COMPSCI762: Foudnations of Machine Learning

Regression

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Today we will cover...

Regression

Linear Regression

Least Squares

Different Notation

Summary

Partially based on Slides from University of British Columbia

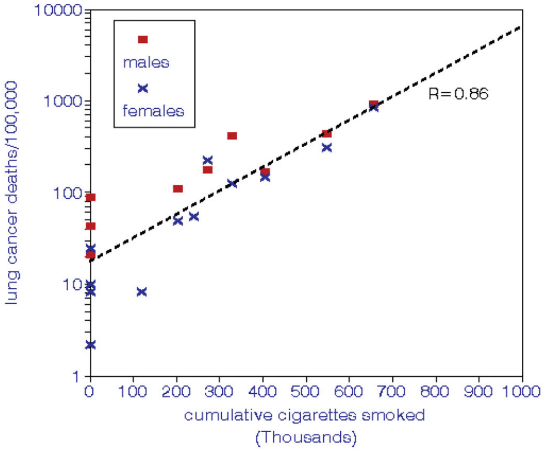
Regression

Supervised Learning Round 2: Regression

- We are going to revisit supervised learning
- Previously, we considered classification
  - We assumed y_i was discrete: $y_i = spam$ or $y_i = not\ spam$
- Now we are going to consider regression
  - We allow y_i to be numerical, for example $y_3 = 10.34cm$

Example: Dependent vs. Explanatory Variables

- We want to discover relationship between numerical variables
  - Does number of lung cancer deaths change with number of cigarettes?
  - Does number of skin cancer deaths change with latitude?
  - Do people in big cities walk faster?
  - Is the universe expanding or shrinking or staying the same size?
  - Does number of gun deaths change with gun ownership?
  - Does number violent crimes change with violent video games?



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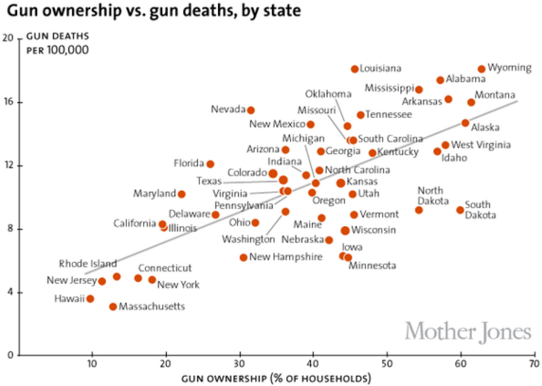

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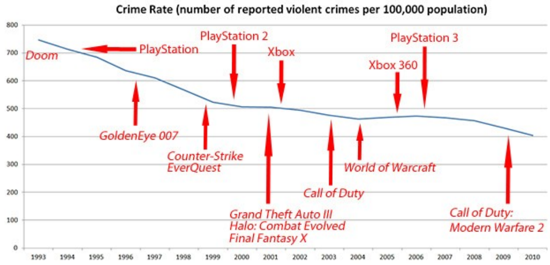
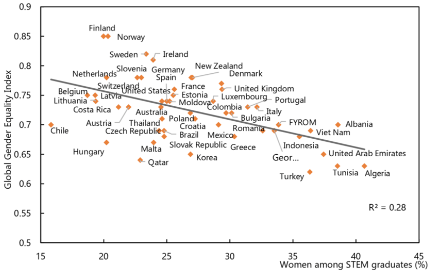


Example: Dependent vs. Explanatory Variables

- We want to discover relationship between numerical variables
  - Does higher gender equality index lead to more women STEM grads?
- Not that we're doing supervised learning
  - Trying to predict value of 1 variable (the y_i values) – instead of measuring correlation between 2
- Supervised learning does not give causality
  - OK: Higher gender equality index is correlated with lower graduation rate
  - OK: Higher gender equality index helps predict lower graduation rate
  - BAD: Higher gender equality index leads to lower graduation rate



Handling Numerical Labels

- One way to handle numerical y_i: discretize
  - E.g., for 'age' could we use $age \leq 20$, $20 < age \leq 30$, $age > 30$
  - Now we can apply methods for classification to do regression
  - But coarse discretization loses resolution
  - And fine discretization requires lots of data
- There exist regression versions of classification methods:
  - Regression trees, probabilistic models, non-parametric models
  - Today: one of oldest, but still most popular/important methods
    - Linear regression based on squared error
    - Interpretable and the building block for more-complex methods

Linear Regression

Linear Regression in 1 Dimension

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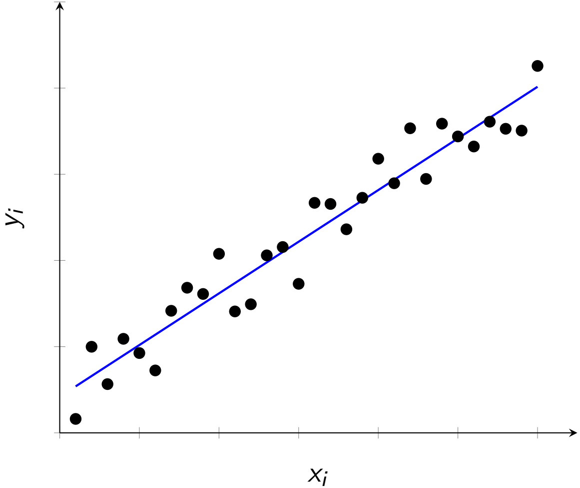
- Assume we only have 1 feature ($d = 1$)
  - E.g., x_i is number of cigarettes and y_i is number of lung cancer deaths
- Linear regression makes predictions $\hat{y}_i$ using a linear function of x_i

$$\hat{y}_i = wx_i$$

- The parameter w is the weight or regression coefficient of x_i
  - We are temporarily ignoring the y-intercept
- As x_i changes, slope w affects the rate that $\hat{y}_i$ increases/decreases
  - Positive w: $\hat{y}_i$ increase as x_i increases
  - Negative w: $\hat{y}_i$ decreases as x_i increases

Linear Regression in 1 Dimension



line $\hat{y}_i = wx_i$ for a particular slope w

Least Squares

Least Squares Objective

- Our linear model is given by
$$\hat{y}_i = wx_i$$
- So we make predictions for a new example by using
$$\hat{y}_i = w\tilde{x}_i$$
- But we can't use the same error as before
  - It is unlikely to find a line where $\hat{y}_i = y_i$ exactly for many points
    - Due to noise, relationship not being quite linear or just floating-point issues
  - Best model may have $|\hat{y}_i - y_i|$ is small but not exactly 0

Least Squares Objective

- Instead of *exact* y_i, we evaluate size of the error in prediction
- Classic way is setting slope w to minimize sum of squared errors

Prediction $\hat{y}_i$ True value of y_i

$$f(w) = \sum_{i=1}^{n} (wx_i - y_i)^2$$

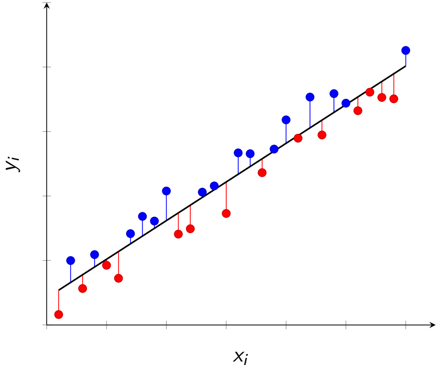
Sum over all training examples

Squared difference between prediction and true value for example x_i

- There are some justifications for this choice
  - A probabilistic interpretation is coming later in the course
- But usually, it is done because it is easy to minimize

Least Squares Objective

- Classic way to set slope w is minimizing sum of squared errors
$$f(w) = \sum_{i=1}^{n}(wx_i - y_i)^2$$



- "Error" is the sum of the squared values of these vertical distances between the line (wx_i) and the targets (y_i)
- If this error is small then our predictions are close to the target

Minimizing a Differential Function

- Simple approach to minimizing a differentiable function f
  1. Take the derivative of f
  2. Find points w where the derivative $f'(w)$ is equal to 0
  3. Choose the smallest one (and check that $f''(w)$ is positive).
- Note that this problem: $f(w) = \sum_{i=1}^{n}(wx_i - y_i)^2$
- Has the same set of minimizers as this problem: $f(w) = \frac{1}{2}\sum_{i=1}^{n}(wx_i - y_i)^2$
- And these also have the same minimizers: $f(w) = \frac{1}{n}\sum_{i=1}^{n}(wx_i - y_i)^2$, $f(w) = \frac{1}{2n}\sum_{i=1}^{n}(wx_i - y_i)^2 + 1000$
- We can multiply f by any positive constant and not change solution
  - Derivative will still be zero at the same locations
  - We will use this trick a lot!

Finding Least Squares Solution

- Finding w that minimizes the sum of squared errors

$$
\begin{aligned}
f(w) = \frac{1}{2}\sum_{i=1}^{n}(wx_i - y_i)^2 &= \frac{1}{2}\sum_{i=1}^{n}\left[w^2x_i^2 - 2wx_iy_i + y_i^2\right] \\
&= \frac{w^2}{2}\sum_{i=1}^{n}x_i^2 - w\sum_{i=1}^{n}x_iy_i + \frac{1}{2}\sum_{i=1}^{n}y_i^2 \\
&= \frac{w^2}{2}a - wb + c \\
\mathit{Take\ derivative}\ f'(w) &= wa - b + 0
\end{aligned}
$$

Setting $f'(w) = 0$ and solving gives

$$
w = \frac{b}{a} = \frac{\sum_{i=1}^{n} x_iy_i}{\sum_{i=1}^{n} x_i^2}
$$

Finding Least Squares Solution

- Finding w that minimizes sum of squared errors

$$w = \frac{b}{a} = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$$

- Let's check that this is a minimizer by checking the second derivative

$$f'(w) = w \sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} x_i y_i$$

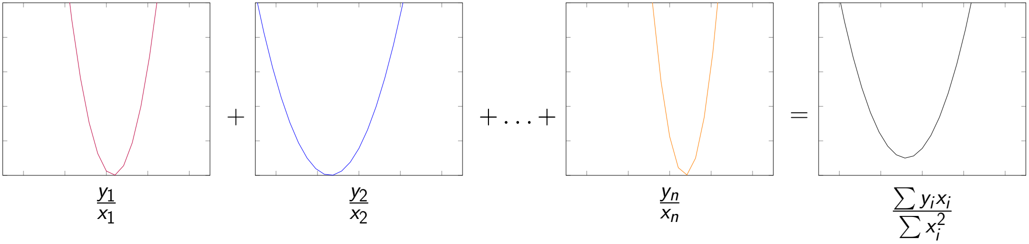
$$f''(w) = \sum_{i=1}^{n} x_i^2$$

  - Since $(anything)^2$ is non-negative and $(anything\ non - zero)^2 > 0$, if we have one non-zero feature then $f''(w) > 0$ and this is a minimizer

Least Squares Objective / Solution (Another View)

- Least squares minimizes a quadratic that is a sum of quadratics

$$f(w) = (wx_1 - y_1)^2 + (wx_2 - y_2)^2 + \ldots + (wx_n - y_n)^2$$



Motivation: Combining Explanatory Variables

- Smoking is not the only contributor to lung cancer
  - For example, there environmental factors like exposure to asbestos
- How can we model the combined effect of smoking and asbestos?
- A simple way is with a 2-dimensional linear function

$$\hat{y} = w_1 x_{i1} + w_2 x_{i2}$$

- We have a weight w_1 for feature 1 and w_2 for feature 2

$$\hat{y}_i = 10(\#cigarettes) + 25(\#asbestos)$$

Different Notation

Different Notations for Least Squares

- If we have d features, the d-dimensional linear model is

$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2} + \ldots + w_d x_{id}$$

  - In words, the output of our model is a weighted sum of the inputs
- We can re-write this in summation notation

$$\hat{y}_i = \sum_{j=1}^{d} w_j x_{ij}$$

- We can also re-write this in vector notation

$$\hat{y}_i = w^T x_i$$

Notation

- In my lectures, all vectors are assumed to be column-vectors

$$w = \begin{bmatrix} w_1 \\ w_2 \\ \cdots \\ w_d \end{bmatrix} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_n \end{bmatrix} \quad x_i = \begin{bmatrix} x_{i_1} \\ x_{i_2} \\ \cdots \\ x_{i_d} \end{bmatrix}$$

- So $w^T x_i$ is a scalar

$$w^T x_i = \begin{bmatrix} w_1 & w_2 & \cdots & w_d \end{bmatrix} \begin{bmatrix} x_{i1} \\ x_{i2} \\ \cdots \\ x_{id} \end{bmatrix} = w_1 x_{i1} + w_2 x_{i2} + \ldots + w_d x_{id} = \sum_{j=1}^{d} w_j x_{ij}$$

- So rows of X are actually transpose of column-vector x

$$X = \begin{bmatrix} x_1^T \\ x_2^T \\ \cdots \\ x_n^T \end{bmatrix}$$

Least Squares in d-Dimensions

- The linear least squares model in d-dimensions minimizes

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(wx_i - y_i)^2$$

  - w is now a vector
  - $w^T x_i$ (prediction) is inner product of w and x_i (linear combination of features)
  - $\sum_{i=1}^{n}(wx_i - y_i)^2$ (error) is still the sum of squared differences between true y_i and our prediction $w^T x_i$
- Dates back to 1801: Gauss used it to predict location of Ceres
- How do we find the best vector w in d dimensions?
  - Can we set the partial derivative of each variable to 0

Summary

Summary

- Regression considers the case of a numerical y_i
- Least squares is a classic method for fitting linear models
- With 1 feature, it has a simple closed-form solution
- Can be generalized to d features
  - What does the regression look like in 2 dimensions?
- There are many more regression models
  - Model trees, regression trees

Literature

- Machine Learning – Tom Mitchell
- Pattern Recognition and Machine Learning – Christopher Bishop
- Data Mining – Jiawei Han, Micheline Kamber, Jian Pei
- Data Mining – Ian Witten, Eibe Frank, Mark Hall, Christopher Pal

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Thank you for your attention!

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