Introduction to Machine Learning – Dimension Reduction

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Slides based off slides courtesy of Jordan Crouser (https://jcrouser.github.io/)

Plan for Today

- Dimension Reduction:
  - Principle components regression
  - Partial least squares
- Linear Models and Regularization Lab

Warm Up: Ri...

- **Ridge Regression-** Find coefficients that minimize:

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2$$

- **The Lasso-** Find coefficients that minimize:

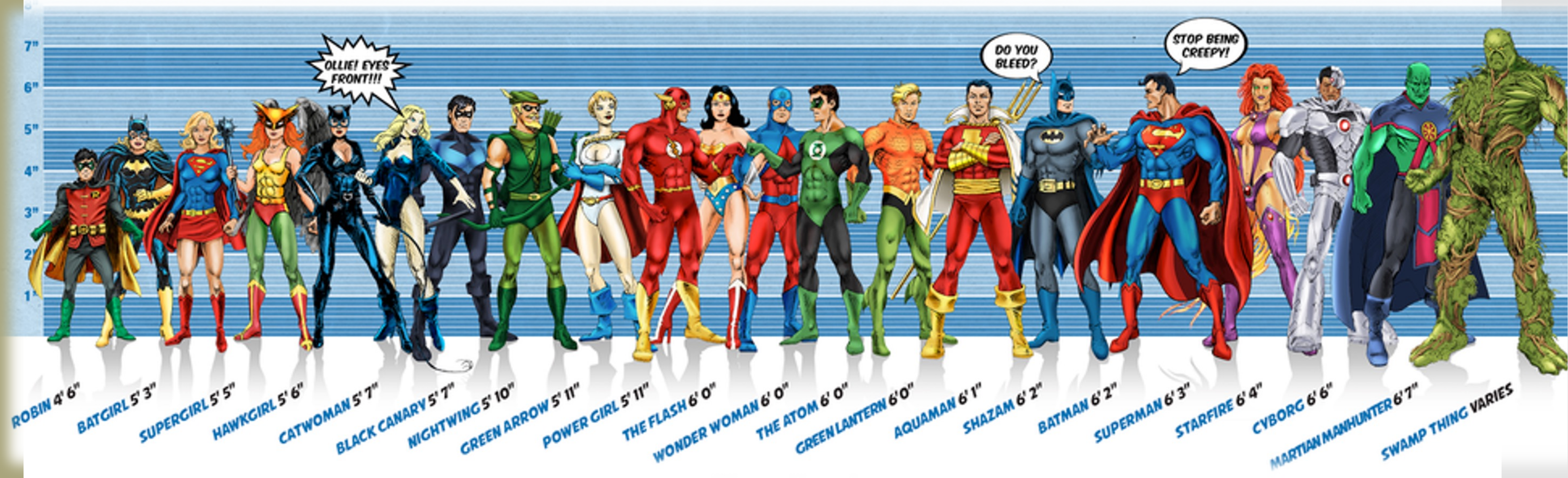
$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\mathrm{B}_j|$$

Suppose you want to predict **Salary** based on **Hits** for baseball players using this data:

Player	Salary	Hits
Alan Ashby	475.0	81
Alvin Davis	480.0	130
Andre Dawson	500.0	141

Write out the equations you need to minimize for ridge regression and the lasso. Once you have the equations use Wolfram Alpha to find the β_0 and β_1 that minimize the equations for $\lambda = 0.5$ and $\lambda = 100$. What do you notice?

Flashback: superheroes



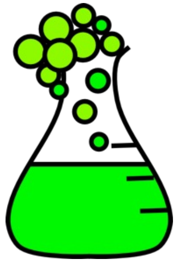
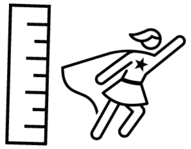
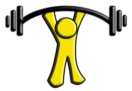
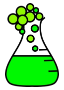
$height = \beta_1$ () $+ \beta_2$ () $+ \beta_3$ ()

Image credit: Ming Malaykham

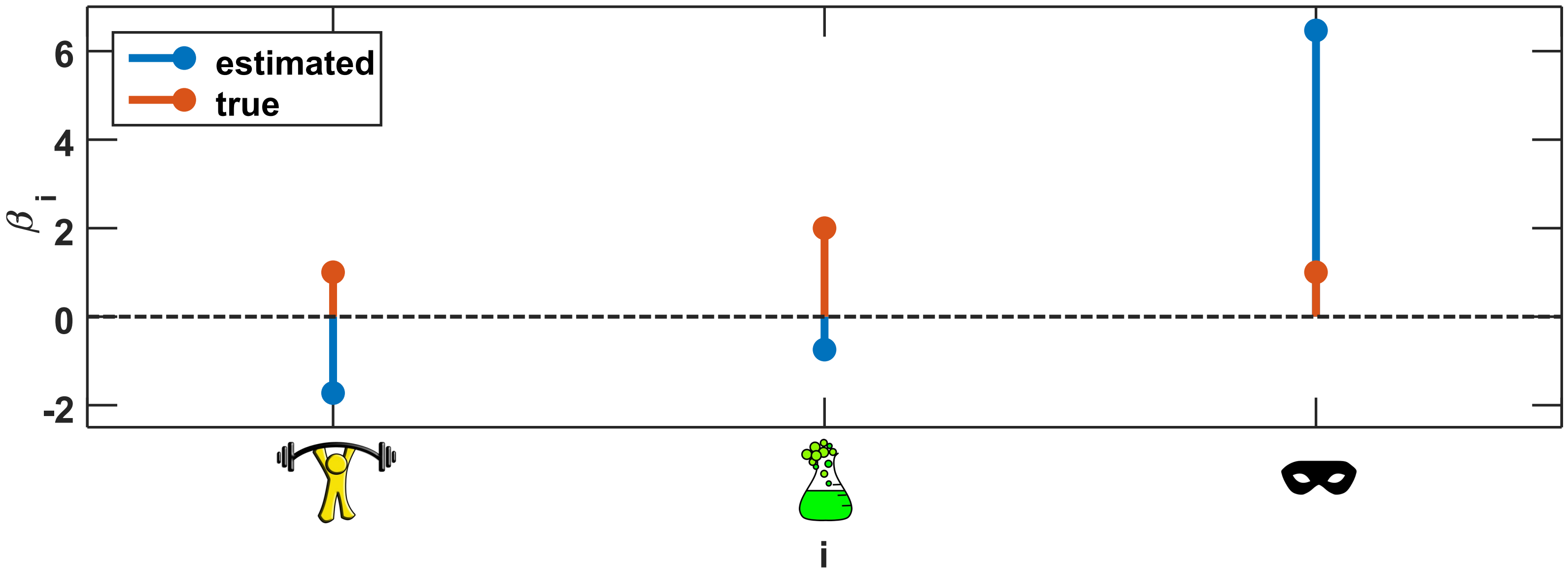
Estimating Height

$$\begin{bmatrix} 232.03 \\ 156.29 \\ 113.82 \\ 229.07 \\ 287.72 \end{bmatrix} = 1\begin{bmatrix} 63.9 \\ 28.9 \\ 54.3 \\ 69.8 \\ 50.4 \end{bmatrix} + 2\begin{bmatrix} 54.0 \\ 45.1 \\ 13.3 \\ 49.5 \\ 85.4 \end{bmatrix} + 1\begin{bmatrix} 59.1 \\ 36.9 \\ 33.7 \\ 59.7 \\ 67.9 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \end{bmatrix}$$

Estimate for β

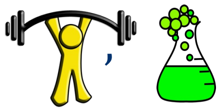
When we try to estimate coefficients using OLS, we get the following:



Notice the (relatively) big difference between actual and estimated coefficients.

What's going on here?

$$\begin{bmatrix}232.03\\156.29\\113.82\\229.07\\287.72\end{bmatrix} = 1\begin{bmatrix}63.9\\28.9\\54.3\\69.8\\50.4\end{bmatrix} + 2\begin{bmatrix}54.0\\45.1\\13.3\\49.5\\85.4\end{bmatrix} + 1\begin{bmatrix}\boxed{\begin{matrix}59.1\\36.9\\33.7\\59.7\\67.9\end{matrix}}\end{bmatrix} + \begin{bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\\\varepsilon_4\\\varepsilon_5\end{bmatrix}$$

$\approx avg$ ()

Some dimensions are redundant

- Little information in 3rd dimension not captured by the first two
- In linear regression, redundancy causes noise to be **amplified**

Dimension reduction

- **Current situation**: our data live in *p*-dimensional space, but not all *p* dimensions are equally useful
- **Subset selection**: throw some out
  - Pro: pretty easy to do
  - Con: lose some information

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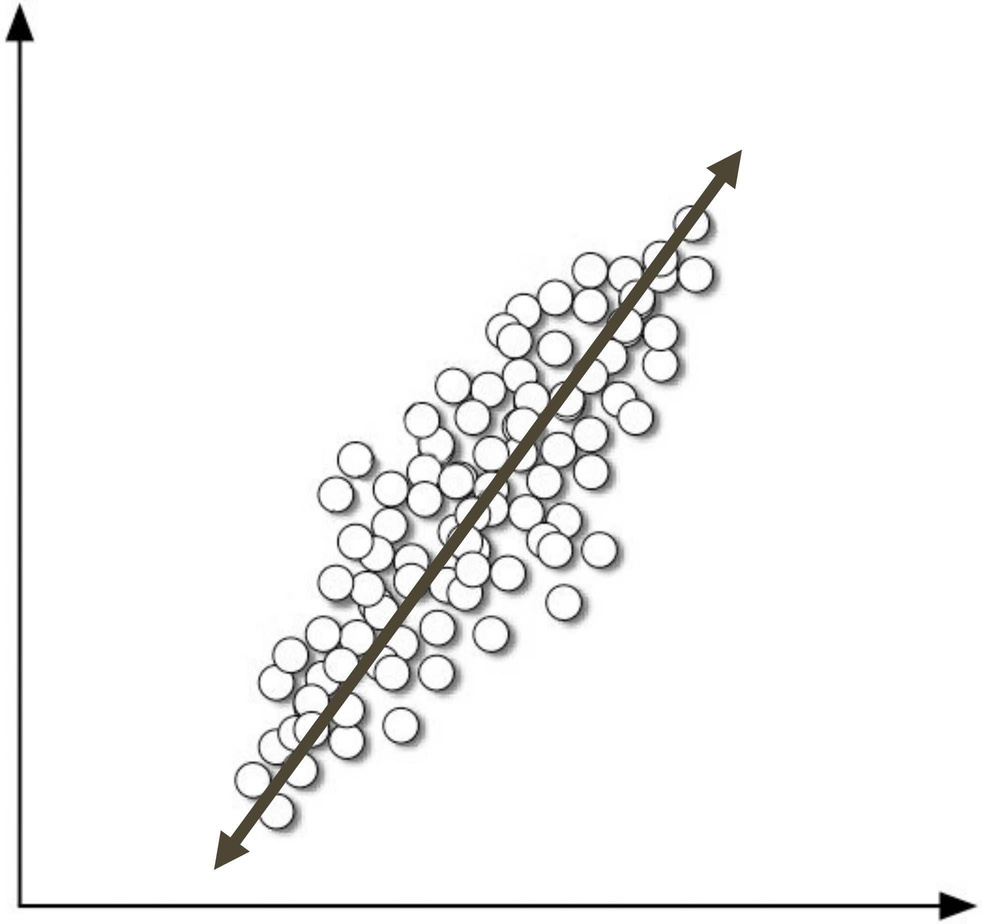
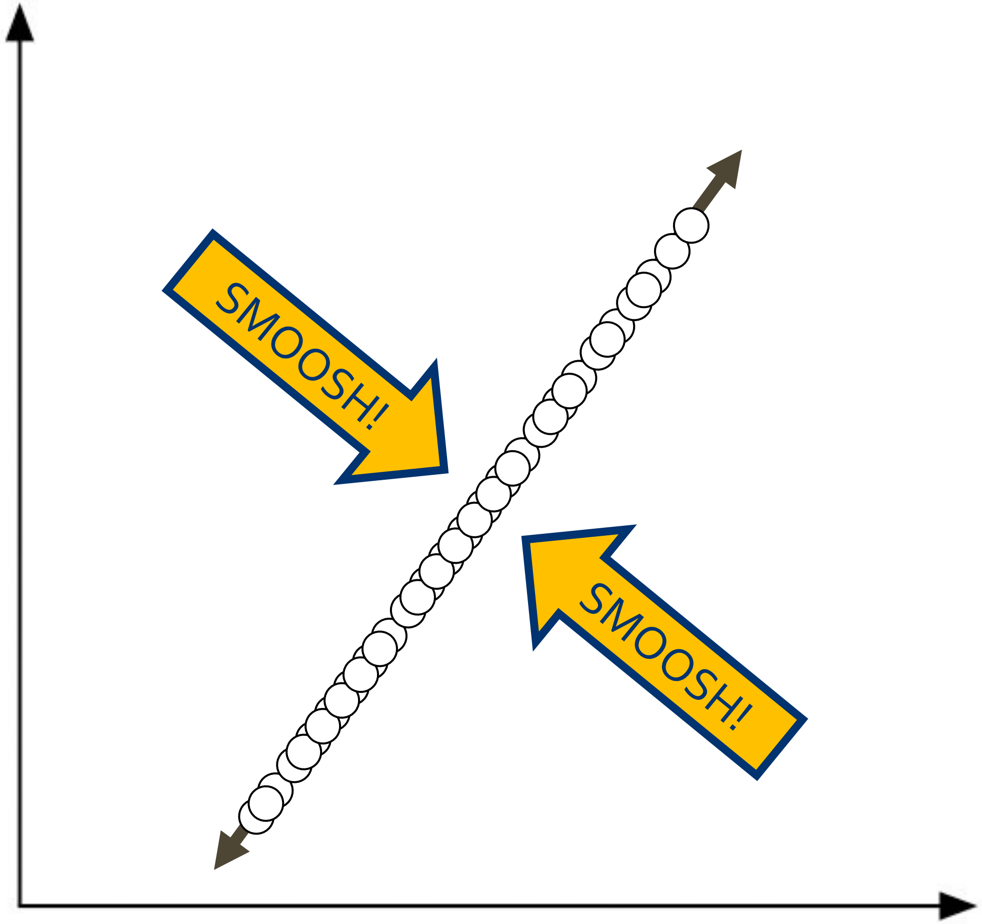
- **Alternate approach**: create **new** features that are combinations of the old ones
  - In other words: We can ***project*** the data into a new feature space to reduce variance in the estimate of coefficients

Projection



Projection



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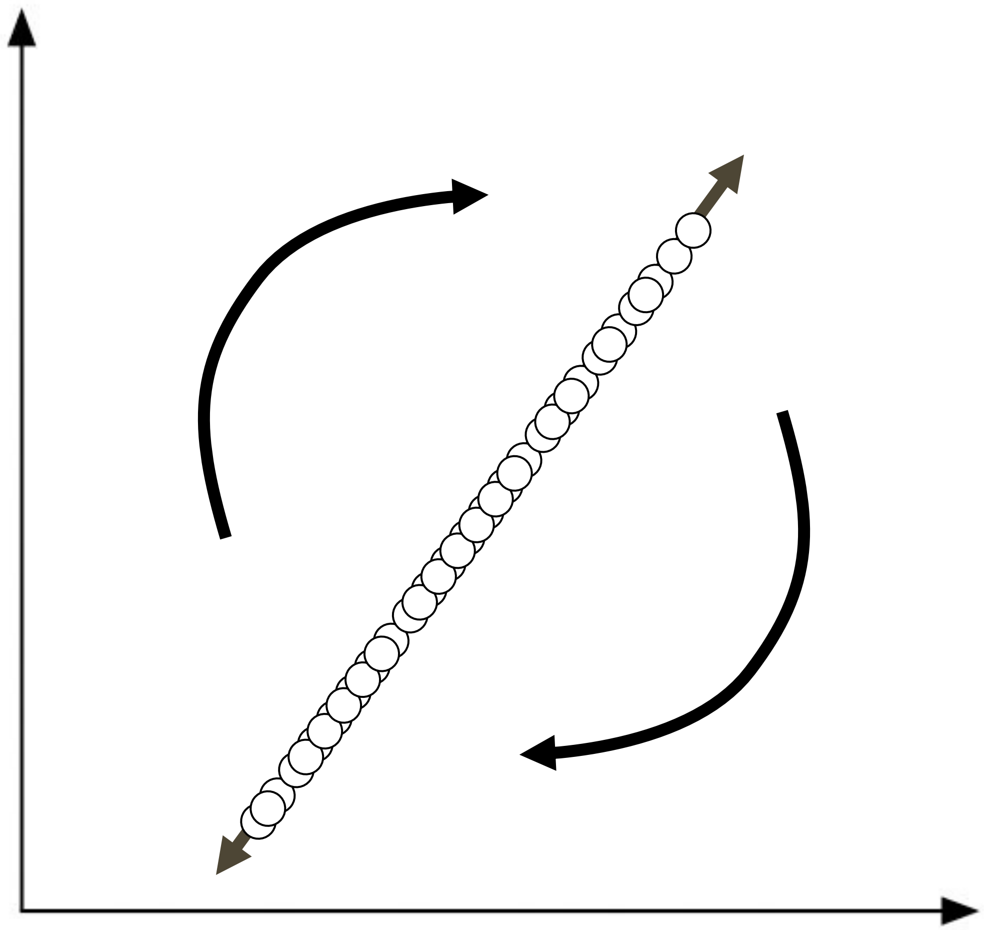


Dimension reduction via projection

- **Big idea**: *transform* the data before performing regression

$$[X_1 \quad X_2 \quad X_3 \quad X_4 \quad X_5] \mapsto [Z_1 \quad Z_2]$$

- Then instead of:

$$Y = \beta_0 + \sum_{i=1}^{p} \beta_i X_i + \varepsilon$$

we solve:

$$Y = \theta_0 + \sum_{i=1}^{m} \theta_i Z_i + \varepsilon$$

Linear projection

- New features are **linear combinations** of original data:

$$Z_j = \sum_{i}^{m} \theta_{ij} X_i$$

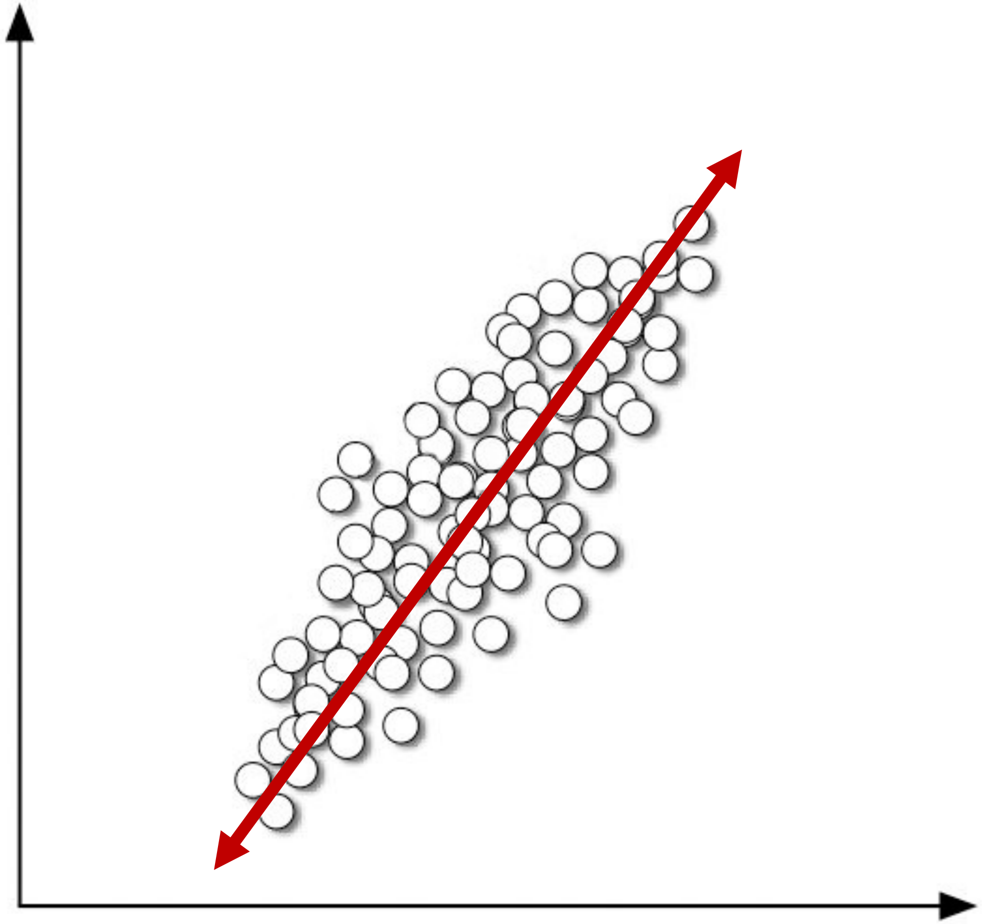
- We get them by multiplying the *data matrix* by a *projection matrix*

$$[Z_1 \quad Z_2] = [X_1 \quad X_2 \quad X_3 \quad X_4 \quad X_5] \boxed{\begin{bmatrix} \varphi_{1,1} & \varphi_{1,2} \\ \varphi_{2,1} & \varphi_{2,2} \\ \varphi_{3,1} & \varphi_{3,2} \\ \varphi_{4,1} & \varphi_{4,2} \\ \varphi_{5,1} & \varphi_{5,2} \end{bmatrix}}$$

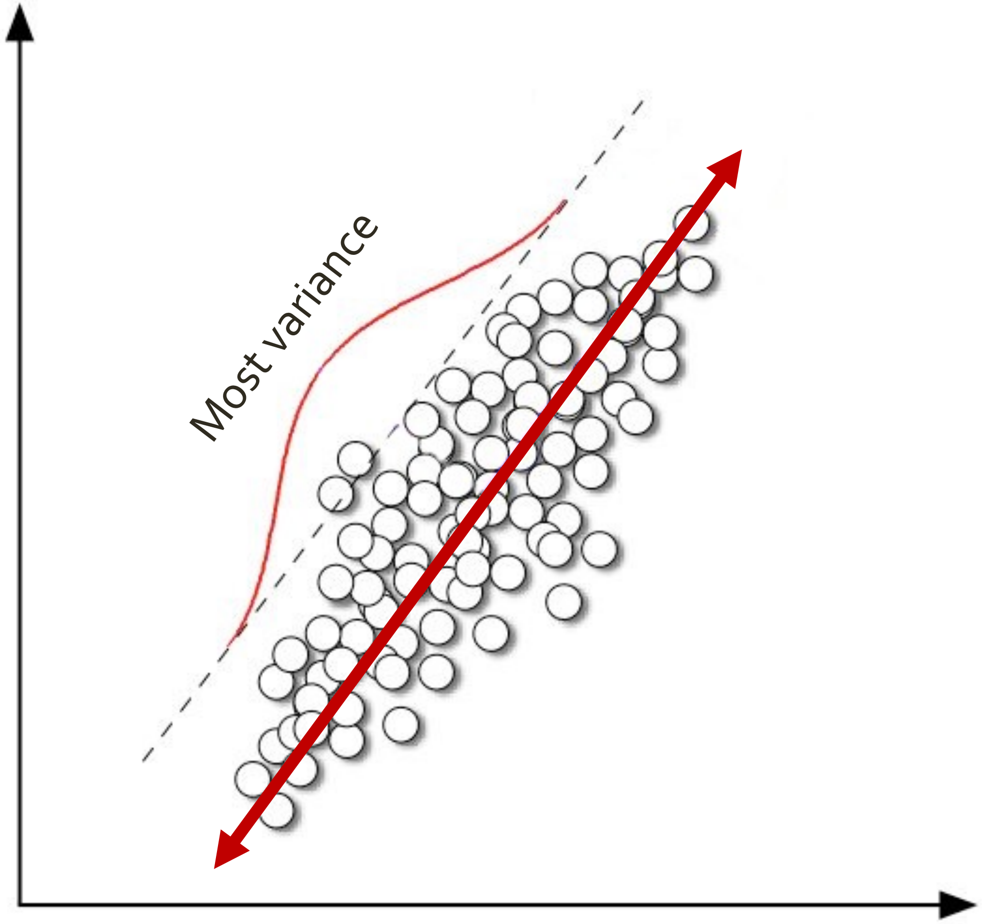
What's the deal with projection?

- Data can be rotated, scaled, and translated without changing the **underlying relationships**
- This means you're allowed to look at the data from whatever angle makes your life easier…

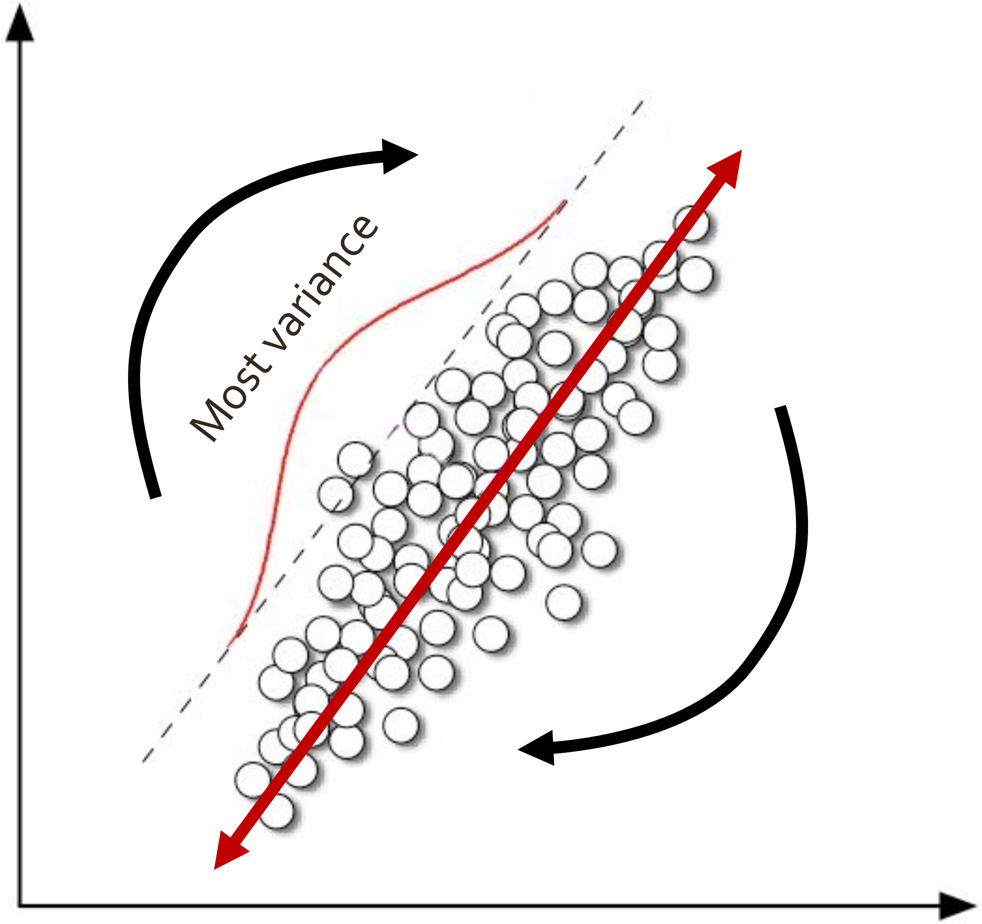
Flashback: why did we pick this line?



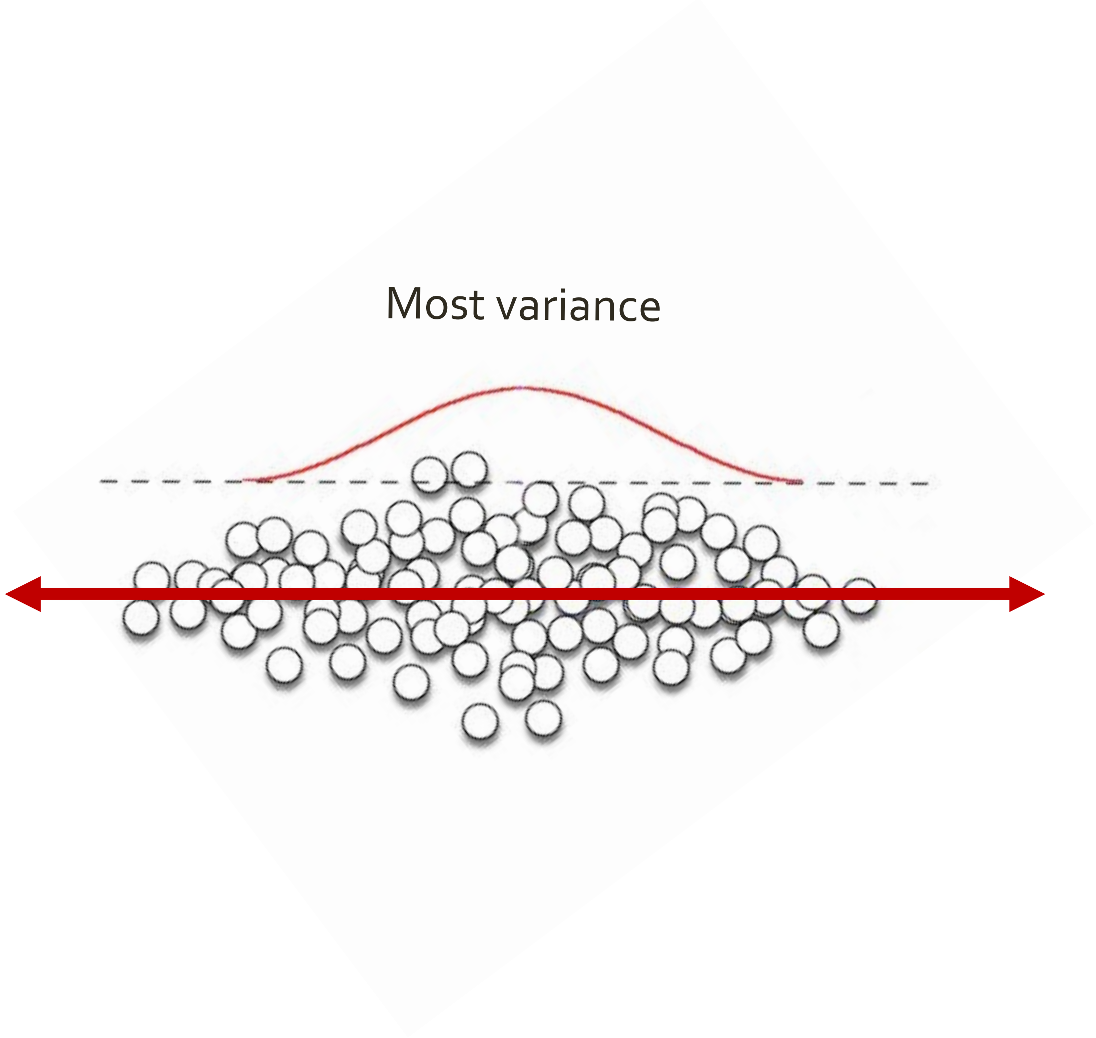
Explains the most **variance** in the data



Imagine this line as a new dimension…



“Principal component”



Mathematically

- The 1^{st} **principal component** is the normalized* linear combination of features:

$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \cdots + \phi_{p1}X_p$$

that has the largest variance

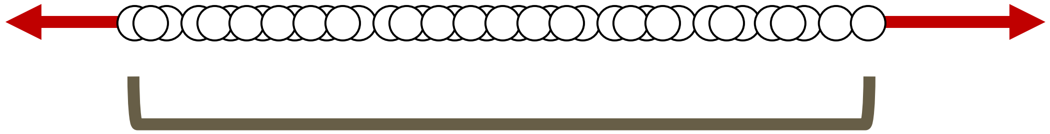
- $\phi_{11}, \ldots, \phi_{p1}$: the **loadings** of the 1^{st} principal component

* By **normalized** we mean: $\sum_{j=1}^{p} \phi_{j1}^2 = 1$

Using loadings to project

Multiply by loading vector to project ("smoosh") each observation onto the line:

$$z_{i1} = \phi_{11}x_{i1} + \phi_{21}x_{i2} + \cdots + \phi_{p1}x_{ip}$$



These values are called the **scores** of the 1st principal component

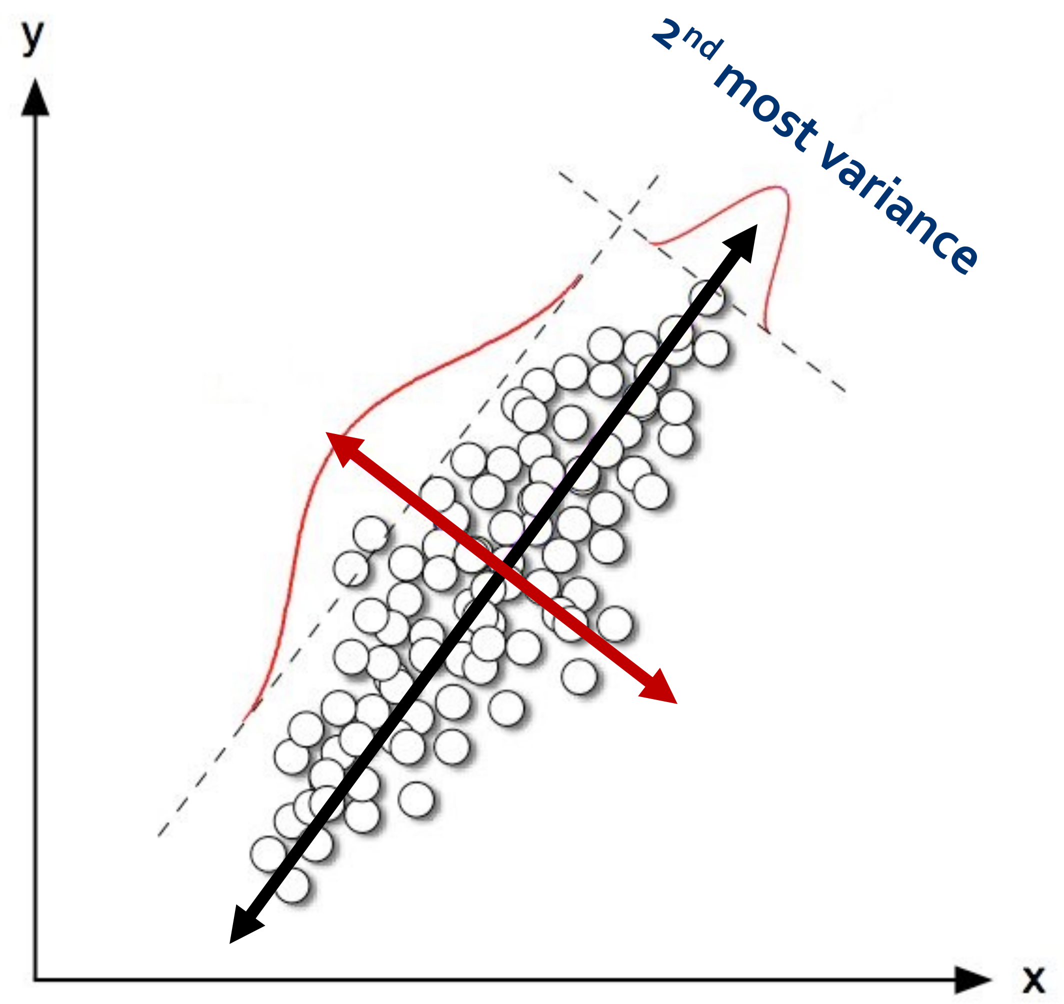
Additional principal components

- The **2nd principal component** is the normalized linear combination of the features

$$Z_2 = \phi_{12}X_1 + \phi_{22}X_2 + \cdots + \phi_{p2}X_p$$

that has maximal variance out of all linear combinations that are **uncorrelated** with Z_1

Principal components are orthogonal



Generating additional principal components

- We can think of this recursively
- To find the M^{th} principal component . . .
  - Find the first $(M-1)$ principal components
  - Subtract the projection into that space
  - Maximize the variance in the remaining *complementary* space

Regression in the principal components

- **Original objective**: solve for β in

$$Y = \beta_0 + \sum_{i}^{p} \beta_i X_i + \varepsilon$$

(that's still our goal)

- Now we're going to work in the new feature space:

$$Y = \theta_0 + \sum_{i}^{M} \theta_i Z_i + \varepsilon$$

Regression in the principal components

- *Remember*: the new features are **related** to the old ones:

$$Z_j = \sum_{i=1}^{p} \phi_{ij} X_i$$

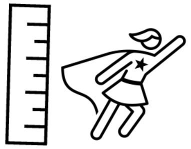
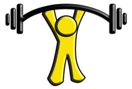
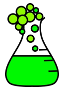
- So we're computing:

$$Y = \theta_0 + \sum_{j=1}^{M} \theta_j Z_j + \varepsilon$$

$$= \theta_0 + \sum_{j=1}^{M} \theta_j \sum_{i=1}^{p} \phi_{ij} X_i + \varepsilon$$

$$\mapsto \beta_i = \sum_{j=1}^{M} \theta_j \phi_{ij}$$

Back to estimating height

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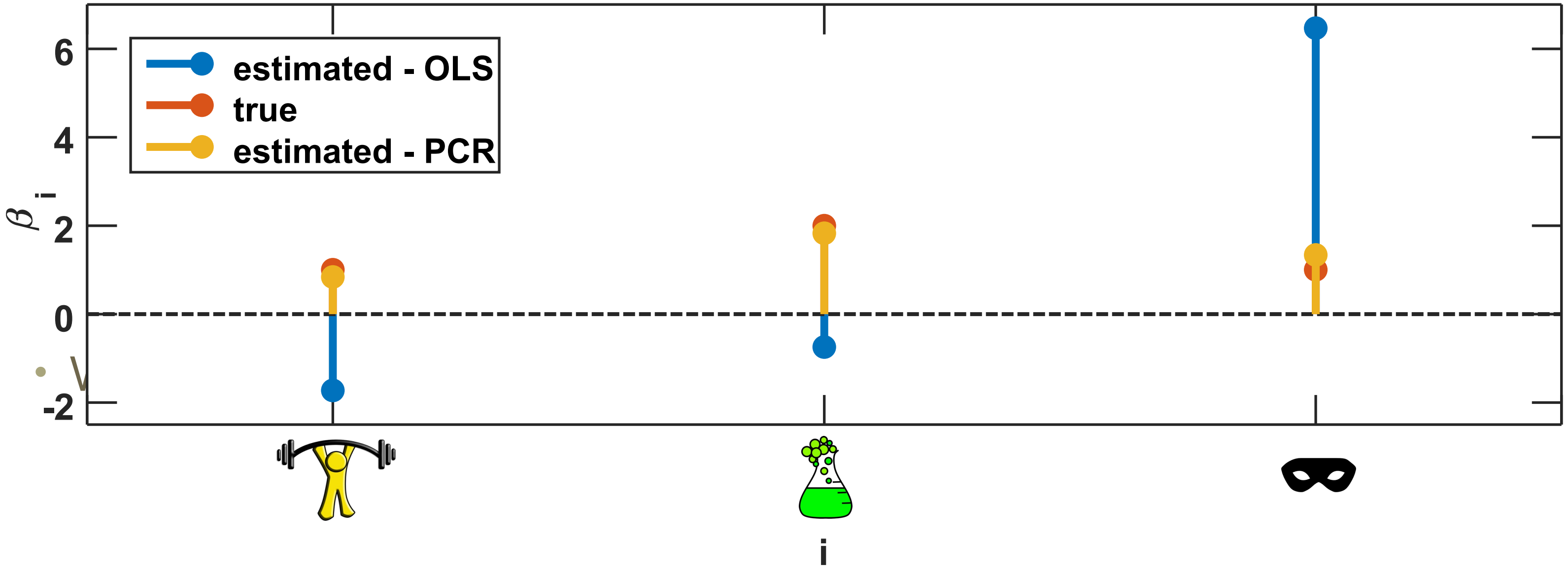
Back to the Guardians



Using principle components dramatically increases our estimates.

Comparison with ridge regression and the lasso

What similarities do you see between principle component regression and ridge regression and the lasso?

Problems with PCR

- We selected principal components based on predictors (not what we're trying to predict!)

Why could this be problematic?

Partial least squares (PLS)

- A *supervised* form of PCR
- Feature derivation algorithm is similar:
  - Find the (M-1) ~~principal~~ **most correlated** components
  - Subtract the projection into that space
  - Maximize the ~~variance~~ **correlation with the response** in the remaining *complementary* space
- As before, we perform least squares on the new features
- We still use the formulation

$$Z_j = \sum_{i=1}^{p} \phi_{ij} X_i$$

- But now ϕ is computed by applying linear regression to *each* predictor

Wrapping up: PCR/PLS comparison

- Both derive a small number of orthogonal predictors for linear regression
- PCR is more biased
  - Emphasizes stability at the expense of versatility
- PLS estimates have higher variance
  - May build new features that aren't as stable
  - But high variance is better than infinite variance