

# Logistic Regression Part 2

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# Content

- Part 1:
  - Classification With Logistic Regression
  - Model Evaluation For Classification
- Part 2:
  - Overfitting and Underfitting
- Part 3:
  - Practical Issues With Classification

## Content - Part 2

- Overfitting and Underfitting
  - Introduction
  - The Concept of Regularization
  - Regularized Linear Regression
  - Regularized Logistic Regression

# Overfitting and Underfitting

## Introduction

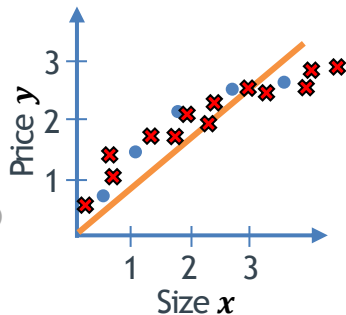
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- Overfitting and Underfitting
  - Introduction
  - The Concept of Regularization
  - Regularized Linear Regression
  - Regularized Logistic Regression

## Introduction

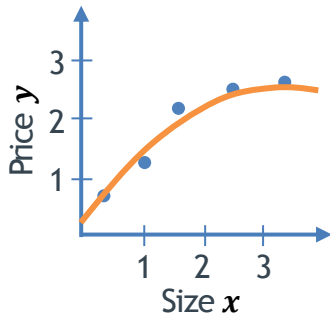
- Underfitting and overfitting are problems that can arise that cause a model (either regression or classification) to perform very poorly on test (new) examples
- We'll describe these problems and then describe how we can mitigate them using a technique called "Regularization"

# Introduction - Overfitting and Underfitting in Linear Regression



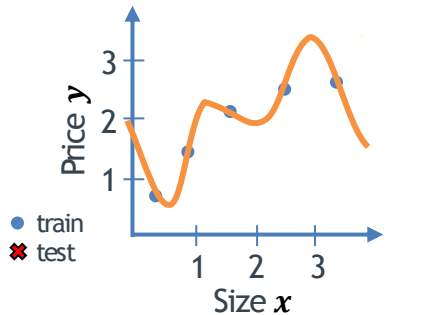
$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

Underfitting  
“High Bias”



$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2$$

“Just right”

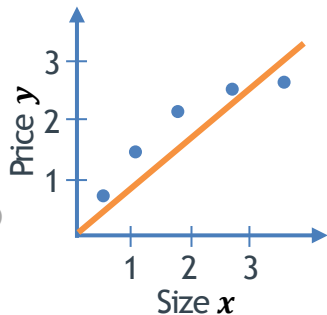


$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

Overfitting  
“High Variance”

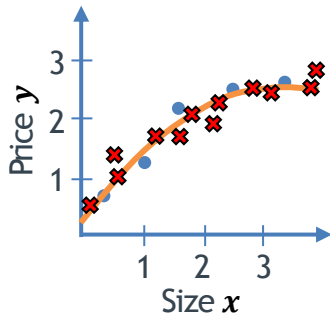
- Underfitting: The model  $h_{\theta}(x)$  is too simple (too few features) and doesn't fit the training examples very well or even at all (so  $J(\theta)$  is very large) and so the model will also not reflect reality and doesn't fit new (test) examples well either
- The model has high “bias” i.e. it has a biased (rigid, inflexible) nature

# Introduction - Overfitting and Underfitting in Linear Regression



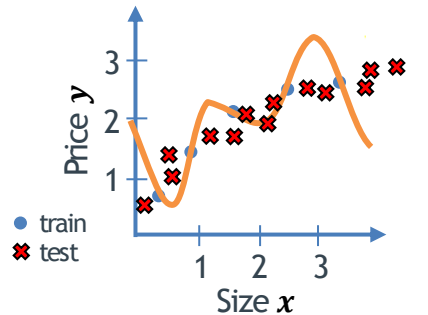
$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

Underfitting  
“High Bias”



$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2$$

“Just right”

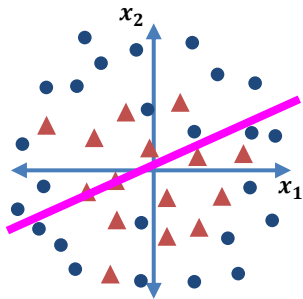


$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

Overfitting  
“High Variance”

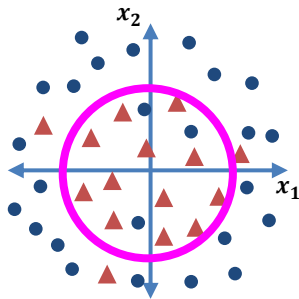
- Overfitting: The model  $h_{\theta}(x)$  is too complex (too many features) and fits the training examples very well or even perfectly (so  $J(\theta) \approx 0$ ) but the model doesn't reflect reality and doesn't fit the test examples very well (or at all)
- The model has “high variance” i.e. it has a “too flexible” / “too variant” nature

## Introduction - Overfitting and Underfitting in Logistic Regression



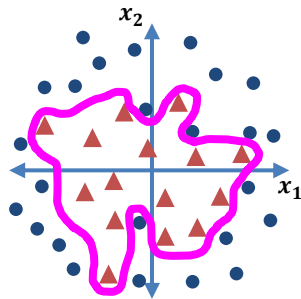
$$h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

Underfitting  
“High Bias”



$$h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$$

“Just right”



$$h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \dots)$$

Overfitting  
“High Variance”



## Introduction - Addressing High Bias and Variance

- To address high bias:
  - Increase the number of features i.e. new types of features, high-order features, combination of features
- To address high variance, there are two main methods:
  1. Reduce the Features
    - Manually (pain-stakingly) select and remove features
    - Use train-cv-test sets to compare various models and select the best one
    - Works well when you have relatively fewer features and/or you have specific ideas about models to use/compare
  2. Apply Regularization
    - Use as complex of a model as you like (number of features, high-order terms, combination of features)
    - Apply regularization to reduce the impact of these features towards predicting  $y$  by adjusting/reducing all of the  $\theta$  parameters
    - Works well when you have a LOT of features and manual selection will be hard

# Overfitting and Underfitting

## The Concept of Regularization

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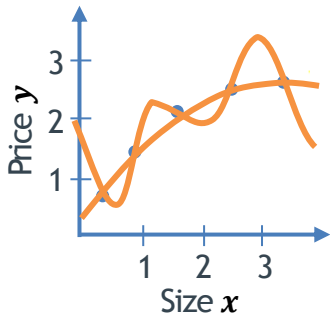
- Overfitting and Underfitting
  - Introduction
  - The Concept of Regularization
  - Regularized Linear Regression
  - Regularized Logistic Regression

## Regularization - Concept

- If we minimize  $J(\theta)$  with this hypothesis, we'll get a  $h_\theta(x)$  that overfits
- Suppose that we penalize  $\theta_3$  and  $\theta_4$  to make them really small by modifying the cost function as follows:

$$\underset{\theta}{\text{minimize}} \frac{1}{2m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)})^2 + 100 \theta_3^2 + 100 \theta_4^2$$

- With everything else the same, the only way to reduce (and minimize) the cost in the same way as before is to ensure that  $\theta_3$  and  $\theta_4$  become really really small
  - Has the effect of setting  $\theta_3$  and  $\theta_4$  such that  $+ 100 \theta_3^2 + 100 \theta_4^2$  is set to 0 to get back the original cost i.e. setting  $\theta_3$  and  $\theta_4$  close to 0
  - Also the effect of almost excluding the third and fourth order terms in  $h_\theta(x)$



$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \underbrace{\theta_3 x^3}_{\approx 0} + \underbrace{\theta_4 x^4}_{\approx 0}$$

## Regularization - Intuition



- Intuition 2: Hamburger shop:

- As the manager of a hamburger joint, you're selling 10 200g hamburgers per day @ R10 per hamburger
- The "cost" of a burger is:

$$\begin{aligned}\text{Cost} &= P_{\text{Meat}} + P_{\text{Veggies}} + P_{\text{Roll}} \\ &= 3.50 + 1.20 + 1.50 = \text{R}6.20\end{aligned}$$

- At this cost, the boss is making a handsome R2000 per day in profits
- Life is good

## Regularization - Intuition



- Intuition 2: Hamburger shop:
  - Suddenly, the centre announces that they are supporting “animal rights” or some weird thing like that
  - They are imposing an extra “cost” on every kg of meat you sell
  - They will charge you 1cent for every 1g of meat you sell (basically the weight of the meat)
  - The “cost” of a burger now changes:

$$\begin{aligned}\text{Cost} &= P_{\text{Meat}} + P_{\text{Veggies}} + P_{\text{Roll}} \\ &= 3.50 + 1.20 + 1.50\end{aligned}$$

- Unfortunately, the boss says he’s not willing to accept that much less profit and orders you to reduce the new cost down to R6.50 **somehow**.
- You’ve got to reduce your cost somehow to keep profits constant
- The prices at which you’re buying meat, veggies and rolls are also still the same
- What can you change to keep the cost the same as it was before?
  - Reducing the “weight” of the burger

## Regularization - Intuition



- Intuition 2: Hamburger shop:
  - Here's what needs to happen to get the new cost down from R8.20 to R6.50:

$$\text{Cost} = P_{\text{Meat}} + P_{\text{Veggies}} + P_{\text{Roll}} + \theta_{\text{Meat}} \times 0.01$$

$$6.50 = 3.50 + 1.20 + 1.50 + \theta_{\text{Meat}} \times 0.01$$

$$\theta_{\text{Meat}} = \frac{6.50 - (3.50 + 1.20 + 1.50)}{0.01}$$

$$\theta_{\text{Meat}} = \frac{6.50 - (3.50 + 1.20 + 1.50)}{0.01}$$

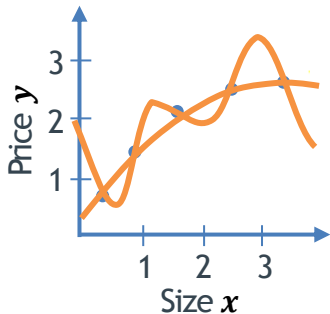
$$\theta_{\text{Meat}} = 30\text{g of meat}$$

## Regularization - Concept

- If we minimize  $J(\theta)$  with this hypothesis, we'll get a  $h_\theta(x)$  that overfits
- Suppose that we penalize  $\theta_3$  and  $\theta_4$  to make them really small by modifying the cost function as follows:

$$\underset{\theta}{\text{minimize}} \frac{1}{2m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)})^2 + 100 \theta_3^2 + 100 \theta_4^2$$

- With everything else the same, the only way to reduce (and minimize) the cost in the same way as before is to ensure that  $\theta_3$  and  $\theta_4$  become really really small
  - Has the effect of setting  $\theta_3$  and  $\theta_4$  such that  $+ 100 \theta_3^2 + 100 \theta_4^2$  is set to 0 to get back the original cost i.e. setting  $\theta_3$  and  $\theta_4$  close to 0
  - Also the effect of almost excluding the third and fourth order terms in  $h_\theta(x)$



$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \underbrace{\theta_3 x^3}_{\approx 0} + \underbrace{\theta_4 x^4}_{\approx 0}$$

## Regularization - Concept

- In the example we saw: we knew which terms were higher-order i.e.  $\theta_3$  and  $\theta_4$
- Adding those specific terms to the cost function reduced their weights
- In practice: we aren't always sure which features we need to regularize
  - We regularize ALL of the weights (except  $\theta_0$ ) equally
  - We add all of them to the cost function

$$J_{\text{reg}}(\theta) = J(\theta) + \frac{\lambda}{2m} \sum_{j=1}^n \theta_j^2$$

- $J(\theta)$  is the normal cost function that we had before (either for linear or logistic regression)
- We don't regularize  $\theta_0$  so  $j$  starts from 1, not 0.
- The parameter  $\lambda$  is the regularization parameter which helps control how much to regularize:
  - Setting  $\lambda = 0$  means that the whole regularization term falls away i.e. no regularization at all - potential **overfitting** - **high variance**
  - Setting  $\lambda > 0$  means increasing amount of regularization by penalizing all  $\theta_j$  (except  $\theta_0$ ) at the same time - moving towards **underfitting** - **high bias**



# Overfitting and Underfitting

## Regularized Linear Regression

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## Regularized Linear Regression

- What we arrived at previously:

$$J_{\text{reg}}(\theta) = J(\theta) + \frac{\lambda}{2m} \sum_{j=1}^n \theta_j^2$$

- So for linear regression:

$$J_{\text{reg}}(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m} \sum_{j=1}^n \theta_j^2$$

$$J_{\text{reg}}(\theta) = \frac{1}{2m} \left[ \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^n \theta_j^2 \right]$$

## Regularized Linear Regression

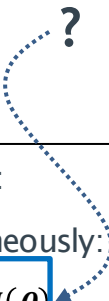
- With the new cost function, we can simply apply gradient descent (or any other optimization/minimization technique) as before
- This involves making continuous updates to all  $\theta_j$  to minimize the cost

$$J(\theta) = \frac{1}{2m} \left[ \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^n \theta_j^2 \right]$$

- We'll be updating  $\theta_j$  using the same update rules as before
- One thing has changed here:  $\frac{\partial}{\partial \theta_j} J(\theta)$  because the  $J(\theta)$  has changed

Repeat until convergence:

Update all  $\theta_j$  simultaneously:

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$


## Regularized Linear Regression

- For any parameter  $\theta_j$ :

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \cdot \frac{1}{2m} \left[ \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^n \theta_j^2 \right]$$

Repeat until convergence:

Update all  $\theta$  simultaneously:

$$\theta_0 \leftarrow \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (\theta^T x^{(i)} - y^{(i)}) \cdot x_0^{(i)}$$

$$\theta_j \leftarrow \theta_j - \alpha \left[ \frac{1}{m} \sum_{i=1}^m (\theta^T x^{(i)} - y^{(i)}) \cdot x_1^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

## Regularized Linear Regression

- The update rule for  $\theta_0$  is exactly the same as before: we're not regularizing it
- The update rules for all other  $\theta_j$  are different; they now have an added term

$$\theta_j \leftarrow \theta_j - \alpha \left[ \frac{1}{m} \sum_{i=1}^m (\theta^T x^{(i)} - y^{(i)}) \cdot x_1^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

- If we slightly restructure this update rule, something interesting emerges:

$$\theta_j \leftarrow \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m (\theta^T x^{(i)} - y^{(i)}) \cdot x_1^{(i)} - \alpha \frac{\lambda}{m} \theta_j$$

$$\theta_j \leftarrow \theta_j - \alpha \frac{\lambda}{m} \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m (\theta^T x^{(i)} - y^{(i)}) \cdot x_1^{(i)}$$


$$\theta_j \leftarrow \left( 1 - \alpha \frac{\lambda}{m} \right) \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m (\theta^T x^{(i)} - y^{(i)}) \cdot x_1^{(i)}$$

- Given that  $m$  will usually be larger than  $\alpha\lambda$ , the term  $0 < \alpha \frac{\lambda}{m} < 1$  e.g. 0.01
- Therefore, also  $0 < \left( 1 - \alpha \frac{\lambda}{m} \right) < 1$  e.g. 0.99
- Multiplying this by  $\theta_j$  has the effect of shrinking by e.g. 1% it before the update

## Regularized Linear Regression - Using sklearn

- Now that we know the details, we can use sklearn to fit a regularized model as follows:

```
from sklearn.linear_model import Ridge  
  
model = Ridge(alpha=10)  
  
model.fit(X,y)
```



A diagram consisting of a dotted line that originates from the value '10' inside a light blue rectangular box in the code 'model = Ridge(alpha=10)'. The line curves upwards and to the right, ending at the text ' $\lambda = 10$ ', indicating that the 'alpha' parameter in sklearn's Ridge class is equivalent to the ' $\lambda$ ' regularization parameter in the mathematical formulation of Ridge regression.

- Note that X should **not** contain the extra column of 1s for feature  $x_0$ .
- The Ridge class has other parameters: find out what they are/do

## Normal Equation With Regularization

- Given a feature matrix  $X$ , and the corresponding output matrix  $y$
- The following equation solves for  $\theta$  that best fits the data with regularization:

$$\theta = \left( X^T X + \lambda I \right)^{-1} X^T y$$

- Where
  - the matrix added is an  $(n + 1) \times (n + 1)$  and
  - has a diagonal of 1s (apart from the top-left entry) and 0s everywhere else
- E.g.

	Size	#Rms	Age	#Grgs		Price
$X =$	1	460	4	12	2	6639
	1	70	1	5	0	1681
	1	155	3	8	2	3969
	1	429	6	10	3	5095

$$y = \begin{bmatrix} 6639 \\ 1681 \\ 3969 \\ 5095 \end{bmatrix}$$

# Overfitting and Underfitting

## Regularized Logistic Regression

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## Regularized Logistic Regression

- What we arrived at previously:

$$J_{\text{reg}}(\theta) = J(\theta) + \frac{\lambda}{2m} \sum_{j=1}^n \theta_j^2$$

- So for linear regression:

$$J_{\text{reg}}(\theta) = -\frac{1}{m} \sum_{i=1}^m \left[ y^{(i)} \ln(h_{\theta}(x^{(i)})) + (1 - y^{(i)}) \ln(1 - h_{\theta}(x^{(i)})) \right] + \frac{\lambda}{2m} \sum_{j=1}^n \theta_j^2$$

- Where:

$$h_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$$

## Regularized Logistic Regression

- With the new cost function, we can simply apply gradient descent (or any other optimization/minimization technique) as before
- This involves making continuous updates to all  $\theta_j$  to minimize the cost

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^m \left[ y^{(i)} \ln(h_{\theta}(x^{(i)})) + (1 - y^{(i)}) \ln(1 - h_{\theta}(x^{(i)})) \right] + \frac{\lambda}{2m} \sum_{j=1}^n \theta_j^2$$

$$h_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$$

- We'll be updating  $\theta_j$  using the same update rules as before
- One thing has changed here:  $\frac{\partial}{\partial \theta_j} J(\theta)$  because the  $J(\theta)$  has changed

Repeat until convergence:

Update all  $\theta_j$  simultaneously:

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

?

## Regularized Logistic Regression

- For any parameter  $\theta_j$ :

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j$$

Repeat until convergence:

Update all  $\theta$  simultaneously:

$$\theta_0 \leftarrow \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x_0^{(i)}$$

$$\theta_j \leftarrow \theta_j - \alpha \left[ \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x_1^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

- Algorithm appears to be identical to gradient descent for regularized linear regression
  - It is NOT! The hypothesis here is that of logistic regression

$$h_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$$

## Regularized Logistic Regression Using Adv. Optim. Algorithms

- Implemented in SciPy's optimize library:

```
from scipy.optimize import minimize

theta = np.zeros(X.shape[1]) #Initialize all thetas to zeros
result = minimize(costFunc, theta, args=(X,y), method='BFGS', jac=gradientFunc,
options={'maxiter' : 400, 'disp': True})

print(result.x)
```

- costFunc is a function that returns the cost as per:

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^m \left[ y^{(i)} \ln(h_{\theta}(x^{(i)})) + (1 - y^{(i)}) \ln(1 - h_{\theta}(x^{(i)})) \right] + \frac{\lambda}{2m} \sum_{j=1}^n \theta_j^2$$

- gradientFunc is a function that returns a list/vector of the gradients of all the  $\theta_j$  as per:

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j$$

## Regularized Logistic Regression Using Adv. Optim. Algorithms

- Implemented in SciPy's optimize library:

```
from scipy.optimize import minimize
```

```
theta = np.zeros(X.shape[1]) #Initialize all thetas to zeros
```

```
result = minimize(costFunc, theta, args=(X,y), method='BFGS', jac=gradientFunc,  
options={'maxiter' : 400, 'disp': True})
```

```
print(result.x)
```

- result.x will contain the optimal  $\theta$  values
- Note that X must contain an extra column of zeros representing feature  $x_0$
- Predictions can then be made by applying  $\mathbf{h}_{\theta}(\mathbf{x}) = g(\theta^T \mathbf{x})$

## Regularized Logistic Regression Using sklearn

- Implemented in sklearn specifically for Logistic Regression:

```
from sklearn.linear_model import LogisticRegression
```

```
clf = LogisticRegression(random_state=0, solver='lbfgs', multi_class='auto', C = 10 )
```

```
clf.fit(X, y)
```

$$C = \frac{1}{\lambda} = 10$$

So here:

$$\lambda = \frac{1}{C} = 0.1$$

- Regularization in the LogisticRegression class is specified differently: it is specified via a parameter  $C$  which is the inverse of  $\lambda$ .

$$C = \frac{1}{\lambda} \quad \text{so} \quad \lambda = \frac{1}{C}$$

- $C$  has the same goal as, but opposite effect to,  $\lambda$  i.e.:
  - Setting  $C$  very small means setting  $\lambda$  very large i.e. **more** regularization
  - Setting  $C$  very large means setting  $\lambda$  very small i.e. **less** regularization

**THE END**

Of Logistic Regression Part 2

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