

Ridge Regression:

Regulating overfitting when
using many features

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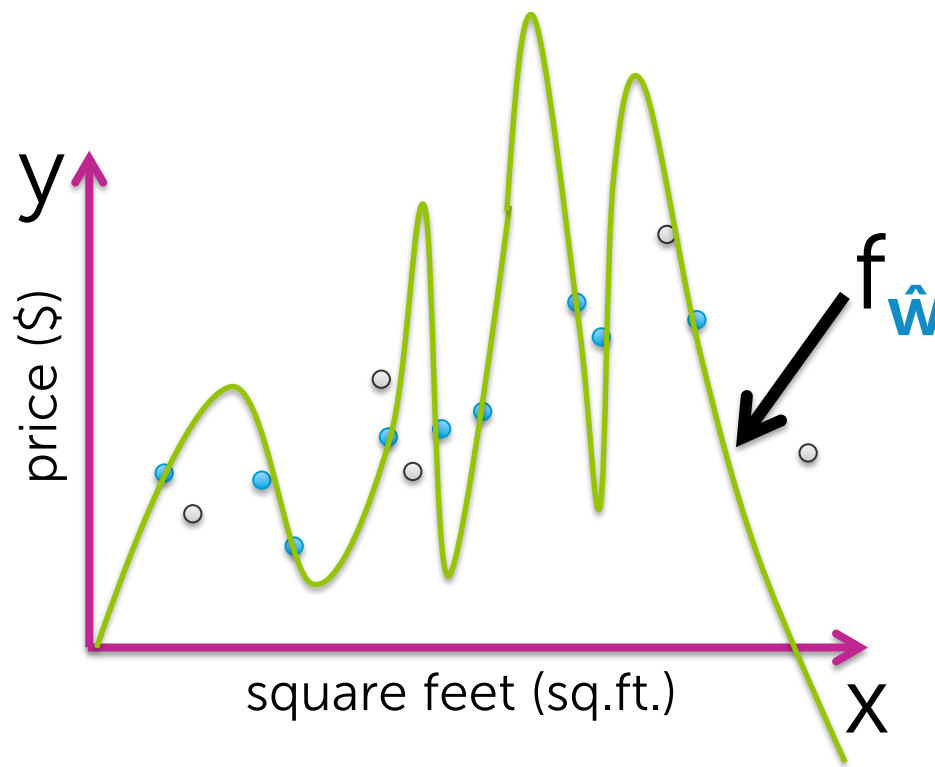
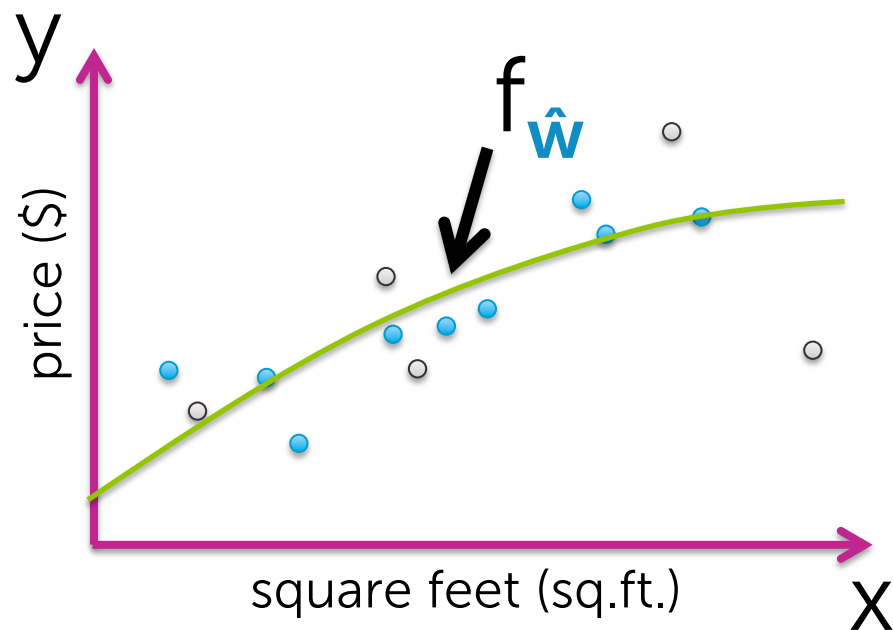
Machine Learning Specialization

University of Washington

Overfitting of polynomial regression

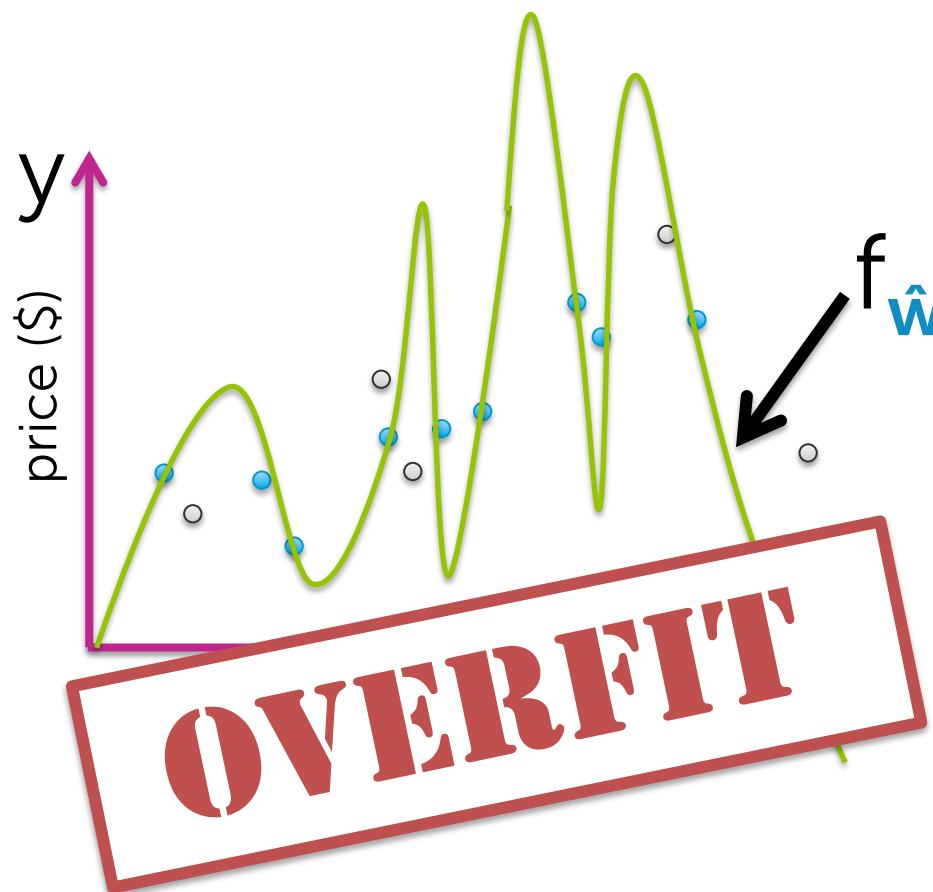
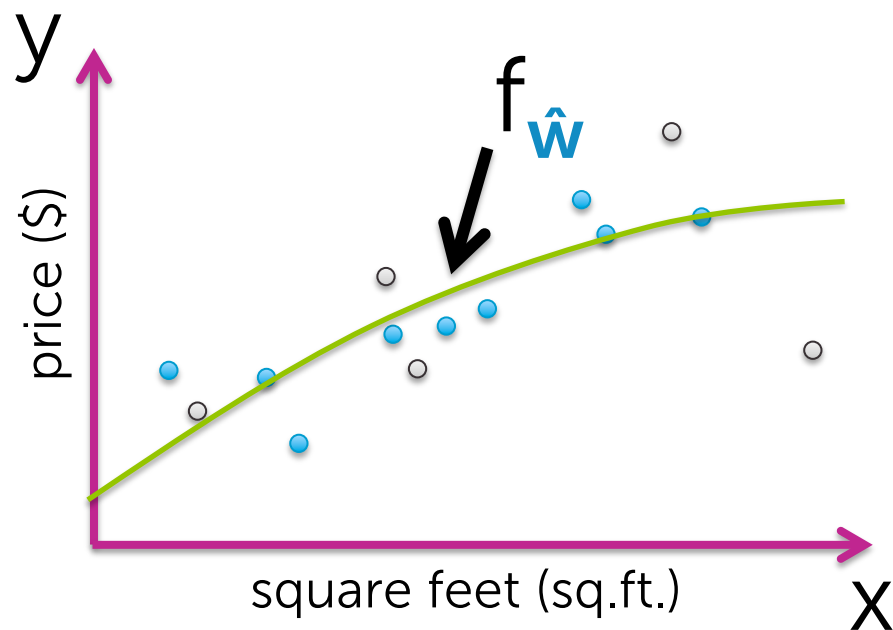
Flexibility of high-order polynomials

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



Flexibility of high-order polynomials

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Symptom of overfitting

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

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**)

$$y_i = \sum_{j=0}^D \mathbf{w}_j h_j(\mathbf{x}_i) + \epsilon_i$$

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

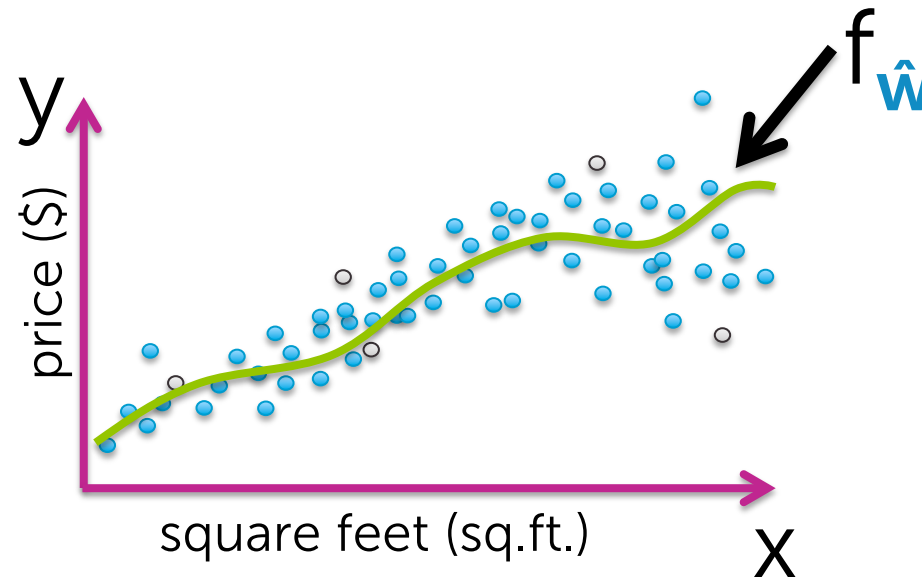
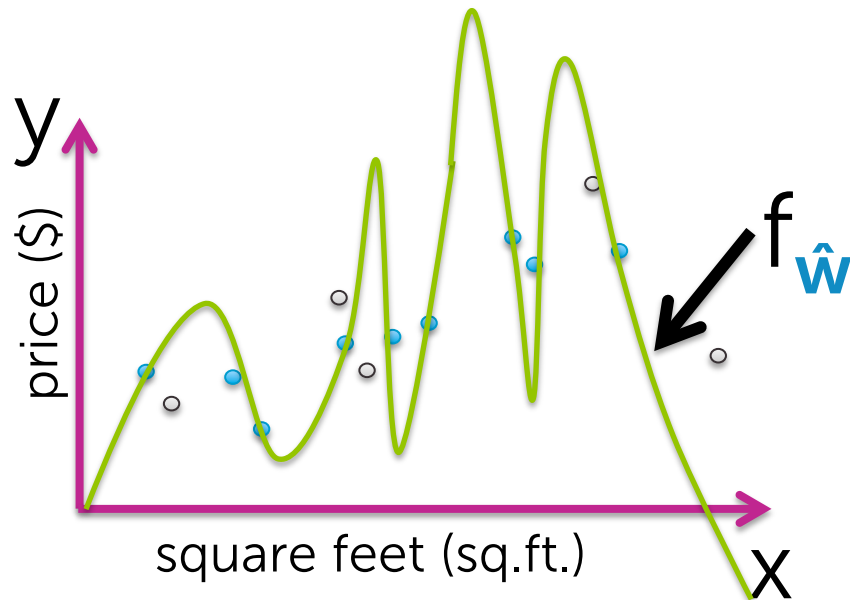
How does # of observations influence overfitting?

Few observations (N small)

→ rapidly overfit as model complexity increases

Many observations (N very large)

→ harder to overfit

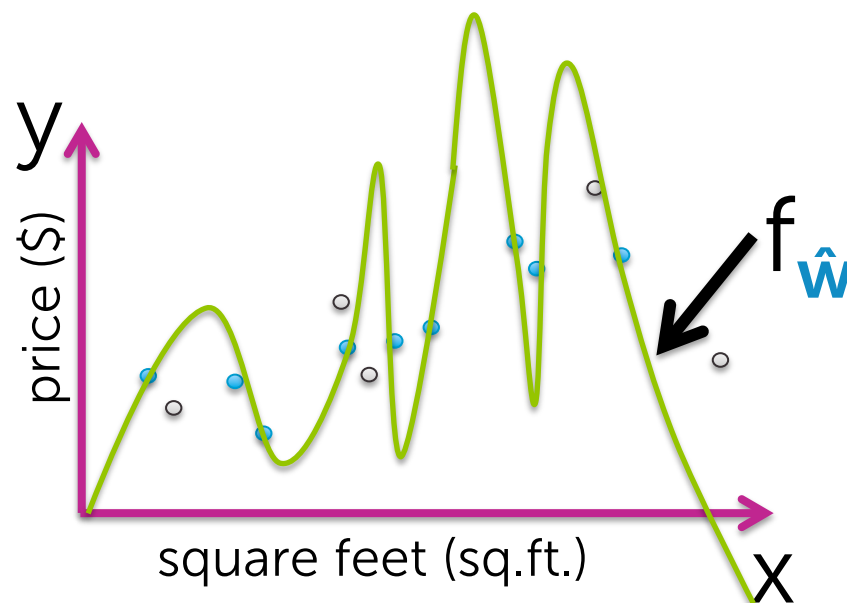


How does # of inputs influence overfitting?

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

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

HARD

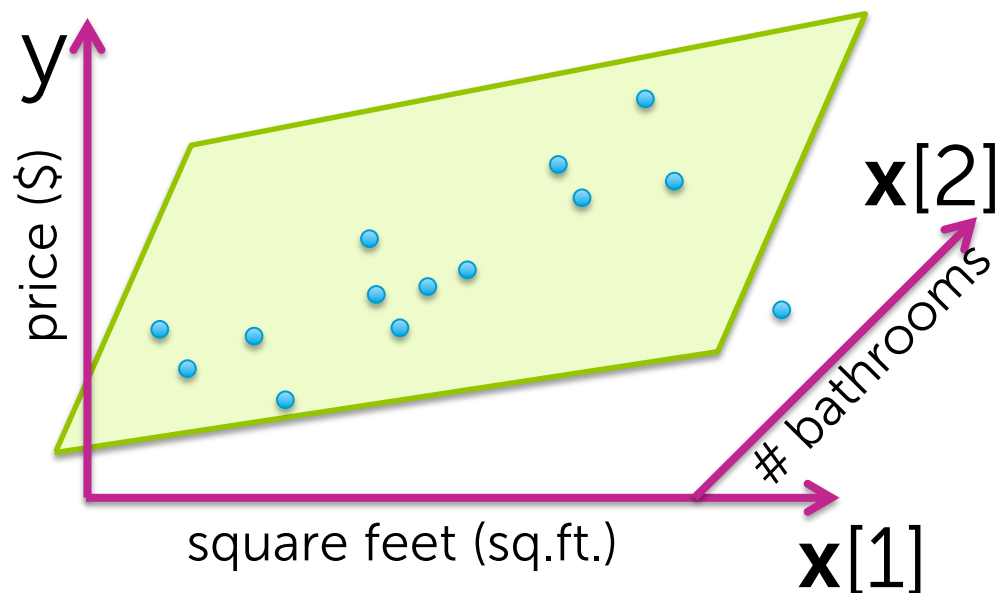


How does # of inputs influence overfitting?

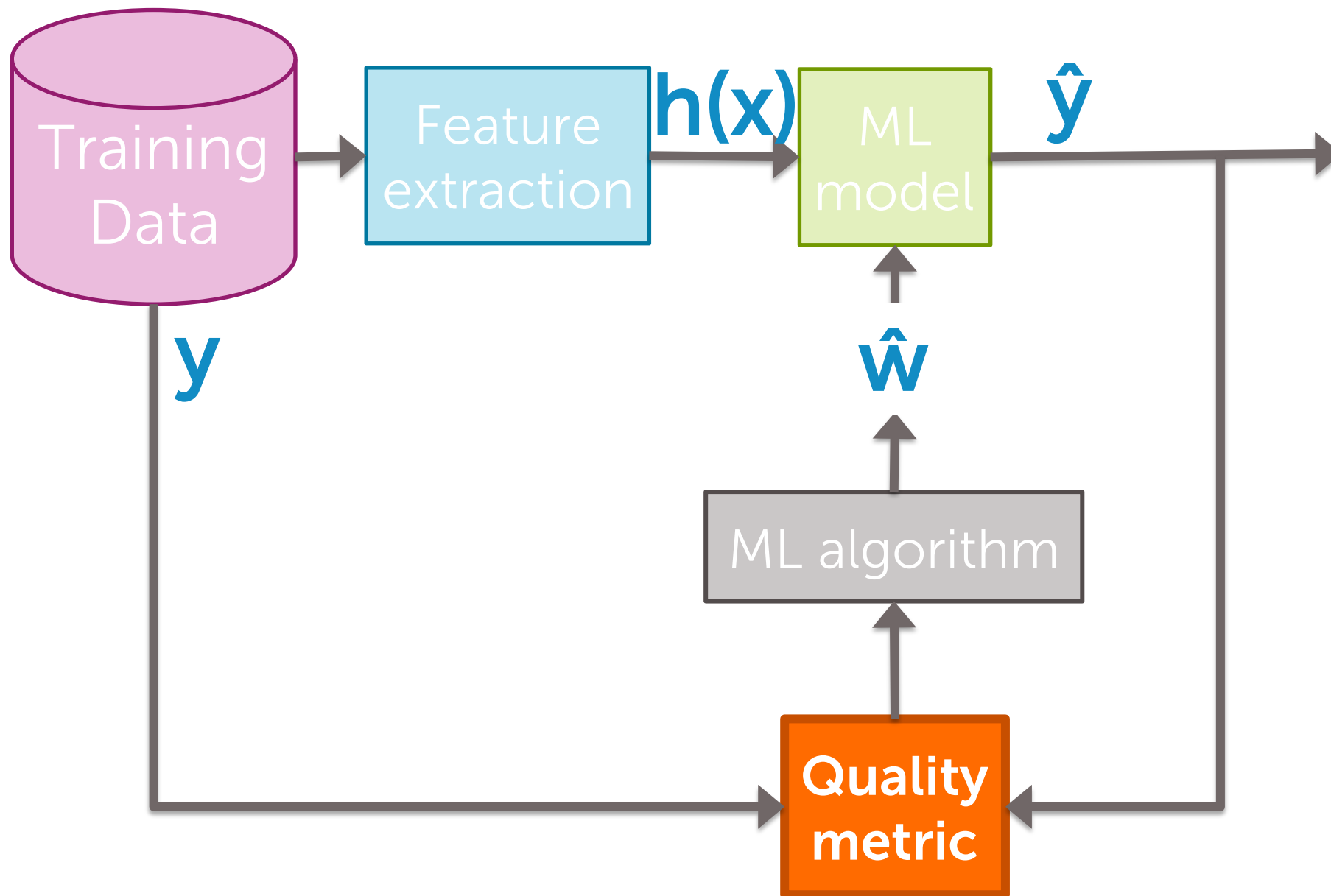
d inputs (e.g., sq.ft., #bath, #bed, lot size, year,...):

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

**MUCH!!!
HARDER**



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



Desired total cost format

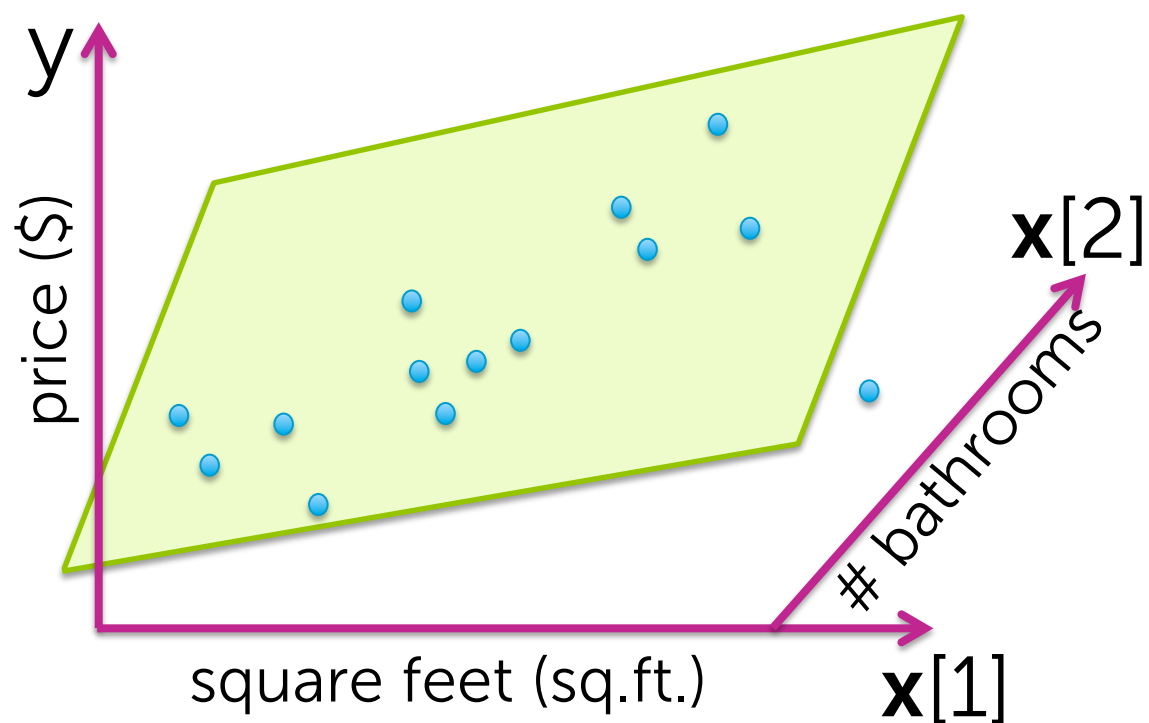
Want to balance:

- i. How well function fits data
- ii. Magnitude of coefficients

Total cost = $\text{measure of fit} + \text{measure of magnitude of coefficients}$

(Annotations: "measure quality of fit" points to "measure of fit"; "want to balance" points to both terms; "small # = good fit to training data" points to "measure of fit"; "small # = not overfit" points to "measure of magnitude of coefficients")

Measure of fit to training data



$$\begin{aligned} \text{RSS}(\mathbf{w}) &= \sum_{i=1}^N (y_i - h(\mathbf{x}_i)^T \mathbf{w})^2 \\ &= \sum_{i=1}^N (y_i - \hat{y}_i(\mathbf{w}))^2 \end{aligned}$$

pred. value using \mathbf{w}

small RSS \rightarrow model fitting training data well

Measure of magnitude of regression coefficient

What summary # is indicative of size of regression coefficients?

– Sum? $w_0 = 1,527,301$ $w_1 = -1,605,253$

No.

$$w_0 + w_1 = \text{small } \#$$

– Sum of absolute value?

$$|w_0| + |w_1| + \dots + |w_D| = \sum_{j=0}^D |w_j| \triangleq \|\mathbf{w}\|_1$$

bold $w \rightarrow$ vector

L_1 norm

reasonable choice

... discuss more in next module

– Sum of squares (L_2 norm)

$$w_0^2 + w_1^2 + \dots + w_D^2 = \sum_{j=0}^D w_j^2 \triangleq \|\mathbf{w}\|_2^2$$

L_2 norm

focus of this module

Consider specific total cost

Total cost =

measure of fit + measure of magnitude
of coefficients

Consider specific total cost

Total cost =

measure of fit + measure of magnitude
of coefficients

$$\text{RSS}(\mathbf{w}) + \|\mathbf{w}\|_2^2$$

Consider resulting objective

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

$$\text{RSS}(\mathbf{w}) + \lambda \|\mathbf{w}\|_2^2$$

 tuning parameter = balance of fit and magnitude

If $\lambda = 0$:

reduces to minimizing $\text{RSS}(\mathbf{w})$, as before (old solution) $\rightarrow \hat{\mathbf{w}}^{\text{LS}} \leftarrow \text{least squares}$

If $\lambda = \infty$:

For solutions where $\hat{\mathbf{w}} \neq 0$, then total cost is ∞
If $\hat{\mathbf{w}} = 0$, then total cost = $\text{RSS}(0)$ \rightarrow solution is $\hat{\mathbf{w}} = 0$

If λ in between: Then $0 \leq \|\hat{\mathbf{w}}\|_2 \leq \|\hat{\mathbf{w}}^{\text{LS}}\|_2$

Consider resulting objective

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

$$\text{RSS}(\mathbf{w}) + \lambda \|\mathbf{w}\|_2^2$$

 tuning parameter = balance of fit and magnitude

Ridge regression
(a.k.a L_2 regularization)

Bias-variance tradeoff

Large λ :

high bias, low variance

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

In essence, λ
controls model
complexity

Small λ :

low bias, high variance

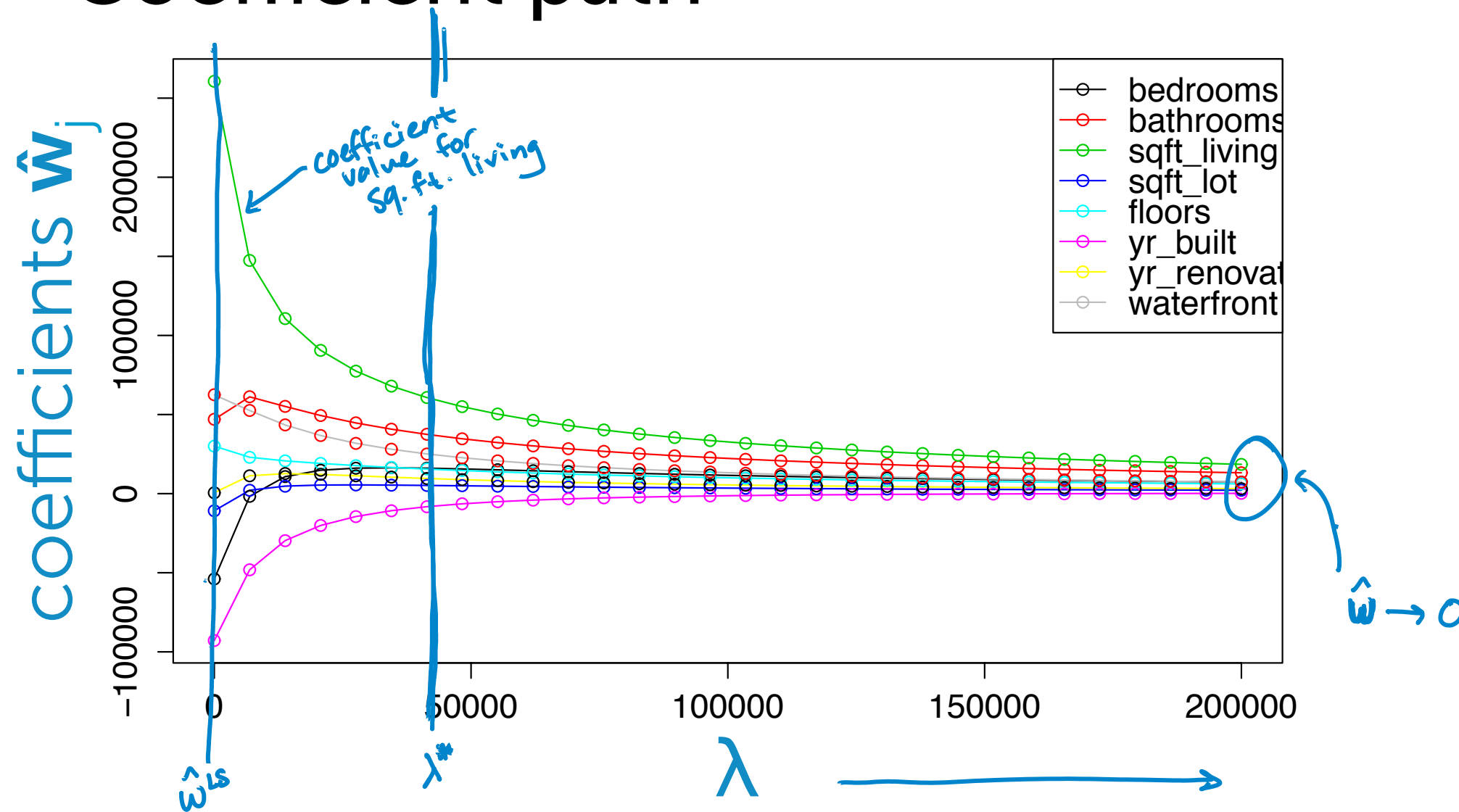
(e.g., standard least squares (RSS) fit of
high-order polynomial for $\lambda = 0$)

Revisit polynomial fit demo

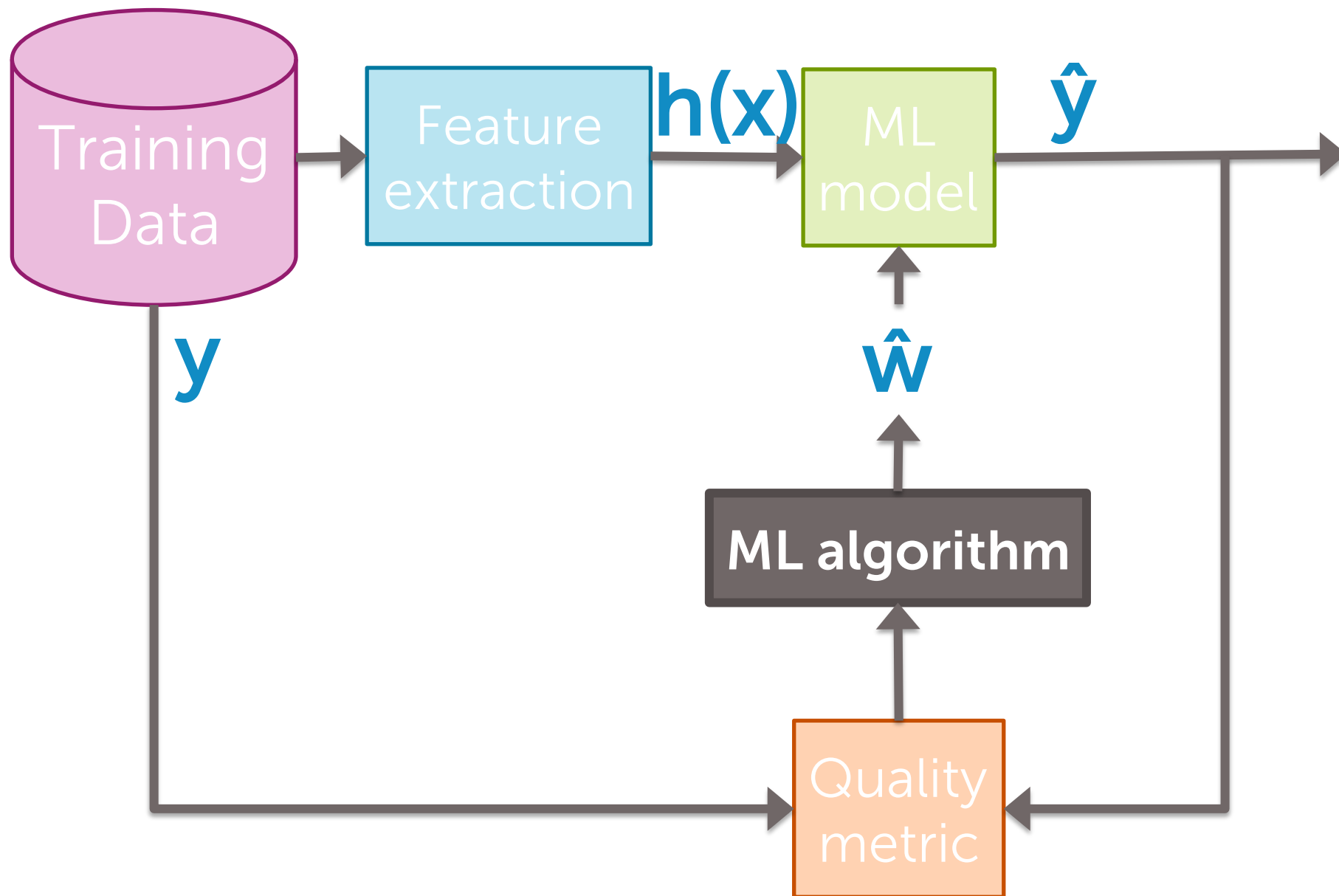
What happens if we refit our high-order polynomial, but now using **ridge regression**?

Will consider a few settings of λ ...

Coefficient path



Fitting the ridge regression model (for given λ value)

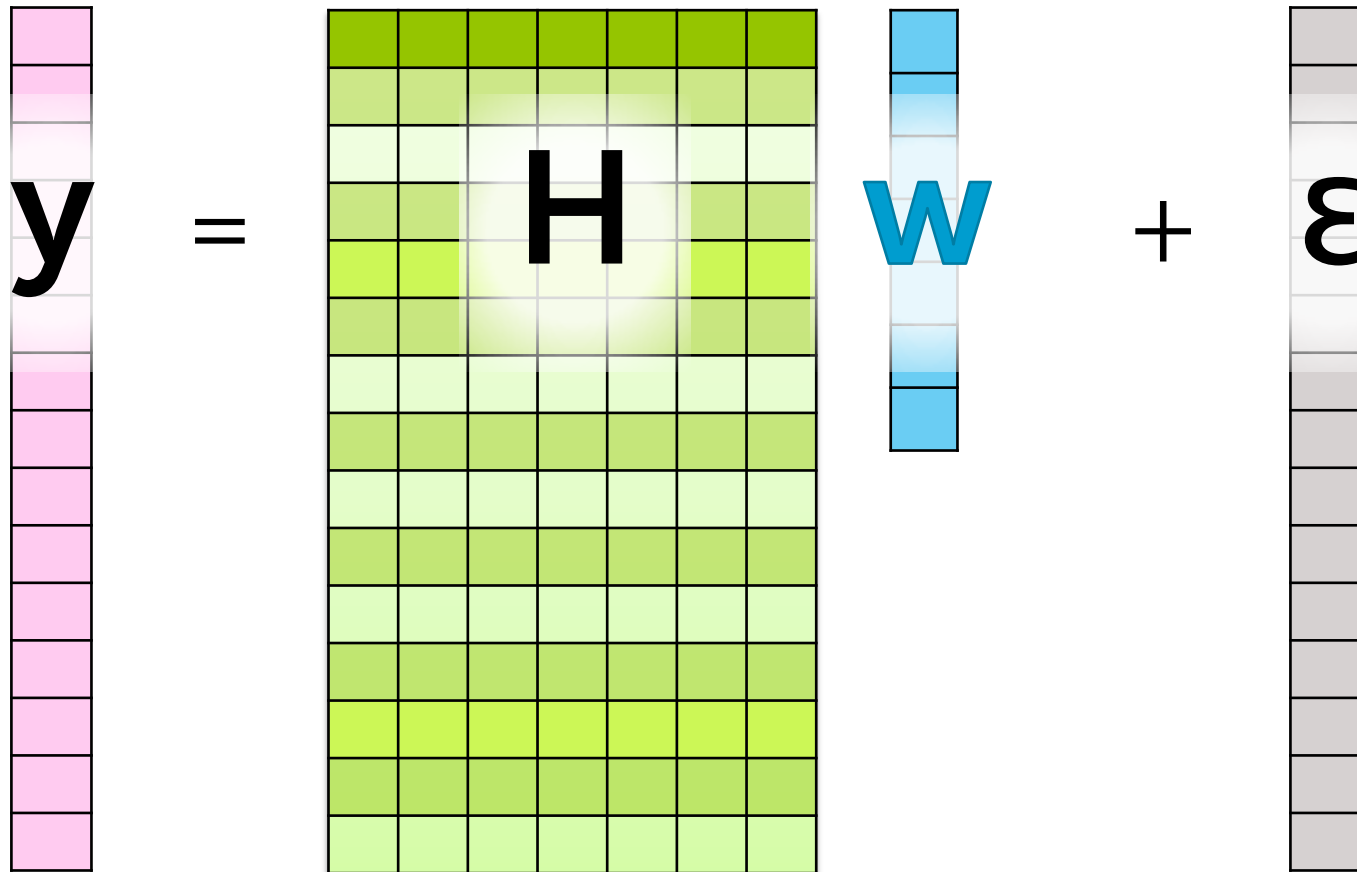


Step 1:

Rewrite total cost in matrix notation

Recall matrix form of RSS

Model for all N observations together



A diagram illustrating the matrix form of the model for all N observations together. It shows the equation $y = Hw + \epsilon$. The variable y is represented by a vertical column of 15 pink squares. The matrix H is a 15x7 grid of squares with a color gradient from light green to dark green. The variable w is a vertical column of 7 light blue squares. The error term ϵ is a vertical column of 15 light gray squares. The equation is written as $y = Hw + \epsilon$.

Recall matrix form of RSS

$$\begin{aligned}\text{RSS}(\mathbf{w}) &= \sum_{i=1}^N (y_i - \mathbf{h}(\mathbf{x}_i)^\top \mathbf{w})^2 \\ &= (\mathbf{y} - \mathbf{H}\mathbf{w})^\top (\mathbf{y} - \mathbf{H}\mathbf{w})\end{aligned}$$

Rewrite magnitude of coefficients in vector notation

$$\|\mathbf{w}\|_2^2 = w_0^2 + w_1^2 + w_2^2 + \dots + w_D^2$$

$$= \begin{array}{ccccccc} \boxed{} & \boxed{} & \boxed{} & \boxed{} & \boxed{} & \boxed{} & \boxed{} \\ w_0 & w_1 & w_2 & \dots & & & w_D \end{array} \quad \begin{array}{c} \boxed{} \\ \boxed{} \\ \boxed{} \\ \boxed{} \\ \boxed{} \\ \boxed{} \\ \boxed{} \end{array} \begin{array}{c} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_D \end{array}$$

$$= \mathbf{w}^T \mathbf{w}$$

Putting it all together

In matrix form, ridge regression cost is:

$$\begin{aligned} \text{RSS}(\mathbf{w}) + \lambda \|\mathbf{w}\|_2^2 \\ = (\mathbf{y} - \mathbf{H}\mathbf{w})^\top (\mathbf{y} - \mathbf{H}\mathbf{w}) + \lambda \mathbf{w}^\top \mathbf{w} \end{aligned}$$

Step 2:

Compute the gradient

Gradient of ridge regression cost

$$\begin{aligned}\nabla [\text{RSS}(\mathbf{w}) + \lambda \|\mathbf{w}\|_2^2] &= \nabla [(\mathbf{y} - \mathbf{H}\mathbf{w})^\top (\mathbf{y} - \mathbf{H}\mathbf{w}) + \lambda \mathbf{w}^\top \mathbf{w}] \\ &= \underbrace{\nabla [(\mathbf{y} - \mathbf{H}\mathbf{w})^\top (\mathbf{y} - \mathbf{H}\mathbf{w})]}_{-2\mathbf{H}^\top (\mathbf{y} - \mathbf{H}\mathbf{w})} + \lambda \underbrace{\nabla [\mathbf{w}^\top \mathbf{w}]}_{2\mathbf{w}}\end{aligned}$$

Why? By analogy to 1d case...

$\mathbf{w}^\top \mathbf{w}$ analogous to w^2 and derivative of $w^2 = 2w$

Step 3, Approach 1:
Set the gradient = 0

Aside:

Refresher on identity matrices

$$I_1 = [1], \quad I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \dots, \quad I_n = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$$

Fun facts:

$$\begin{array}{cccc} \overset{n \times n}{\mathbf{I}} \overset{n \times 1}{\mathbf{v}} = \mathbf{v} & \overset{n \times n}{\mathbf{I}} \overset{n \times m}{\mathbf{A}} = \mathbf{A} & \overset{n \times n}{\mathbf{A}^{-1}} \overset{n \times n}{\mathbf{A}} = \mathbf{I} & \overset{n \times n}{\mathbf{A}} \overset{n \times n}{\mathbf{A}^{-1}} = \mathbf{I} \end{array}$$

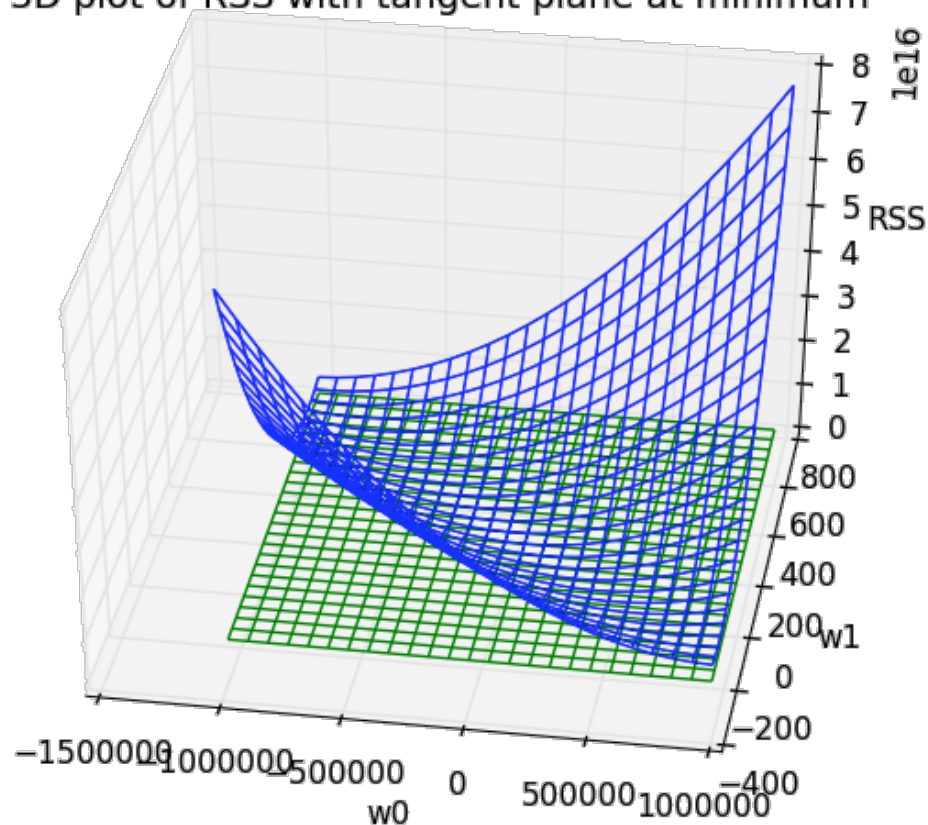
Handwritten notes:

- Under $\mathbf{Iv} = \mathbf{v}$: \uparrow vector
- Under $\mathbf{IA} = \mathbf{A}$: \uparrow matrix, $\mathbf{AI} = \mathbf{A}$
- Under $\mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$: \uparrow by definition of matrix inverse
- Under $\mathbf{AA}^{-1} = \mathbf{I}$: $\mathbf{A} = \mathbf{A} \checkmark$

$$\begin{aligned} \nabla \text{cost}(\mathbf{w}) &= -2\mathbf{H}^T(\mathbf{y} - \mathbf{H}\mathbf{w}) + 2\lambda \mathbf{w} \\ &= -2\mathbf{H}^T(\mathbf{y} - \mathbf{H}\mathbf{w}) + 2\lambda \mathbf{I}\mathbf{w} \end{aligned} \quad \boxed{\text{equivalent}}$$

Ridge closed-form solution

3D plot of RSS with tangent plane at minimum



$$\nabla \text{cost}(\mathbf{w}) = -2\mathbf{H}^T(\mathbf{y} - \mathbf{H}\mathbf{w}) + 2\lambda\mathbf{I}\mathbf{w} = 0$$

Solve for \mathbf{w} : $-\mathbf{H}^T\mathbf{y} + \mathbf{H}^T\mathbf{H}\hat{\mathbf{w}} + \lambda\mathbf{I}\hat{\mathbf{w}} = 0$

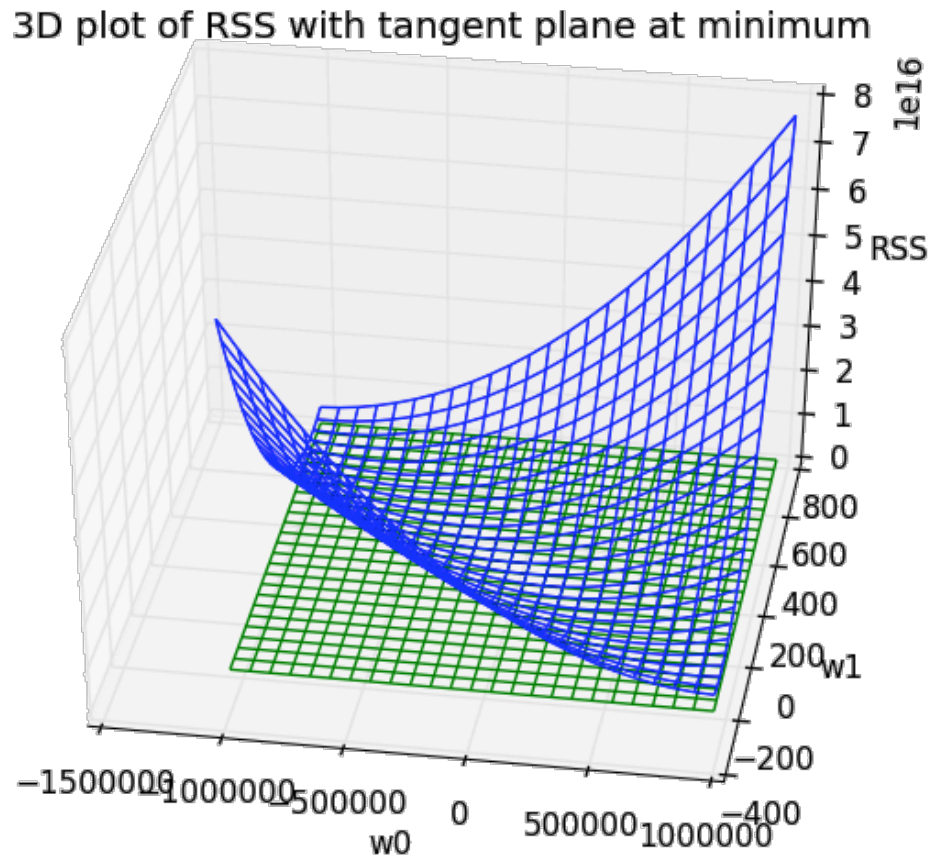
$$\mathbf{H}^T\mathbf{H}\hat{\mathbf{w}} + \lambda\mathbf{I}\hat{\mathbf{w}} = \mathbf{H}^T\mathbf{y}$$

$$(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I})\hat{\mathbf{w}} = \mathbf{H}^T\mathbf{y}$$

$$\hat{\mathbf{w}}^{\text{ridge}} = (\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I})^{-1}\mathbf{H}^T\mathbf{y}$$

$\hat{\mathbf{w}}^{\text{ridge}}$ indicates it's the ridge regression solution for a specific value of λ .

Interpreting ridge closed-form solution



$$\hat{\mathbf{w}}^{\text{ridge}} = (\mathbf{H}^T \mathbf{H} + \lambda \mathbf{I})^{-1} \mathbf{H}^T \mathbf{y}$$

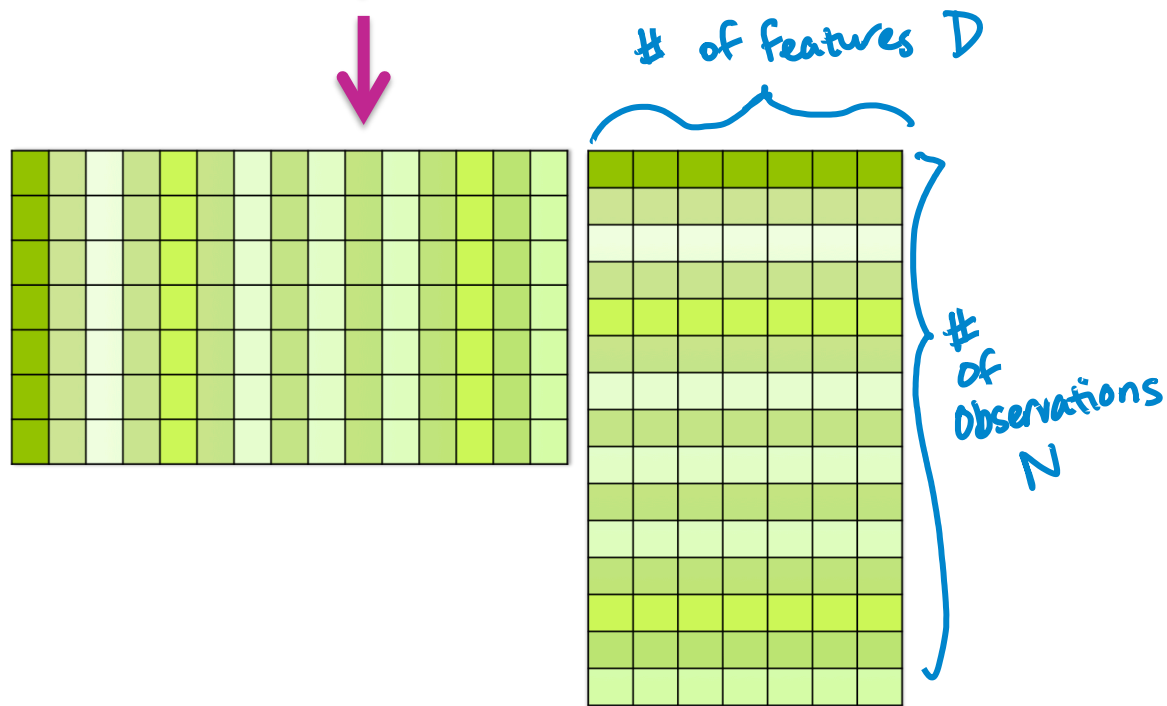
If $\lambda = 0$: $\hat{\mathbf{w}}^{\text{ridge}} = (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \mathbf{y} = \hat{\mathbf{w}}^{\text{LS}}$ ← old solution!

If $\lambda = \infty$: $\hat{\mathbf{w}}^{\text{ridge}} = \mathbf{0}$ ← because it's like dividing by ∞



Recall discussion on previous closed-form solution

$$\hat{\mathbf{w}}^{\text{LS}} = (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \mathbf{y}$$



Invertible if:

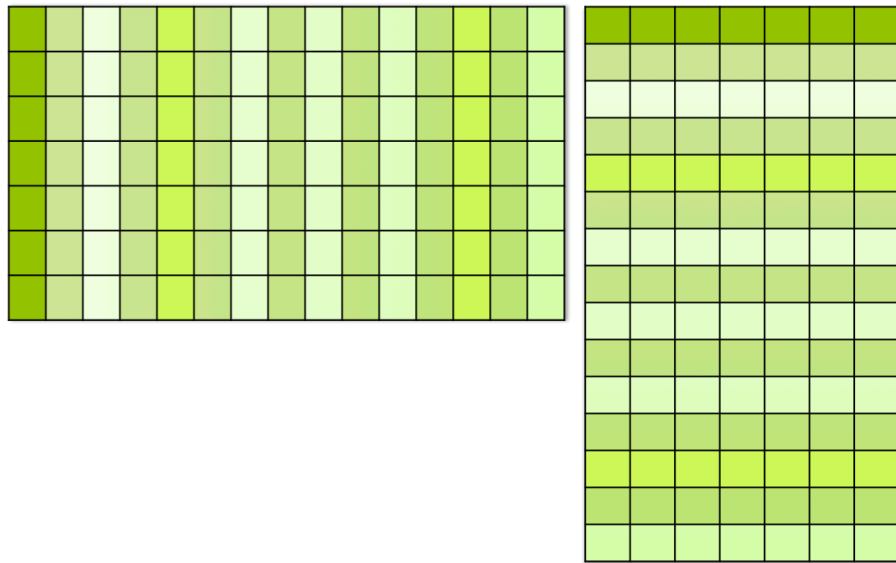
In general,
(# linearly independent obs)
 $N > D$

Complexity of inverse:

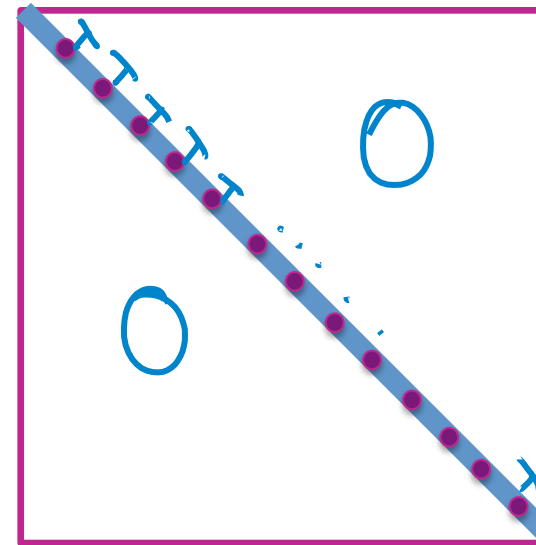
$O(D^3)$

Discussion of ridge closed-form solution

$$\hat{\mathbf{w}} = (\underbrace{\mathbf{H}^T \mathbf{H}} + \underbrace{\lambda \mathbf{I}})^{-1} \mathbf{H}^T \mathbf{y}$$



+



really important for large D
(lots of features)

Invertible if:

Always if $\lambda > 0$,
even if $N < D$

Complexity of
inverse:

$O(D^3)$...

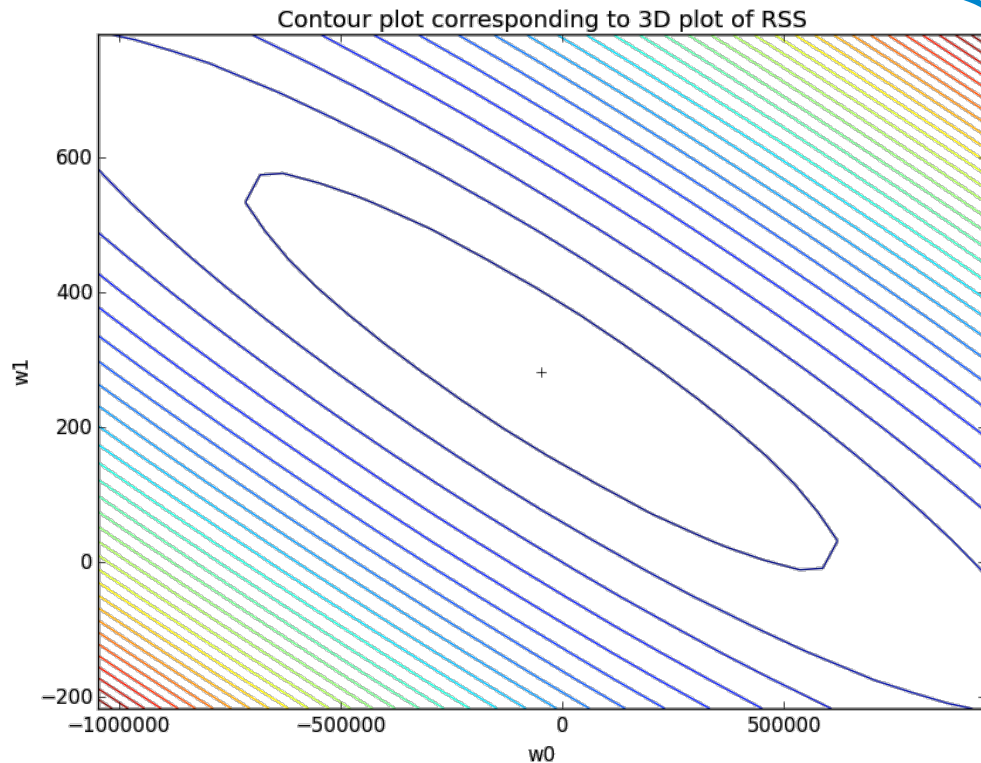
big for large D !

$\lambda \mathbf{I}$ is making $\mathbf{H}^T \mathbf{H} + \lambda \mathbf{I}$ more "regular"
→ "regularized"

Step 3, Approach 2: Gradient descent

Elementwise ridge regression gradient descent algorithm

$$\nabla \text{cost}(\mathbf{w}) = -2\mathbf{H}^T(\mathbf{y} - \mathbf{H}\mathbf{w}) + 2\lambda\mathbf{w}$$



Update to j^{th} feature weight:

$$w_j^{(t+1)} \leftarrow \underline{w_j^{(t)}} - \eta *$$

Same as before (from RSS term) $\rightarrow 2 \sum_{i=1}^N \mathbf{x}_i (y_i - \hat{y}_i(\mathbf{w}^{(t)}))$

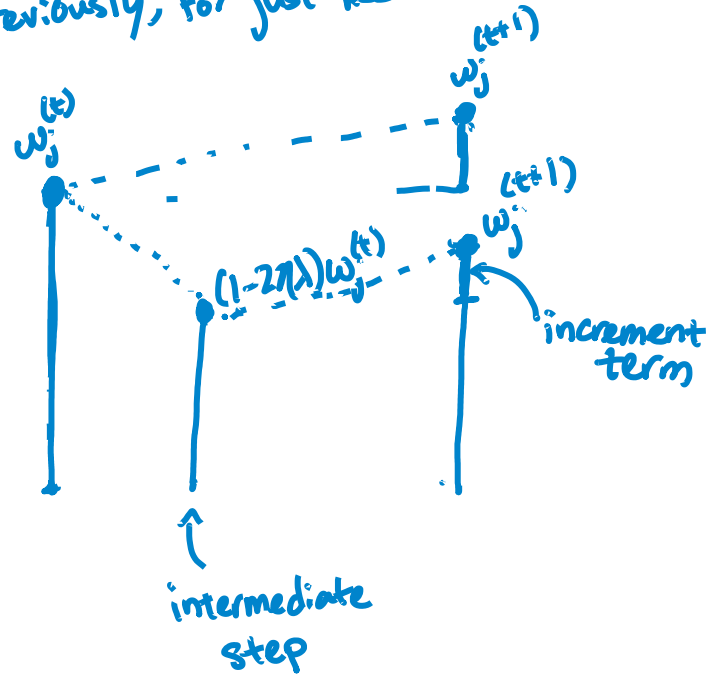
$$+ 2\lambda \underline{w_j^{(t)}}]$$

new term, comes from the j^{th} component of $2\lambda\mathbf{w}$

Elementwise ridge regression gradient descent algorithm

$$\nabla \text{cost}(\mathbf{w}) = -2\mathbf{H}^T(\mathbf{y} - \mathbf{H}\mathbf{w}) + 2\lambda\mathbf{w}$$

previously, for just RSS



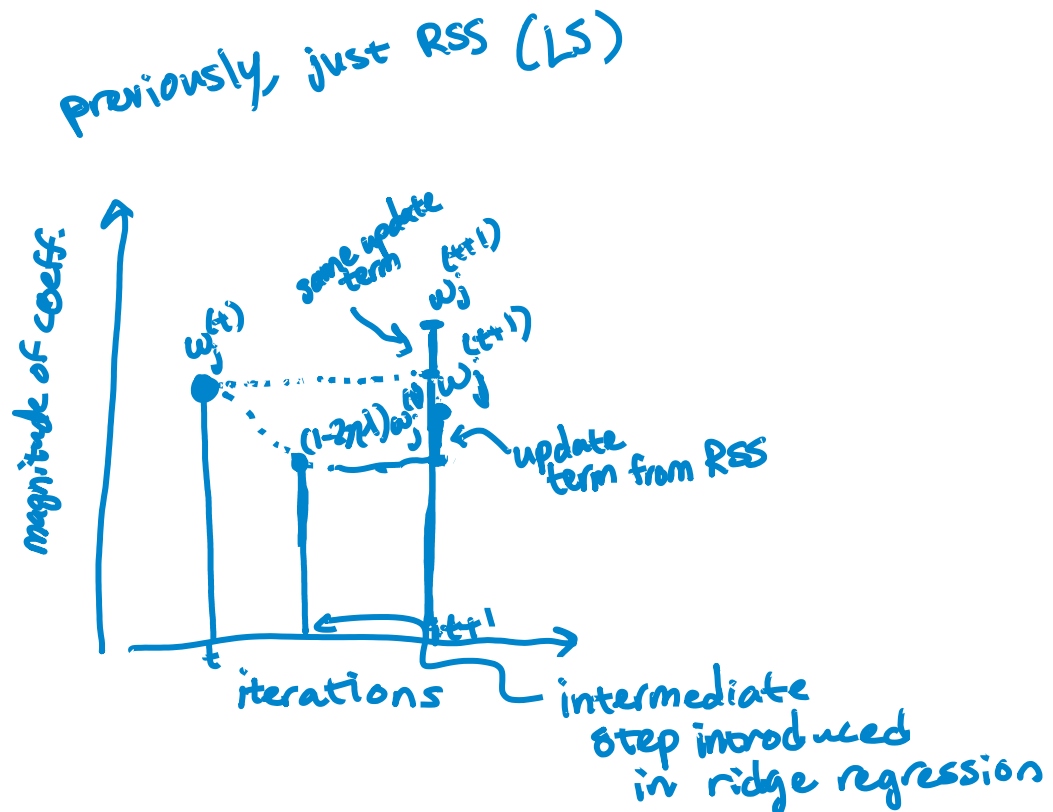
$1 - 2\eta\lambda$, where $\eta > 0$ and $\lambda \geq 0$, which make it ≤ 1 .
To enforce the result > 0 , make sure $2\eta\lambda < 1$.
 $w_j(t)$ shrinks multiplied by $1 - 2\eta\lambda$

Equivalently:

$$w_j^{(t+1)} \leftarrow \underbrace{(1 - 2\eta\lambda)}_{\leq 1} w_j^{(t)} + 2\eta \underbrace{\sum_{i=1}^N h_{ij}(x_i)(y_i - \hat{y}_i(\mathbf{w}^{(t)}))}_{\text{increment term}}$$

Elementwise ridge regression gradient descent algorithm

$$\nabla \text{cost}(\mathbf{w}) = -2\mathbf{H}^T(\mathbf{y} - \mathbf{H}\mathbf{w}) + 2\lambda\mathbf{w}$$



Equivalently:

$$w_j^{(t+1)} \leftarrow \underbrace{(1 - 2\eta \lambda)}_{\leq 1} w_j^{(t)} + 2\eta \underbrace{\sum_{i=1}^N \mathbf{x}_i (y_i - \hat{y}_i(\mathbf{w}^{(t)}))}_{\text{update term from RSS}}$$

Handwritten notes: $2\eta\lambda < 1$ and $\lambda^0 \lambda^0$ above the λ in the first term.

Recall previous algorithm

init $\mathbf{w}^{(1)} = 0$ (or randomly, or smartly), $t = 1$

while $\|\nabla \text{RSS}(\mathbf{w}^{(t)})\| > \epsilon$

for $j = 0, \dots, D$

partial[j] = $-2 \sum_{i=1}^N (\mathbf{x}_i)_j (y_i - \hat{y}_i(\mathbf{w}^{(t)}))$

$\mathbf{w}_j^{(t+1)} \leftarrow \mathbf{w}_j^{(t)} - \eta \text{partial}[j]$

$t \leftarrow t + 1$

Summary of ridge regression algorithm

init $\mathbf{w}^{(1)} = 0$ (or randomly, or smartly), $t = 1$

while $|| \nabla \text{RSS}(\mathbf{w}^{(t)}) || > \epsilon$

for $j = 0, \dots, D$

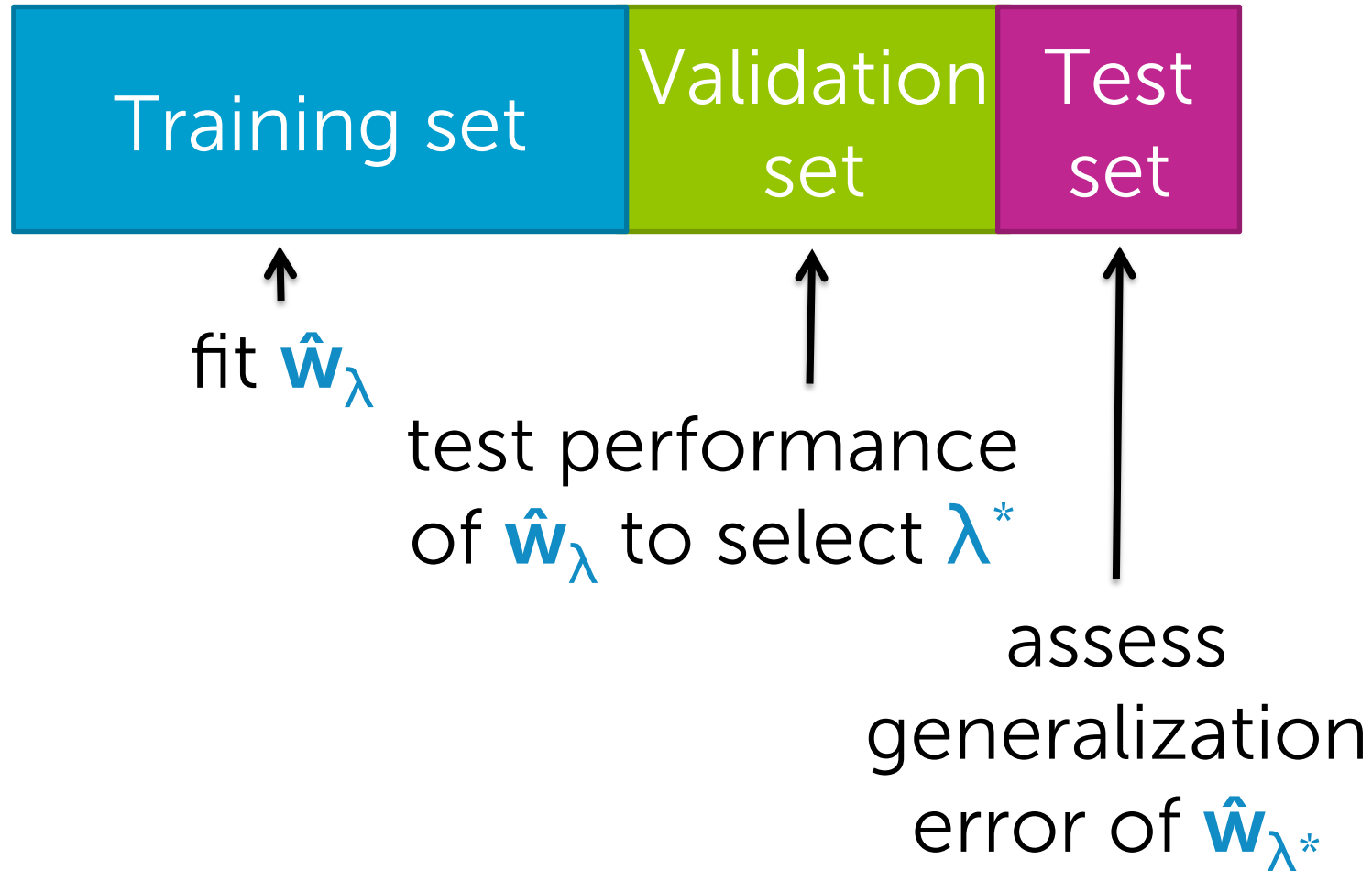
partial[j] = $-2 \sum_{i=1}^N (\mathbf{x}_i)_j (y_i - \hat{y}_i(\mathbf{w}^{(t)}))$

$w_j^{(t+1)} \leftarrow (1 - 2\eta\lambda) w_j^{(t)} - \eta \text{partial}[j]$

$t \leftarrow t + 1$

How to choose λ

If sufficient amount of data...



Start with smallish dataset



All data

Still form test set and hold out



How do we use the other data?

Rest of data



use for both training and
validation, but not so naively

Recall naïve approach



↑
small validation set

Is validation set enough to compare performance of \hat{w}_λ across λ values?

No

Small set, not representative of the space of things we might see.

Choosing the validation set



small validation set

Didn't have to use the last data points tabulated to form validation set

Can use **any data subset**

Choosing the validation set



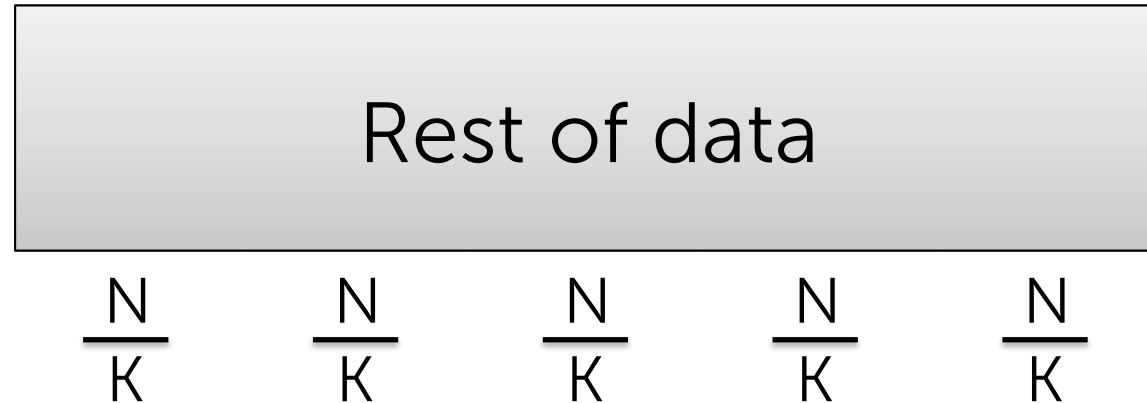
↑
small validation set

Which subset should I use?

ALL!

average
performance
over all
choices

K-fold cross validation

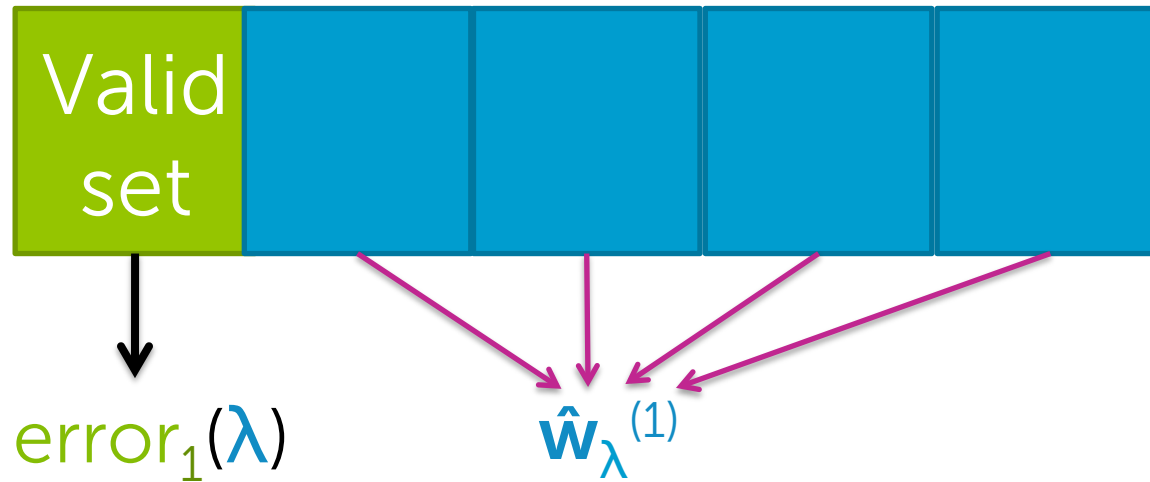


Preprocessing:

Randomly assign data to K groups

(use same split of data for all other steps)

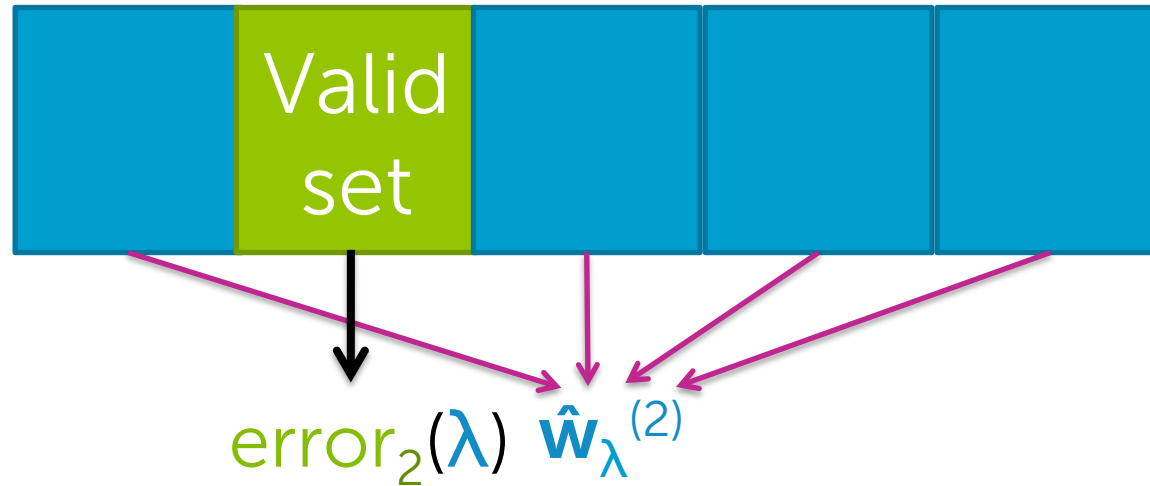
K-fold cross validation



For $k=1, \dots, K$

1. Estimate $\hat{\mathbf{w}}_{\lambda}^{(k)}$ on the training blocks
2. Compute error on validation block: $\text{error}_k(\lambda)$

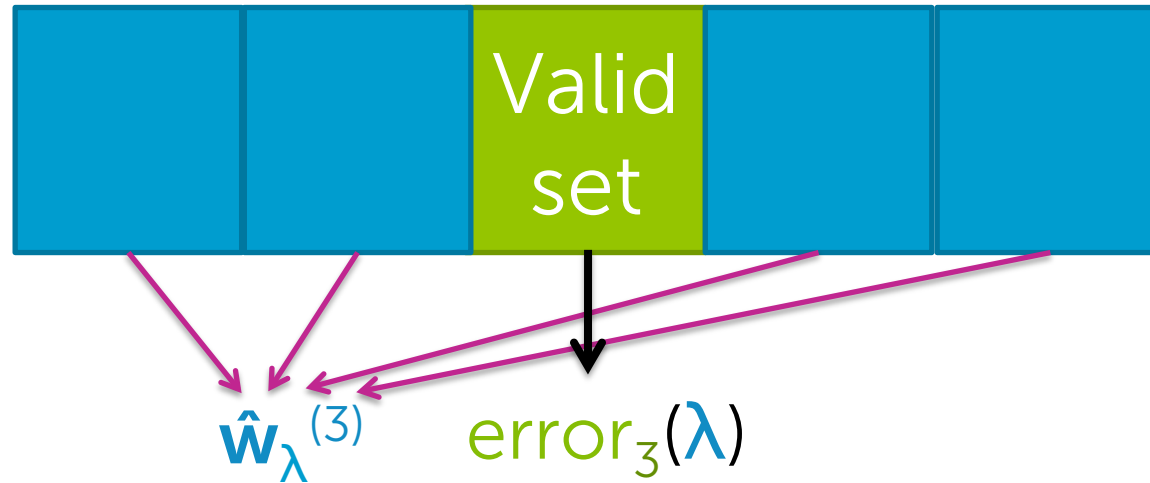
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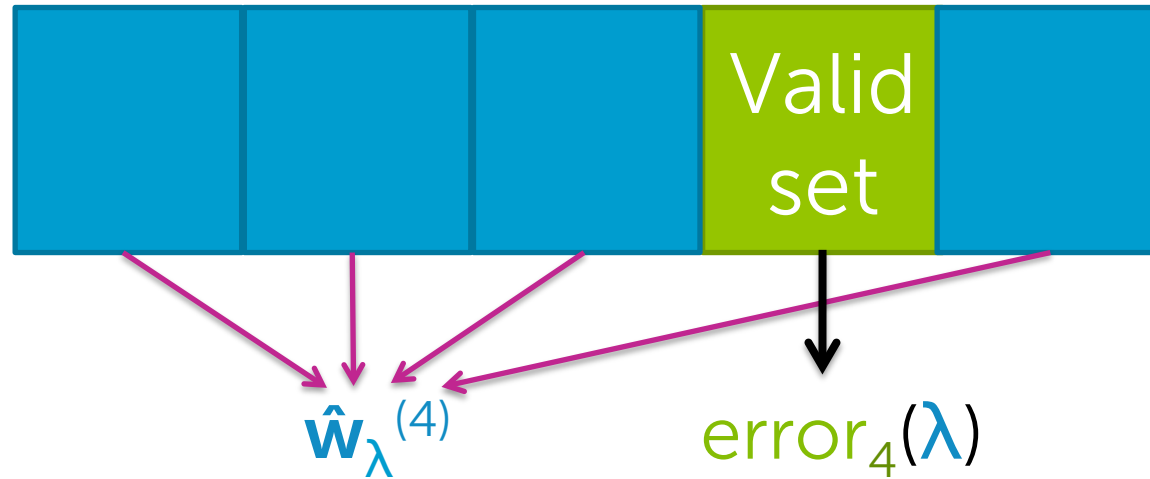
K-fold cross validation



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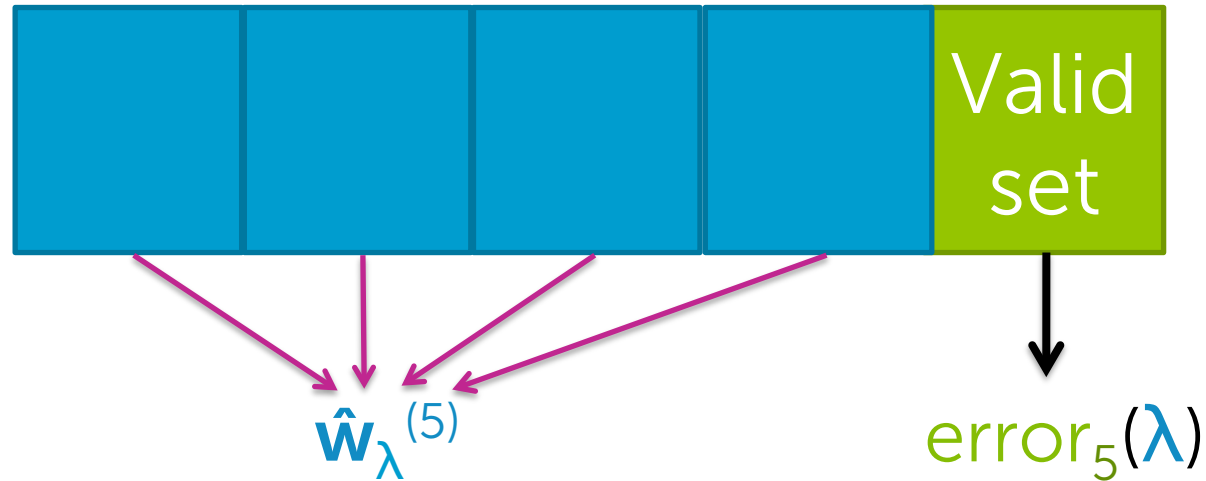
K-fold cross validation



For $k=1, \dots, K$

1. Estimate $\hat{\mathbf{w}}_{\lambda}^{(k)}$ on the training blocks
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K-fold cross validation

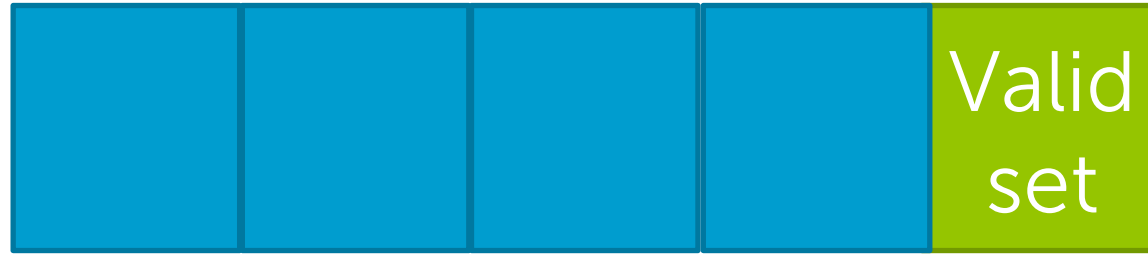


For $k=1, \dots, K$

1. Estimate $\hat{\mathbf{w}}_{\lambda}^{(k)}$ on the training blocks
2. Compute error on validation block: $\text{error}_k(\lambda)$

Compute average error: $\text{CV}(\lambda) = \frac{1}{K} \sum_{k=1}^K \text{error}_k(\lambda)$

K-fold cross validation



Repeat procedure for each choice of λ

Choose λ^* to minimize $CV(\lambda)$

What value of K?

Formally, the **best approximation** occurs for validation sets of size 1 ($K=N$)

leave-one-out
cross validation

Computationally intensive

- requires computing N fits of model per λ

Typically, $K=5$ or 10

5-fold CV

10-fold CV

How to handle the intercept

Recall multiple regression model

Model:

$$y_i = w_0 h_0(\mathbf{x}_i) + w_1 h_1(\mathbf{x}_i) + \dots + w_D h_D(\mathbf{x}_i) + \varepsilon_i$$
$$= \sum_{j=0}^D w_j h_j(\mathbf{x}_i) + \varepsilon_i$$

feature 1 = $h_0(\mathbf{x})$...often 1 (constant)

feature 2 = $h_1(\mathbf{x})$... e.g., $\mathbf{x}[1]$

feature 3 = $h_2(\mathbf{x})$... e.g., $\mathbf{x}[2]$

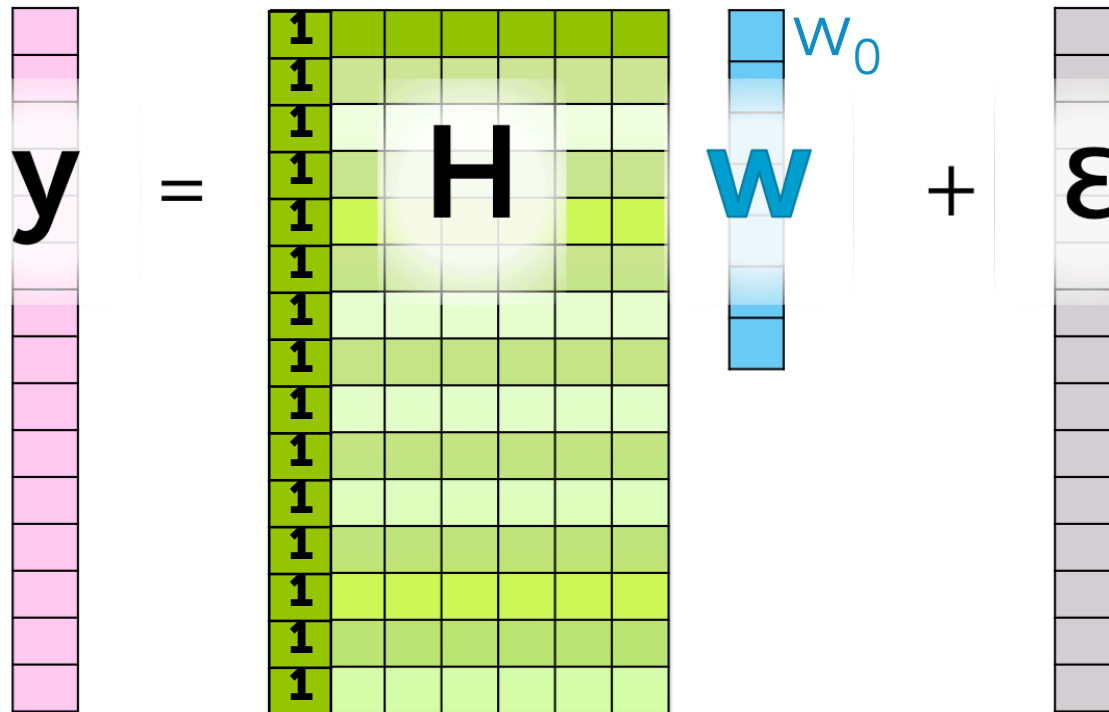
...

feature D+1 = $h_D(\mathbf{x})$... e.g., $\mathbf{x}[d]$

If constant feature...

$$y_i = w_0 + w_1 h_1(\mathbf{x}_i) + \dots + w_D h_D(\mathbf{x}_i) + \varepsilon_i$$

In matrix notation for N observations:



The diagram illustrates the matrix notation for N observations. It shows a vertical vector y (pink) equal to a matrix H (green) multiplied by a vector w (blue) plus a vector ε (grey). The matrix H has 15 rows and 6 columns. The first column of H contains 15 ones, representing the constant feature. The vector w has 6 elements, with the first element labeled w_0 . The vector ε has 15 elements.

$$\mathbf{y} = \mathbf{H} \mathbf{w} + \boldsymbol{\varepsilon}$$

Do we penalize intercept?

Standard ridge regression cost:

$$\text{RSS}(\mathbf{w}) + \lambda \|\mathbf{w}\|_2^2$$

 strength of penalty

Encourages intercept w_0 to also be small

Do we want a small intercept?

Conceptually, not indicative of overfitting...

Option 1: Don't penalize intercept

Modified ridge regression cost:

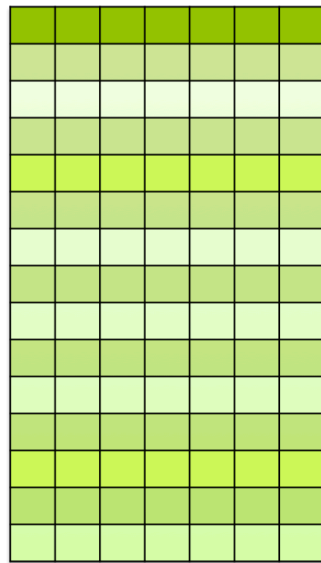
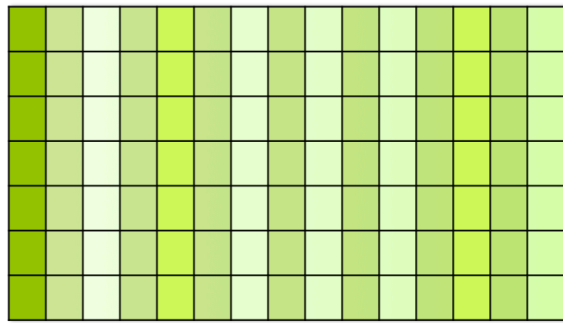
$$\text{RSS}(\mathbf{w}_0, \mathbf{w}_{\text{rest}}) + \lambda \|\mathbf{w}_{\text{rest}}\|_2^2$$

How to implement this in practice?

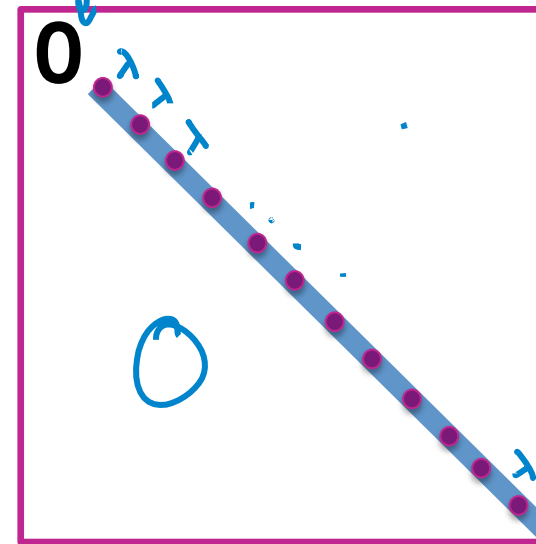
Option 1: Don't penalize intercept

- Closed-form solution –

$$\hat{\mathbf{w}} = (\underbrace{\mathbf{H}^T \mathbf{H}} + \underbrace{\lambda \mathbf{I}^{\text{mod}}})^{-1} \mathbf{H}^T \mathbf{y}$$



+



new penalty:
 $\lambda \mathbf{w}_{\text{res}}^T \mathbf{w}_{\text{res}}$

gradient:

$$2\lambda \mathbf{w}_{\text{res}} = 2\lambda \mathbf{I}^{\text{mod}} \mathbf{w}_{\text{res}} \rightarrow 2\lambda \begin{bmatrix} 0 & & \\ & \ddots & \\ & & 1 \end{bmatrix} \begin{bmatrix} w_0 \\ \mathbf{w}_{\text{res}} \end{bmatrix}$$

Option 1: Don't penalize intercept

- Gradient descent algorithm –

while $\|\nabla \text{RSS}(\mathbf{w}^{(t)})\| > \varepsilon$

for $j=0, \dots, D$

partial[j] = $-2 \sum_{i=1}^N \mathbf{x}_i(j) (y_i - \hat{y}_i(\mathbf{w}^{(t)}))$

if $j=0$

$w_0^{(t+1)} \leftarrow w_0^{(t)} - \eta \text{partial}[j]$

← old LS update
(no shrinkage to w_0)

else ← for all other features

$w_j^{(t+1)} \leftarrow (1 - 2\eta\lambda)w_j^{(t)} - \eta \text{partial}[j]$

← ridge update

$t \leftarrow t + 1$

Option 2: Center data first

If data are first **centered about 0**, then favoring small intercept not so worrisome

Step 1: Transform y to have 0 mean

Step 2: Run ridge regression as normal
(closed-form or gradient algorithms)

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
- Estimate ridge regression parameters:
 - In closed form
 - Using an iterative gradient descent algorithm
- Implement K-fold cross validation to select the ridge regression tuning parameter λ