CS M148 –

Data Science Fundamentals

Lecture #15: Neural Networks

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Announcements

HW 2

- Grades are posted
- Regrade requests close 3/6 11pm

HW 4 (last one!)

- Posted, due Monday March 7 at 2pm

Project 3 (last one!)

- Posted, due Monday March 14 at 11:59pm

Thank you!

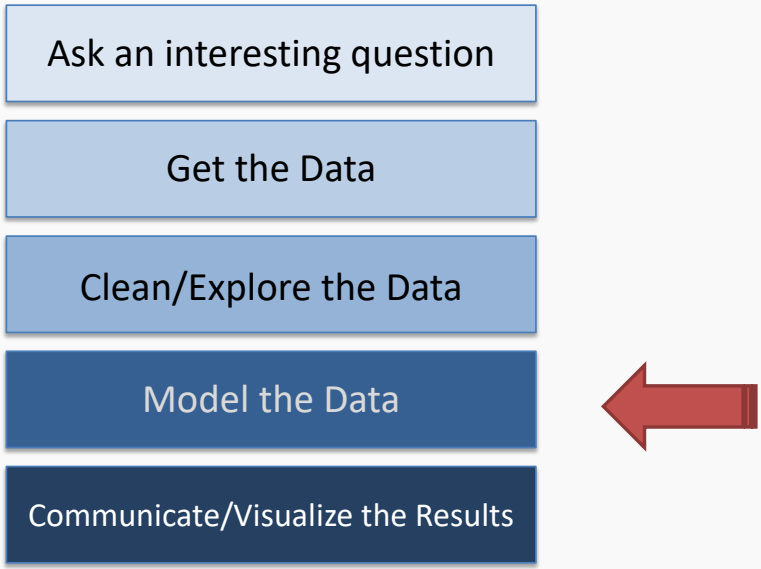
Thank you for your kind answers to the survey

- Especially the last question!

Let’s quickly review what we saw last time

Still here!

The Data Science Process



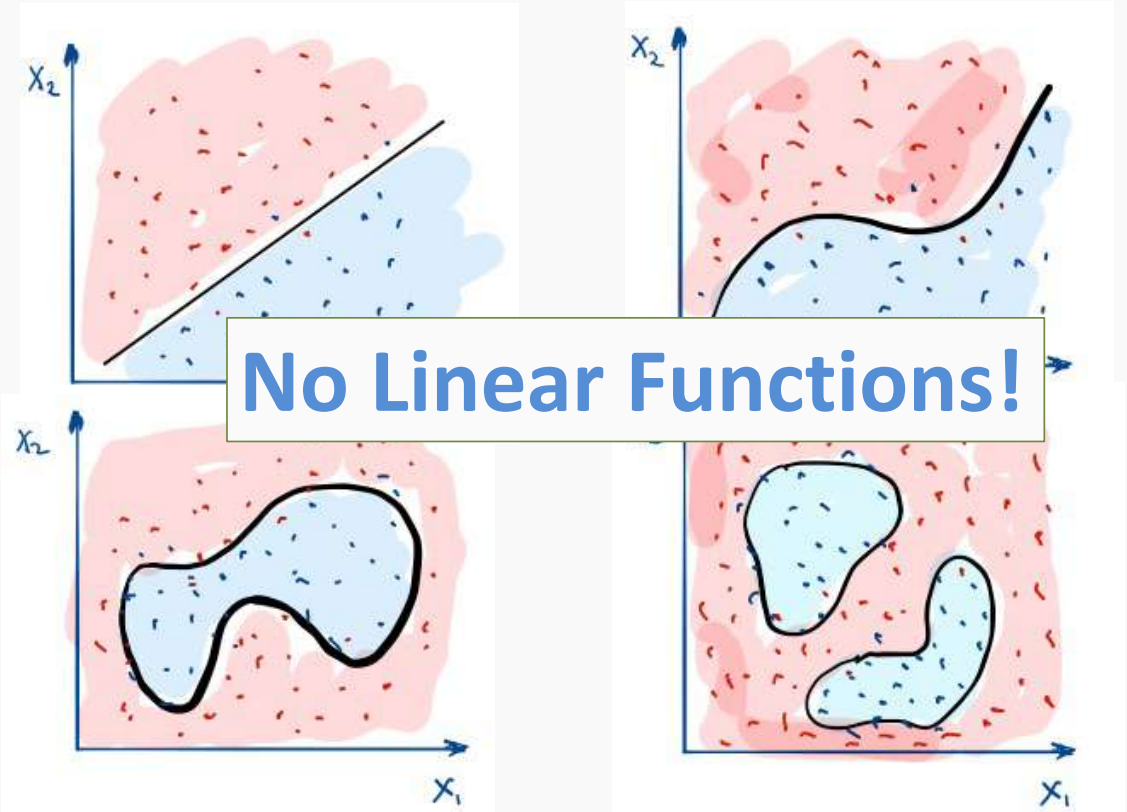
Classification & Regression

Neural Networks

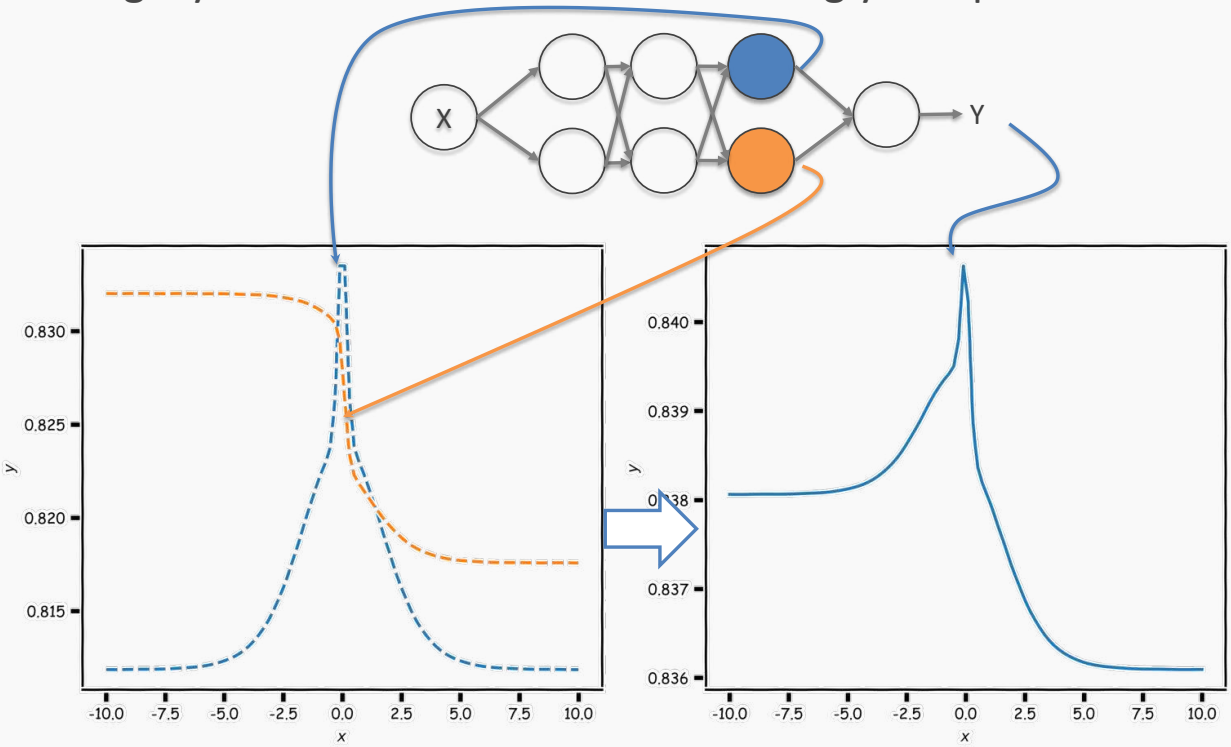
Outline

1. Review of basic concepts
2. Optimization
3. Regularization

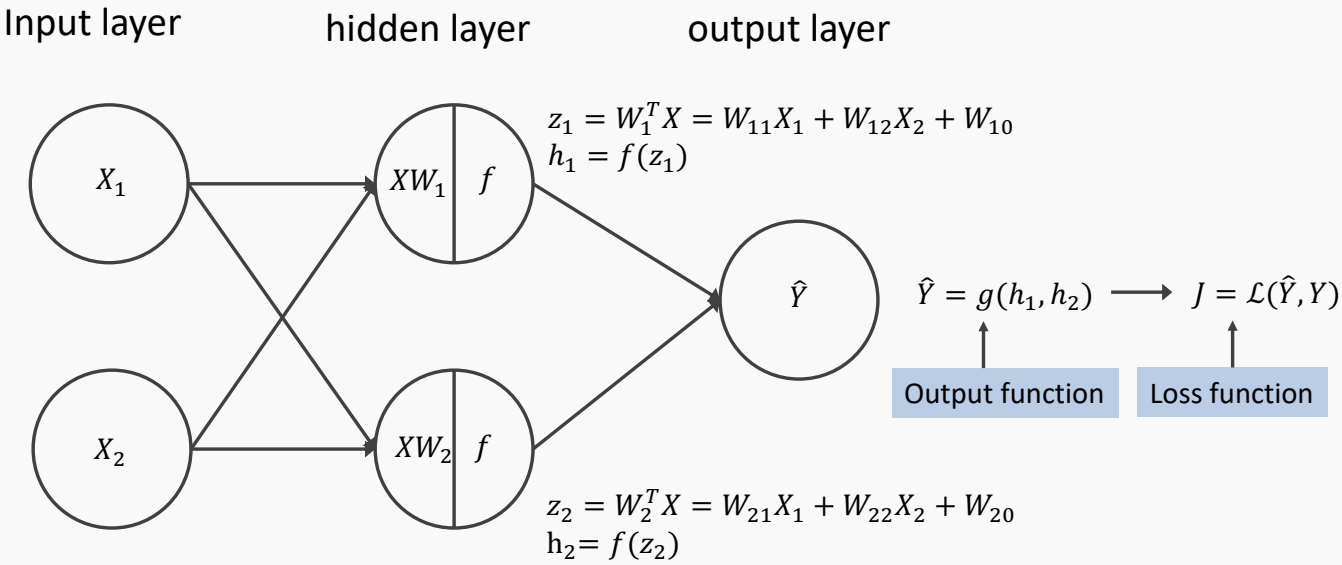
So what's the big deal about Neural Networks?



Adding layers allows us to model increasingly complex functions

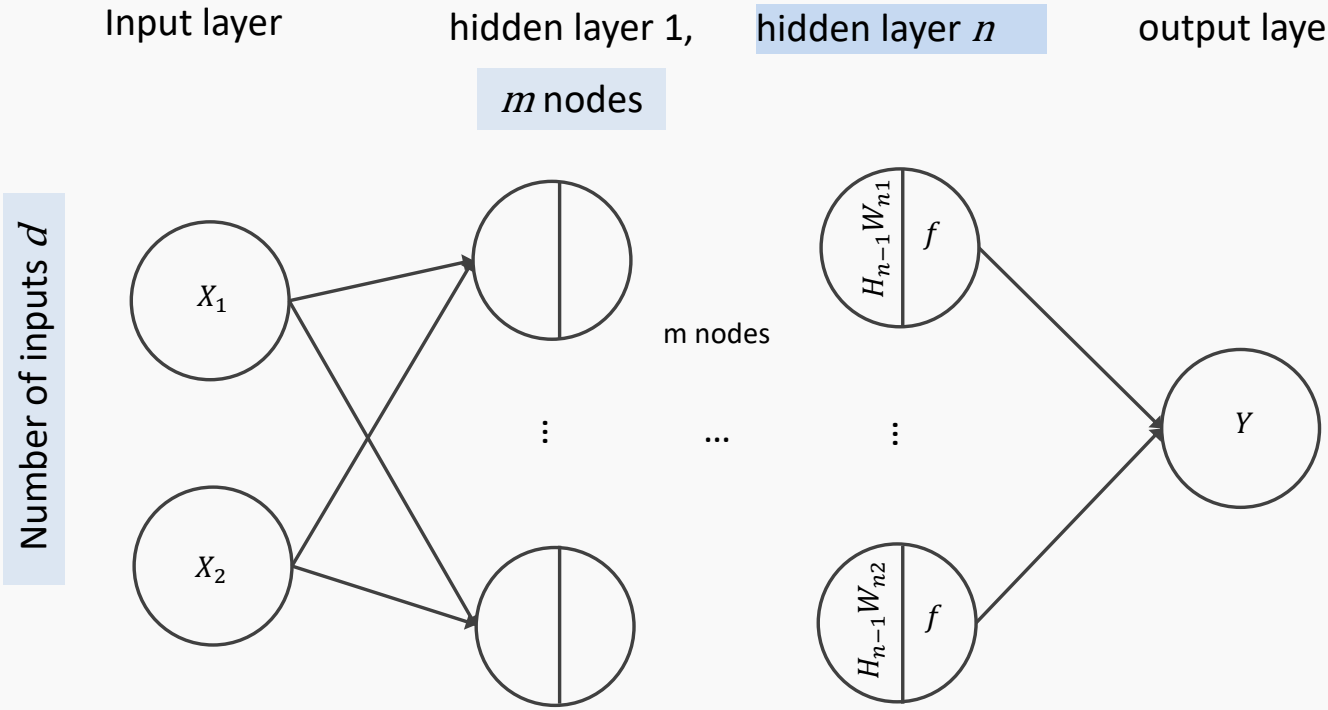


Anatomy of artificial neural network (ANN)



We will talk later about the choice of the output layer and the loss function. So far we consider sigmoid as the output and log-bernoulli.

Anatomy of artificial neural network (ANN)



Number of inputs is specified by the data

Output Units

Output Type	Output Distribution	Output layer	Cost Function
Binary	Bernoulli	Sigmoid	Binary Cross Entropy
Discrete	Multinoulli	Softmax	Cross Entropy
Continuous	Gaussian	Linear	MSE
Continuous	Arbitrary	-	GANS

Probabilistic modeling

Likelihood for a given measurement:

$$p(y_i|W;x_i)$$

Assume **independency**, likelihood for all measurements:

$$L(W;X,Y) = p(Y|W;X) = \prod_i p(y_i|W;x_i)$$

Maximize the likelihood, or equivalently minimizing the –ve log-likelihood:

$$\mathcal{L}(W;X,Y) = -\log L(W;X,Y) = \sum_i \log p(y_i|W;x_i)$$

Loss Function

Do not need to design separate loss functions if we follow the probabilistic modeling approach, i.e. minimize the –ve likelihood function.

Examples:

- Distribution is **Normal** then –ve log-likelihood is **MSE** :

$$p(y_i|W;x_i) = \frac{1}{\sqrt{\{2\pi^2\sigma\}}} e^{-\frac{(y_i-\hat{y}_i)^2}{2\sigma^2}}$$

$$\mathcal{L}(W;X,Y) = \sum_i (y_i - \hat{y}_i)^2$$

- Distribution is **Bernoulli** then –ve log-likelihood is **Binary Cross-Entropy**:

$$p(y_i|W;x_i) = p_i^{y_i}(1-p_i)^{1-y_i}$$

$$\mathcal{L}(W;X,Y) = -\sum_i [y_i \log p_i + (1-y_i)\log(1-p_i)]$$

Loss Function

- For y that follow **Multinoulli,** then likelihood is:

$$p(y_i|W;x_i) = \prod_k p\,(y_i = k)^{\mathbb{I}(y_i=k)}$$

Cross-Entropy

$$\mathcal{L}(W;X,Y) = -\sum_i \sum_k \mathbb{I}(y_i = k)\log p(y_i = k)$$

where k is the class and $\mathbb{I}(y_i = k)$ is the indicator function.

Optimizer: Learning/Training Neural Networks

Learning the coefficients

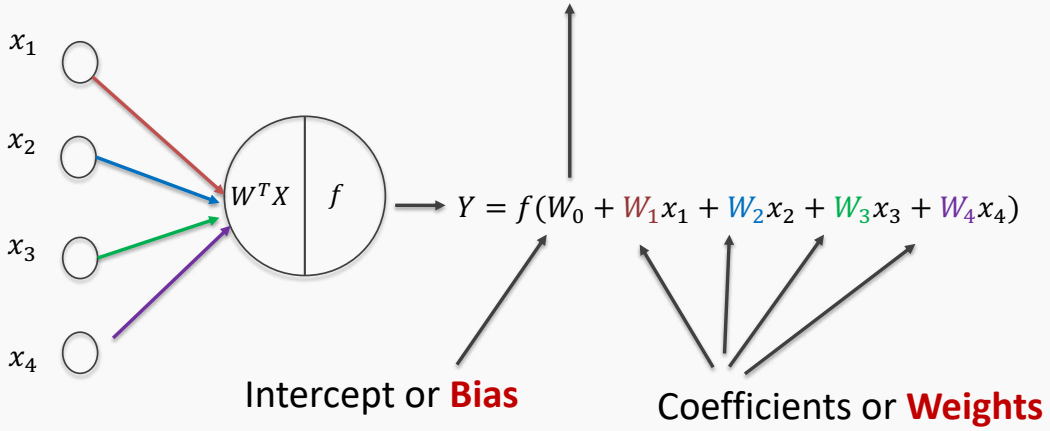
Start with single neuron

Classification

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

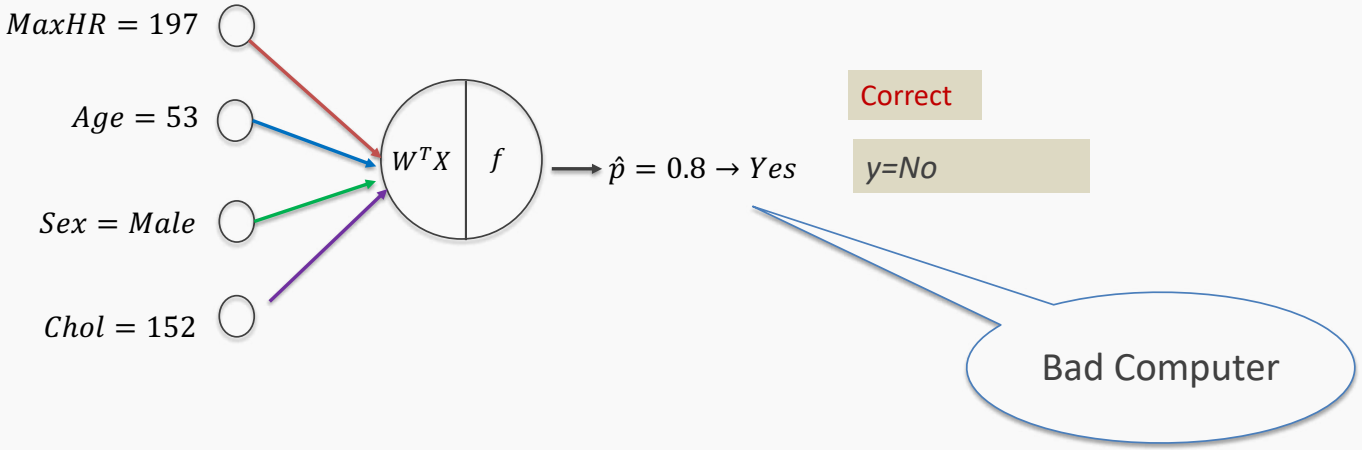
Regression

$f(X) = W^T X$



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.



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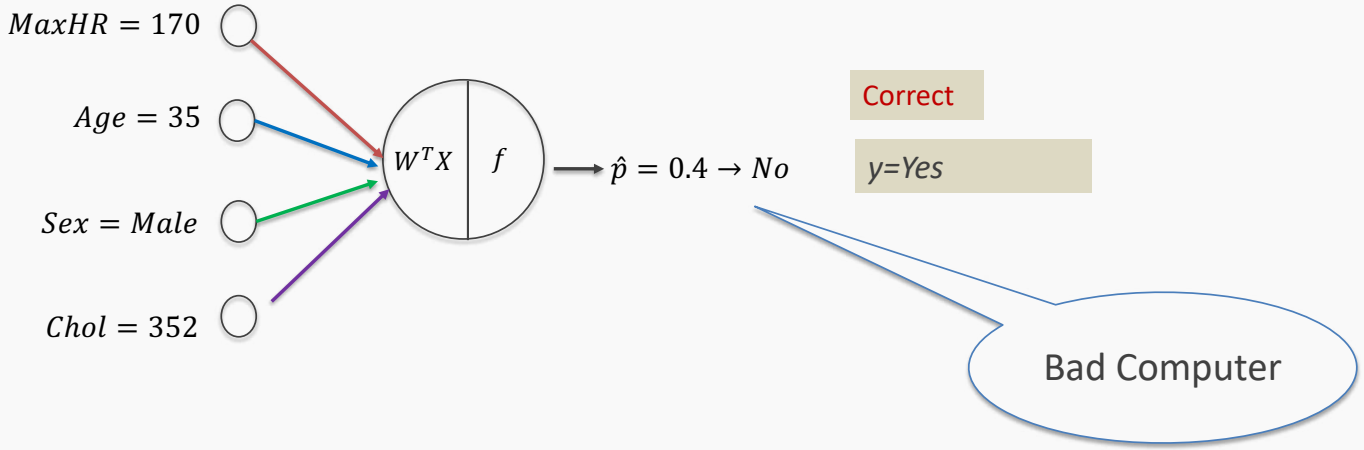


But what is the idea?

- **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: $\mathcal{L}(w_0, w_1, w_2, w_3, w_4)$

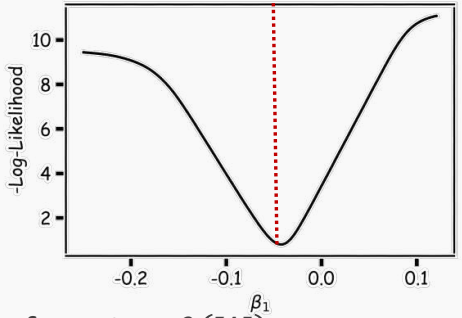
For now let's only consider a single weight, $\mathcal{L}(w_1)$

Outline

- Gradient Descent
- Stochastic Gradient Descent

Minimizing the Loss function

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

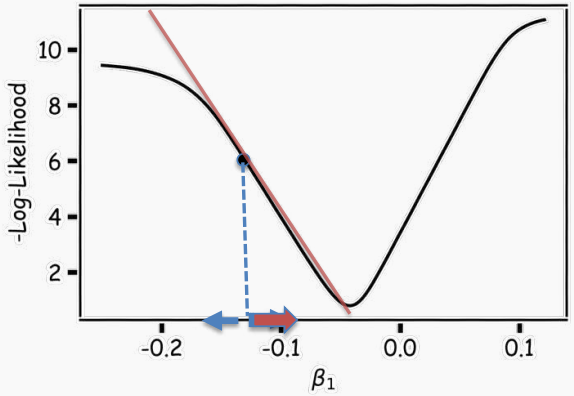


To find the optimal point of a function $\mathcal{L}(W)$

$$\frac{d\mathcal{L}(W)}{dW} = 0 \qquad \text{solve for } W^* = \text{argmin}_W \mathcal{L}(W)$$

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

Minimization of the Loss Function

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

Derivative

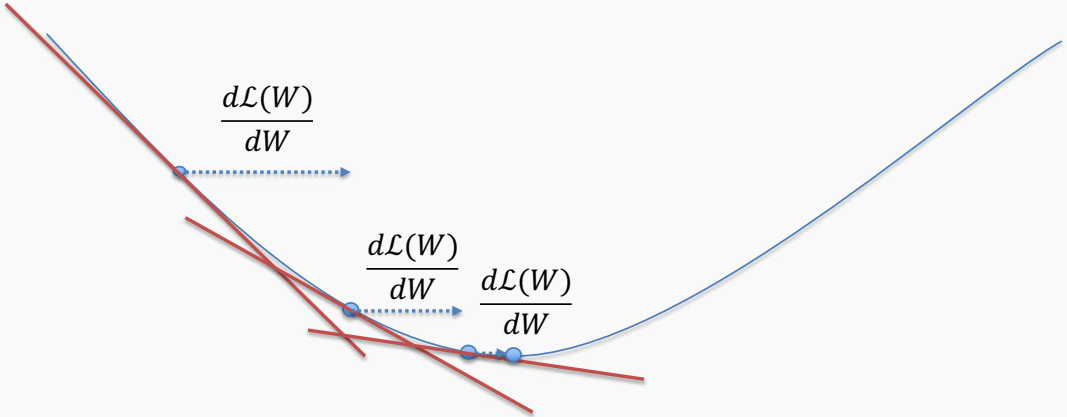
Question: How do we generalize this to more than one predictor?

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

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

Gradient Descent (cont.)

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



Gradient Descent (cont.)

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

Making a step means:

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

Step size is proportional to derivative

Opposite direction of the derivative means:

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

Learning Rate

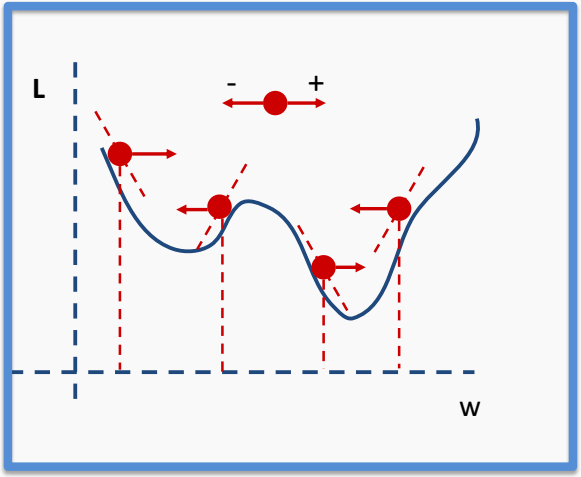
Change to more conventional notation:

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

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 η.

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



Outline

- Gradient Descent
- Stochastic Gradient Descent

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.

Chain Rule

Chain rule for computing gradients:

$$y = g(x) \qquad z = f(y) = f\big(g(x)\big)$$

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

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

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

- For longer chains:

$$\frac{\partial z}{\partial x_i} = \sum_{j_1} \cdots \sum_{j_m} \frac{\partial z}{\partial y_{j_1}} \cdots \frac{\partial y_{j_m}}{\partial x_i}$$

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:

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

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

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

$$-X\sigma(h)\big(1 - \sigma(h)\big)\left[y\frac{1}{p}\right]$$

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

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

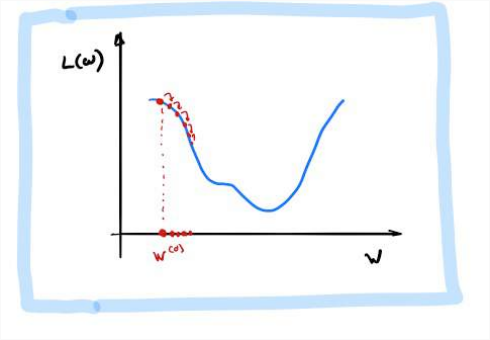
$$-X\sigma(h)\big(1-\sigma(h)\big)[(1-y)\frac{1}{1-p}]$$

Considerations

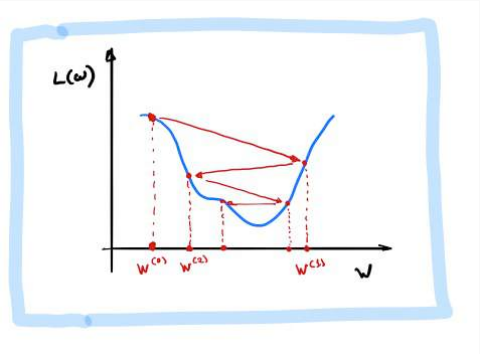
- We still need to calculate the derivatives.
- **We need to know what is the learning rate or how to set it.**
- Local vs global minima.
- The full likelihood function includes summing up all individual '*errors'.* Unless you are a statistician, sometimes this includes hundreds of thousands of examples.

Learning Rate

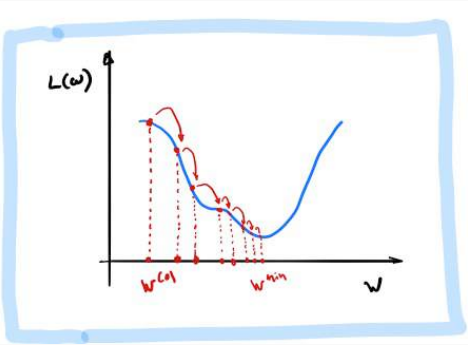
Our choice of the learning rate has a significant impact on the performance of gradient descent.



When η is too small, the algorithm makes very little progress.

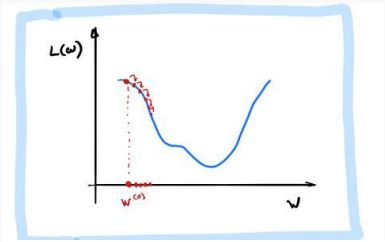


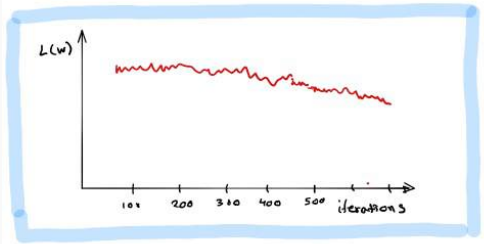
When η is too large, the algorithm may overshoot the minimum and has crazy oscillations.



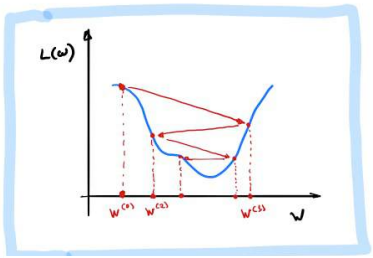
When η is appropriate, the algorithm will find the minimum. The algorithm **converges**!

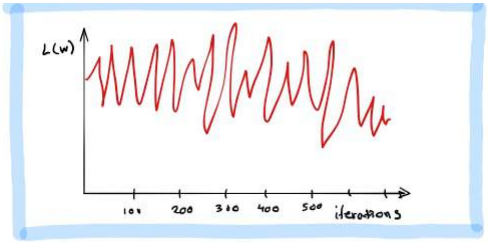
How can we tell when gradient descent is converging? We visualize the loss function at each step of gradient descent. This is called the **trace plot**.



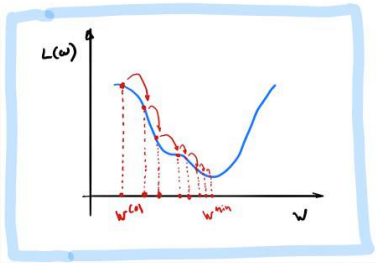


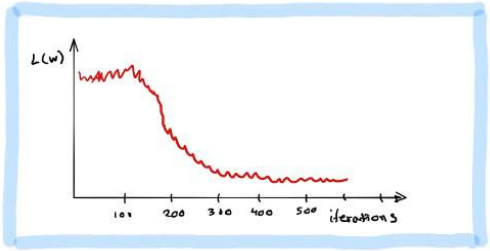
While the loss is decreasing throughout training, it does not look like descent hit the bottom.





Loss is mostly oscillating between values rather than converging.





The loss has decreased significantly during training. Towards the end, the loss stabilizes and it can't decrease further.

Learning Rate

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.

We may talk more about this later.

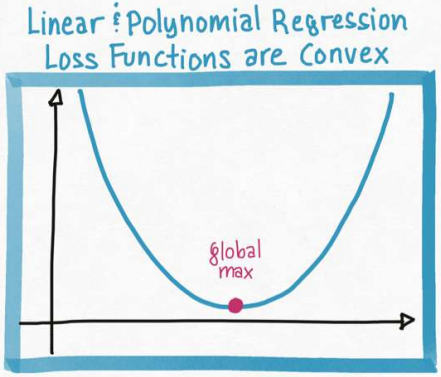
Considerations

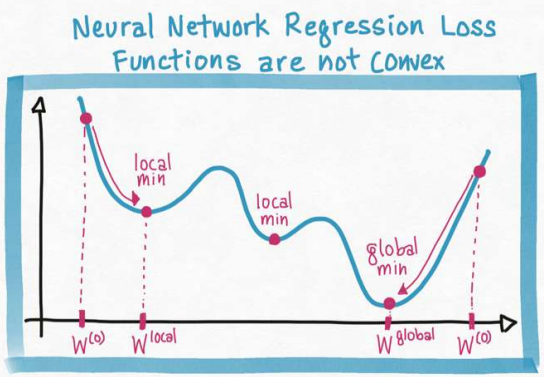
- We still need to calculate the derivatives.
- We need to know what is the learning rate or how to set it.
- **Local vs global minima.**
- The full likelihood function includes summing up all individual '*errors'.* Unless you are a statistician, sometimes this includes hundreds of thousands of examples.

Local vs Global Minima

If we choose η correctly, then gradient descent will converge to a stationary point. But will this point be a **global minimum**?

If the function is convex then the stationary point will be a global minimum.





Local vs Global Minima

No guarantee that we get the global minimum.

Question: What would be a good strategy?

- Random restarts
- Add noise to the loss function

Considerations

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- 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.

DATA

Calculate $L_1 \Rightarrow \frac{\partial L_1}{\partial w} \Rightarrow w^* = w - \eta \frac{\partial L_1}{\partial w}$

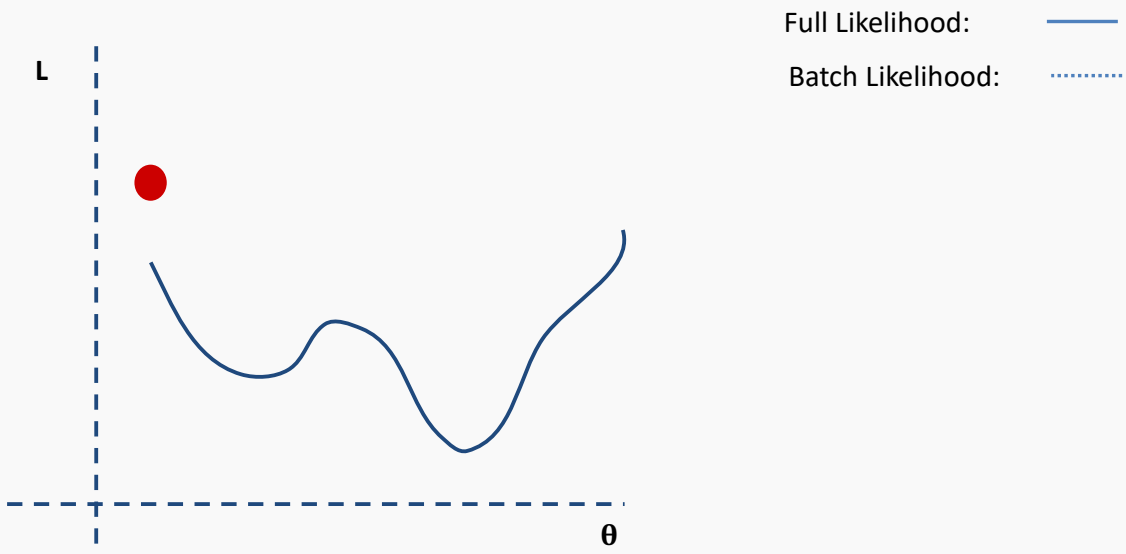
Calculate $L_2 \Rightarrow \frac{\partial L_2}{\partial w} \Rightarrow w^* = w - \eta \frac{\partial L_2}{\partial w}$

$L_B \Rightarrow \frac{\partial L_B}{\partial w} \Rightarrow w^* = w - \eta \frac{\partial L_B}{\partial w}$

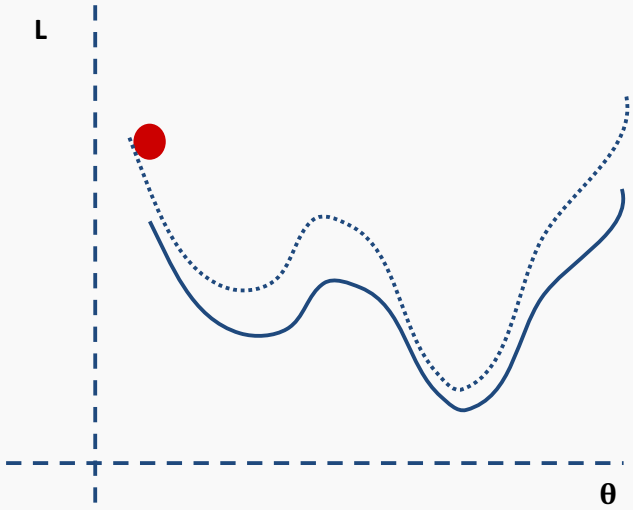
COMPLETE DATA $\Rightarrow$ ONE EPOCH

RESHUFFLE DATA AND REPEAT

Batch and Stochastic Gradient Descent



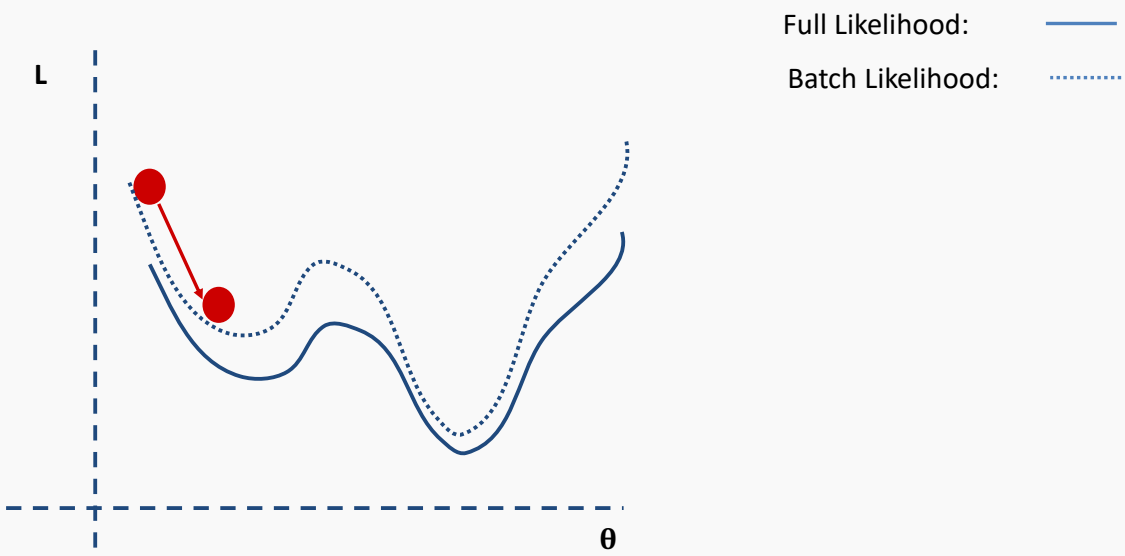
Batch and Stochastic Gradient Descent



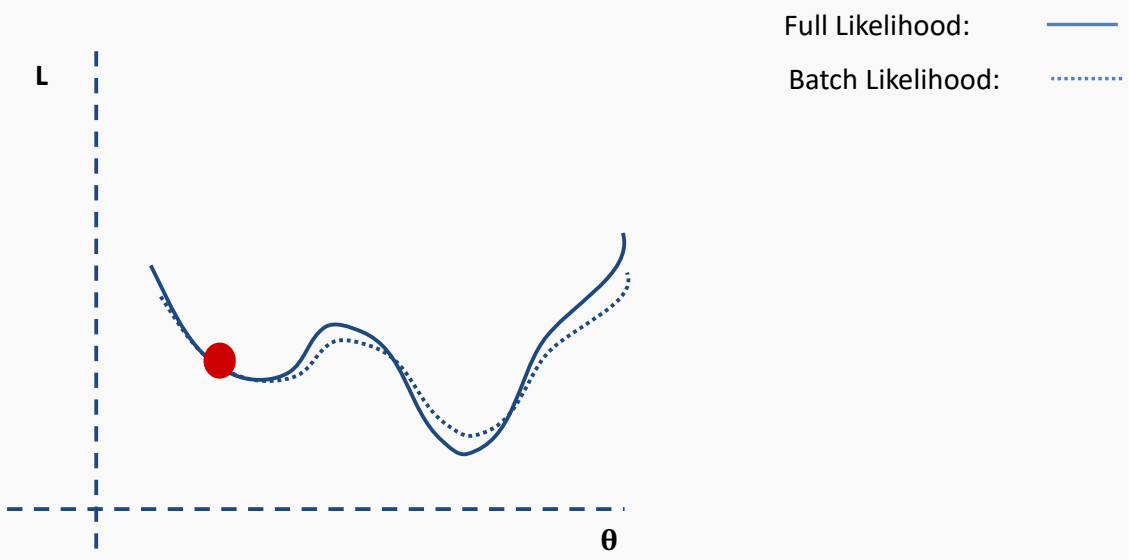
Full Likelihood:

Batch Likelihood:

Batch and Stochastic Gradient Descent



Batch and Stochastic Gradient Descent



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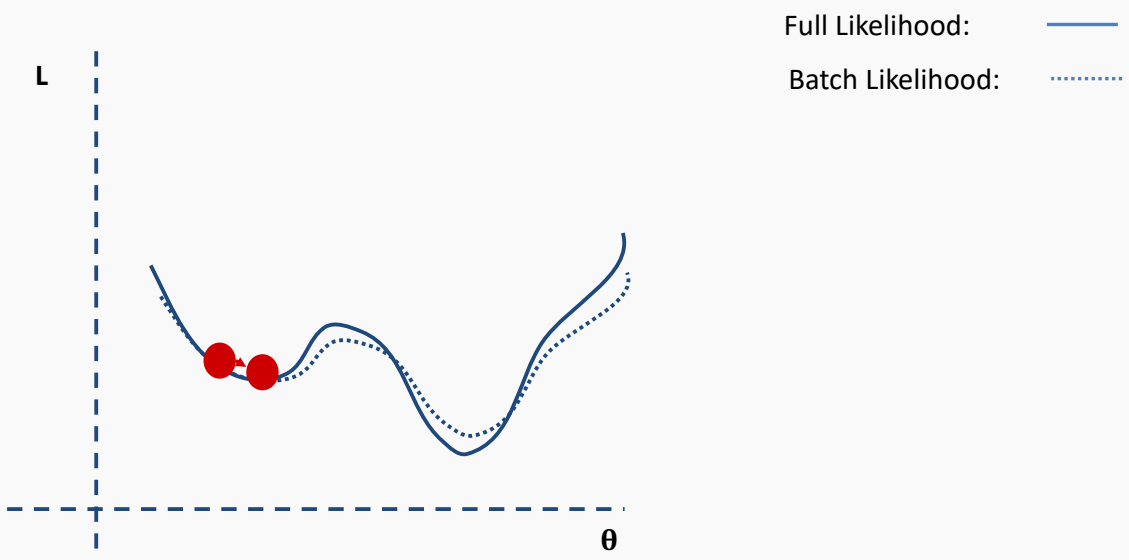
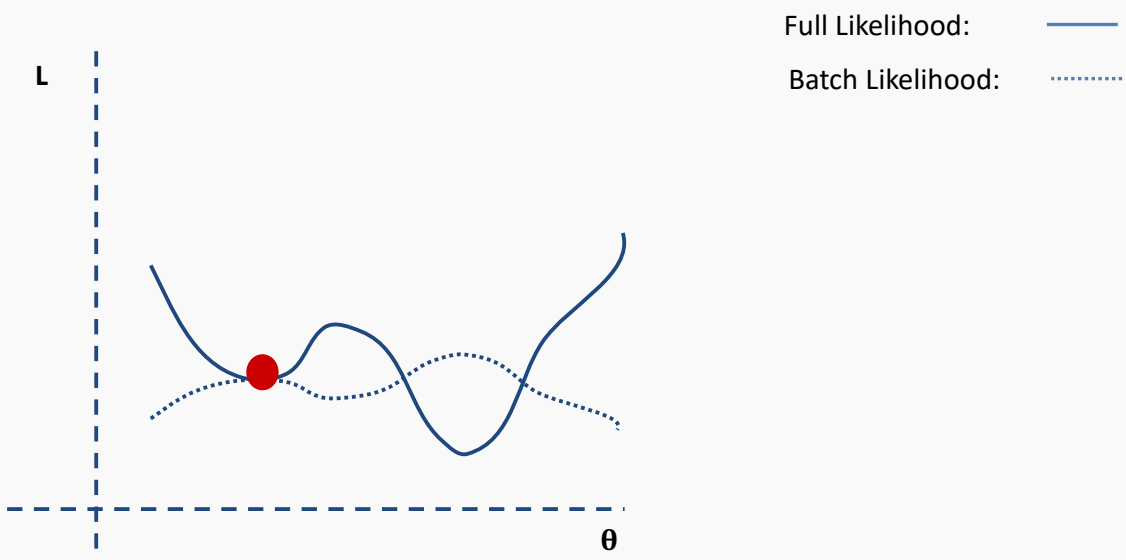
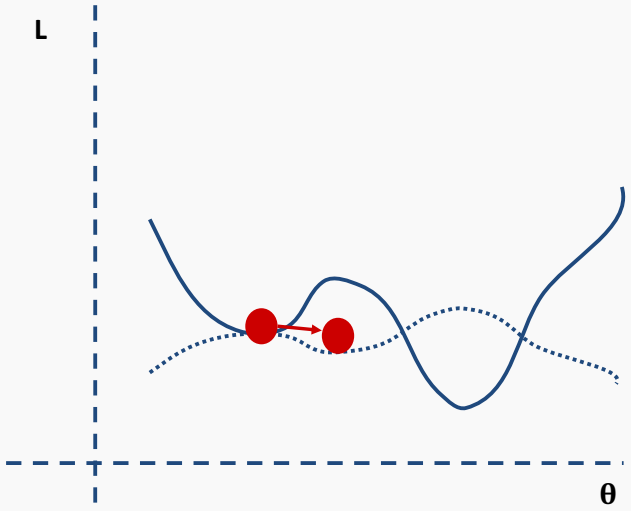


Batch and Stochastic Gradient Descent



Batch and Stochastic Gradient Descent



Full Likelihood:

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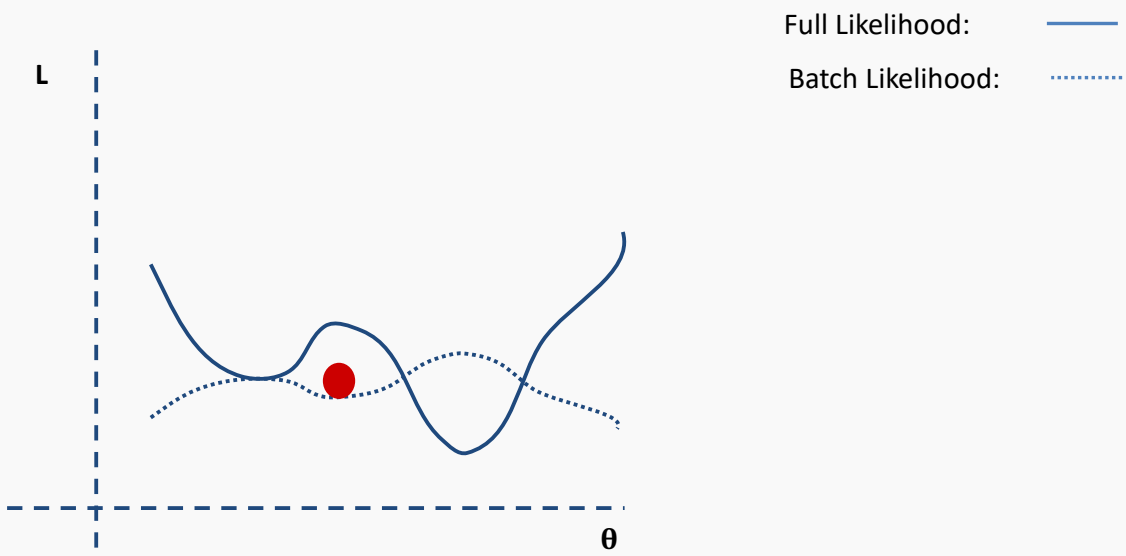
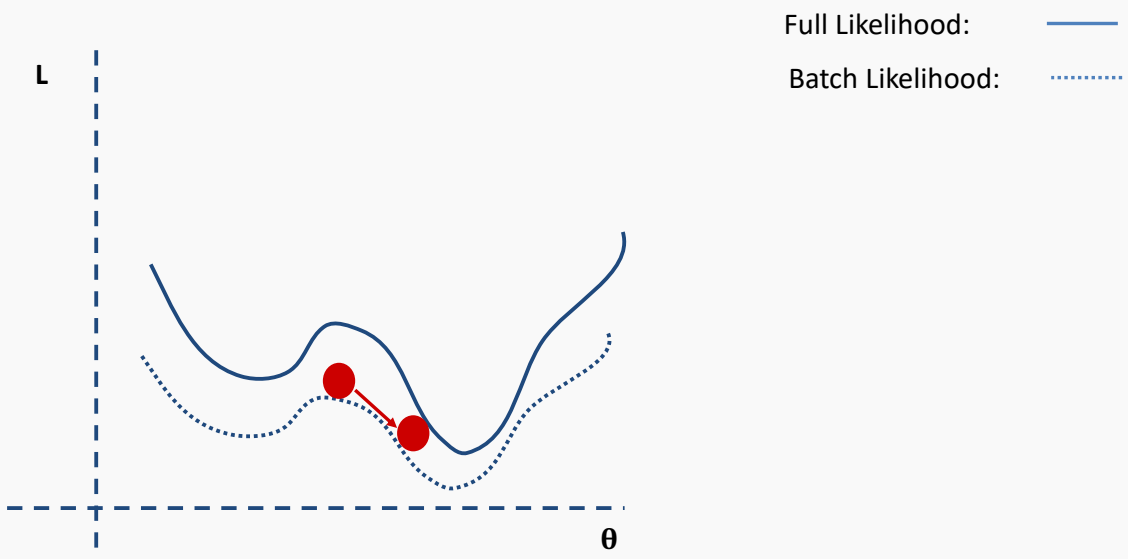
Batch and Stochastic Gradient Descent

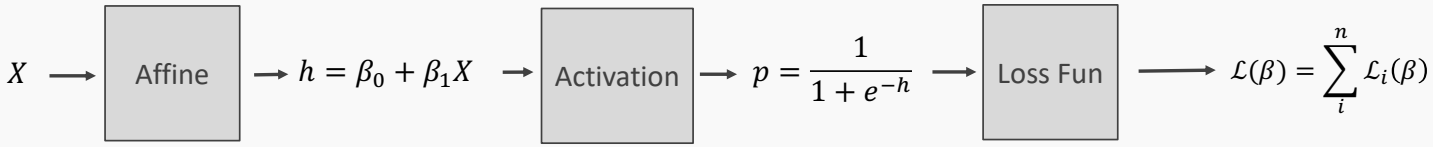


Batch and Stochastic Gradient Descent



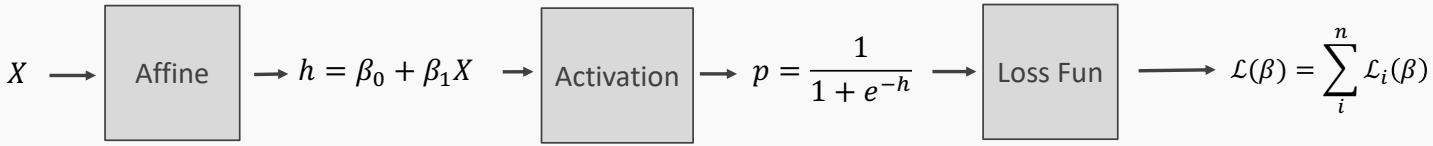
Backpropagation

Backpropagation: Logistic Regression Revisited



Backpropagation: Logistic Regression Revisited

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



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

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

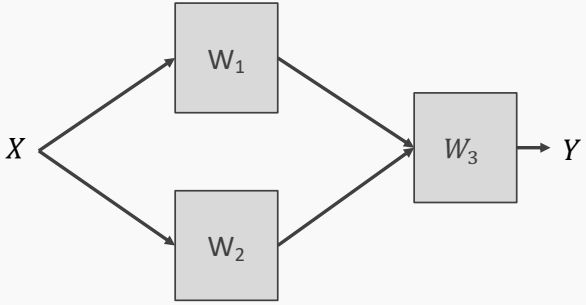
$$\frac{\partial \mathcal{L}}{\partial \beta_1} = -X\sigma(h)\big(1 - \sigma(h)\big)[y\frac{1}{p} + (1 - y)\frac{1}{1 - p}]$$

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

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



Backpropagation

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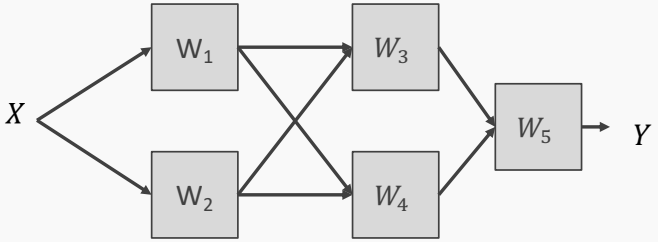


Backpropagation

Need to find a formalism to calculate the derivatives of the loss w.r.t. weights that is:

1. Flexible enough that adding a node or a layer or changing something in the network will not require re-deriving 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	$-3e^{-9}$
$\xi_4 = \frac{1}{\xi_3} = \frac{1}{1 + e^{-W^T X}} = p$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\xi_3^2}$	$\frac{1}{1 + e^{-9}}$	$\left(\frac{1}{1 + e^{-9}}\right)^2$	$-3e^{-9}\left(\frac{1}{1+e^{-9}}\right)^2$
$\xi_5 = \log \xi_4 = \log p = \log \frac{1}{1 + e^{-W^T}}$	$\frac{\partial \xi_5}{\partial \xi_4} = \frac{1}{\xi_4}$	$\log \frac{1}{1 + e^{-9}}$	$1 + e^{-9}$	$-3e^{-9}\left(\frac{1}{1+e^{-9}}\right)$
$\mathcal{L}_i^A = -y\xi_5$	$\frac{\partial \mathcal{L}}{\partial \xi_5} = -y$	$-\log \frac{1}{1 + e^{-9}}$	-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	$-3e^{-9}$
$\xi_4 = \frac{1}{\xi_3} = \frac{1}{1 + e^{-W^T X}} = p$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\xi_3^2}$	$\frac{1}{1 + e^{-9}}$	$\left(\frac{1}{1 + e^{-9}}\right)^2$	$-3e^{-9}\left(\frac{1}{1+e^{-9}}\right)^2$
$\xi_5 = \log \xi_4 = \log p \ = \log \frac{1}{1 + e^{-W^T X}}$	$\frac{\partial \xi_5}{\partial \xi_4} = \frac{1}{\xi_4}$	$\log \frac{1}{1 + e^{-9}}$	$1 + e^{-9}$	$-3e^{-9}\left(\frac{1}{1+e^{-9}}\right)$
$\mathcal{L}_i^A = -y\xi_5$	$\frac{\partial \mathcal{L}}{\partial \xi_5} = -y$	$-\log \frac{1}{1 + e^{-9}}$	-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

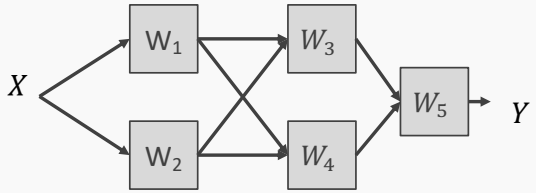
Basic functions

Notice though those are basic functions that everybody 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

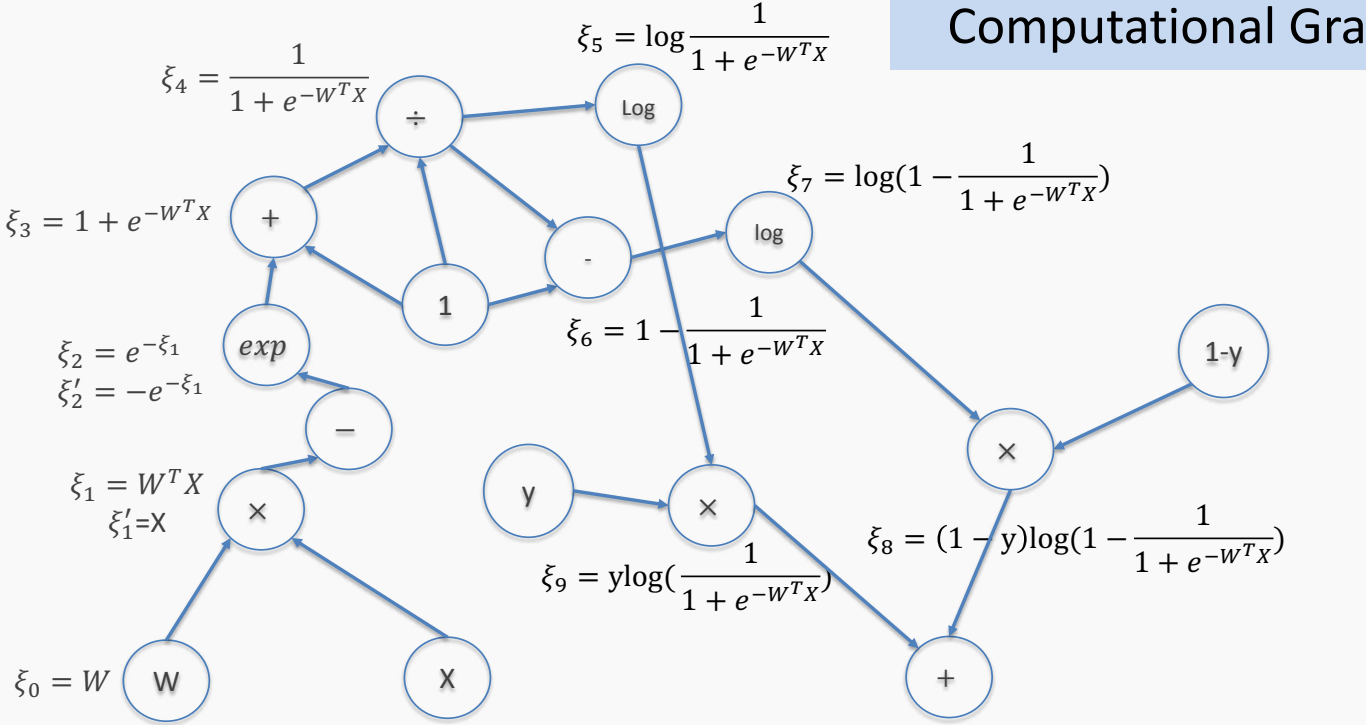
1. We specify the network structure



2. Following the computational graph …

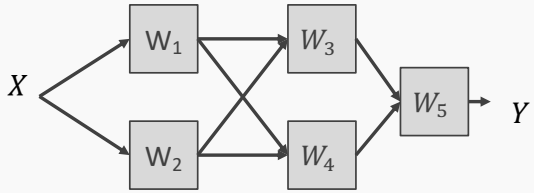
What is computational graph?

Computational Graph



Putting it altogether

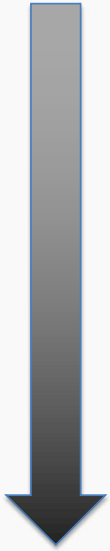
1. We specify the network structure



- Envision the computational graph (only needed for the reverse mode).
- 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.

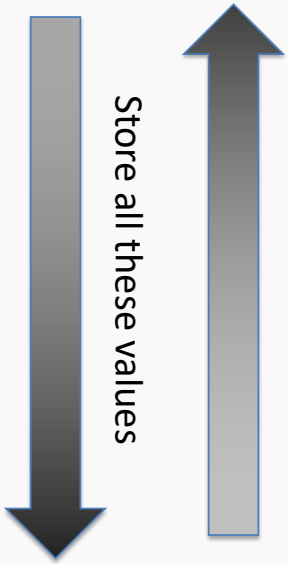
Forward mode: Evaluate the derivative at: $X=\{3\}, y=1, W=3$

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	$-3e^{-9}$
$\xi_4 = \frac{1}{\xi_3} = \frac{1}{1+e^{-W^T X}} = p$	$\frac{\partial \xi_4}{\partial \xi_3} = -\frac{1}{\xi_3^2}$	$\frac{1}{1+e^{-9}}$	$\left(\frac{1}{1+e^{-9}}\right)^2$	$-3e^{-9}\left(\frac{1}{1+e^{-9}}\right)^2$
$\xi_5 = \log \xi_4 = \log p = \log \frac{1}{1+e^{-W^T X}}$	$\frac{\partial \xi_5}{\partial \xi_4} = \frac{1}{\xi_4}$	$\log \frac{1}{1+e^{-9}}$	$1+e^{-9}$	$-3e^{-9}\left(\frac{1}{1+e^{-9}}\right)$
$\mathcal{L}_i^A = -y\xi_5$	$\frac{\partial \mathcal{L}}{\partial \xi_5} = -y$	$-\log \frac{1}{1+e^{-9}}$	-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



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.



Check this: https://autoed.herokuapp.com

Outline

Regularization of NN

- Norm Penalties
- Early Stopping
- Data Augmentation
- Dropout

Regularization

Regularization is any modification we make to a learning algorithm that is intended to **reduce its generalization error** but not its training error.

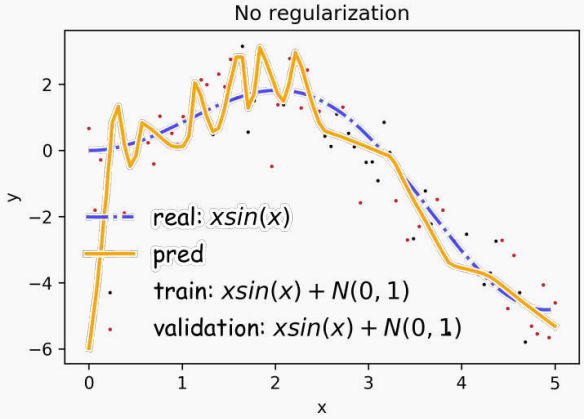
Outline

Regularization of NN

- **Norm Penalties**
- Early Stopping
- Data Augmentation
- Dropout

Overfitting

Fitting a deep neural network with 5 layers and 100 neurons per layer can lead to a very good prediction on the training set but poor prediction on validations set.



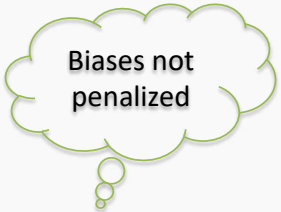
Norm Penalties

We used to optimize:

$$L(W; X, y)$$

Change to …

$$L_R(W; X, y) = L(W; X, y) + \alpha\Omega(W)$$



L_2 regularization:

- Weights decay
- MAP estimation with Gaussian prior

$$\Omega(W) = \frac{1}{2} \| W \|_2^2$$

L_1 regularization:

- encourages sparsity
- MAP estimation with Laplacian prior

$$\Omega(W) = \frac{1}{2} \| W \|_1$$

Norm Penalties

We used to optimize:

$$W^{(i+1)} = W^{(i)} - \lambda \frac{\partial L}{\partial W}$$

Change to:

$$L_R(W; X, y) = L(W; X, y) + \frac{1}{2}\alpha \parallel W \parallel_2^2$$

$$W^{(i+1)} = W^{(i)} - \lambda \frac{\partial L}{\partial W} - \lambda\alpha\, W^{(i)}$$

Weights decay in proportion to size

Biases not penalized

L_2 regularization:

- **Decay of weights**
- MAP estimation with Gaussian prior

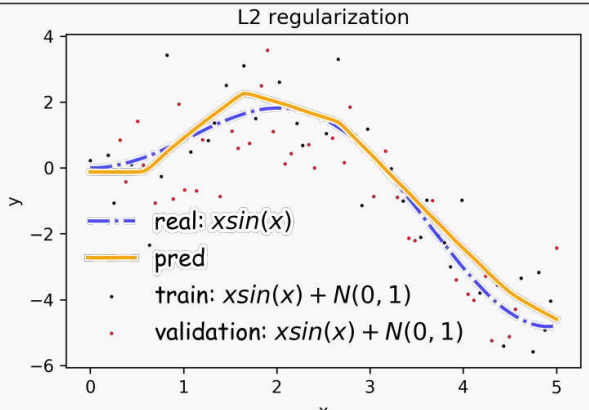
$$\Omega(W) = \frac{1}{2} \parallel W \parallel_2^2$$

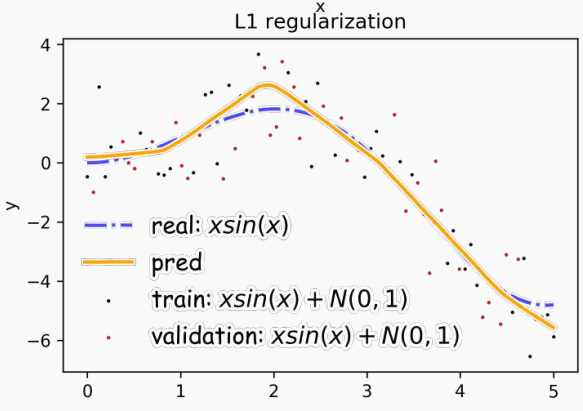
L_1 regularization:

- encourages sparsity
- MAP estimation with Laplacian prior

$$\Omega(W) = \frac{1}{2} \parallel W \parallel_1$$

Norm Penalties





$$\Omega(W) = \frac{1}{2} \| W \|_2^2$$

$$\Omega(W) = \frac{1}{2} \| W \|_1$$

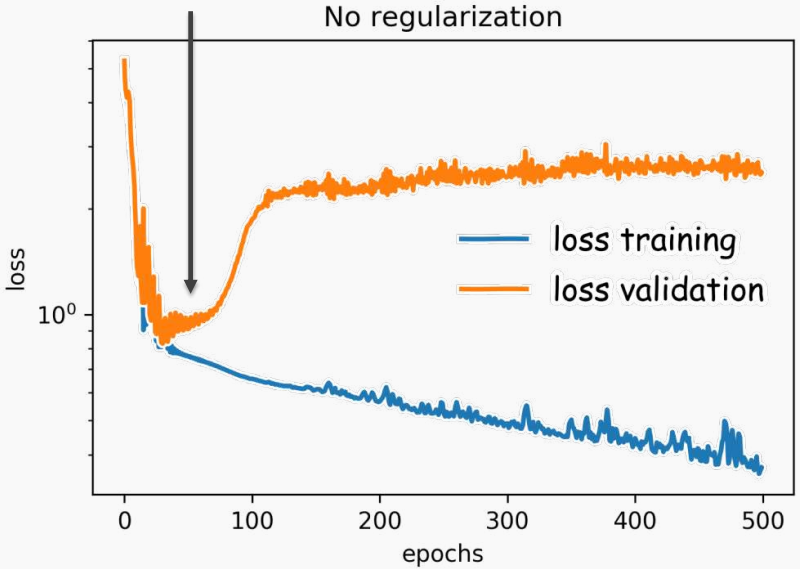
Outline

Regularization of NN

- Norm Penalties
- **Early Stopping**
- Data Augmentation
- Dropout

Early Stopping

Early stopping: terminate while validation set performance is better. Sometimes is worth waiting a little before stopping. This is called `patience`.



Patience is defined as the number of epochs to wait before early stop if no progress on the validation set.

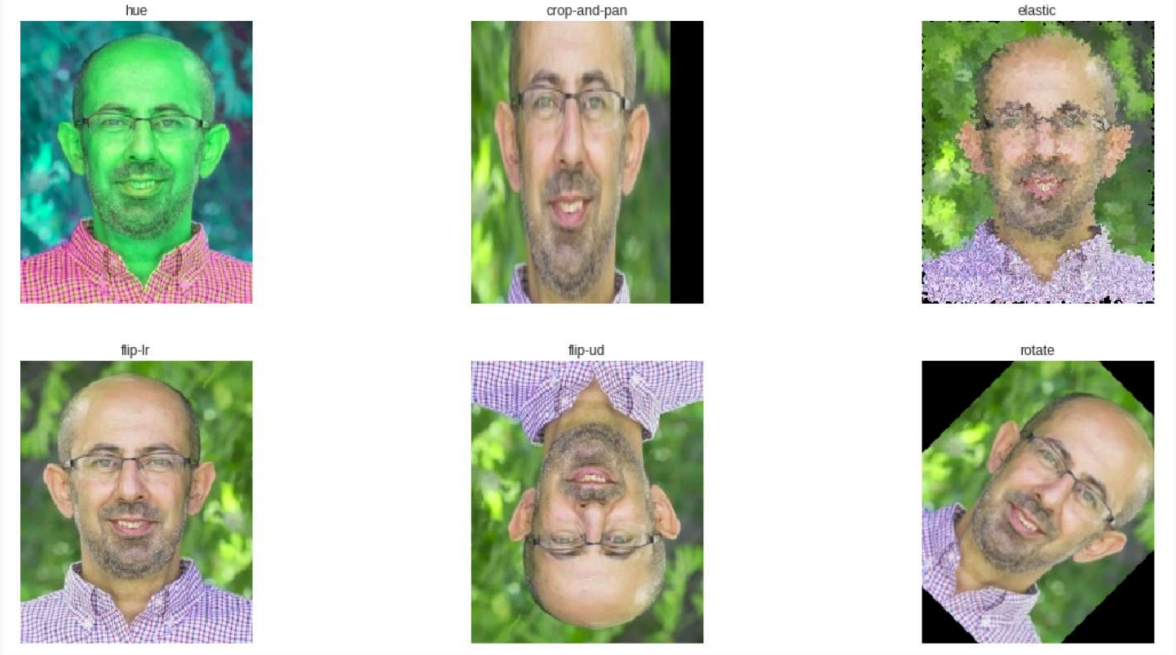
The patience is often set somewhere between 10 and 100 (10 or 20 is more common), but it really depends on the dataset and network.

Outline

Regularization of NN

- Norm Penalties
- Early Stopping
- **Data Augmentation**
- Dropout

Data Augmentation



Data Augmentation: dos and don'ts

We use ImageDataGenerator to augment the dataset

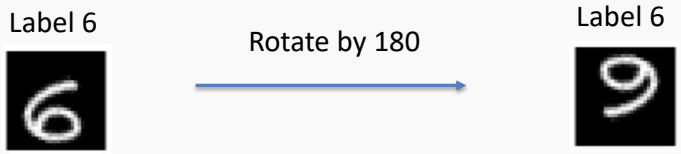
```
def get_generator():
    # create duplicate images
    BATCHES_PER_EPOCH = 300//BATCH_SIZE
    classes = ['pavlos', 'not-pavlos']
    for img_class in classes:
        img = Image.open((f'{DATA_DIR}/{img_class}.jpeg'))
        for i in range(1, BATCH_SIZE*BATCHES_PER_EPOCH//2+1):
            img.thumbnail(TARGET_SIZE, Image.ANTIALIAS)
            img.save(f'{DATA_DIR}/{img_class}/{img_class}{i:0>3}.jpeg', "JPEG")

    data_gen = ImageDataGenerator(
            rescale=1./255,
            height_shift_range=0.5,
            width_shift_range=0.5)

    img_generator = data_gen.flow_from_directory(
            DATA_DIR,
            target_size=(TARGET_SIZE),
            batch_size=BATCH_SIZE,
            classes=classes,
            class_mode='binary')
    return img_generator
```

Data Augmentation: dos and don'ts

Carefully choose your transformations. Not all transformations are valid.



Data Augmentation does not work for tabular data and not as nicely for time series.

Outline

Regularization of NN

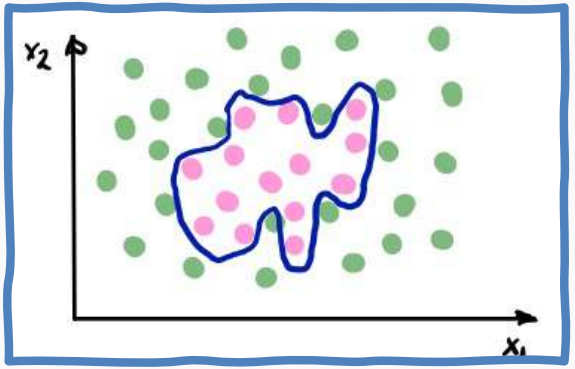
- Norm Penalties
- Early Stopping
- Data Augmentation
- **Dropout**

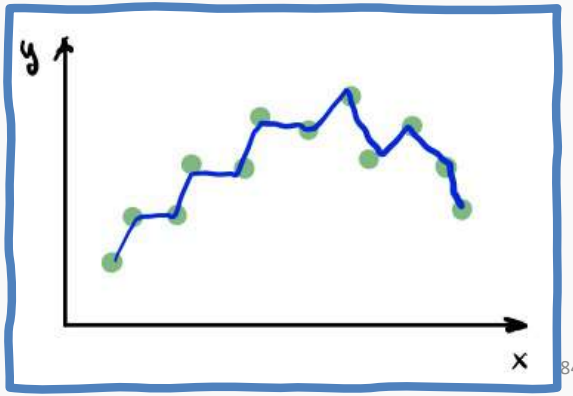
Co-adaptation

Overfitting occurs when the model is sensitive to slight variations on the input and therefore it fits the noise.

L1 and L2 regularizations ‘shrink’ the weights to avoid this problem.

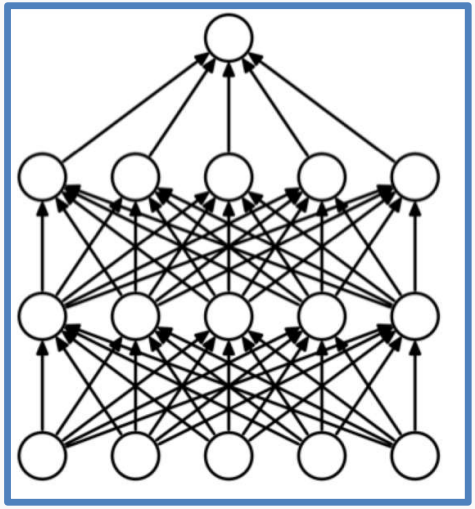
However in a large network many units can collaborate to respond to the input while the weights can remain relatively small. This is called co-adaptation.



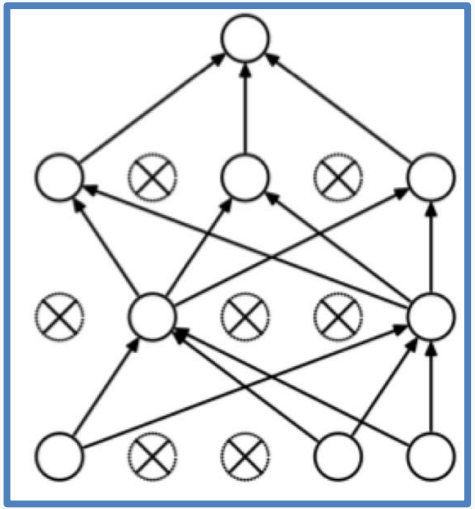


Dropout

- Randomly set some neurons and their connections to zero (i.e. “dropped”)
- Prevent overfitting by reducing co-adaptation of neurons
- Like training many random sub-networks



Standard Neural Network



After applying dropout

https://arxiv.org/pdf/1207.0580.pdf

Dropout: Training

For each new example in a mini-batch (could be for one mini-batch depending on the implementation):

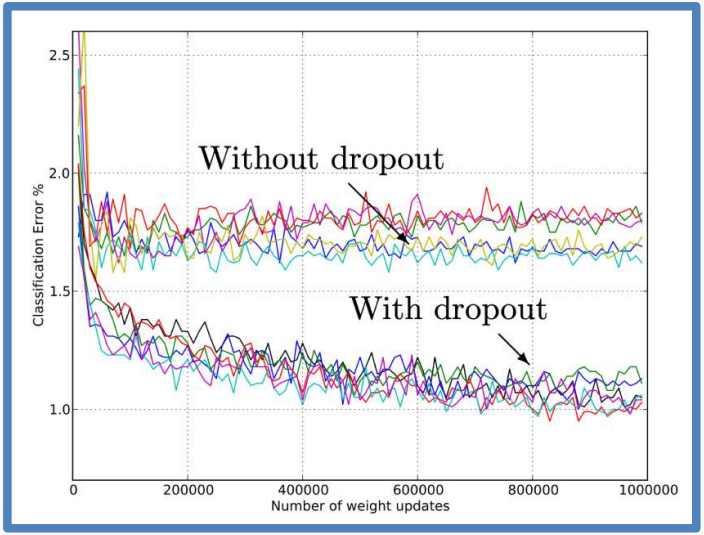
- Randomly sample a binary mask μ independently, where μ_i indicates if input/hidden node i is included
- Multiply output of node i with μ_i, and perform gradient update

Typically:

- Input nodes are included with prob=0.8 (as per original paper, but rarely used)
- Hidden nodes are included with prob=0.5

Dropout

- Widely used and highly effective



Test error for different architectures with and without dropout.

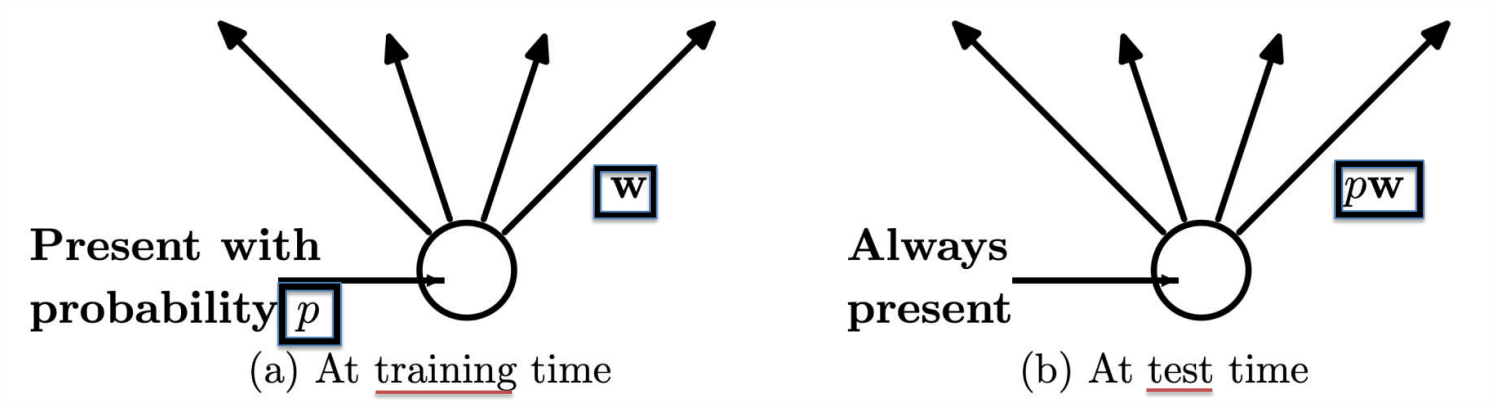
The networks have 2 to 4 hidden layers each with 1024 to 2048 units.

- Proposed as an alternative to ensemble methods, which is too expensive for neural nets

http://jmlr.org/papers/volume15/srivastava14a/srivastava14a.pdf

Dropout: Prediction

- We can think of dropout as training many of sub-networks
- At **test time**, we can "aggregate" over these sub-networks by **reducing connection weights in proportion to dropout probability, *p***



NOTE: Dropouts can be used for **neural network inference** by dropping during predictions and predicting multiple times to get a distribution