CSE 446
Regularization & Sparsity

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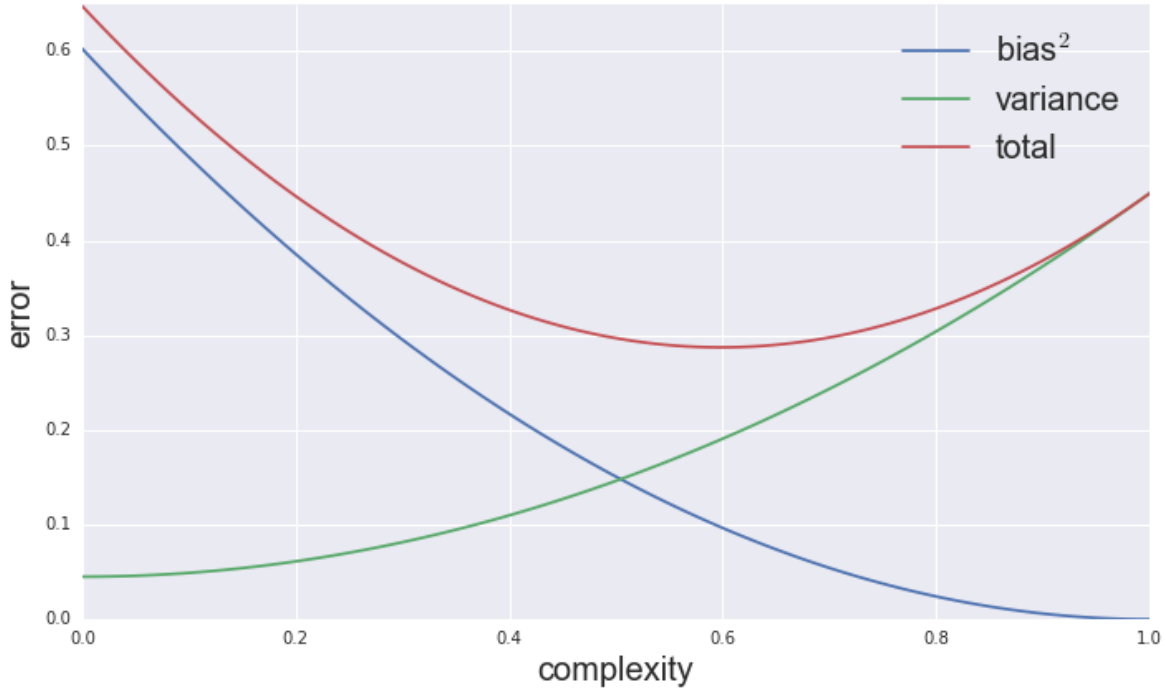
Bias-Variance Tradeoff

$$\underbrace{\mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y-\widehat{f}_{\mathcal{D}}(x))^2]\big|X=x]}_{\text{True generalization error}} = \underbrace{\mathbb{E}_{Y|X}[(Y-\eta(x))^2\big|X=x]}_{\text{irreducible error}}$$

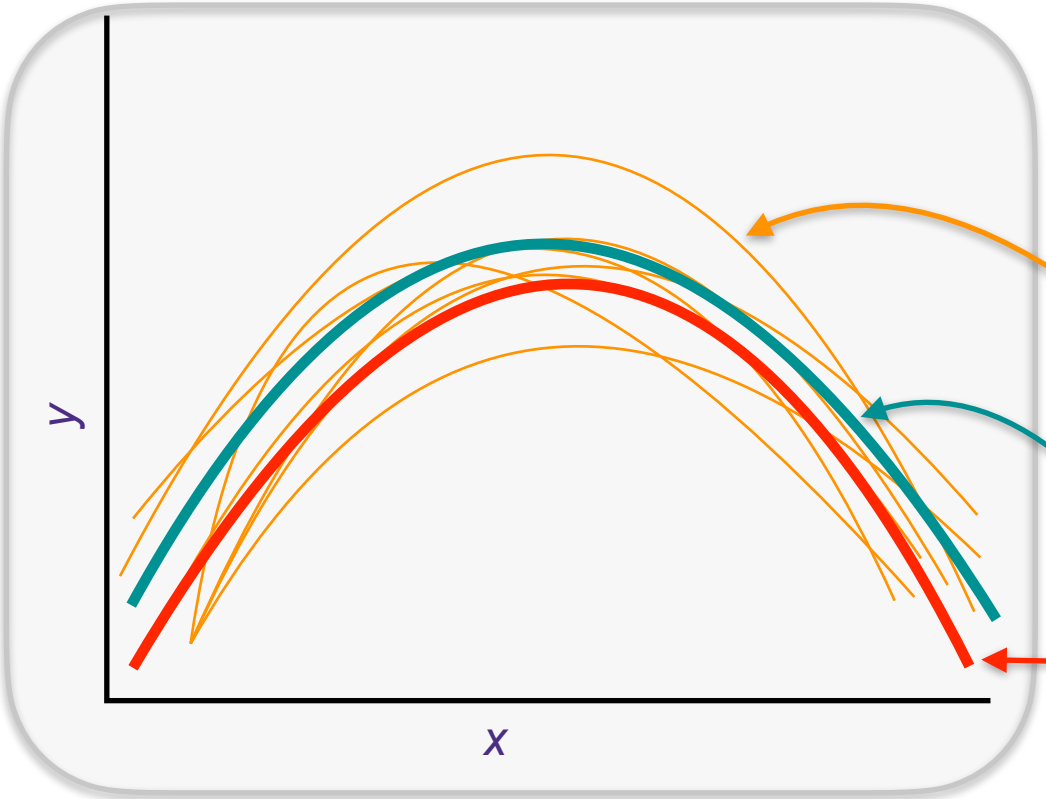
$$+\underbrace{(\eta(x)-\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])^2}_{\text{biased squared}} + \underbrace{\mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)]-\widehat{f}_{\mathcal{D}}(x))^2]}_{\text{variance}}$$



Bias-Variance Tradeoff

$$\mathbb{E}_{\mathcal{D}}[(\eta(x) - \widehat{f}_{\mathcal{D}}(x))^2] = (\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])^2 + \mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]$$

learning error = **biased squared** + **variance**

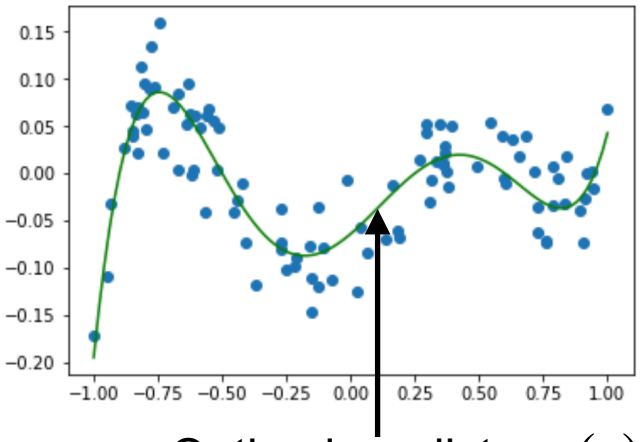


$$\widehat{f} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

$$\mathbb{E}_{\mathcal{D}}[\widehat{f}(x)]$$

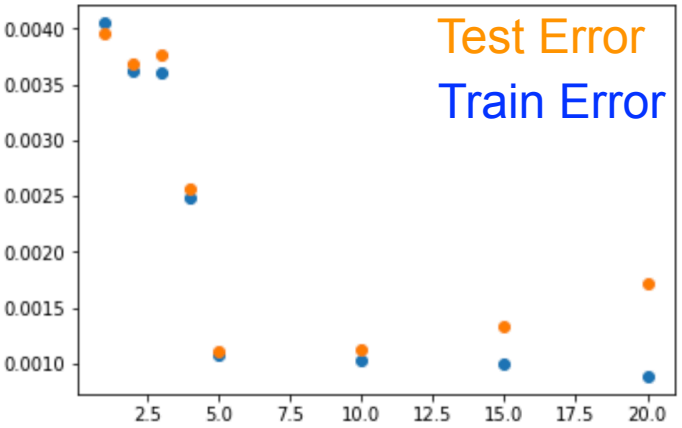
$$\eta(x) = \mathbb{E}_{Y|X}[Y|X = x]$$

Test error vs. model complexity



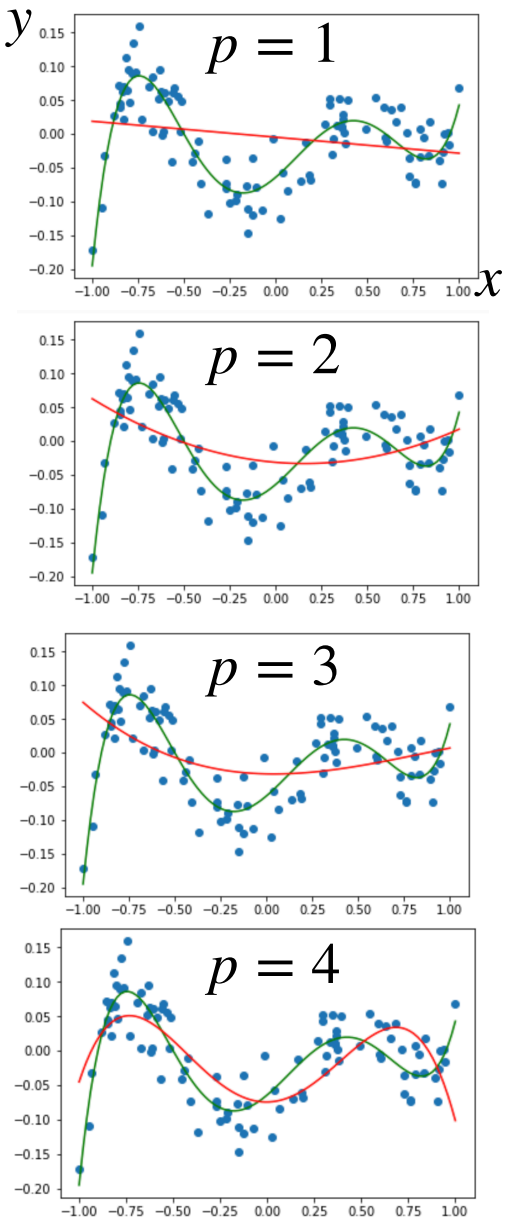
Optimal predictor $\eta(x)$ is degree-5 polynomial

Error

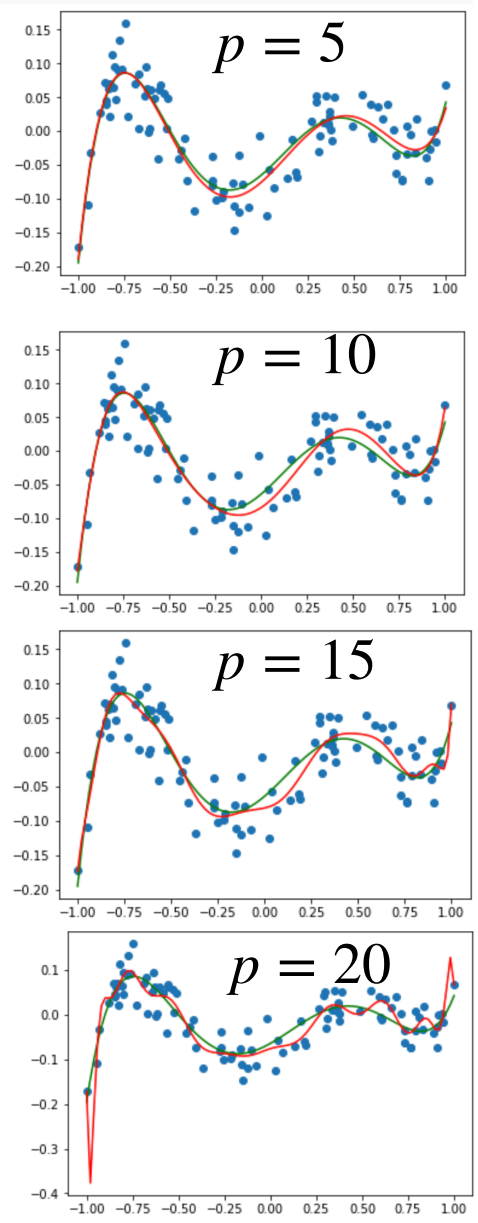


degree p of the polynomial regression

Simple model:
Model complexity is below the complexity of $\eta(x)$

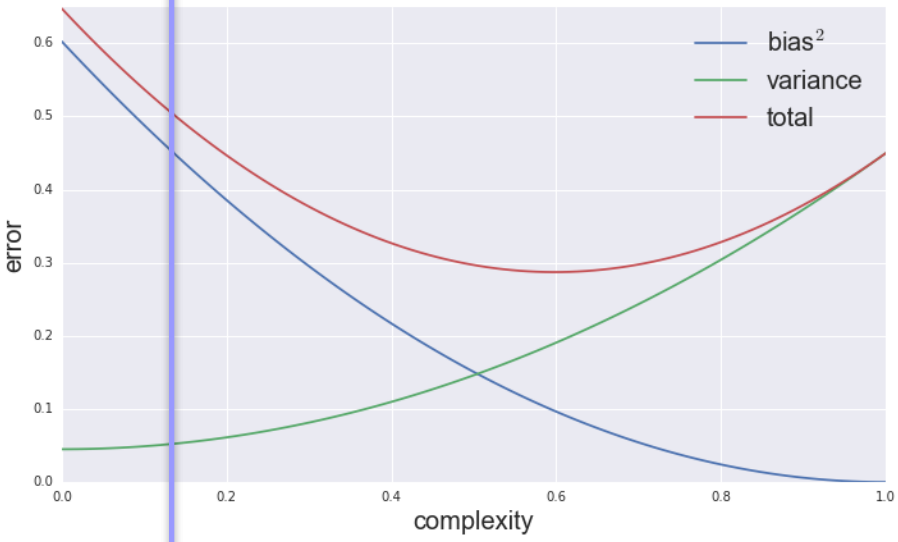


Complex model:
Fits noise in train data, diverging from $\eta(x)$

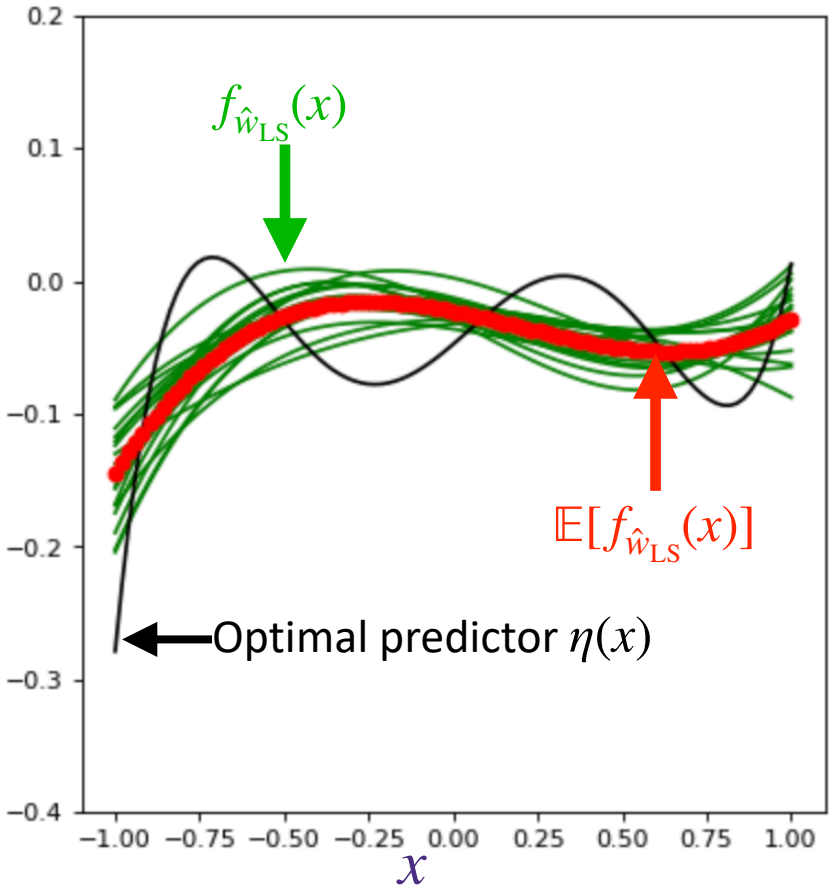


Recap: Bias-variance tradeoff with simple model

(Conceptual) bias variance tradeoff



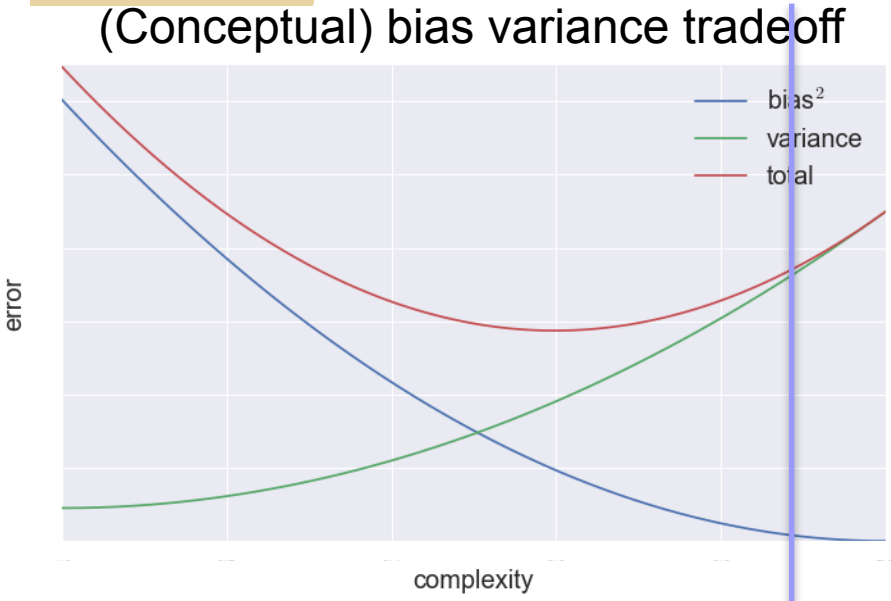
With degree-3 polynomials, we underfit



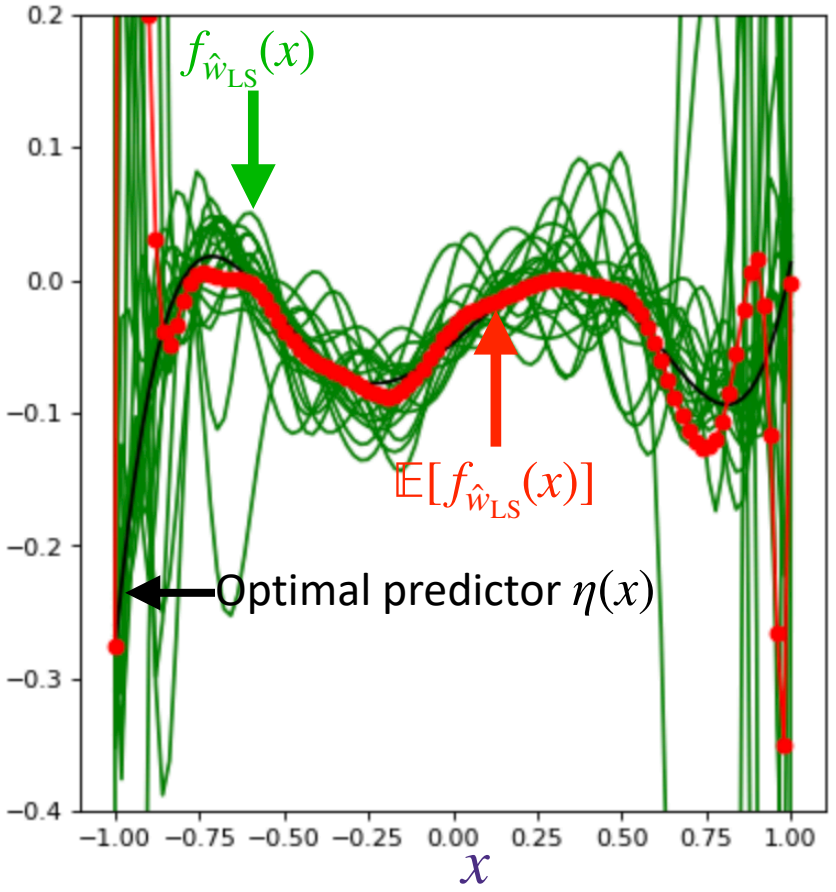
- When model **complexity is low** (lower than the optimal predictor $\eta(x)$)
  - Bias^2 of our predictor, $\left(\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]\right)^2$, is large
  - Variance of our predictor, $\mathbb{E}_{\mathcal{D}}\left[\left(\mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - \hat{f}_{\mathcal{D}}(x)\right)^2\right]$, is small
  - **If we have more samples (larger n), then**
    - What happens to bias?
    - What happens to variance?
    - What happens to overall test error?

Recap: Bias-variance tradeoff with complex model

(Conceptual) bias variance tradeoff



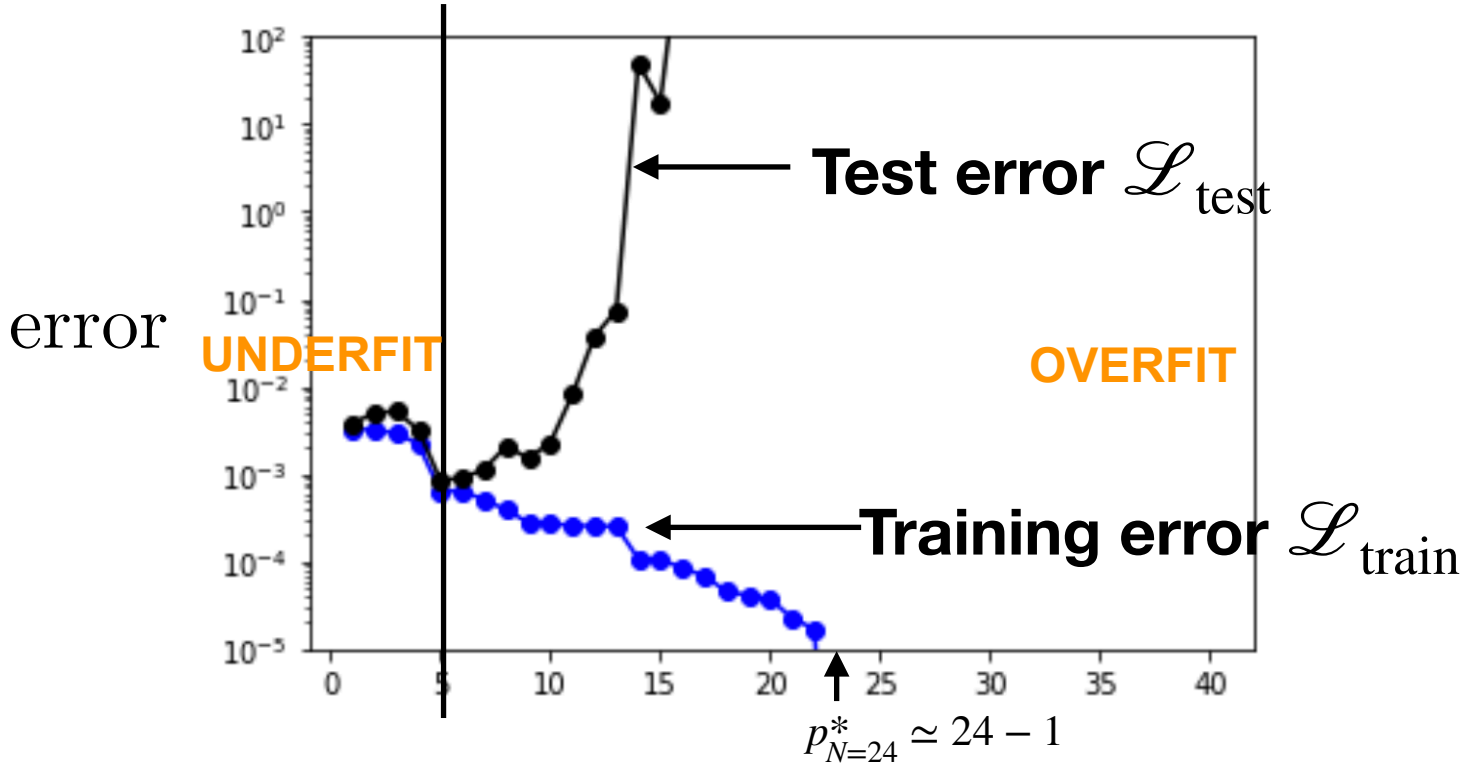
With degree-20 polynomials, we overfit



- When model complexity is high (higher than the optimal predictor $\eta(x)$)
  - Bias of our predictor, $\left(\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]\right)^2$, is small
  - Variance of our predictor, $\mathbb{E}_{\mathcal{D}}\left[\left(\mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - \hat{f}_{\mathcal{D}}(x)\right)^2\right]$, is large
- **If we have more samples (larger n), then**
  - What happens to bias?
  - What happens to variance?
  - What happens to overall test error?

Optimal model complexity depends on dataset size

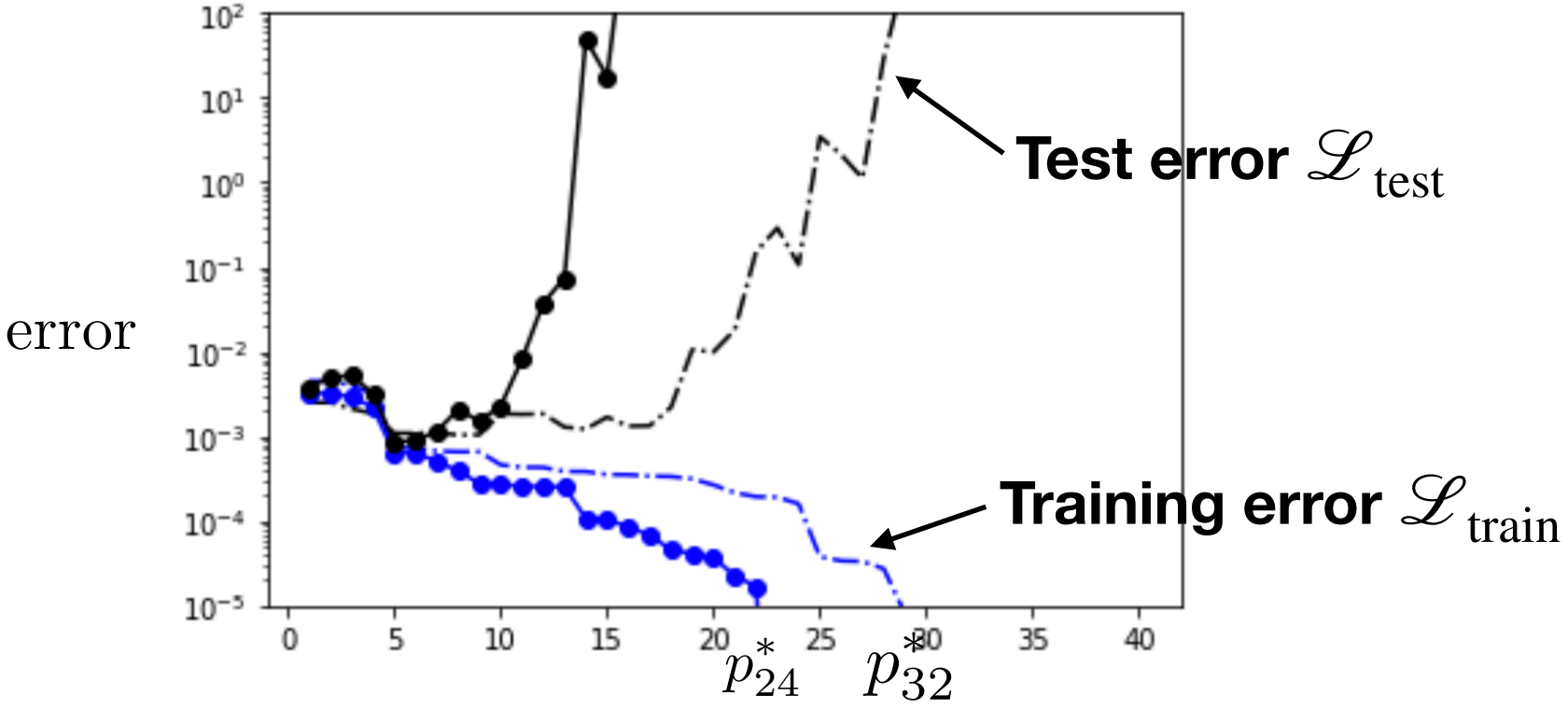
- Assume ***N=30***



- Given sample size N there is a threshold, p^*_N, where training error is zero
- Training error is **always** monotonically non-increasing
- Test error has a trend of going down and then up, but fluctuates

Variance decreases with more data, letting you fit more complex models

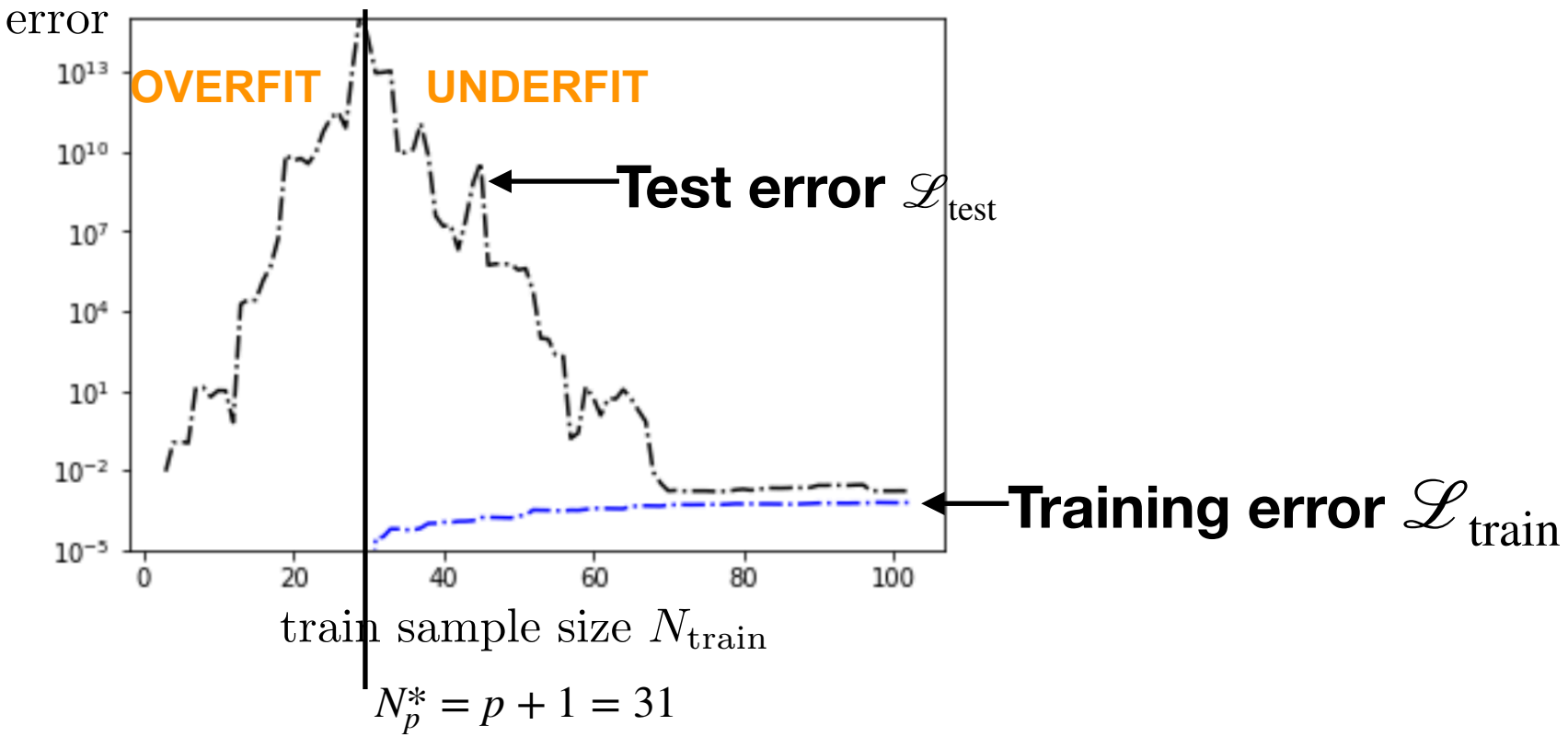
- Now compare ***N=40*** *to previous* ***N=30*** *case*



- **The threshold, p^*_N, moves right as dataset size increases**
- Training error tends to increase, because more points need to fit
- Test error tends to decrease, because Variance decreases

Variance decreases with more data, letting you fit more complex models

- Choose model complexity ***p=30***, **vary dataset size n**



- There is a threshold, N_p^*, below which training error is zero (extreme overfit)
- Above the threshold, test error tends to decrease
- Training error tends to increase (harder to fit so much data with simple model)

Regularization helps avoid overfitting

Ridge Regression

Regularization in Linear Regression

Recall Least Squares:

$$\widehat{w}_{LS} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$$

$$= \arg\min_{w} (\mathbf{y} - \mathbf{X}w)^T (\mathbf{y} - \mathbf{X}w)$$

when $(\mathbf{X}^T\mathbf{X})^{-1}$ exists….

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

Regularization in Linear Regression

Recall Least Squares:

$$\begin{aligned}\widehat{w}_{LS} &= \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 \\ &= \arg\min_w (\mathbf{y} - \mathbf{X}w)^T(\mathbf{y} - \mathbf{X}w) \\ &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}\end{aligned}$$

when $(\mathbf{X}^T\mathbf{X})^{-1}$ exists….

What if $x_i \in \mathbb{R}^d$ and $d > n$?

Regularization in Linear Regression

Recall Least Squares: $$\widehat{w}_{LS} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$$

When $x_i \in \mathbb{R}^d$ and $d > n$ the objective function is flat in some directions:

Regularization in Linear Regression

Recall Least Squares: $\widehat{w}_{LS} = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$

When $x_i \in \mathbb{R}^d$ and $d > n$ the objective function is flat in some directions:

Implies optimal solution is *not unique* and unstable due to lack of curvature*:*

- small changes in training data result in large changes in solution
- often the *magnitudes* of *w* are "very large"

Regularization imposes "simpler" solutions by a "complexity" penalty

Sensitivity increases overfitting

- For a linear model,
  $$y \simeq b + w_1 x_1 + w_2 x_2 + \cdots + w_d x_d$$
  if $|w_j|$ is large then the prediction is **sensitive** to small changes in x_j
- Large ***sensitivity*** leads to overfitting and poor generalization, and equivalently models that overfit tend to have large weights
- Note that b is a constant and hence there is no sensitivity for the offset b

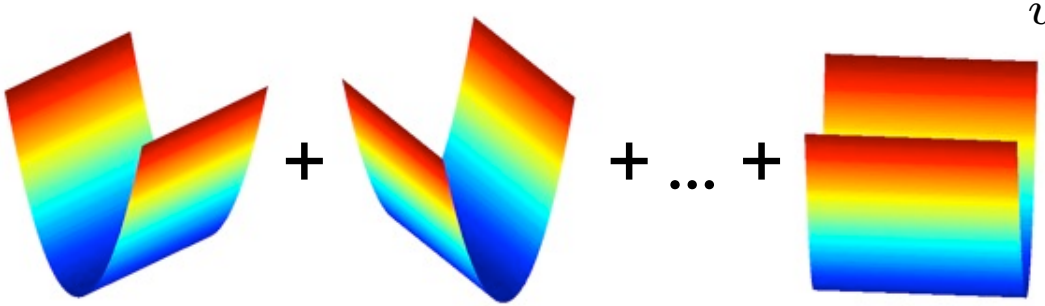
- In ***Ridge Regression***, we use a regularizer $\|w\|_2^2$ to measure and control the sensitivity of the predictor
- And optimize for small loss and small sensitivity, by adding a ***regularizer*** in the objective (assume no offset for now)

$$\hat{w}_{\text{ridge}} = \arg\min_{w} \left\{ \sum_{i=1}^{n} (y_i - x_i^T w)^2 + \lambda \|w\|_2^2 \right\}$$

Ridge Regression

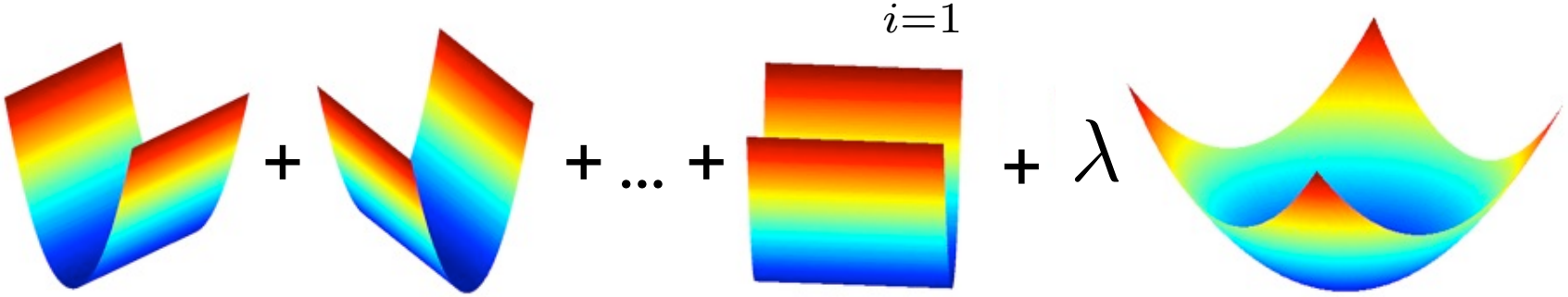
- Old Least squares objective:

$$\widehat{w}_{LS} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$$



- Ridge Regression objective:

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$



Minimizing the Ridge Regression Objective

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

Scalar derivative			Vector derivative		
$f(x)$	$\rightarrow$	$\frac{\mathrm{d}f}{\mathrm{d}x}$	$f(\mathbf{x})$	$\rightarrow$	$\frac{\mathrm{d}f}{\mathrm{d}\mathbf{x}}$
bx	$\rightarrow$	b	$\mathbf{x}^T\mathbf{B}$	$\rightarrow$	$\mathbf{B}$
bx	$\rightarrow$	b	$\mathbf{x}^T\mathbf{b}$	$\rightarrow$	$\mathbf{b}$
x^2	$\rightarrow$	$2x$	$\mathbf{x}^T\mathbf{x}$	$\rightarrow$	$2\mathbf{x}$
bx^2	$\rightarrow$	$2bx$	$\mathbf{x}^T\mathbf{B}\mathbf{x}$	$\rightarrow$	$2\mathbf{B}\mathbf{x}$

from Varun's notes in Week 1 Section notes

Shrinkage Properties

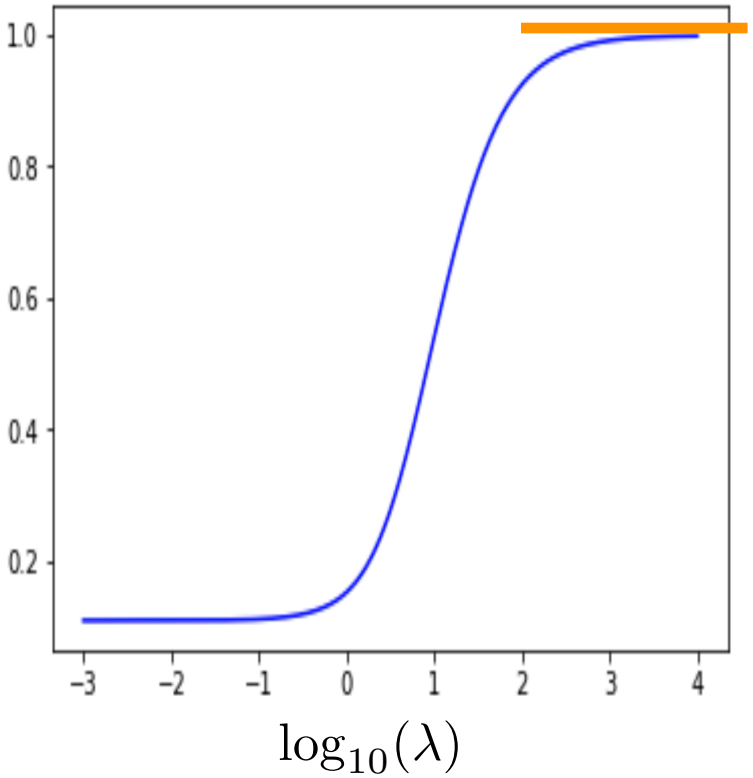
$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

$$= (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

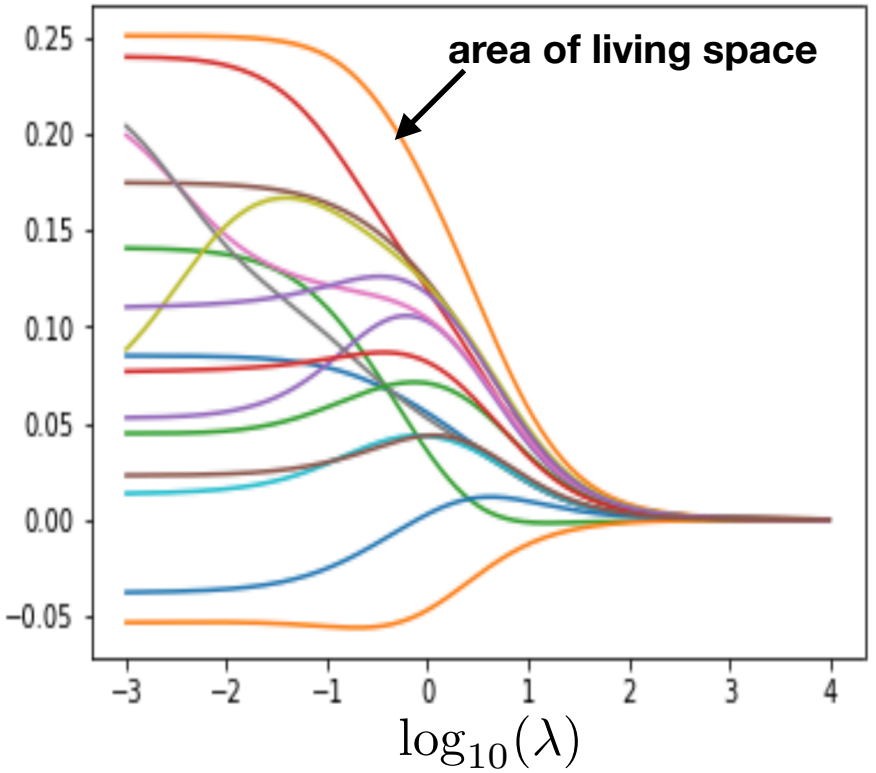
- When $\lambda = 0$, this gives the least squares model
- This defines a family of models hyper-parametrized by λ
- Large λ means more regularization and simpler model
- Small λ means less regularization and more complex model

Ridge regression: minimize $\sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_2^2$

training MSE $\frac{1}{n} \sum_{i=1}^{n} (y_i - x_i^T \hat{w}_{\text{ridge}}^{(\lambda)})^2$

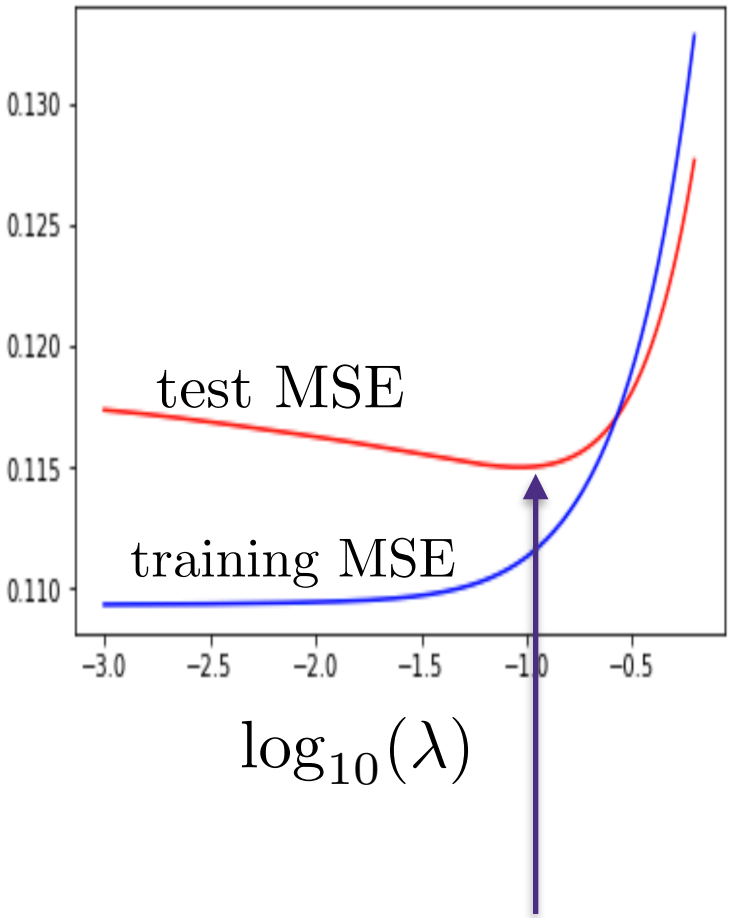


Housing price predictor $w_i's$



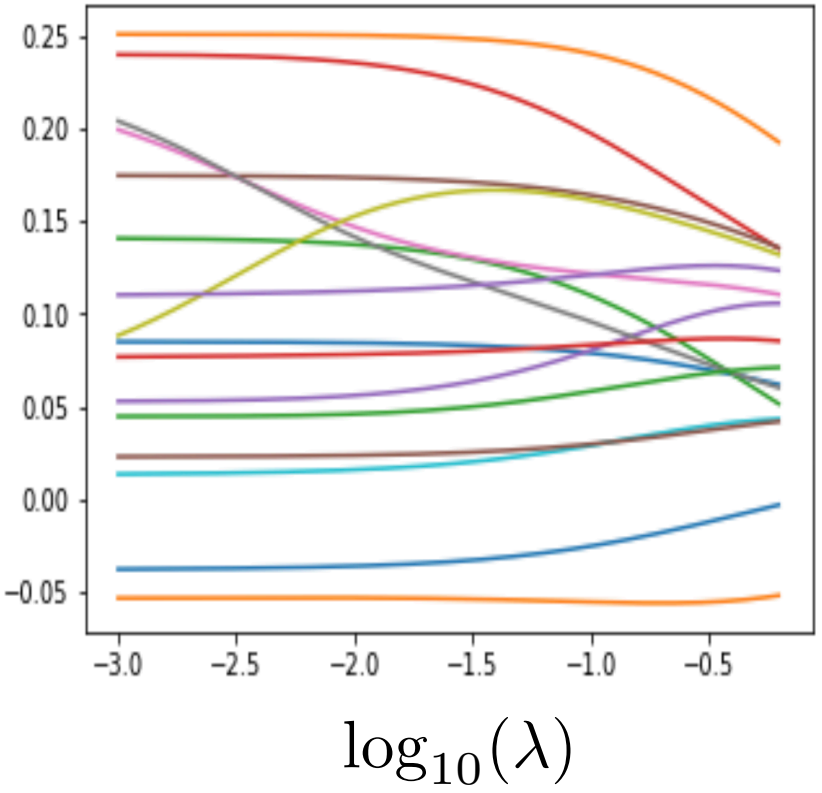
- Left plot: leftmost training error is with no regularization: 0.1093
- Left plot: rightmost training error is variance of the training data: 0.9991
- Right plot: called **regularization path**

Ridge regression: minimize $\sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_2^2$



- this gain in test MSE comes from shrinking w's to get a less sensitive predictor
(which in turn reduces the variance)

Housing price predictor $w_i's$



- this is the role of regularizer

Bias-Variance Properties

- Recall: $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$
- To analyze bias-variance tradeoff, we need to assume probabilistic generative model: $x_i \sim P_X, \;\; \mathbf{y} = \mathbf{X}w + \epsilon, \;\; \epsilon \sim \mathcal{N}(0,\sigma^2\mathbf{I})$ for some ground truth model parameter w
- The true error at a sample with feature x is $\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$

Bias-Variance Properties

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$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$$= \underbrace{\mathbb{E}_{y|x}[(y - \mathbb{E}[y\,|\,x])^2 \,|\, x]}_{\text{Irreducible Error}} + \underbrace{\mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}[y\,|\,x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]}_{\text{Learning Error}}$$

Bias-Variance Properties

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&\quad = \mathbb{E}_{y|x}[(y - x^Tw)^2 \,|\, x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^Tw - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]
\end{aligned}$$

Bias-Variance Properties

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$$= \mathbb{E}_{y|x}[(y - x^Tw)^2 \,|\, x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^Tw - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$$= \sigma^2 + (x^Tw - \mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x])^2 + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

Irreduc. Error — Bias-squared — Variance

Bias-Variance Properties

- Recall: $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$
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Irreduc. Error — Bias-squared — Variance

Suppose $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$, then $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T(\mathbf{X}w + \epsilon)$

$$= \frac{n}{n+\lambda}w + \frac{1}{n+\lambda}\mathbf{X}^T\epsilon$$

Bias-Variance Properties

Suppose $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$, then

$$\hat{w}_{\text{ridge}} = \frac{n}{n+\lambda} w + \frac{1}{n+\lambda}\mathbf{X}^T\epsilon$$

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&= \sigma^2 + (x^Tw - \mathbb{E}_{\mathcal{D}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x])^2 + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]
\end{aligned}$$

(verify at home)

$$= \sigma^2 + \frac{\lambda^2}{(n+\lambda)^2}(w^Tx)^2 + \frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2$$

Irreduc. Error | Bias-squared | Variance

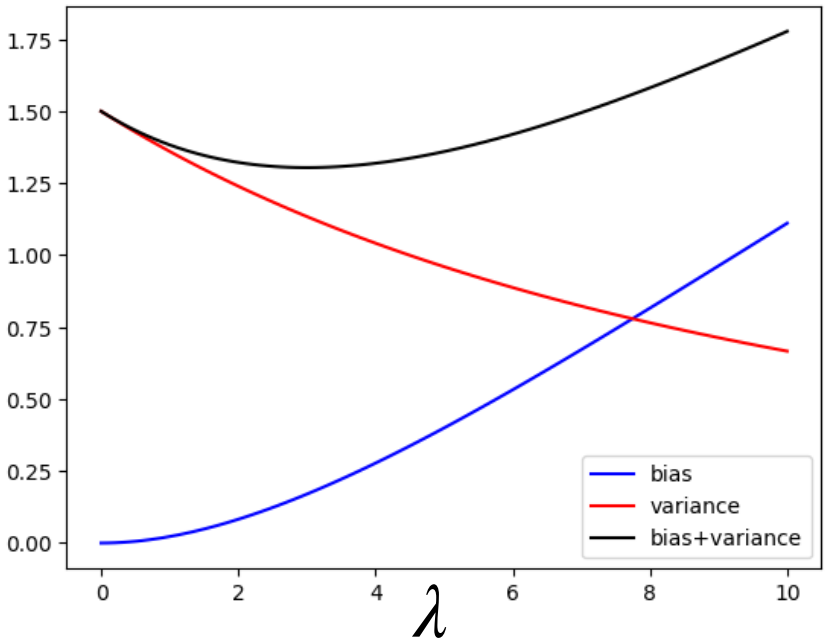
Bias-Variance Properties

Suppose $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$,

- Ridge regressor: $\hat{w}_{ridge} = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$
- True error

$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x] = \sigma^2 + \underbrace{\frac{\lambda^2}{(n+\lambda)^2}(w^T x)^2}_{\text{Bias-squared}} + \underbrace{\frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2}_{\text{Variance}}$$

d=10, n=20, $\sigma^2 = 3.0, \|w\|_2^2 = 10$



as $\lambda \to 0$,
$\hat{w}_{\text{ridge}} \to \hat{w}_{\text{LS}}$

as $\lambda \to \infty$
$\hat{w}_{\text{ridge}} \to 0$

What you need to know…

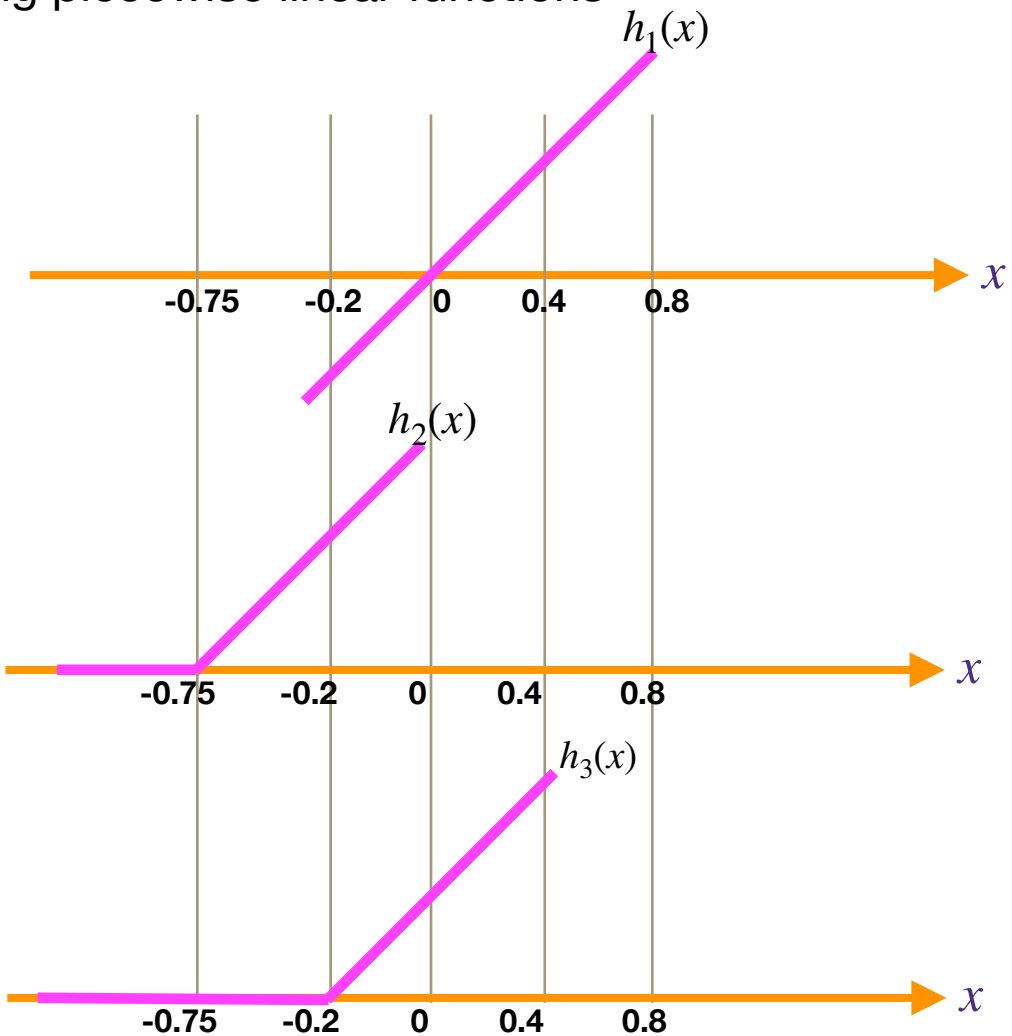
- Regularization
  - Penalizes complex models towards preferred, simpler models
- Ridge regression
  - L_2 penalized least-squares regression
  - Regularization parameter trades off model complexity with training error
  - Never regularize the offset!

Example: piecewise linear fit

- we fit a linear model:
  $f(x) = b + w_1 h_1(x) + w_2 h_2(x) + w_3 h_3(x) + w_4 h_4(x) + w_5 h_5(x)$
- with a specific choice of features using piecewise linear functions

$$h(x) = \begin{bmatrix} h_1(x) \\ h_2(x) \\ h_3(x) \\ h_4(x) \\ h_5(x) \end{bmatrix} = \begin{bmatrix} x \\ [x + 0.75]^+ \\ [x + 0.2]^+ \\ [x - 0.4]^+ \\ [x - 0.8]^+ \end{bmatrix}$$

$$[a]^+ \triangleq \max\{a, 0\}$$



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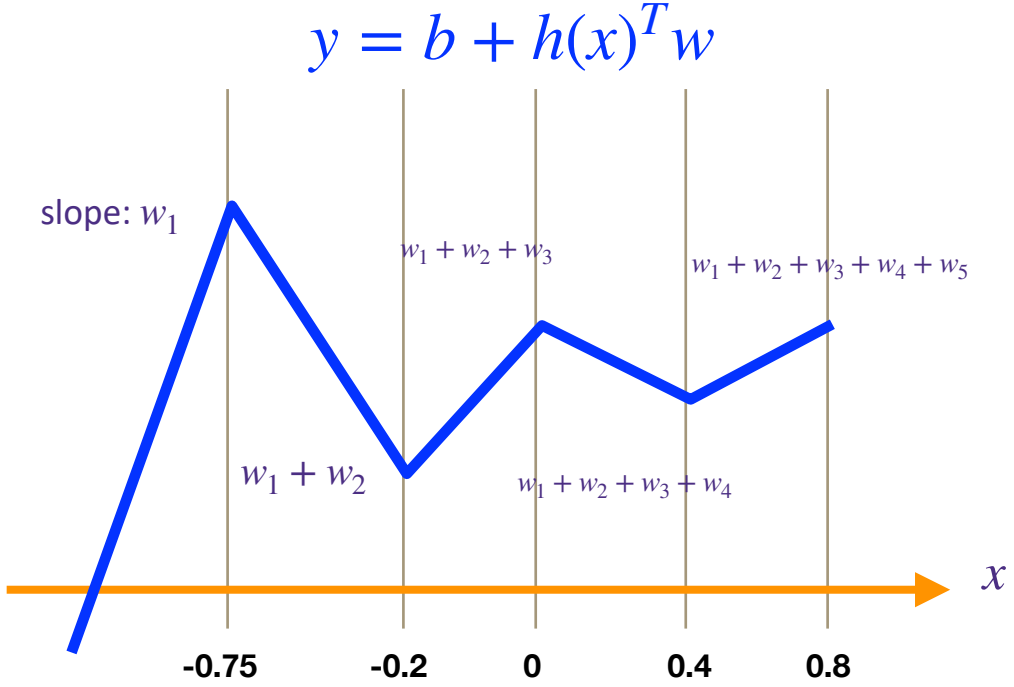
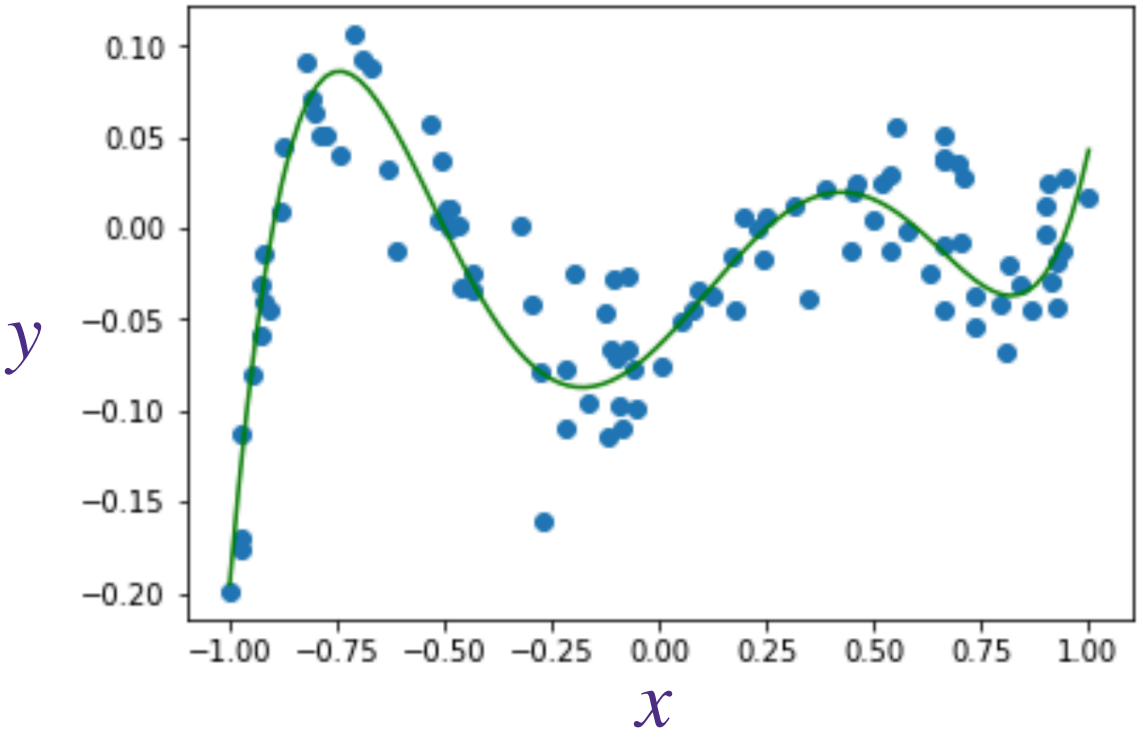


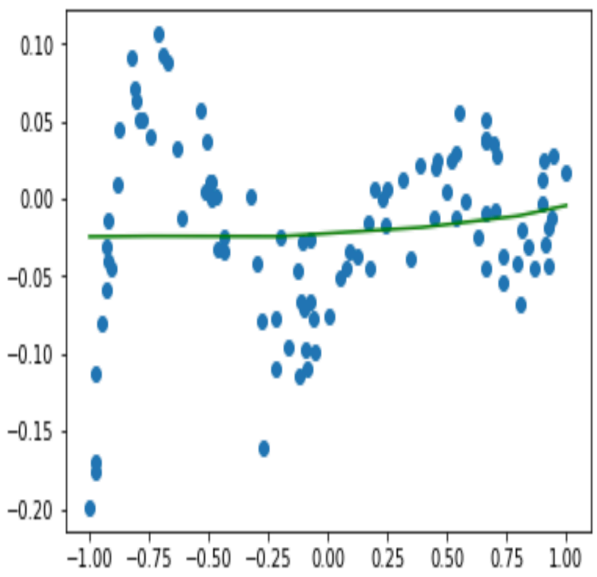
the weights capture the change in the slopes

Example: piecewise linear fit

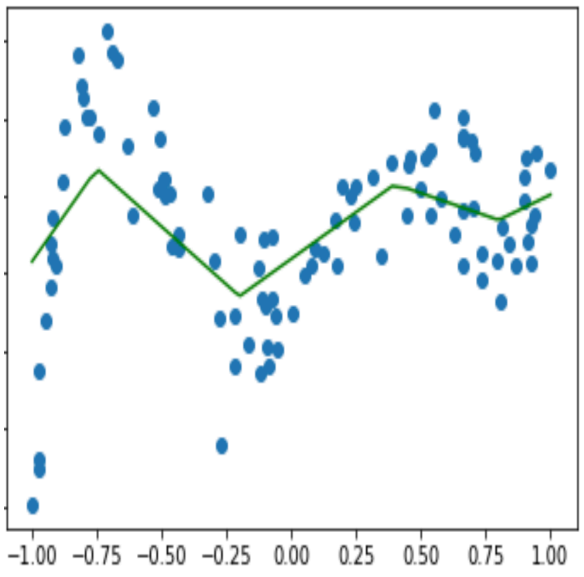
- we fit a linear model:
  $f(x) = b + w_1 h_1(x) + w_2 h_2(x) + w_3 h_3(x) + w_4 h_4(x) + w_5 h_5(x)$
- with a specific choice of features using piecewise linear functions



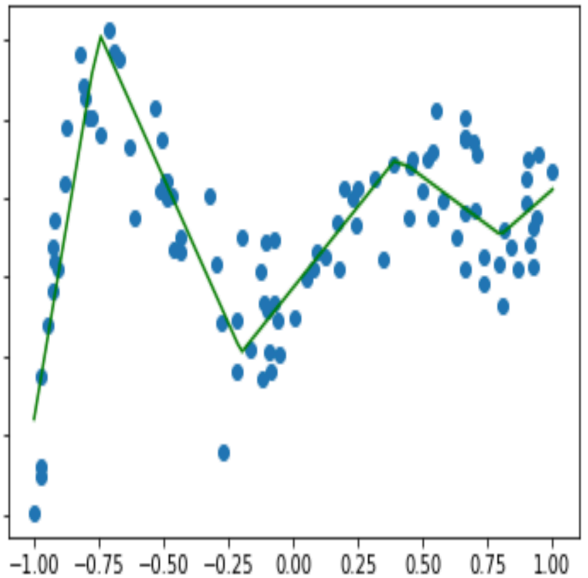
Example: piecewise linear fit (ridge regression)



$\lambda = 1$



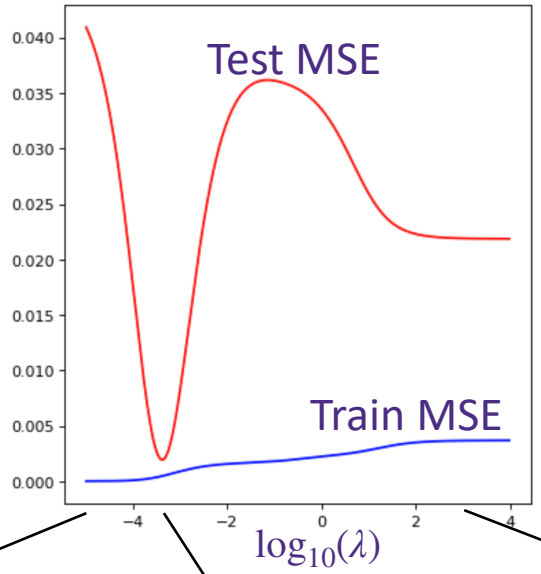
$\lambda = 0.005$

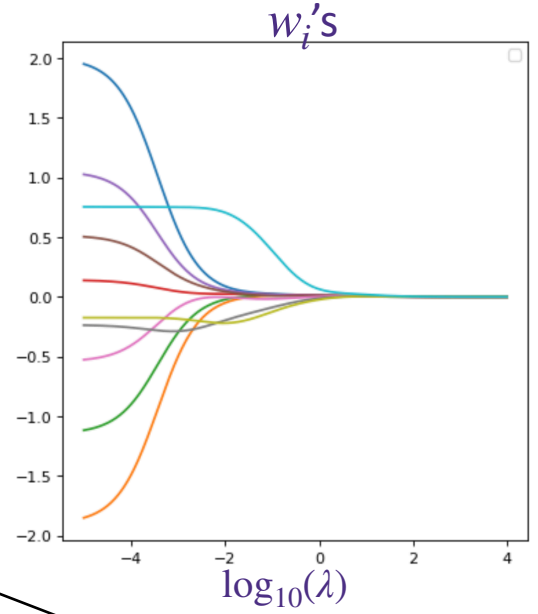


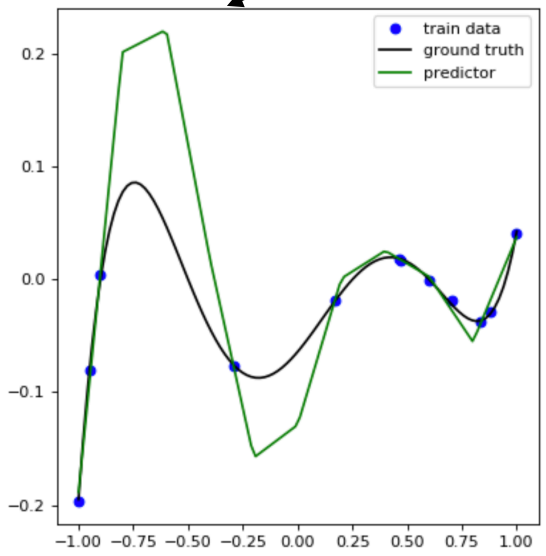
$\lambda = 0.000001$

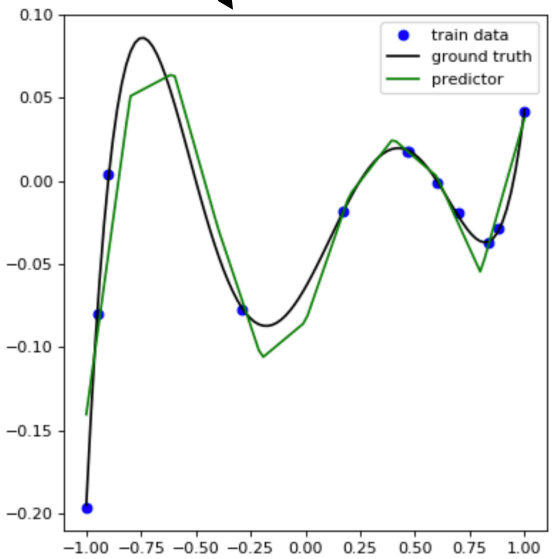
We do not observe overfitting, as d=5 << n=100

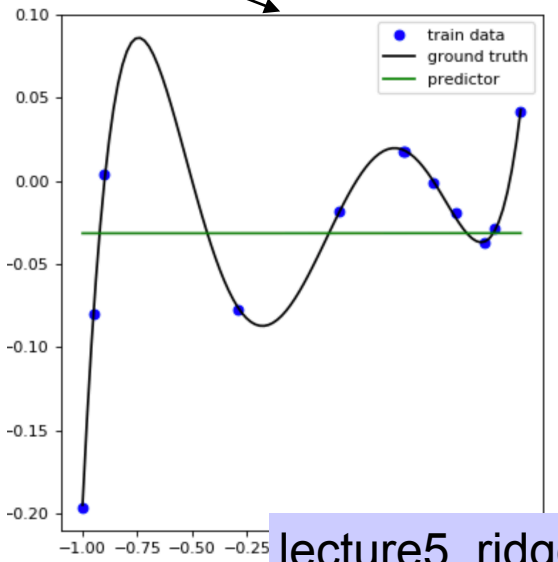
Piecewise linear with $w \in \mathbb{R}^{10}$ and n=11 samples











lecture5_ridge.ipynb

Sparsity & the LASSO

How to make the model compact and interpretable

UNIVERSITY of WASHINGTON

Sparsity

$$\widehat{w}_{LS} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$$

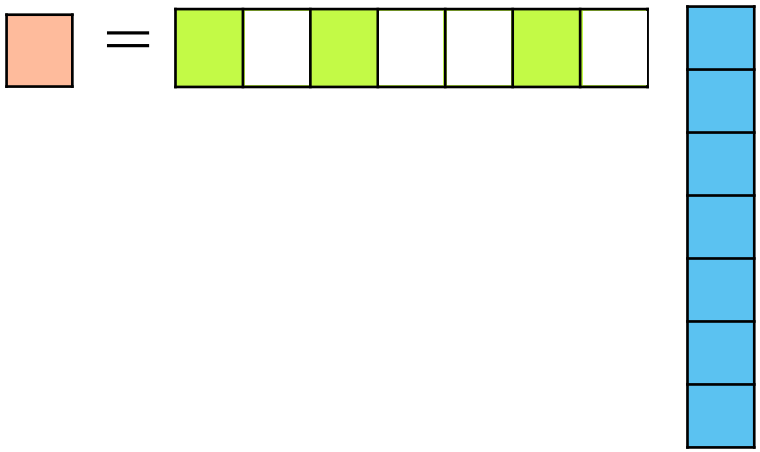
- We learned to measure ***sensitivity*** by the size of weights: $\|w\|_2^2$
- Vector w is ***sparse***, if many entries are zero
  - A vector w is said to be k-sparse if at most k entries are non-zero
  - We are interested in k-sparse w with $k \ll d$
  - Why do we prefer sparse vector w in practice?

Sparsity

$$\widehat{w}_{LS} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$$

- Vector w is **sparse**, if many entries are zero
  - **Efficiency**: If size(w) = 100 Billion, each prediction $w^T x$ is expensive:
    - If w is sparse, prediction computation only depends on number of non-zeros in w

$$\widehat{y}_i = \widehat{w}_{\text{LS}}^T x_i$$



$$= \sum_{j=1}^{d} \widehat{w}_{\text{LS}}[j] \times x_i[j] = \sum_{j:w_{\text{LS}}[j]\neq 0} \widehat{w}_{\text{LS}}[j] \times x_i[j]$$

Computational complexity decreases from $2d$ to $2k$ for k-sparse $\widehat{w}_{\text{LS}}$

Sparsity

$$\widehat{w}_{LS} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$$

- Vector w is **sparse**, if many entries are zero
  - **Interpretability**: What are the relevant features to make a prediction?

Lot size	Dishwasher
Single Family	Garbage disposal
Year built	Microwave
Last sold price	Range / Oven
Last sale price/sqft	Refrigerator
Finished sqft	Washer
Unfinished sqft	Dryer
Finished basement sqft	Laundry location
# floors	Heating type
Flooring types	Jetted Tub
Parking type	Deck
Parking amount	Fenced Yard
Cooling	Lawn
Heating	Garden
Exterior materials	Sprinkler System
Roof type	
Structure style	

- How do we find "best" subset of features useful in predicting the price among all possible combinations?

Finding best subset of features that explain the outcome/label: Exhaustive

- Try all subsets of size 1, 2, 3, … and one that minimizes validation error
  - Problem?
  - Any Ideas?

Finding best subset: Greedy

Forward stepwise:
Starting from simple model and iteratively add features most useful to fit

Forward Greedy

1: $T \leftarrow \emptyset$

2: **For** $j = 1, \ldots, k$ **do**

3: $j^* \leftarrow \arg\min_{\ell} \min_{w} \sum_{i=1}^{n} \left(y_i - \sum_{j \in T \cup \{\ell\}} w[j] \times x_i[j] \right)^2$

4: $T \leftarrow T \cup \{j^*\}$

Backward stepwise:
Start with full model and iteratively remove features least useful to fit

Combining forward and backward steps:
In forward algorithm, insert steps to remove features no longer as important

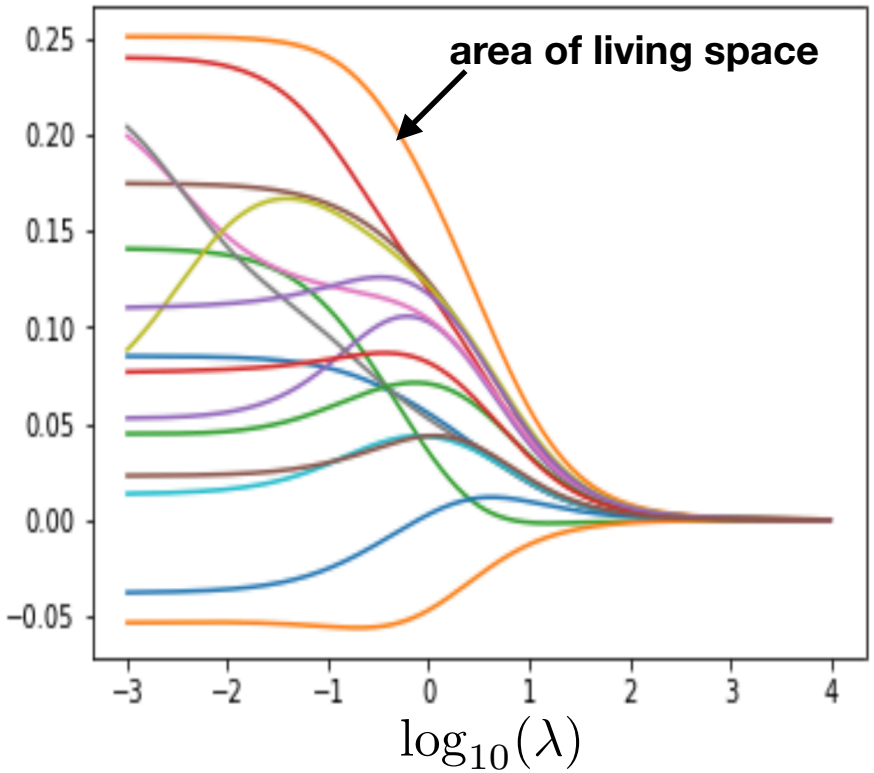
Lots of other variants, too.

Finding best subset: Regularize

Recall that Ridge regression makes coefficients small

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

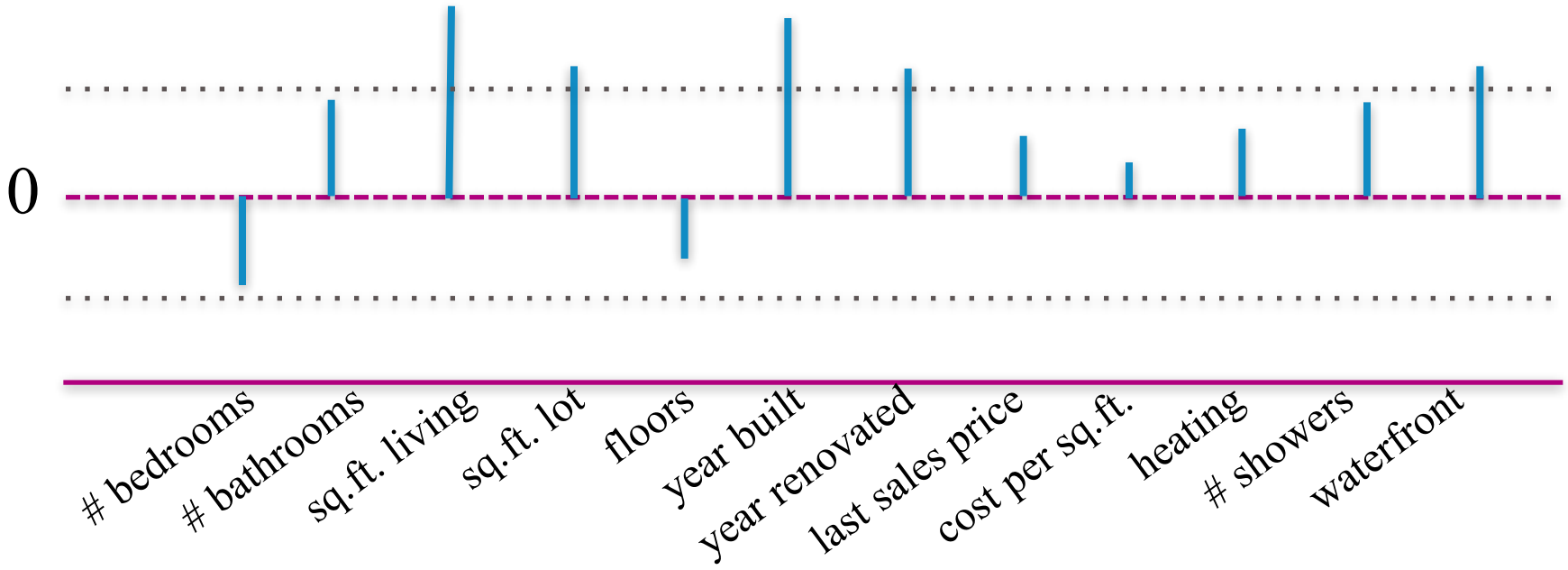
w_i's



Thresholded Ridge Regression

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

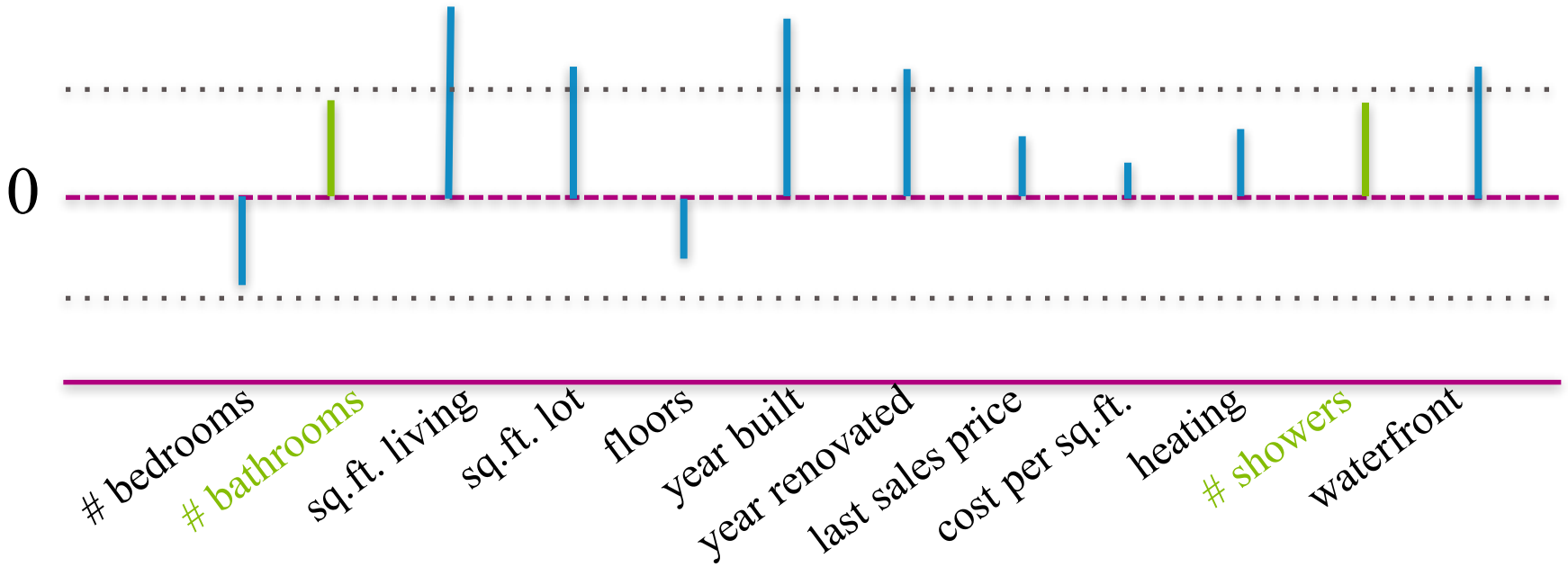
- Why don't we just set **small** ridge coefficients to 0?
  - Any issues?



Thresholded Ridge Regression

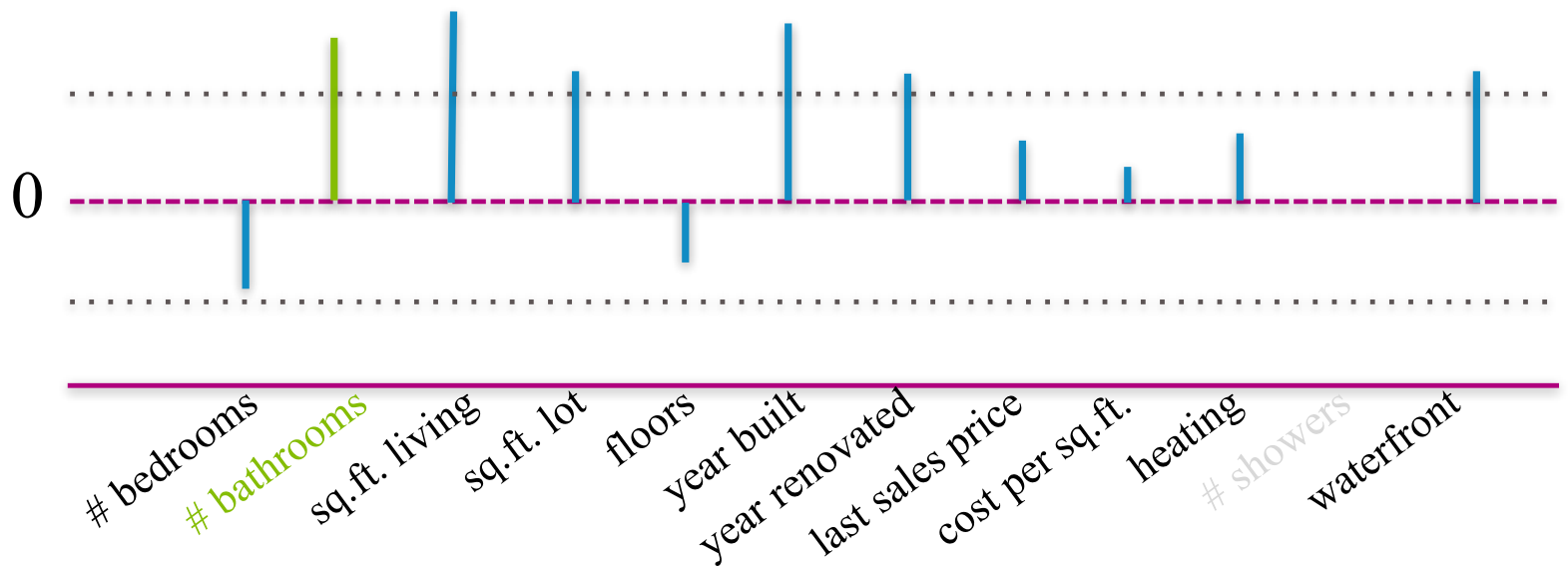
$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

- Consider two related features (bathrooms, showers)
- Consider $w[\text{bath}] = 1$ and $w[\text{shower}] = 1$, and
  $w[\text{bath}] = 2$ and $w[\text{shower}] = 0$,
  which one does ridge regression choose?
  (assuming #bathroom=#showers in every house)



Thresholded Ridge Regression

- What if we **didn't** include showers? Weight on bathrooms increases!
- We want a feature selection scheme that selects one of (#bathroom) or (#showers) automatically, using the fact that if you delete #showers #bathroo is an important feature

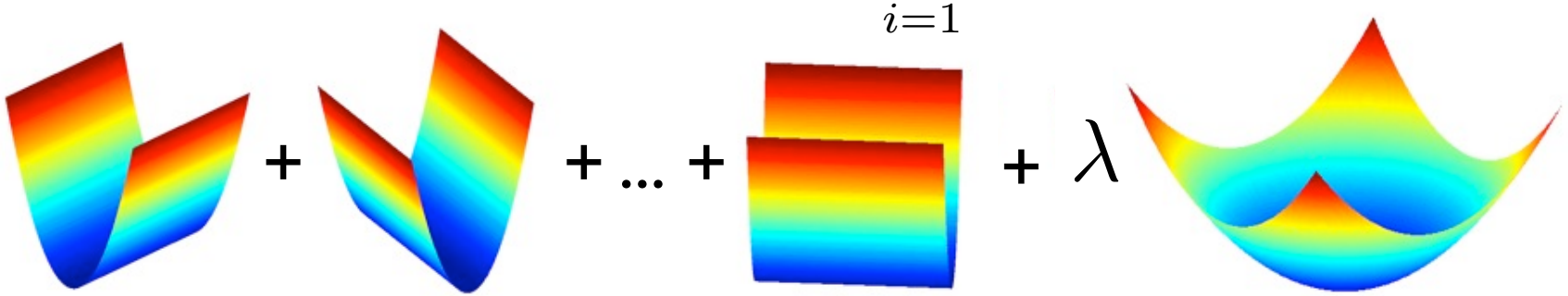


Can another regularizer perform selection automatically?

Ridge vs. Lasso Regression

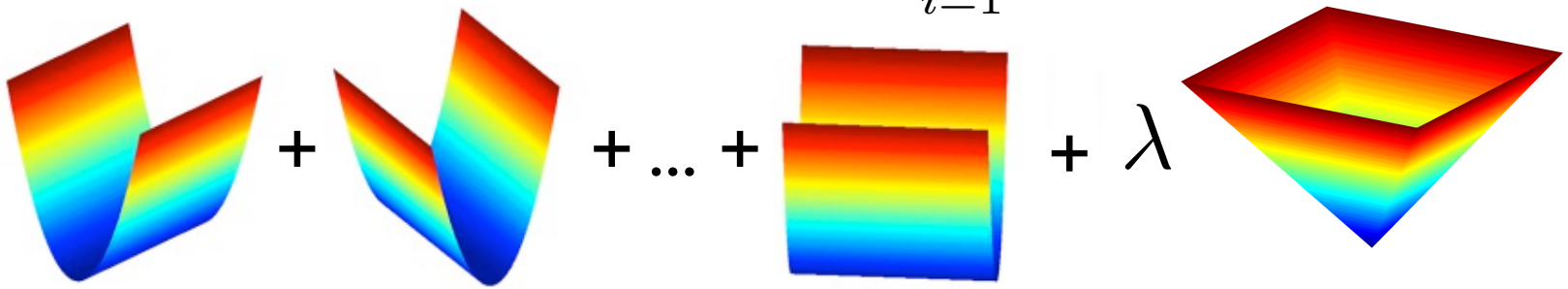
- Ridge Regression objective:

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$



- Lasso objective:

$$\widehat{w}_{lasso} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_1$$



Ridge vs. LASSO Regression

LASSO = Least Absolute Shrinkage and Selection Operator

- Recall Ridge Regression objective:

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

- sensitivity of a model w is measured in squared ℓ_2 norm $\|w\|_2^2$
- A principled method to get sparse model is **Lasso** with regularized objective:

$$\widehat{w}_{lasso} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_1$$

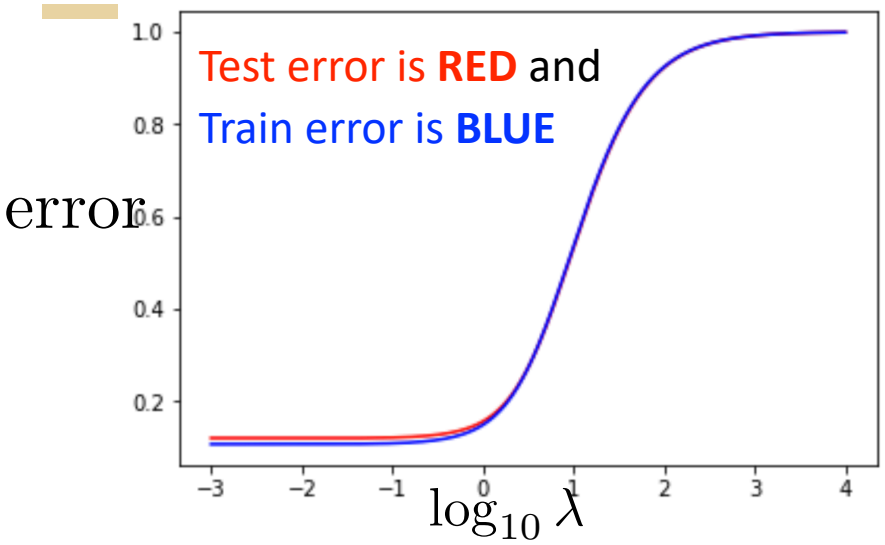
- sensitivity of a model w is measured in ℓ_1 norm:

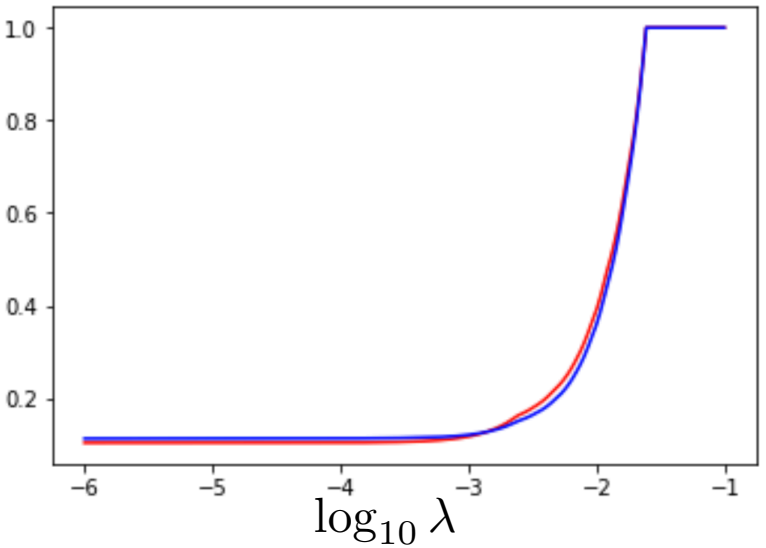
$$\|w\|_1 = \sum_{j=1}^{d} \left|w[j]\right|$$

ℓ_p-norm of a vector $w \in \mathbb{R}^d$ is

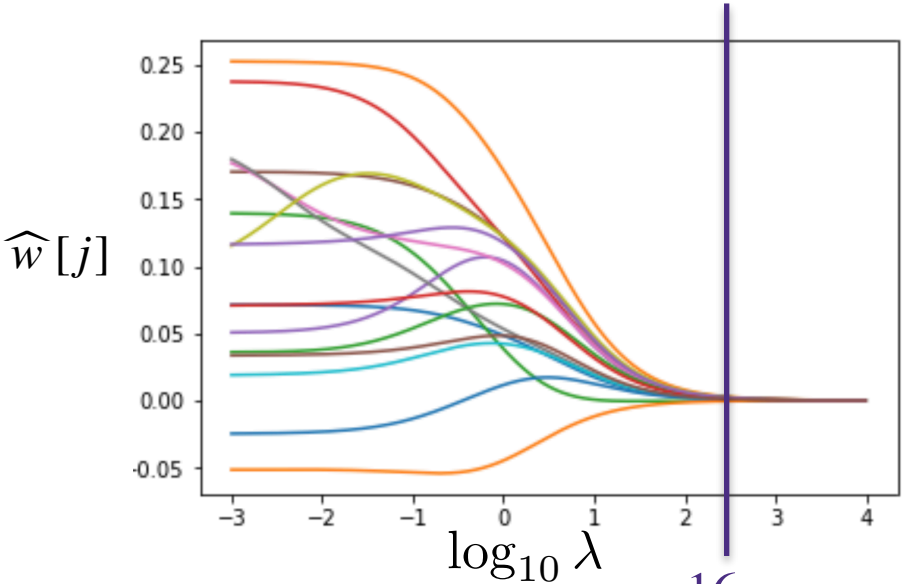
$$\|w\|_p \triangleq \left(\sum_{j=1}^{d} |w[j]|^p\right)^{1/p}$$

Example: house price with 16 features

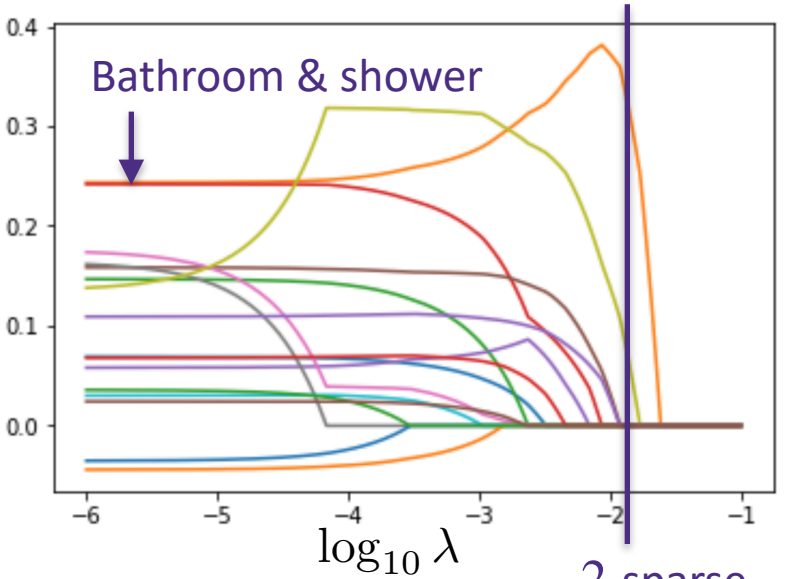




- Regularization path for LASSO shows that weights drop to exactly zero as λ increases



Ridge regression



Lasso regression

LASSO regression naturally gives sparse features

- ***Feature selection*** with LASSO regression
  1. **Model selection**: choose λ based on cross validation error
  2. **Feature selection**: keep only those features with non-zero (or not-too-small) parameters in w at optimal λ
  3. **retrain** with the sparse model and $\lambda = 0$

  why do we need to retrain?

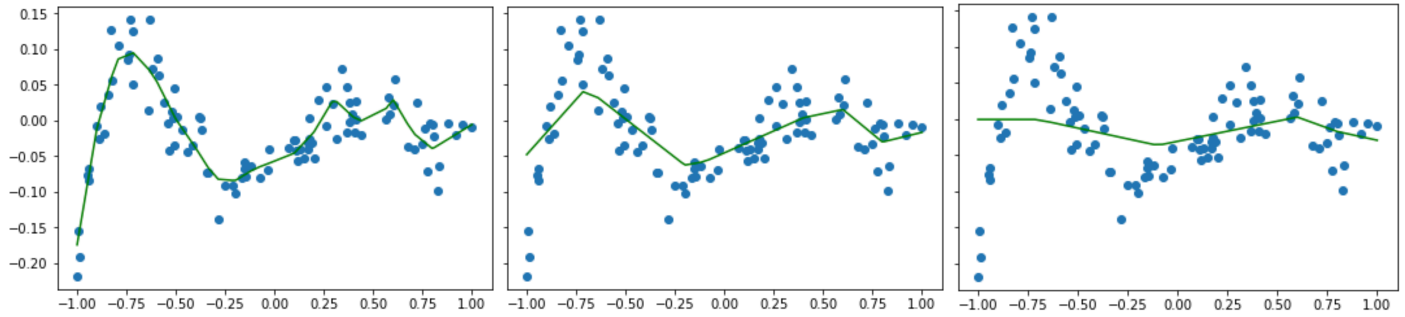
Example: piecewise-linear fit

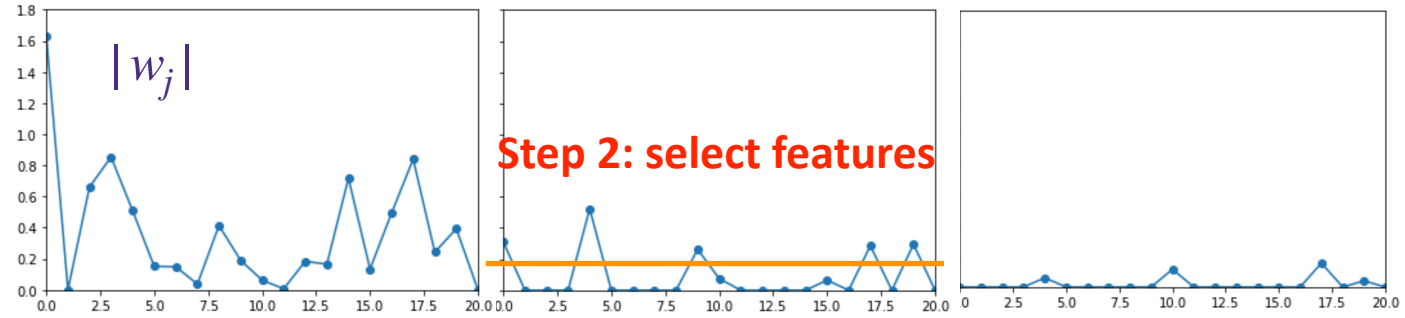
$$h_0(x) = 1$$
$$h_i(x) = [x + 1.1 - 0.1i]^+$$

- We use LASSO on the piece-wise linear example

Step 1: find optimal λ^*

$$\text{minimize}_w \quad \mathscr{L}(w) + \lambda \|w\|_1$$





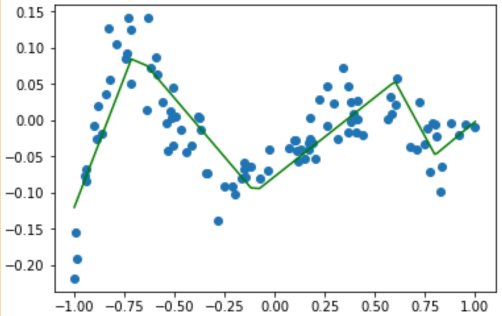
Step 2: select features

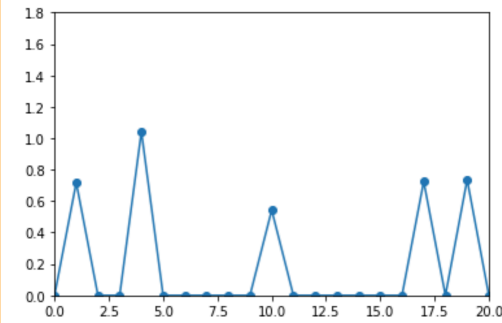
$\lambda = 10^{-8}$ $\lambda = 10^{-4}$ $\lambda = 2 \times 10^{-4}$

- de-biasing (via re-training) is critical!

Step 3: retrain

$$\text{minimize}_w \quad \mathscr{L}(w)$$





$\lambda = 0$

but only use selected features

Regularized Least Squares

$$\text{Ridge} : r(w) = ||w||_2^2 \qquad \text{Lasso} : r(w) = ||w||_1$$

$$\widehat{w}_r = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda r(w)$$

Regularized Least Squares

- Regularized optimization:

$$\hat{w}_r = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda r(w)$$

$$\text{Ridge} : r(w) = ||w||_2^2$$
$$\text{Lasso} : r(w) = ||w||_1$$

- For any $\lambda^* \geq 0$ for which $\hat{w}_r$ achieves the minimum, there exists a $\mu^* \geq 0$ such that the solution of the constrained optimization, $\widehat{w}_c$, is the same as the solution of the regularized optimization , $\widehat{w}_r$, where

$$\widehat{w}_C = \arg\min_w \sum_{i=1}^{n} (y_i - x_i^T w)^2 \qquad \text{subject to } r(w) \leq \mu^*$$

- so there are pairs of (λ, μ) whose optimal solution $\widehat{w}_r$ are the same for the regularizes optimization and constrained optimization

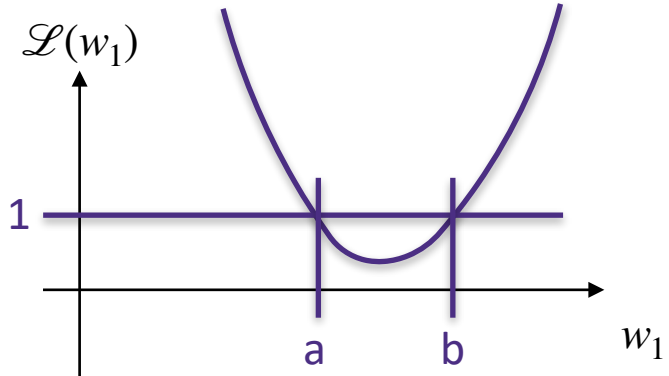
Why does LASSO give sparse solutions?

$$\text{minimize}_w \quad \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

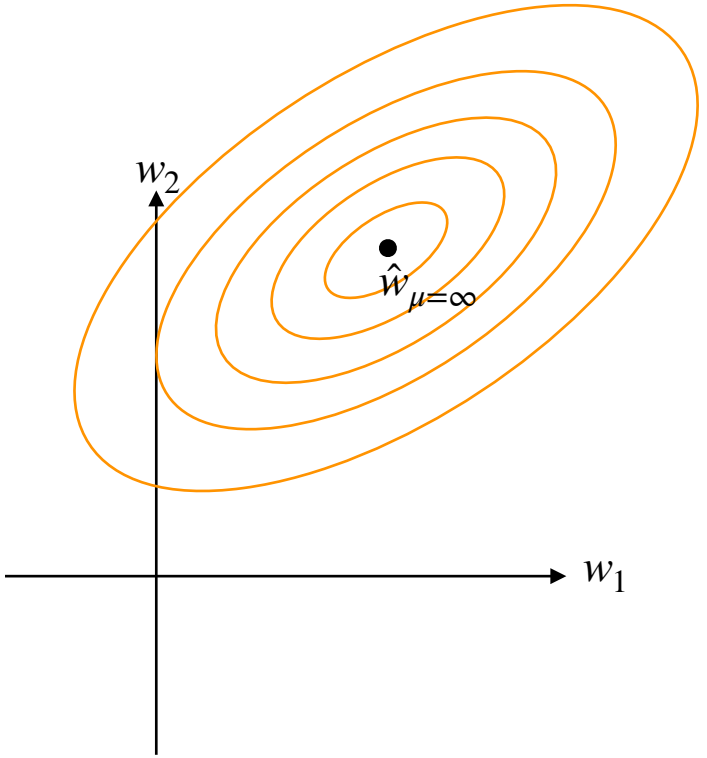
$$\text{subject to} \quad \|w\|_1 \leq \mu$$

- the ***level set*** of a function $\mathscr{L}(w_1, w_2)$ is defined as the set of points (w_1, w_2) that have the same function value
- the level set of a quadratic function is an oval
- the center of the oval is the least squares solution $\hat{w}_{\mu=\infty} = \hat{w}_{\text{LS}}$

1-D example with quadratic loss



Level set of $\mathscr{L}(w_1)$ at value 1 is {a,b}



Why does Lasso give sparse solutions?

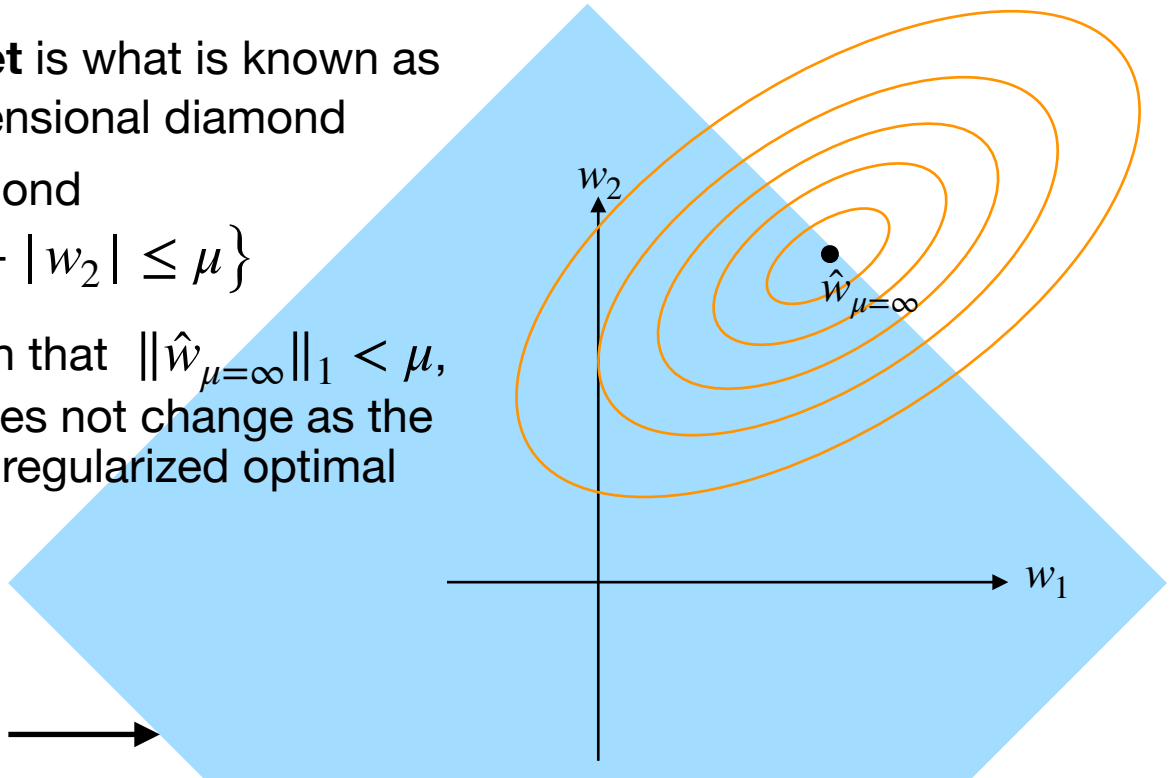
$$\text{minimize}_w \quad \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

$$\text{subject to} \quad \|w\|_1 \leq \mu$$

- as we decrease μ from infinity, the feasible set becomes smaller
- the shape of the **feasible set** is what is known as L_1 ball, which is a high dimensional diamond
- In 2-dimensions, it is a diamond

$$\{(w_1, w_2) \mid |w_1| + |w_2| \leq \mu\}$$

- when μ is large enough such that $\|\hat{w}_{\mu=\infty}\|_1 < \mu$, then the optimal solution does not change as the feasible set includes the un-regularized optimal solution



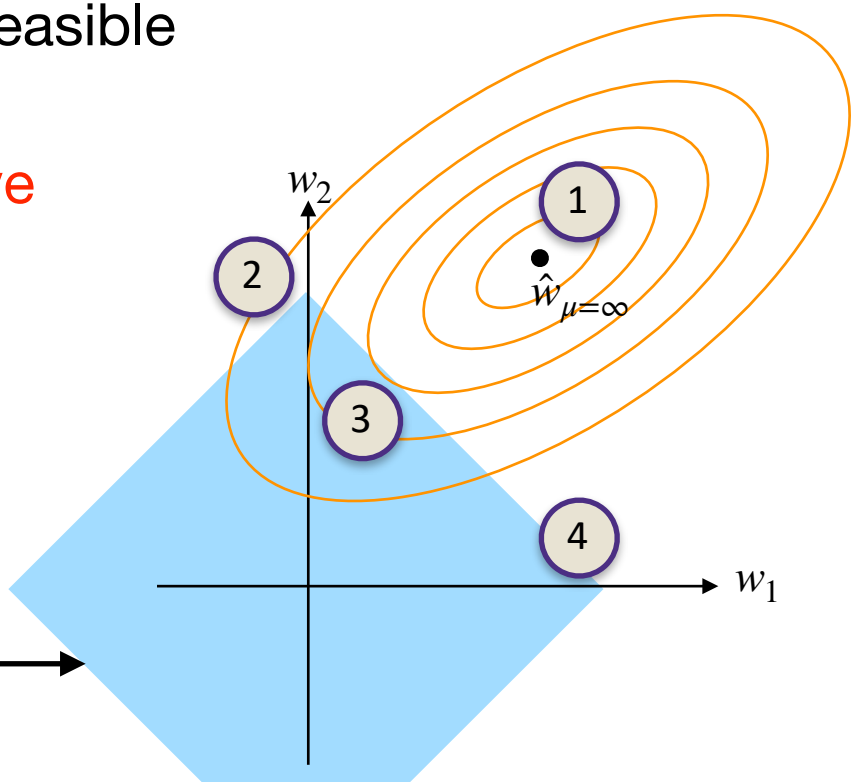
feasible set: $\{w \in \mathbb{R}^2 \mid \|w\|_1 \leq \mu\}$ ⟶

Why does Lasso give sparse solutions?

$$\text{minimize}_w \quad \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

$$\text{subject to} \quad \|w\|_1 \leq \mu$$

- As μ decreases (which is equivalent to increasing regularization λ) the feasible set (blue diamond) shrinks
- The optimal solution of the above optimization is ?



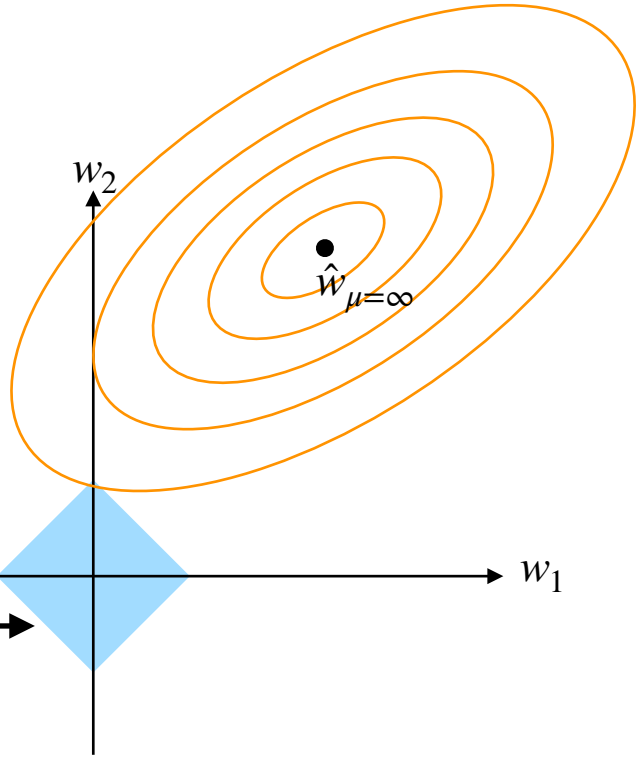
feasible set: $\{w \in \mathbb{R}^2 \mid \|w\|_1 \leq \mu\}$

Why does Lasso give sparse solutions?

$$\text{minimize}_w \quad \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

$$\text{subject to} \quad \|w\|_1 \leq \mu$$

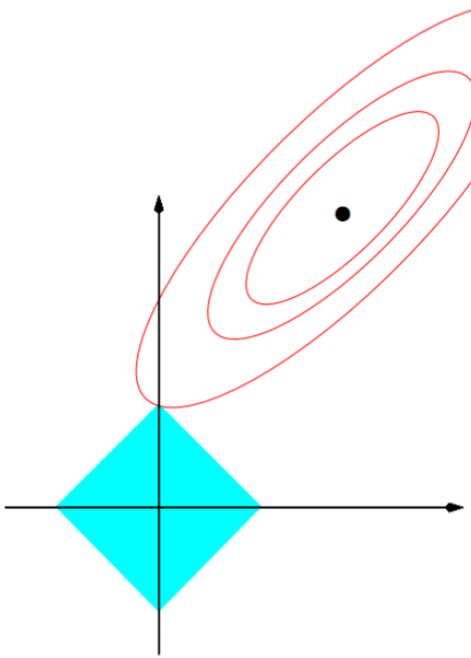
- For small enough μ, the optimal solution becomes **sparse**
- This is because the L_1-ball is "pointy",i.e., has sharp edges aligned with the axes

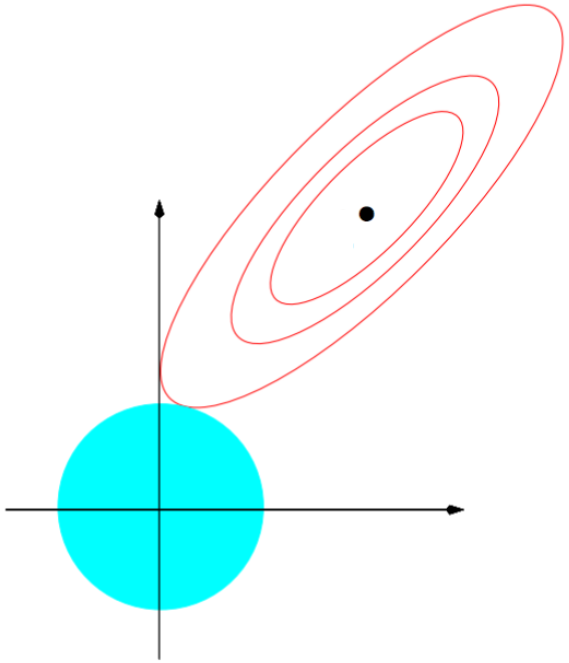


feasible set: $\{w \in \mathbb{R}^2 \mid \|w\|_1 \leq \mu\}$

Constrained Least Squares

- LASSO regression finds sparse solutions, as L_1-ball is "pointy"
- Ridge regression finds dense solutions, as L_2-ball is "smooth"





$$\text{minimize}_w \sum_{i=1}^{n} (w^T x_i - y_i)^2 \quad \text{subject to} \quad \|w\|_1 \leq \mu$$

$$\text{minimize}_w \sum_{i=1}^{n} (w^T x_i - y_i)^2 \quad \text{subject to} \quad \|w\|_2^2 \leq \mu$$

L1 Ball in Higher Dimensions

> L1 ball 3 dimensions