EECE5645
Parallel Processing for Data Analytics

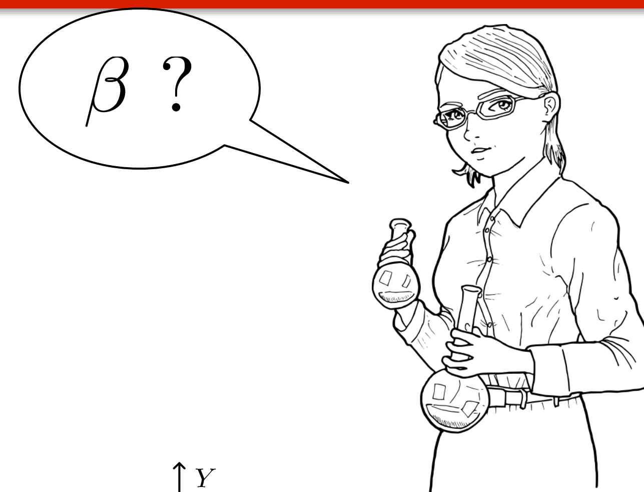
Lecture 10: Feature Selection

Linear Regression

$x_i \in \mathbb{R}^d$ $\qquad$ $y_i \in \mathbb{R}$

n

Height	Weight	Age	Blood Pressure
1.8m	40K	19ys	3.1
1.9m	55K	34ys	1.2
⋮			
1.5m	90K	24ys	2.5

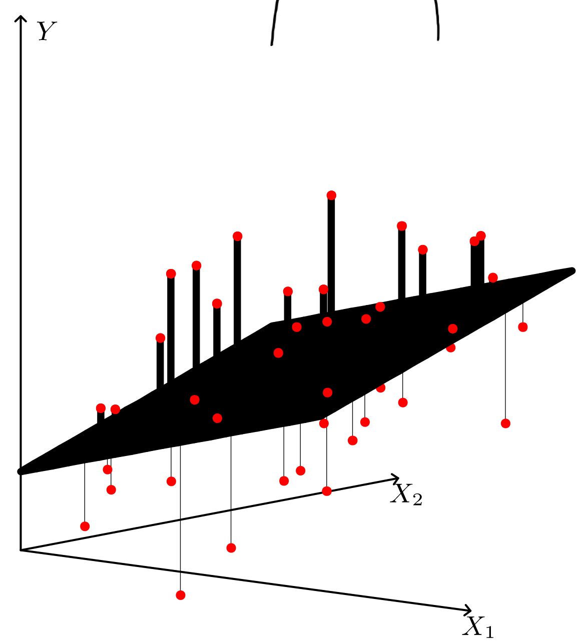


$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

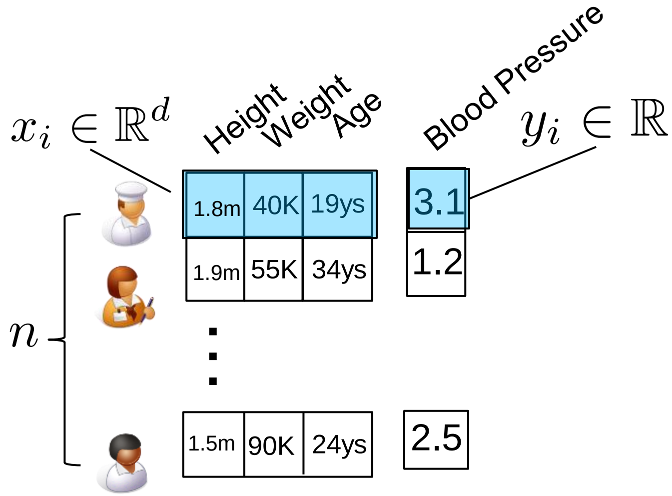
Learn by minimizing Residual-Sum-of-Squares (RSS):

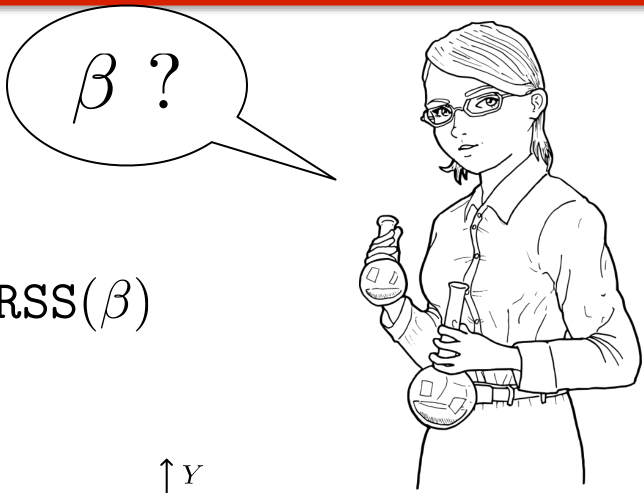
$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^d} \mathrm{RSS}(\beta) = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \langle \beta, x_i \rangle)^2$$

$$= (X^T X)^{-1} X^T y$$

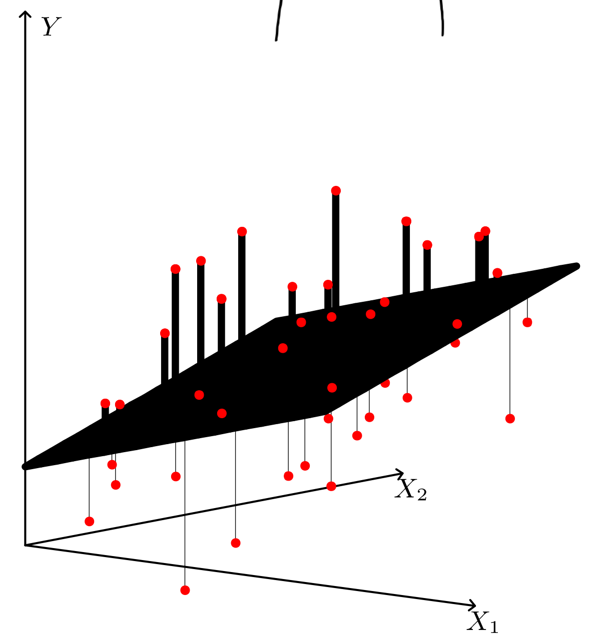


Linear Regression





$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^d} \text{RSS}(\beta)$$

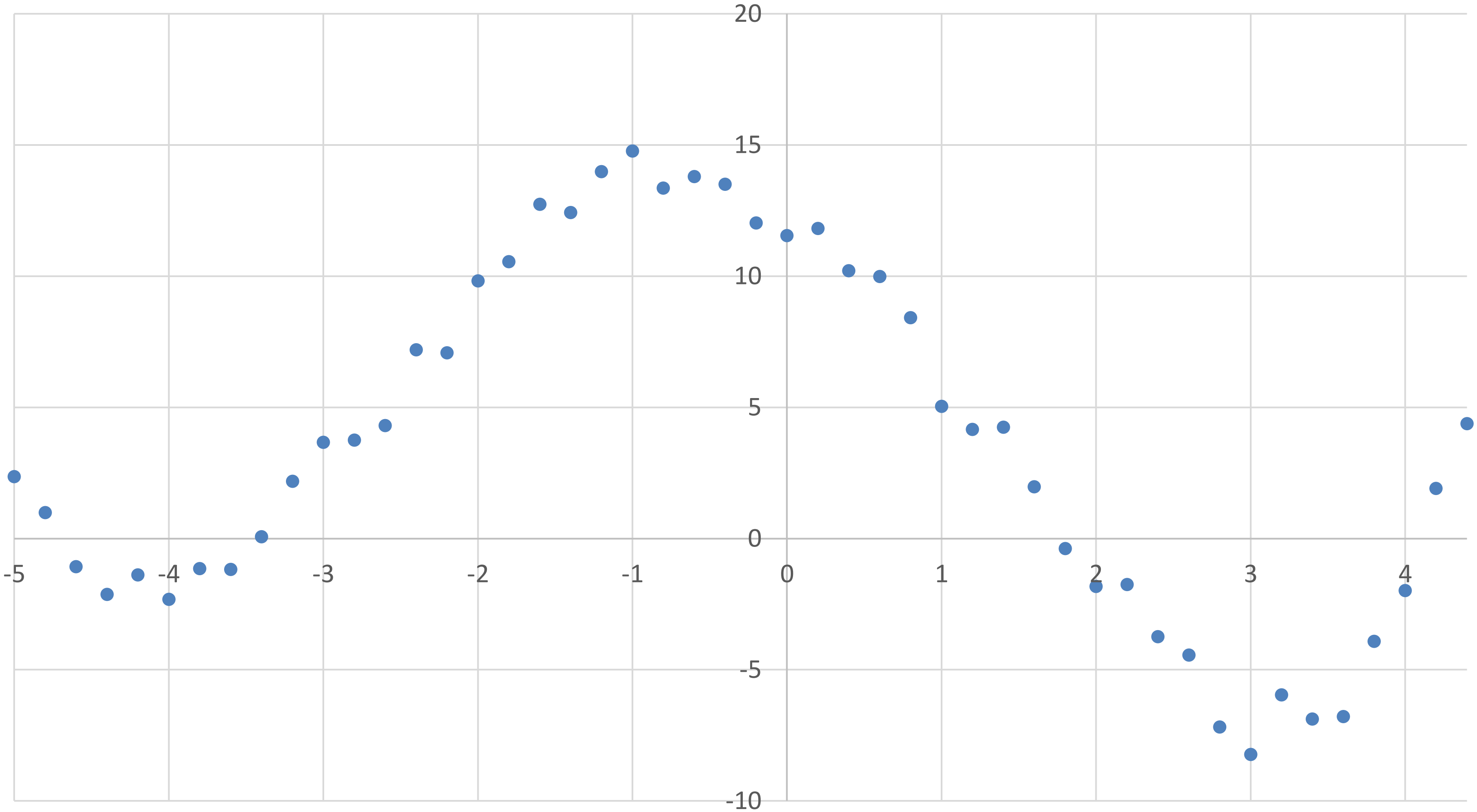


$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

Expected Prediction Error:

$$\text{EPE} \quad \approx \sigma^2 + \sigma^2 \frac{d}{n}$$

What if Data is Not Linear?



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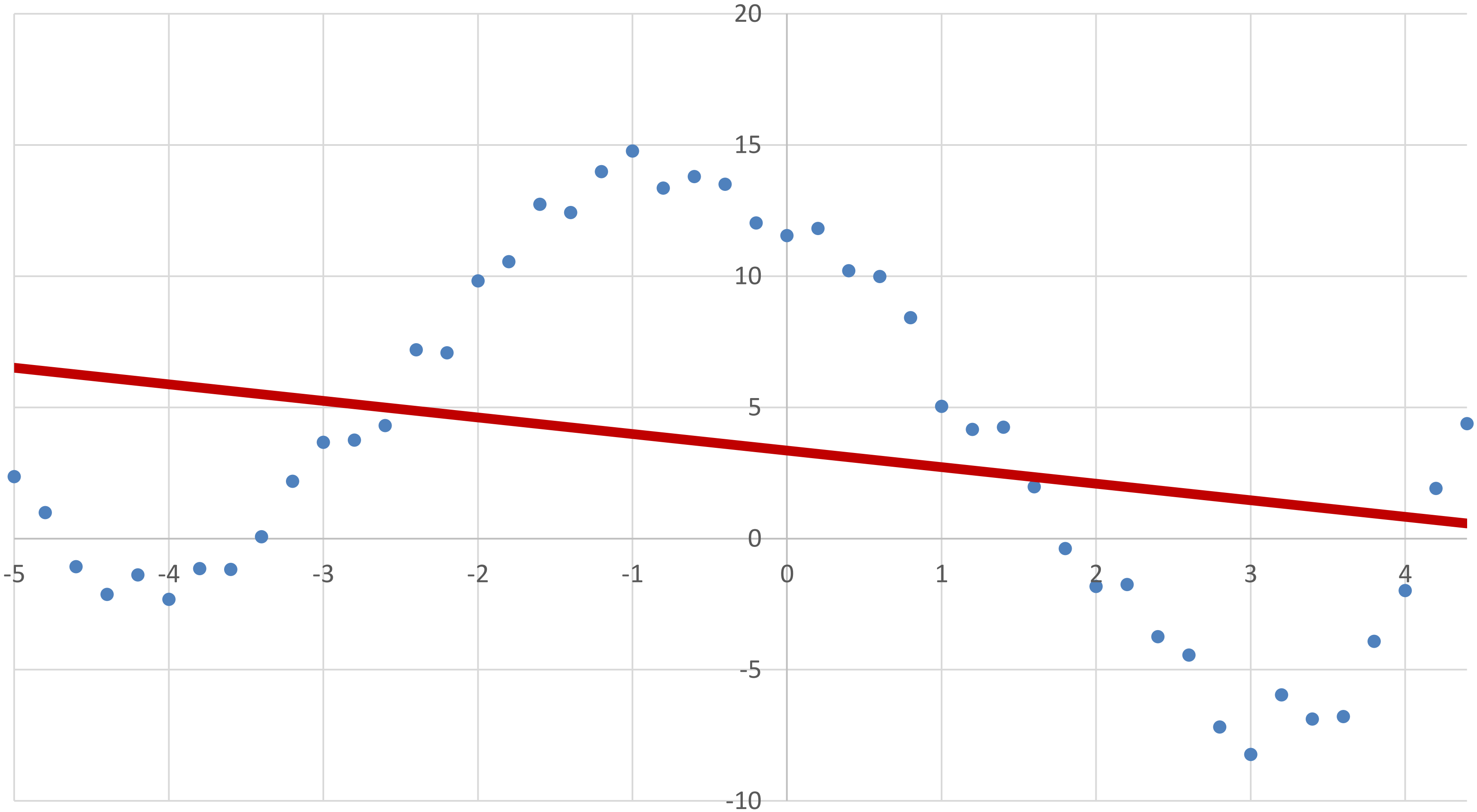
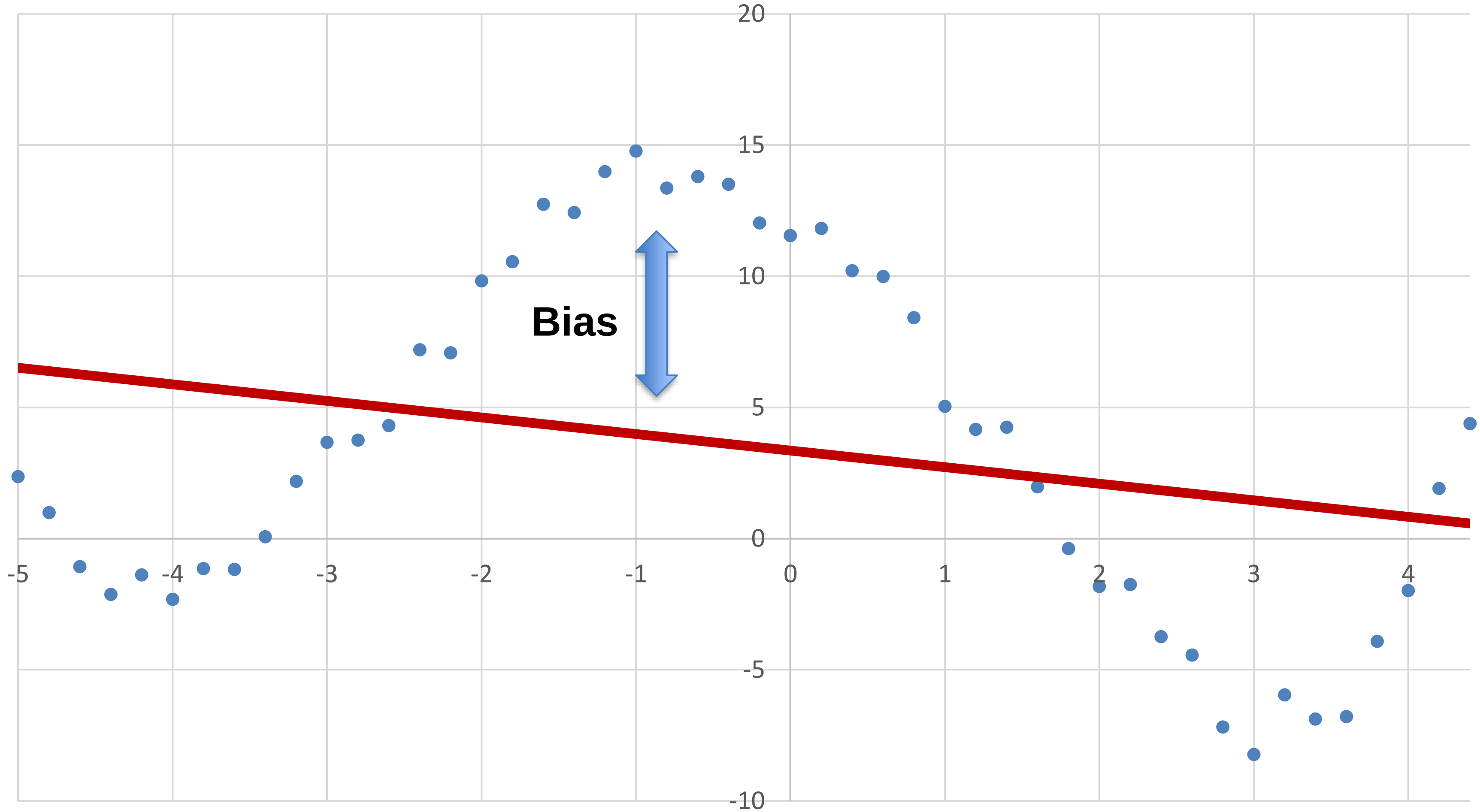
What if Data is Not Linear?

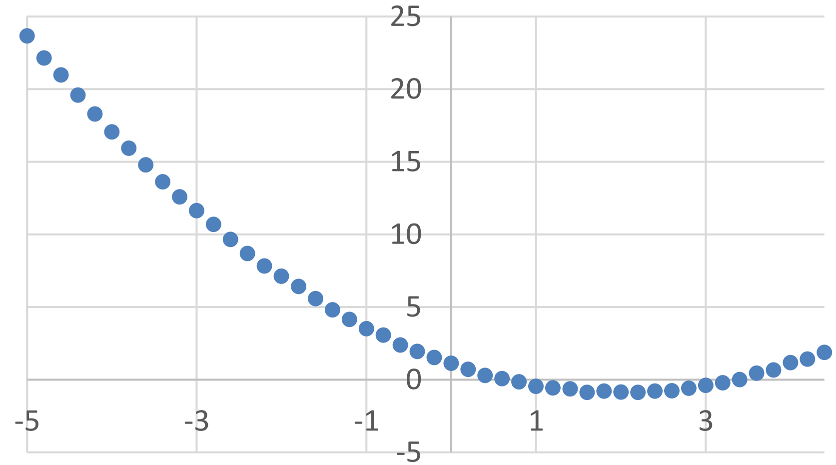


What if Data is Not Linear?



Fitting Quadratic Functions

- Suppose f is quadratic:

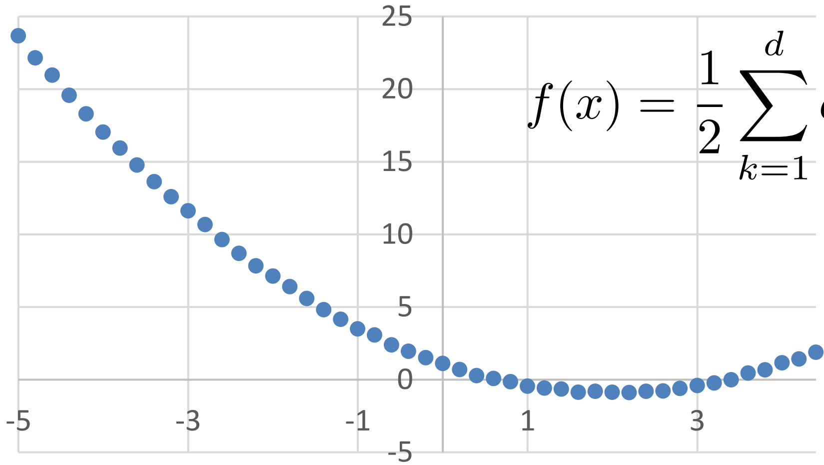


$$f(x) = \frac{1}{2}x^\top Q x + b^\top x + c$$

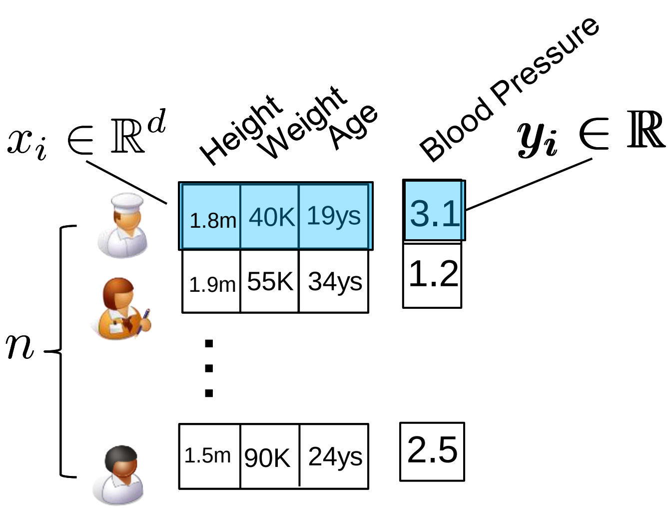
$$= \frac{1}{2}\sum_{k=1}^{d}\sum_{k'=1}^{d} q_{kk'}x_k x_{k'} + \sum_{k=1}^{d} b_k x_k + c$$

$$= \frac{1}{2}\sum_{k=1}^{d} q_{kk}x_k^2 + \sum_{k=1}^{d}\sum_{k'>k}^{d} q_{kk'}x_k x_{k'} + \sum_{k=1}^{d} b_k x_k + c$$

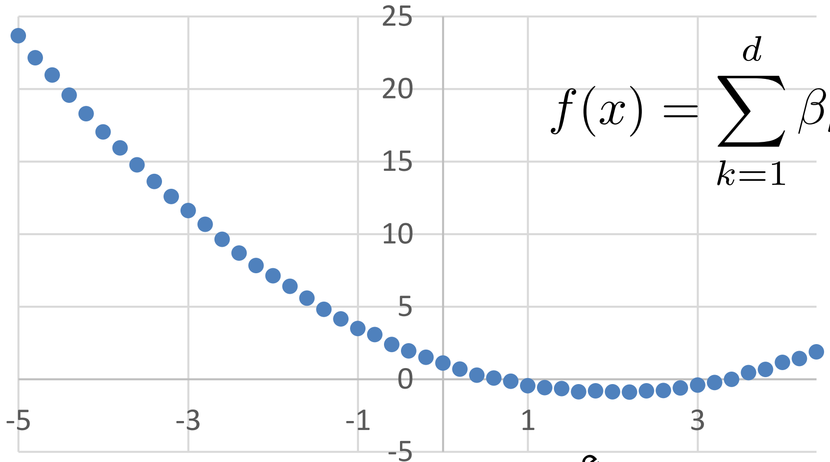
Fitting Quadratic Functions



$$f(x) = \frac{1}{2}\sum_{k=1}^{d} q_{kk} x_k^2 + \sum_{k=1}^{d}\sum_{k'>k}^{d} q_{kk'} x_k x_{k'} + \sum_{k=1}^{d} b_k x_k + c$$

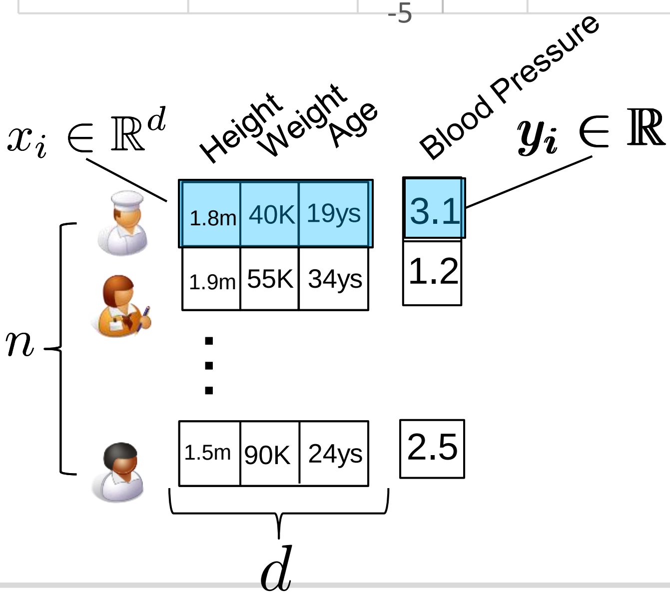


Fitting Quadratic Functions

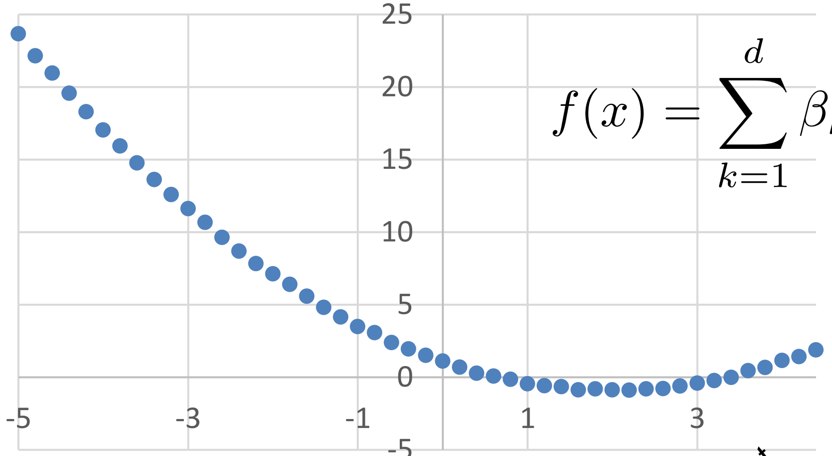


$$f(x) = \sum_{k=1}^{d} \beta_{kk} x_k^2 + \sum_{k=1}^{d} \sum_{k'>k}^{d} \beta_{kk'} x_k x_{k'} + \sum_{k=1}^{d} \beta_k x_k + \beta_0$$

$$\beta \in \mathbb{R}^{\frac{d(d-1)}{2}+2d+1}$$

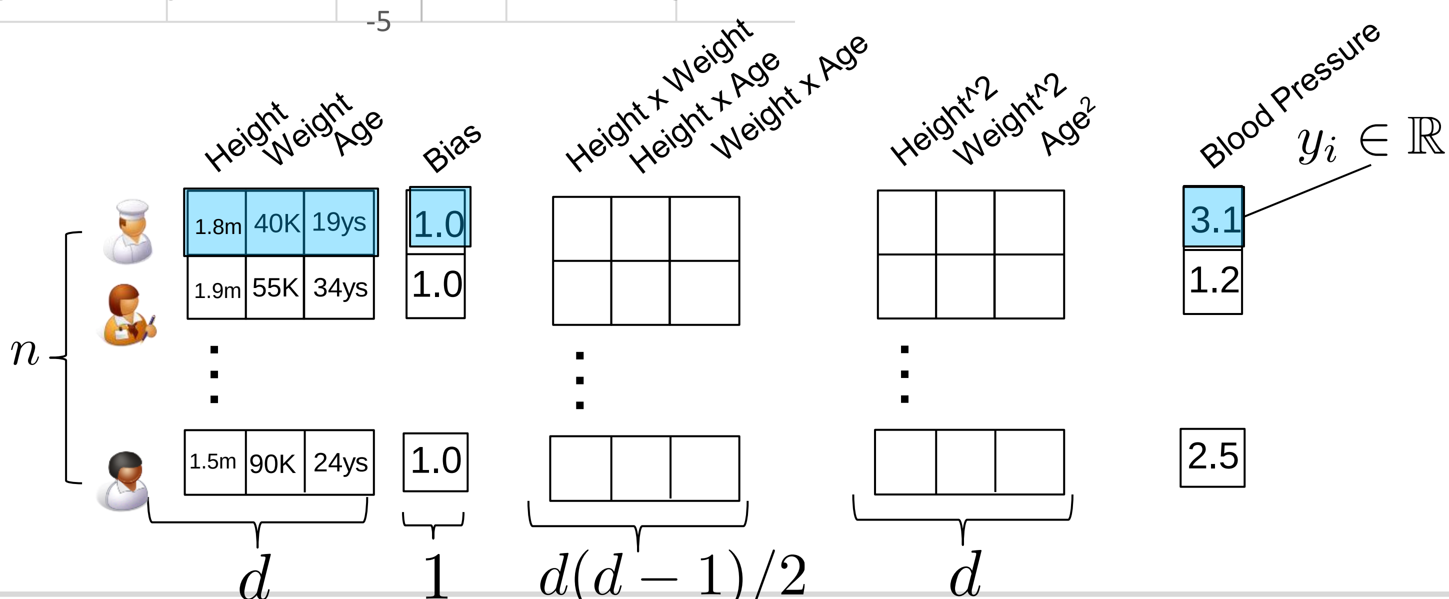


Fitting Quadratic Functions



$$f(x) = \sum_{k=1}^{d} \beta_{kk} x_k^2 + \sum_{k=1}^{d} \sum_{k'>k}^{d} \beta_{kk'} x_k x_{k'} + \sum_{k=1}^{d} \beta_k x_k + \beta_0$$

Learn $\beta \in \mathbb{R}^{\frac{d(d-1)}{2}+2d+1}$ **through LSE!**



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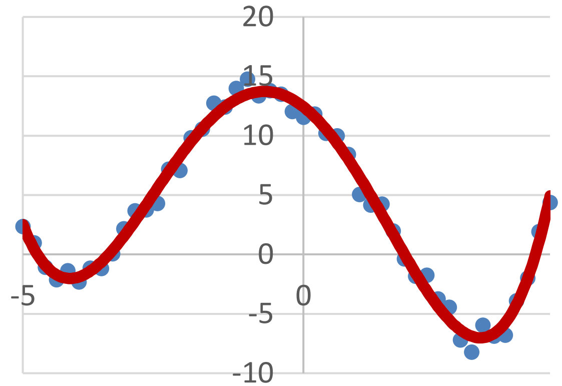
Fitting Polynomials

To learn a polynomial f of degree

$$k = 2, 3, \ldots :$$



- Produce new features containing all monomials:

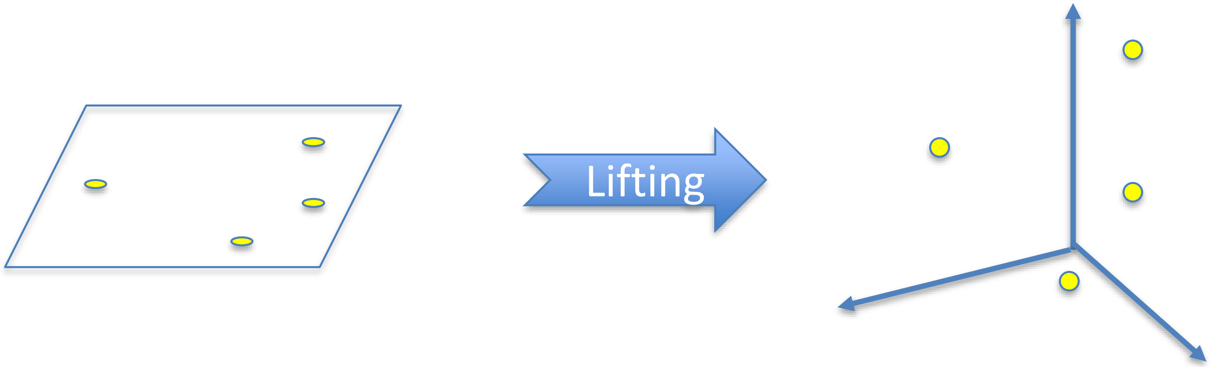
$$\prod_{i=1}^{d} x_i^{k_i} = x_1^{k_1} x_2^{k_2} \ldots x_d^{k_d}$$

where $k_1 + k_2 + \ldots + k_d \leq k$.

- Perform linear regression on resulting new set of features

Lifting

- Affine in $\mathbb{R}^d$ = Linear in $\mathbb{R}^{d+1}$
- Quadratic in $\mathbb{R}^d$ = Linear in $\mathbb{R}^{d(d-1)/2+2d+1} = \mathbb{R}^{O(d^2)}$
- Polynomial of degree k in $\mathbb{R}^d$ = Linear in $\mathbb{R}^{O(d^k)}$



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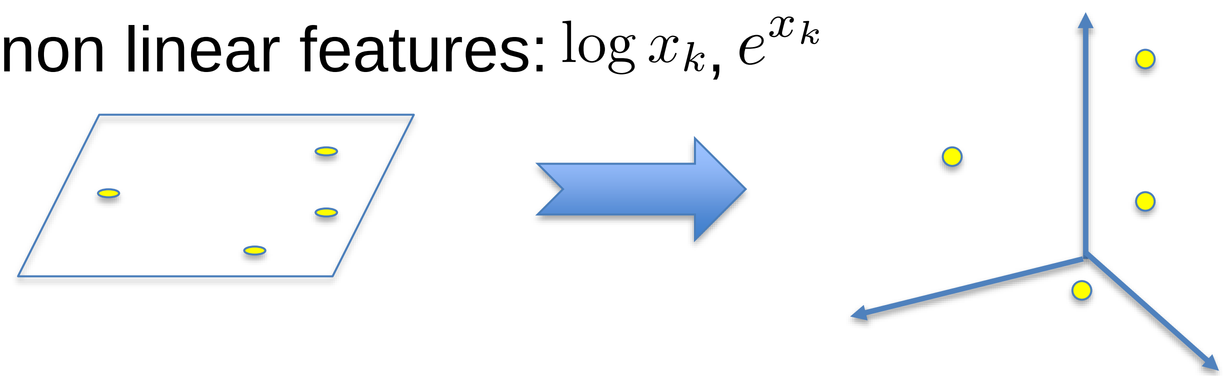
Different Basis Functions

Coefficients to be learned

Known **basis** functions

$$f(x) = \sum_{\ell=1}^{m} \beta_\ell f_\ell(x)$$

- Polynomials: basis functions are monomials
- Periodic functions: $\sin(\ell \frac{x}{T}), \cos(\ell \frac{x}{T}), \ell \in \mathbb{N}, x \in [0, T]$
- Other non linear features: $\log x_k$, e^{x_k}



$(x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$ $\qquad$ $(f_1(x), f_2(x), \ldots, f_m(x)) \in \mathbb{R}^m$

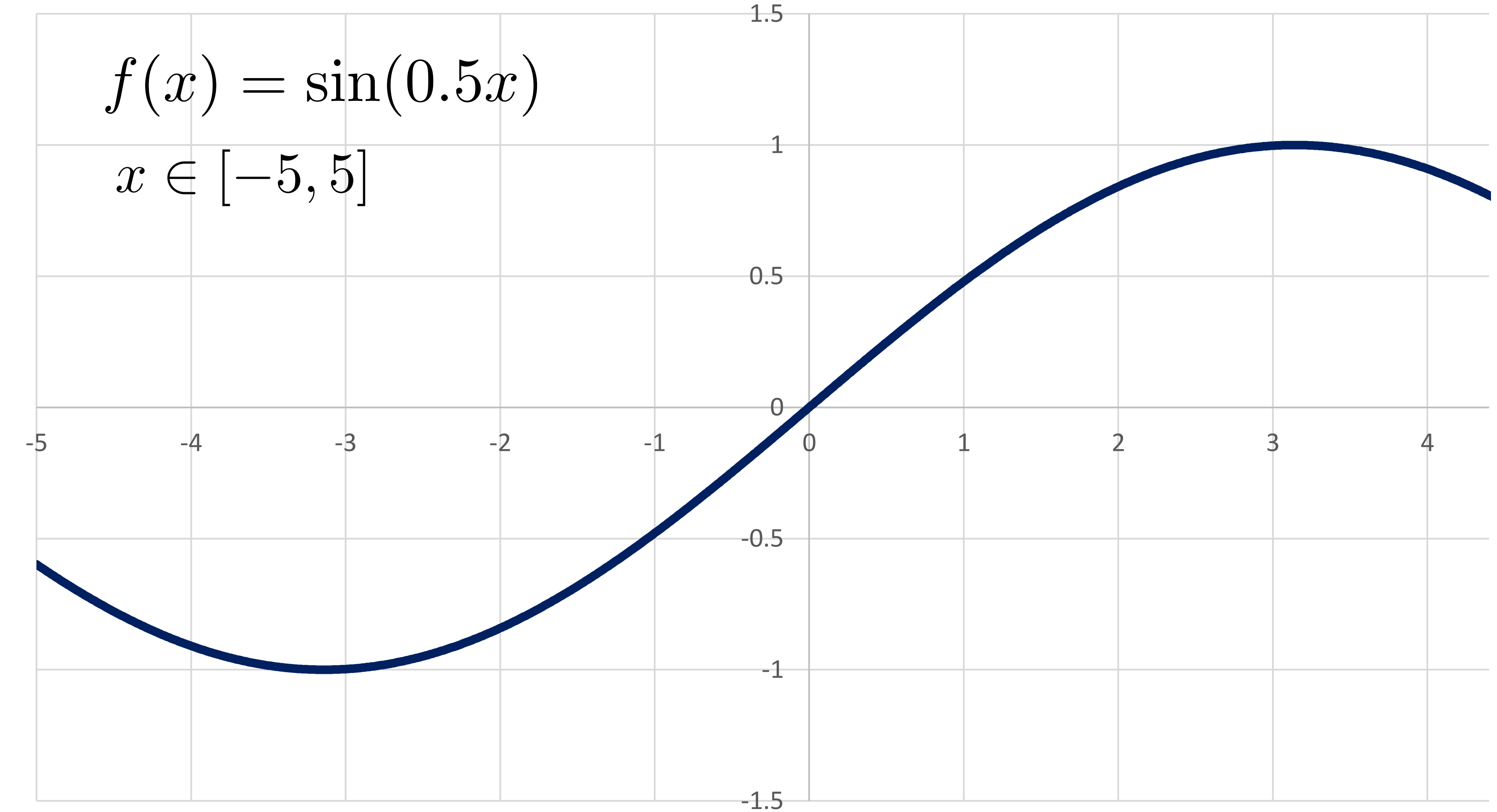
Stone-Weierstrass Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a continuous function defined over a closed and bounded set $A \subset \mathbb{R}^d$. Then, for any $\delta > 0$, there exists a polynomial $p : \mathbb{R}^d \to \mathbb{R}$ such that:

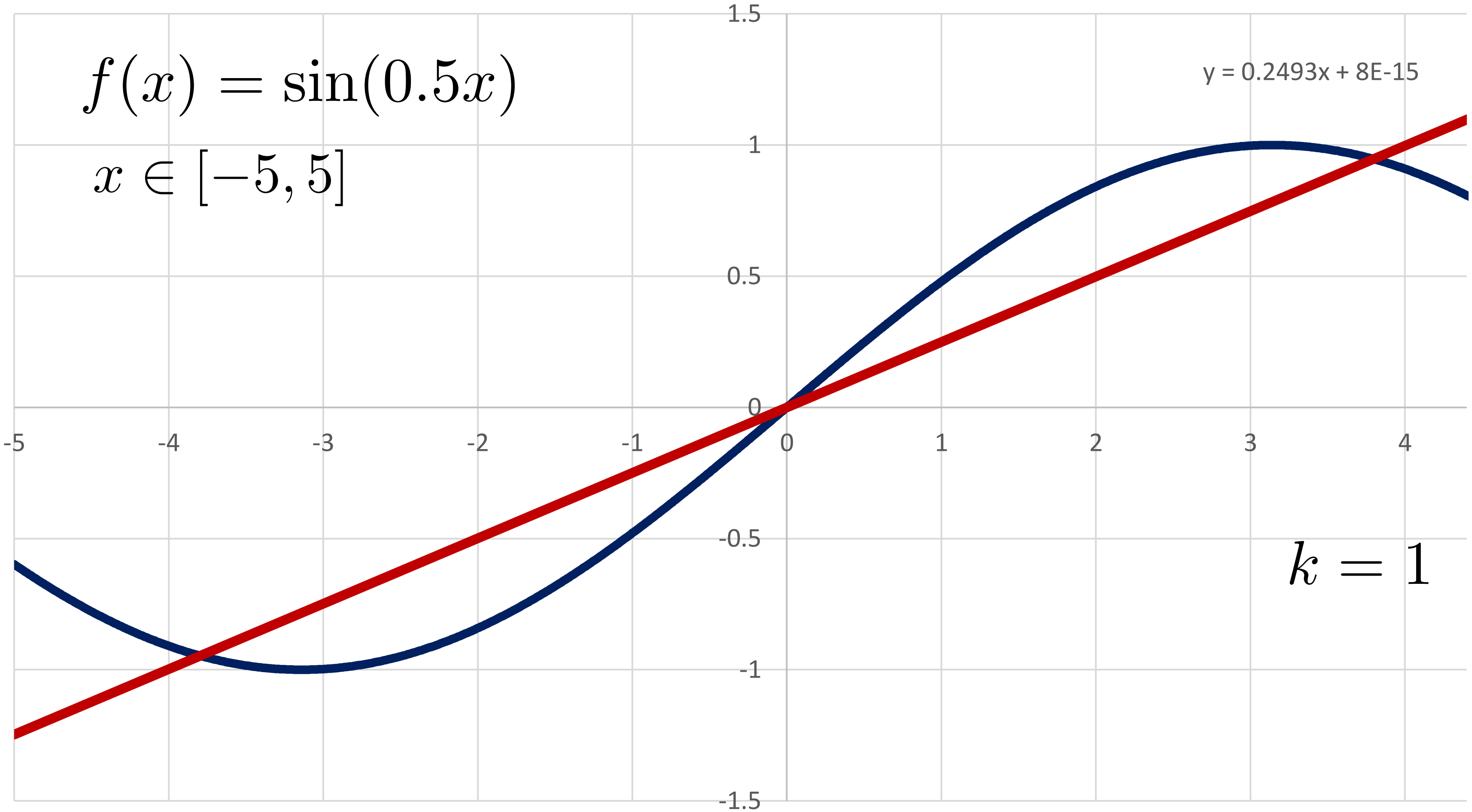
$$|f(x) - p(x)| \leq \delta$$

for all $x \in A$.

Stone-Weierstrass in Action



Stone-Weierstrass in Action



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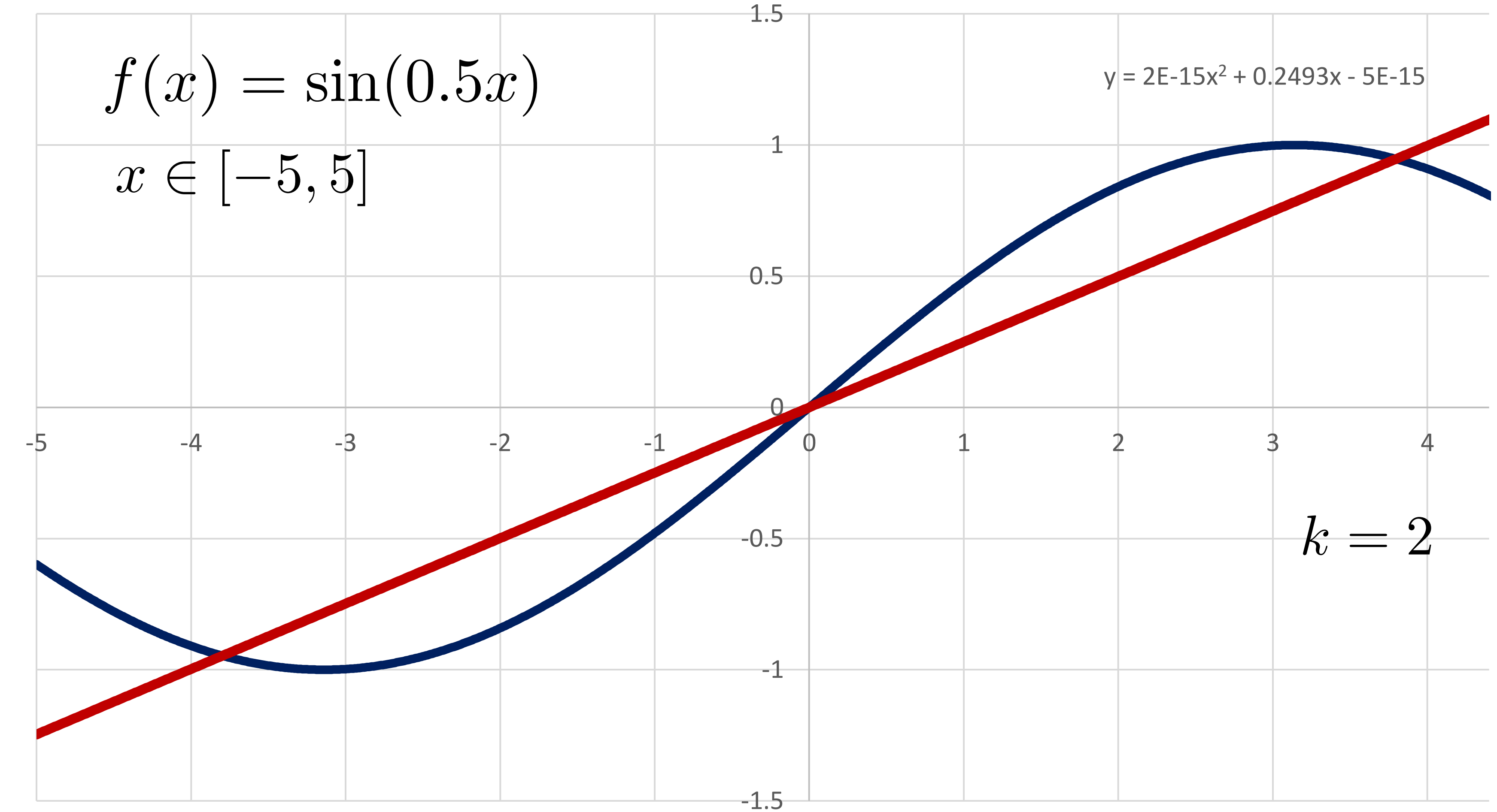
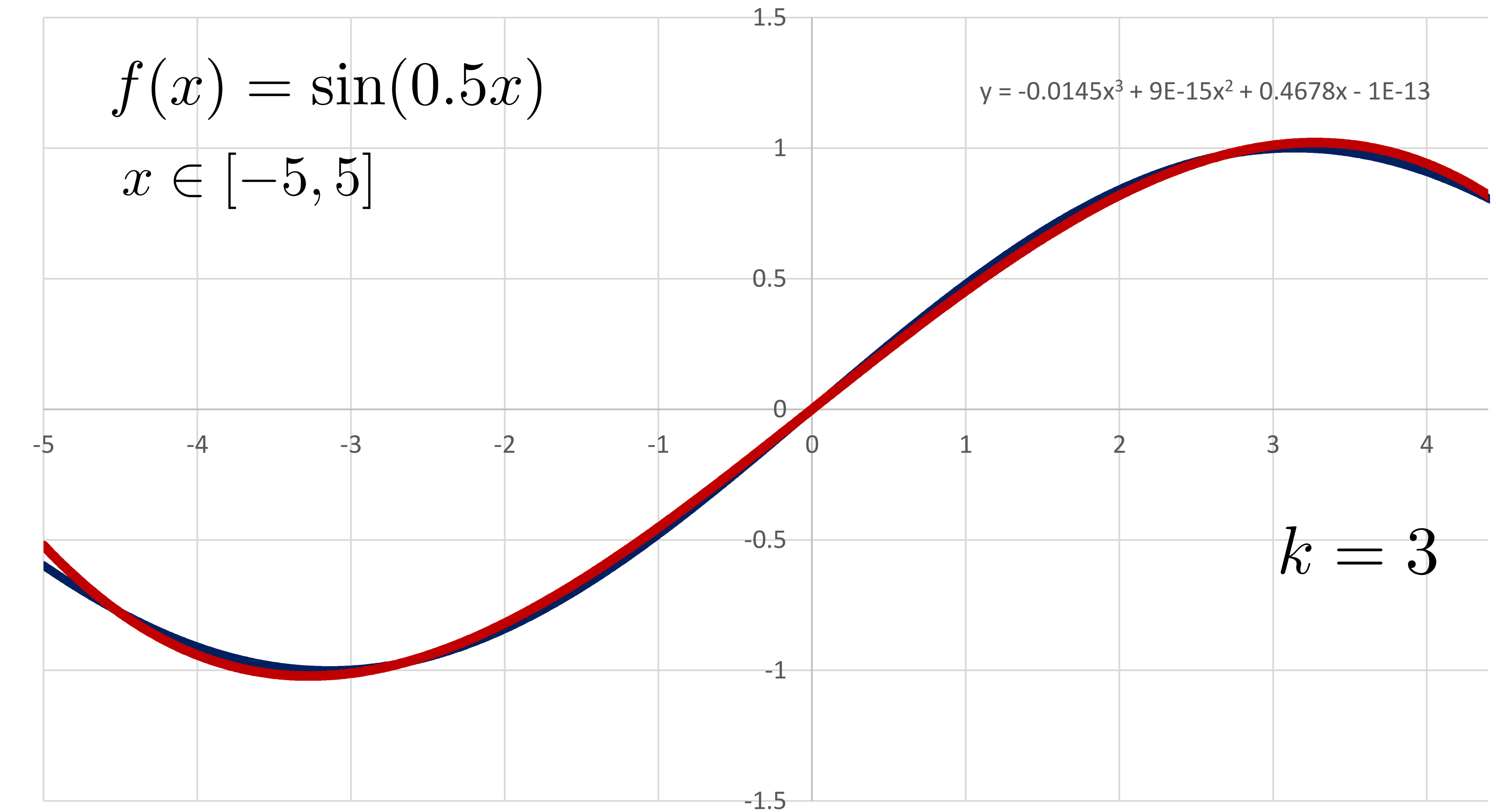
Stone-Weierstrass in Action



Stone-Weierstrass in Action



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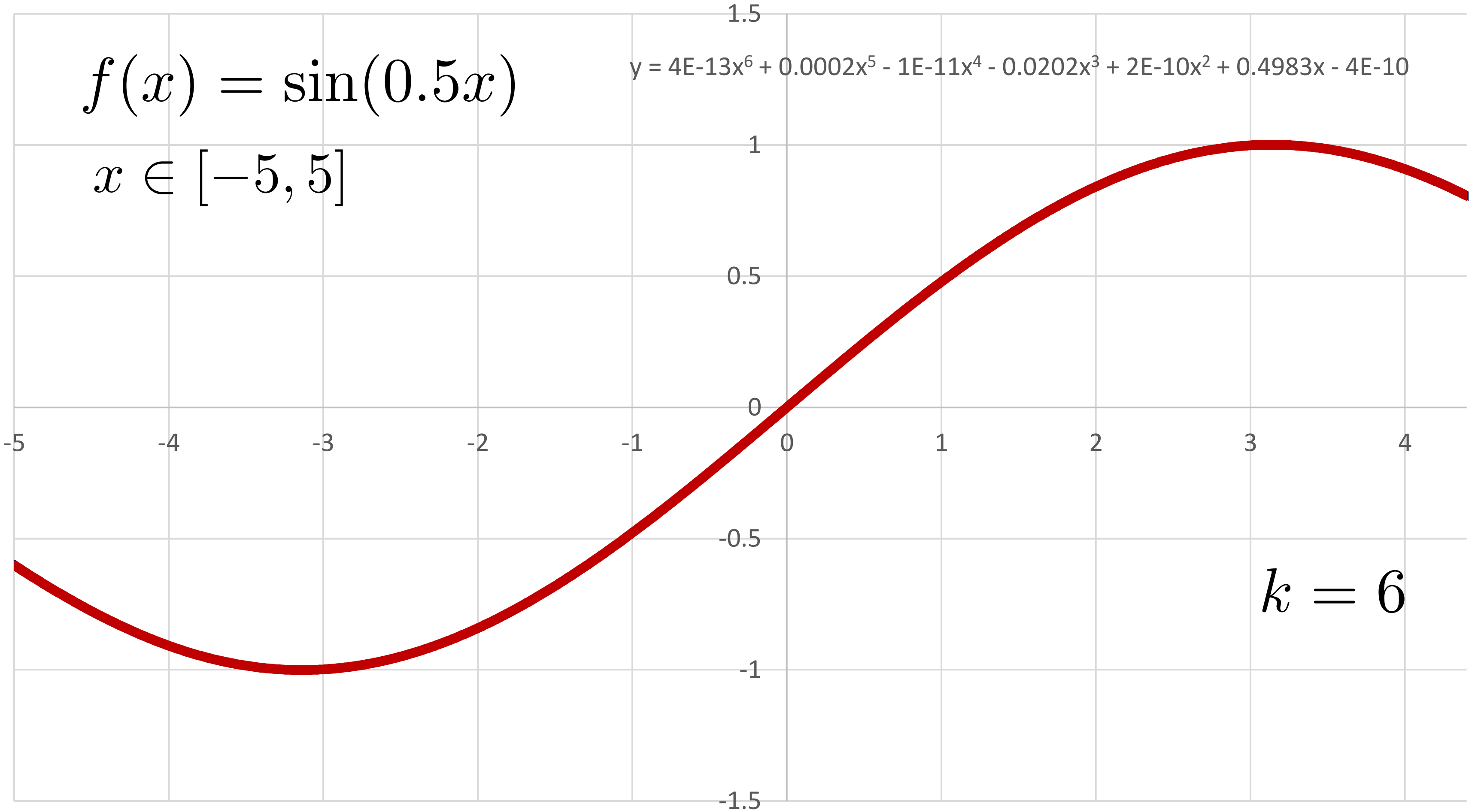
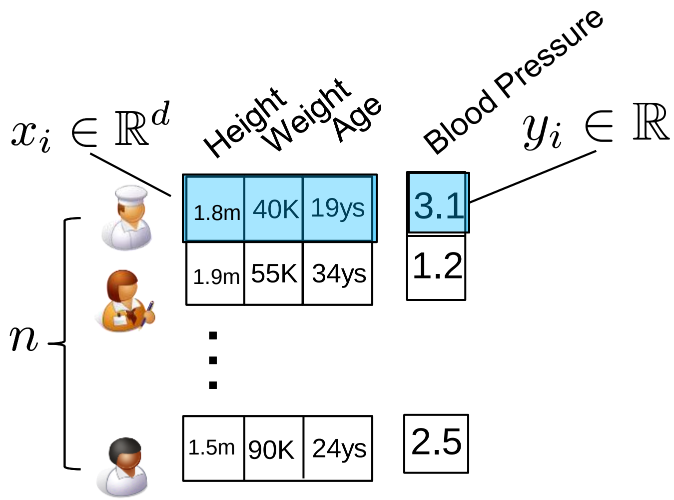
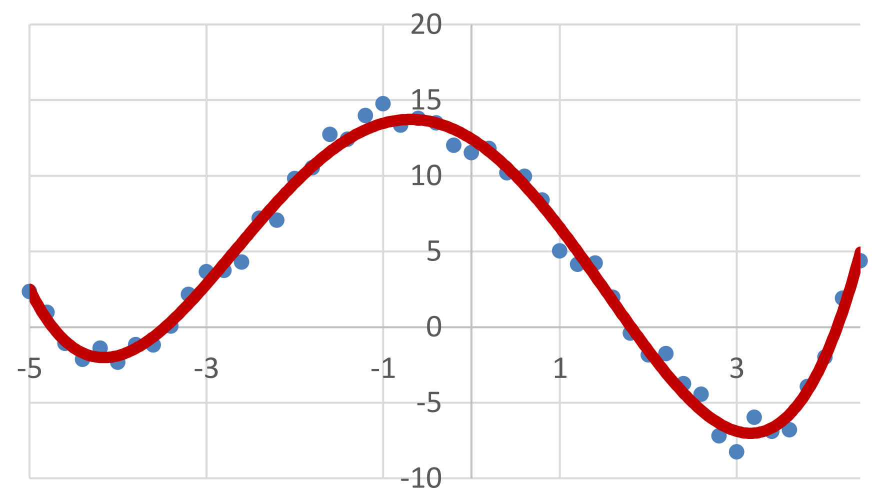
Stone-Weierstrass in Action



What Does This Imply?





$$y_i = f(x_i) + \varepsilon_i, \quad i = 1, \ldots, n$$

Suppose features x_i are in in $[0, 100]^d$, and $f : \mathbb{R}^d \to \mathbb{R}$ is a continuous function.

Then, we can learn a polynomial that is **arbitrarily close to** f using linear regression!

Wait…what?

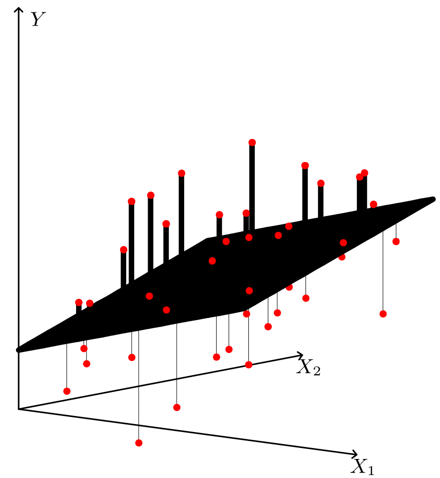
kNN

- $f : \mathbb{R}^d \to \mathbb{R}$ is continuous

Curse of dimensionality

Linear Regression

- $f : \mathbb{R}^d \to \mathbb{R}$ is linear.



No curse: we have assumed it away!

Wait…what?

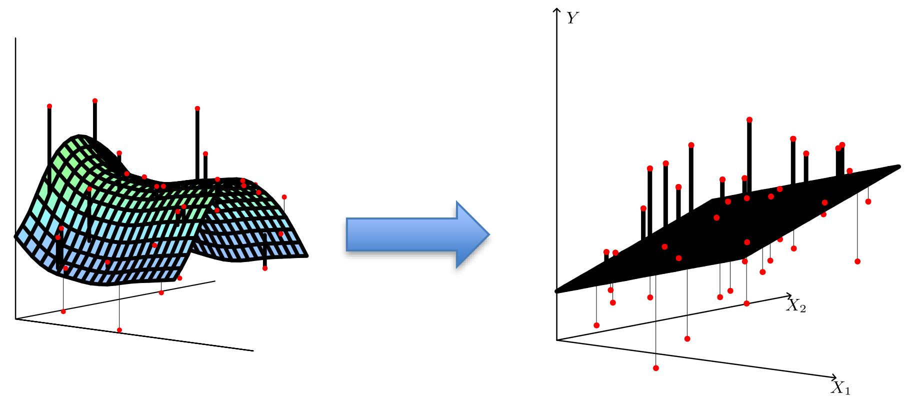
kNN

- ❑ $f : \mathbb{R}^d \to \mathbb{R}$ is continuous

Curse of dimensionality

Linear Regression

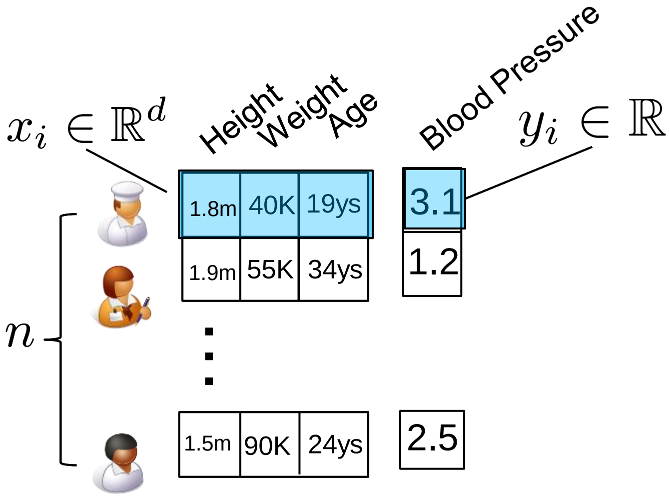
- ❑ $f : \mathbb{R}^d \to \mathbb{R}$ is continuous



Learn f through appropriate lifting.

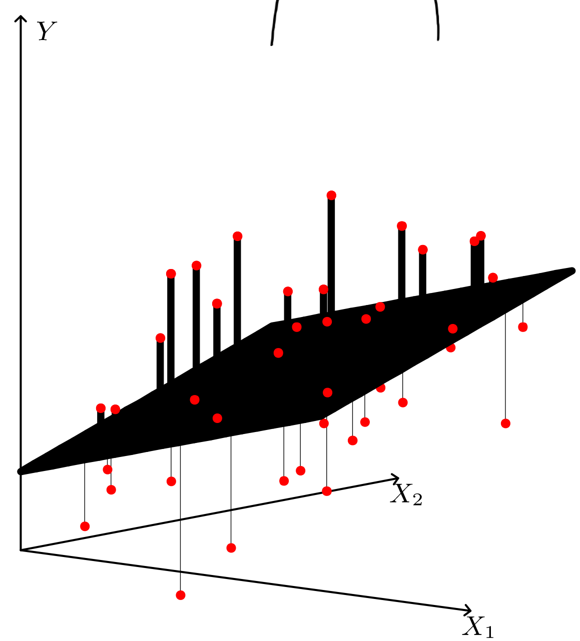
Did we escape the curse?!?

No, We Did Not.



$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

$$\boxed{n \geq \frac{d\sigma^2}{\epsilon}}$$



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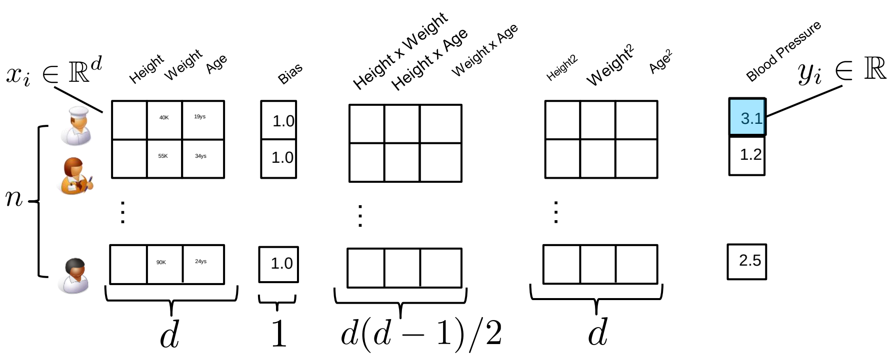
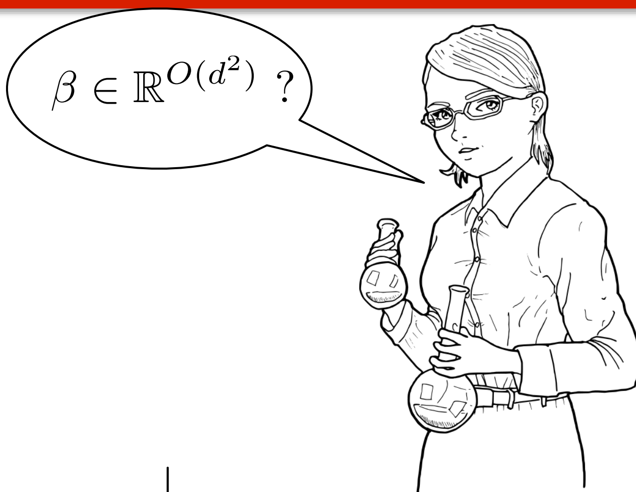
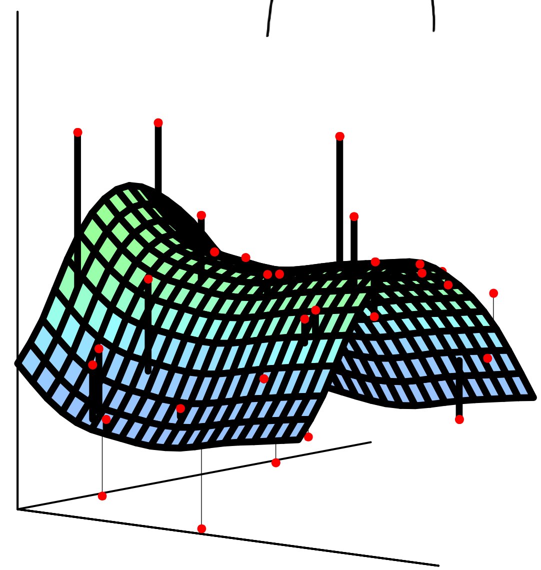


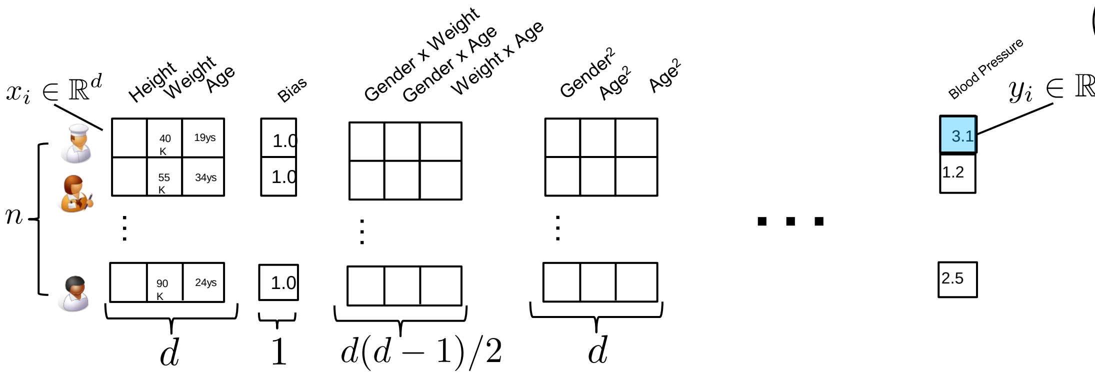


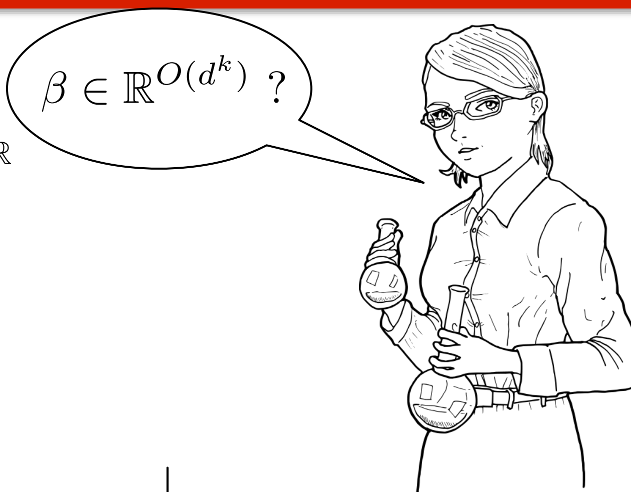
$$f(x) = \sum_{k=1}^{d} \beta_{kk} x_k^2 + \sum_{k=1}^{d} \sum_{k'>k}^{d} \beta_{kk'} x_k x_{k'} + \sum_{k=1}^{d} \beta_k x_k + \beta_0$$



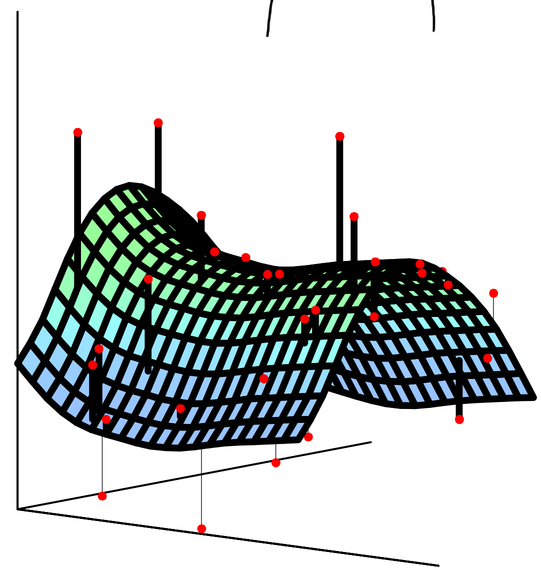
$$n \geq \frac{d^2 \sigma^2}{\epsilon}$$

No, We Did Not.



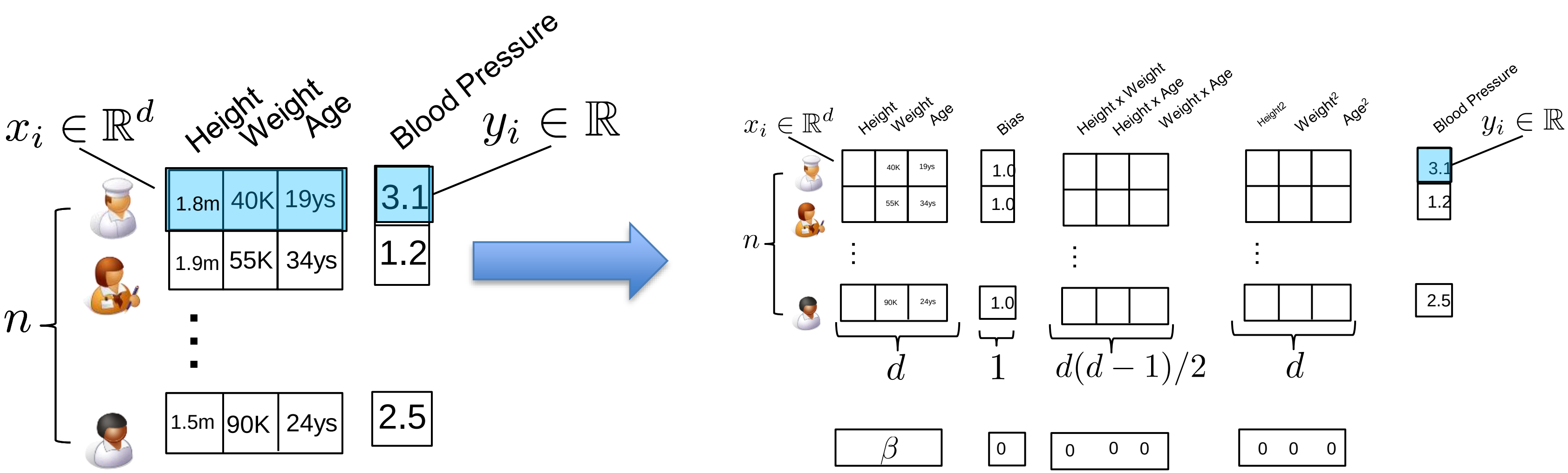


$$f(x) = \sum_{k_1,k_2,\ldots,k_n : \sum_{i=1}^n k_i \le k} \beta_{k_1,k_2,\ldots,k_n} \prod_{i=1}^n x_i^{k_i}.$$



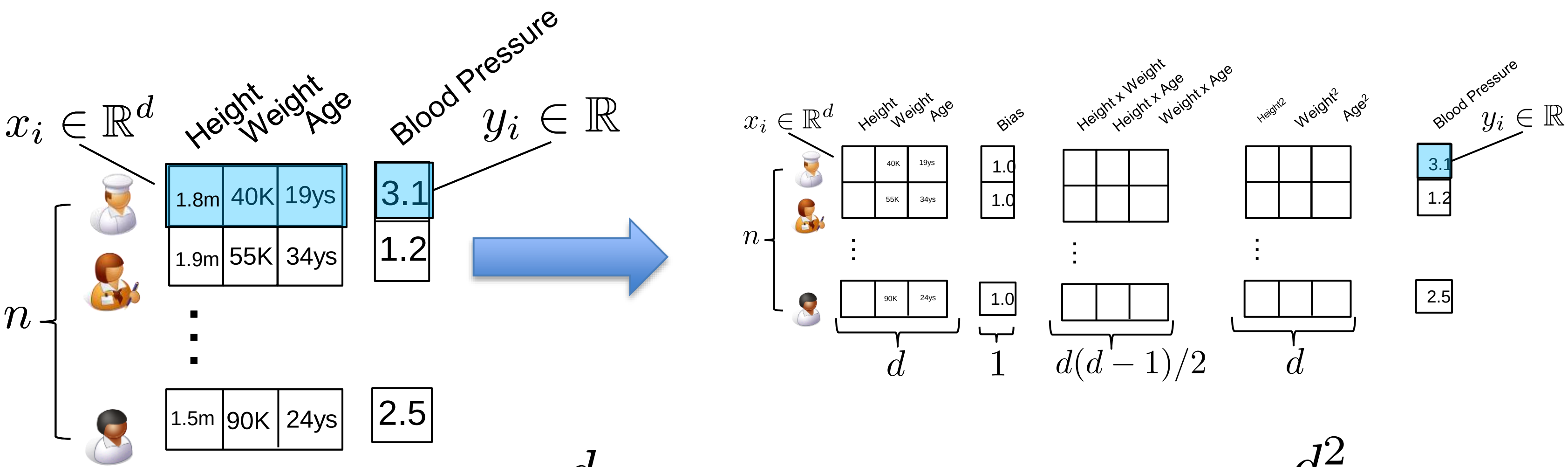
$$n \geq \frac{d^k \sigma^2}{\epsilon}$$

To Lift or Not to Lift?



- If f is **quadratic**, we want to lift
- If f is **linear** and then LSE should still learn a linear model

Lifting Can Lead to Redundant Features

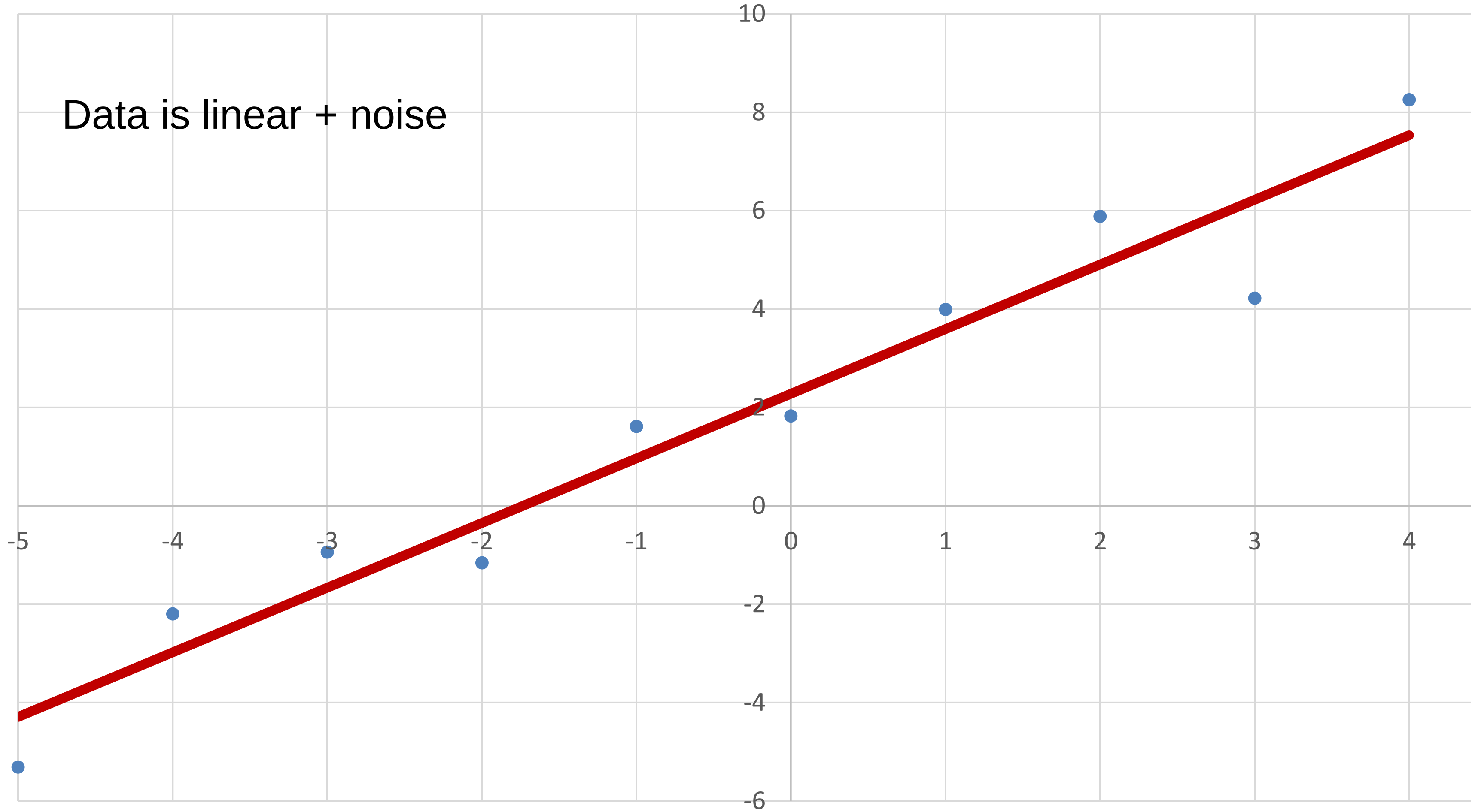


$$\mathbb{E}[\text{EPE}] \approx \sigma^2 + \sigma^2 \frac{d}{n}$$

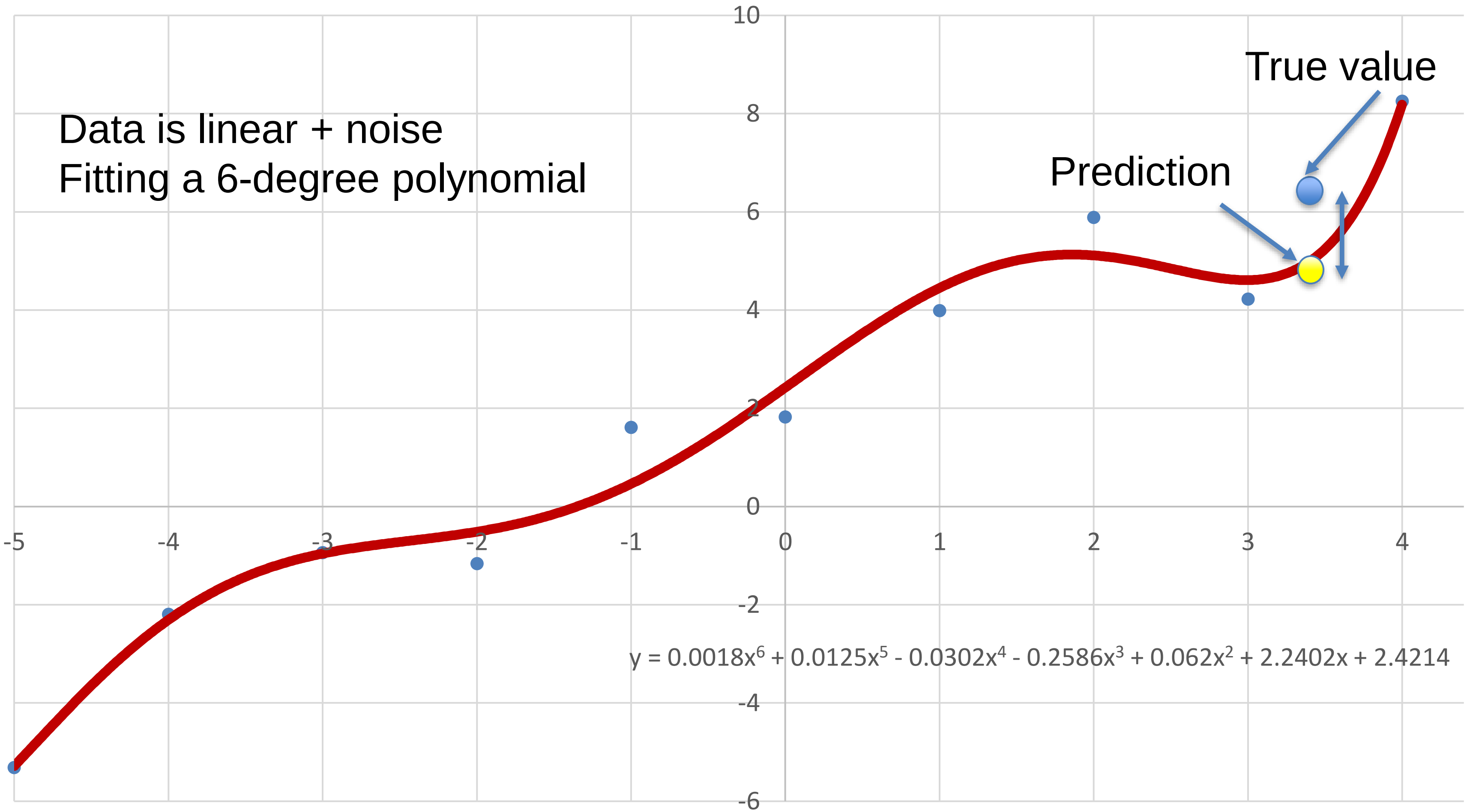
$$\mathbb{E}[\text{EPE}] \approx \sigma^2 + \sigma^2 \frac{d^2}{n}$$

- If f is linear, quadratic features are **redundant/irrelevant**
- Lifting will make EPE increase compared to not lifting!

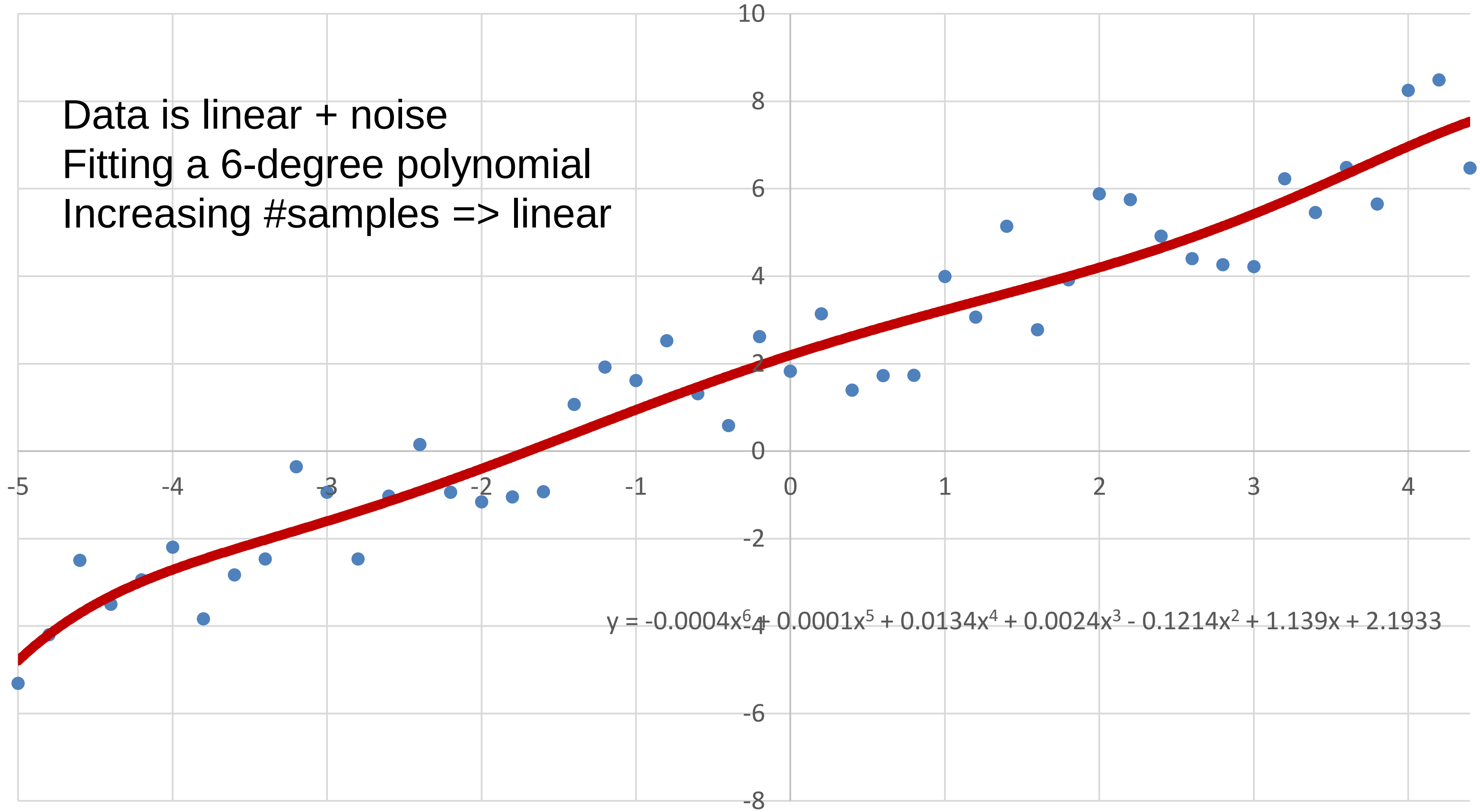
Over-fitting



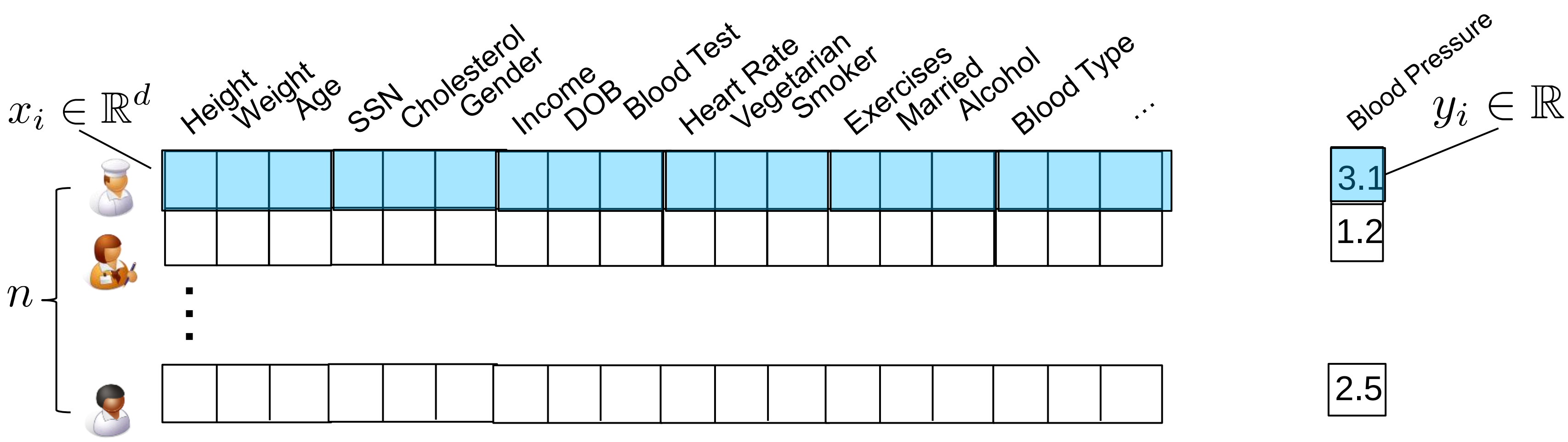
Over-fitting



Over-fitting



Redundant Features May Exist in Data!



$$\beta = \begin{bmatrix} 0 & 0.2 & 0 & 0 & 0 & 0 & -0.3 & 0 & 0 & 0 & 1.4 & 0 & 0 & 2.1 & 0 & 0 & 0 & -2.7 \end{bmatrix}$$

Only $d' \ll d$ features actually affect blood pressure!

Linear Regression needs:

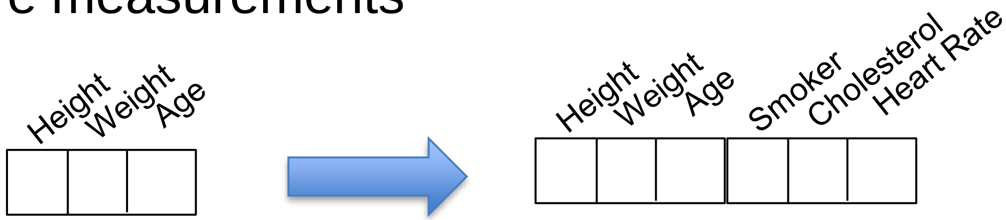
$$n = O(d) \gg O(d')$$

to learn β

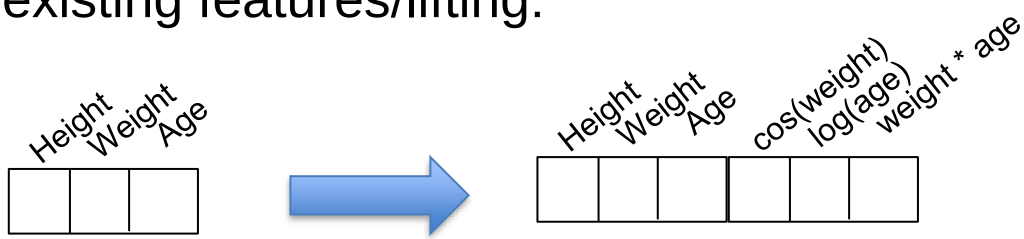
Summary

One can increase number of features by:

- ❑ Collecting more measurements



- ❑ Transforming existing features/lifting:



- ❑ If features are redundant, regression will set corresponding weight to zero, but…

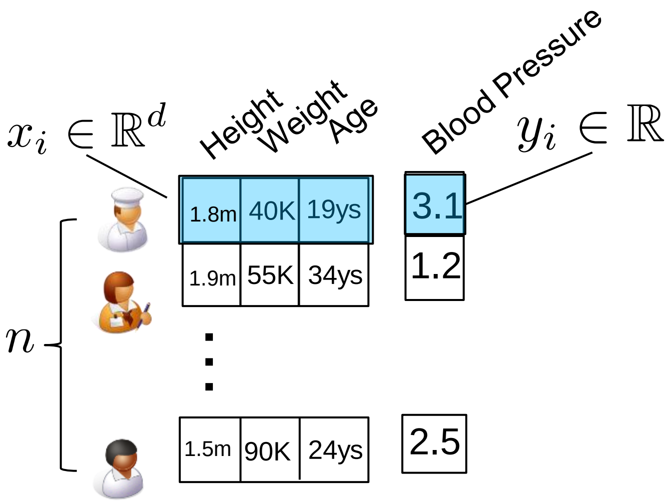
- ❑ ..it will require more samples to do this!!!

A New Challenge

- In practice, we are often just given a dataset

- We cannot increase n: we need to work with what we have

A New Challenge



$$y_i \approx f(x_i), \quad i = 1, \dots, n$$

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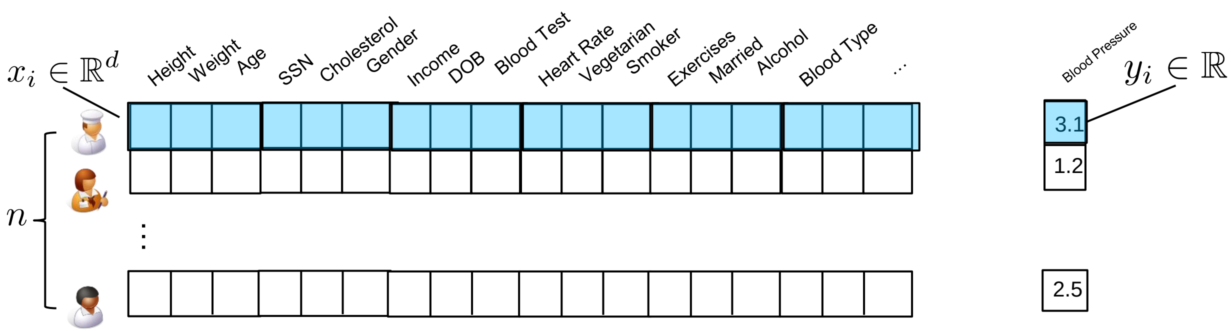
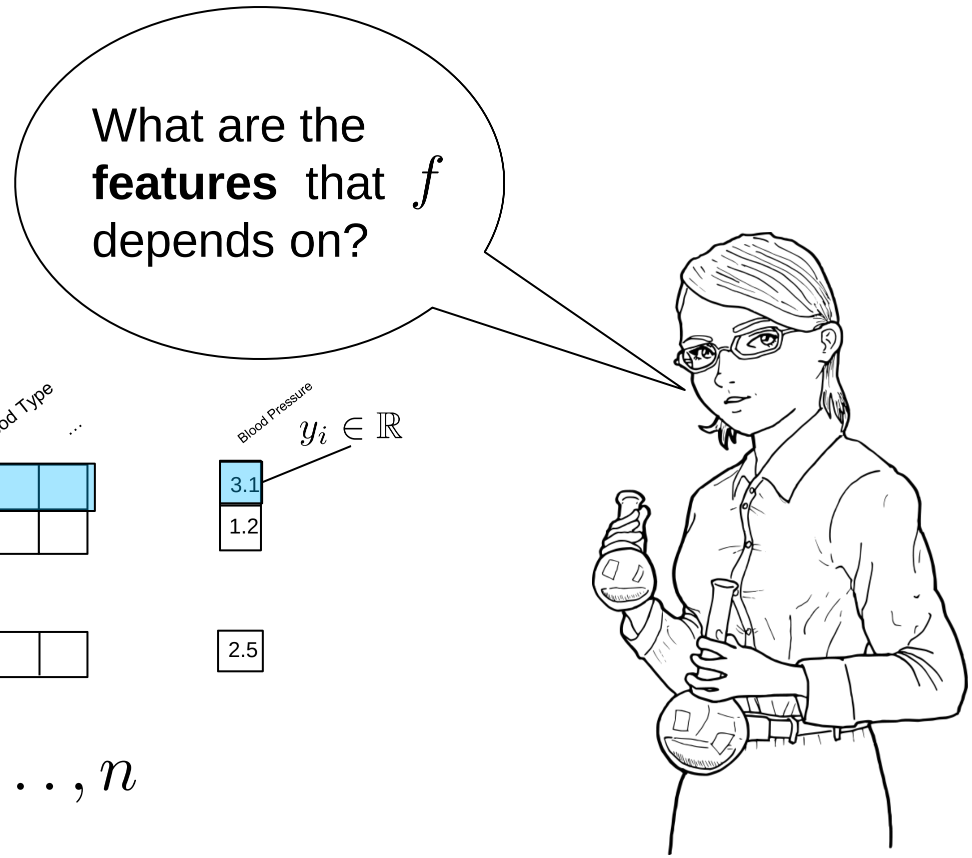
A New Challenge





$$y_i \approx f(x_i), \quad i = 1, \ldots, n$$

Feature Selection!!!

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Q: How can we find out which features matter?

0	0.2	0	0	0	0	-0.3	0	0	0	1.4	0	0	2.1	0	0	0	-2.7	⋰

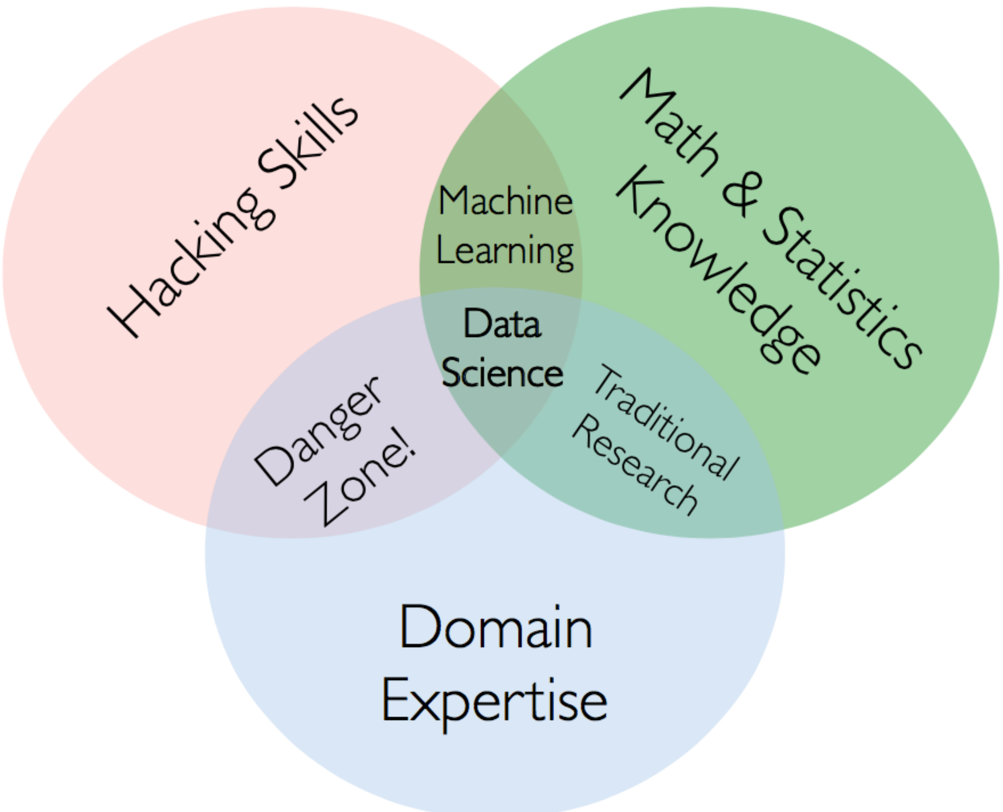
A Simple Solution: Just ask!!!

Experts

What causes high blood pressure?

Statistician/Data Analyst

Revisiting Venn Diagram



http://drewconway.com/zia/2013/3/26/the-data-science-venn-diagram

Ok, but can we do this from data alone?

- No experts
- Experts do not know either
- Discover features experts do not know
- …

Feature Selection

We actually need two things:

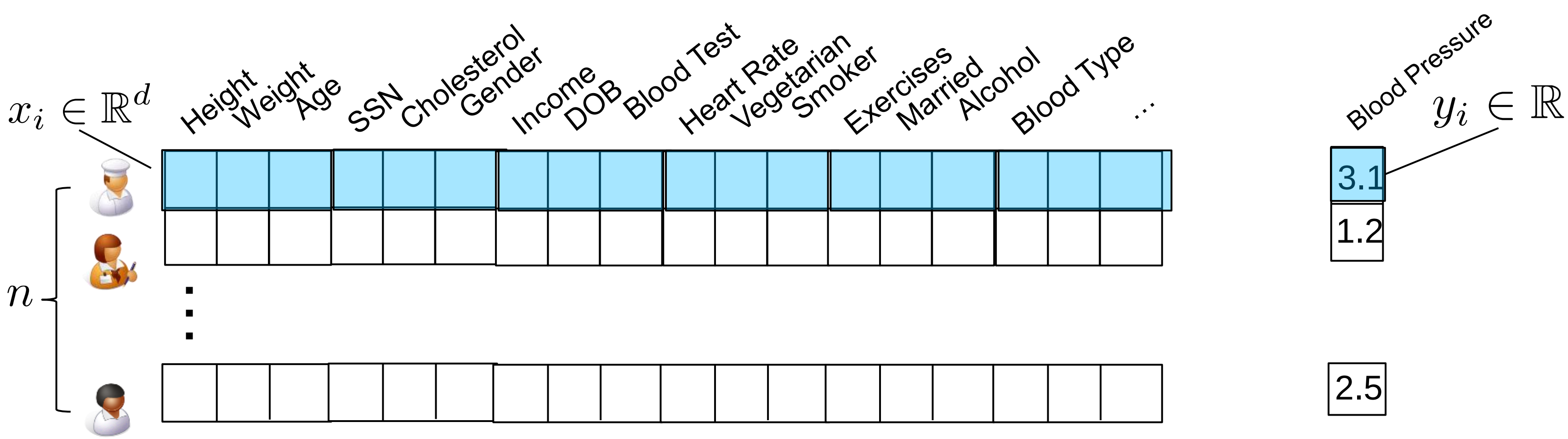
- A procedure for selecting features
- A way of measuring whether this selection is good

Feature Selection

We actually need two things:

- A procedure for selecting features
- **A way of measuring whether this selection is good**

How can I tell if I have a good set of features?

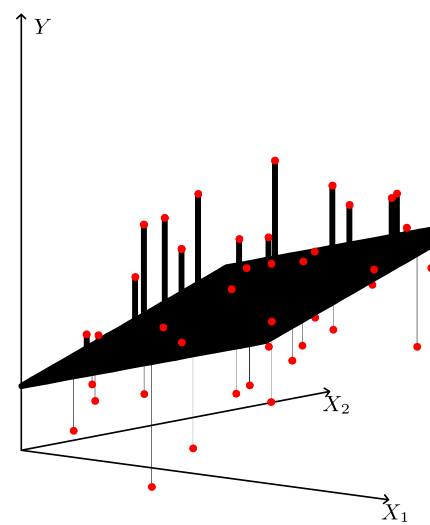


Least-Squares Estimator (LSE)

Residual Sum of Squares

$\mathrm{RSS}(\beta)$

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \langle \beta, x_i \rangle)^2$$
$$= \arg\min_{\beta \in \mathbb{R}^d} \|X\beta - y\|_2^2$$



Q: Can I use RSS to see if I have a good set of features?

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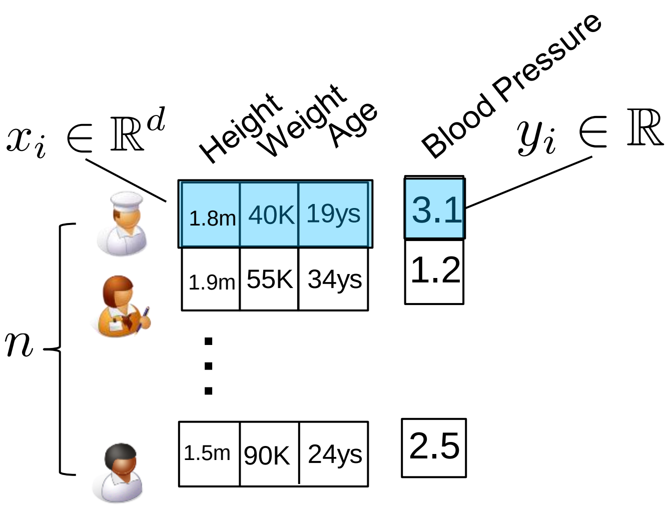
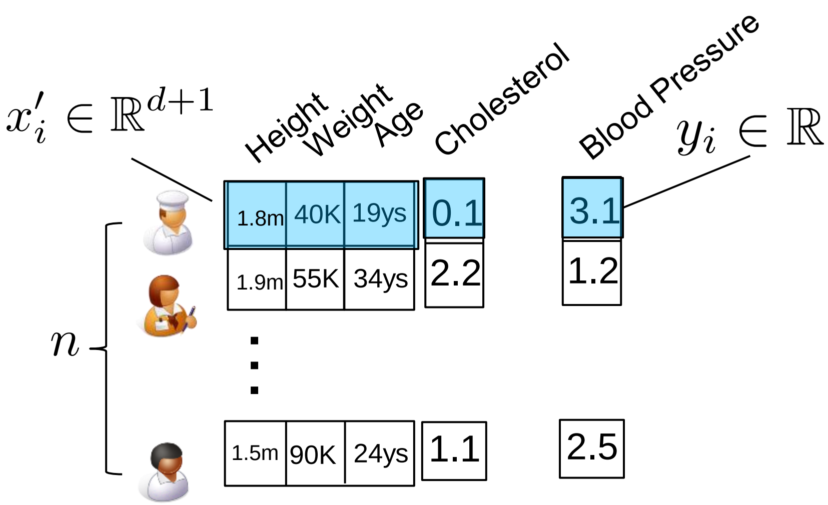
Residual Sum of Squares



$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \langle \beta, x_i \rangle)^2$$

$$\mathrm{RSS}(\hat{\beta}) = \sum_{i=1}^{n} (y_i - \hat{\beta}^\top x_i)$$

Residual Sum of Squares: Adding a New Feature



$$\hat{\beta}' = \arg\min_{\beta \in \mathbb{R}^{d+1}} \sum_{i=1}^{n} (y_i - \beta^\top x'_i)^2$$

$$\mathrm{RSS}(\hat{\beta}') = \sum_{i=1}^{n} (y_i - \hat{\beta}'^\top x'_i)$$

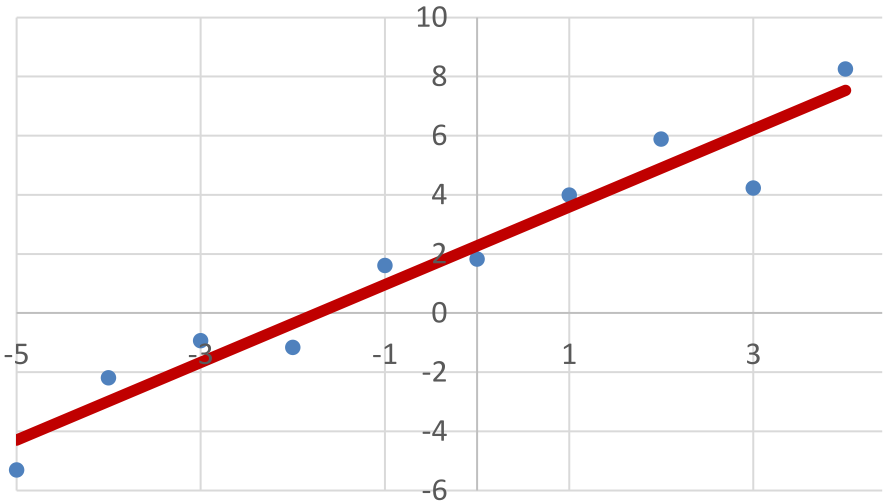
$$\overset{?}{\lessgtr} \mathrm{RSS}(\hat{\beta})$$

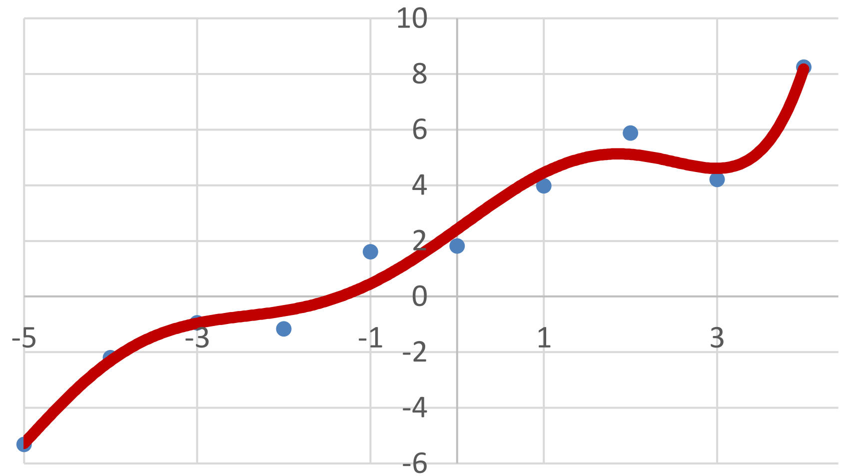
Adding Features Decreases RSS

Proof:

$$\begin{aligned}
\mathtt{RSS}(\hat\beta') &= \min_{\beta\in\mathbb{R}^{d+1}} \mathtt{RSS}(\beta) \\
&\leq \mathtt{RSS}\big((\hat\beta, 0.0)\big) \\
&= \sum_{i=1}^{n}\left(y_i - (\hat\beta, 0.0)^\top x_i'\right)^2 \\
&= \sum_{i=1}^{n}\left(y_i - \hat\beta^\top x_i\right)^2 \\
&= \mathtt{RSS}(\hat\beta)
\end{aligned}$$

Same Principle As Overfitting!





RSS(linear) > RSS(poly(6))

Illustration: Best-Subset Selection

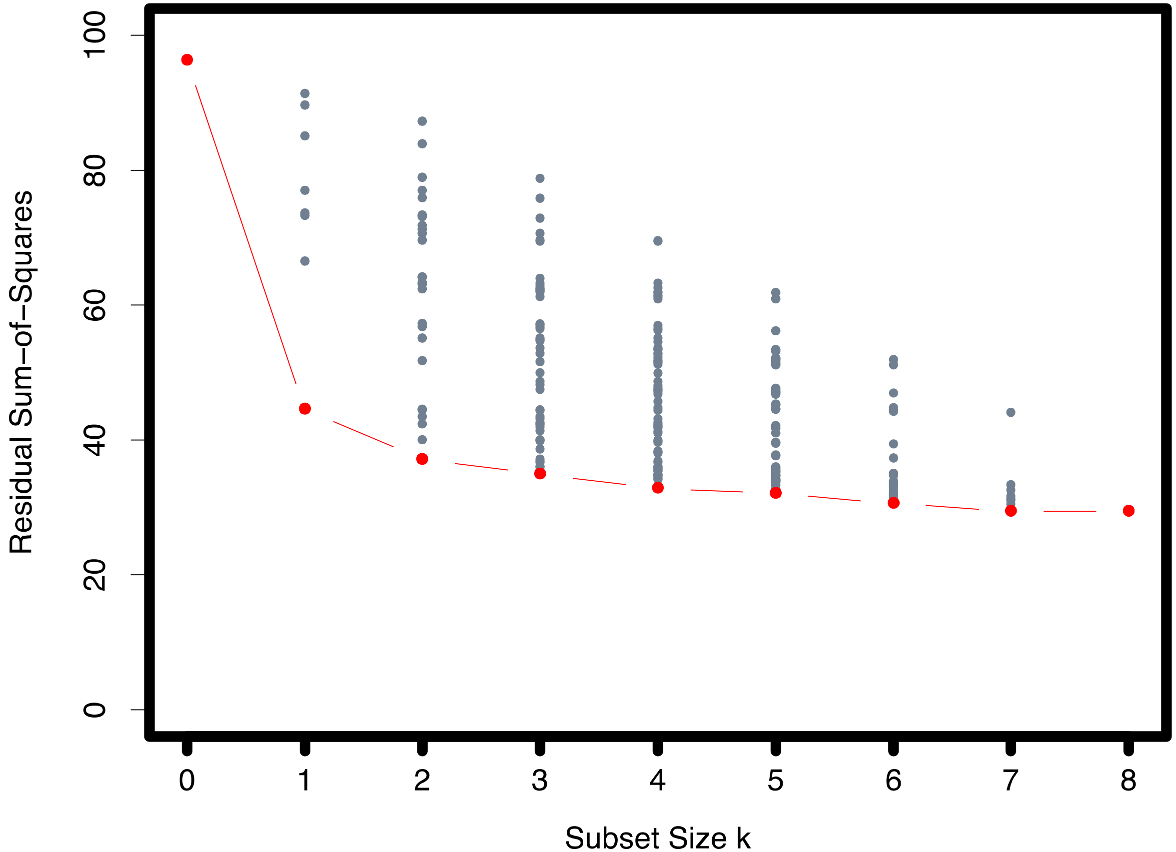
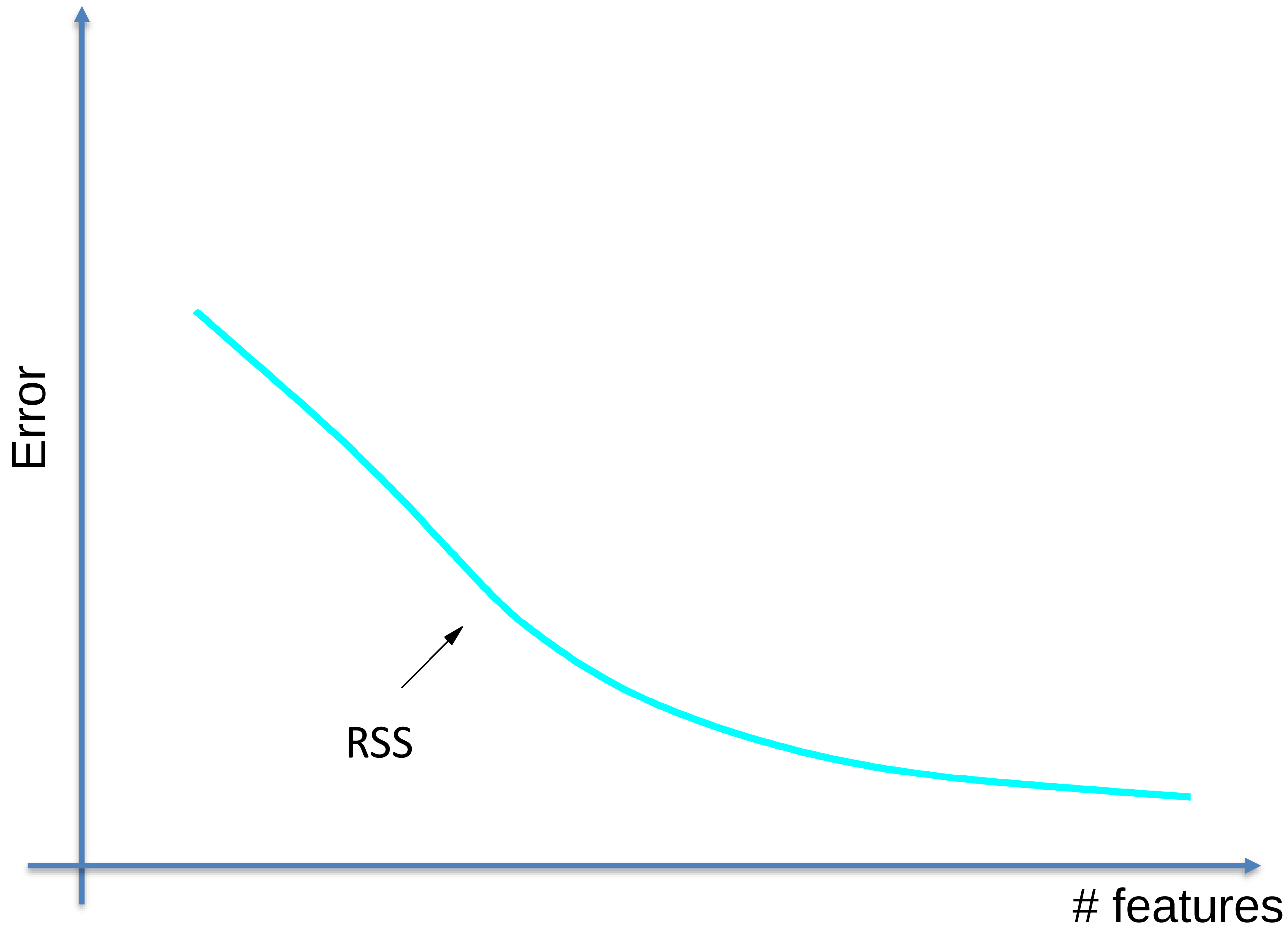


FIGURE 3.5. *All possible subset models for the prostate cancer example. At each subset size is shown the residual sum-of-squares for each model of that size.*

Solution: EPE



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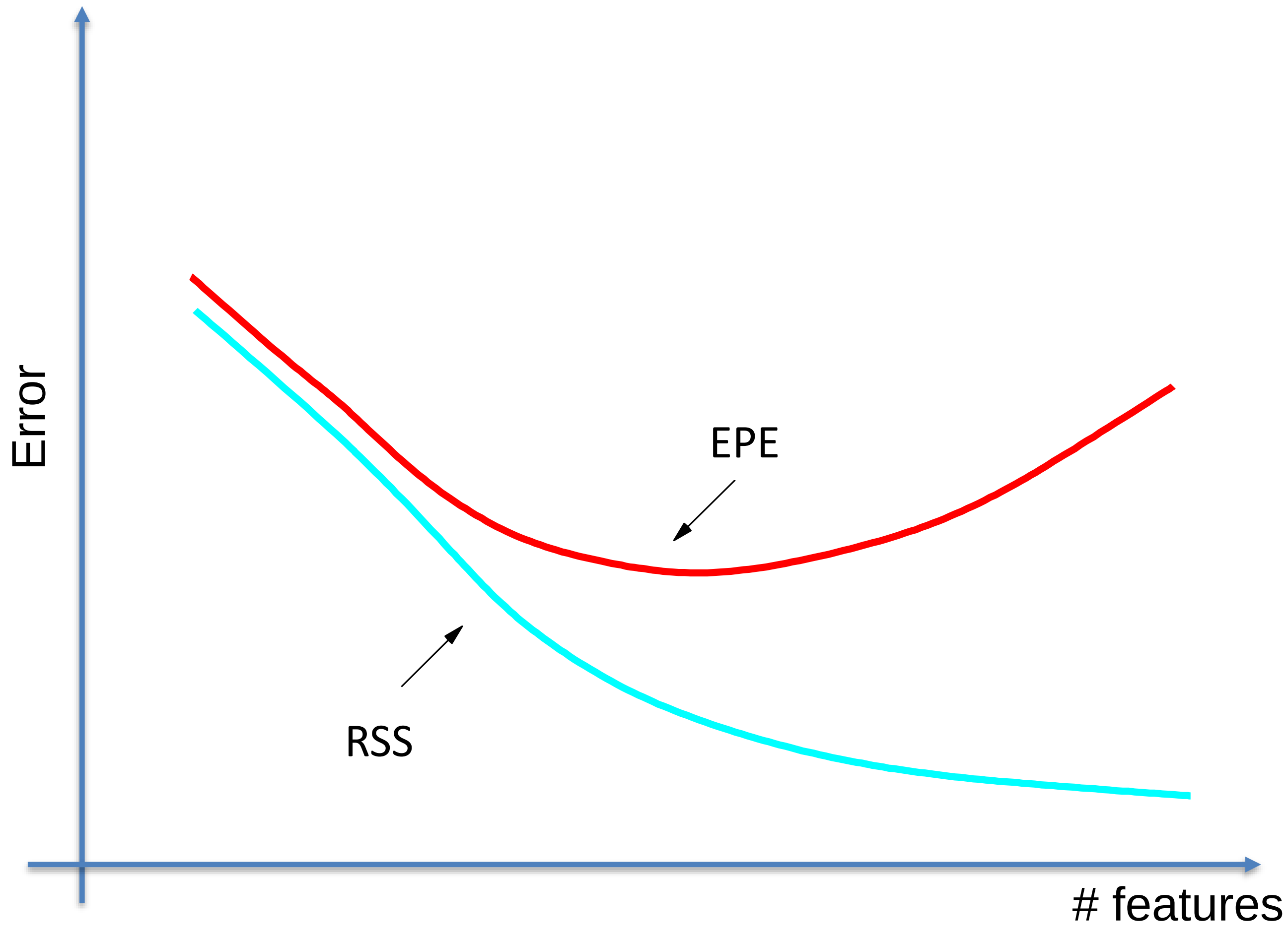
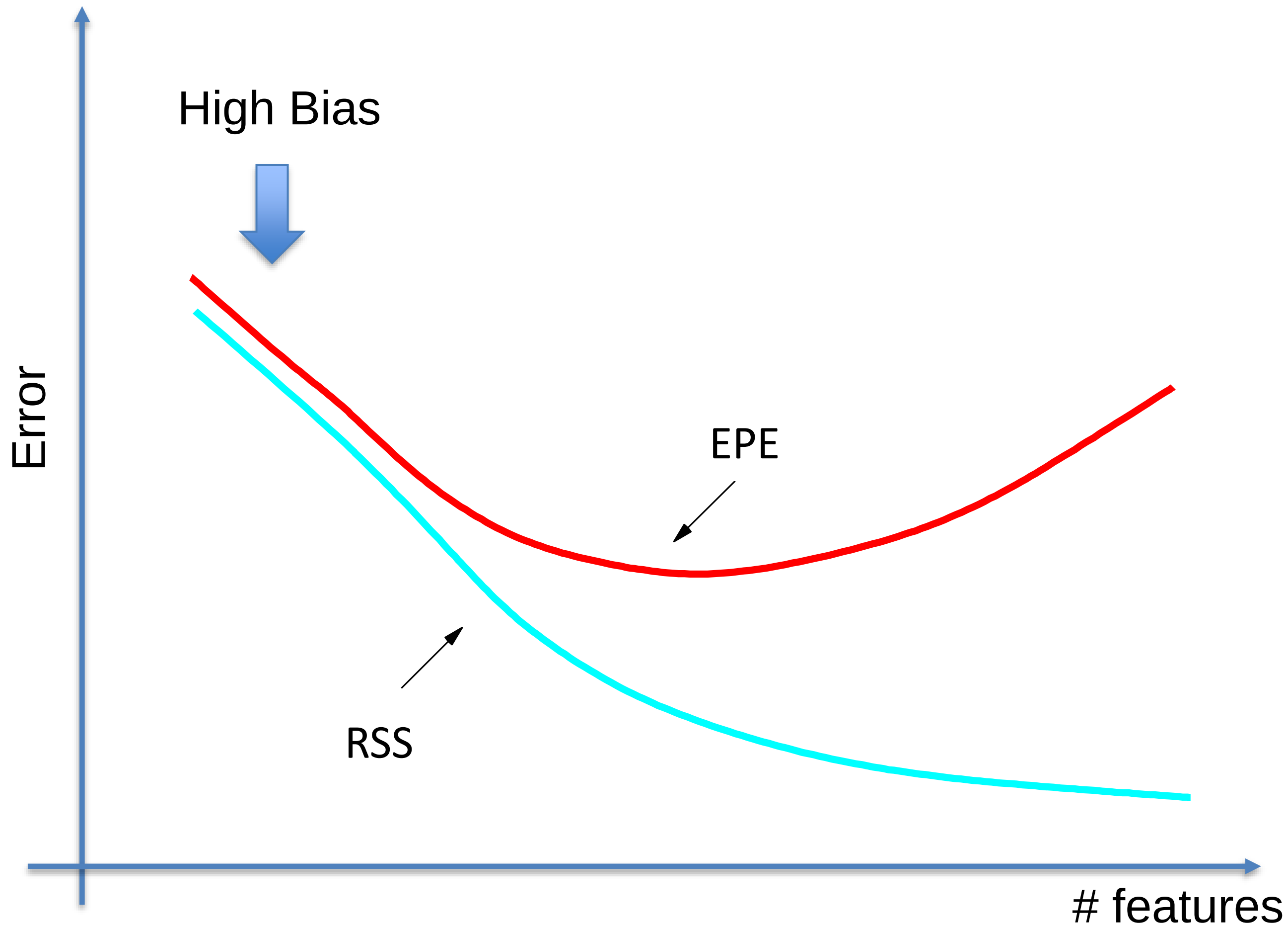
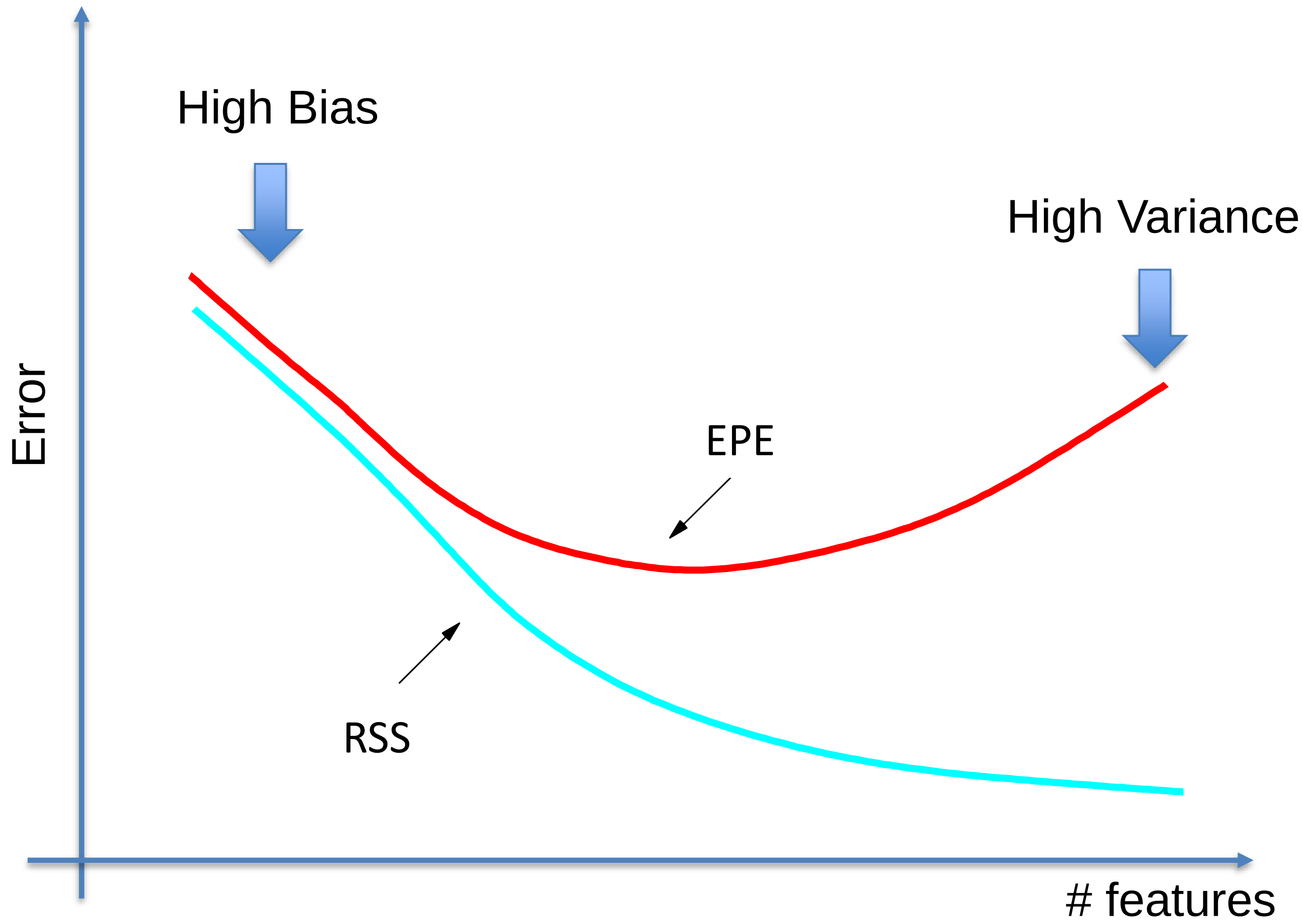
Solution: EPE



Solution: EPE



Solution: EPE



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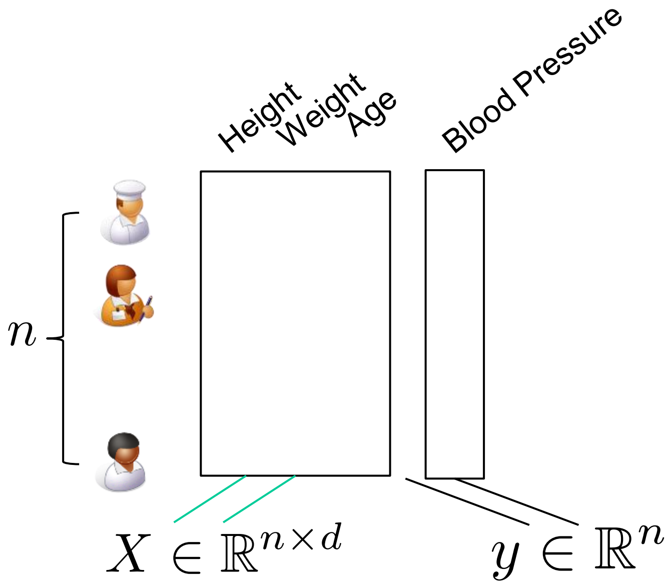
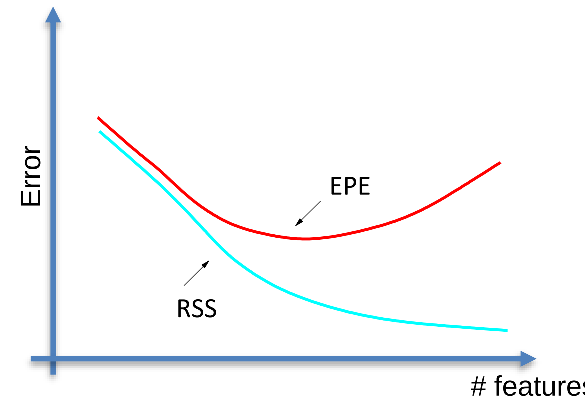
What Was EPE Again?

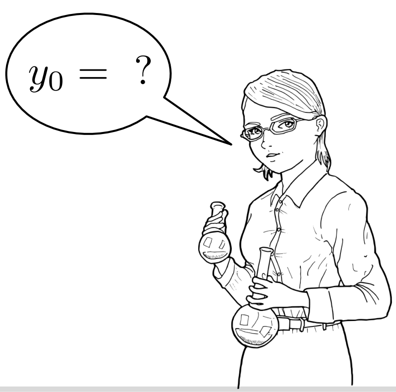




$x_0 =$

1.8m	90K	24ys

$$y_0 = \beta^\top x_0 + \varepsilon_0$$



Estimate: $\hat{y}_0 = \hat{\beta}^\top x_0$

EPE:
$$\begin{aligned}\mathbb{E}[(y_0 - \hat{y}_0)^2] &= \mathbb{E}[(y_0 - \beta^\top x_0)^2] + \mathbb{E}[(\beta^\top x_0 - \hat{\beta}^\top x_0)^2] \\ &= \sigma^2 + {x_0}^\top \mathbb{E}[(\beta - \hat{\beta})(\beta - \hat{\beta})^\top] x_0 \\ &= \sigma^2 + {x_0}^\top \mathrm{Cov}(\hat{\beta}) x_0\end{aligned}$$

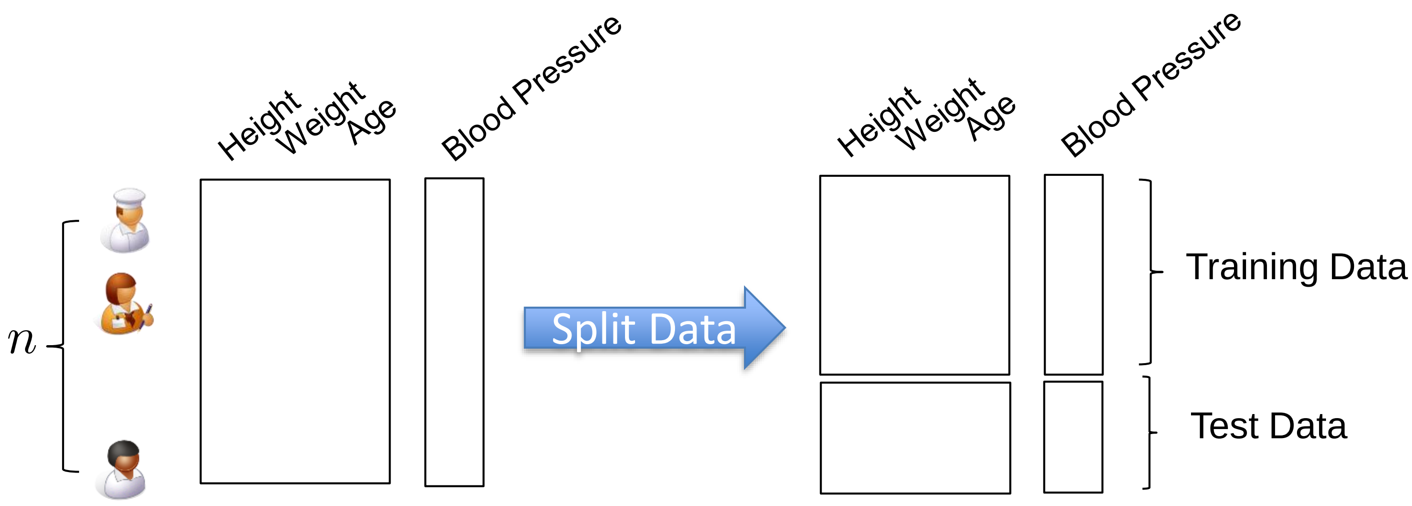
If $x_i, x \in \mathbb{R}^d$ are sampled from the same distribution, then:

$$\mathbb{E}\,[\text{EPE}] \approx \sigma^2 + \sigma^2 \frac{d}{n}$$

Problem: We don't know the distribution!

Solution: use data!!!

Estimating EPE



- **Train** $\hat{\beta}$ by minimizing:

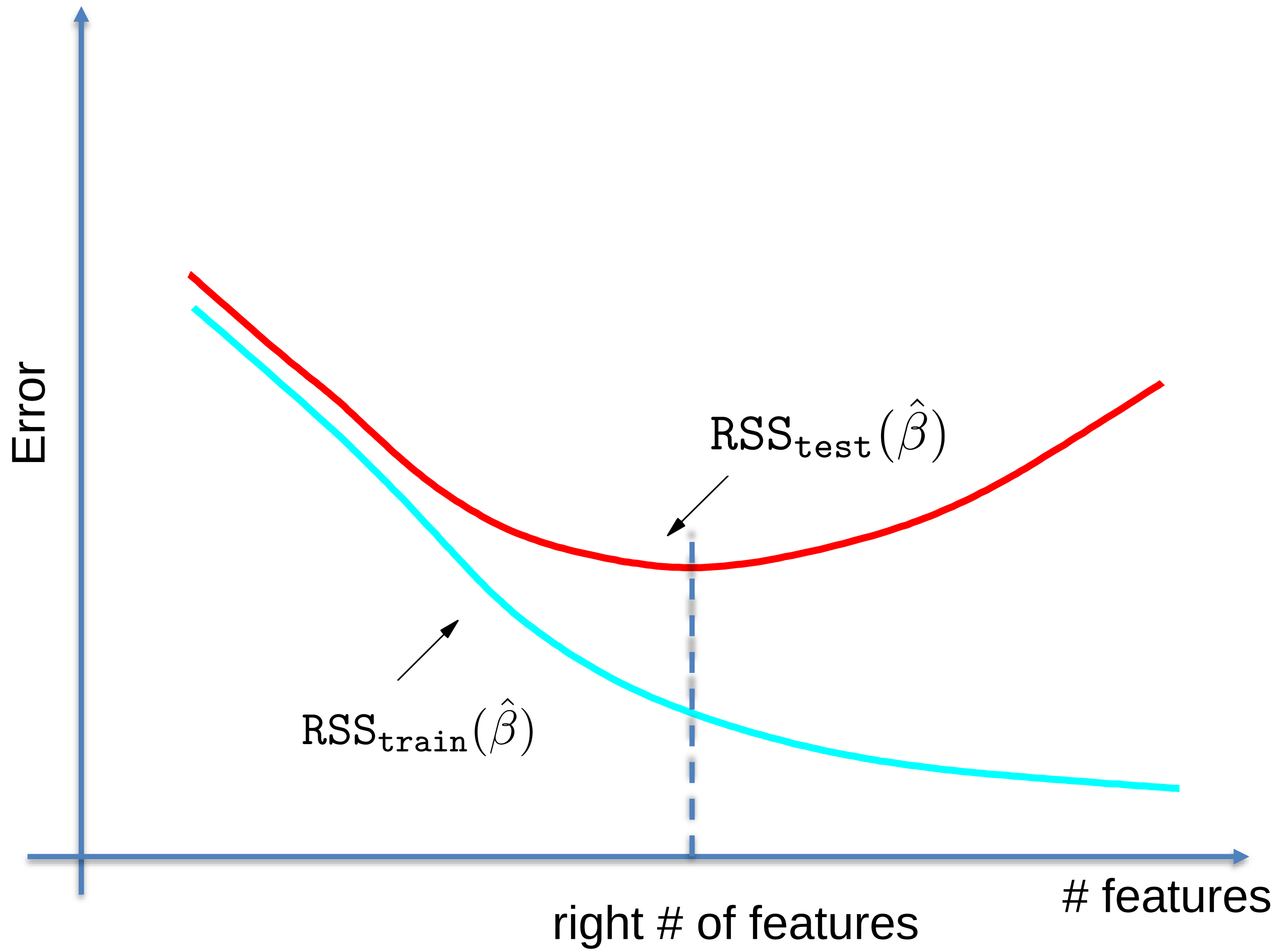
$$\mathrm{RSS}_{\mathtt{train}}(\beta) = \sum_{i \in \mathtt{train}} (y_i - \beta^\top x_i)^2$$

- **Test** $\hat{\beta}$ by evaluating:

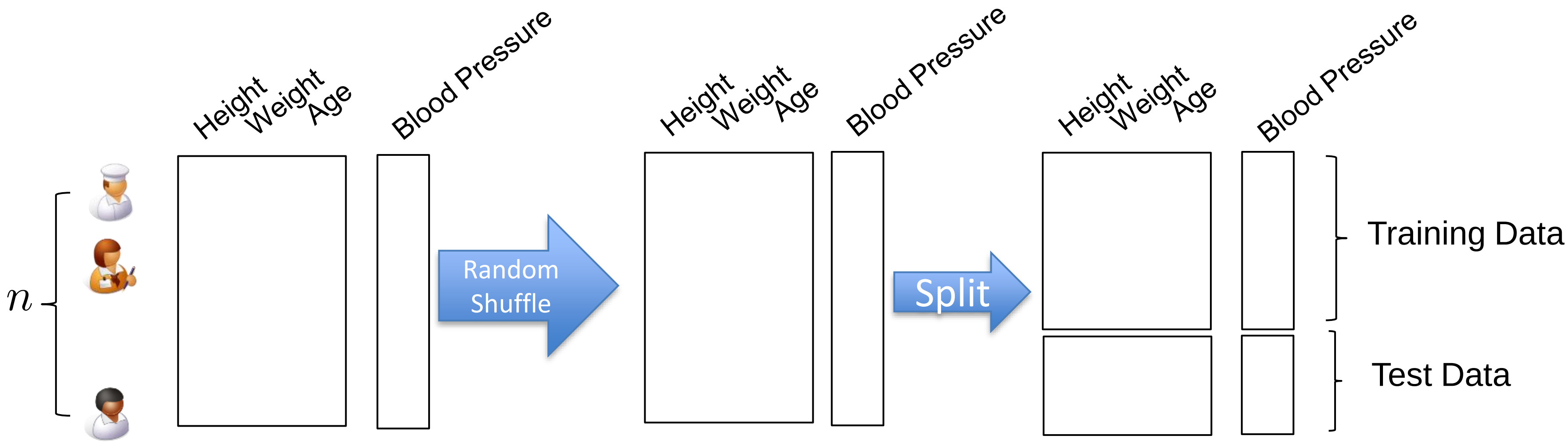
$$\mathrm{RSS}_{\mathtt{test}}(\hat{\beta}) = \sum_{i \in \mathtt{test}} (y_i - \hat{\beta}^\top x_i)^2$$

"Proxy" for EPE!!

Feature Selection Revisited



Improvement #1



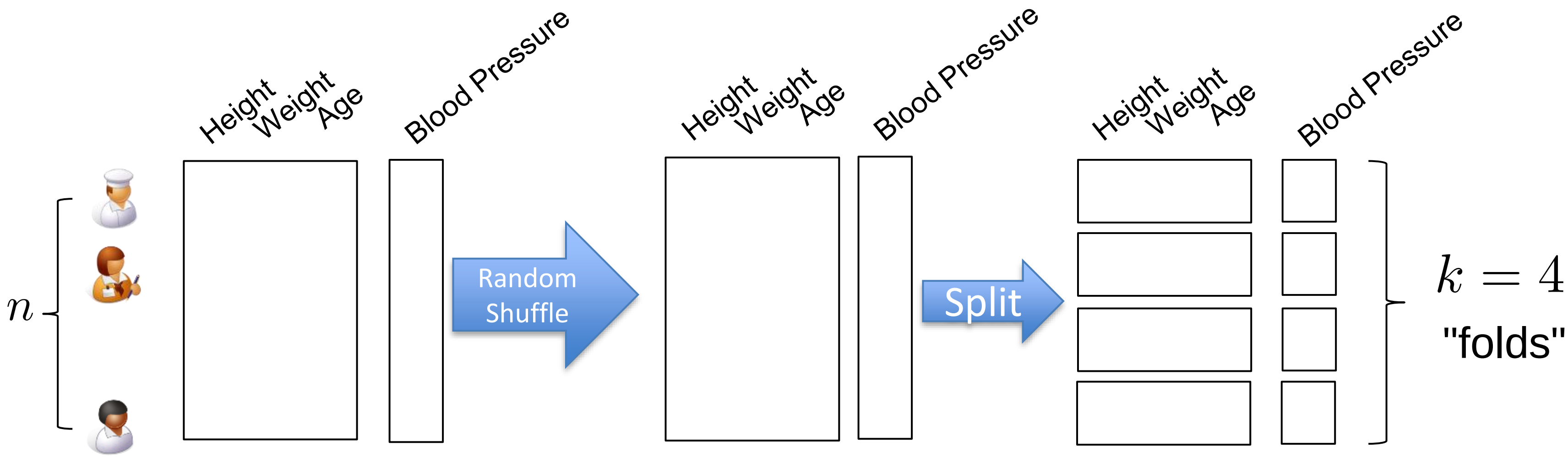
- **Train** $\hat{\beta}$ by minimizing:

$$\mathrm{RSS}_{\mathtt{train}}(\beta) = \sum_{i \in \mathtt{train}} (y_i - \beta^\top x_i)^2$$

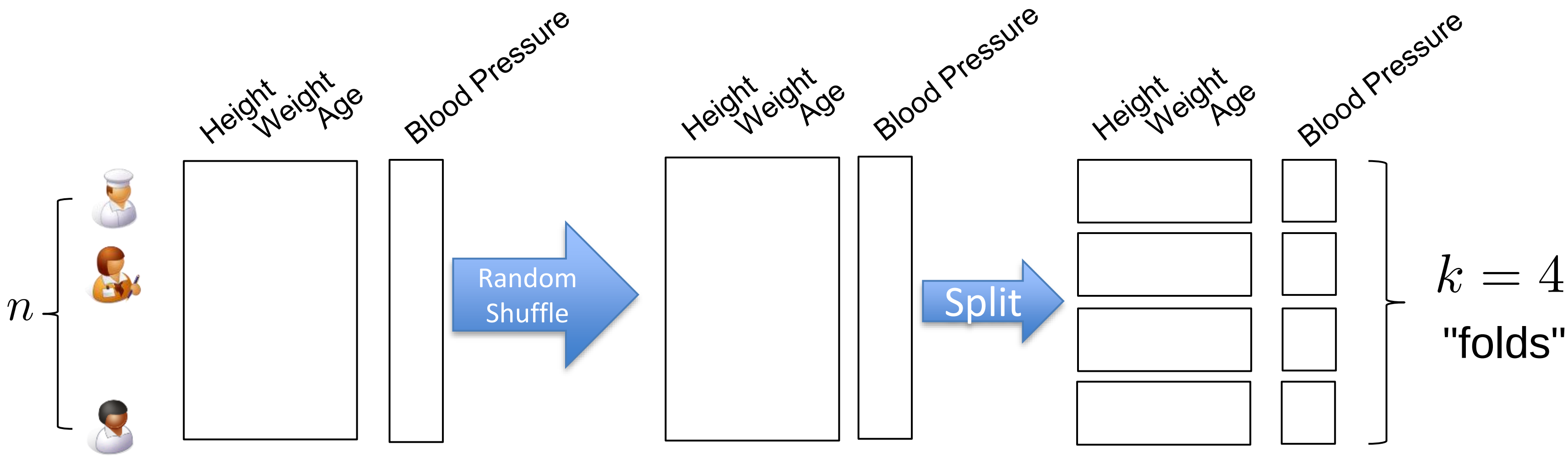
- **Test** $\hat{\beta}$ by evaluating:

$$\mathrm{RSS}_{\mathtt{test}}(\hat{\beta}) = \sum_{i \in \mathtt{test}} (y_i - \hat{\beta}^\top x_i)^2$$

Improvement #2: k-fold Cross Validation

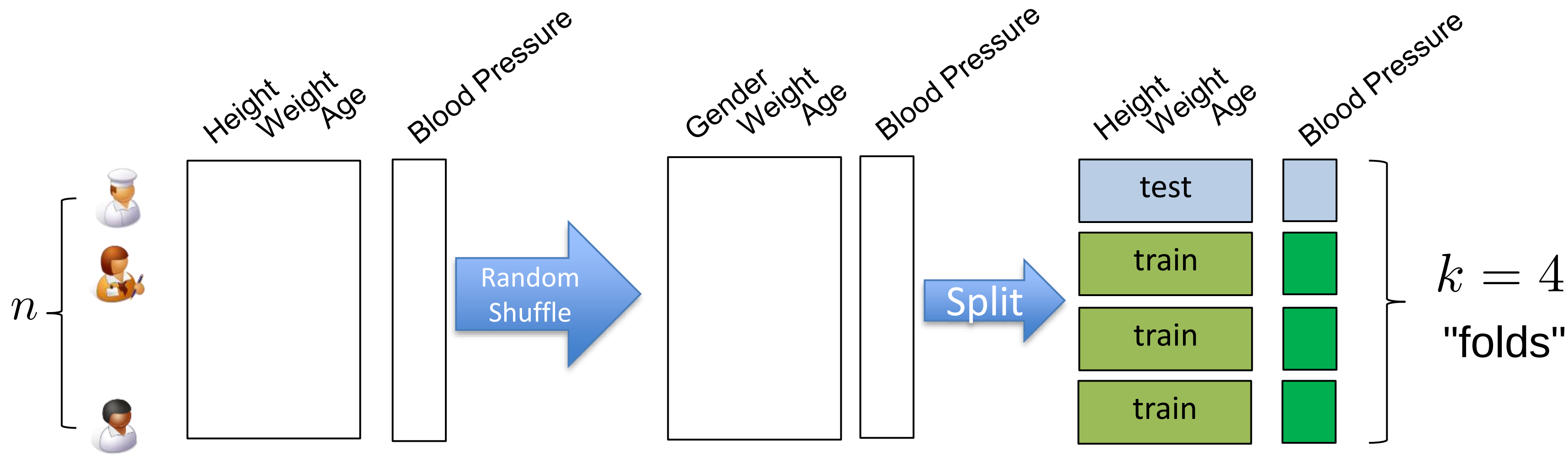


Improvement #2: k-fold Cross Validation



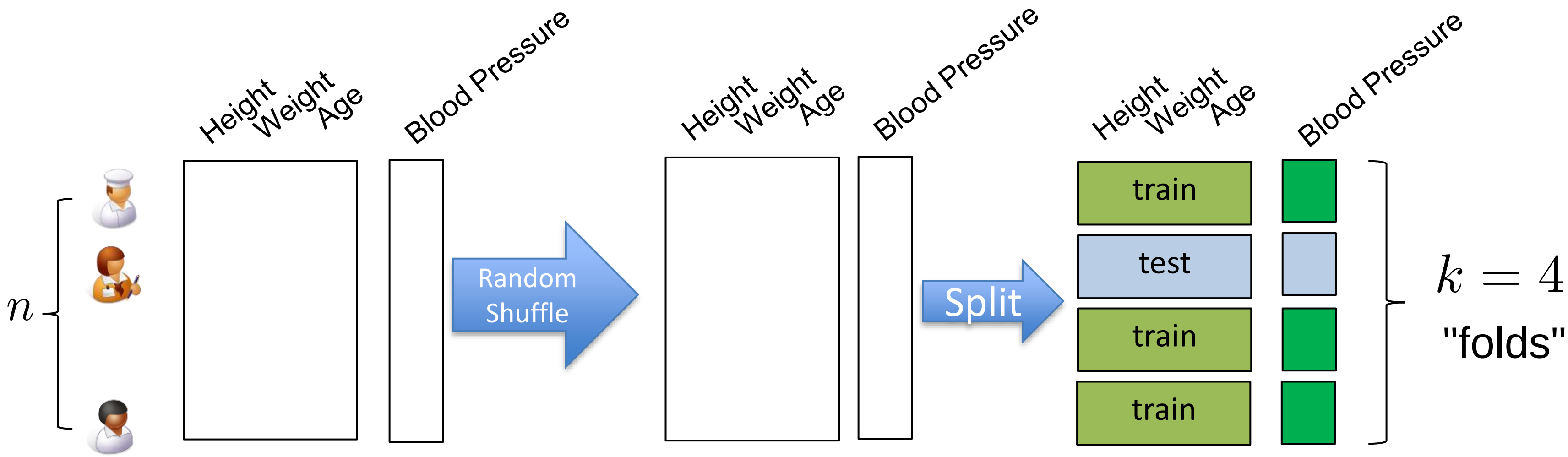
- For each fold $\ell = 1, \ldots, k$:
  - Set $\texttt{test}_\ell$ to include all data in fold ℓ.
  - Put remaining folds in $\texttt{train}_\ell$

Improvement #2: k-fold Cross Validation



- For each fold $\ell = 1, \ldots, k$:
  - Set $\texttt{test}_\ell$ to include all data in fold ℓ.
  - Put remaining folds in $\texttt{train}_\ell$
  - **Train** $\hat{\beta}$ by minimizing: $\text{RSS}_{\texttt{train}_\ell}(\beta) = \sum_{i \in \texttt{train}_\ell} (y_i - \beta^\top x_i)^2$
  - **Test** $\hat{\beta}$ by evaluating: $\text{RSS}_{\texttt{test}_\ell}(\hat{\beta}) = \sum_{i \in \texttt{test}_\ell} (y_i - \hat{\beta}^\top x_i)^2$

Improvement #2: k-fold Cross Validation



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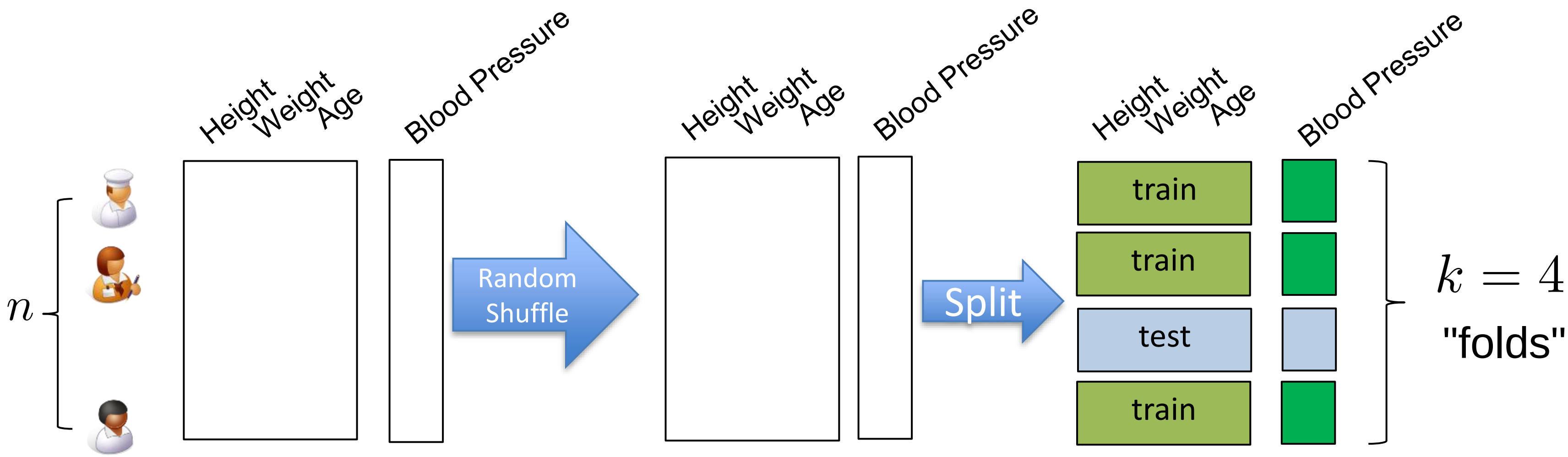

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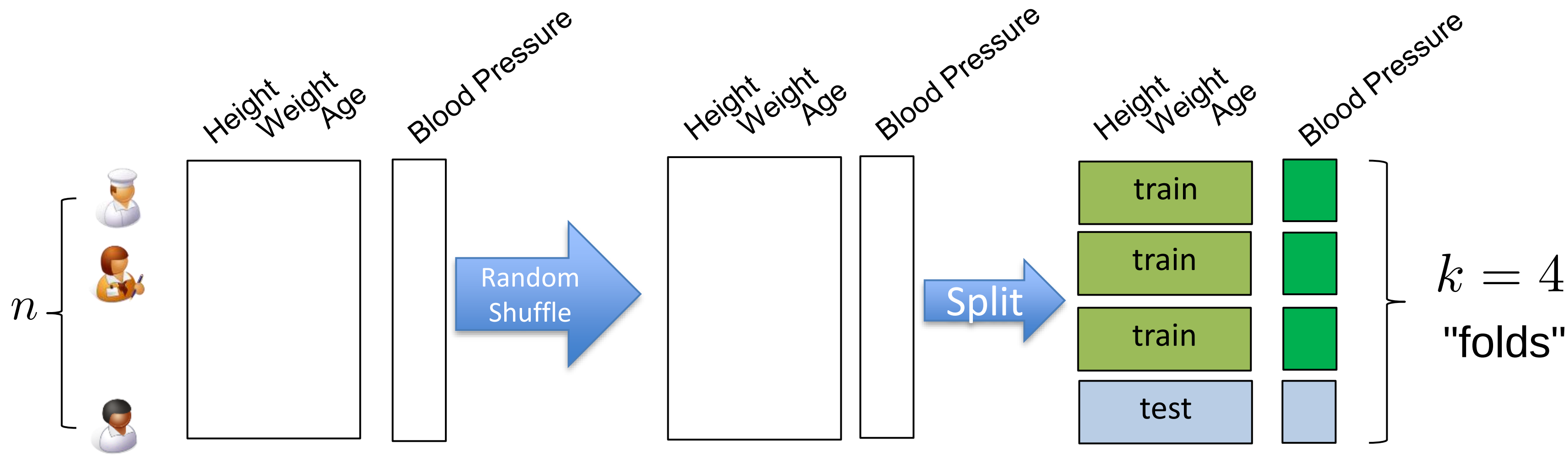
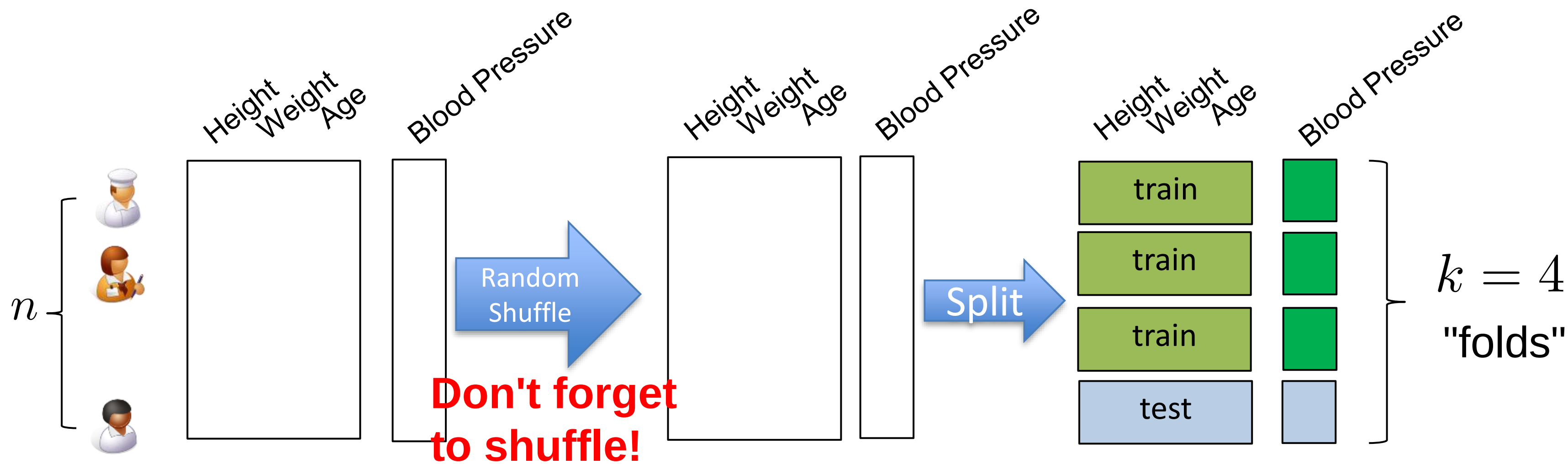
Improvement #2: k-fold Cross Validation



- For each fold $\ell = 1, \ldots, k$:
  - Set $\texttt{test}_\ell$ to include all data in fold ℓ.
  - Put remaining folds in $\texttt{train}_\ell$
  - **Train** $\hat{\beta}$ by minimizing: $\mathrm{RSS}_{\texttt{train}_\ell}(\beta) = \sum_{i \in \texttt{train}_\ell} (y_i - \beta^\top x_i)^2$
  - **Test** $\hat{\beta}$ by evaluating: $\mathrm{RSS}_{\texttt{test}_\ell}(\hat{\beta}) = \sum_{i \in \texttt{test}_\ell} (y_i - \hat{\beta}^\top x_i)^2$
- Quality of solution: $\overline{\mathrm{RSS}} = \frac{1}{k} \sum_{\ell=1}^{k} \mathrm{RSS}_{\texttt{test}_\ell}$

"Proxy" for EPE!!

k-fold Cross Validation

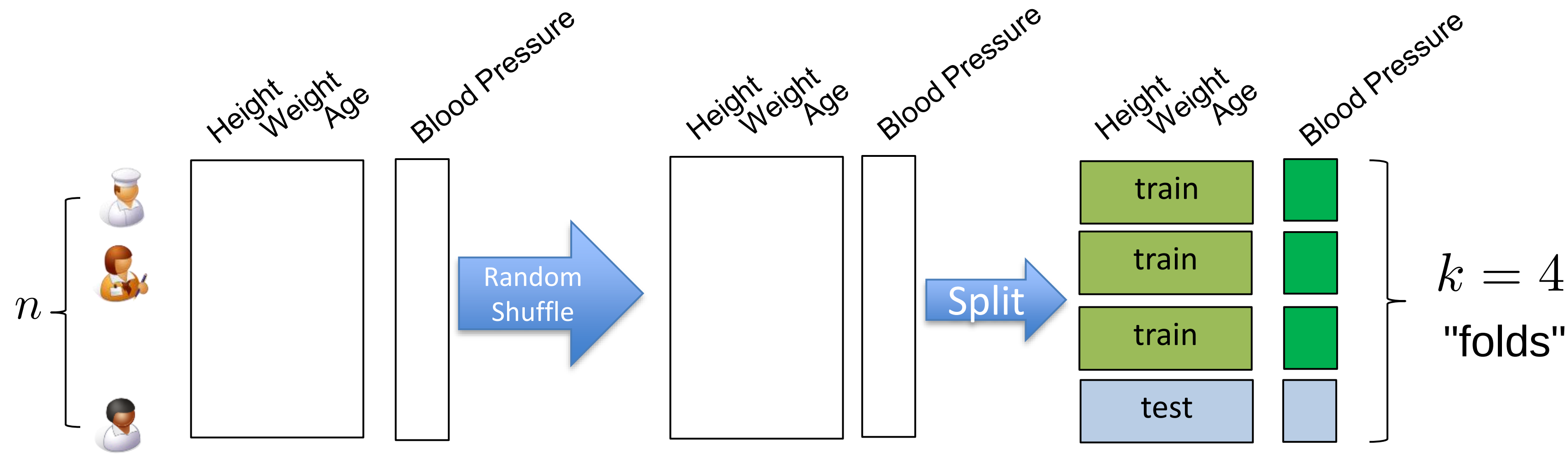


Cross-validation error:

$$\overline{\mathrm{RSS}} = \frac{1}{k}\sum_{\ell=1}^{k} \mathrm{RSS}_{\mathtt{test}_\ell}$$

- ❑ **Less sensitive** to how split happens than train/test
- ❑ Can be applied to **other metrics** (accuracy, precision, recall, AUC)…
- ❑ Can be applied to **pick other parameters** of estimation procedure:
  - ❑ Feature selection
  - ❑ Number of iterations
  - ❑ …
- ❑ Can be used to compute **standard deviation, confidence intervals, etc.**

k-fold Cross Validation



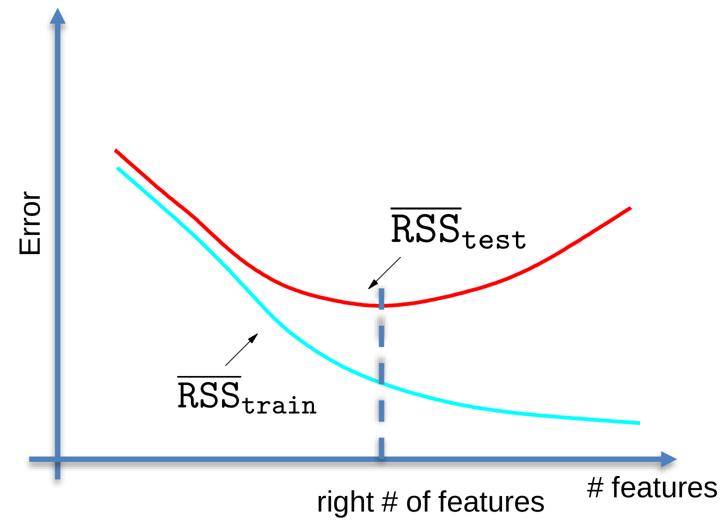
Cross-validation error:

$$\overline{\mathrm{RSS}} = \frac{1}{k} \sum_{\ell=1}^{k} \mathrm{RSS}_{\mathtt{test}_\ell}$$

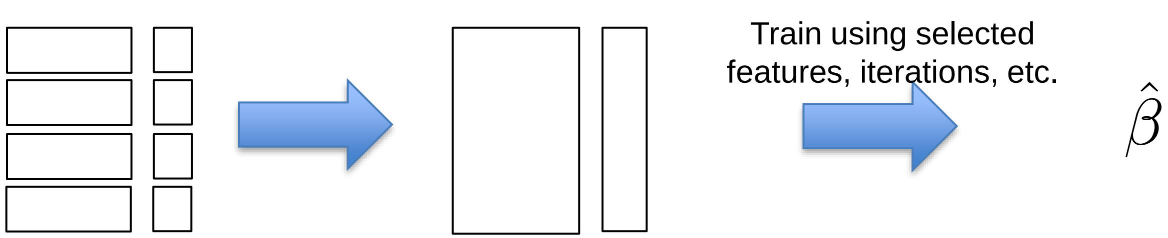
THIS IS AN EXTREMELY IMPORTANT TOPIC!!! IF YOU ONLY REMEMBER A SINGLE THING FROM ENTIRE CLASS, PLEASE REMEMBER TO CROSS-VALIDATE!!!

Finding the Right Features

- Use k-fold CV to find right problem parameters:
  - Features
  - Iterations
  - Regularization parameters (coming up)…



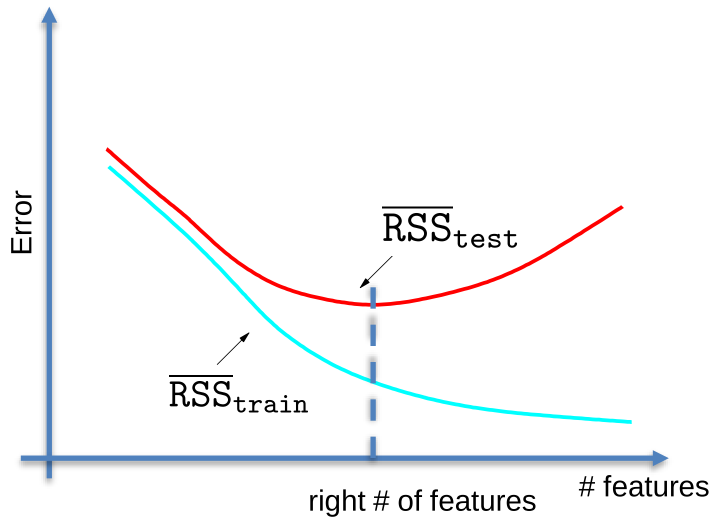
- One model $\hat{\beta}_\ell$ per fold $\ell = 1, \ldots, k$.
  - Fix these parameters and then retrain model **over entire dataset**



Feature Selection

We actually need two things:

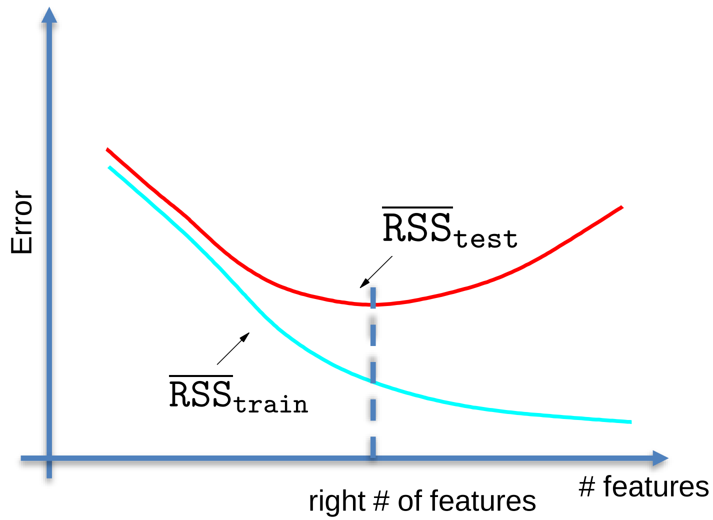
- ❑ A procedure for selecting features
- ❑ A way of measuring whether this selection is good



Feature Selection

We actually need two things:

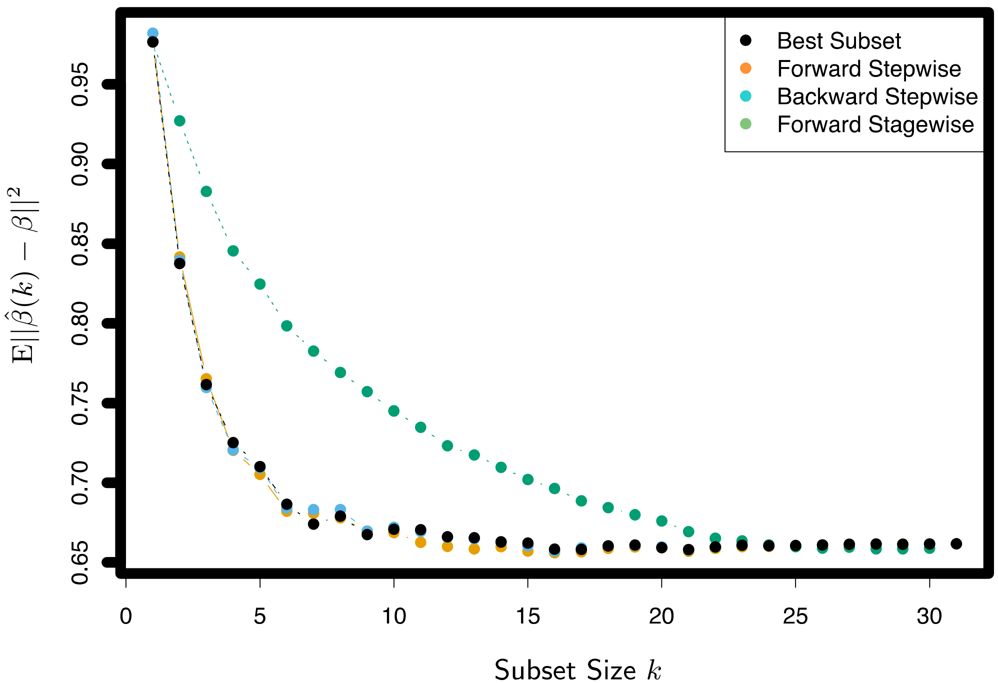
- ❑ **A procedure for selecting features**
- ❑ A way of measuring whether this selection is good



A Few Combinatorial Approaches

Best Subset Selection:

- ❑ Try all subsets of features
- ❑ Too expensive



❑ Greedy approaches:

- ❑ Forward step-wise
- ❑ Backward step-wise
- ❑ Forward stage-wise

❑More efficient

❑Not robust: solutions can change drastically with small changes in data

Northeastern

Shrinkage/Regularization Methods

$x_i \in \mathbb{R}^d$ $\qquad$ $y_i \in \mathbb{R}$

n

Height	Weight	Age	Blood Pressure
1.8m	40K	19ys	3.1
1.9m	55K	34ys	1.2
⋮			
1.5m	90K	24ys	2.5

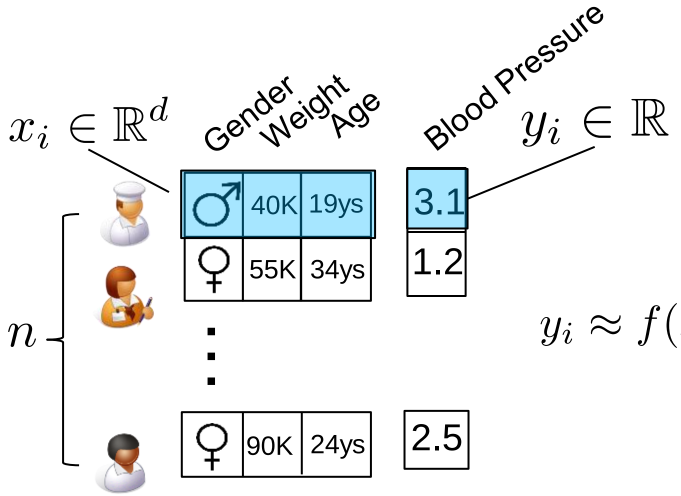
$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^d} \underbrace{\sum_{i=1}^{n} (y_i - \beta^\top x_i)^2}_{\mathrm{RSS}(\beta)} + c(\beta)$$

Penalty if β is "complicated"

Occam's razor, KISS (Keep it Simple, Stratis): among two solutions that produce **the same RSS**, we prefer the one that has **smaller complexity**

Shrinkage/Regularization Methods



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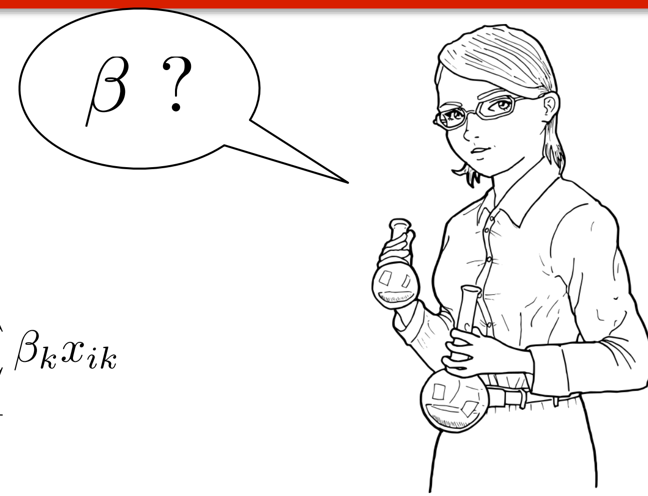


$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_0 \text{ , for some } \lambda > 0$$

$\|\beta\|_0 =$ # of non-zero elements of β (i.e., size of β's **support**)

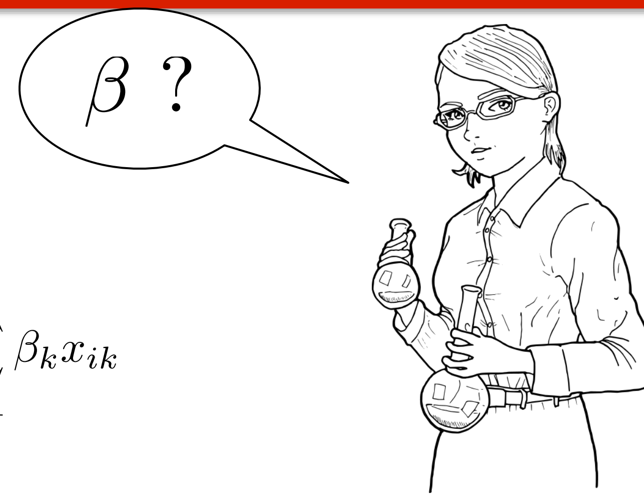
Occam's razor: Between two β with the same RSS, we prefer the one that is **sparser**, i.e., has fewer features.

Shrinkage/Regularization Methods

$x_i \in \mathbb{R}^d$ $\qquad$ $y_i \in \mathbb{R}$

	Height	Weight	Age	Blood Pressure
n	1.8m	40K	19ys	3.1
	1.9m	55K	34ys	1.2
	⋮			
	1.5m	90K	24ys	2.5

$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$



$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_0 \text{ , for some } \lambda > 0$$

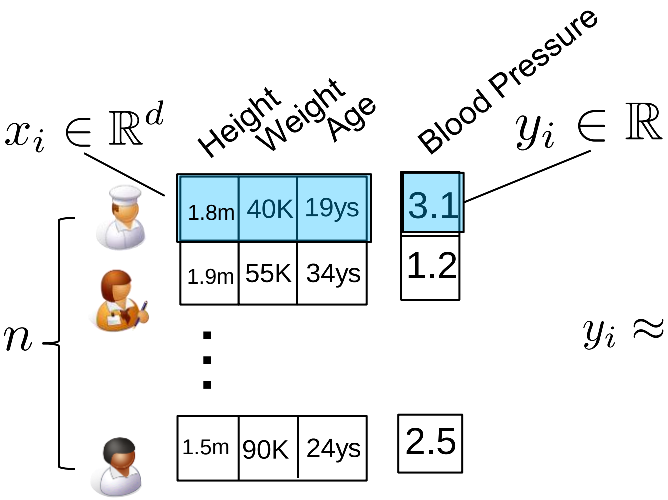
$\|\beta\|_0 =$ # of non-zero elements of β (i.e., size of β's **support**)

$\lambda \gg 0$: optimal solution contains only zeros

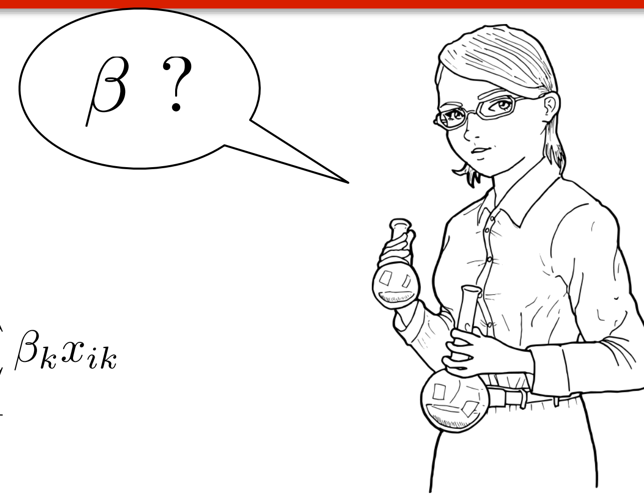
$\lambda = 0$: linear regression

Varying λ can be used for feature selection!

Shrinkage/Regularization Methods



$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$



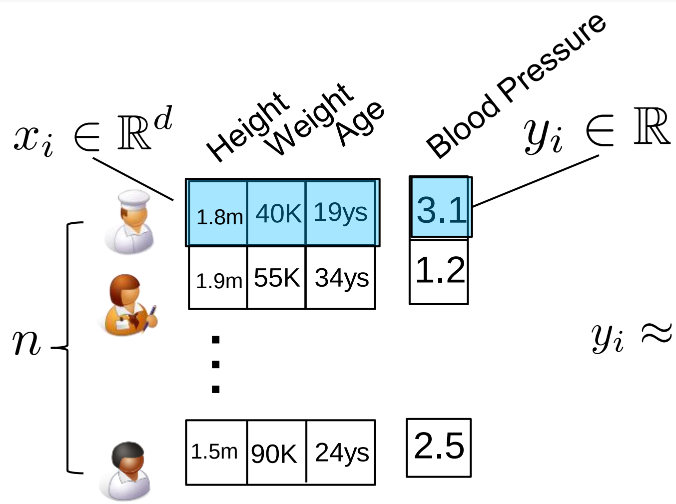
$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_0 \text{ , for some } \lambda > 0$$

Problem: Alas, this is **not a convex objective!**

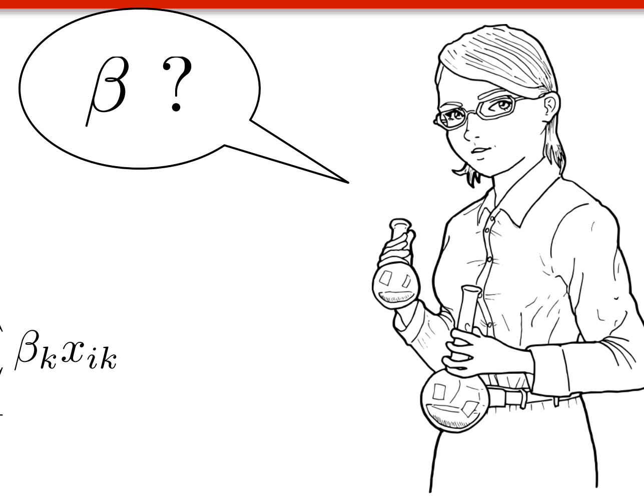
Solution: We replace it with **convex relaxations**

Northeastern

Ridge Regression



$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

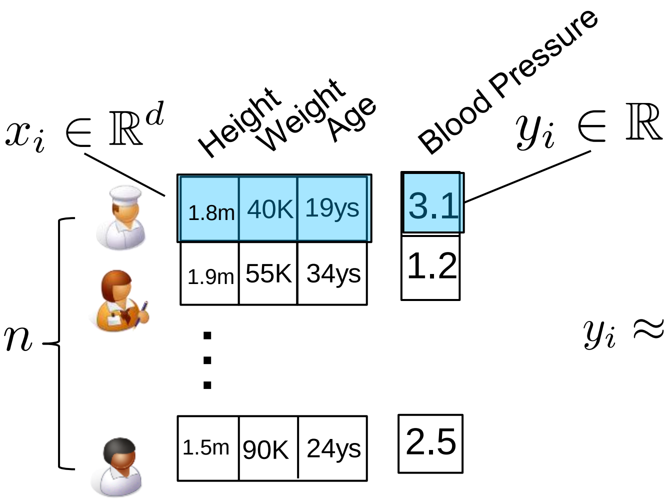


$$\hat{\beta}^{\texttt{ridge}} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_2^2, \text{ for some } \lambda > 0$$

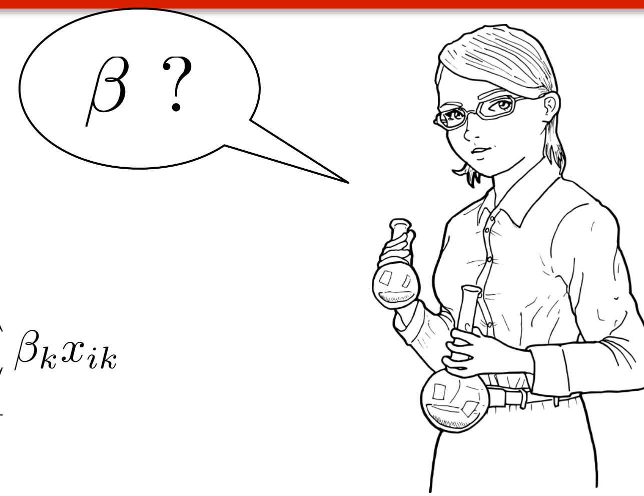
where $\|\beta\|_2^2 = \beta^\top \beta = \sum_{k=1}^{d} \beta_k^2$

Strongly Convex!!!!

Lasso Regression



$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

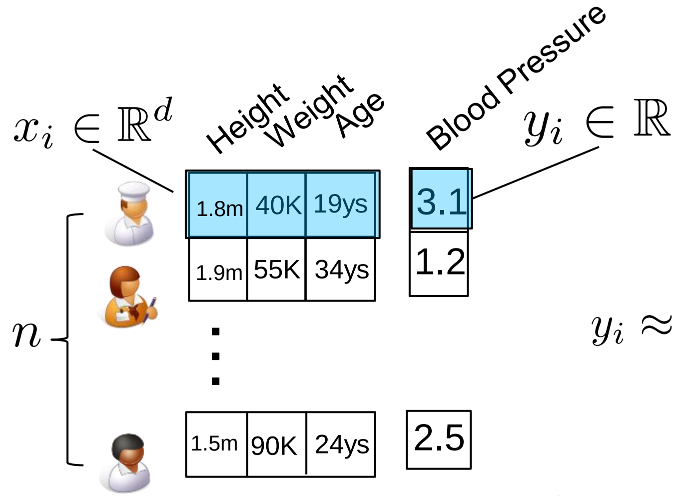


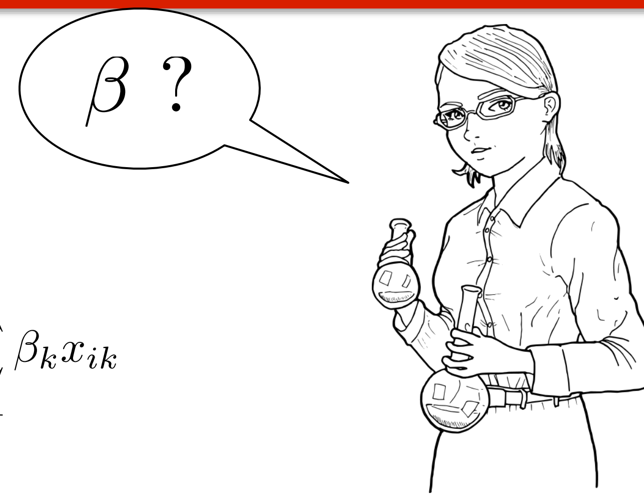
$$\hat{\beta}^{\texttt{lasso}} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_1, \text{ for some } \lambda > 0$$

where $\|\beta\|_1 = \sum_{k=1}^{d} |\beta_k|$

Convex!
(not differentiable)

Ridge Regression





$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

$$\hat{\beta}^{\texttt{ridge}} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \underbrace{\lambda \|\beta\|_2^2}$$, for some $\lambda > 0$

l2-penalty,
ridge penalty,
regularization term,

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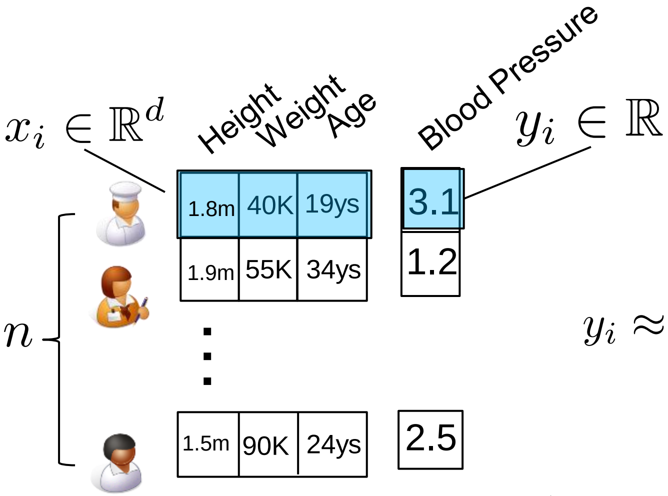
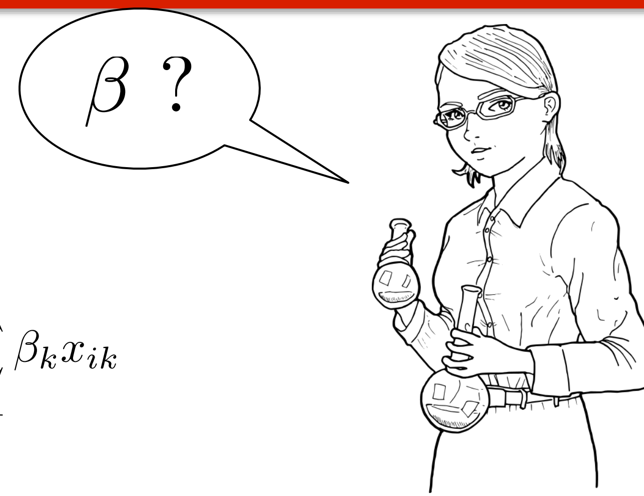
Ridge Regression



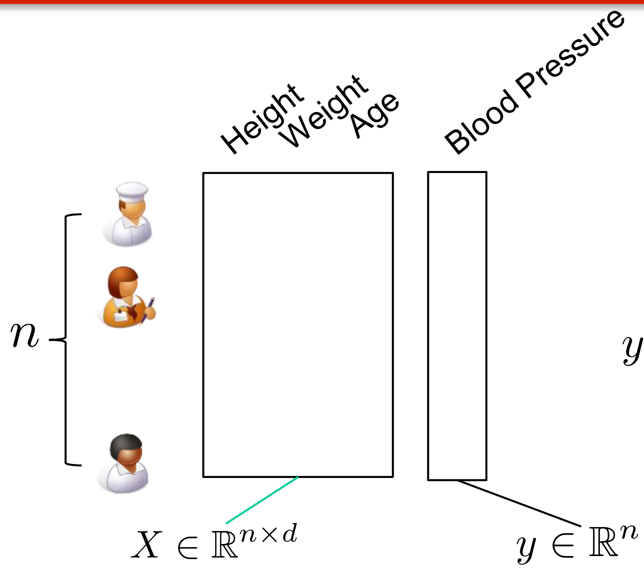


$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

$$\hat{\beta}^{\texttt{ridge}} = \underset{\beta \in \mathbb{R}^d}{\arg\min} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_2^2$$, for some $\lambda > 0$

regularization parameter

Ridge Regression



$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

$$F(\beta) = \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_2^2 \text{ , for some } \lambda > 0$$

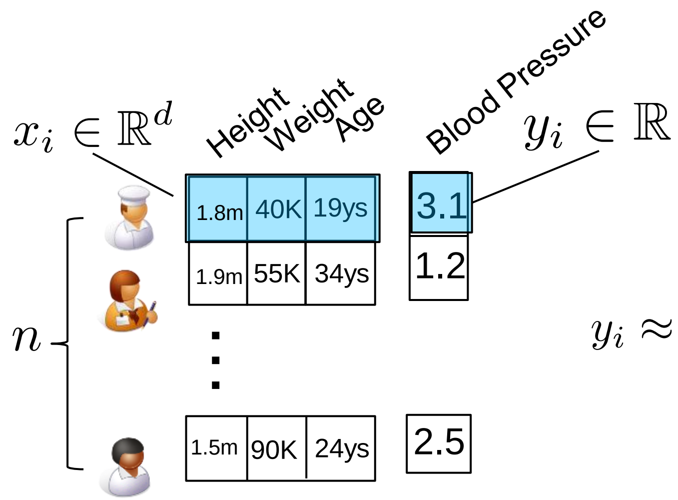
$$= \|X\beta - y\|_2^2 + \lambda \|\beta\|_2^2$$

$$\nabla F(\beta) = 2X^\top X\beta - 2X^\top y + 2\lambda\beta$$

$$\nabla^2 F(\beta) = 2(X^\top X + \lambda I) \succ 0$$

$$\nabla F(\hat{\beta}) = 0 \Leftrightarrow \hat{\beta} = \underbrace{(X^\top X + \lambda I)}_{\text{Invertible for } \lambda > 0!}{}^{-1} X^\top y$$

Ridge Regression: Intuition #1



$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

For every $\lambda \geq 0$, there exists a $t \geq 0$ such that the two problems produce **the same solution**

Minimize: $\sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_2^2$

subject to: $\beta \in \mathbb{R}^d$

Minimize: $\sum_{i=1}^{n} (y_i - \beta^\top x_i)^2$

subject to: $\|\beta\|_2^2 \leq t$

Ridge Regression: Intuition #1

For every $\lambda \geq 0$, there exists a $t \geq 0$ such that the two problems produce **the same solution**

PROBLEM 1

Minimize: $$\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda\|\beta\|_2^2$$

subject to: $$\beta \in \mathbb{R}^d$$

PROBLEM 2

Minimize: $$\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2$$

subject to: $$\|\beta\|_2^2 \leq t$$

Proof: Given a $\lambda \geq 0$, let β^* be an optimal solution to PROBLEM 1.

Let $t = \|\beta^*\|_2^2$. Then, β^* is an optimal solution to PROBLEM 2 for this $t \geq 0$.

Suppose not. Then, there exists a $\beta' \neq \beta^*$ such that $\|\beta'\|_2^2 \leq t$ and

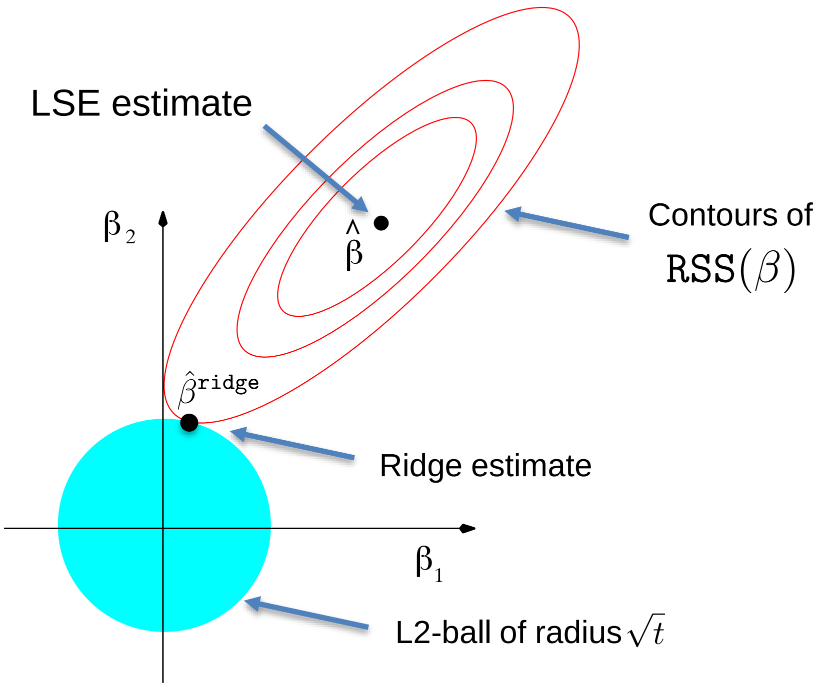
$$\sum_{i=1}^{n}(y_i - {\beta'}^\top x_i)^2 < \sum_{i=1}^{n}(y_i - {\beta^*}^\top x_i)^2$$

But then

$$\sum_{i=1}^{n}(y_i - {\beta'}^\top x_i)^2 + \lambda\|\beta'\|_2^2 \leq \sum_{i=1}^{n}(y_i - {\beta'}^\top x_i)^2 + \lambda t < \sum_{i=1}^{n}(y_i - {\beta^*}^\top x_i)^2 + \lambda t = \sum_{i=1}^{n}(y_i - {\beta^*}^\top x_i)^2 + \lambda\|\beta^*\|_2^2$$

a contradiction, as β^* is an optimal solution to PROBLEM 1 $\square$

Ridge Regression: Intuition #1



PROBLEM 1

Minimize: $$\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda\|\beta\|_2^2$$

subject to: $\beta \in \mathbb{R}^d$

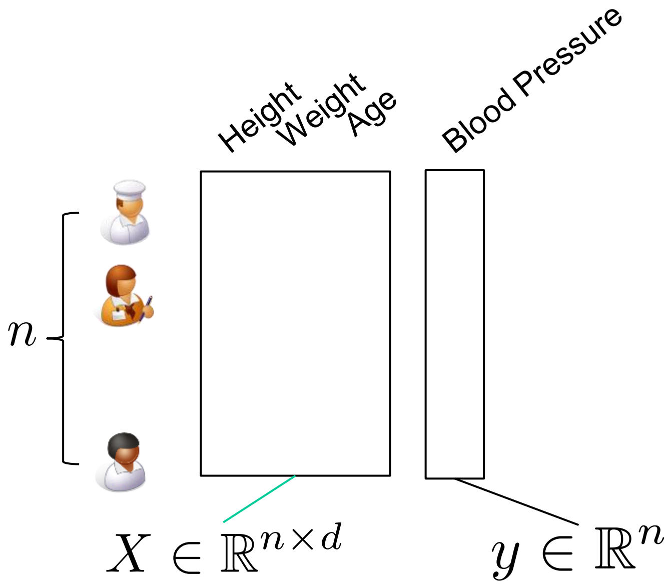
PROBLEM 2

Minimize: $$\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2$$

subject to: $\|\beta\|_2^2 \leq t$

$$\lambda \Uparrow \quad \Rightarrow \quad t \Downarrow$$

Ridge Regression: Intuition #2



$$y_i = \beta^\top x_i + \varepsilon_i, \quad i = 1, \ldots, n$$

ε_i i.i.d., $\mathbb{E}[\varepsilon_i] = 0, \mathbb{E}[\varepsilon_i^2] = \sigma^2 < \infty$

- Suppose, in addition, that

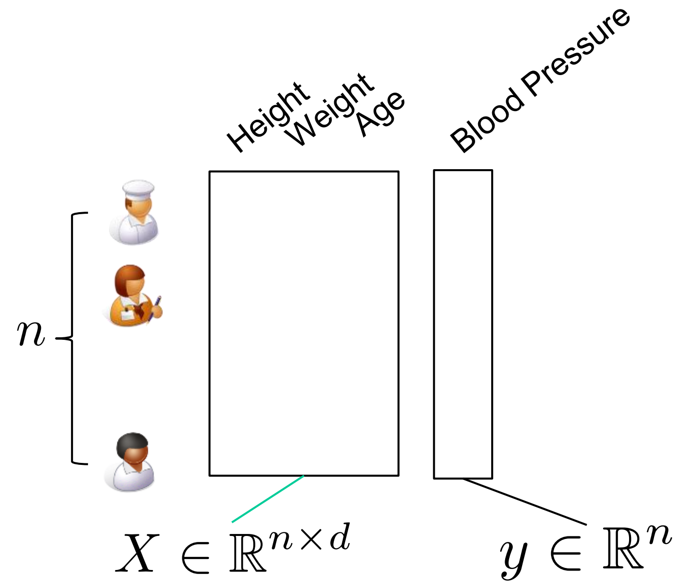
$$\varepsilon_i \sim N(0, \sigma^2)$$

Then, LSE is a **Maximum Likelihood Estimator**:

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \langle \beta, x_i \rangle)^2 = \arg\min_{\beta \in \mathbb{R}^d} \; -\log\left(P\left(y|\beta, X\right)\right)$$

$$= \arg\max_{\beta \in \mathbb{R}^d} \; P\left(y|\beta, X\right)$$

Ridge Regression: Intuition #2



$$y_i = \beta^\top x_i + \varepsilon_i, \quad i = 1, \ldots, n$$

ε_i i.i.d., $\mathbb{E}[\varepsilon_i] = 0, \mathbb{E}[\varepsilon_i^2] = \sigma^2 < \infty$

- Suppose, in addition, that

$$\varepsilon_i \sim N(0, \sigma^2)$$

and

$$\beta \sim N(0, \frac{\sigma^2}{\lambda} I)$$

Bayes prior

Then, Ridge Regression is a **Maximum A-Posteriori (MAP) Estimation**:

The bigger the λ the higher our "prior" belief on small $\|\beta\|_2$

$$\begin{aligned}\hat{\beta}^{\texttt{ridge}} = \arg\min_{\beta\in\mathbb{R}^d} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda\|\beta\|_2^2 &= \arg\min_{\beta\in\mathbb{R}^d} - \log(P(y|\beta)) - \log P(\beta) \\ &= \arg\min_{\beta\in\mathbb{R}^d} - \log(P(y, \beta)) \\ &= \arg\max_{\beta\in\mathbb{R}^d} P(y, \beta) = \arg\max_{\beta\in\mathbb{R}^d} P(\beta|y)P(y) = \arg\max_{\beta\in\mathbb{R}^d} P(\beta|y)\end{aligned}$$

Towards Intuition #3

Gauss

Markov

Best **L**inear **U**nbiased **E**stimator

LSE has the "smallest" covariance among all linear unbiased estimators

What About Ridge Regression?

$$\hat{\beta}^{\texttt{ridge}} = \underset{\beta \in \mathbb{R}^d}{\arg\min} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_2^2$$
$$= \underbrace{(\lambda I + X^\top X)^{-1} X^\top}_{\text{This is a linear estimator!}} y$$

- ❑ Q: Does it have a smaller covariance than LSE?
- ❑ Yes! Because it is **biased!**

Bias of Ridge Regression

$$\hat{\beta}^{\texttt{ridge}} = (\lambda I + X^\top X)^{-1} X^\top y$$

$$\begin{aligned}
\mathbb{E}[\hat{\beta}^{\texttt{ridge}}] &= \mathbb{E}[(\lambda I + X^\top X)^{-1} X^\top y] = (\lambda I + X^\top X)^{-1} X^\top \mathbb{E}[y] \\
&= (\lambda I + X^\top X)^{-1} X^\top X \beta \\
&= (\lambda I + X^\top X)^{-1} X^\top X \beta + \lambda(\lambda I + X^\top X)^{-1}\beta - \lambda(\lambda I + X^\top X)^{-1}\beta \\
&= (\lambda I + X^\top X)^{-1}(X^\top X + \lambda I)\beta - \lambda(\lambda I + X^\top X)^{-1}\beta \\
&= \beta - \lambda(\lambda I + X^\top X)^{-1}\beta
\end{aligned}$$

So the **bias** or the ridge estimator is:

$$\mathtt{b} = \mathbb{E}[\hat{\beta}^{\texttt{ridge}}] - \beta = -\lambda(\lambda I + X^\top X)^{-1}\beta \neq 0$$

Covariance of Ridge Regression

$$\hat{\beta}^{\texttt{ridge}} = (\lambda I + X^\top X)^{-1} X^\top y$$

$$\mathbb{E}[\hat{\beta}^{\texttt{ridge}}] = \beta - \lambda(\lambda I + X^\top X)^{-1}\beta \neq \beta$$

$$\begin{aligned}
\texttt{Cov}\left(\hat{\beta}^{\texttt{ridge}}\right) &= \mathbb{E}\left[\left(\hat{\beta}^{\texttt{ridge}} - \mathbb{E}[\hat{\beta}^{\texttt{ridge}}]\right)\left(\hat{\beta}^{\texttt{ridge}} - \mathbb{E}[\hat{\beta}^{\texttt{ridge}}]\right)^\top\right] \\
&= \ldots \\
&= \sigma^2(\lambda I + X^\top X)^{-1} X^\top X (\lambda I + X^\top X)^{-1}
\end{aligned}$$

So What?

$$\hat{\beta}^{\texttt{ridge}} = (\lambda I + X^\top X)^{-1} X^\top y$$

$$\mathbb{E}[\hat{\beta}^{\texttt{ridge}}] = \beta - \lambda(\lambda I + X^\top X)^{-1}\beta \neq \beta$$

$$\texttt{Cov}(\hat{\beta}^{\texttt{ridge}}) = \sigma^2(\lambda I + X^\top X)^{-1} X^\top X (\lambda I + X^\top X)^{-1}$$

Recall that $X^\top X \succeq 0$

Let $0 \leq \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_d$ be its eigenvalues, and $e_i, i = 1, \ldots, d$ the corresponding eigenvectors.

Then:

$$X^\top X = \sum_{i=1}^{d} \lambda_i e_i e_i^\top \qquad \lambda I + X^\top X = \sum_{i=1}^{d} (\lambda + \lambda_i) e_i e_i^\top \succ X^\top X$$

Hence: $(\lambda I + X^\top X)^{-1} = \sum_{i=1}^{d} \frac{1}{\lambda + \lambda_i} e_i e_i^\top$

So What?

$$X^\top X = \sum_{i=1}^{d} \lambda_i e_i e_i^\top \qquad (\lambda I + X^\top X)^{-1} = \sum_{i=1}^{d} \frac{1}{\lambda + \lambda_i} e_i e_i^\top$$

$$\begin{aligned}
\texttt{Cov}(\hat{\beta}^{\texttt{ridge}}) &= \sigma^2 (\lambda I + X^\top X)^{-1} X^\top X (\lambda I + X^\top X)^{-1} \\
&= \sigma^2 \sum_{i=1}^{d} \frac{1}{\lambda + \lambda_i} e_i e_i^\top \cdot \sum_{i=1}^{d} \lambda_i e_i e_i^\top \cdot \sum_{i=1}^{d} \frac{1}{\lambda + \lambda_i} e_i e_i^\top \\
&= \sigma^2 \sum_{i=1}^{d} \frac{\lambda_i}{(\lambda + \lambda_i)^2} e_i e_i^\top \\
&= \sigma^2 \sum_{i=1}^{d} \frac{1}{\lambda_i + 2\lambda + \frac{\lambda^2}{\lambda_i}} e_i e_i^\top \\
&\prec \sigma^2 \sum_{i=1}^{d} \frac{1}{\lambda_i} e_i e_i^\top = (X^\top X)^{-1} = \texttt{Cov}(\hat{\beta}^{\texttt{LSE}})
\end{aligned}$$

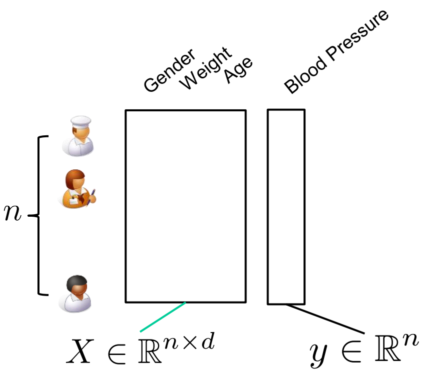
Opposite of What G-M predicts!

$$\mathtt{Cov}(\hat{\beta}^{\mathtt{ridge}}) \prec \mathtt{Cov}(\hat{\beta}^{\mathrm{LSE}})$$

No contradiction with G-M, as ridge estimator **is biased.**

$$\mathtt{Cov}(\hat{\beta}^{\mathtt{ridge}}) = \sigma^2 \sum_{i=1}^{d} \frac{\lambda_i}{(\lambda+\lambda_i)^2} e_i e_i^\top$$

$$\mathtt{b} = -\lambda(\lambda I + X^\top X)^{-1}\beta$$



Predicted Value: $\hat{y}_0 = \langle \hat{\beta}^{\mathtt{ridge}}, x_0 \rangle$

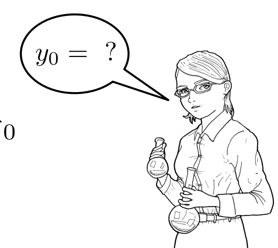
Expected Prediction Error:

$$\mathbb{E}[(y_0-\hat{y}_0)^2] = \mathbb{E}[(y_0-\beta^\top x_0)^2] + \mathbb{E}\left[\left({\beta^{\mathtt{ridge}}}^\top x_0 - \mathbb{E}[\beta^{\mathtt{ridge}}]^\top x_0\right)^2\right] + \left(\mathbb{E}[\beta^{\mathtt{ridge}}]^\top x_0 - \beta^\top x_0\right)^2$$

$$= \underbrace{\sigma^2}_{\text{inherent noise}} + \underbrace{x_0^\top \mathtt{Cov}(\hat{\beta}^{\mathtt{ridge}}) x_0}_{\text{variance}} + \underbrace{(\mathtt{b}^\top x_0)^2}_{\text{bias}}$$

$x_0 =$ [♀ | 90K | 24ys]

$y_0 = \beta^\top x_0 + \varepsilon_0$



λ establishes a bias variance trade-off

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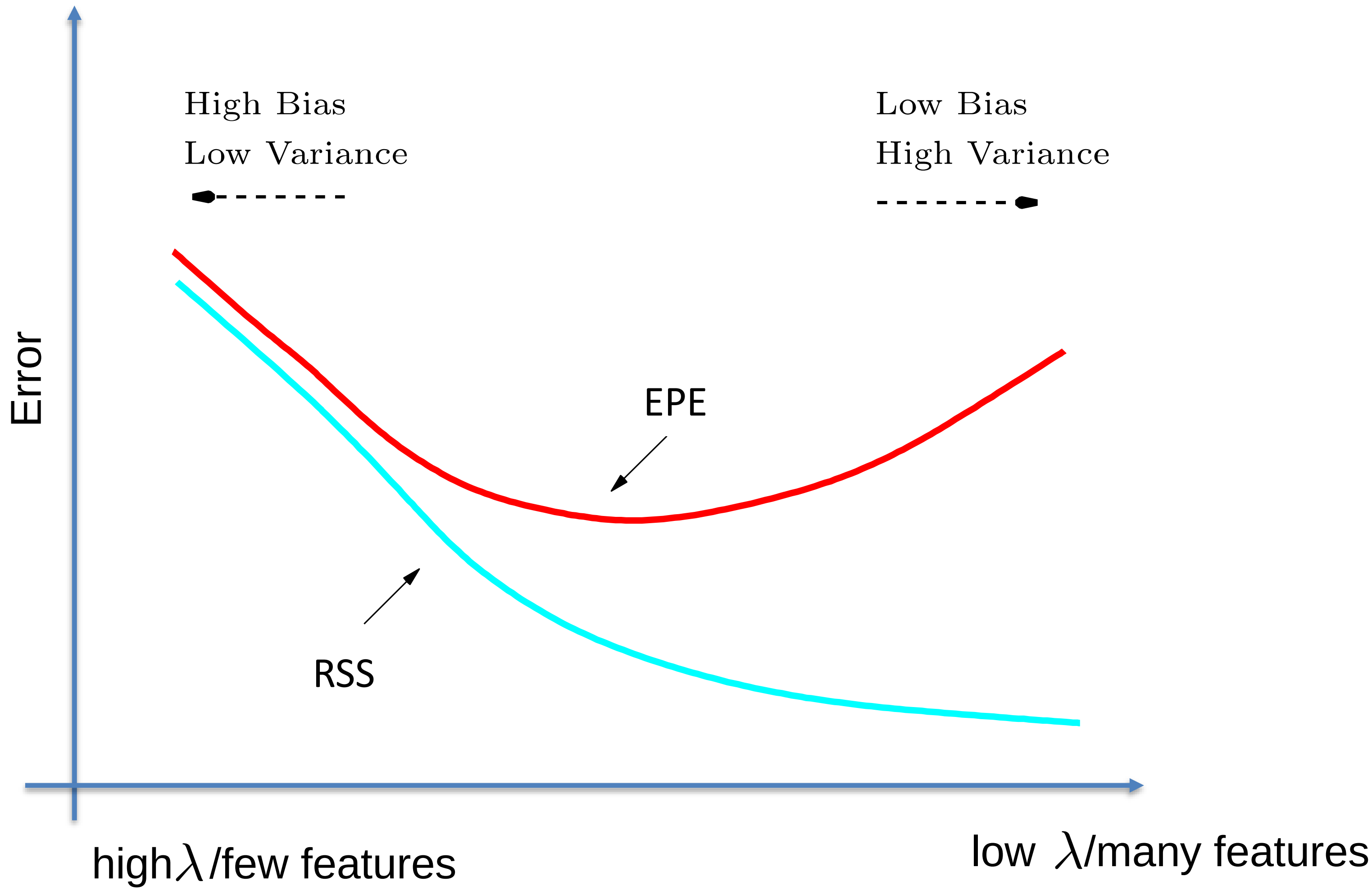
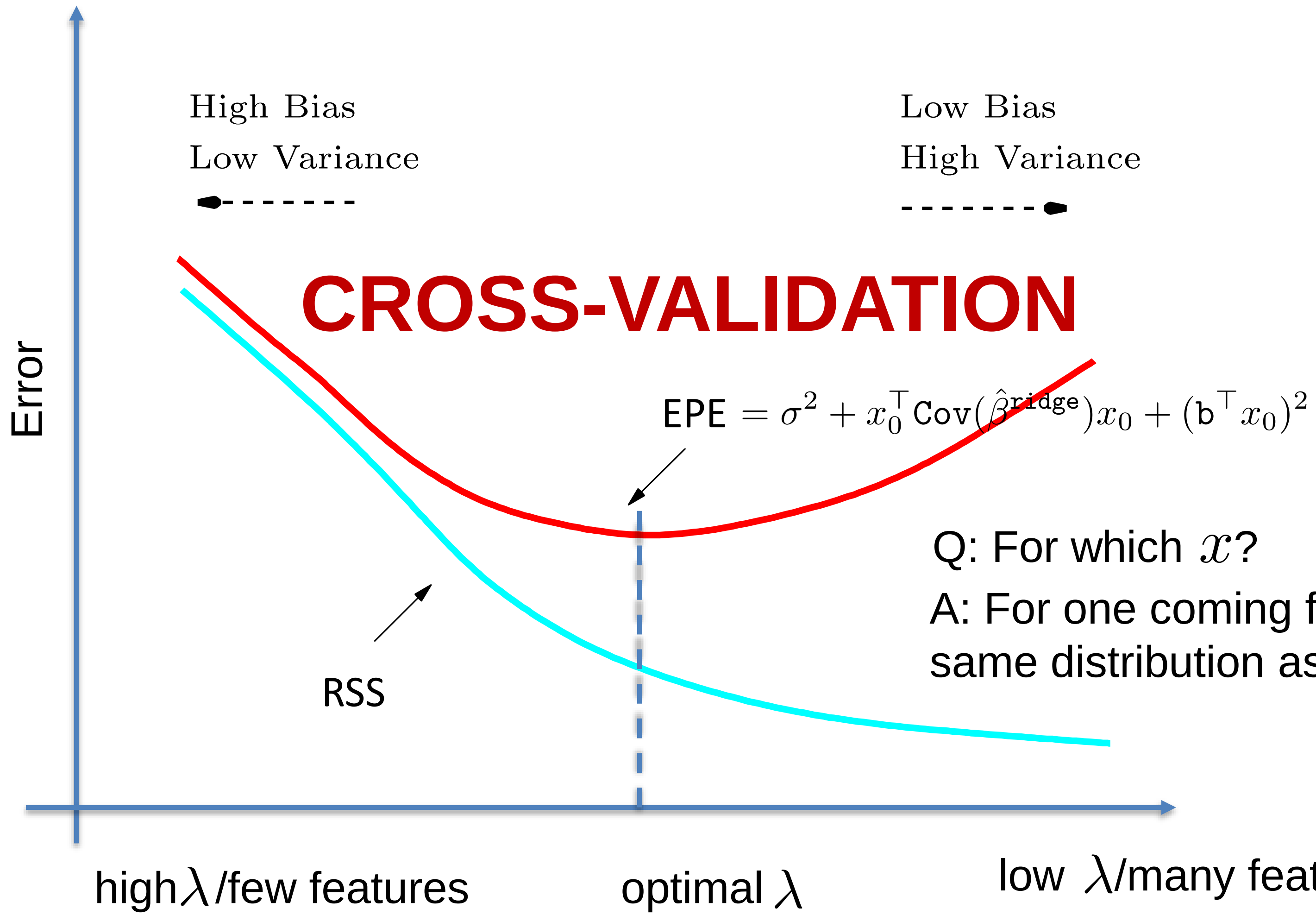
Ridge Regression: Intuition #3



Ridge Regression: Intuition #3

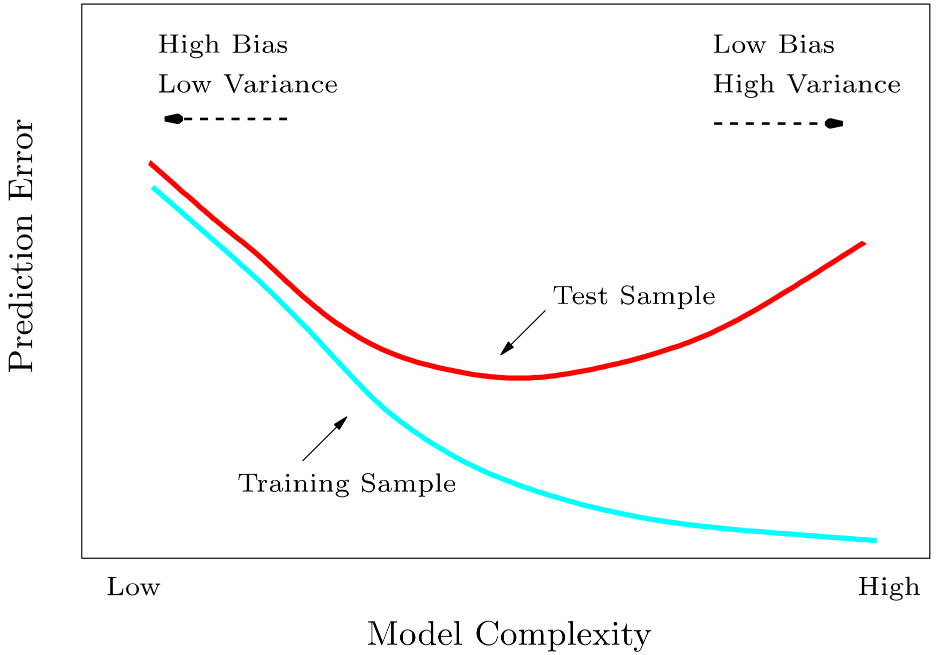


Q: For which x?

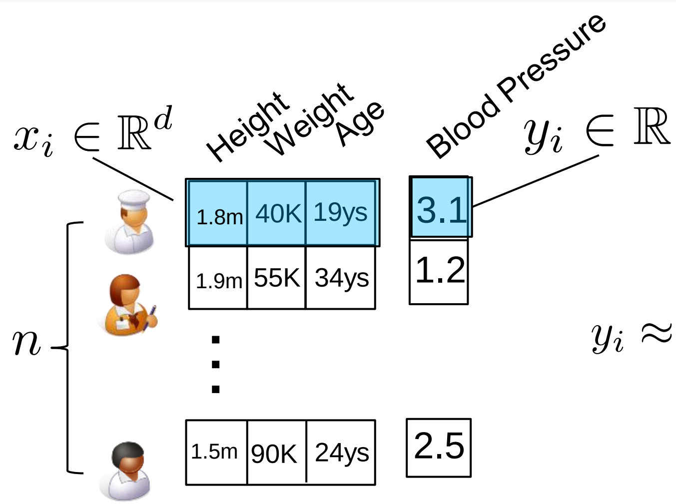
A: For one coming from same distribution as data

Intuition 3 Has a Universal, General Interpretation

- Cross-Validation minimizes EPE, assuming new data comes from **same distribution** as existing data
- When varying **model complexity,** we are establishing a tradeoff between **variance** and **bias**



Lasso Regression



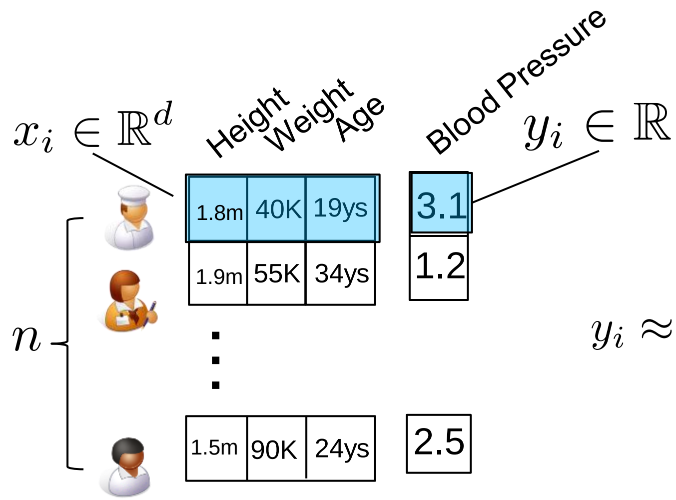
$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

$$\hat{\beta}^{\texttt{lasso}} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_1, \text{ for some } \lambda > 0$$

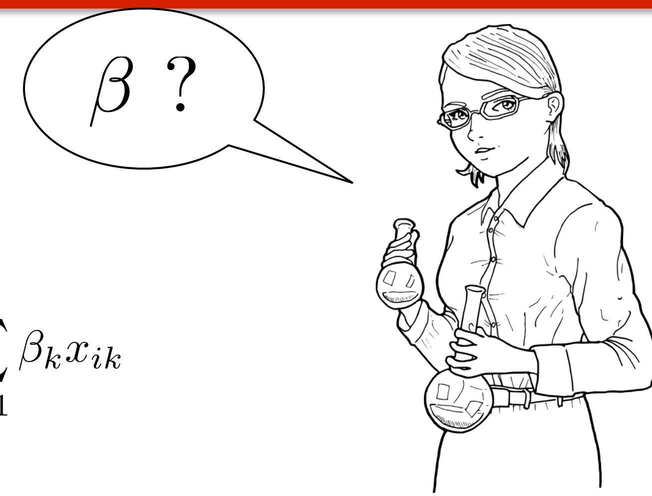
where $\|\beta\|_1 = \sum_{k=1}^{d} |\beta_k|$

Convex!
(not differentiable)

Lasso Regression



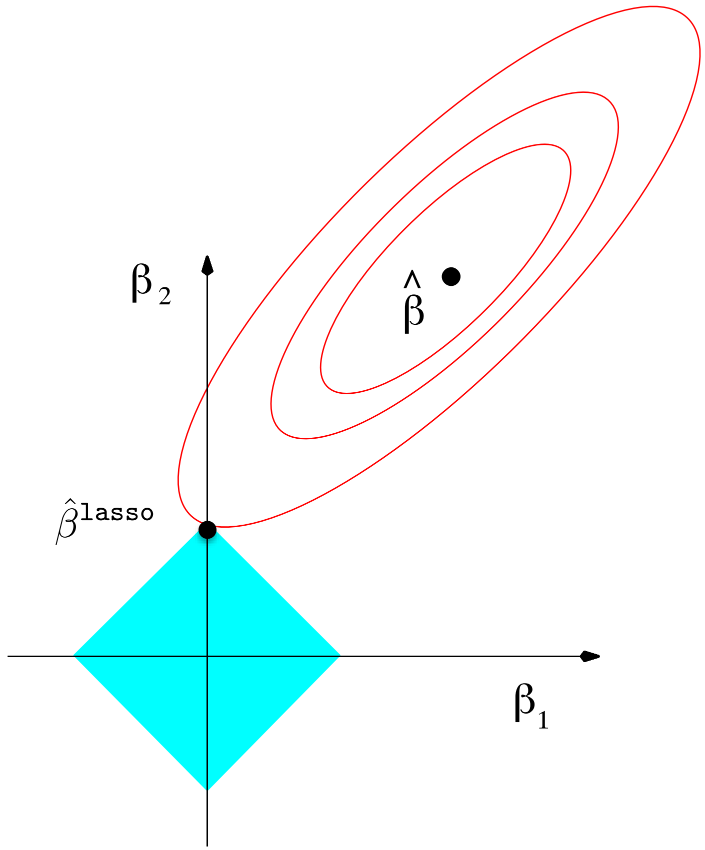
$$y_i \approx f(x_i) = \beta^\top x_i = \sum_{k=1}^{d} \beta_k x_{ik}$$

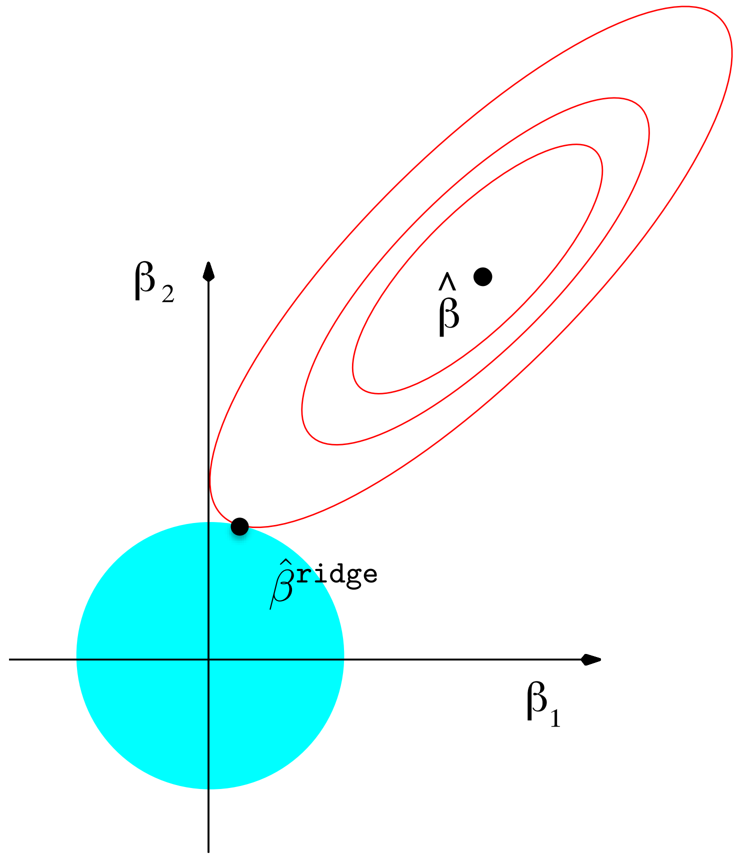


For every $\lambda \geq 0$, there exists a $t \geq 0$ such that the two problems produce **the same solution**

Minimize: $\sum_{i=1}^{n} (y_i - \beta^\top x_i)^2 + \lambda \|\beta\|_1$	Minimize: $\sum_{i=1}^{n} (y_i - \beta^\top x_i)^2$
subject to: $\beta \in \mathbb{R}^d$	subject to: $\|\beta\|_1 \leq t$

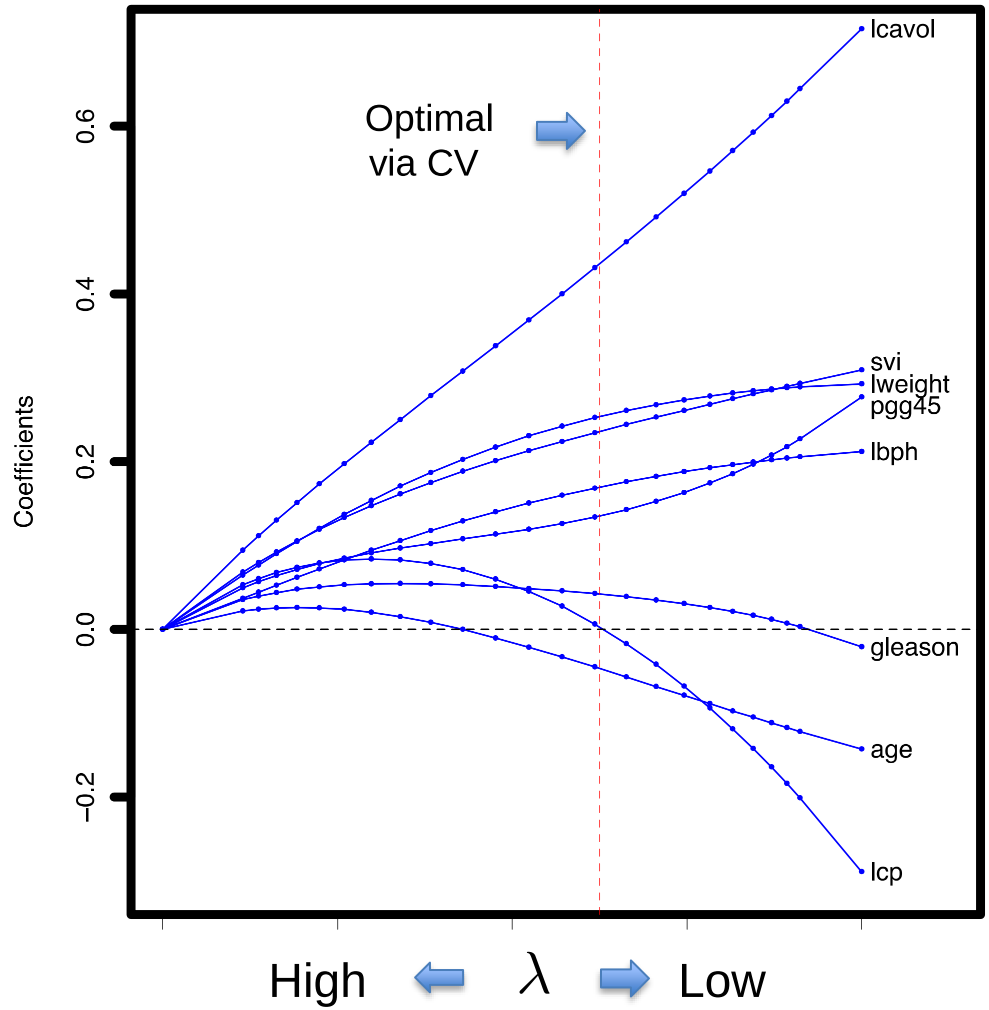
Lasso Regression vs. Ridge Regression





Lasso is more prone to sparse solutions

Varying λ in Ridge Regression



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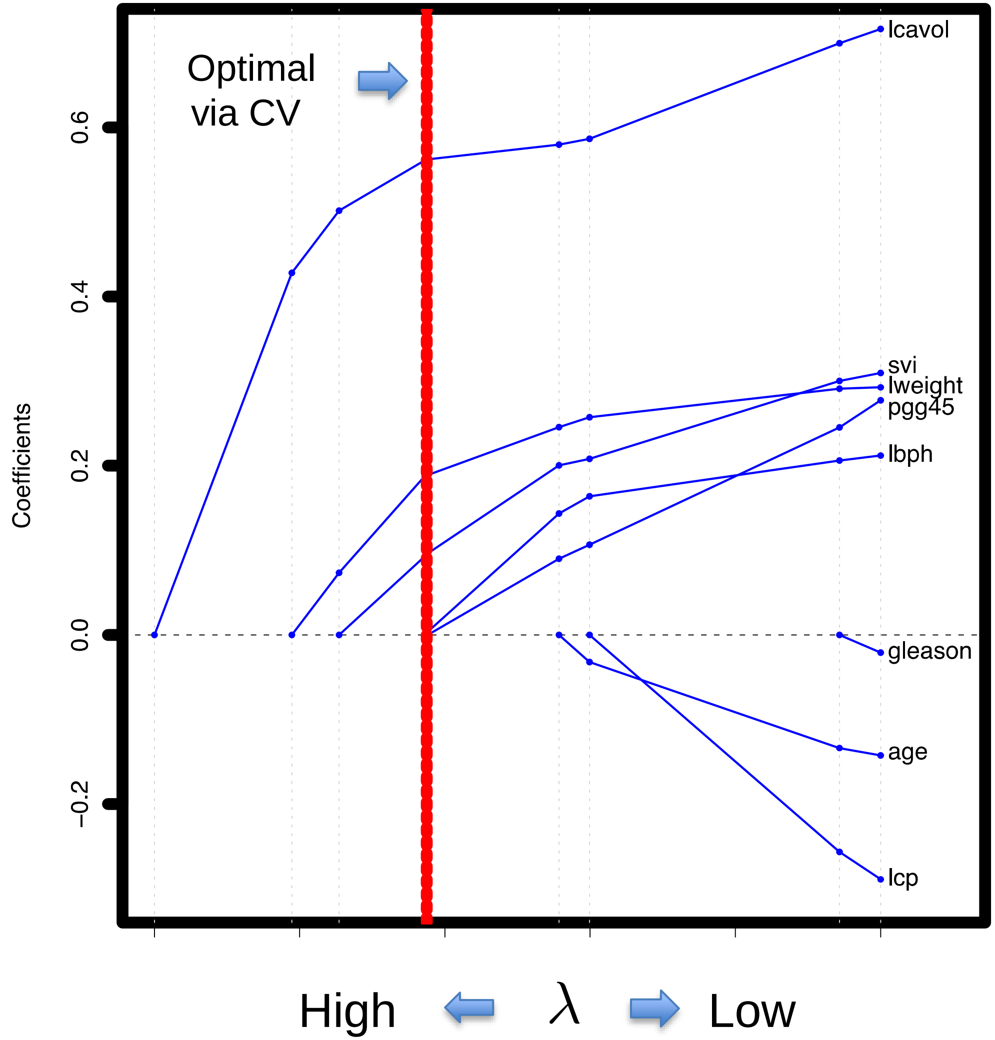
Varying λ in Lasso Regression



Lasso Regression via Constrained Optimization

Minimize: $$\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda \sum_{k=1}^{d} |\beta_k|$$

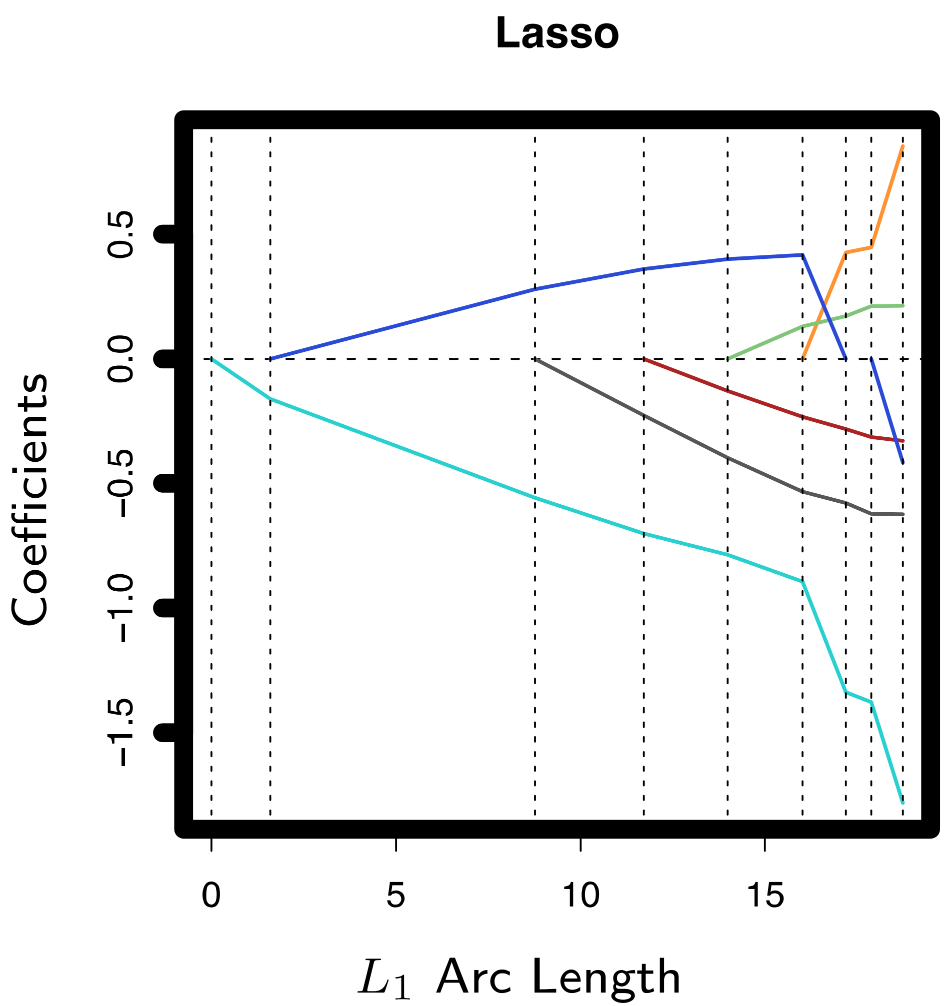
subject to: $$\beta \in \mathbb{R}^d$$

Lasso Regression via Constrained Optimization

Minimize:
$$\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 + \lambda \sum_{k=1}^{d} t_k$$

subject to:
$$\beta_k \leq t_k,$$
$$\beta_k \geq -t_k, \qquad \forall k = 1, \ldots, d$$

Least Angle Regression



- ❑ Computes **entire path** under λ
  - ❑ needed anyway for CV
- ❑ Same complexity as standard linear regression
- ❑ Not that easy to parallelize

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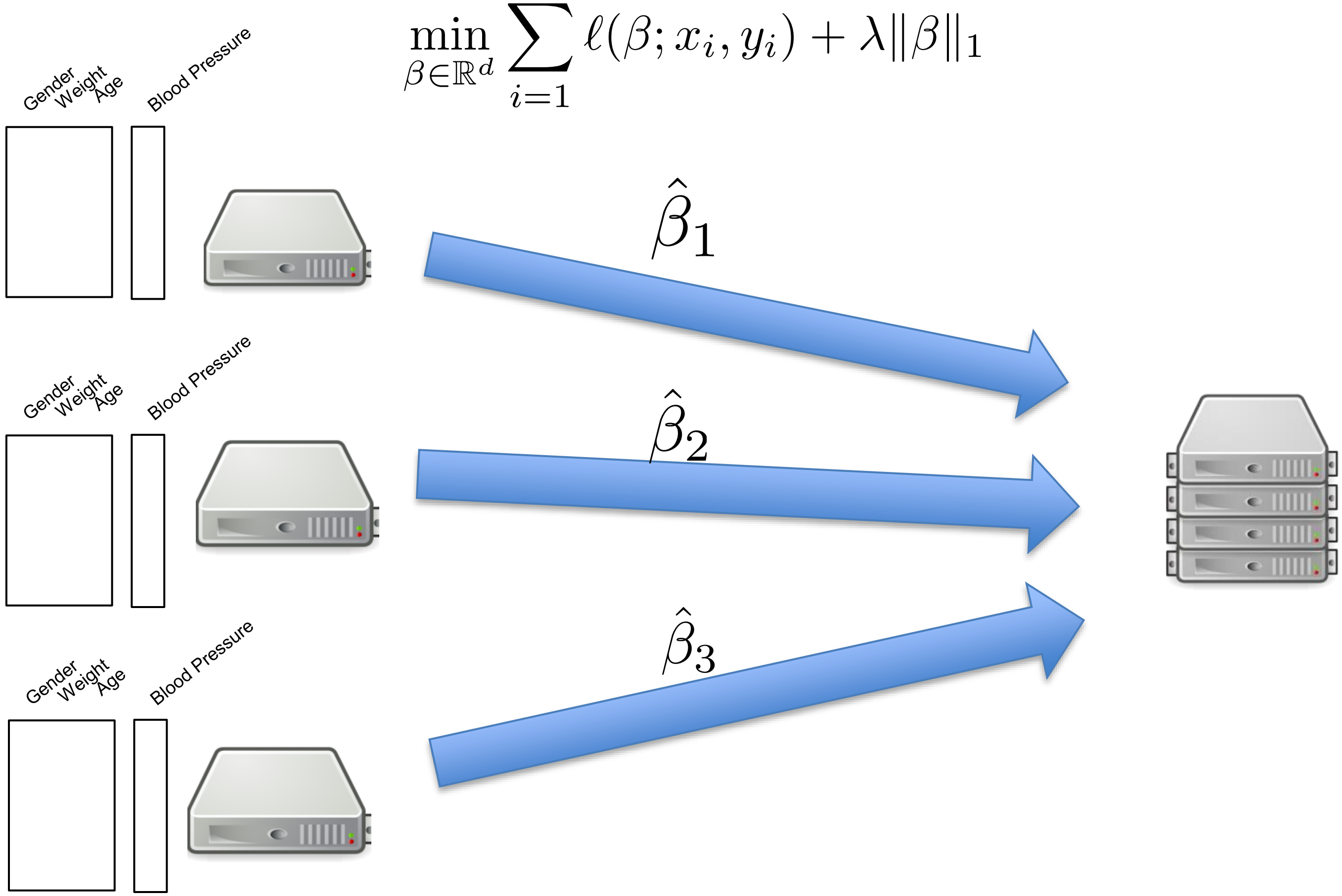
Alternating Directions Method of Multipliers

Distributed optimization and statistical learning via the alternating direction method of multipliers S. Boyd, N. Parikh, E. Chu, B. Peleato, and J. Eckstein, 2011

$$\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} \ell(\beta; x_i, y_i) + \lambda \|\beta\|_1$$

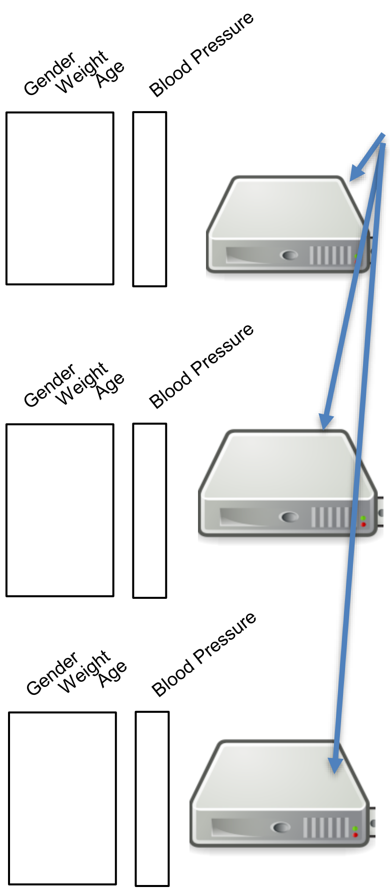


Alternating Directions Method of Multipliers

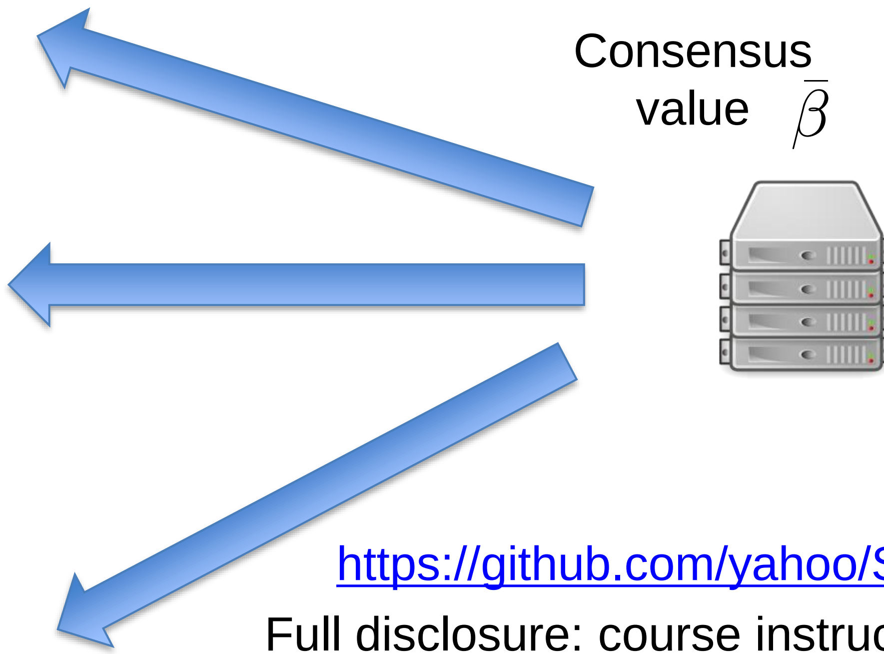
[Distributed optimization and statistical learning via the alternating direction method of multipliers](#) S. Boyd, N. Parikh, E. Chu, B. Peleato, and J. Eckstein, 2011

$$\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^{n} \ell(\beta; x_i, y_i) + \lambda \|\beta\|_1$$

Solve problem again, forcing agreement with $\bar{\beta}$



Consensus value $\bar{\beta}$



https://github.com/yahoo/SparkADMM

Full disclosure: course instructor involved

A Note on Biases and Regularization

"bias"

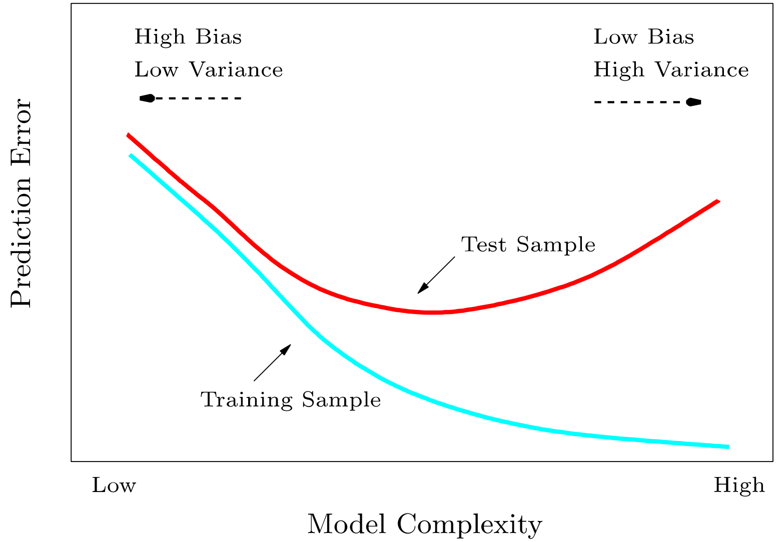
$$\min_{\beta \in \mathbb{R}^d, \beta_0 \in \mathbb{R}} \quad \sum_{i=1}^{n} \|y_i - \beta^\top x_i - \beta_0\|_2^2 + \lambda \|\beta\|_1$$

- Bias is typically **not** regularized
- Intuition: solution should be invariant to shifting the origin of either features or response

Conclusions

- ❑ Learning f ➡ learning right **features**

- ❑ Fitting is not enough! **Cross Validation**



- ❑ Model complexity ⬌ Bias-Variance Tradeoff

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Conclusions: Relaxing $||\cdot||_0$