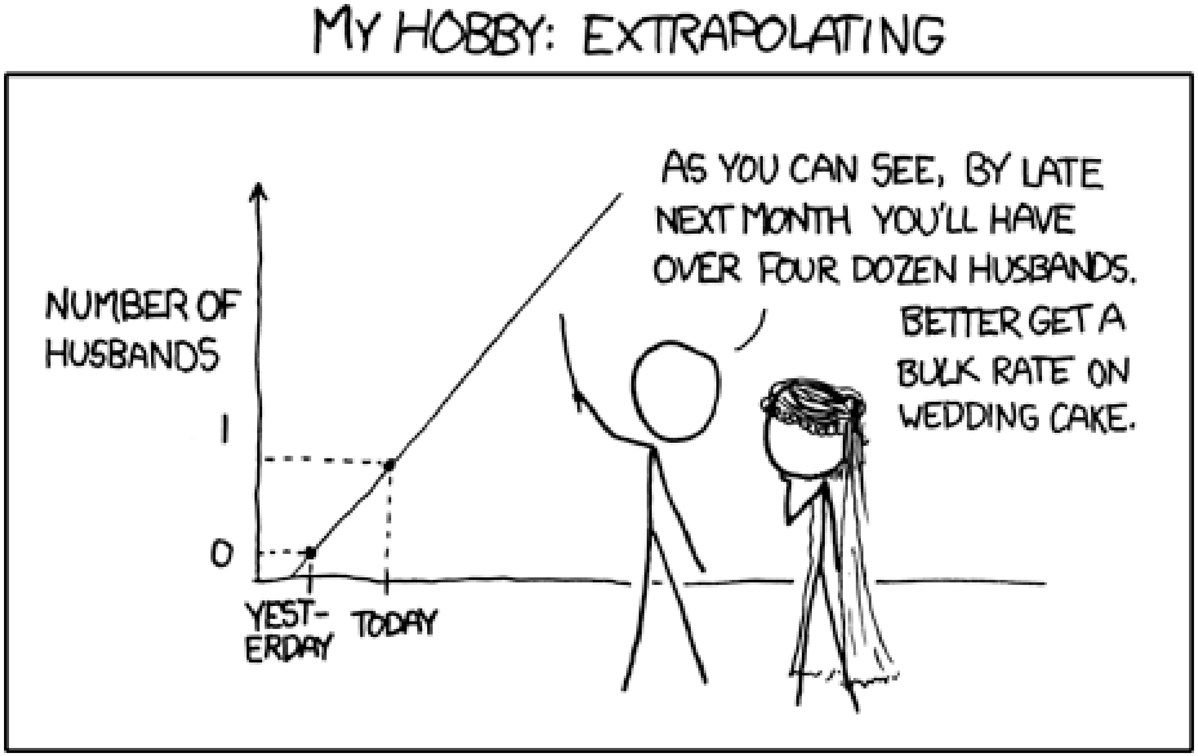
UNIVERSITY of WASHINGTON

Data Science UW Methods for Data Analysis

SVD, More Regression and Intro to Time Series
Lecture 6
Nick McClure


MY HOBBY: EXTRAPOLATING
NUMBER OF HUSBANDS
1
0
YEST-ERDAY
TODAY
AS YOU CAN SEE, BY LATE NEXT MONTH YOU'LL HAVE OVER FOUR DOZEN HUSBANDS.
BETTER GET A BULK RATE ON WEDDING CAKE.

Topics

- Review
- Linear Algebra overview
- Decomposition Methods
- Lasso Regression
- Ridge Regression
- Logistic Regression
- Binary Classification
- Time Series

Review

- Linear Regression
- Multiple Regression
- Introduction to Python / iPython
- Introduction to Graph Theory
  - Gephi Visualization
  - Degree Distribution Tests

Linear Algebra

- Matrix: a rectangular array of values, with dimensions n by m (n rows, m columns).
- Vector: a one dimensional array of values (n or m = 1).
- Square matrix: a n x n matrix.
- Identity matrix: a square matrix with 1’s on the diagonal and 0’s elsewhere.
- R demo.

Linear Algebra

> Algebraic Properties of Matrices:

- Add/subtract matrices: Must be of the same dimensions
- Multiplication of matrices:
  > Inner dimensions must match.

$$\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} \times \begin{bmatrix} j & k & l \\ m & n & o \\ p & q & r \end{bmatrix} =$$

$$\begin{bmatrix} aj + bm + cp & ak + bn + cq & al + bo + cr \\ dj + em + fp & dk + en + fq & dl + eo + fr \\ gj + hm + ip & gk + hn + iq & gl + ho + ir \end{bmatrix}$$

- [n x m] * [m x p] = [n x p]

- Note that matrix multiplication is not commutative

Linear Algebra

> Identity matrix: just like 1 is the multiplicative identity.
  - 5*1=5

$$\begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix}$$

<u>Identity matrix</u>: a square matrix of zeros with 1's on the diagonal. Also written as I_{nxn}

Linear Algebra

- Transpose (given an element in position i,j, the transpose has the same element in position j,i.)
- Inverse:
  - Just like the multiplicative inverse of n is 1/n, matrices also have multiplicative inverses:

$$A_{nxn} \cdot A_{nxn}^{-1} = I_{nxn}$$

$$A_{nxn}^{-1} \cdot A_{nxn} = I_{nxn}$$

$$\begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} \cdot \begin{bmatrix} -2 & \frac{3}{2} \\ 1 & -\frac{1}{2} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Linear Algebra

- For a 2x2 matrix:

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, A^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ c & d \end{bmatrix}$$

- What if (ad-bc) = 0? That means that ad=bc or a/c = b/d.
- If a/c = b/d, then one of the columns is a multiple of the other!
- These columns are dependent on each other.
  - If these were columns in our numerical data frame, then one column would be a multiple of the other.
  - Examples: Using meters and Kilometers as separate predictors.

Linear Algebra

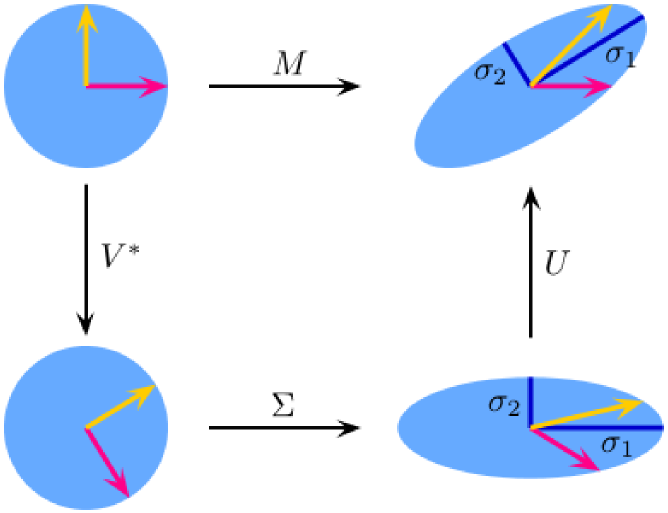
- Eigenvalues: Given a nxn matrix, A, λ is an eigenvalue if there exists a vector X such that:

$$AX = \lambda X$$

- Finding the eigenvectors of A involves lots of computation.
- If A rotates and shifts a vector X, then we can think of eigenvalues as a geometric hinge on which the ‘A’ operation acts.
- Eigenvalues have corresponding eigenvectors.
- This may seem insignificant at the moment, but eigenvalues and eigenvectors play an important role in manipulating our data.

Linear Algebra

- Matrix Decompositions allow us to write a matrix, M, in many different forms.
- The one that is the most used, is Singular Value Decomposition (SVD).
- The SVD is a way to express a transformation from one nxn space (the space M lies in) to another nxn space by writing M as a product of three matrices, say M=VSU.



$$M = U \cdot \Sigma \cdot V^*$$

Linear Algebra

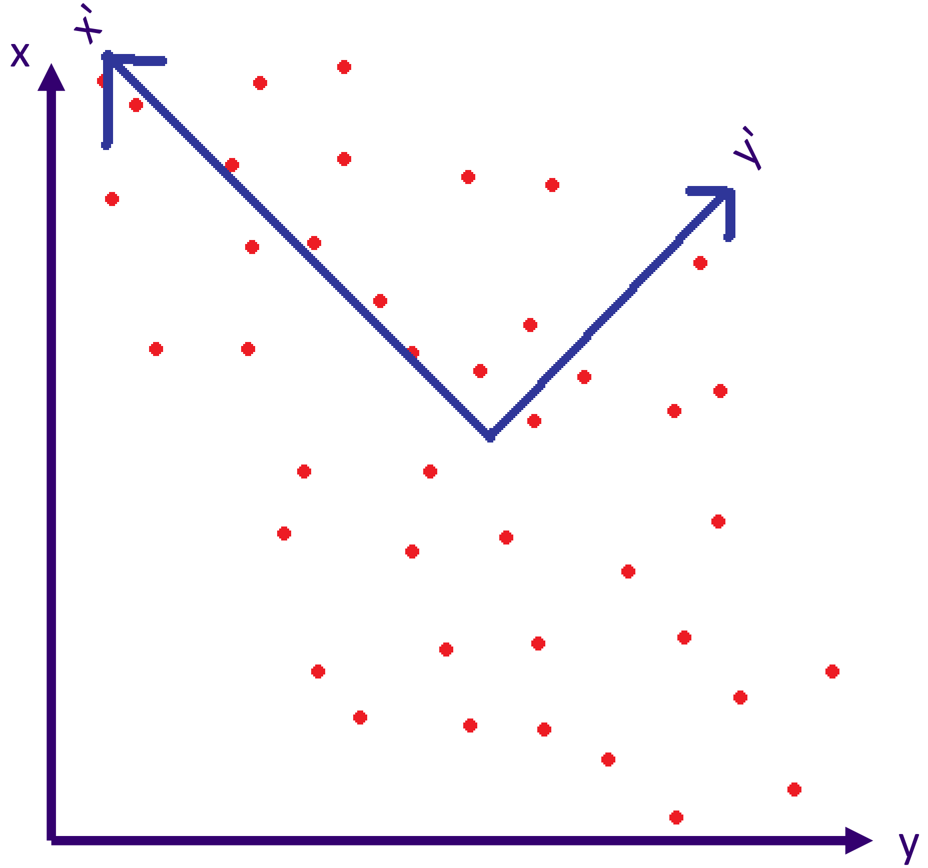
- These three matrices, say, V,S,U, (M = V*S*U), have very specific properties that we can use to our advantage when describing a data set.
- R-demo.

Deriving Independent Features from Dependence

- With larger data sets, we've seen that no matter the quality, we can find a explanatory feature.
- If we consider our data as a matrix, we know that having dependent columns is a problem.
- Solutions:
  - Remove columns that do not contain enough 'information'.
    - Too much missing data.
    - Low Variance.
  - Remove columns that are correlated
  - Maybe we can transform our axes such that our data is more independent?

Possible Axis Transformations

- If two variables are correlated, we can transform both of the axes to directions in which they are not correlated.
- These new axes are called the Principal Components.



SVD

- This transformation is called the Singular Value Decomposition, or SVD.
- It holds true for as many features (dimensions) as we wish to choose, up to the number of original dimensions.
- Each of the new axes is some function of all the old axes.
- The SVD assures us that:
  - The first axis explains the most variation, the second axis the most variation after the first, and so on.
  - All axes are right-angled to each other (orthogonal).
- Usually, we keep less than the original amount of axes, so that we can reduce the amount of dimensions we have to keep track of.

SVD

- Know that instead of our original system:

$$y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots$$

- We now have the system:

$$y_i = \beta_0 + \beta_1 f_1(x_1, x_2, \ldots) + \beta_2 f_2(x_1, x_2, \ldots) + \cdots$$

- The *f* functions are called our principle components.
- The *f* function outputs are guaranteed to be independent of each other.
- We can no longer interpret our linear model coefficients!

SVD

> SVD returns the same amount of components as our number of features.

> Since these are *all* orthogonal, the first few will explain much more variance than the last few axes. How do we decide how many to keep?

> We look at the magnitude of the associated eigenvalues for each principal component.

> R-demo.

SVD

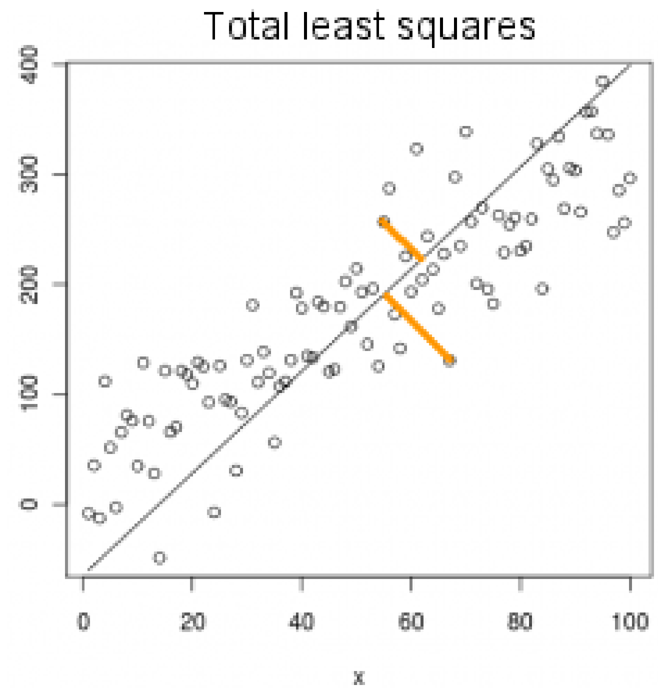
- This seems like an awful lot of work for little improvement and loss of interpretability.
- But note that we lost the dependence in the data set!
- There are other applications as well…

SVD, as a type of regression

> Also, looking at the first principal component, we can consider SVD as a new type of regression, which is called total least squares. (Also called Deming regression or PCA Regression)

Regressing y on x

SVD Primary Principal Component



> R demo

SVD, as a type of regression

- When to use total least squares:
  - If we want to control for error in x as well as y.
  - We are minimizing the distance from the point to the line as opposed to the distance between the y-values.
- R-squared doesn’t really apply here, at least in the way we have defined it.

SVD, as a way to compress information

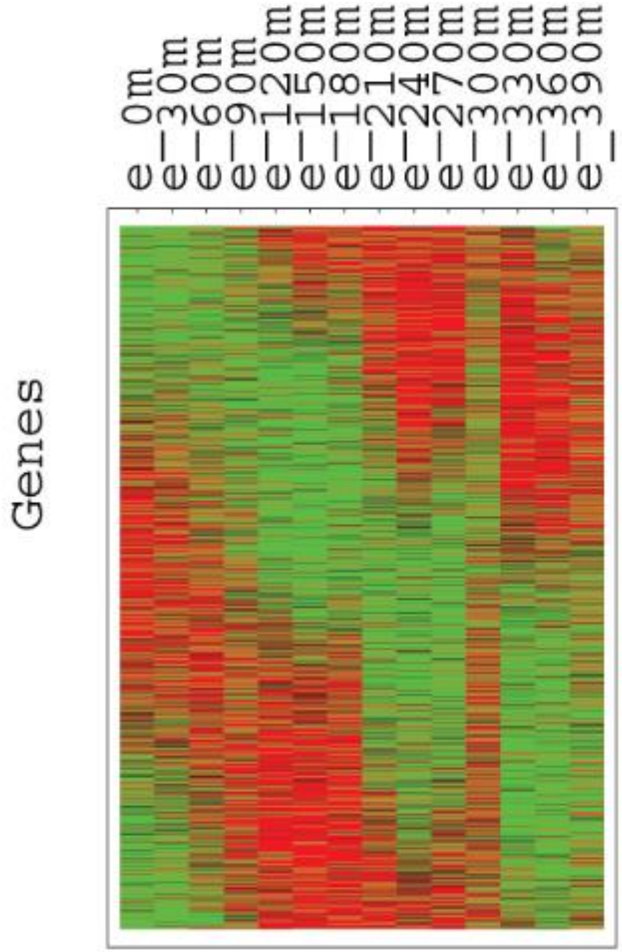
> We can group together similar points via SVD and store them as multiples of principal components.

> R-demo.

SVD, as a way to cluster data

> We can group together similar points via which SVD component is closest to representing original point.

- One of the most common uses is clustering individuals or genes as it pertains to RNA expression.
- In the microarray to the right, red represents absence of expression and green represents over expression.
- Each row is a gene (thousands of them) and each column is a sample (or patient).



Ridge Regression

- Ridge regression is a way to limit the amount of independent variables in the regression.
- Our regular least squares criterion minimizes the least squares of the error plus a regularization term that is a product of a constant and the sum of squared coefficients :

$$\min \sum (y - y_i)^2 + \alpha \sum \beta^2$$

- Essentially this is preventing the partial slope terms from getting too large.

Lasso Regression

- Lasso regression is another way to limit the amount of independent variables in the regression.
- Our regular least squares criterion minimizes the least squares of the error:

$$\min \sum (y - y_i)^2$$

- Lasso regression minimizes the same with the addition of a 'regularization' term:

$$\min \sum \left(y - y_j\right)^2 \quad \text{Such that} \quad \sum |\beta_i| < \lambda$$

- Here, y is the predicted for j points. There are i terms with beta coefficients. Lambda is a fixed value that limits the betas.

Using Linear Regression to Predict Limited Dependent Variables

> Let’s say we wanted to predict if someone evacuated their home during hurricane Katrina.

> R demo.

Logistic Regression

> The purpose of logistic regression is to use linear regression to predict a limited dependent variable.

> Usually our dependent variable has 2 outcomes (1 or 0) or occurrence.

> Examples:
  - Bank gives a yes (1) or no (0) outcome to loan applications.
  - Success/Failures of clinical trials.
  - Morbidity outcomes.
  - Marketing outcomes (will a user click on an add).

> Logistic predictions will result in a probability of success.

Logistic Regression

> Logistic regression is also called the 'logit' model:

> Original model:

$$y_i = \beta_0 + \beta_1 x_1 + \varepsilon_0$$

> Logit model:

$$\underbrace{\ln\left[\frac{p_i}{1-p_i}\right]}_{\text{Log-odds-ratio}} = \beta_0 + \beta_1 x_1 + \varepsilon_0$$

> So estimated probabilities follow: (solving for p)

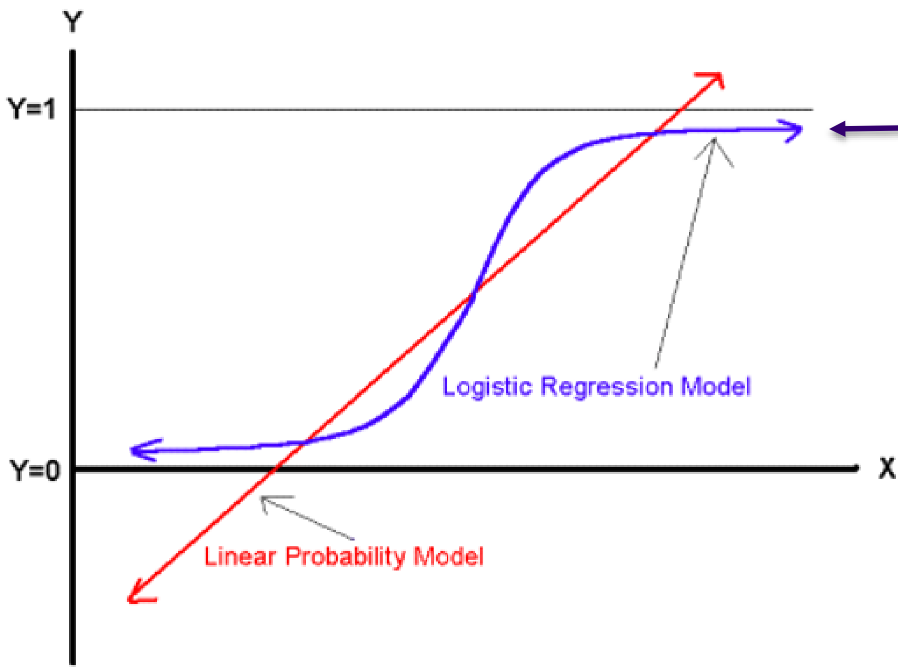
$$p_i = \frac{1}{1+\exp(-(\beta_0 + \beta_1 x_1))}$$

Logistic Regression

$$p_i = \frac{1}{1 + \exp(-(\beta_0 + \beta_1 x_1))}$$

> As $(\beta_0 + \beta_1 x_1)$ gets really big, p approaches 1.

> As $(\beta_0 + \beta_1 x_1)$ gets really small, p approaches 0.



$$\frac{1}{1 + \exp(-x)}$$

Logistic Regression

- Differences between linear and logistic regression.
- Predictions
  - Linear regression outcomes are unbounded.
  - Logistic regression outcomes are bounded between 0 and 1.

$$p_i = \frac{1}{1 + \exp(-(\beta_0 + \beta_1 x_1))}$$

- Error distribution
  - Linear regression errors are normally distributed.
  - Logistic regression errors are Bernoulli distributed.

- R demo

Assignment

- Complete Homework 6:
  - Perform Lasso-Logistic Regression on a subset of Microarray data.
    - Description, dataset and homework hint on Moodle.
  - Data comes from:
    - http://www.ncbi.nlm.nih.gov/pubmed/21532620
  - You should submit:
    - A R-script.
  - Read Introduction to Data Science, Chapter 16.
  - Read two articles about p-values and reproducible research.
  - http://blogs.plos.org/publichealth/2015/06/24/p-values/
  - http://www.science20.com/the_conversation/half_of_biomedical_studies_arent_reproducible_and_what_we_need_to_do_about_that-156696