LECTURE 13:

DIMENSIONALITY REDUCTION

October 25, 2017

SDS 293: Machine Learning

Outline

- Model selection: alternatives to least-squares

✓Subset selection

  ✓Best subset

  ✓Stepwise selection (forward and backward)

  ✓Estimating error using cross-validation

✓Shrinkage methods

  ✓Ridge regression and the Lasso

  – **Dimension reduction**

- Labs for each part

Recap: Ridge Regression and the Lasso

- Both are "shrinkage" methods
- Estimates for the coefficients are ***biased*** toward the origin
  - Biased = "prefers some estimates to others"
  - Does not yield the true value in expectation
- Question: why would we **want** a biased estimate?

Recap: Ridge Regression and the Lasso

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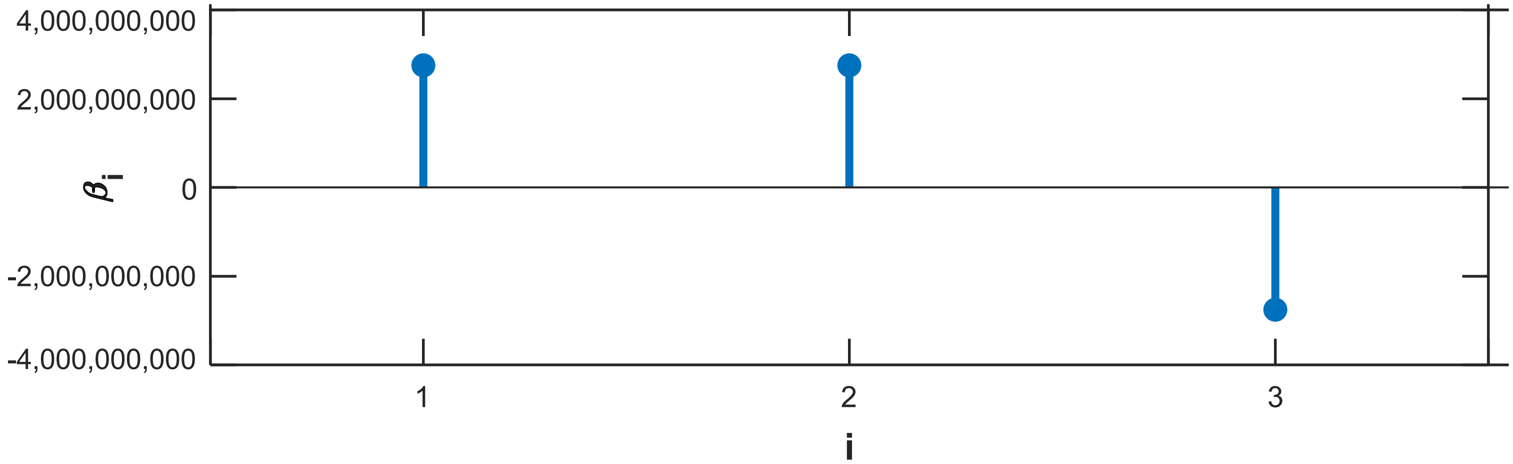
What's wrong with bias?

- What if your unbiased estimator gives you this?



May want to bias our estimate to **reduce variance**

Flashback: superheroes

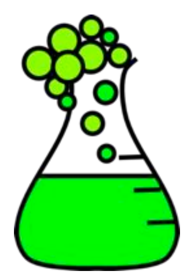
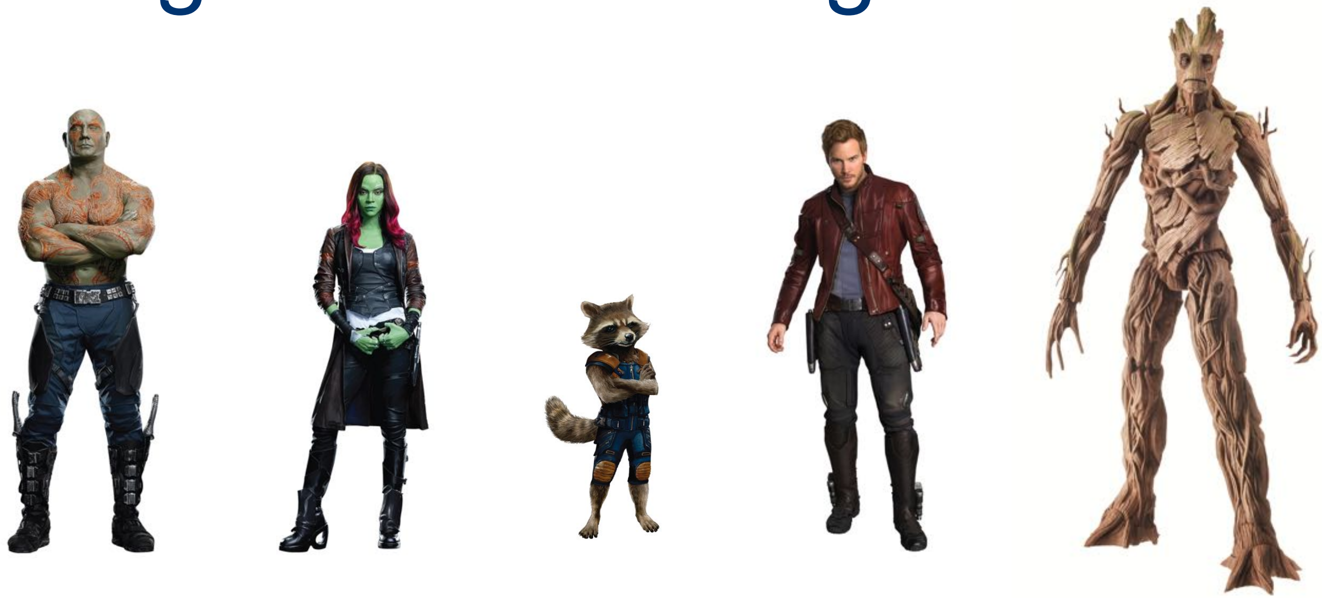
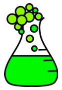
$height = \beta_1 ($  $) + \beta_2 ($  $) + \beta_3 ($  $)$

Image credit: Ming Malaykham

Estimating Guardians' Height



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Estimate for β

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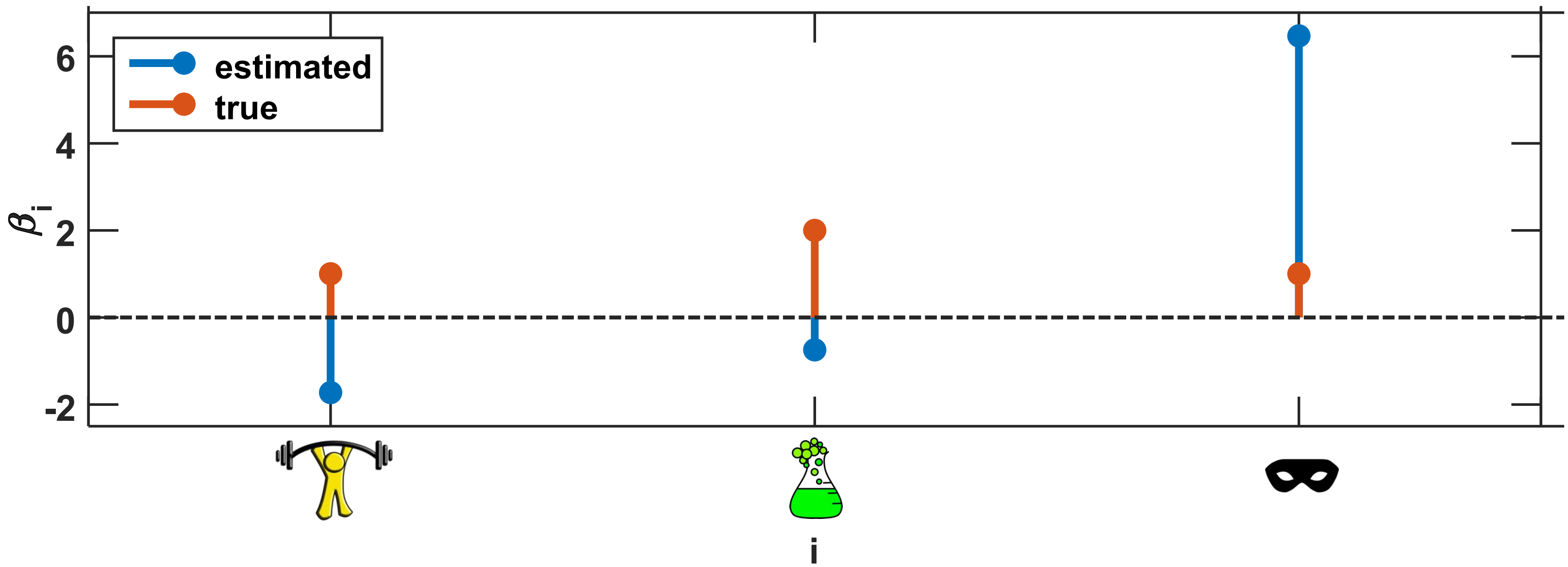
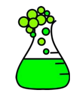


(Relatively) huge difference between actual and estimated coefficients

What's going on here?

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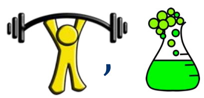
$\approx avg\Big($  $\Big)$

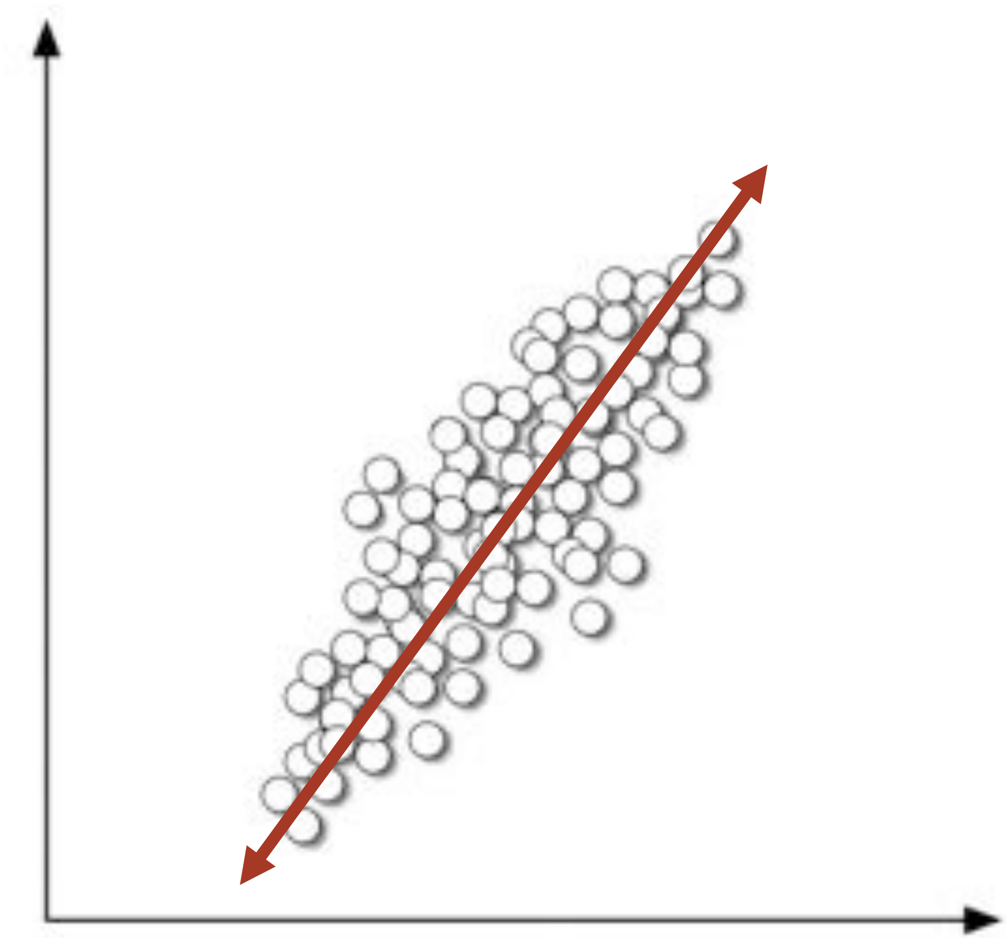
- Some dimensions are redundant
  - Little information in 3rd dimension not captured by the first two
  - In linear regression, redundancy causes noise to be **amplified**

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
- **Alternate approach**: create **new** features that are combinations of the old ones

In other words:
Project the data into a new feature space to reduce variance in the estimate

Projection



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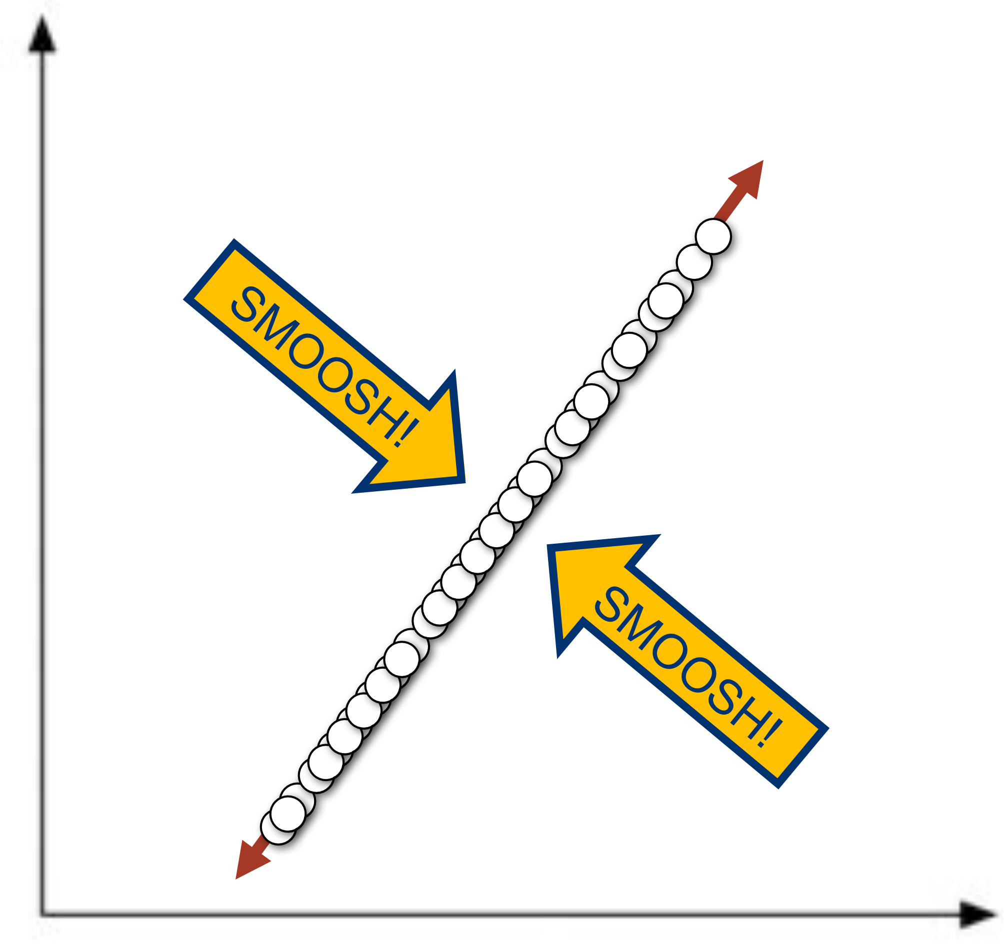

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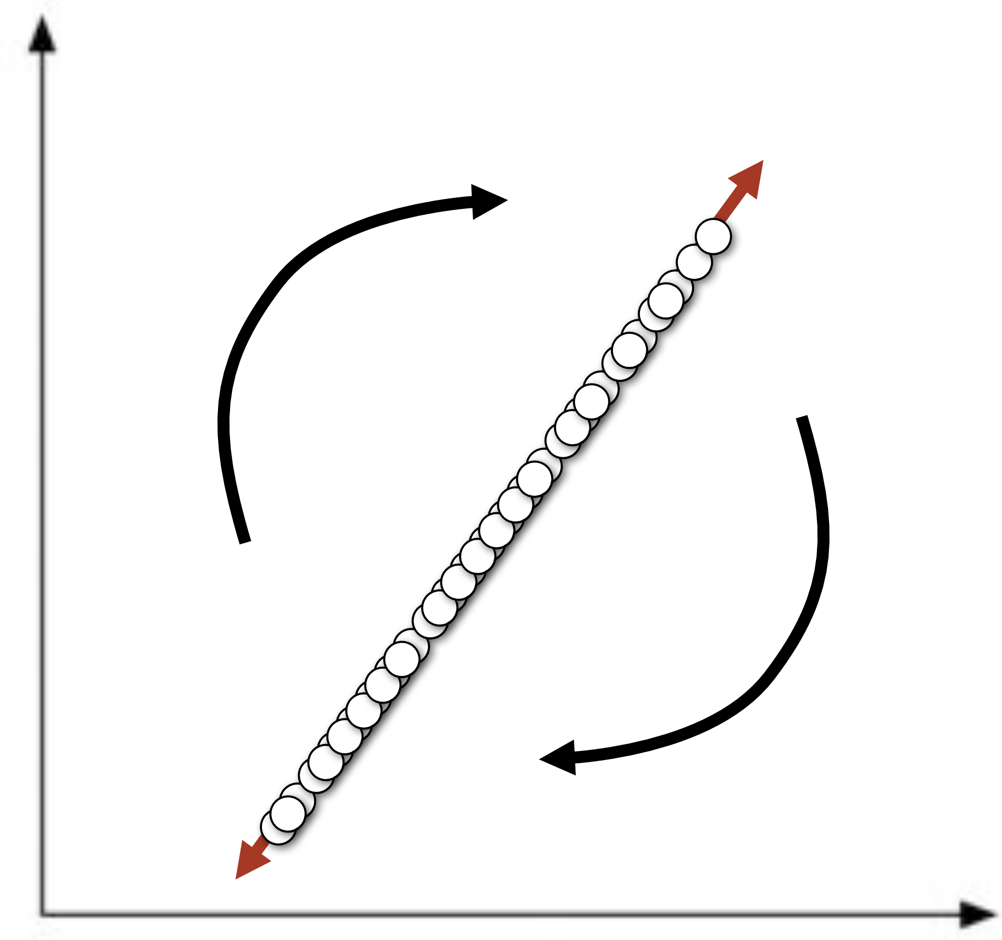


Dimension reduction via projection

- **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:

$$Z_j = \sum_i^m \theta_{ij} X_i$$

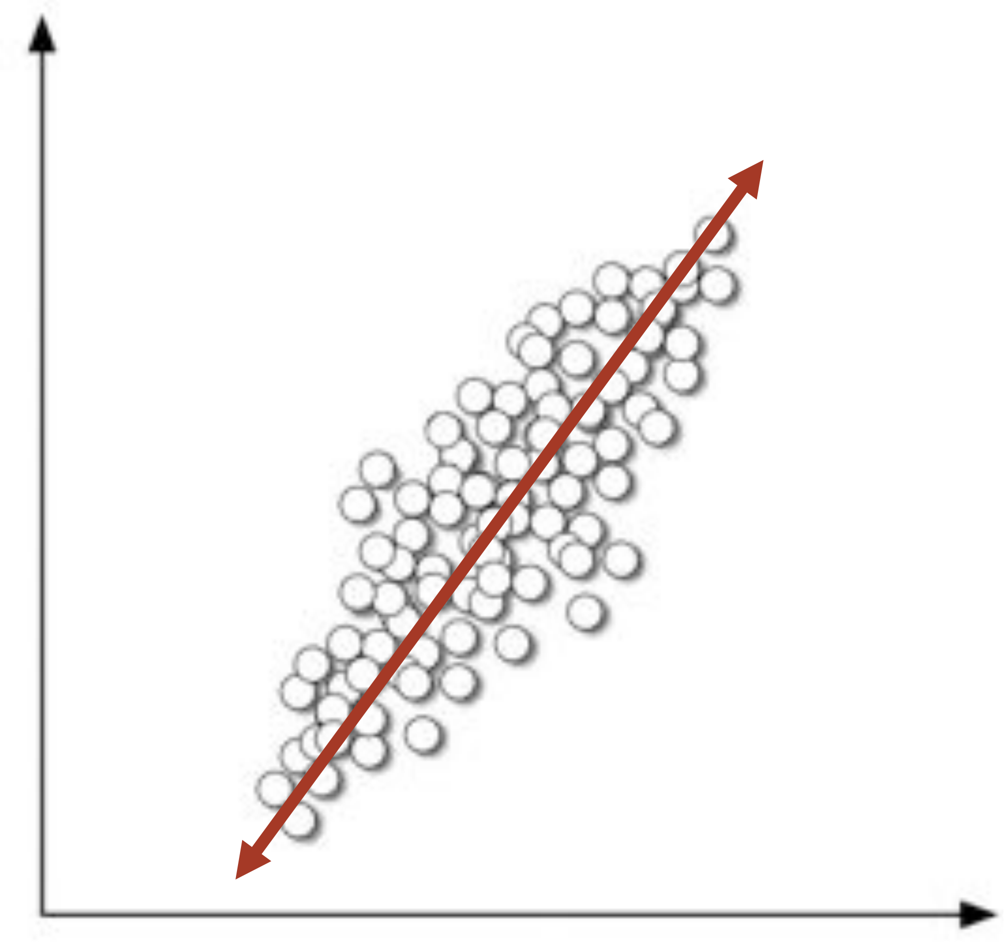
- **MTH211**: multiplying the *data matrix* by a *projection matrix*

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

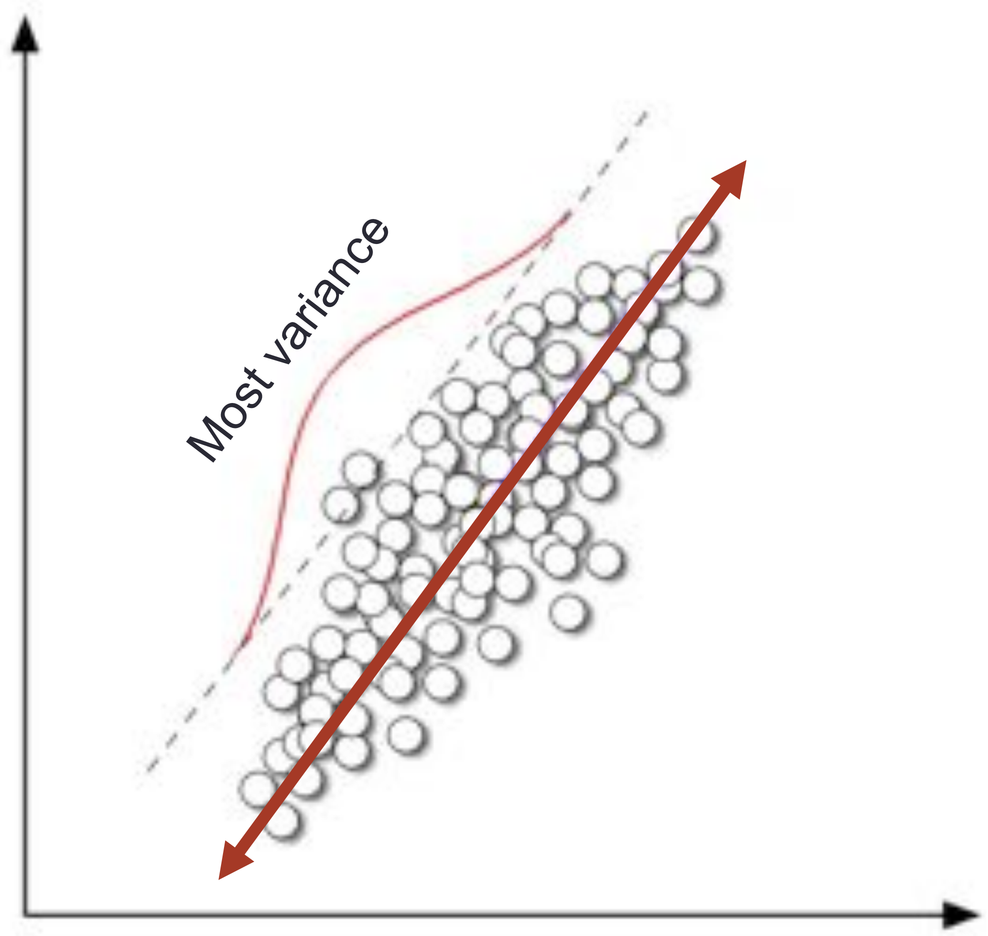
What’s the deal with projection?

- 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…

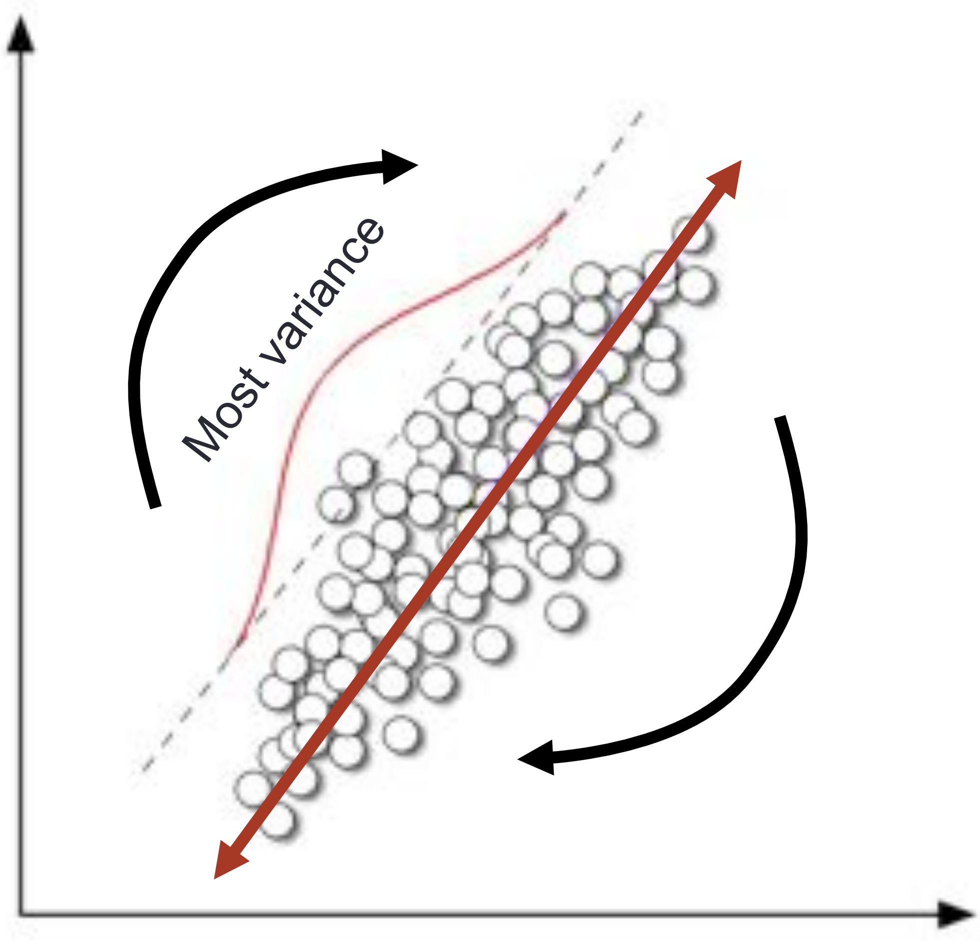
Flashback: why did we pick this line?



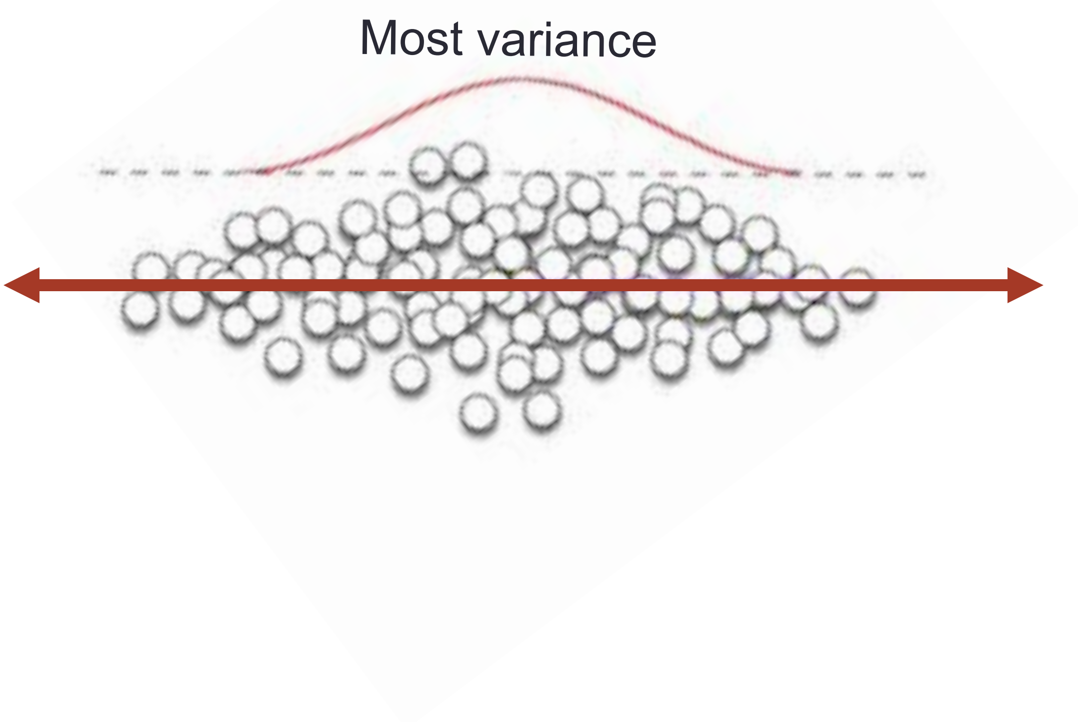
Explains the most **variance** in the data



Imagine this line as a new dimension…



“Principal component”



Mathematically

- The **1st 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

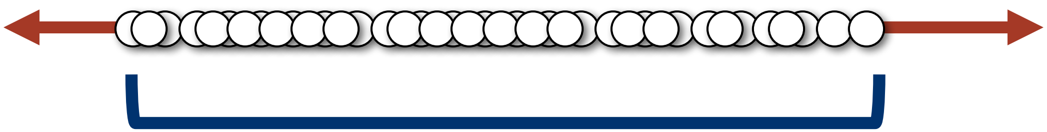
- $\phi_{11}, \ldots, \phi_{p1}$: the **loadings** of the 1st principal component

* 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

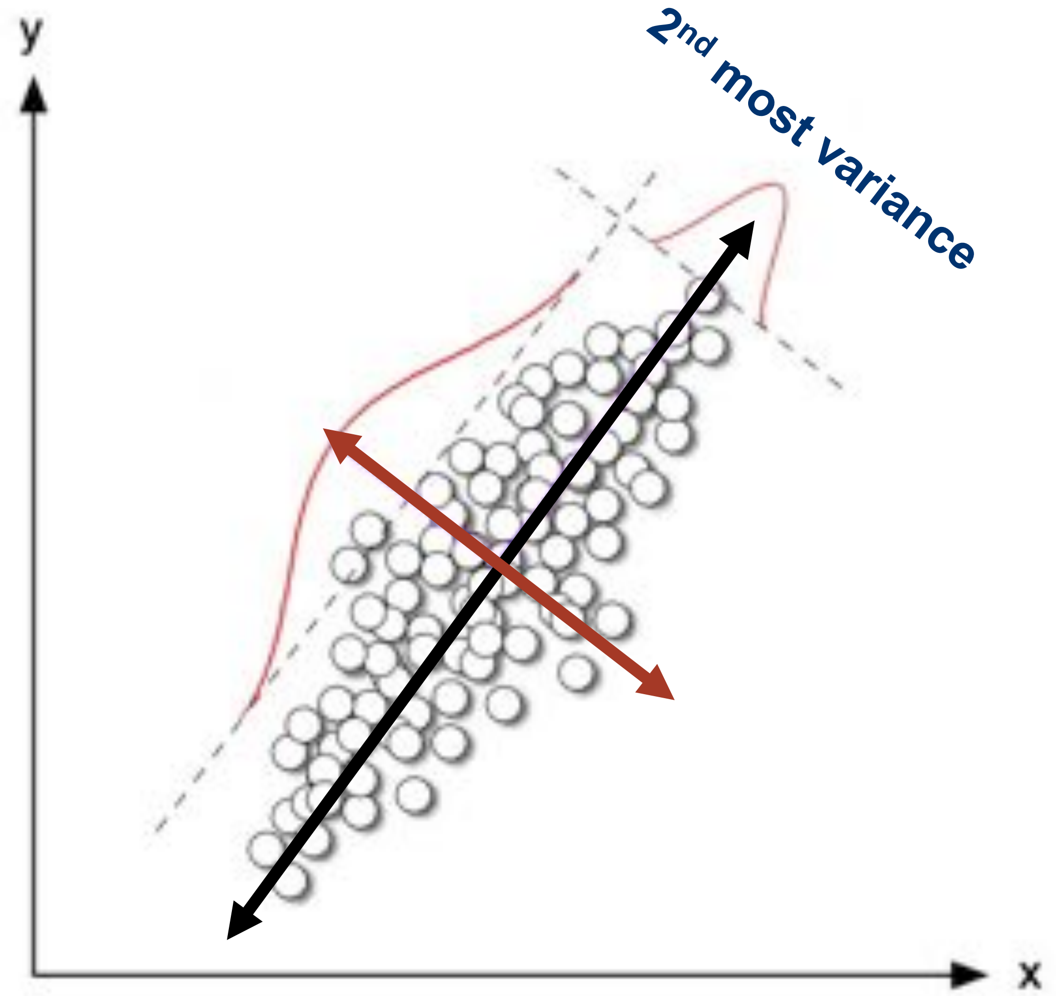
- **2nd principal component** is the normalized linear combination of the features

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

that has maximal variance out of all linear combinations that are **uncorrelated** with Z_1 (why does that matter?)

- Fun fact:

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:

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

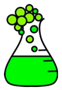
- So we're computing:

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

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

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

Back to the Guardians

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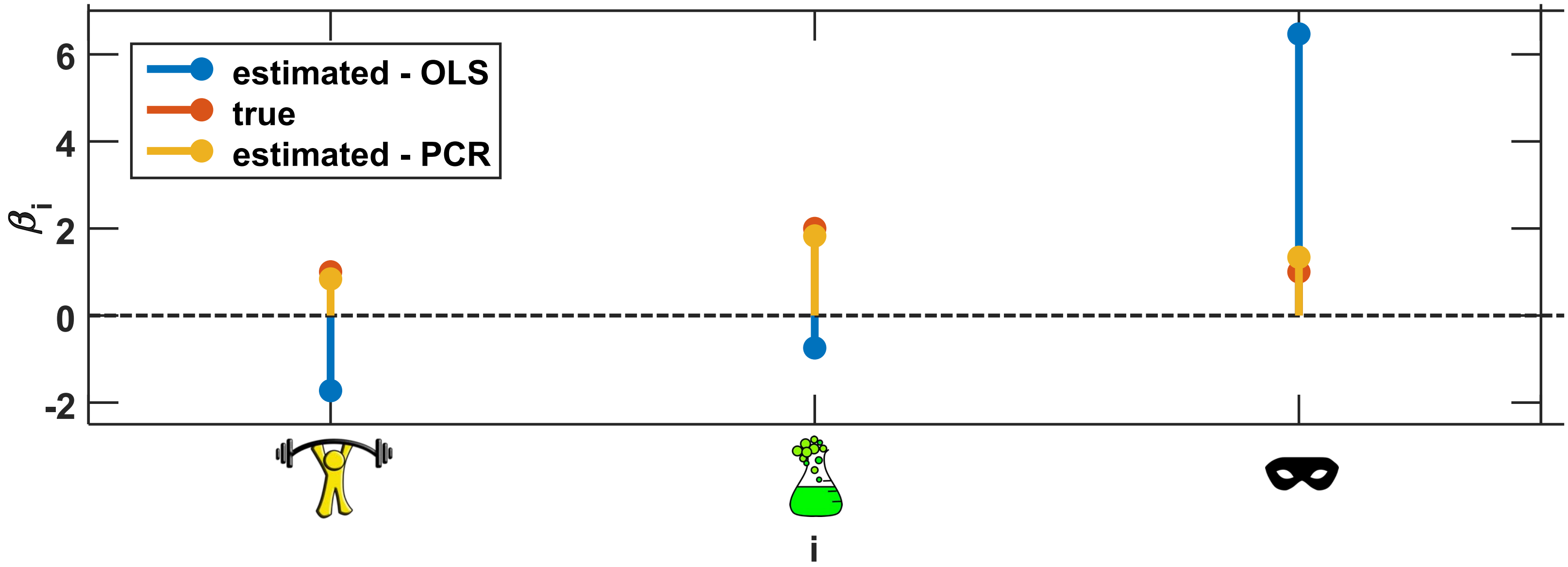
Back to the Guardians

- What happens if we use 2 components instead of 3?



Using only the principal components significantly improves our estimate!

Comparison with ridge regression and the lasso

- What similarities do you see?
  - Reduces dimensionality of the solution space (like Lasso)
  - Finds a solution in the space of all features (like RR)
  - Results can be difficult to interpret (like RR)

Problems with PCR

- We selected principal components based on predictors (not what we're trying to predict!)
- This could be problematic (why?)
  - What if the values you're trying to predict aren't correlated with the first few components?
  - You lose all predictive power!

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

Lab: PCR and PLS

- To do today’s lab in R: **`pls`**
- To do today’s lab in python: <nothing new>
- Instructions and code:

[course website]/labs/lab11-r.html

[course website]/labs/lab11-py.html

- Full version can be found beginning on p. 256 of ISLR

Flashback: superheroes

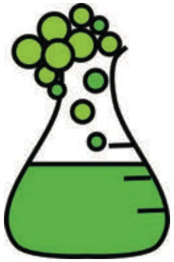
$height = \beta_1$ () $+\beta_2$ () $+\beta_3$ ()

Image credit: Ming Malaykham

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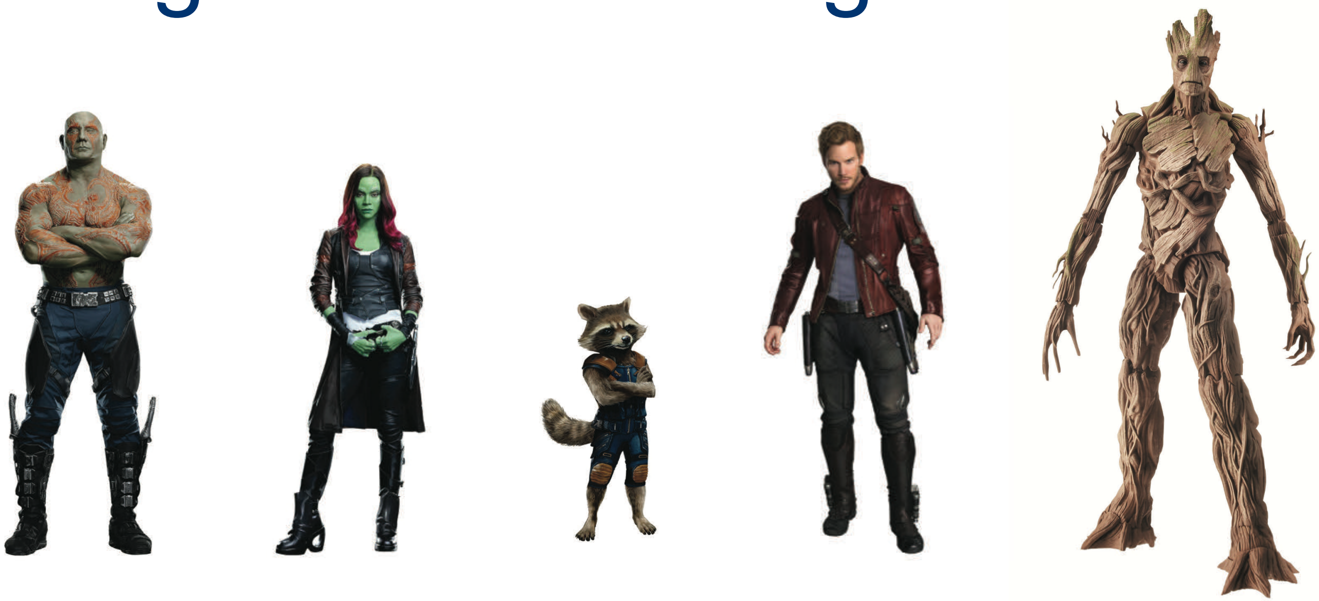

  

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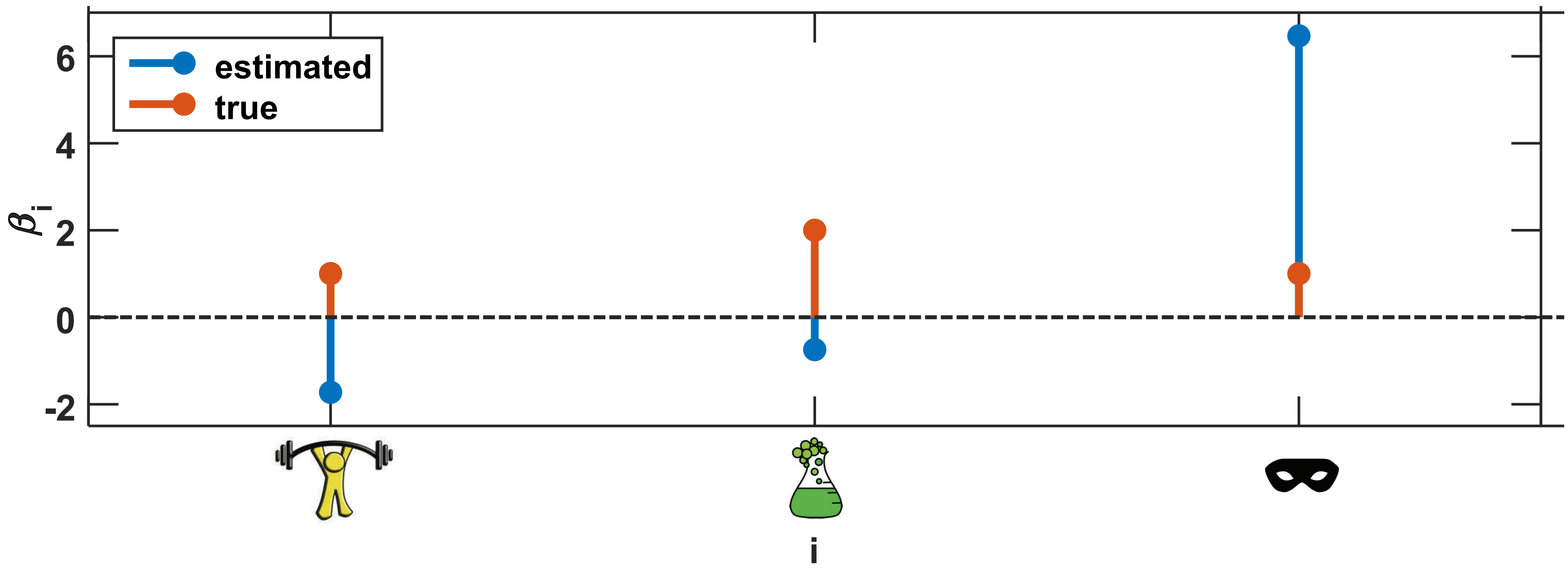

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 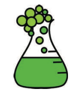 

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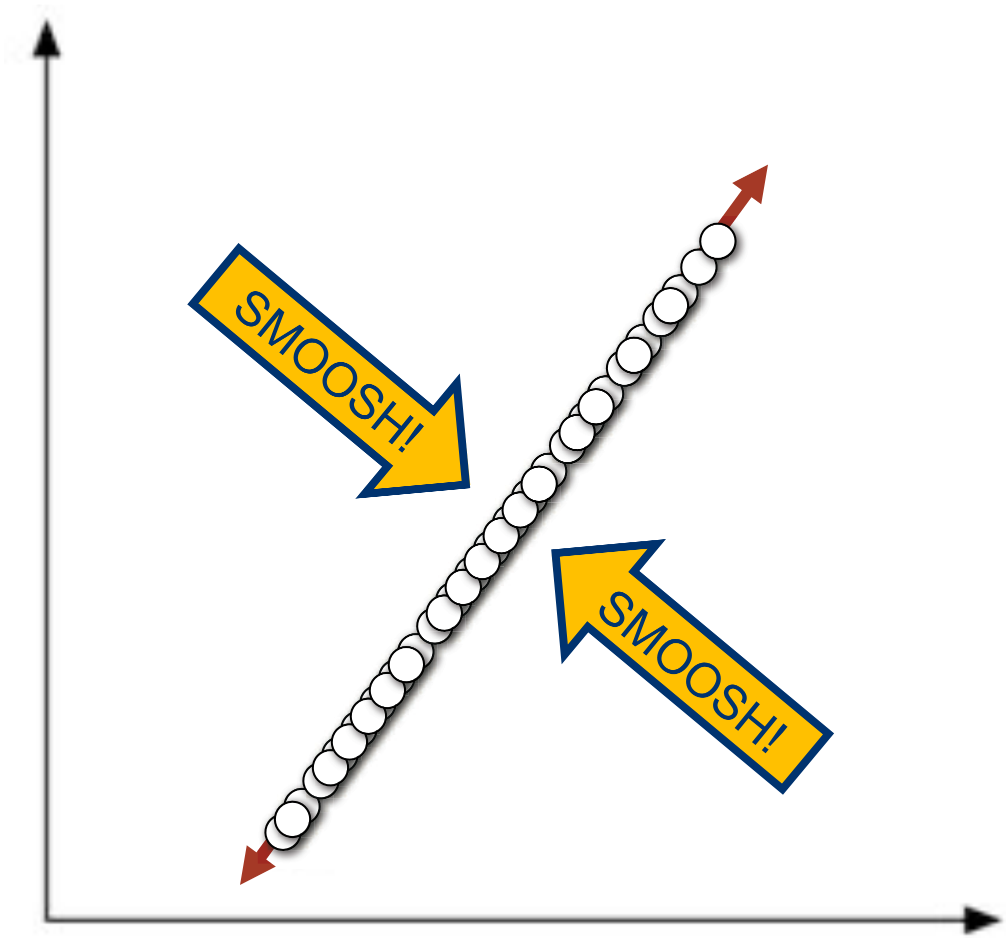

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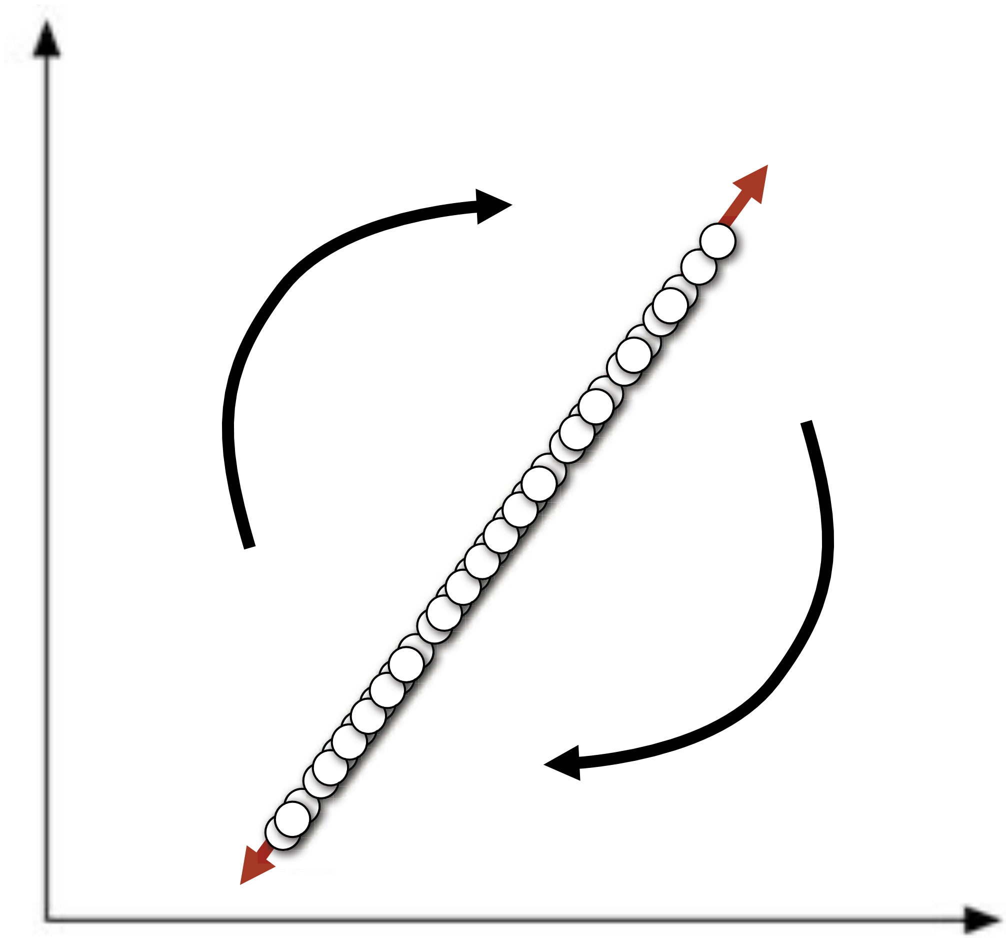

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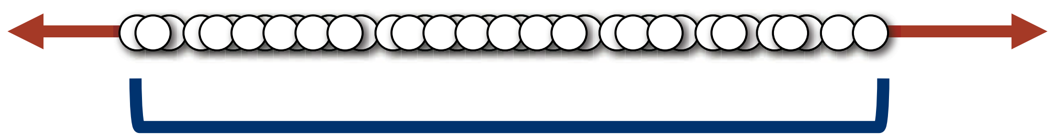

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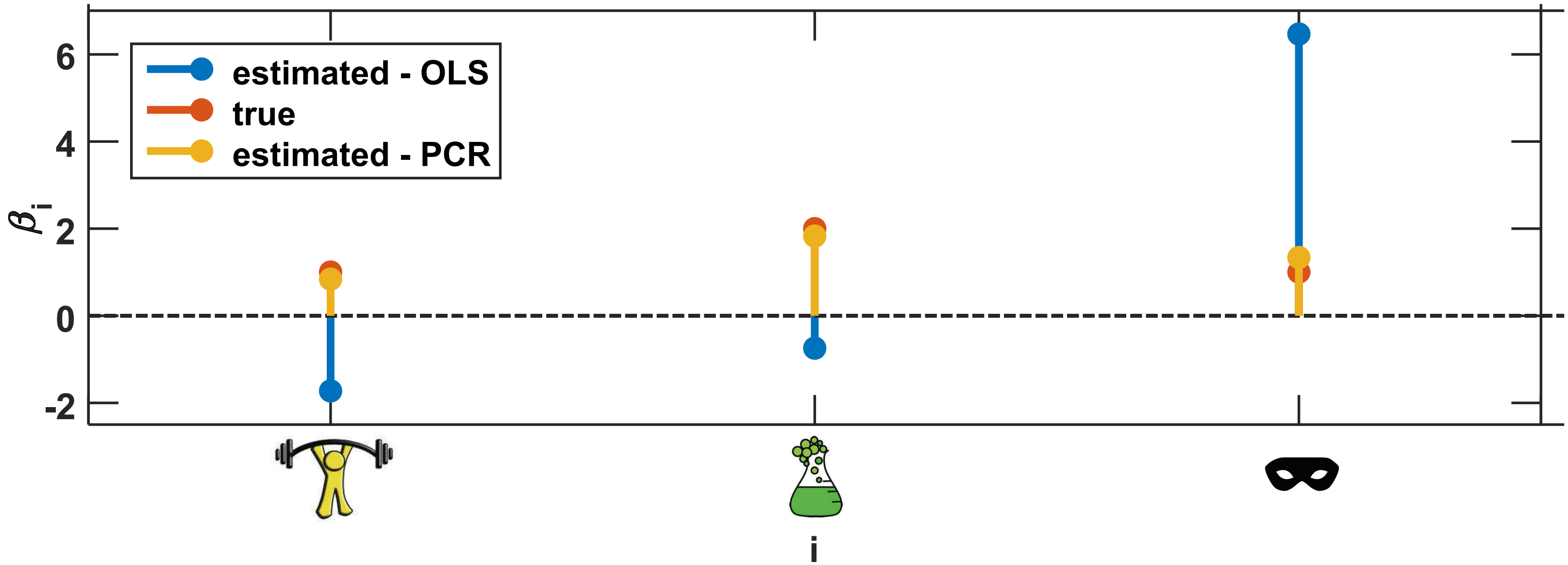

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