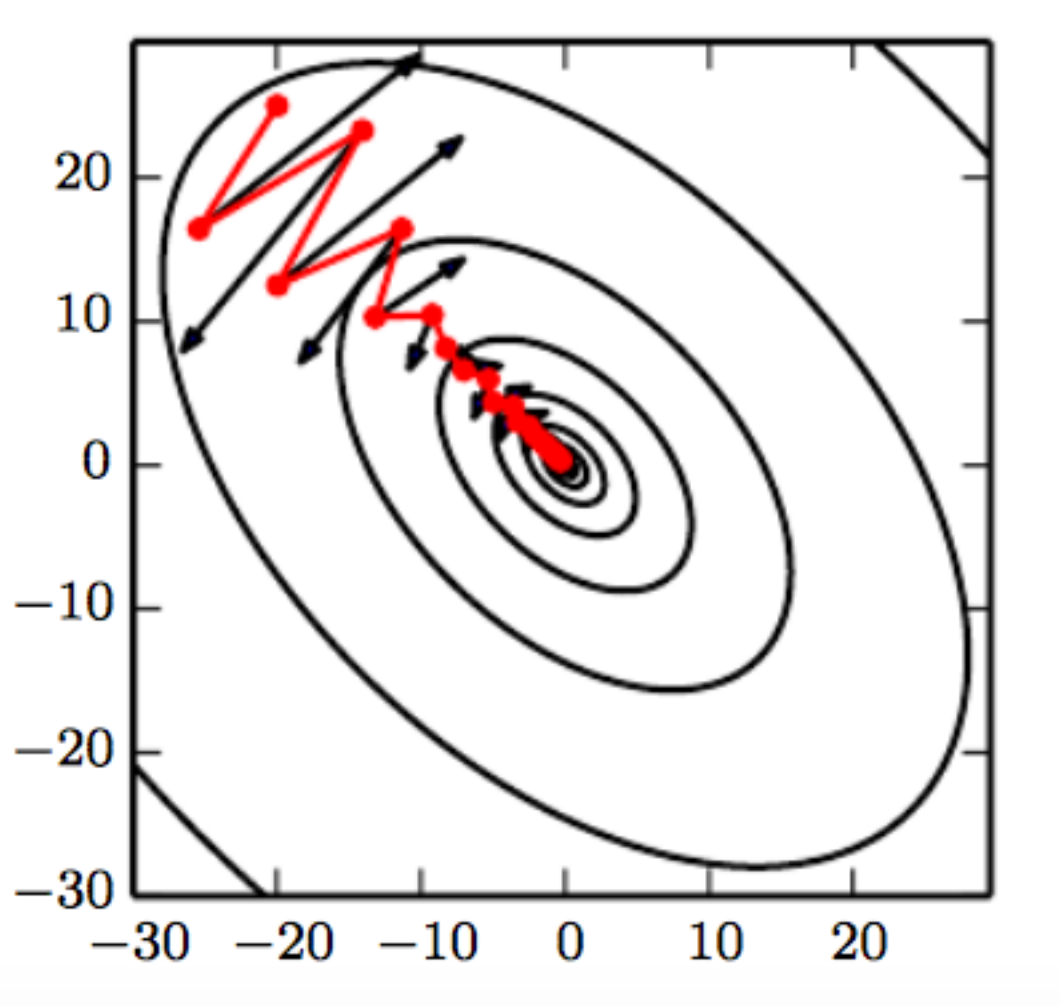
Update parameters:

$$\theta = \theta + v$$

Momentum

$J(\theta)$

Damped oscillations: gradients in opposite directions get cancelled out



Goodfellow et al. (2016)

Nesterov Momentum

Apply an interim update:

$$\tilde{\theta} = \theta + v$$

Perform a correction based on gradient at the interim point:

$$g = \frac{1}{m} \sum_i \nabla_\theta L(f(x^{(i)}; \tilde{\theta}), y^{(i)})$$

$$v = \alpha v - \varepsilon g$$

$$\theta = \theta + v$$

Momentum based on look-ahead slope

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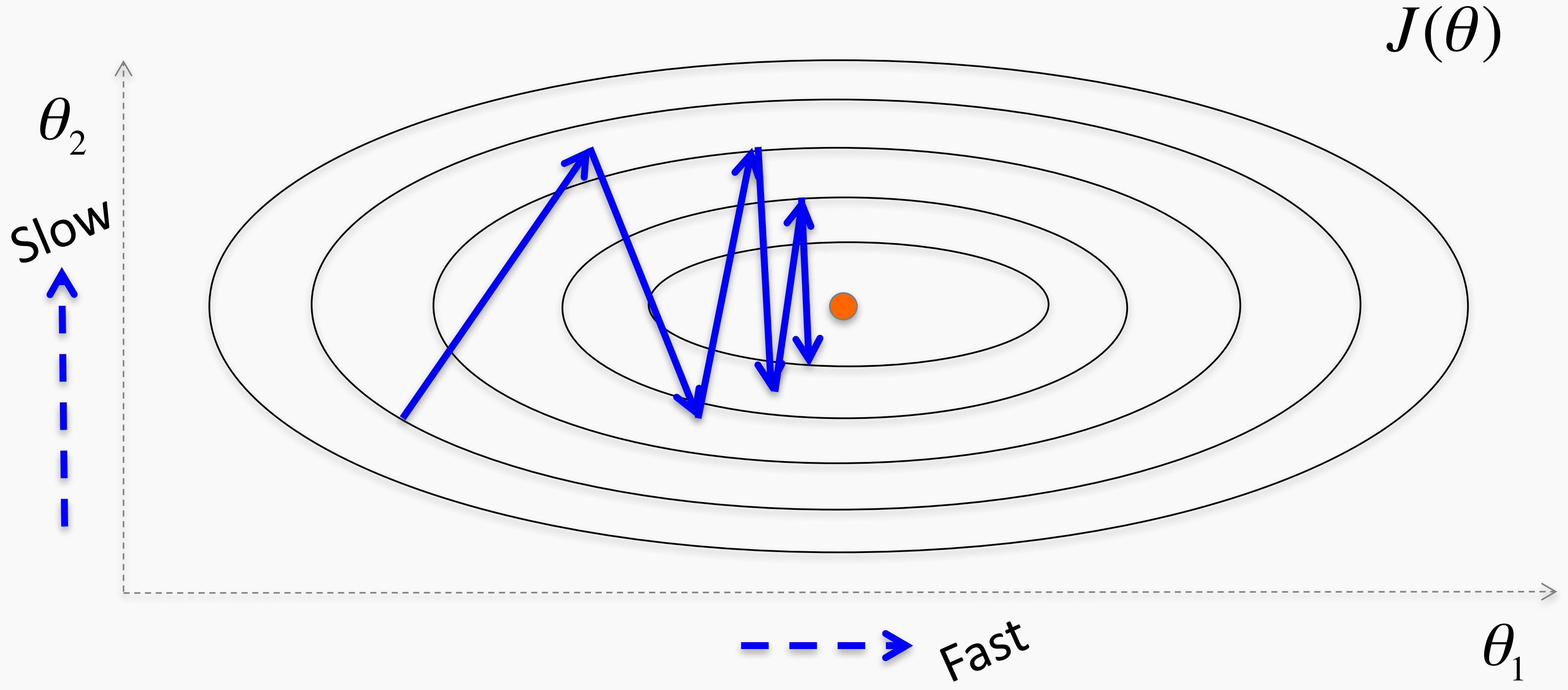
Adaptive Learning Rates



Oscillations along vertical direction

– Learning must be slower along parameter 2

Use a different learning rate for each parameter?

AdaGrad

- Accumulate squared gradients:

$$r_i = r_i + g_i^2$$

- Update each parameter:

$$\theta_i = \theta_i - \frac{\varepsilon}{\delta + \sqrt{r_i}} g_i$$

Inversely proportional to cumulative squared gradient

- Greater progress along gently sloped directions

RMSProp

- For non-convex problems, AdaGrad can prematurely decrease learning rate
- Use exponentially weighted average for gradient accumulation

$$r_i = \rho r_i + (1-\rho) g_i^2$$

$$\theta_i = \theta_i - \frac{\varepsilon}{\delta + \sqrt{r_i}} g_i$$

Adam

- RMSProp + Momentum
- Estimate first moment:

$$v_i = \rho_1 v_i + (1-\rho_1) g_i$$

Also applies bias correction to v and r

- Estimate second moment:

$$r_i = \rho_2 r_i + (1-\rho_2) g_i^2$$

- Update parameters:

$$\theta_i = \theta_i - \frac{\varepsilon}{\delta + \sqrt{r_i}} v_i$$

Works well in practice, is fairly robust to hyper-parameters

Outline

Optimization

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Parameter Initialization

- Goal: break symmetry between units
  - so that each unit computes a different function
- Initialize all weights (not biases) randomly
  - Gaussian or uniform distribution
- Scale of initialization?
  - *Large* -> grad explosion, *Small* -> grad vanishing

Xavier Initialization

- Heuristic for all outputs to have unit variance
- For a fully-connected layer with m inputs:

$$W_{ij} \sim N\left(0,\ \frac{1}{m}\right)$$

- For ReLU units, it is recommended:

$$W_{ij} \sim N\left(0,\ \frac{2}{m}\right)$$

Normalized Initialization

- Fully-connected layer with m inputs, n outputs:

$$W_{ij} \sim U\left(-\sqrt{\frac{6}{m+n}}, \sqrt{\frac{6}{m+n}}\right)$$

- Heuristic trades off between initialize all layers have same activation and gradient variance
- Sparse variant when m is large
  - Initialize k nonzero weights in each unit

Bias Initialization

- Output unit bias
  - Marginal statistics of the output in the training set
- Hidden unit bias
  - Avoid saturation at initialization
  - E.g. in ReLU, initialize bias to 0.1 instead of 0
- Units controlling participation of other units
  - Set bias to allow participation at initialization

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Outline

Challenges in Optimization

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Feature Normalization

Good practice to normalize features before applying learning algorithm:

Feature vector

Vector of mean feature values

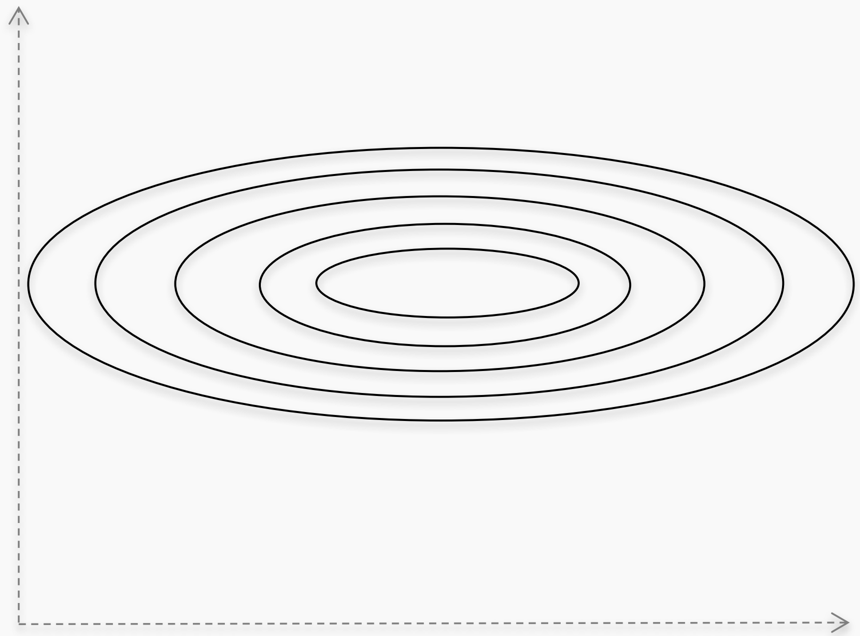
$$x' = \frac{x - \mu}{\sigma}$$

Vector of SD of feature values

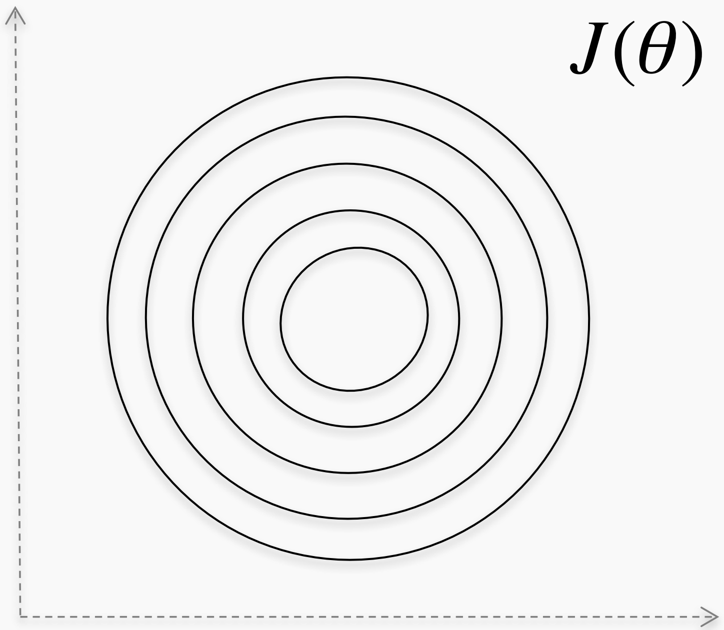
Features in same scale: mean 0 and variance 1

- Speeds up learning

Feature Normalization



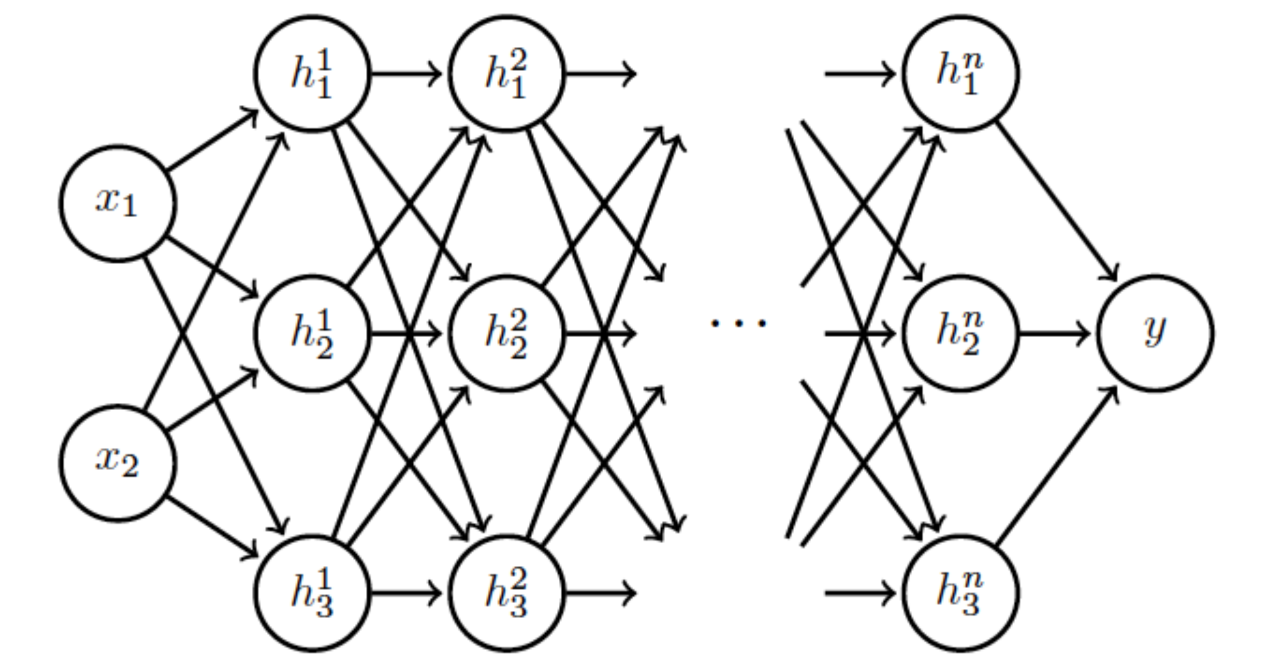
Before normalization



After normalization

Internal Covariance Shift

Each hidden layer changes distribution of inputs to next layer: *slows down learning*



Normalize inputs to layer 2

...

Normalize inputs to layer n

Batch Normalization

Training time:

- Mini-batch of activations for layer to normalize

$$H = \begin{bmatrix} H_{11} & \cdots & H_{1K} \\ \vdots & \ddots & \vdots \\ H_{N1} & \cdots & H_{NK} \end{bmatrix}$$

K hidden layer activations

N data points in mini-batch

Batch Normalization

Training time:

- Mini-batch of activations for layer to normalize

where
$$H' = \frac{H - \mu}{\sigma}$$

$$\mu = \frac{1}{m}\sum_i H_{i,:} \qquad \sigma = \sqrt{\frac{1}{m}\sum_i (H-\mu)_i^2 + \delta}$$

Vector of mean activations across mini-batch

Vector of SD of each unit across mini-batch

Batch Normalization

Training time:

- Normalization can reduce expressive power
- Instead use:

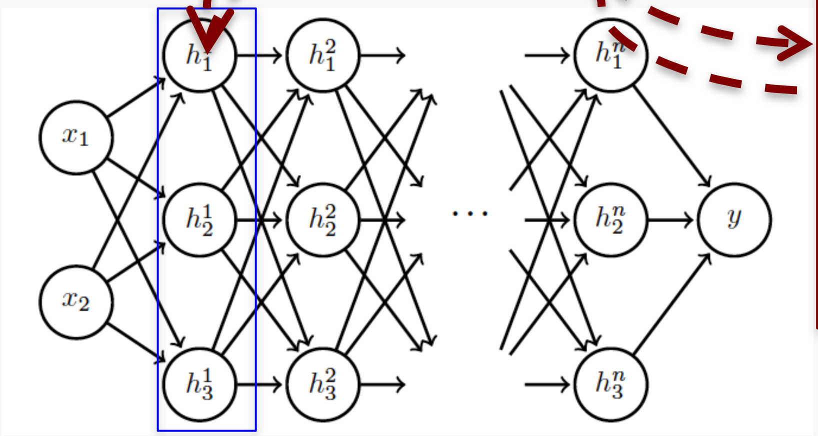
$$\gamma H' + \beta$$

Learnable parameters

- Allows network to control range of normalization

Batch Normalization

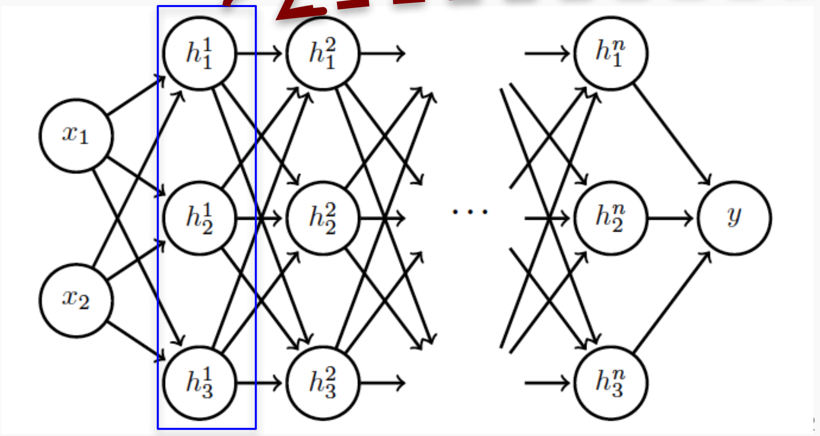
Batch 1



$$\mu^1 = \frac{1}{m}\sum_i H_{i,:}$$

$$\sigma^1 = \sqrt{\frac{1}{m}\sum_i (H-\mu)_i^2 + \delta}$$

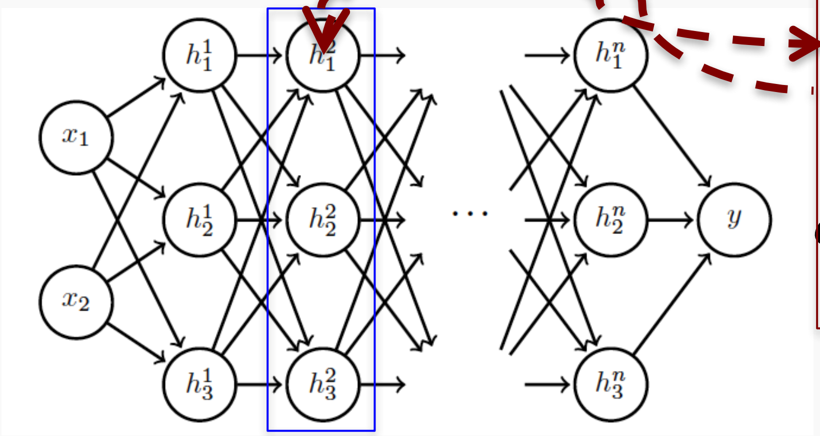
Batch *N*



Add normalization operations for layer 1

Batch Normalization

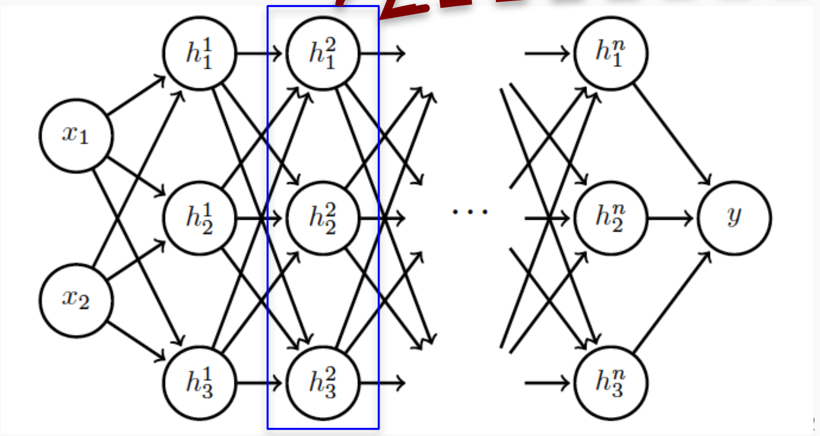
Batch 1



$$\mu^2 = \frac{1}{m}\sum_i H_{i,:}$$

$$\sigma^2 = \sqrt{\frac{1}{m}\sum_i (H-\mu)_i^2 + \delta}$$

Batch *N*



Add normalization operations for layer 2 and so on …

Batch Normalization

Differentiate the joint loss for *N* mini-batches

Back-propagate *through* the norm operations

Test time:

- Model needs to be evaluated on a *single example*
- Replace μ and σ with running averages collected during training