Ridge Regression:

Regulating overfitting when using many features

CS229: Machine Learning

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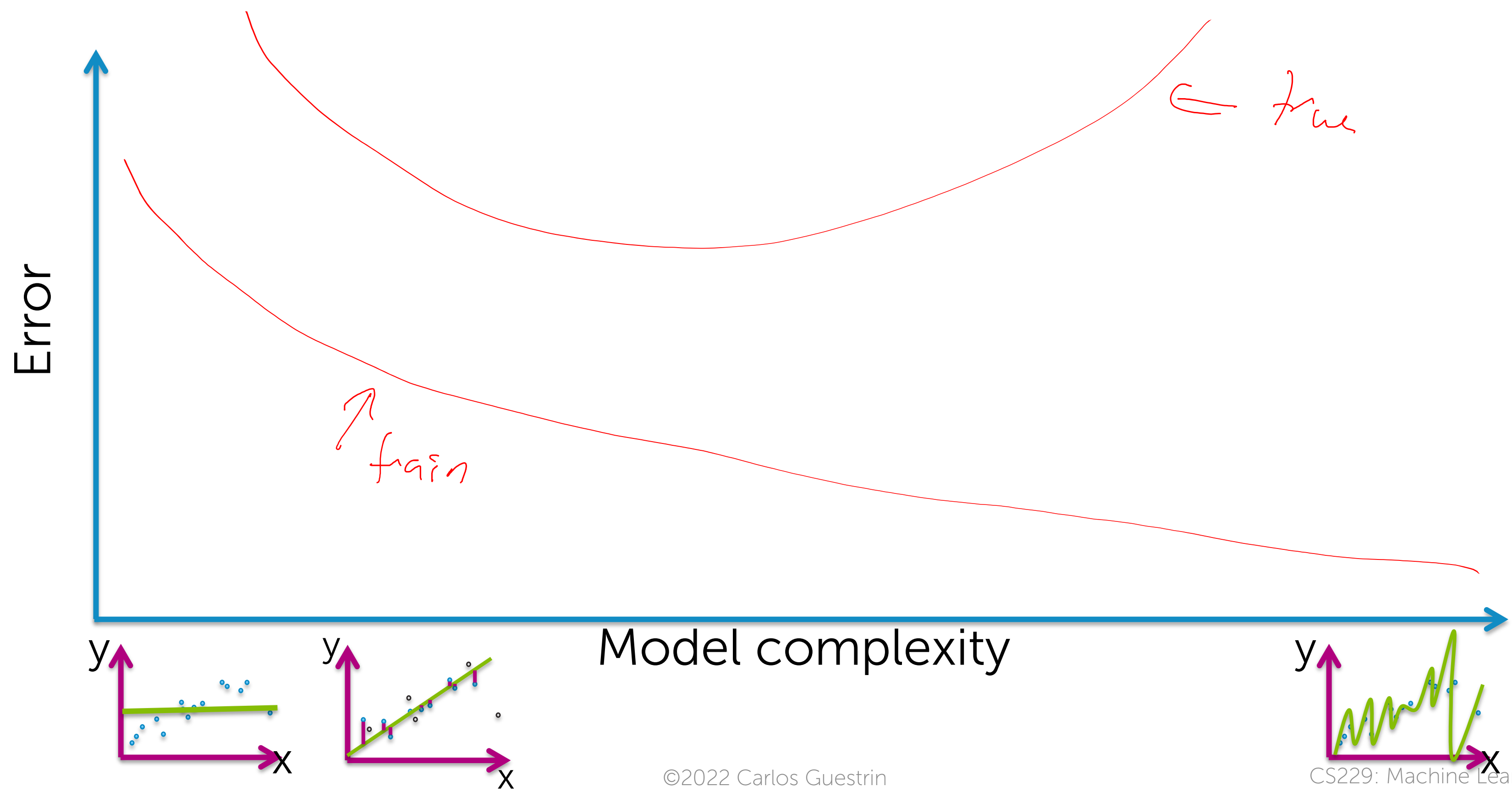
Slides include content developed by and co-developed with Emily Fox

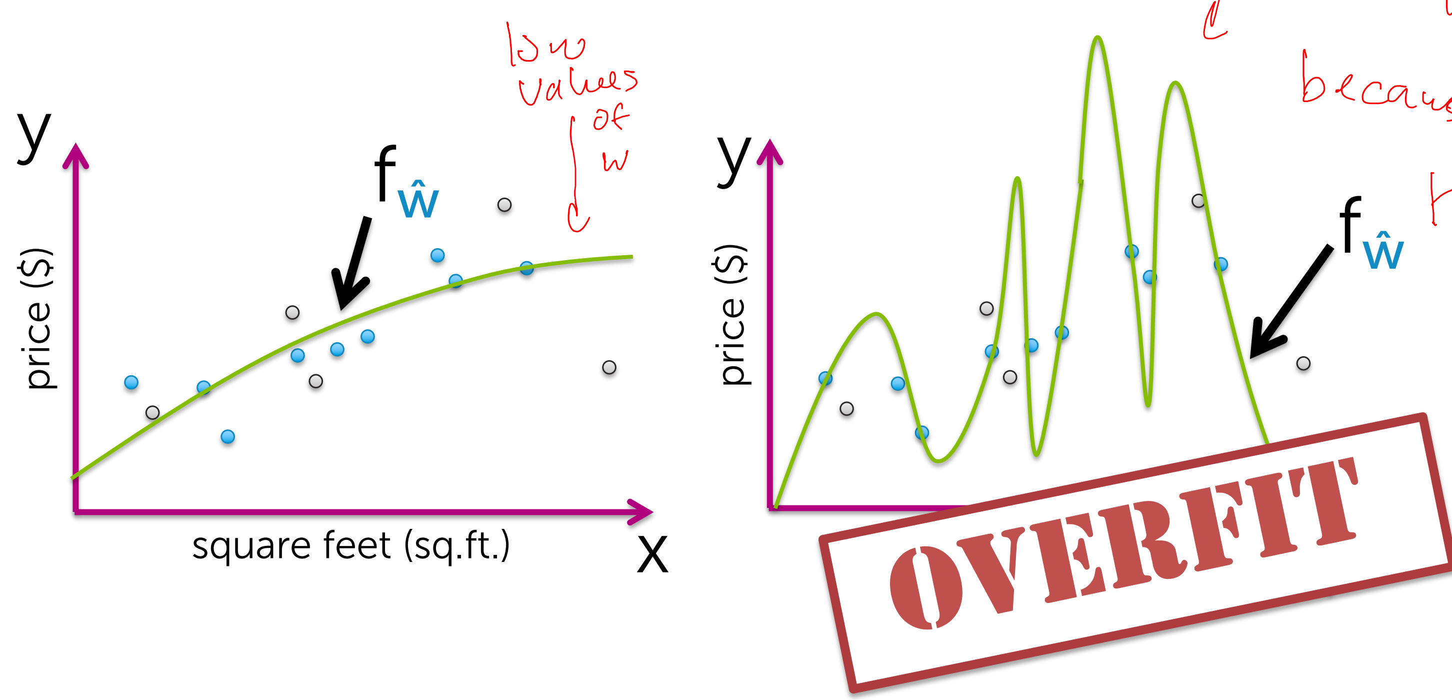
Training, true vs. model complexity



Overfitting of polynomial regression

Flexibility of high-order polynomials

$$y_i = w_0 + w_1 x_i + w_2 x_i^2 + \ldots + w_p x_i^p + \varepsilon_i$$

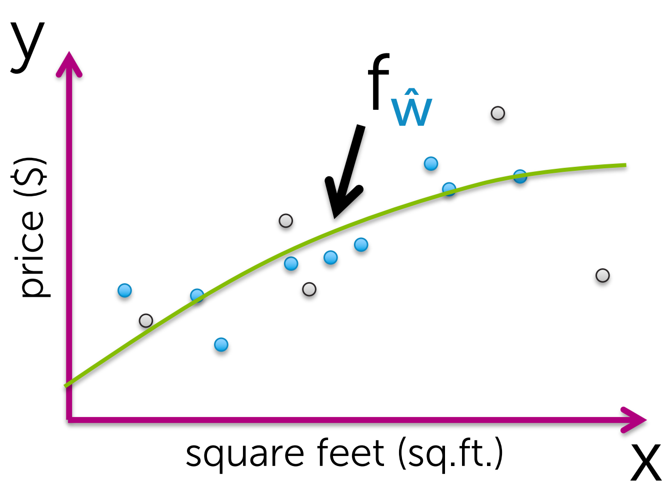


large values of w, because of high curvature

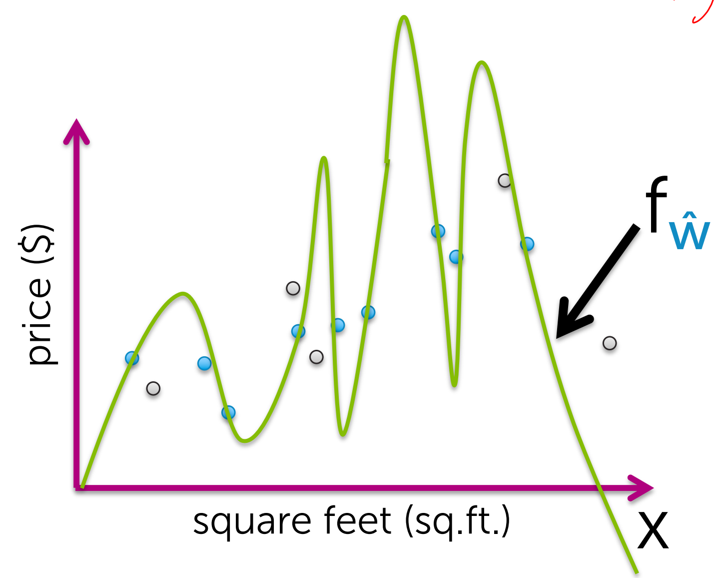
Symptom of overfitting

Often, overfitting associated with very large estimated parameters $\hat{w}$

$||\hat{w}||$ is low

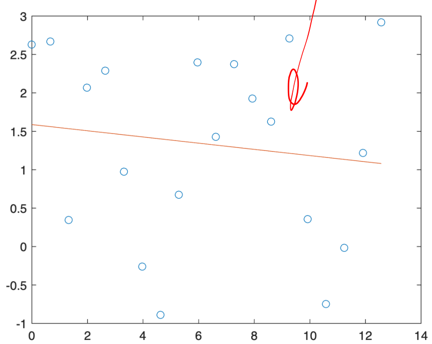


$||\hat{w}||$ is high



Polynomial fit example

bad fit

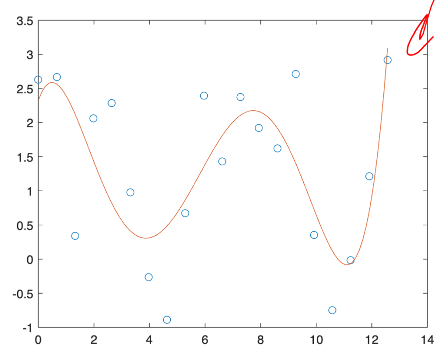


w0 = −0.0403609   w1 = 1.58766

~~Fer~~

small

good fit

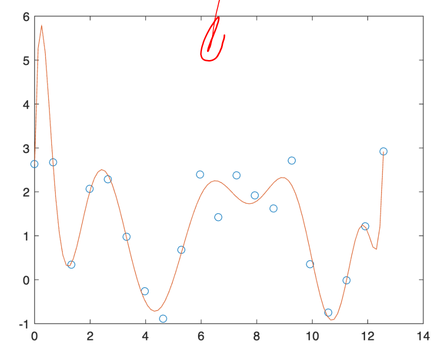


w0 = 0.00142109   w1 = −0.0412048   w2 = 0.402433

w3 = −1.45804   w4 = 1.16305   w5 = 2.32569

reasonable

bad fit



w0 = −3.33355e-09   w1 = 3.24407e-07   w2 = −1.3957e-05   w3 = 0.000351859   w4 = −0.00580734

w5 = 0.0664276   w6 = −0.543967   w7 = 3.24647   w8 = −14.1922   w9 = 44.8987   w10 = −98.886

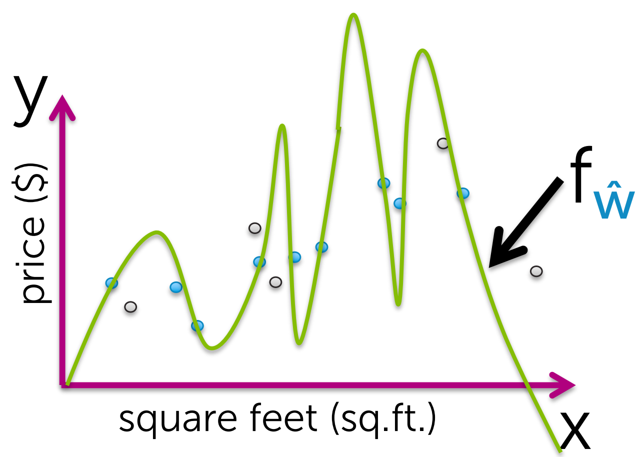
w11 = 139.912   w12 = −109.084   w13 = 32.5699   w14 = 2.62986

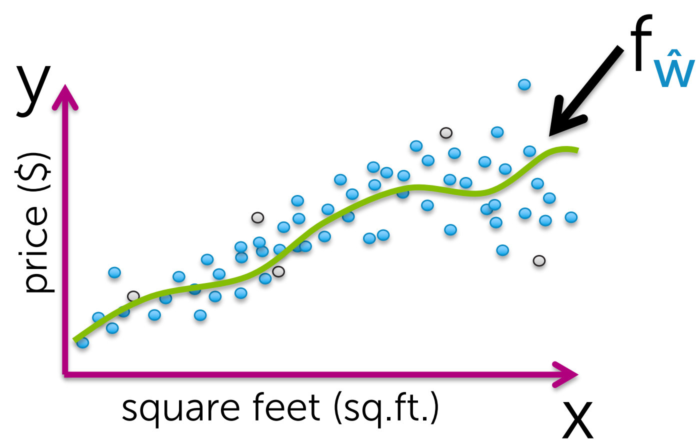
large

How does # of observations influence overfitting?

Few observations (N small)
→ rapidly overfit as model complexity increases

Many observations (N very large)
→ harder to overfit





Overfitting of linear regression models more generically

Overfitting with many features

Not unique to polynomial regression,
but also if **lots of inputs** (d large)

Or, generically,
lots of features (D large)

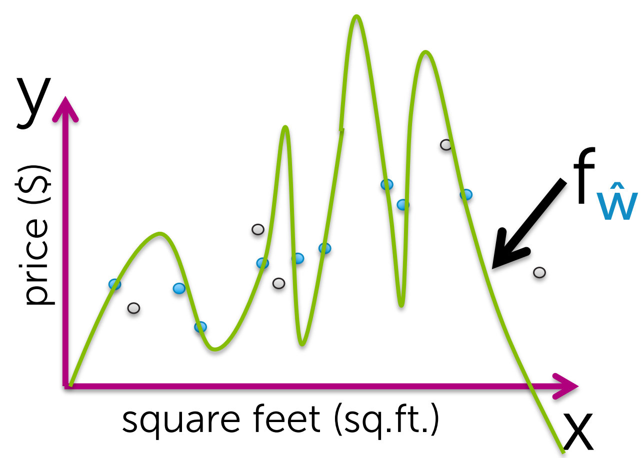
$$y = \sum_{j=0}^{D} w_j h_j(\mathbf{x}) + \varepsilon$$

- Square feet
- # bathrooms
- # bedrooms
- Lot size
- Year built
- ...

How does # of inputs influence overfitting?

1 input (e.g., sq.ft.):

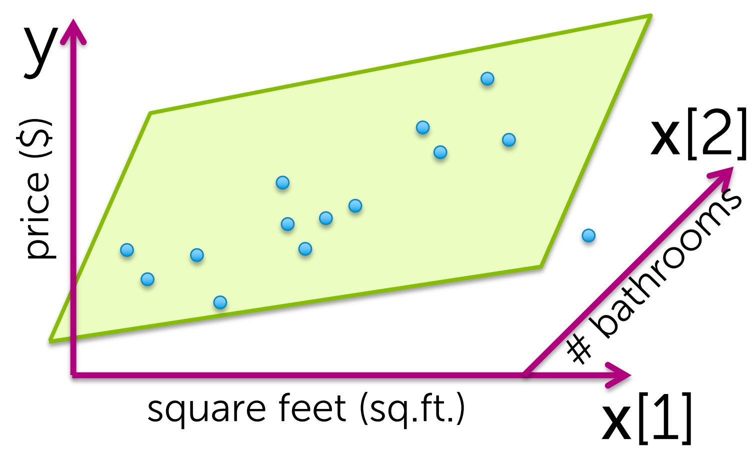
Data must include representative examples of all possible (sq.ft., $) pairs to avoid overfitting



How does # of inputs influence overfitting?

d inputs (e.g., sq.ft., #bath, #bed, lot size, year,…):

Data must include examples of all possible (sq.ft., #bath, #bed, lot size, year,…., $) combos to avoid overfitting



Regularization:
Adding term to cost-of-fit
to prefer small coefficients

Desired total cost format

Want to balance:

i. How well function fits data

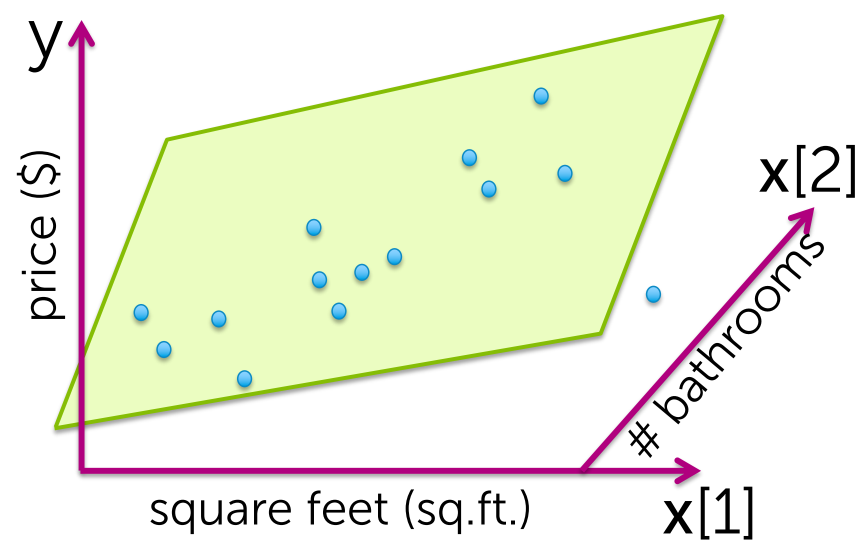
ii. Magnitude of coefficients

Total cost =

$$\underbrace{\text{measure of fit}}_{\text{e.g., RSS}} + \underbrace{\text{measure of magnitude of coefficients}}_{\text{penalty for large parameter values}}$$

force me to find simpler models

Measure of fit to training data



$$\mathrm{RSS}(\mathbf{w}) = \sum_{i=1}^{N} (y_i - h(\mathbf{x}_i)^T \mathbf{w})^2$$

Measure of magnitude of regression coefficient

What summary # is indicative of size of regression coefficients?

– Sum? $w_0 + w_1 + w_2 + \dots$ typically bad idea!! (negative w)

– Sum of absolute value? $||w||_1 = |w_0| + |w_1| + |w_2| + \dots$ (Lasso)

– **Sum of squares (L_2 norm)**

$||w||_2^2 = w_0^2 + w_1^2 + w_2^2 + \dots$ (ridge regression)

Consider specific total cost

Total cost =

measure of fit + measure of magnitude of coefficients

$RSS(w) \quad + \quad \lambda \quad \|w\|_2^2$

magic tradeoff parameter

Ridge Regression (aka L_2 regularization)

What if $\hat{w}$ selected to minimize

$$RSS(w) + \lambda \; ||w||_2^2$$

If λ=0: $\hat{w}_{ridge} = \hat{w}_{RSS}$

If λ=∞: $\hat{w}_{ridge} = 0$

If λ in between: $||\hat{w}_{ridge}||_2^2 < ||w_{RSS}||_2^2$

Bias-variance tradeoff

Large λ:

high bias, low variance

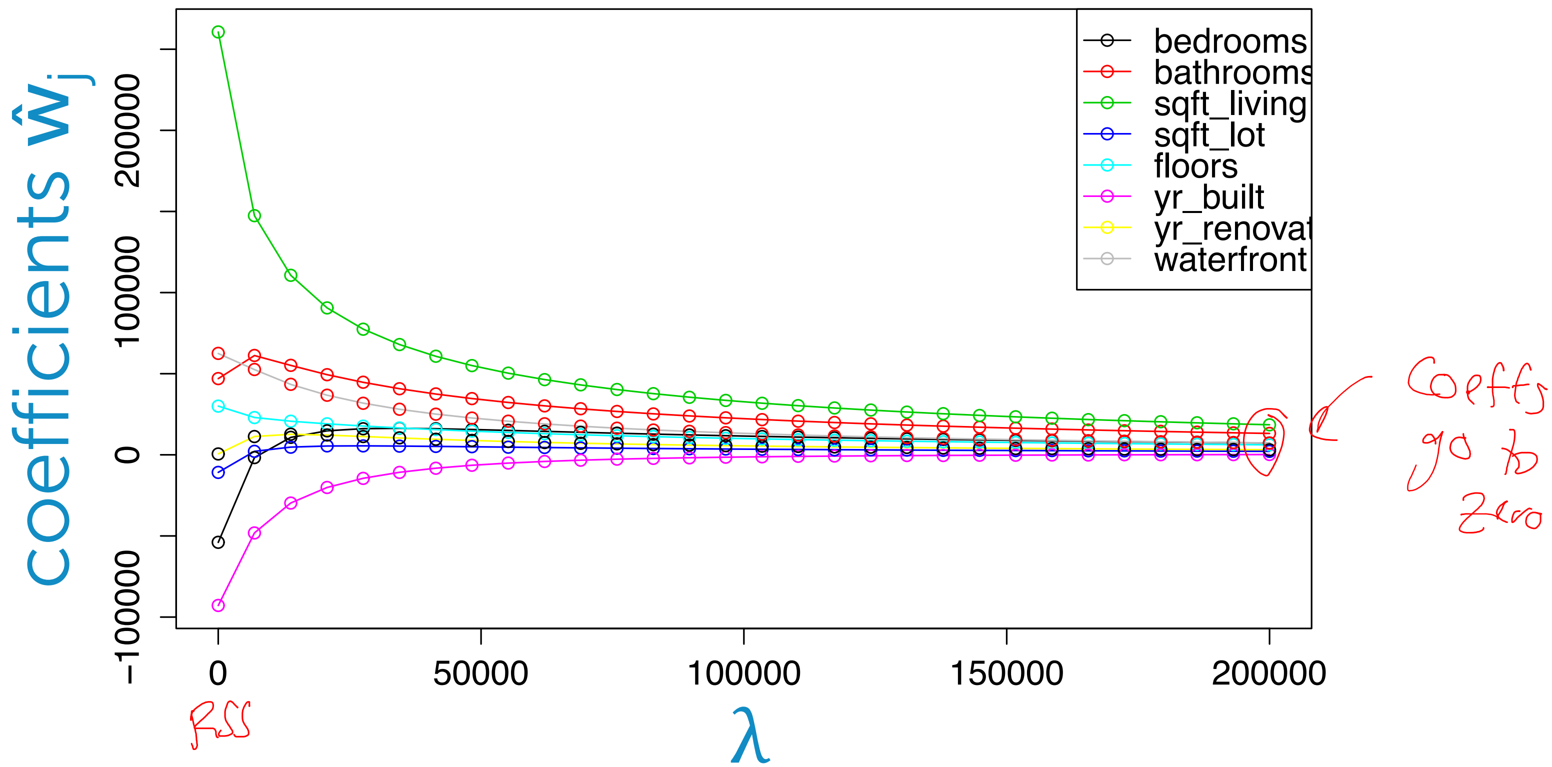
(e.g., $\hat{w} = 0$ for $\lambda = \infty$)

Small λ:

low bias, high variance

(e.g., standard least squares (RSS) fit of high-order polynomial for $\lambda = 0$)

Coefficient path



How to choose λ

The regression/ML workflow

1. **Model selection**
   Need to choose tuning parameters λ controlling model complexity

   choose λ

2. **Model assessment**
   Having selected a model, assess generalization error

Hypothetical implementation 1

1. **Model selection**

For each considered λ :

i. Estimate parameters $\hat{w}_\lambda$ on **training data**
ii. Assess performance of $\hat{w}_\lambda$ on **training data**
iii. Choose λ^* to be λ with lowest train error

2. **Model assessment**

Compute test error of $\hat{w}_{\lambda^*}$ (fitted model for selected λ^*) to approx. true error

Hypothetical implementation 1

Issue: Both λ and $\hat{w}$ selected on training data then $\lambda^* = 0$

- λ^* was selected to minimize training error (i.e., λ^* was fit on training data)
- Most complex model will have lowest training error

Hypothetical implementation 2

1. **Model selection**

For each considered λ :

i. Estimate parameters $\hat{w}_\lambda$ on **training data**
ii. Assess performance of $\hat{w}_\lambda$ on **test data**
iii. Choose λ^* to be λ with lowest test error

2. **Model assessment**

Compute test error of $\hat{w}_{\lambda^*}$ (fitted model for selected λ^*) to approx. true error

Hypothetical implementation 2

Issue: Just like fitting $\hat{w}$ and assessing its performance both on training data

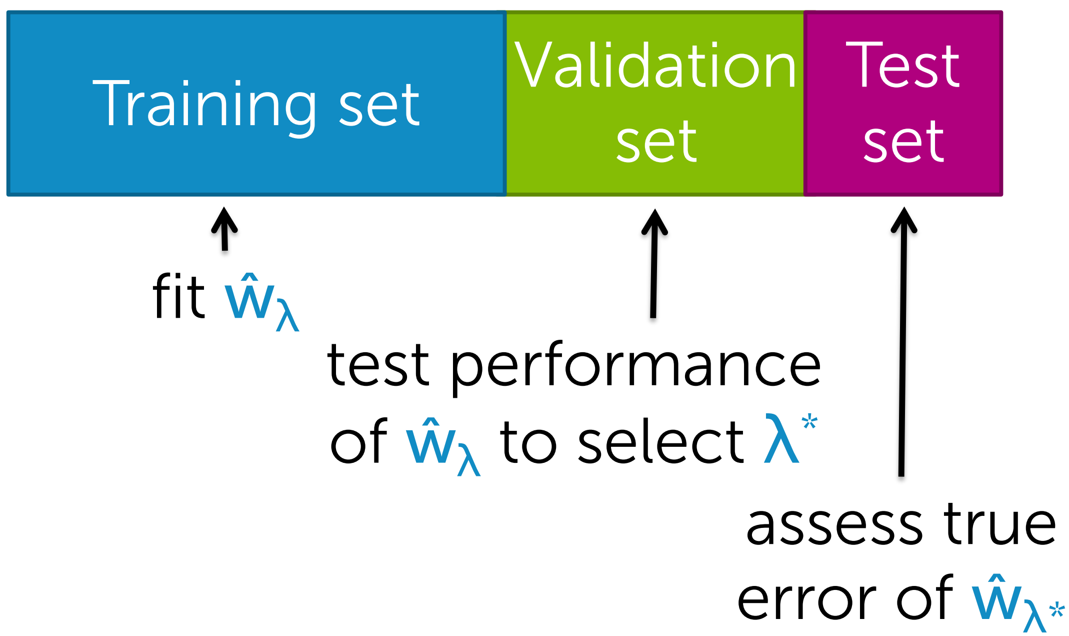
- λ^* was selected to minimize test error (i.e., λ^* was fit on test data)
- If test data is not representative of the whole world, then $\hat{w}_{\lambda^*}$ will typically perform worse than test error indicates

Practical implementation

Solution: Create two "test" sets!

1. Select λ^* such that $\hat{w}_{\lambda^*}$ minimizes error on validation set
2. Approximate true error of $\hat{w}_{\lambda^*}$ using test set

Practical implementation



Feature normalization

Normalizing features

Scale training **columns** (not rows!) as:

$$\underline{h}_j(x_k) = \frac{h_j(x_k)}{\boxed{\sqrt{\sum_{i=1}^{N} h_j(x_i)^2}}}$$

Normalizer:
z_j

Apply same training scale factors to test data:

$$\underline{h}_j(x_k) = \frac{h_j(x_k)}{\boxed{\sqrt{\sum_{i=1}^{N} h_j(x_i)^2}}}$$

Normalizer:
z_j

apply to
test point

summing over training points

Summary for ridge regression

What you can do now…

- Describe what happens to magnitude of estimated coefficients when model is overfit
- Motivate form of ridge regression cost function
- Describe what happens to estimated coefficients of ridge regression as tuning parameter λ is varied
- Interpret coefficient path plot
- Use a validation set to select the ridge regression tuning parameter λ
- Handle intercept and scale of features with care