# Regression

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### Outline

• Linear regression

• Logistic regression

### Problem setting

- Example: How likely is a user clicking an online ad?
  - Inputs: User's profile, Ad's profile
- Regression on probability
  - But actually a classification problem
  - Can be applied to many binary classification

Product: Tennis shoe Color: Grey Price: Medium Pr(Click) = ??



Will this user click this ad?



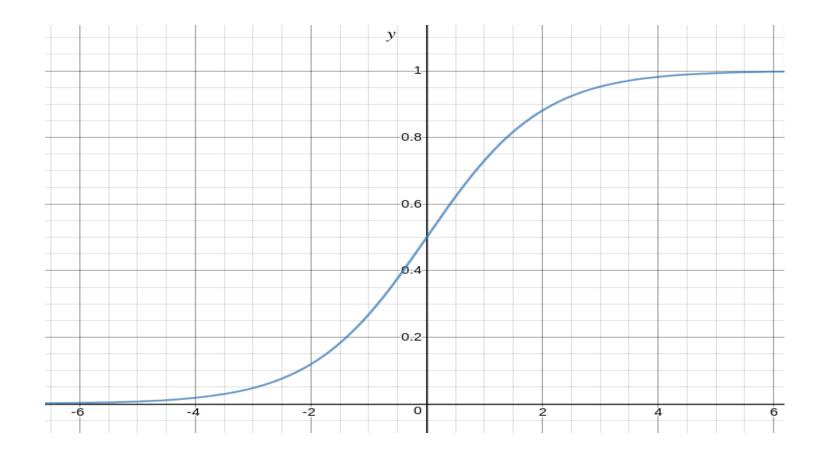
Non-athletic, likes green, big spender

# Modeling probability

• What function ALWAYS produces value in range [0, 1]?

Can replace this with any function of x

Logistic function 
$$\sigma(x) = \frac{1}{1 + \exp(-x)} = \frac{\exp(x)}{1 + \exp(x)}$$



# Modeling probability

• Why not use a more expressive form for x?

$$\sigma(x) = \frac{1}{1 + \exp(-g(x))}, g(x) = \theta_1 x + \theta_0$$

• Multi-variate input x:

$$g(x) = \theta_1^T x + \theta_0$$

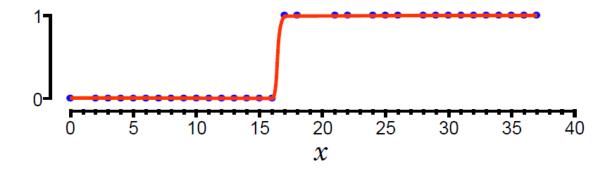
• Rearranging the terms, we can see

$$\log \frac{\sigma(x)}{1 - \sigma(x)} = \theta_1^T x + \theta_0$$

• Linear regression on log-odds (well, sort of...)

#### How to train

- Typical regression algorithms are trained to minimize the residual
  - In logistic regression, the ground-truths are either 0 or 1
  - So should we just find the best-fit logistic curve using MSE?



- What's wrong with this?
  - It's not really regression if there are only two target values
  - MSE is not related to accuracy
  - We wish to model the *probability* of success: Need probabilistic interpretation of the model

### Training via maximum likelihood

- Given the training data  $D = \{(x_i, y_i) | x_i \in \mathbb{R}, y_i \in \{0,1\}\}$ 
  - What is the log likelihood of D under our logistic regression model?

$$\log \Pr(D; \theta) = \sum_{i|y_i=1} \log \sigma(x_i) + \sum_{i|y_i=0} \log \left(1 - \sigma(x_i)\right)$$

- We should find the parameters that maximize this (log) likelihood
- Differentiate!

$$\Pr((x_i, y_i = 0)) = \Pr(y_i = 0 | x_i) = 1 - \sigma(\theta_1 x_i + \theta_0)$$

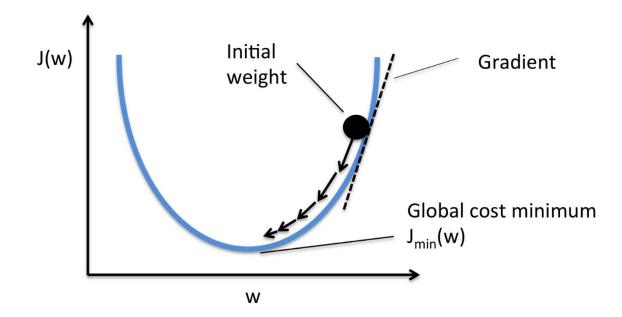
$$\frac{\partial \log \Pr(D;\theta)}{\partial \theta_1} = \sum_{y_i=1} (1 - \sigma(x_i)) x_i + \sum_{y_i=0} \sigma(x_i) x_i = 0,$$

$$\frac{\partial \log \Pr(D;\theta)}{\partial \theta_0} = \sum_{y_i=1} (1 - \sigma(x_i)) + \sum_{y_i=0} \sigma(x_i) = 0$$
System of non-linear equations that don't always yield closed-form solutions

Need to use iterative methods (e.g., gradient descent)

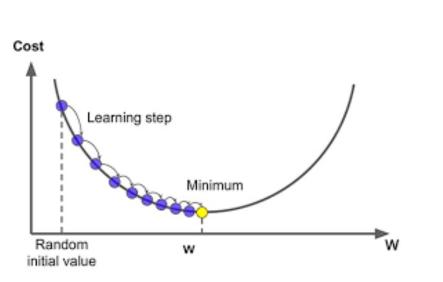
# Optimization

- Since we can't find a closed-form solution, we use iterative methods
  - Also called "Numerical methods", since relies on numerical analysis
- Gradient descent
  - Gradually move in the direction of steepest descent (i.e., opposite of gradient)

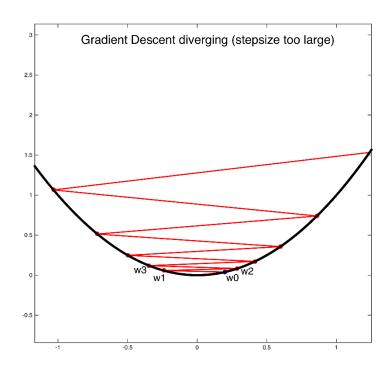


#### Gradient descent

- As always, we wish to find the minimum of our loss (cost) function
- If we move in the direction of gradient, we have better hope of finding the minimum
  - But if we move TOO much, we might overshoot



https://saugatbhattarai.com.np/what-is-gradient-descent-in-machine-learning/



### Gradient descent pseudocode

- In pseudocode:
- 1. Let  $J(\theta)$  be the cost function
- 2. Initialize  $\theta^*$
- 3. While not converged:

1. 
$$\theta^* \leftarrow \theta^* - \gamma \frac{\partial J}{\partial \theta}$$

2. Adjust step  $\overline{\text{size }} \gamma$  (if necessary)

//Update w\* in the direction that decreases the loss the most, but only by a small amount

Python example (Thank you Wikipedia)

```
next x = 6 # We start the search at x=6
gamma = 0.01 # Step size multiplier
precision = 0.00001 # Desired precision of result
max iters = 10000 # Maximum number of iterations
# Derivative function
def df(x):
    return 4 * x**3 - 9 * x**2
for _i in range(max_iters):
    current_x = next_x
    next_x = current_x - gamma * df(current_x)
    step = next_x - current_x
    if abs(step) <= precision:</pre>
        break
print("Minimum at {}".format(next_x))
```

### Where the decision boundary lies

- How do we predict?
  - If the probability is >0.5, we say "yes", otherwise, "no"
- To see the boundary, simply set the probability to 0.5, and see what happens:

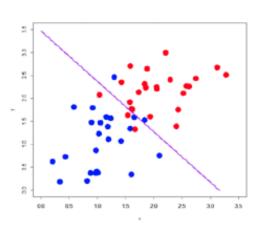
$$\frac{1}{1 + \exp(-x\theta_1 - \theta_0)} = \frac{1}{2}$$

$$\exp(-x\theta_1 - \theta_0) = 1$$

$$\Phi$$

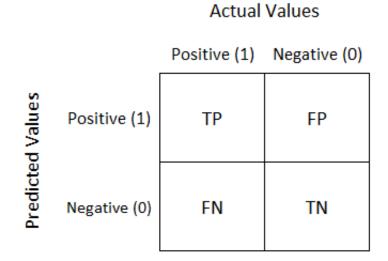
$$x\theta_1 + \theta_0 = 0$$

- This is just a linear function!
- Logistic regression is a linear classifier



#### How well did we do?

- Sometimes, it's not all about getting the right answer
  - We also have to successfully reject the wrong answers



- Precision: How many of the found items are correct?
  - True positive / (True positive + False positive)
- Recall: How many of the relevant items did we find?
  - True positive / (False negative + True positive)

| GT | PD |    |
|----|----|----|
| 1  | 0  | FN |
| 0  | 0  | TN |
| 0  | 0  | TN |
| 1  | 1  | TP |
| 1  | 1  | TP |
| 1  | 1  | TP |
| 1  | 0  | FN |
| 0  | 1  | FP |
| 0  | 0  | TN |
| 0  | 0  | TN |
|    |    |    |

Precision: 0.75

Recall: 0.6

F1: 0.667

Accuracy: 0.7

#### How well did we do?

- Useful for class imbalance
  - If 70% of your data has label '1', you can still get 70% accuracy by just saying '1'
  - But that will drastically lower the precision

Precision = True positive / (True positive + False positive)

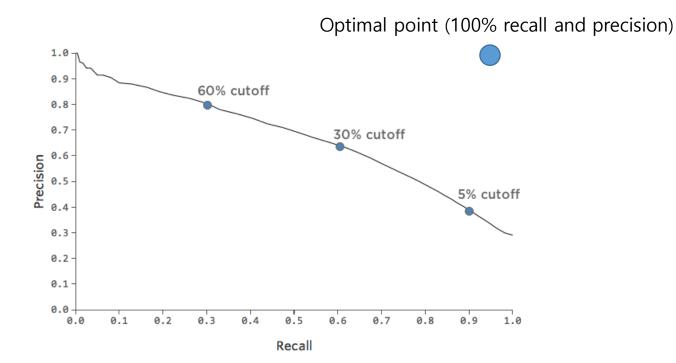
Combined measure: F1 score

$$F1 = 2\frac{PR}{P+R}$$

- Harmonic mean of precision and recall
- Both precision and recall have to be high

#### How well did we do?

- Precision-recall curve
  - Recall that our decision rule is: IF p(x) > 0.5 THEN '1' ELSE '0'
  - We can see how the results change if we vary the threshold 0.5
  - Collect and plot the (recall, precision) points for many different threshold values



c.f., ROC curve (Receiver operating characteristic curve)

#### We want more than two

- How do we extend beyond binary classification? (K classes, K > 2)
- Setting: D =  $\{(x_i, y_i) | x_i \in \mathbb{R}, y_i \in [K]\}$
- Main idea:
  - Run multiple binary regressions on each class independently
  - i.e., set a parameter for each class (plus one for bias)

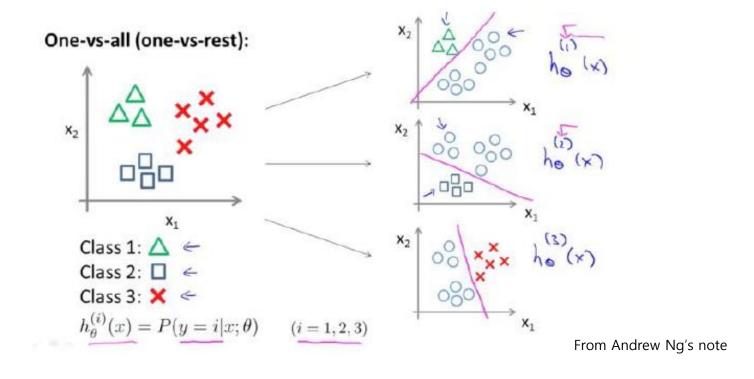
$$\Pr(Y_i = k | X_i) \propto \exp(\theta_k X_i + \theta_0)$$

- Why do we use an exponential?
  - i) good way to ensure non-negativity
  - ii) Log-linear interpretation

$$\Pr(Y_i = k) = \frac{\exp(\theta_k X_i + \theta_0)}{\sum_i \exp(\theta_i X_i + \theta_0)}$$
 A.K.A., "Softmax regression"

### We want more than two

- One-vs-All
  - Also common in multi-class classification problems
- To predict among K classes, train K binary logistic regressors
  - Choose the class that yields highest probability



### What about multi-class precision/recall? (Macro avg.)

- Construct a confusion matrix as follows
  - Each entry is the # of predictions made

|        |    | Ground-truth labels |    |    |    |    |    |
|--------|----|---------------------|----|----|----|----|----|
|        |    | L1                  | L2 | L3 | L4 | L5 | L6 |
| L2     | L1 | 3                   | 3  | 4  | 1  | 3  | 3  |
|        | L2 | 0                   | 15 | 2  | 0  | 0  | 0  |
|        | L3 | 3                   | 2  | 10 | 0  | 2  | 0  |
| labels | L4 | 1                   | 1  | 1  | 14 | 0  | 0  |
|        | L5 | 0                   | 0  | 4  | 1  | 12 | 0  |
|        | L6 | 0                   | 0  | 0  | 0  | 0  | 17 |

Prec(L1) = 3 / (3+3+4+1+3+3) = 3/17

Simply average row-by-row and column-by-column



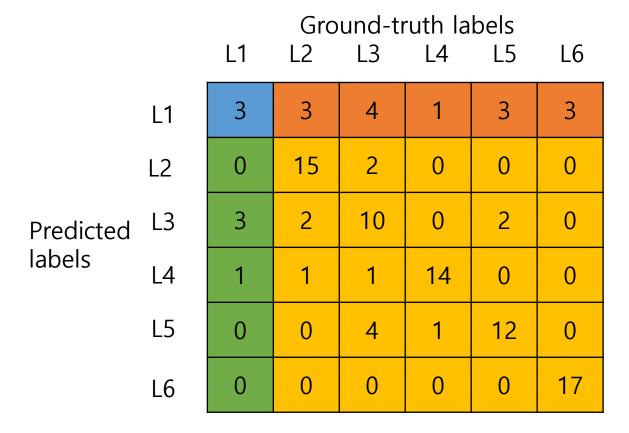
Then average over all labels for the final precision/recall

$$Prec = Avg(Prec(L1), ..., Prec(L6))$$
  
 $Rec = Avg(Rec(L1), ..., Rec(L6))$ 

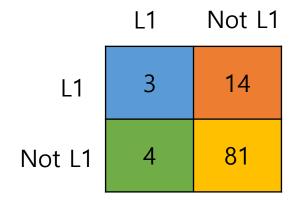
$$Rec(L1) = 3 / (3+0+3+1+0+0) = 3/7$$

### What about multi-class precision/recall? (Micro avg.)

- Construct a confusion matrix as follows
  - Each entry is the # of predictions made

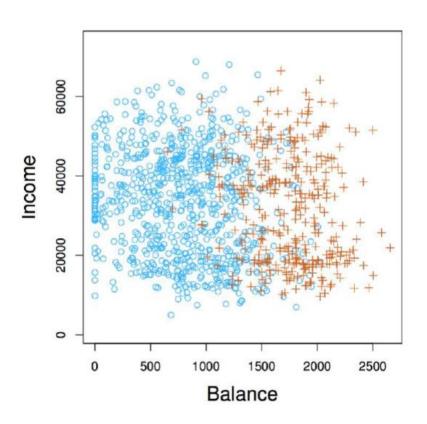


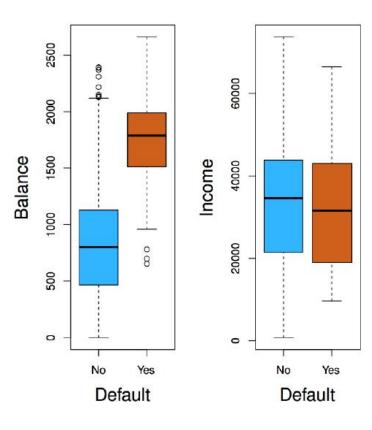
Construct a confusion matrix for each label with 1-vs-all criterion



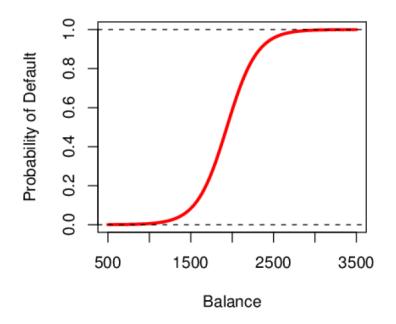
Then construct the aggregate confusion matrix by summing over all confusion matrices before computing the prec./rec. in the usual manner.

- Will a given customer default on his/her payment?
  - Customer features: Annual income, or monthly credit card balance
  - Output: Yes / No





- Since 'balance' is more decisive, we'll use that as an input
- Learned model:



|           | Coefficient | Std. Error | Z-statistic | P-value  |
|-----------|-------------|------------|-------------|----------|
| Intercept | -10.6513    | 0.3612     | -29.5       | < 0.0001 |
| balance   | 0.0055      | 0.0002     | 24.9        | < 0.0001 |

Coefficient for 'balance' is positive

→ default probability increases with balance

- Let's use more information
  - Balance, income, and student-ness
  - Student-ness is a binary variable that's 1 for student, 0 for not
- Learned model

|              | Coefficient | Std. Error | Z-statistic | P-value  |
|--------------|-------------|------------|-------------|----------|
| Intercept    | -10.8690    | 0.4923     | -22.08      | < 0.0001 |
| balance      | 0.0057      | 0.0002     | 24.74       | < 0.0001 |
| income       | 0.0030      | 0.0082     | 0.37        | 0.7115   |
| student[Yes] | -0.6468     | 0.2362     | -2.74       | 0.0062   |

• What if we isolate 'student'?

Learned model

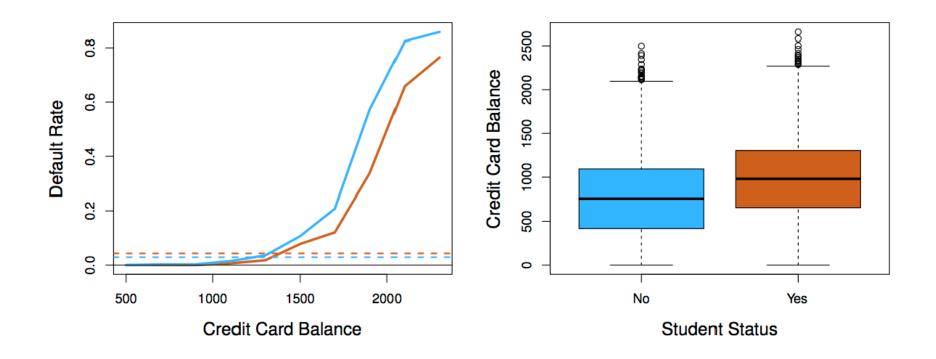
|              | Coefficient | Std. Error | Z-statistic | P-value  |
|--------------|-------------|------------|-------------|----------|
| Intercept    | -3.5041     | 0.0707     | -49.55      | < 0.0001 |
| student[Yes] | 0.4049      | 0.1150     | 3.52        | 0.0004   |

Positive

• But wait...

|              | Coefficient | Std. Error | Z-statistic | P-value  |
|--------------|-------------|------------|-------------|----------|
| Intercept    | -10.8690    | 0.4923     | -22.08      | < 0.0001 |
| balance      | 0.0057      | 0.0002     | 24.74       | < 0.0001 |
| income       | 0.0030      | 0.0082     | 0.37        | 0.7115   |
| student[Yes] | -0.6468     | 0.2362     | -2.74       | 0.0062   |

• Student vs. non-student



Default more likely for non-students (Possibly because of more spending?)

### Summary

- Regression is used to predict continuous outcomes for each input
  - Classification is used to predict categorical outcomes
- Linear regression assumes a linear relationship between input-output
  - 'Y = aX + b', where the trainable parameters are {a, b}
  - Admits closed-form solution (OLS)
  - General enough to model many other functions (polynomial, sinusoidal, etc.)
- Logistic regression tries to predict the *probability* of a categorical outcome
  - Mostly used as a classification model, despite its name
  - Doesn't have closed-form solution (must rely on iterative numerical methods)
  - Produces linear decision boundary