CSE 4/587 Data Intensive Computing

Dr. Eric Mikida epmikida@buffalo.edu 208 Capen Hall

Dr. Shamshad Parvin shamsadp@buffalo.edu 313 Davis Hall

Models and Algorithms

Intro to Modeling Algorithms

- At this point, we have clean data, we have some intuition about it, and we've extracted just the parts of the data we are interested in
- Now, we can move to modeling to start getting useful information out of our data
- Two different types of algorithms/models
 - Optimization algorithms for parameter estimation
 - Machine learning algorithms

Optimization Algorithms

- These algorithms attempt to determine the parameters of the process from which the data is generated
- Once we have the parameters, we can use the resulting functions to predict new outcomes
- These algorithms also attempt to quantify the uncertainty; they attempt to give a measure of how good the prediction is
- Examples: Least squares, newton's methods, stochastic gradient descent

Machine Learning Algorithms

- These algorithms attempt to predict, classify, and cluster data
- Don't often make any claims about the degree of uncertainty
- Basis of Al

"Models" vs "Algorithms"?

- Distinction between the two is fuzzy at best
- Models come from the math side (statistics)...sort of
 - Equations which attempt to model the actual process at hand
 - Come with some measure of uncertainty
- Algorithms come from the computer science side (ML)...sort of
 - Set of steps required to achieve some result
 - Not designed (generally) to capture the underlying process, just to predict the outcome with the most accuracy

- Very simple conceptually
- Expresses the relationship between two (or more) variables/attributes
- Assume a linear relationship between an outcome variable (also called dependent variable, response variable or label) and the predictor variable(s) (aka independent variables, features, explanatory variables)
- What if the relationship isn't linear?
 - Linear is a good starting point...
 - o ...but we can also look at other relationships after we get the basics down

• Specifically, we assume the underlying data is related in the real world by a function of the form: $y = f(x) = \beta_0 + \beta_1 x$

• Specifically, we assume the underlying data is related in the real world by a function of the form: $y = f(x) = \beta_0 + \beta_1 x$

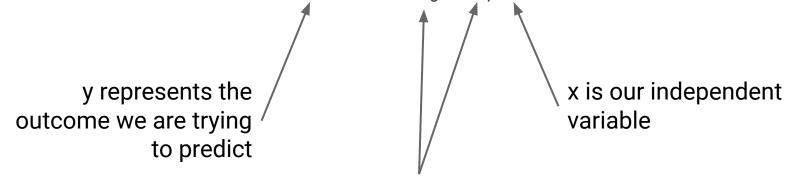
y represents the outcome we are trying to predict

• Specifically, we assume the underlying data is related in the real world by a function of the form: $y = f(x) = \beta_0 + \beta_1 x$

y represents the outcome we are trying to predict

x is our independent variable

• Specifically, we assume the underlying data is related in the real world by a function of the form: $y = f(x) = \beta_0 + \beta_1 x$



 β_0 and β_1 are the parameters we are trying to solve for

Subscriber Revenue

Take the following table of monthly revenue and subscriber

count:

Subscribers (x)	Revenue (y)
5	125
10	250
15	375
20	500

Subscriber Revenue

Take the following table of monthly revenue and subscriber

count:

Subscribers (x)	Revenue (y)
5	125
10	250
15	375
20	500

In this case it's clear that y=25x.

Notice that in this case, we actually know the truth of the model. The website charges \$25 for a subscription.

The model is attempting to capture that.

Friends vs Time Spent

Now take the following table:

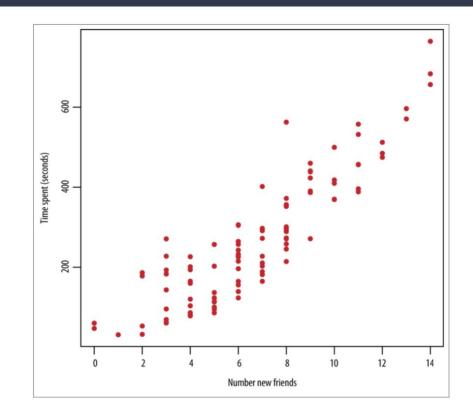
New Friends (x)	Time Spent (y)
7	276
3	43
4	83
6	136
10	417

In this case, the data represents the amount of time a user spends on a social media site, compared to the number of new friends they've added this week.

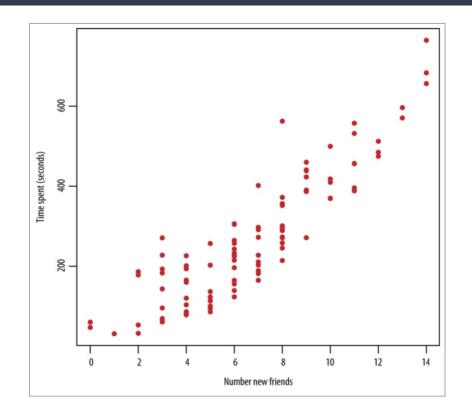
What does our intuition say?

What does the data look like?

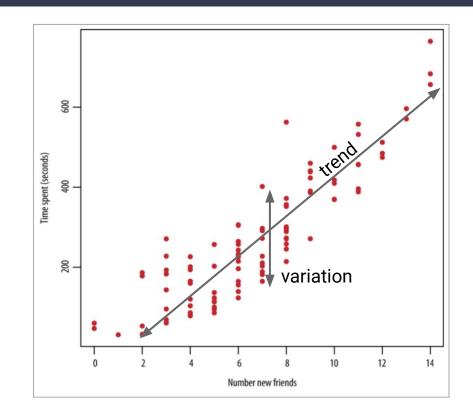
- The right shows a plot of the dataset where the table came from
- We do see a generally linear looking relationship
- This time the model isn't deterministic...but can we estimate it?



- We want to capture 2 factors: trend and variation
- Assume a linear relationship $(y=\beta_0 + \beta_1 x)$
- Now we must "fit" the model use an algorithm to find the best values of β_0 and β_1



- We want to capture 2 factors: trend and variation
- Assume a linear relationship $(y=\beta_0 + \beta_1 x)$
- Now we must "fit" the model use an algorithm to find the best values of β_0 and β_1

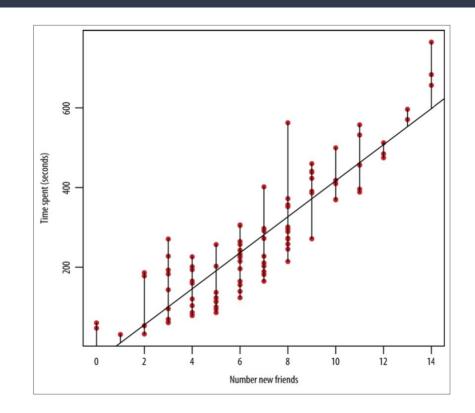


Fitting a Model

- Find the values of β_0 and β_1 that yield the "best" line
- What do we mean by "best"?
 - For now, the line that is on average closest to all the points
 - Closeness measured as vertical distance squared
- Therefore, we want the function that minimizes the sum of the squares for all points
 - This is called, unsurprisingly, least squares estimation

Fitting Our Example

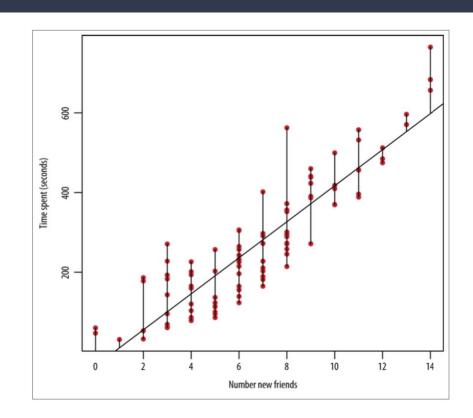
- Running the data through a solver yields $\beta_0 = -32.08$ and $\beta_1 = 45.92$
- How confident are we in this model?
- If we have a new user, with 5 new friends, can we predict how much time they'll spend?



Fitting Our Example

- Running the data through a solver yields $\beta_0 = -32.08$ and $\beta_1 = 45.92$
- How confident are we in this model?
- If we have a new user, with 5 new friends, can we predict how much time they'll spend?

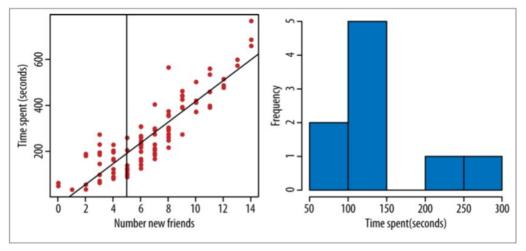
...This, afterall, is the whole goal for modeling in the first place, right?



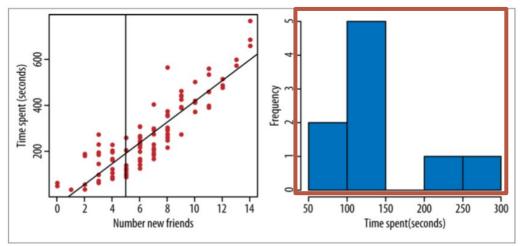
Next Steps...

- We have an initial model, how can we build on it?
 - Evaluate our model and add error terms
 - Add in more predictors
 - Transform the predictors

- With our model so far, predictions are deterministic
 - We claim that for a given x, the outcome will be y
 - However, our data has some amount of variability



- With our model so far, predictions are deterministic
 - We claim that for a given x, the outcome will be y
 - However, our data has some amount of variability



How do we capture this variability?

- Add in an error term, ϵ : $y = \beta_0 + \beta_1 x + \epsilon$
 - Referred to as noise
 - Represents relationships you have not accounted for
 - This term captures the difference between our observations, and the true regression line

- Add in an error term, ϵ : $y = \beta_0 + \beta_1 x + \epsilon$
 - Referred to as noise
 - Represents relationships you have not accounted for
 - This term captures the difference between our observations, and the true regression line

Remember, our data is just a trace of the real world. It is incomplete. It has uncertainty. We can only estimate the true regression line.

Noise attempts to capture this fact.

Finding Noise

- A common first assumption is that noise follows a normal distribution
 - \circ $\epsilon \sim N(0, \sigma^2)$
 - It then follows that $p(y|x) \sim N(\beta_0 + \beta_1 x, \sigma^2)$
 - \circ We have already found $β_0$ and $β_1$
 - \circ σ^2 is the mean squared error (roughly the sum of all of the observed error squared, divided by n-2)

Finding Noise

- A common first assumption is that noise follows a normal distribution
 - \circ $\epsilon \sim N(0, \sigma^2)$
 - It then follows that $p(y|x) \sim N(\beta_0 + \beta_1 x, \sigma^2)$
 - \circ We have already found $β_0$ and $β_1$
 - \circ σ^2 is the mean squared error (roughly the sum of all of the observed error squared, divided by n-2)

 $\beta_0 + \beta_1 x$

Our prediction now becomes: Given x = 5, we predict y is a random variable with the distribution shown to the right.

Evaluating Our Model

- How can we be certain our model is good?
- Many solvers will compute a few heuristics to help
 - o R² captures the amount of the variance explained by our model
 - High R² means we've captured most of the variance
 - p-values captures the likelihood that our coefficients are "unimportant"
 - Low p-values means our coefficients are likely significant
- We can also cross validate ourselves!
 - Divide the data into training data and test data.
 - \circ Fit the model on the training data to find β and ϵ
 - Calculate mean squared error on the test data and see if it's consistent

Extending Our Model

- Add more predictors...
 - $o y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \epsilon$
 - Fit using the package of your choice
 - May even have interaction between predictors
- Transformation on predictors
 - Why did we assume linear...what about $y = \beta_0 + \beta_1 x + \beta_2 x^2 + ...$
 - We can still use linear regression:
 - \blacksquare assume $z = x^2$
 - Now do a linear regression based on z