Lecture 8: Regression Trees

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Outline

1. Regression
2. Linear Regression
3. Regression Trees

Regression and Linear Regression

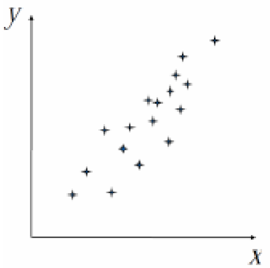
Supervised Learning

- **Dataset:**
  - Training (labeled) data: $D = \{(x_i, y_i)\}$
  - $x_i \in \mathbb{R}^d$
  - Test (unlabeled) data: $x_0 \in \mathbb{R}^d$
- **Tasks:**
  - Classification: $y_i \in \{1, 2, \ldots, C\}$
  - Regression: $y_i \in \mathbb{R}$
- **Objective:** Given x_0, predict y_0
- **Supervised** learning as y_i was given during training

Regression

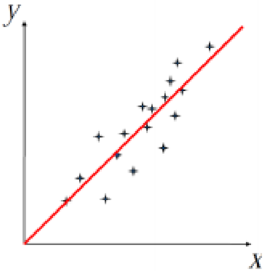
- Predict cost of house from details
- Predict job salary from job description
- Predict SAT, GRE scores
- Predict future price of Petrol from past prices
- Predict future GDP of a country, valuation of a company

Linear Regression : One-dimensional Case



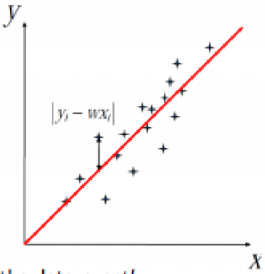
- **Given:** a set of N input-response pairs
- The inputs (x) and the responses (y) are one dimensional scalars
- **Goal:** Model the relationship between x and y

Linear Regression : One-dimensional Case



- Let's assume the relationship between x and y is linear
- Linear relationship can be defined by a straight line with *parameter* w
- Equation of the straight line: $y = wx$

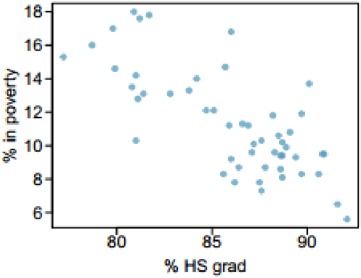
Linear Regression : One-dimensional Case



- The line may not fit the data *exactly*
- But we can try making the line a reasonable approximation
- Error for the pair (x_i, y_i) pair: $e_i = y_i - wx_i$
- The total squared error: $E = \sum_{i=1}^{N} e_i^2 = \sum_{i=1}^{N} (y_i - wx_i)^2$
- The best fitting line is defined by w minimizing the total error E
- Just requires a little bit of calculus to find it (take derivative, equate to zero..)

Linear Regression: Poverty vs HS Graduation Rate

The *scatterplot* below shows the relationship between HS graduate rate in all 50 US states and DC and the % of residents who live below the poverty line (income below $23,050 for a family of 4 in 2012).



Response variable?

% in poverty

Explanatory variable?

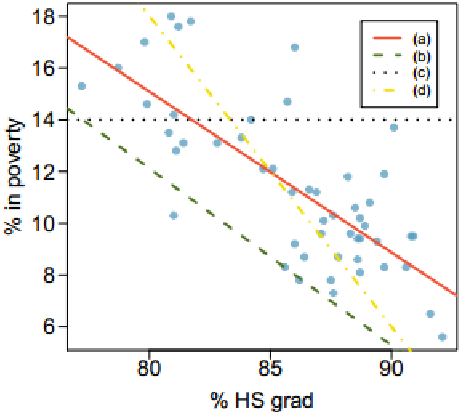
% HS grad

Relationship?

linear, negative, moderately strong

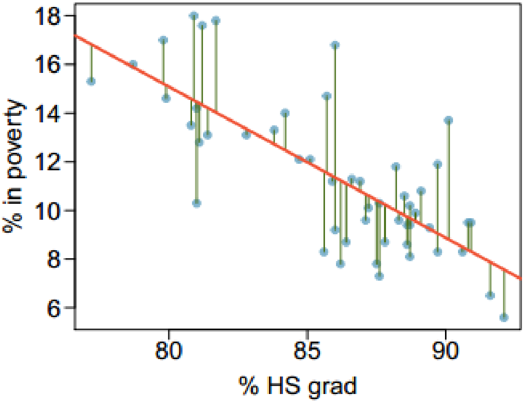
Linear Regression: Poverty vs HS Graduation Rate

Which of the following appears to be the line that best fits the linear relationship between % in poverty and % HS grad? Choose one.



Residuals

Residuals are the leftovers from the model fit: Data = Fit + Residual

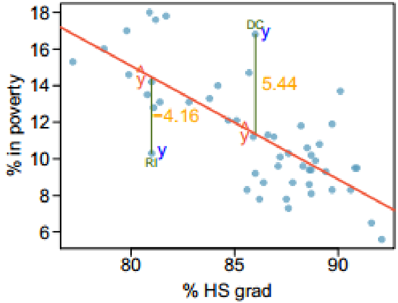


Residuals

Residual

Residual is the difference between the observed (y_i) and predicted $\hat{y}_i$.

$$e_i = y_i - \hat{y}_i$$



- % living in poverty in DC is 5.44% more than predicted.
- % living in poverty in RI is 4.16% less than predicted.

A measure for the best line

- We want a line that has small residuals:
  1. Option 1: Minimize the sum of magnitudes (absolute values) of residuals

$$|e_1| + |e_2| + \cdots + |e_n|$$

  2. Option 2: Minimize the sum of squared residuals – *least squares*

$$e_1^2 + e_2^2 + \cdots + e_n^2$$

- Why least squares?
  1. Most commonly used
  2. Easier to compute by hand and using software
  3. In many applications, a residual twice as large as another is usually more than twice as bad

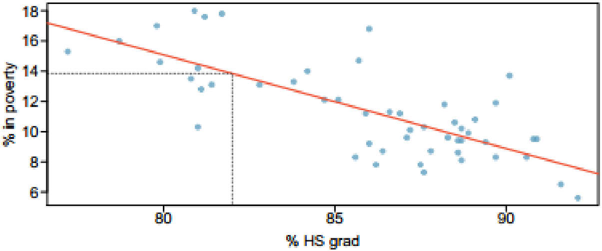
Least Squares Line

$$\hat{y} = \beta_0 + \beta_1 x$$

predicted y *intercept* *slope* *explanatory variable*

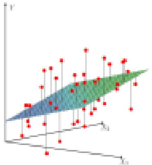
Prediction

- Using the linear model to predict the value of the response variable for a given value of the explanatory variable is called *prediction*, simply by plugging in the value of x in the linear model equation.
- There will be some uncertainty associated with the predicted value.



Linear Regression in Higher Dimensions

- **Analogy to line fitting:** In higher dimensions, we will fit hyperplanes
- For 2-dim. inputs, linear regression fits a 2-dim. plane to the data



- Many planes are possible. Which one is the best?
- **Intuition:** Choose the one which is (on average) closest to the responses Y
  - Linear regression uses the sum-of-squared error notion of closeness
- Similar intuition carries over to higher dimensions too
  - Fitting a D-dimensional hyperplane to the data
  - Hard to visualize in pictures though..
- The hyperplane is defined by parameters $\mathbf{w}$ (a $D \times 1$ weight vector)

Linear Regression in Higher Dimensions

- Given training data $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$
- Inputs $\mathbf{x}_i$: D-dimensional vectors ($\mathbb{R}^D$), responses y_i: scalars ($\mathbb{R}$)
- The linear model: response is a linear function of the model parameters

$$y = f(\mathbf{x}, \mathbf{w}) = b + \sum_{j=1}^{M} w_j \phi_j(\mathbf{x})$$

- w_j's and b are the model parameters (b is an offset)
    - Parameters define the mapping from the inputs to responses
- Each ϕ_j is called a basis function
    - Allows change of representation of the input $\mathbf{x}$ (often desired)

Linear Regression in Higher Dimensions

The linear model:

$$y = b + \sum_{j=1}^{M} w_j \phi_j(\mathbf{x}) = b + \mathbf{w}^T \phi(\mathbf{x})$$

- $\phi = [\phi_1, \ldots . \phi_M]$
- $\mathbf{w} = [w_1, \ldots, w_M]$, the **weight vector** (to learn using the training data)
- We consider the simplest case: $\phi(\mathbf{x}) = \mathbf{x}$
  - $\phi_j(\mathbf{x})$ is the j-th feature of the data (total D features, so $M = D$)
- The linear model becomes

$$\boxed{y = b + \sum_{j=1}^{D} w_j x_j = b + \mathbf{w}^T \mathbf{x}}$$

- **Note:** Nonlinear relationships between $\mathbf{x}$ and y can be modeled using suitably chosen ϕ_j's (more when we cover Kernel Methods)

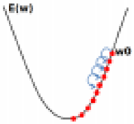
Linear Regression: Objective Function

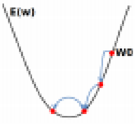
- Parameter $\mathbf{w}$ that satisfies $y_i = \mathbf{w}^T \mathbf{x}_i$ *exactly* for each i may not exist
- So we look for the closest approximation
- Specifically, $\mathbf{w}$ that minimizes the following sum-of-squared-differences between the truth (y_i) and the predictions ($\mathbf{w}^T \mathbf{x}_i$), just as we did for the one-dimensional case:

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

Linear Regression: Gradient Descent based Solution

- The least-squares linear regression objective is a convex function
  - It has a unique minimum
  - Gradient descent will find the unique minimum (or get very close it to, depending in the learning rate α)
  - For general functions, GD can only find a local minimum
- Effect of the learning rate α (left: small α, right: large α)

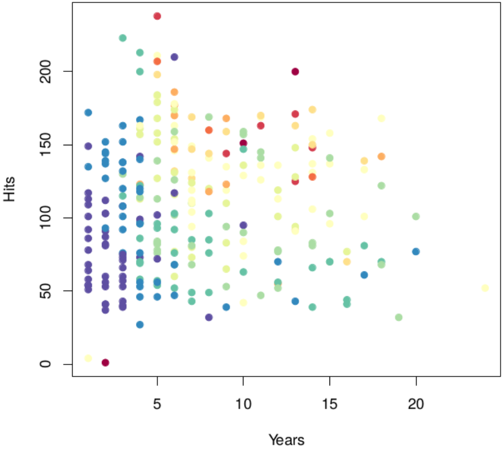




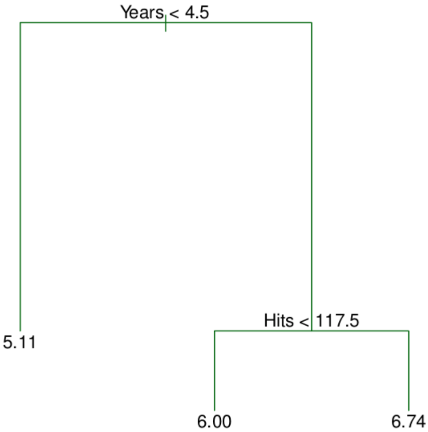
Regression Trees

Predicting Baseball salary data

Salary is color-coded from low (blue, green) to high (yellow,red)

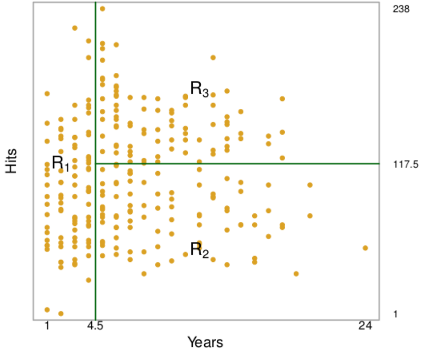


Decision tree for Baseball Salary Prediction

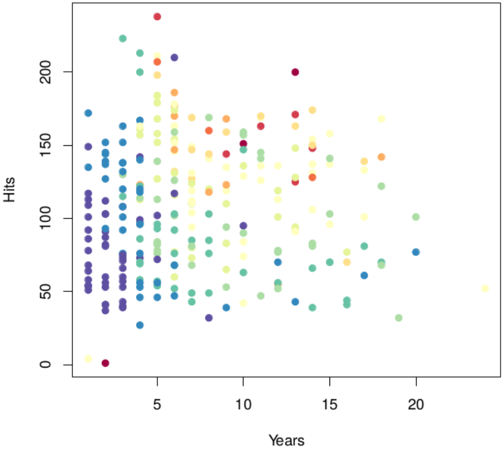


Decision tree for Baseball Salary Prediction

- Overall, the tree stratifies or segments the players into three regions of predictor space: R_1 ={X | `Years`< 4.5}, R_2 ={X | `Years`>=4.5, `Hits`<117.5}, and R_3 ={X | `Years`>=4.5, `Hits`>=117.5}.



Interpreting the Decision Tree



Interpreting the Decision Tree

- Years is the most important factor in determining Salary, and players with less experience earn lower salaries than more experienced players.
- Given that a player is less experienced, the number of Hits that he made in the previous year seems to play little role in his Salary .
- But among players who have been in the major leagues for five or more years, the number of Hits made in the previous year does affect Salary , and players who made more Hits last year tend to have higher salaries.
- Surely an over-simplification, but compared to a regression model, it is easy to display, interpret and explain

High Level Idea

- We divide the feature space into J distinct and non-overlapping regions $R_1, R_2, \dots, R_J$
- For every observation that falls into the region R_i, we make same prediction, which is simply the mean of the response values for the training observations in R_i
- **Objective:** Find boxes $R_1, R_2, \dots, R_J$ that minimizes Residual Sum of Square (RSS)

$$RSS = \sum_{i=1}^{J} \sum_{j \in R_i} (y_j - \widehat{y_{R_i}})^2$$

where $\widehat{y_{R_i}}$ is the mean response for the training in the i-th box.

Building Regression Trees

- We first select the feature X_i and the cutpoint s such that splitting the feature space into the regions $\{X|X_i < s\}$ and $\{X|X_i \geq s\}$ leads to the greatest possible reduction in RSS.
- Next, we repeat the process, looking for the best attribute and best cutpoint in order to split the data further so as to minimize the RSS within each of the resulting regions.
- The process continues until a stopping criterion is reached; for instance, we may continue until no region contains more than five observations.

Summary

Major Concepts:

- Geometric interpretation of Classification
- Decision trees

Slide Material References

- Slides from ISLR book
- Slides by Piyush Rai
- Slides from OpenIntro Statistics book (http://www.webpages.uidaho.edu/~stevel/251/slides/os2_slides_07.pdf)
- See also the footnotes