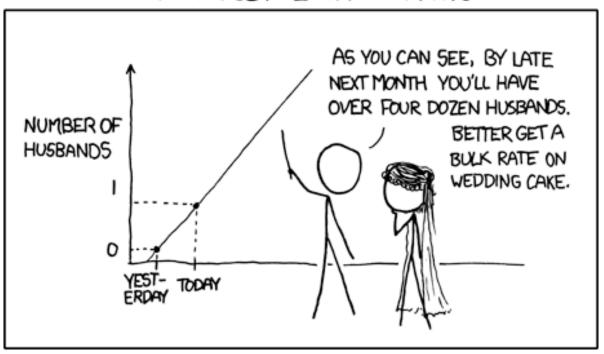
Data Science UW Methods for Data Analysis

SVD and more Regression Lecture 6 Nick McClure



MY HOBBY: EXTRAPOLATING





Topics

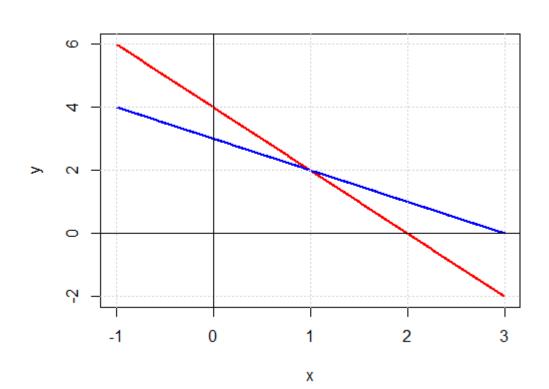
- > Review
- > Linear Algebra overview
- > Decomposition Methods
- > Lasso Regression
- > Ridge Regression
- > Logistic Regression
- > Binary Classification



Motivation

> Consider the system of equations

$$y = -2x + 4$$
$$y = -x + 3$$





Matrix Notation

> When we consider multiple equations, we can write it in short-hand matrix notation.

$$y = -2x + 4$$

$$y = -x + 3$$

$$y = \begin{bmatrix} -2 \\ -1 \end{bmatrix} x + \begin{bmatrix} 4 \\ 3 \end{bmatrix}$$

$$y = \mathbf{M}x + \mathbf{B}$$

> **M**, and **B** are matrices that both have dimension (2x1).



- 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.



> Matrix Transpose: Change rows into columns and viceversa.

$$A = \begin{bmatrix} 1 & 3 & -1 \\ 0 & 1 & 2 \end{bmatrix} \qquad A^T = \begin{bmatrix} 1 & 0 \\ 3 & 1 \\ -1 & 2 \end{bmatrix}$$

$$(A_{n \times m} B_{m \times p})^T = B_{p \times m}^T A_{m \times n}^T$$

> Matrix Trace (square matrices only): sum of the diagonals.

$$A = \begin{bmatrix} 1 & 3 & 2 \\ 0 & 3 & -1 \\ -2 & 1 & 0 \end{bmatrix}$$

$$tr(A) = 1 + 3 + 0 = 4$$



> Matrix addition/subtraction

$$A = \begin{bmatrix} 1 & 3 & -1 \\ 0 & 1 & 2 \end{bmatrix}$$
$$B = \begin{bmatrix} 2 & -1 & 1 \\ -3 & 2 & 0 \end{bmatrix}$$

$$A + B = \begin{bmatrix} 3 & 2 & 0 \\ -3 & 3 & 2 \end{bmatrix}, A - B = \begin{bmatrix} -1 & 4 & -2 \\ 3 & -1 & 2 \end{bmatrix}$$



> Matrix multiplication

 1st matrix row multiplied element wise with 2nd matrix column, then added up.

$$A = \begin{bmatrix} 1 & 3 & -1 \\ 0 & 1 & 2 \end{bmatrix}$$

$$B^T = \begin{bmatrix} 2 & -3 \\ -1 & 2 \\ 1 & 0 \end{bmatrix}$$

$$A \cdot B^T = \begin{bmatrix} 1 \cdot 2 + 3 \cdot -1 + (-1) \cdot 1 & 1 \cdot -3 + 3 * 2 + (-1) * 0 \\ 0 \cdot 2 + 1 \cdot -1 + 2 \cdot 1 & 0 \cdot -3 + 1 \cdot 2 + 2 \cdot 0 \end{bmatrix}$$

$$A \cdot B^T = \begin{bmatrix} -2 & 3\\ 1 & 2 \end{bmatrix}$$

$$A_{(2\times3)} \cdot B_{(3\times2)}^T = [A \cdot B^T]_{(2\times2)}$$



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

$$\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} x \begin{bmatrix} j & k & 1 \\ m & n & o \\ p & q & r \end{bmatrix} =$$

- $[n \times m] * [m \times p] = [n \times p]$
- Note that matrix multiplication is not commutative

$$A \times B \neq B \times A$$



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

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

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



> Matrix Identity
$$\begin{bmatrix} 1 & 2 & -1 \\ -2 & 0 & 1 \\ 3 & 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 2 & -1 \\ -2 & 0 & 1 \\ 3 & 1 & 1 \end{bmatrix}$$

$$A \cdot I = A$$

> Matrix Inverse

$$\begin{bmatrix} 4 & 3 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & -3 \\ -1 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$
$$A \cdot A^{-1} = I$$

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

- > Matrix Division is not Defined.
- > R examples of Matrix operations.



> 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.



$$A \times X$$

Siven a sequence of data points in a matrix, X, which has dimensions 2xn:

$$X = \begin{bmatrix} 1 & 2 & 0 \\ -2 & 3 & 1 \end{bmatrix}$$

> If we multiply by another matrix A (2x2):

$$A_{2x2} \times \begin{bmatrix} 1 & 2 & 0 \\ -2 & 3 & 1 \end{bmatrix}$$

- > Then we can consider A, a matrix that transforms the points in X.
 - More on this later.



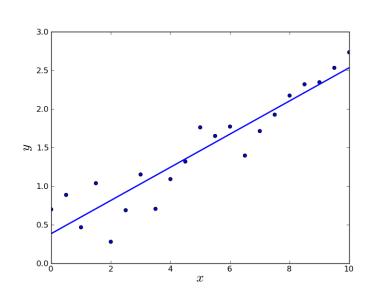
Linear Regression with Matrices

> Consider our linear regression formula.

$$y_i = mx_i + b + \epsilon_i, \epsilon_i \sim N(0, \sigma^2)$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} mx_1 + b \\ \vdots \\ mx_n + b \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

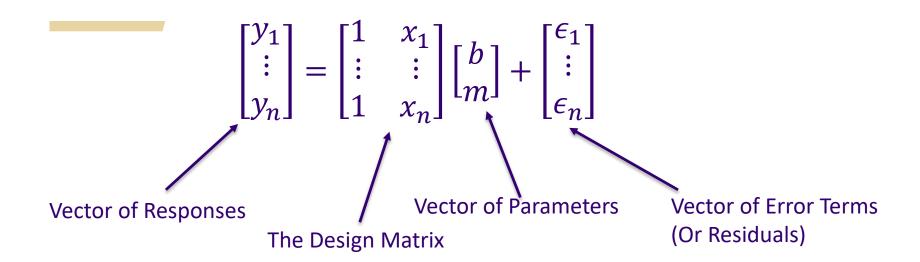


> Matrix Dimensions must agree:

$$(nx1)=(nx2)*(2x1) + (nx1)$$



Linear Regression with Matrices



> In a succinct form:

$$Y = X\beta + \epsilon$$



Consider two points for linear regression. (3,4),(1,1)

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix} \\
\begin{bmatrix} 4 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\
\begin{bmatrix} 1 & 3 \\ 1 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 4 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 1 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 3 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} \\
\begin{bmatrix} 1 & 3 \\ 1 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 4 \\ 1 \end{bmatrix} = \begin{bmatrix} b \\ m \end{bmatrix} \\
\begin{bmatrix} -0.5 & 1.5 \\ 0.5 & -0.5 \end{bmatrix} \begin{bmatrix} 4 \\ 1 \end{bmatrix} = \begin{bmatrix} b \\ m \end{bmatrix} \\
\begin{bmatrix} -0.5 \\ 1.5 \end{bmatrix} = \begin{bmatrix} b \\ m \end{bmatrix}$$



Consider two points for linear regression. (3,4),(3,1)

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$
$$\begin{bmatrix} 4 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

> We run into issues!!!! (ad=bc, which means no inverse).



Consider multiple points for linear regression.

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$Y = X\beta + \epsilon$$
$$Y - X\beta = \epsilon$$

- > How to solve for β ? (Problem when X is not square!)
- > Solution: Minimize ϵ^2 , because $\epsilon^2 = \epsilon^T \epsilon$ is square.



> Solution: Minimize ϵ^2 :

$$\epsilon^{2} = (Y - X\beta)^{T} (Y - X\beta)$$

$$\epsilon^{2} = (Y^{T} - (X\beta)^{T})(Y - X\beta)$$

$$\epsilon^{2} = Y^{T}Y - (X\beta)^{T}Y - Y^{T}X\beta + (X\beta)^{T}X\beta$$

$$\epsilon^{2} = Y^{T}Y - (X\beta)^{T}Y - Y^{T}X\beta + (X\beta)^{T}X\beta$$

> Note that the middle two terms end up being 1d-vectors.

$$\epsilon^{2} = Y^{T}Y - 2(X\beta)^{T}Y + (X\beta)^{T}X\beta$$

$$\epsilon^{2} = Y^{T}Y - 2\beta^{T}X^{T}Y + \beta^{T}X^{T}X\beta$$

> To minimize, 'derivative' set to zero.

$$0 = 2X^{T}Y + 2X^{T}X\beta$$
$$2X^{T}X\beta = 2X^{T}Y$$
$$\beta = (X^{T}X)^{-1}X^{T}Y$$



> Numerical Verification

$$\beta = (X^{T}X)^{-1}X^{T}Y$$

$$\begin{bmatrix} b \\ m \end{bmatrix} = \begin{pmatrix} \begin{bmatrix} 1 & 3 \\ 1 & 1 \end{bmatrix}^{T} \begin{bmatrix} 1 & 3 \\ 1 & 1 \end{bmatrix} \end{pmatrix}^{-1} \begin{bmatrix} 1 & 3 \\ 1 & 1 \end{bmatrix}^{T} \begin{bmatrix} 4 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} 2 & 4 \\ 4 & 10 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} 2.5 & -1 \\ -1 & 0.5 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} -0.5 & 1.5 \\ 0.5 & -0.5 \end{bmatrix} \begin{bmatrix} 4 \\ 1 \end{bmatrix} = \begin{bmatrix} -0.5 \\ 1.5 \end{bmatrix}$$



> This works with higher dimensions as well.

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$Y_{n\times 1} = X_{n\times 2}\beta_{2\times 1} + \epsilon_{n\times 1}$$

$$\beta_{2\times 1} = (X^T_{2\times n} X_{n\times 2})^{-1} X^T_{2\times n} Y_{n\times 1}$$



Multiple Linear Regression

- > This works with Multiple Linear Regression as well.
- > n points, F features.

$$y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_F x_F + \epsilon_i$$

> Remember that a data point for this regression is:

$$(x_1, x_2, \dots, x_F, y)$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{F1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{1n} & \cdots & x_{Fn} \end{bmatrix} \begin{vmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_F \end{vmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$Y_{n\times 1} = X_{n\times F}\beta_{F\times 1} + \epsilon_{n\times 1}$$

$$\beta_{F\times 1} = (X^T_{F\times n}X_{n\times F})^{-1}X^T_{F\times n}Y_{n\times 1}$$



Why Independent Columns?

> Consider the 2x2 inverse formula:

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

- > Even if $ad \neq bc$, and $ad \sim bc$, then we run into very large numbers and the inverse is hard to compute.
- > This holds true for inverses of any size square matrix, when the columns are linearly dependent on each other, the inverse doesn't exist.



The Determinant

> Consider the 2x2 inverse formula:

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

- > The number: ad bc is called the determinant.
- > The determinant is very special and important.
 - It governs when a matrix has an inverse.
 - It tells us how linearly related columns are.
 - It is physically linked to the volume of the 'unit' box which we apply the matrix as a transformation.
 - > The identity matrix is exactly the unit box and has a determinant of 1.
 - > If we multiply a row by a constant, the determinant is multiplied by that constant. (physically expanding or shrinking the box).
 - > This is also used in physics to keep conservation laws by
 - > forcing a volume to stay at 1.

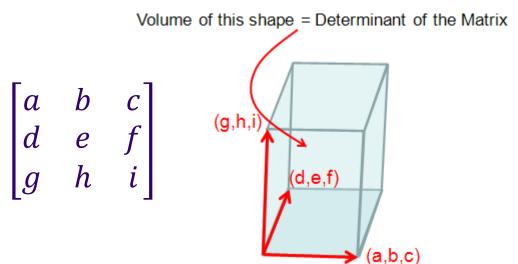


The Determinant

> Consider the 2x2 inverse formula:

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

> The number: ad - bc is called the determinant.





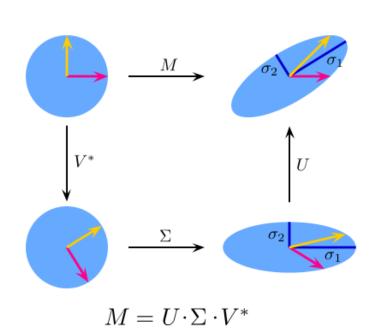
> Eigenvalues: Given a nxn matrix, A, λ is an eigenvalue if there exists a vector X such that:

$$AX = \lambda X$$

- > 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.



- 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.





- > 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.



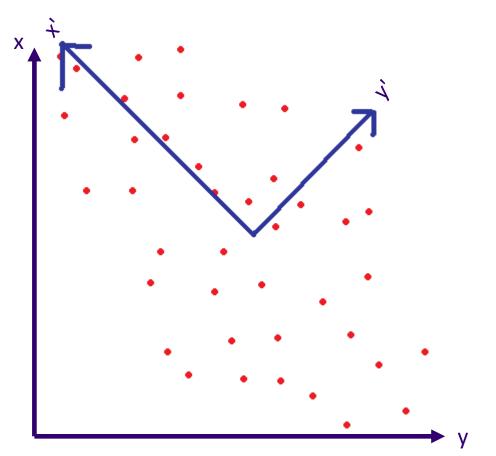
Deriving Independent Features from Dependence

- > 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 data such that our data is more independent?



Possible Data Transformations

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





- > 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.



> 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:

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

- 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 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.



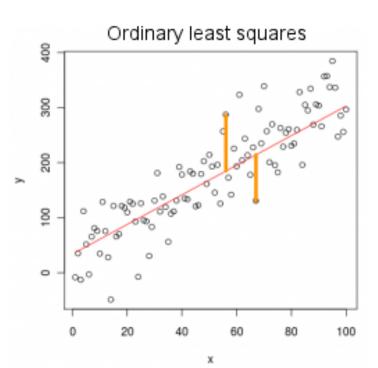
- > This seems like an awful lot of work for little improvement and loss of interpretability.
- > But note that we lost the dependence in the data set!
- > There are other applications as well...



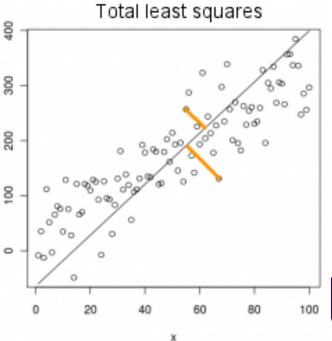
SVD, as a type of regression

 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





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.

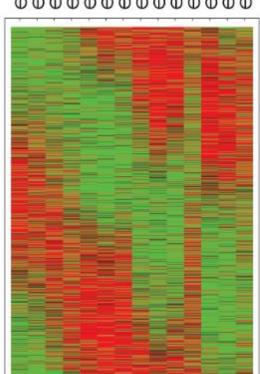


SVD, as a way to cluster data

> 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).





Genes

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:

$$\min \sum (y-y_j)^2$$
 Such that $\sum |\beta_i| < \lambda$

> 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.



- > 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 is also called the 'logit' model:
- > Original model:

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

> Logit model:

$$\ln\left[\frac{p_i}{1-p_i}\right] = \beta_0 + \beta_1 x_1 + \varepsilon_0$$

$$\uparrow$$
Log-odds-ratio

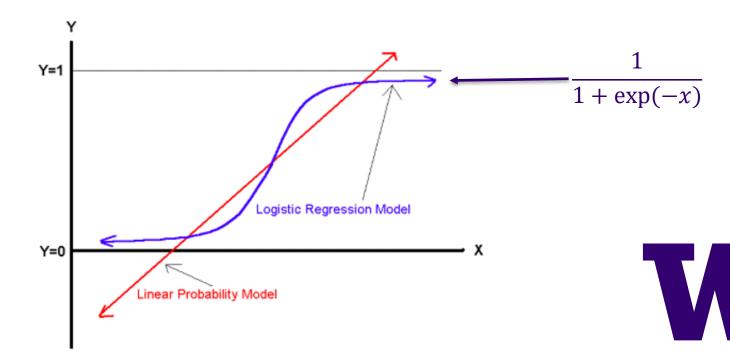
So estimated probabilities follow: (solving for p)

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



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

- > 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.



- > 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 SVD regression on Crime-community data.
 - You should submit:
 - > A R-script (PRODUCTION) and a text/log write up.
 - 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_t hat-156696

