INTRODUCTION TO DATA SCIENCE

This lecture is
based on course by E. Fox and C. Guestrin, Univ of Washington

9/10, 16/10, 23/10 2024

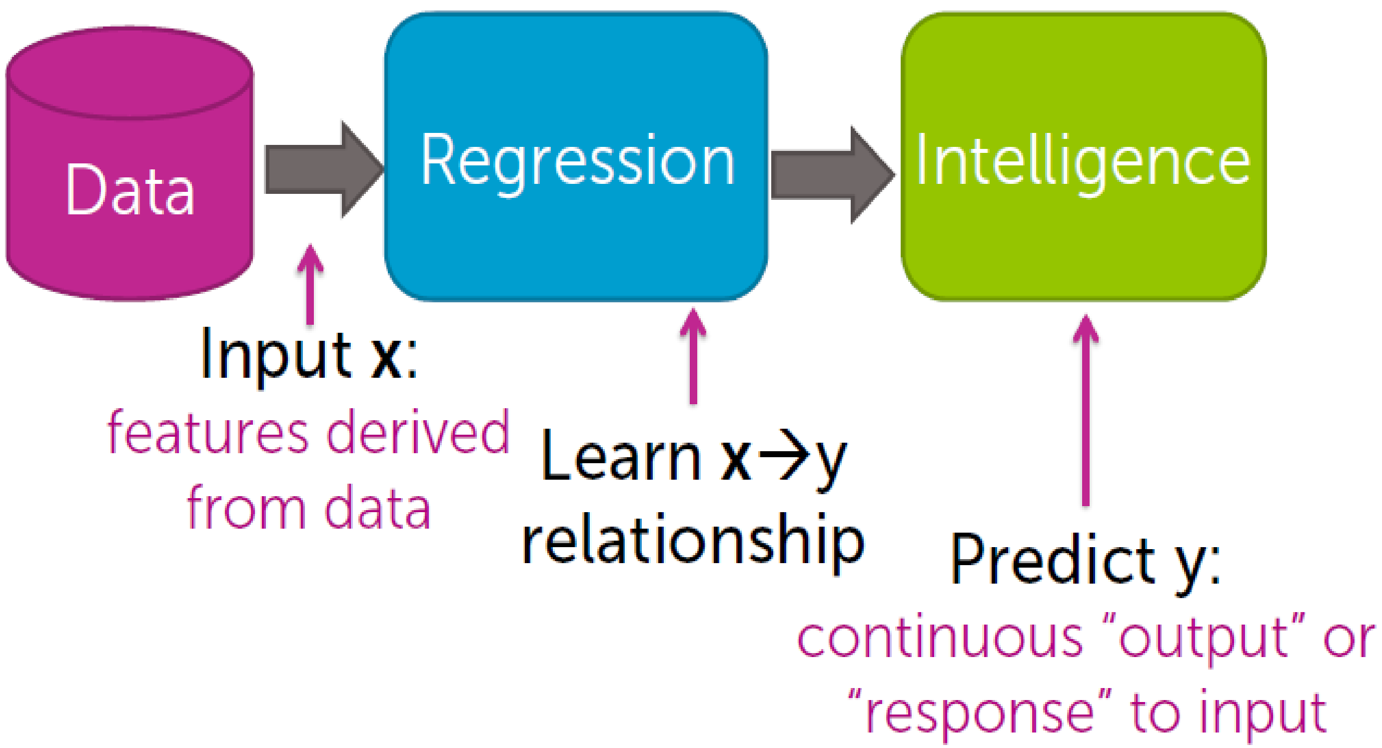
WFAiS UJ, Informatyka Stosowana
I stopień studiów

Regression for predictions

- **Simple regression**
- **Multiple regression**
- **Accesing performance**
- **Ridge regression**
- **Feature selection and lasso regression**
- **Nearest neighbor and kernel regression**

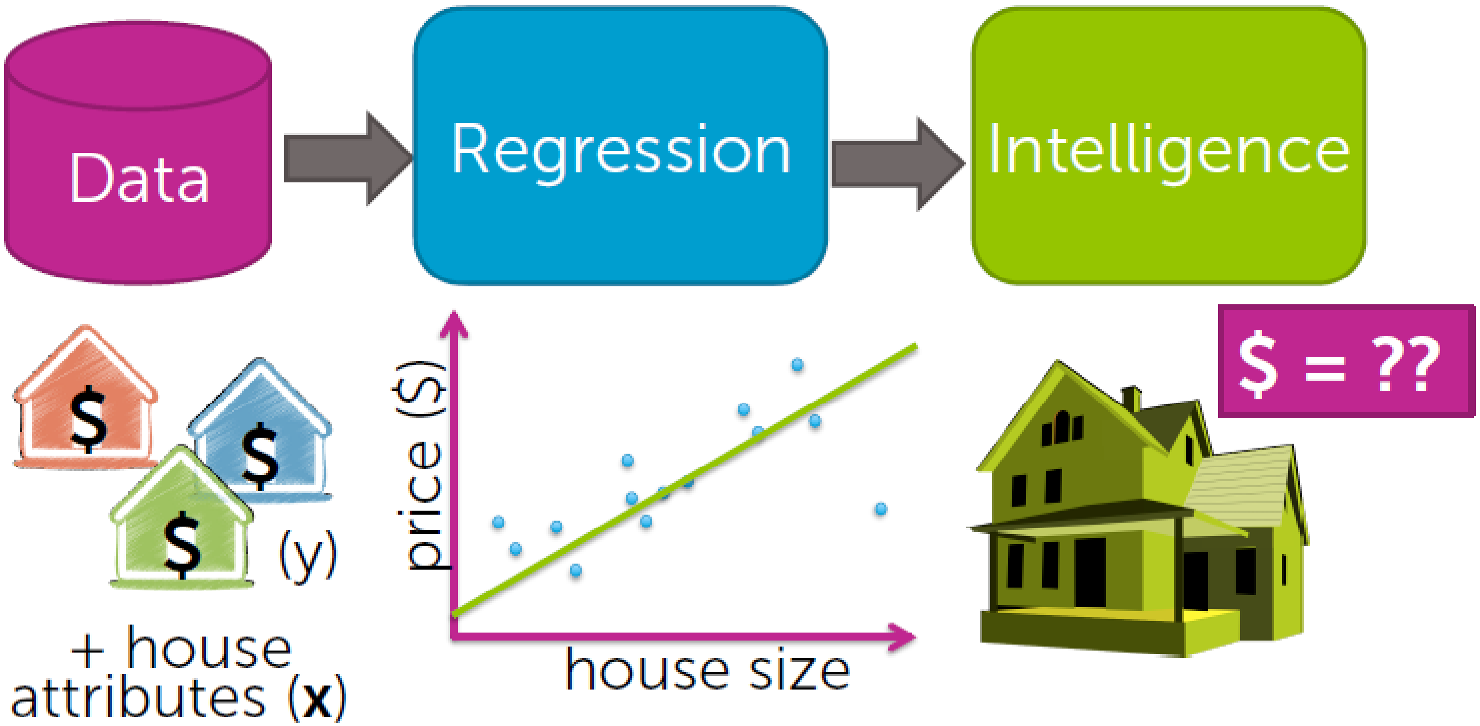
What is regression?

From features to predictions



Case study

Predicting house prices



Data

input *output*

$(x_1 = \text{sq.ft.}, \mathbf{y}_1 = \$)$

$(x_2 = \text{sq.ft.}, \mathbf{y}_2 = \$)$

$(x_3 = \text{sq.ft.}, \mathbf{y}_3 = \$)$

$(x_4 = \text{sq.ft.}, \mathbf{y}_4 = \$)$

$(x_5 = \text{sq.ft.}, \mathbf{y}_5 = \$)$

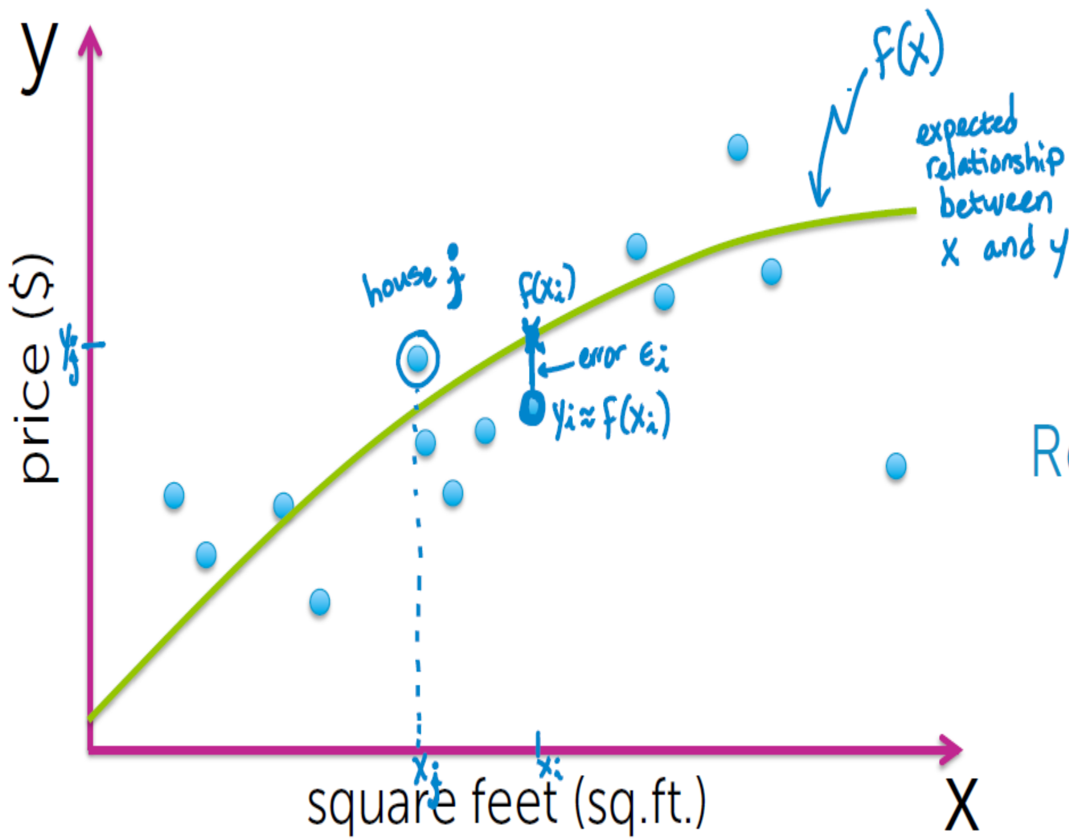
⋮

Input vs output

- **y is quantity of interest**
- **assume y can be predicted from x**

Model: assume functional relationship

„Essentially, all models are wrong but some are usefull.” George Box, 1987.



Regression model:

$$y_i = f(x_i) + \epsilon_i$$

$E[\epsilon_i] = 0$ ← equally likely that error is + or −

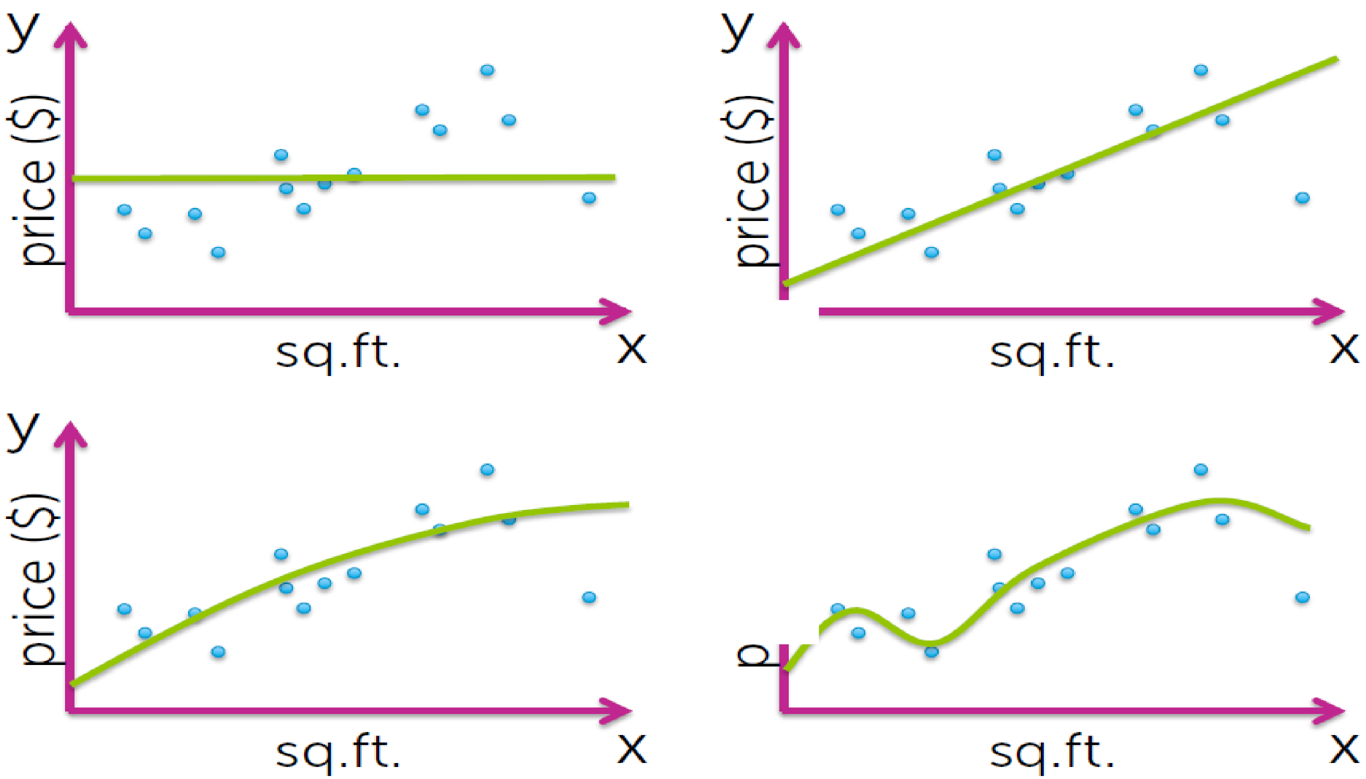
↑ expected value

⇓

y_i is equally likely to be above or below $f(x_i)$

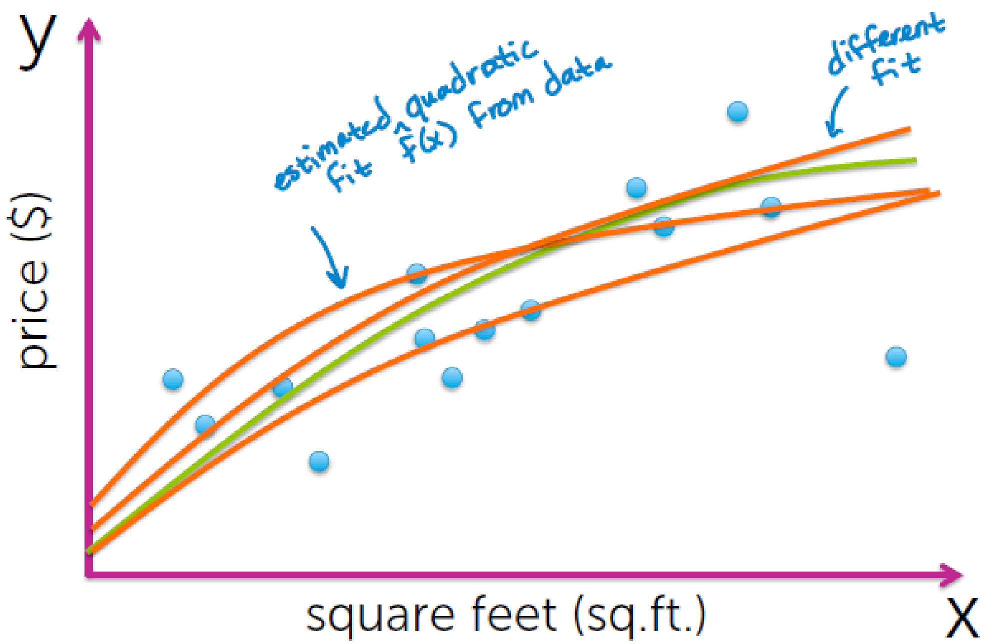
Task 1:

Which model to fit?



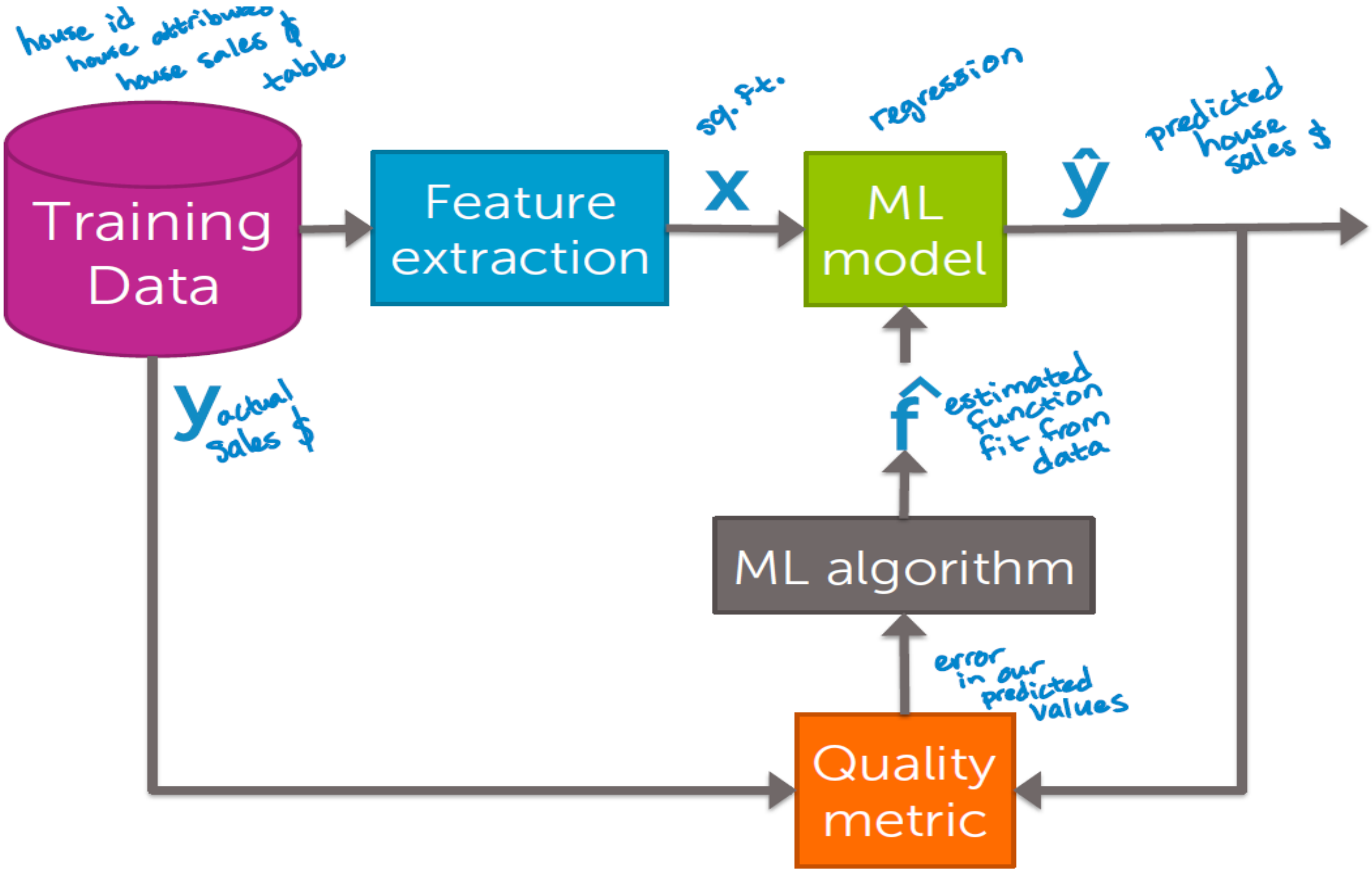
Task 2:

For a given model f(x) estimate function $\hat{f}(x)$ from data



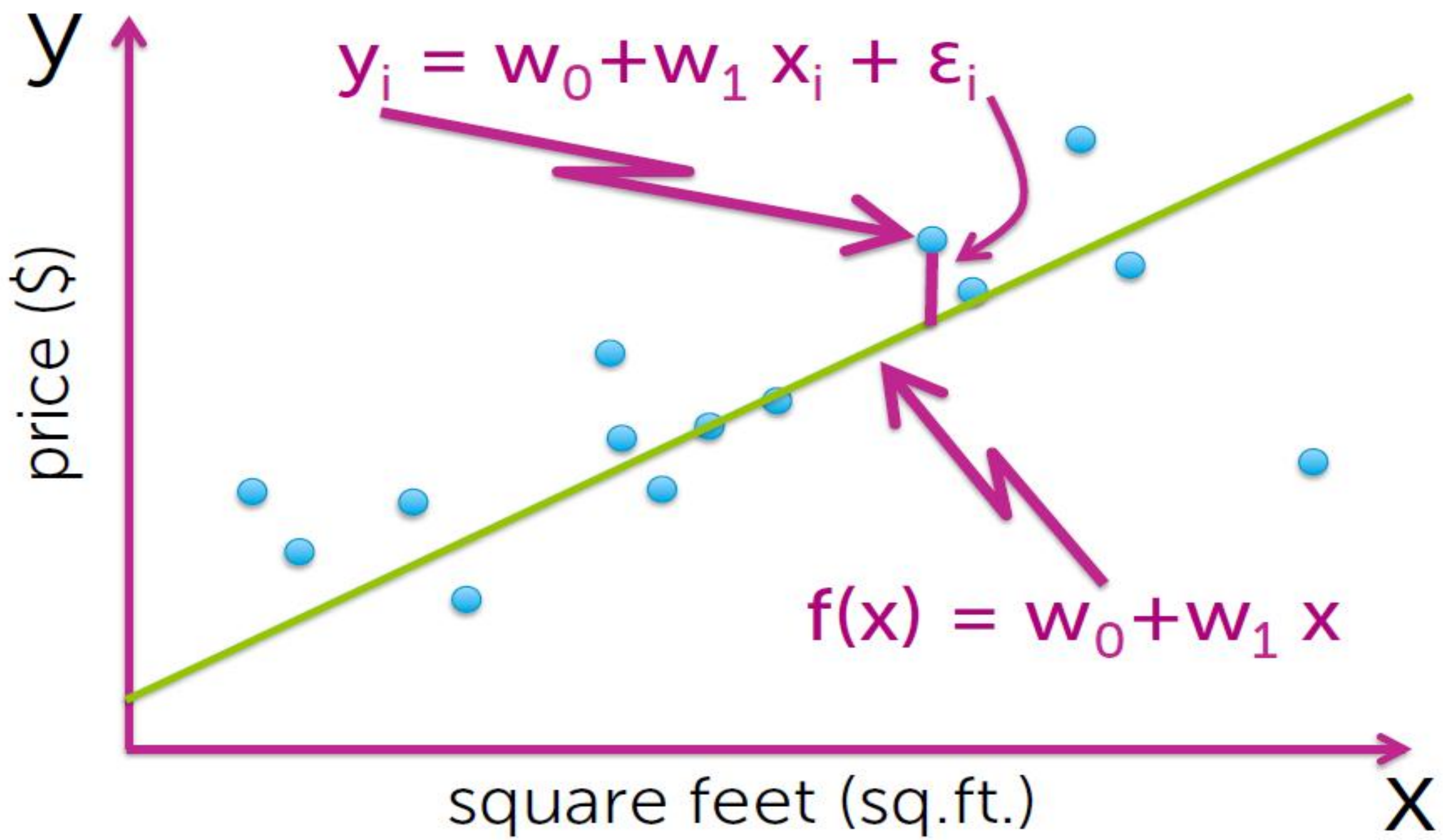
Assume model f(x) is a quadratic function

How it works: baseline flow chart



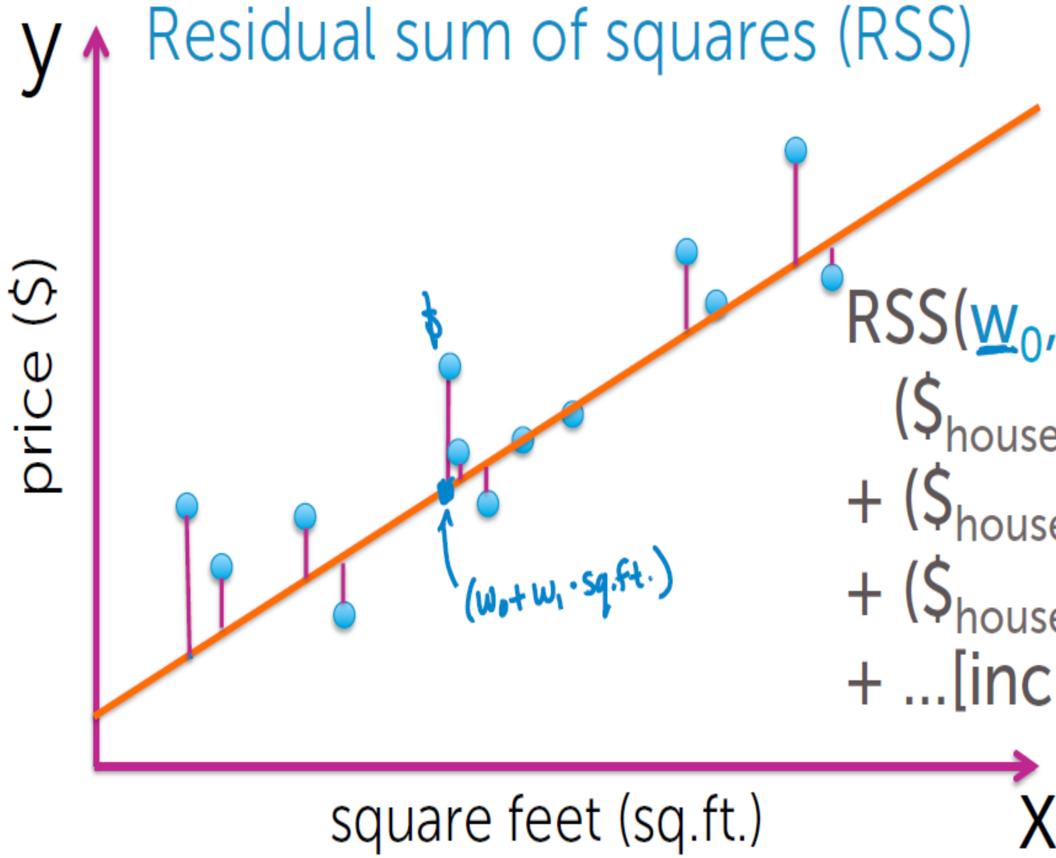
SIMPLE LINEAR REGRESSION

Simple linear regression model



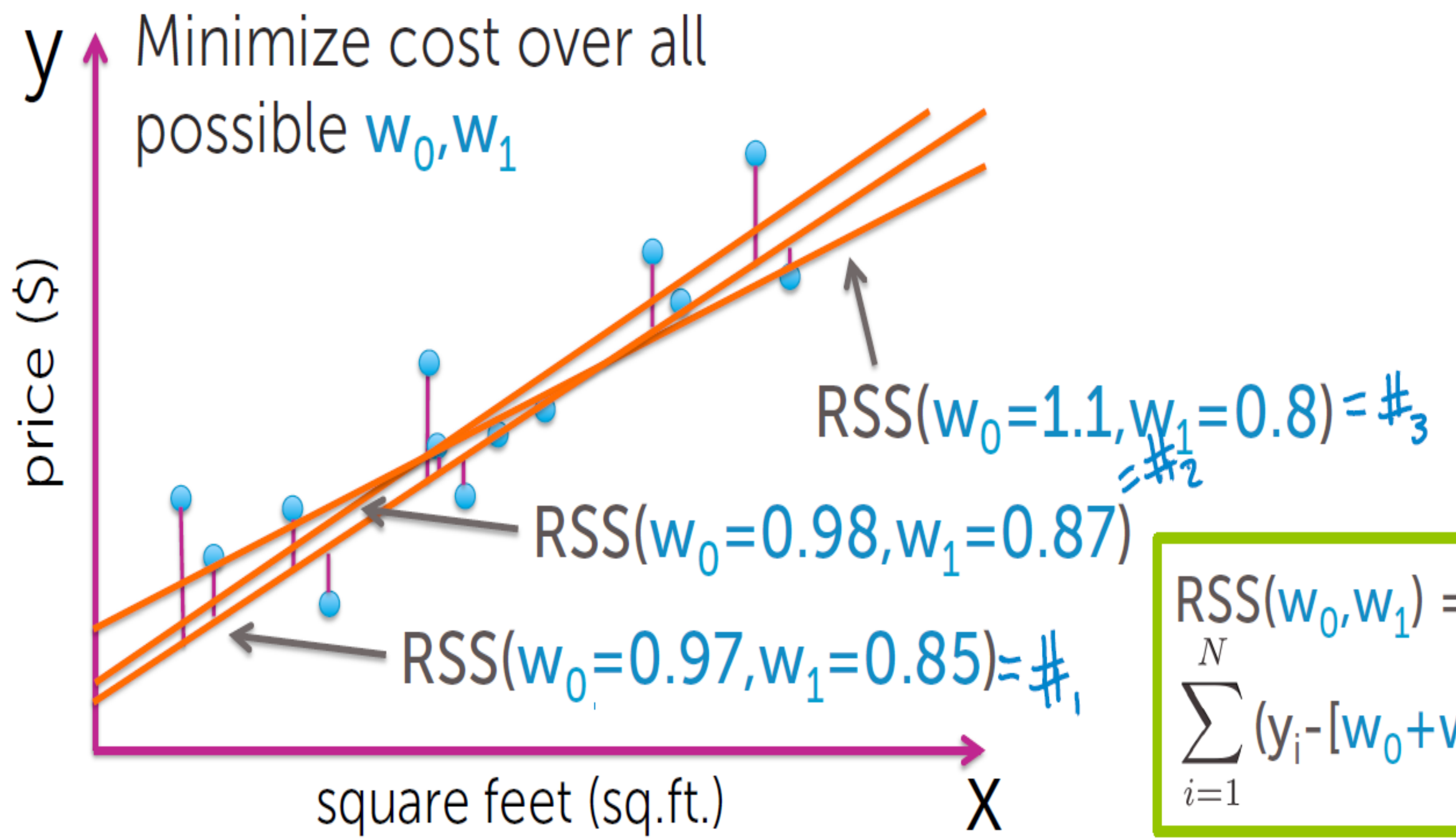
The cost of using a given line

Residual sum of squares (RSS)



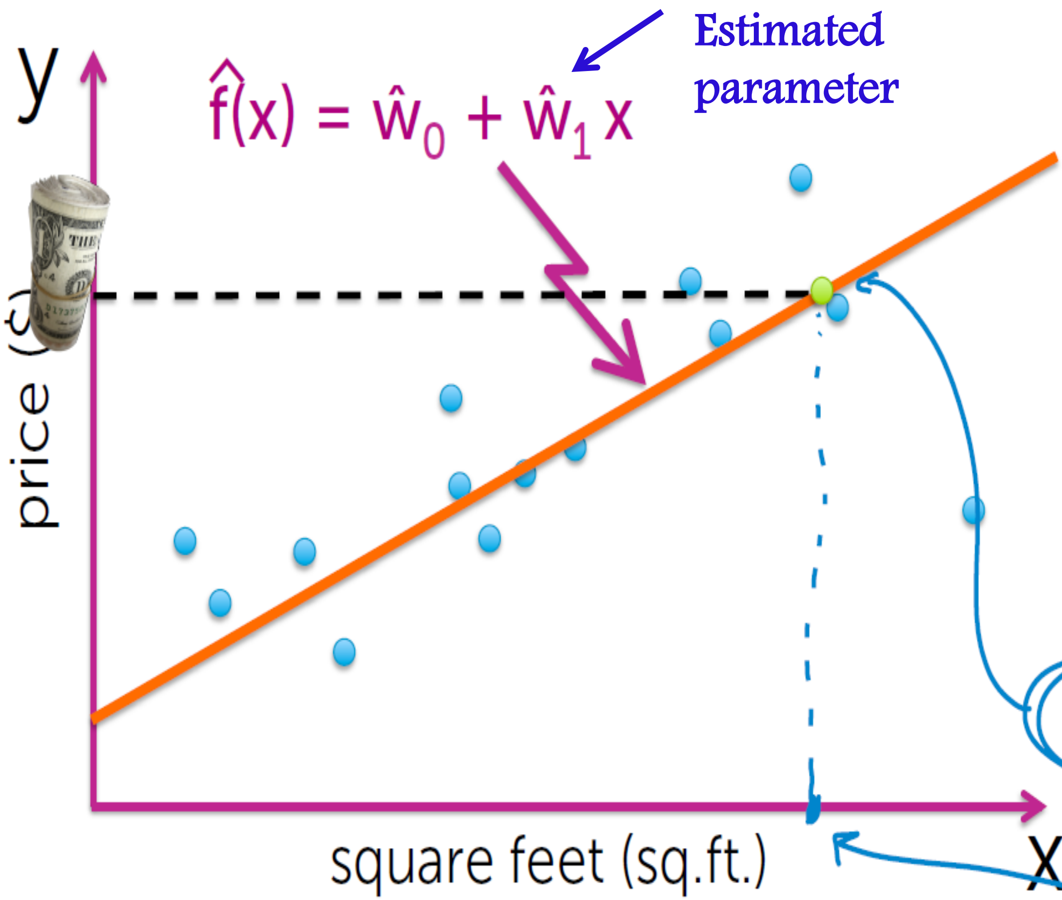
$$\begin{aligned}\mathrm{RSS}(\underline{w_0},\underline{w_1}) = \; & (\$_{\text{house }1} - [w_0 + w_1 \text{sq.ft.}_{\text{house }1}])^2 \\ & + (\$_{\text{house }2} - [w_0 + w_1 \text{sq.ft.}_{\text{house }2}])^2 \\ & + (\$_{\text{house }3} - [w_0 + w_1 \text{sq.ft.}_{\text{house }3}])^2 \\ & + \ldots\underline{\text{[include all training houses]}}\end{aligned}$$

Find „best” line



$$RSS(w_0,w_1) = \sum_{i=1}^{N} (y_i-[w_0+w_1x_i])^2$$

Predicting size of house you can afford



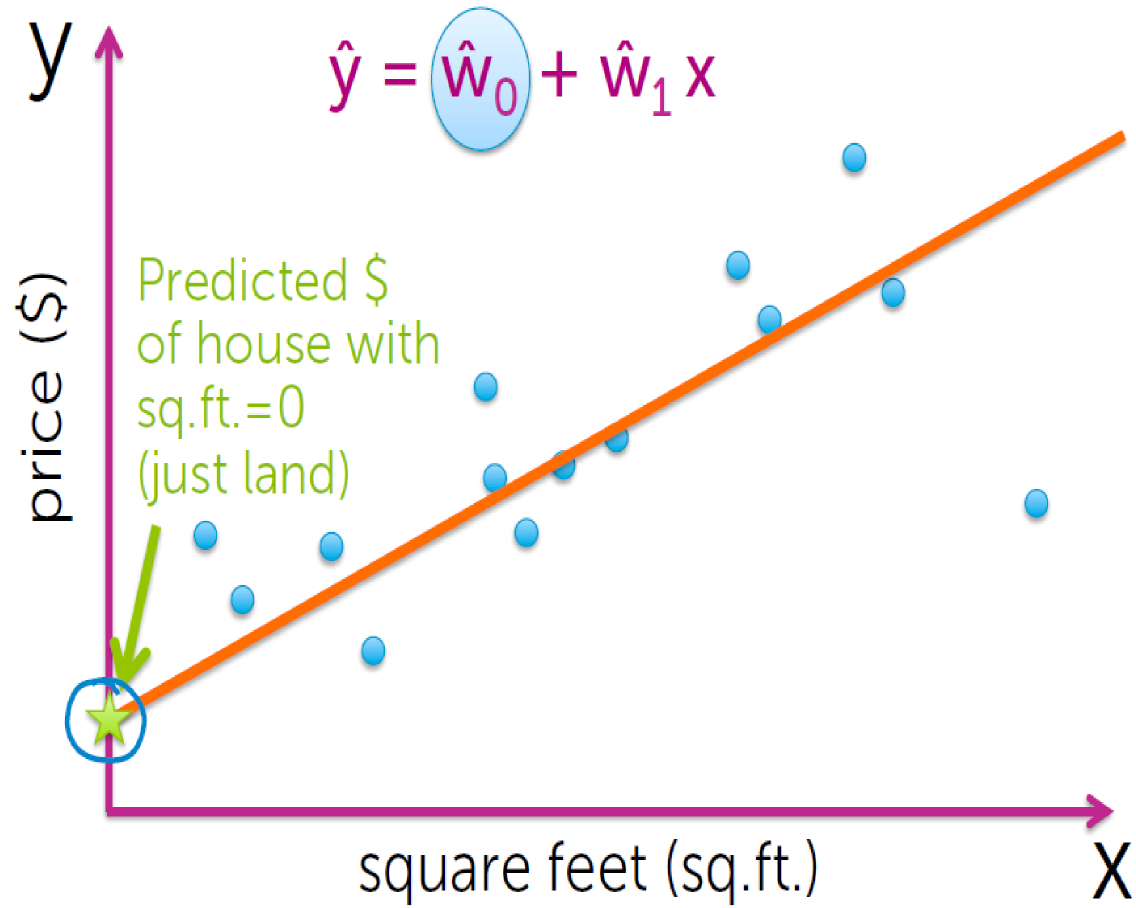
Regression model:

$$y_i = w_0 + w_1 x_i + \varepsilon_i$$

Best guess of size of house you can afford:

$$\$_{\text{in bank}} = \hat{w}_0 + \hat{w}_1 \widehat{\text{sq.ft.}}$$

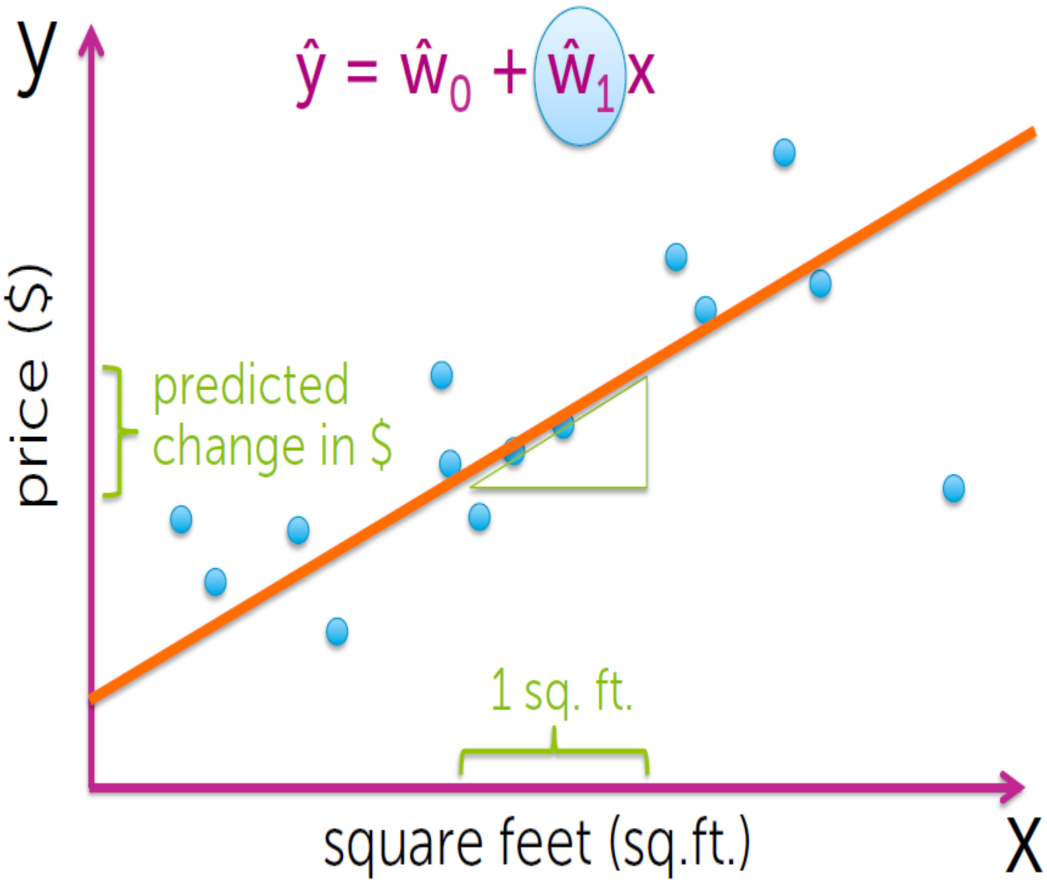
Interpreting the coefficients



$\hat{y} = \hat{w}_0$ when $x = 0$

not very meaningful

Interpreting the coefficients

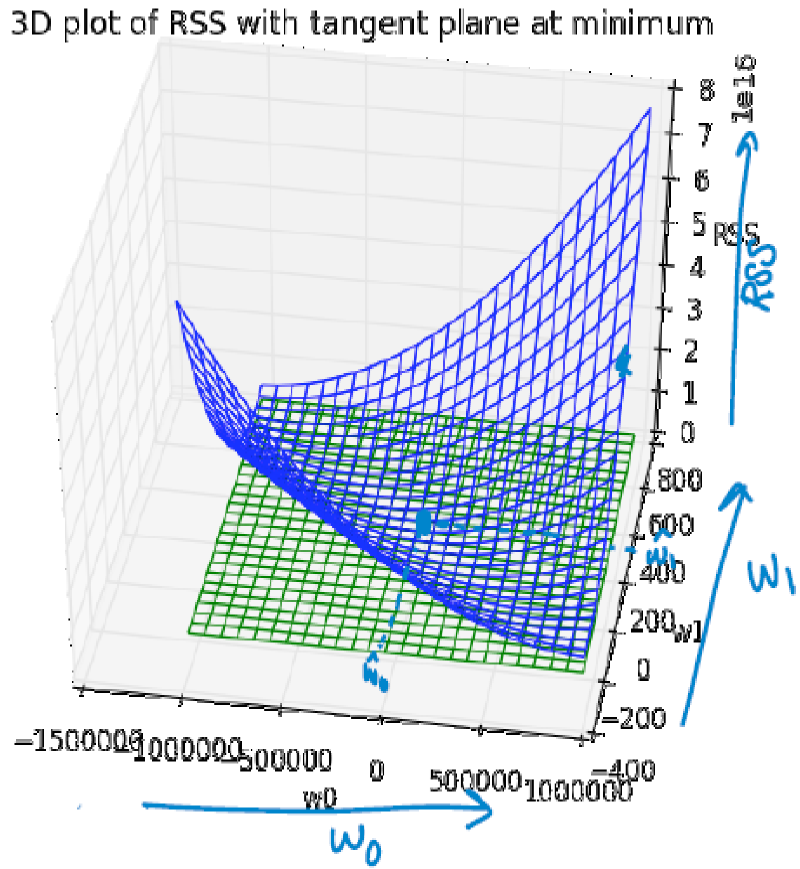


Magnitude of fit parameters depend on the units of both features and observations

$$\hat{\$}_{1001\ sq.ft.} - \hat{\$}_{1000\ sq.ft.}$$
$$= \cancel{\hat{w}_0} + \hat{w}_1 \cdot 1001\ sq.ft.$$
$$- (\cancel{\hat{w}_0} + \hat{w}_1\, 1000\ sq.ft.)$$
$$= \hat{w}_1$$

predicted change in the output per unit change in input

ML algorithm: minimasing the cost



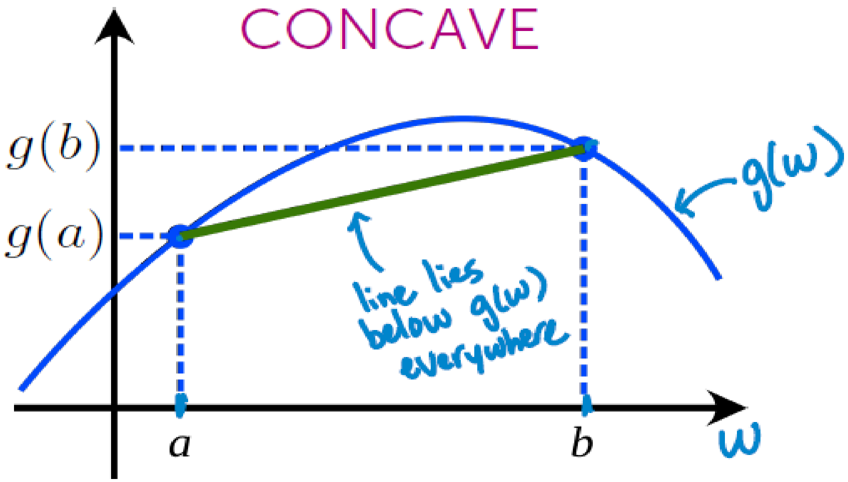
Minimize function over all possible w_0, w_1

$$\boxed{\min_{w_0, w_1}} \underbrace{\sum_{i=1}^{N} (y_i - [w_0 + w_1 x_i])^2}$$

RSS(w_0,w_1) is a function of 2 variables $= g(w_0, w_1)$

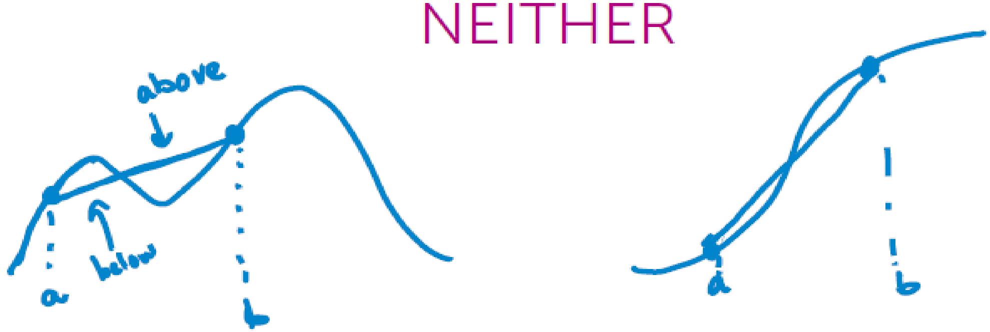
Convex/concave function

CONCAVE



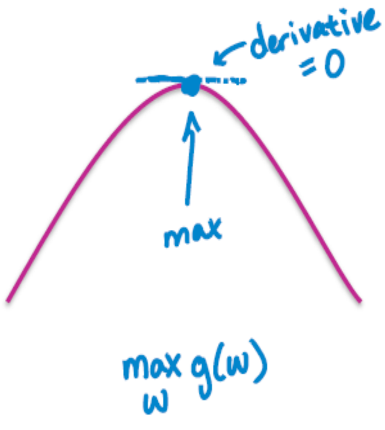
CONVEX

NEITHER



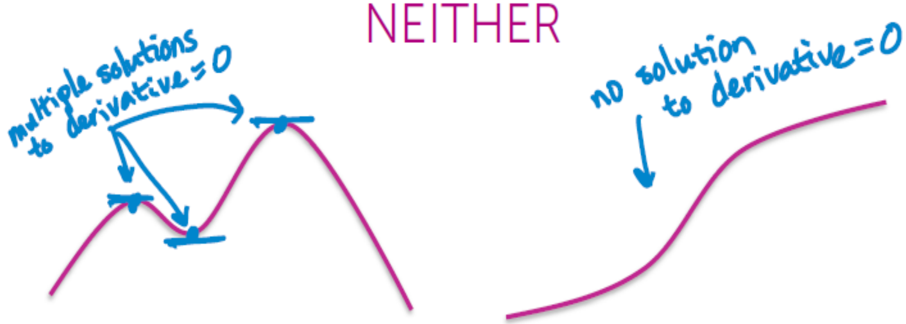
Finding max/min analytically

CONCAVE



CONVEX

NEITHER



Example:

$g(w) = 5\text{-}(w\text{-}10)^2$

$$\frac{dg(w)}{dw} = 0 - 2(w-10)^1 \cdot 1$$

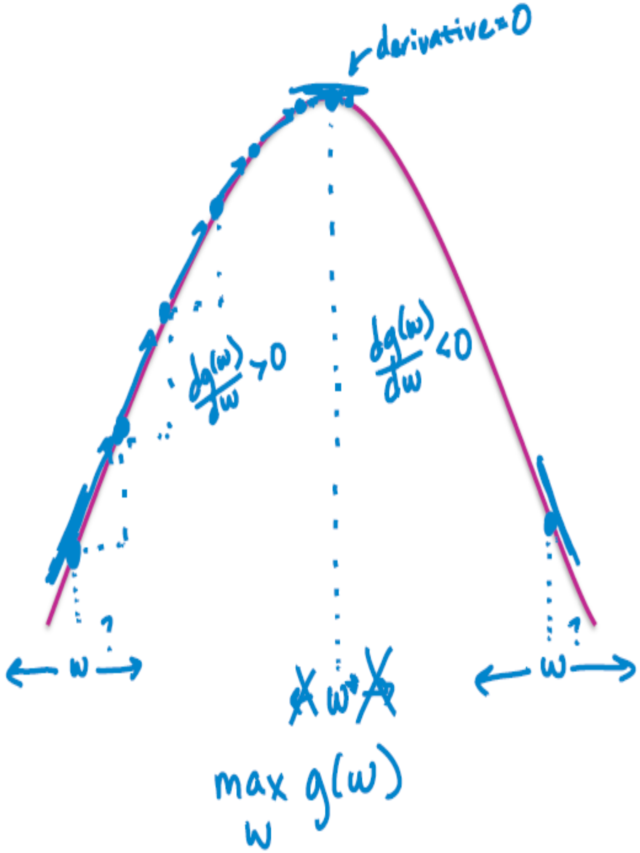
$$= -2w + 20$$

set derivate = 0:

$$-2w+20=0$$

$$w = 10$$

Finding the max via hill climbing



Sign of the derivative is saying me what I want to do :move left or right or stay where I am

How do we know whether to move w to right or left ? (inc. or dec. the value of w?)

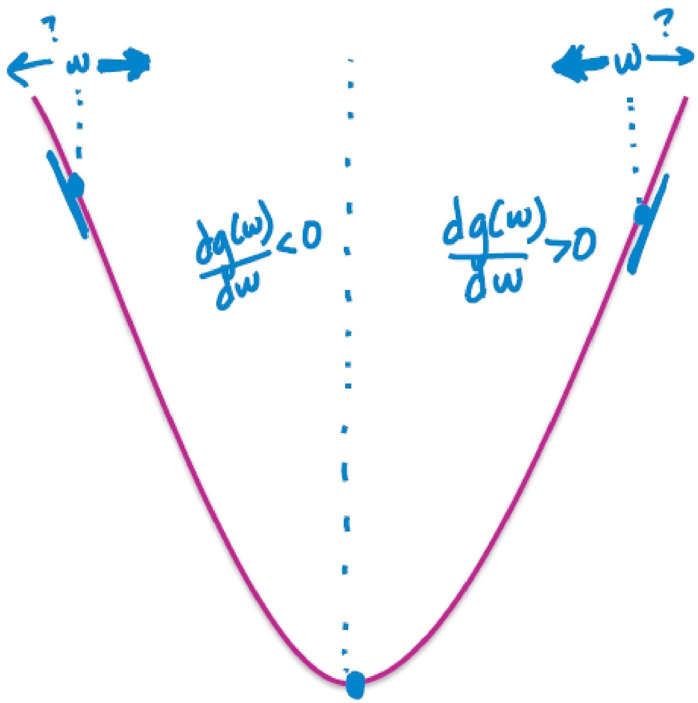
while not converged

$$w^{(t+1)} \leftarrow w^{(t)} + \eta \frac{dg(w)}{dw}$$

iteration t

stepsize

Finding the min via hill descent



$\min_w g(w)$

when derivative is positive, we want to decrease w
and when derivative is negative, we want to increase w

Algorithm:

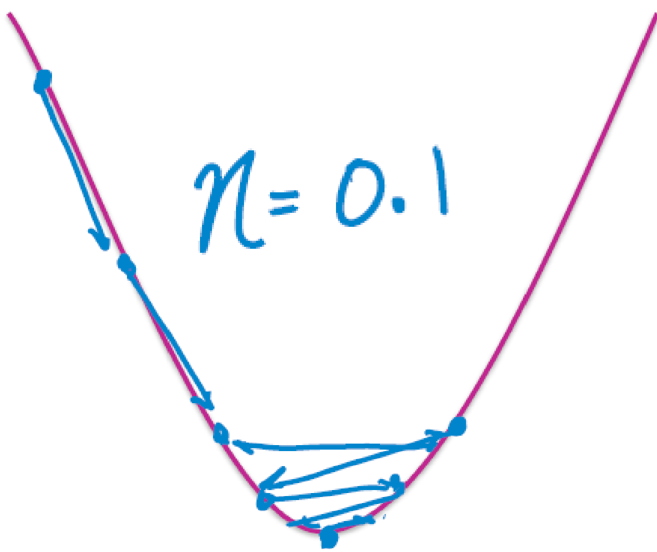
while not converged

$$w^{(t+1)} \leftarrow w^{(t)} - \eta \left.\frac{dg}{dw}\right|_{w^{(t)}}$$

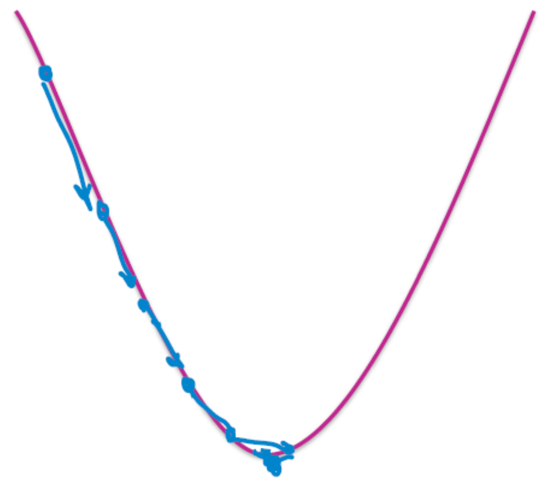
Choosing the step size (stepsize schedule)

Fixed

Works well for strongly convex functions



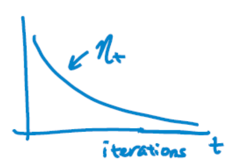
Varying



Common choices:

$$\eta_t = \frac{\alpha}{t}$$

$$\eta_t = \frac{\alpha}{\sqrt{t}}$$



Try not to decrease η too fast

Convergence criteria

For convex functions,

optimum occurs when

$$\frac{dg(w)}{dw} = 0$$

In practice, stop when

$$\left|\frac{dg(w)}{dw}\right| < \epsilon$$

threshold to be set

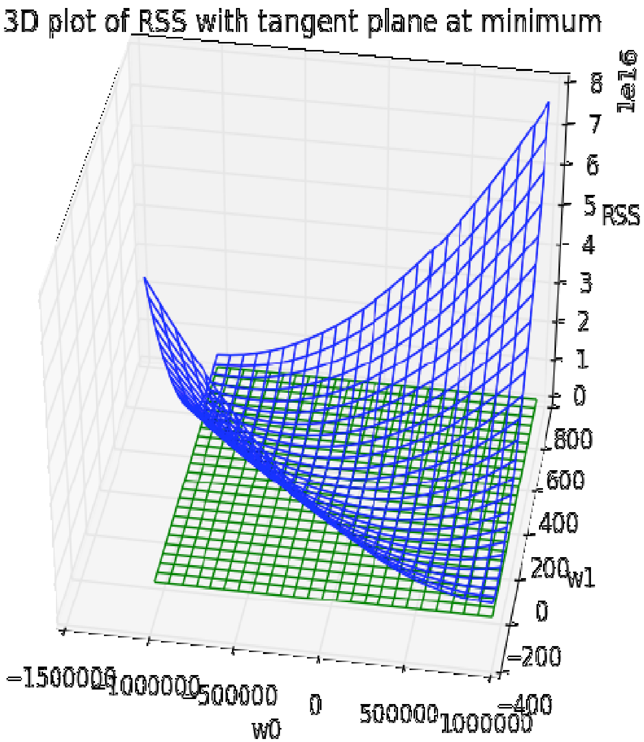
That will be „good enough"
value of ε depends on the data we are looking at

Algorithm:

while not converged

$$w^{(t+1)} \leftarrow w^{(t)} - \eta \left.\frac{dg}{dw}\right|_{w^{(t)}}$$

Moving to multiple dimensions



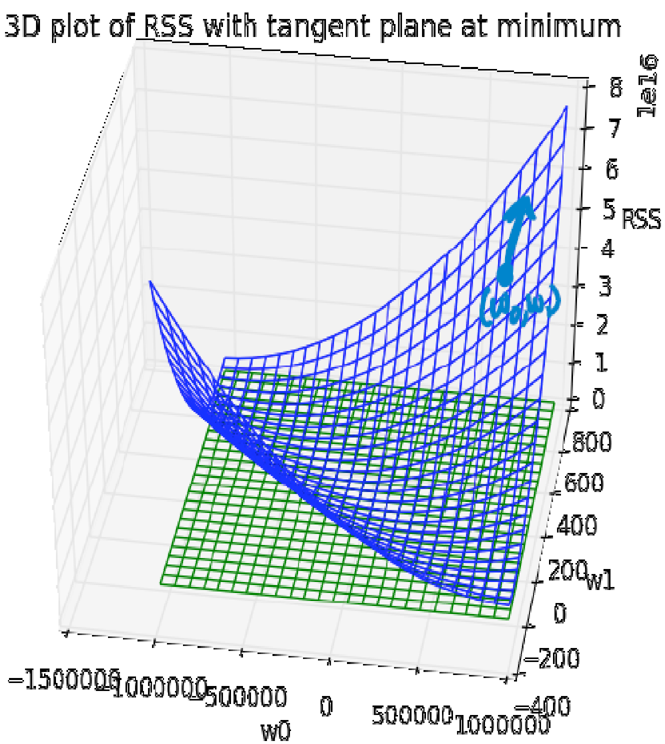
$$\nabla g(w) = \begin{bmatrix} \frac{\partial g}{\partial w_0} \\ \frac{\partial g}{\partial w_1} \\ \vdots \\ \frac{\partial g}{\partial w_p} \end{bmatrix} \left.\vphantom{\begin{bmatrix} a \\ a \\ a \\ a \end{bmatrix}}\right\} \text{(p+1)-dimensional vector}$$

gradient

$[w_0, w_1, \dots, w_p]$

partial derivative is like a derivate with respect to w_1 treating all other variables as constants

Gradient example



$$g(w) = 5w_0 + \underline{10}\,\underline{w}_0 w_1 + 2w_1^2$$

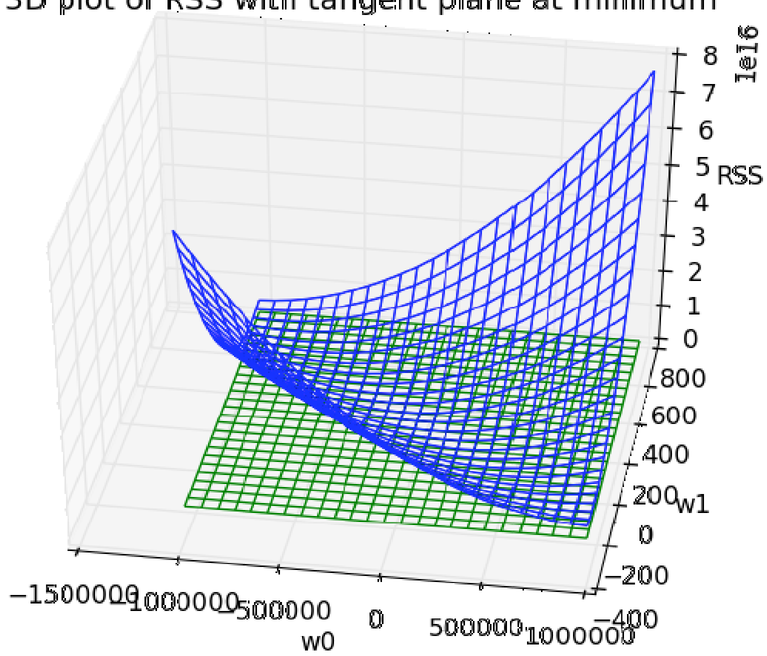
$$\frac{\partial g}{\partial w_0} = 5 + 10w_1$$

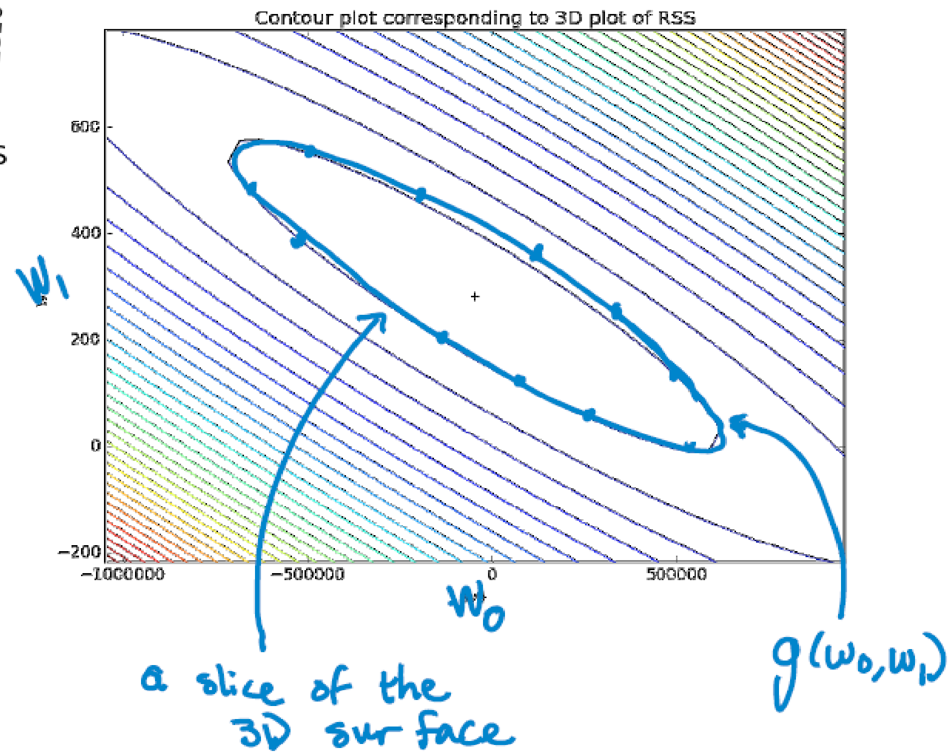
$$\frac{\partial g}{\partial w_1} = 10w_0 + 4w_1$$

$$\nabla g(w) = \begin{bmatrix} 5 + 10w_1 \\ 10w_0 + 4w_1 \end{bmatrix}$$

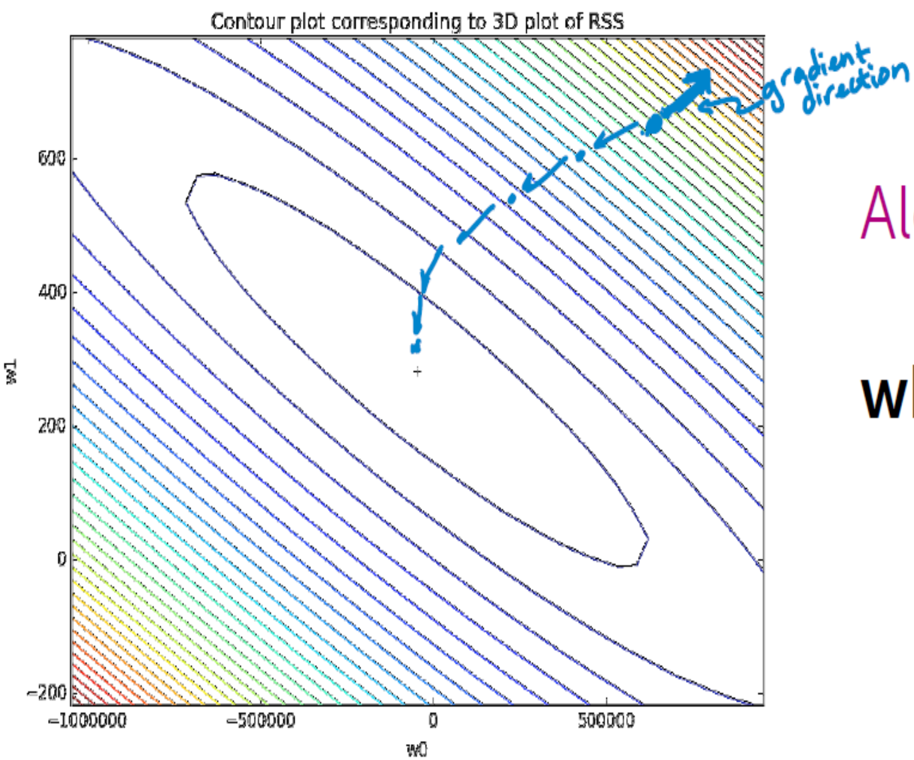
Contour plots

bird's eye view





Gradient descent



Algorithm:

while not converged

$$w^{(t+1)} \leftarrow w^{(t)} - \eta \nabla \underline{g(w^{(t)})}$$

$$\begin{bmatrix} \vdots \end{bmatrix} \leftarrow \begin{bmatrix} \vdots \end{bmatrix} - \eta \begin{bmatrix} \vdots \end{bmatrix}$$

$$\boxed{\text{Convergence: } \|\nabla g(w)\| < \epsilon}$$

Compute the gradient

$$RSS(w_0,w_1) = \sum_{i=1}^{N} (y_i-[w_0+w_1x_i])^2$$

Taking the derivative w.r.t. w_0

$$\sum_{i=1}^{N} 2(y_i - [w_0+w_1x_i])^1 \cdot (-1)$$

$$= -2\sum_{i=1}^{N} (y_i - [w_0+w_1x_i])$$

Taking the derivative w.r.t. w_1

$$\sum_{i=1}^{N} 2(\underline{y_i - [w_0+w_1x_i]})^1 \cdot (-x_i)$$

$$= -2\sum_{i=1}^{N} (y_i - [w_0+w_1x_i])\underline{x_i}$$

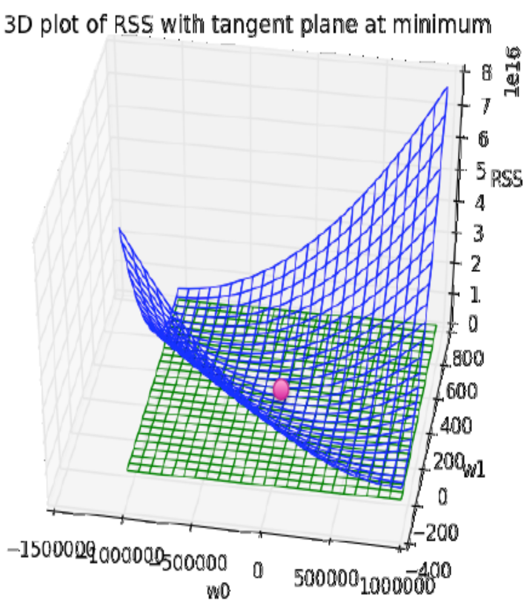
Putting it together:

$$\nabla RSS(w_0,w_1) = \begin{bmatrix} -2\sum_{i=1}^{N}[y_i - (w_0+w_1x_i)] \\ -2\sum_{i=1}^{N}[y_i - (w_0+w_1x_i)]x_i \end{bmatrix}$$

Approach 1: set gradient to 0

$$\nabla RSS(w_0, w_1) = \begin{bmatrix} -2\sum_{i=1}^{N}[y_i - (w_0 + w_1 x_i)] \\ -2\sum_{i=1}^{N}[y_i - (w_0 + w_1 x_i)]x_i \end{bmatrix}$$

This method is called „Closed form solution"



top term:

average house sales price

estimate of the slope

average sq. ft.

$$\hat{w}_0 = \frac{\sum_{i=1}^{N} y_i}{N} - \hat{w}_1 \frac{\sum_{i=1}^{N} x_i}{N}$$

bottom term:

$$\sum y_i x_i - \hat{w}_0 \sum x_i - \hat{w}_1 \sum x_i^2 = 0$$

plug in

$$\hat{w}_1 = \frac{\sum y_i x_i - \frac{\sum y_i \sum x_i}{N}}{\sum x_i^2 - \frac{\sum x_i \sum x_i}{N}}$$

Note:

$\sum_{i=1}^{N} y_i$

$\sum_{i=1}^{N} x_i$

$\sum_{i=1}^{N} y_i x_i$

$\sum_{i=1}^{N} x_i^2$

Approach 2: gradient descent

Interpreting the gradient:

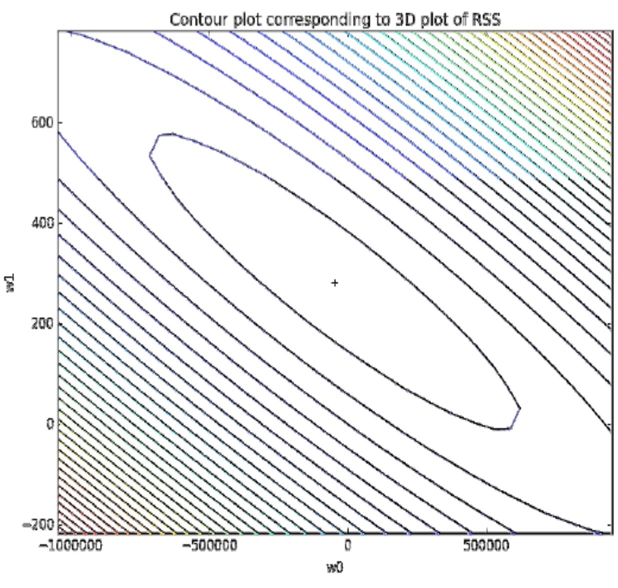
actual house sales observation

predicted value $\hat{y}_i(w_0, w_1)$

$$\nabla RSS(w_0,w_1) = \begin{bmatrix} -2\sum_{i=1}^{N}[y_i - (w_0+w_1x_i)] \\ -2\sum_{i=1}^{N}[y_i - (w_0+w_1x_i)]x_i \end{bmatrix} = \begin{bmatrix} -2\sum_{i=1}^{N}[y_i - \hat{y}_i(w_0,w_1)] \\ -2\sum_{i=1}^{N}[y_i - \hat{y}_i(w_0,w_1)]x_i \end{bmatrix}$$

Approach 2: gradient descent

$$\nabla RSS(w_0,w_1) = \begin{bmatrix} -2\sum_{i=1}^{N} [y_i - \hat{y}_i(w_0,w_1)] \\ -2\sum_{i=1}^{N} [y_i - \hat{y}_i(w_0,w_1)]x_i \end{bmatrix}$$



while not converged $(-2)\cdot(-\eta)$

$$\begin{bmatrix} w_0^{(t+1)} \\ w_1^{(t+1)} \end{bmatrix} \leftarrow \begin{bmatrix} w_0^{(t)} \\ w_1^{(t)} \end{bmatrix} + 2\eta \begin{bmatrix} \sum_{i=1}^{N} [y_i - \hat{y}_i(w_0^{(t)}, w_1^{(t)})] \\ \sum_{i=1}^{N} [y_i - \hat{y}_i(w_0^{(t)}, w_1^{(t)})]x_i \end{bmatrix}$$

If overall, under predicting $\hat{y}_i$, then $\Sigma[y_i - \hat{y}_i]$ is positive

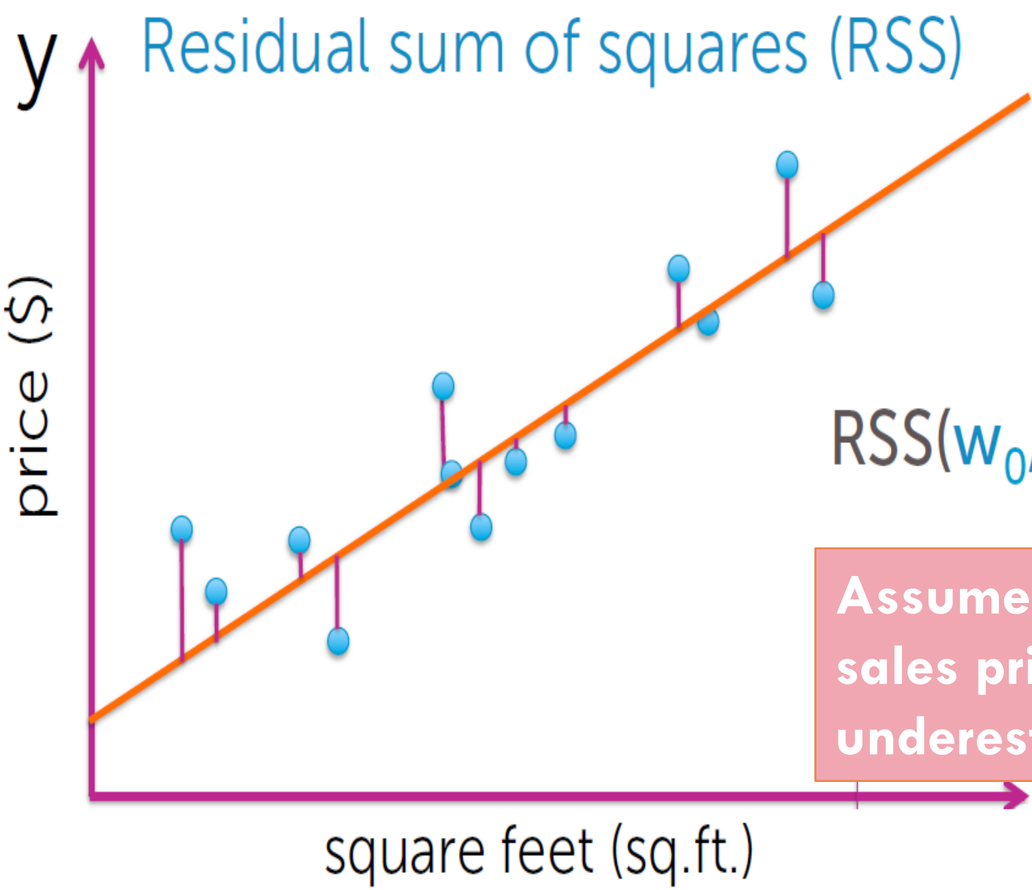
→ w_0 is going to increase

similar intuition for w_1, but multiply by x_i

Comparing the approaches

- For most ML problems, cannot solve gradient = 0
- Even if solving gradient = 0 is feasible, gradient descent can be more efficient
- Gradient descent relies on choosing stepsize and convergence criteria

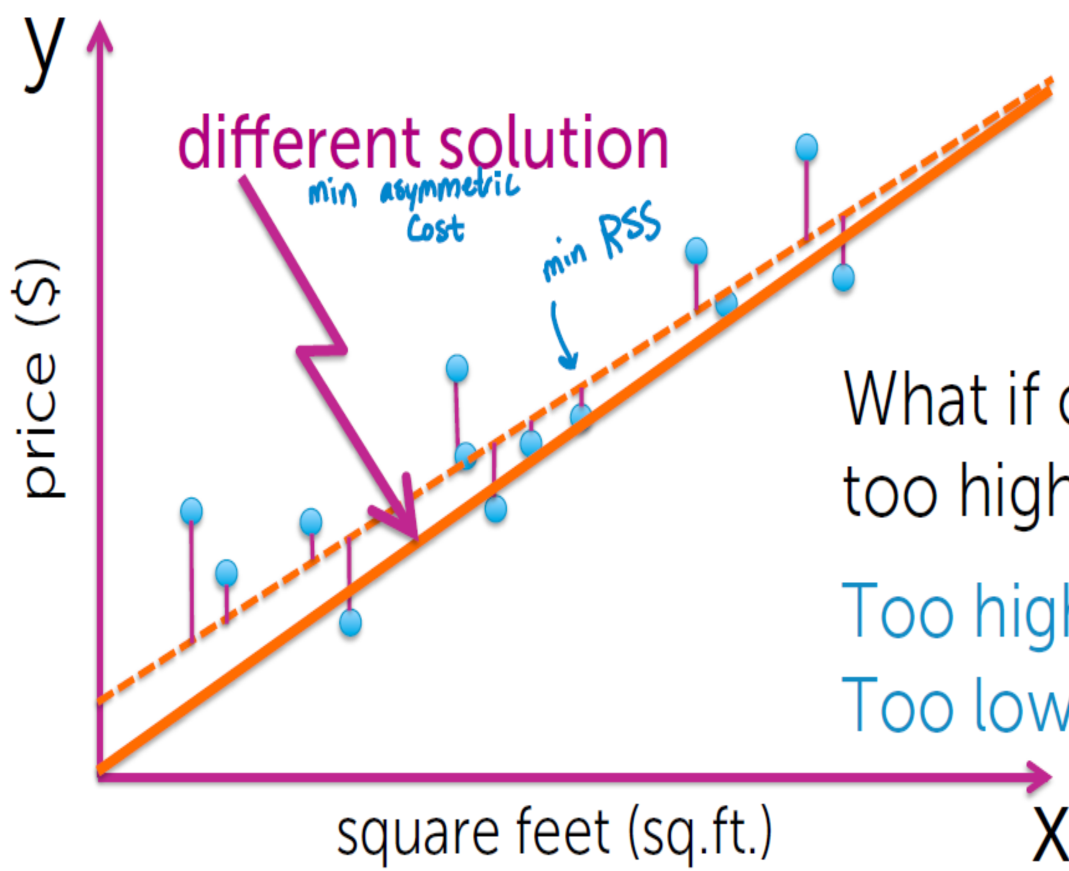
Symmetric cost function



$$RSS(w_0,w_1) = \sum_{i=1}^{N}(y_i-[w_0+w_1x_i])^2$$

Assumes error of overestimating sales price is the same as underestimating it

Asymmetric cost functions



We can weight differently positive and negative errors in RSS calculations.

What if cost of listing house too high has **bigger cost**?

Too high → no offers ($=0)

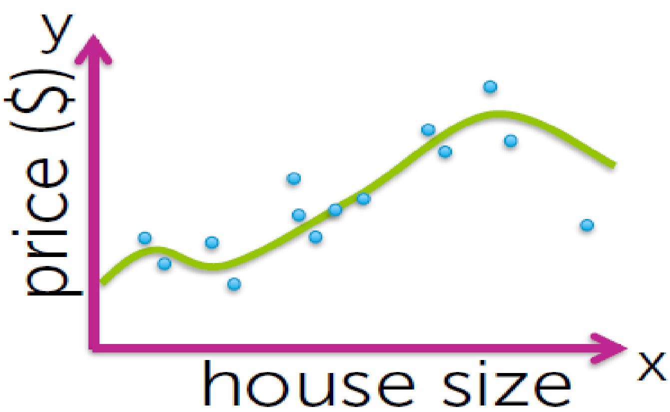
Too low → offers for lower $

What you can do now

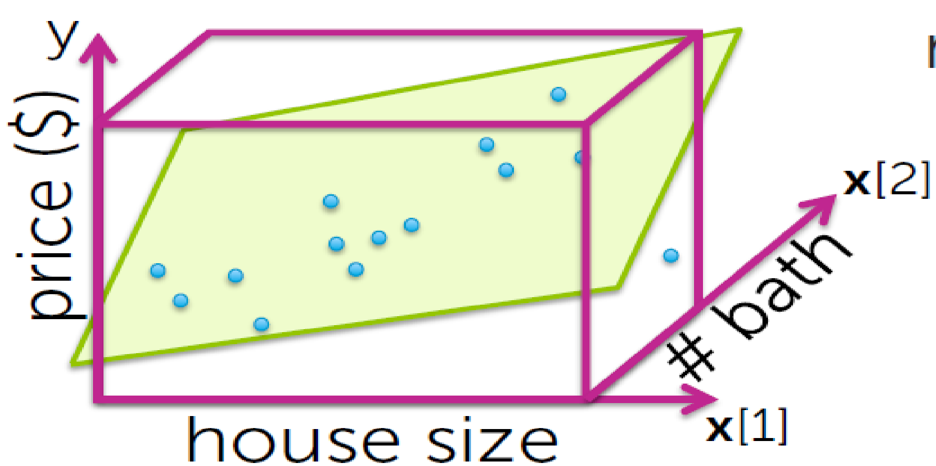
- Describe the input (features) and output (real-valued predictions) of a regression model
- Calculate a goodness-of-fit metric (e.g., RSS)
- Estimate model parameters to minimize RSS using gradient descent
- Interpret estimated model parameters
- Exploit the estimated model to form predictions
- Discuss the possible influence of high leverage points
- Describe intuitively how fitted line might change when assuming different goodness-of-fit metrics

MULTIPLE REGRESSION

Multiple regression



Fit more complex relationships than just a line



Incorporate more inputs

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

Polynomial regression

Model:

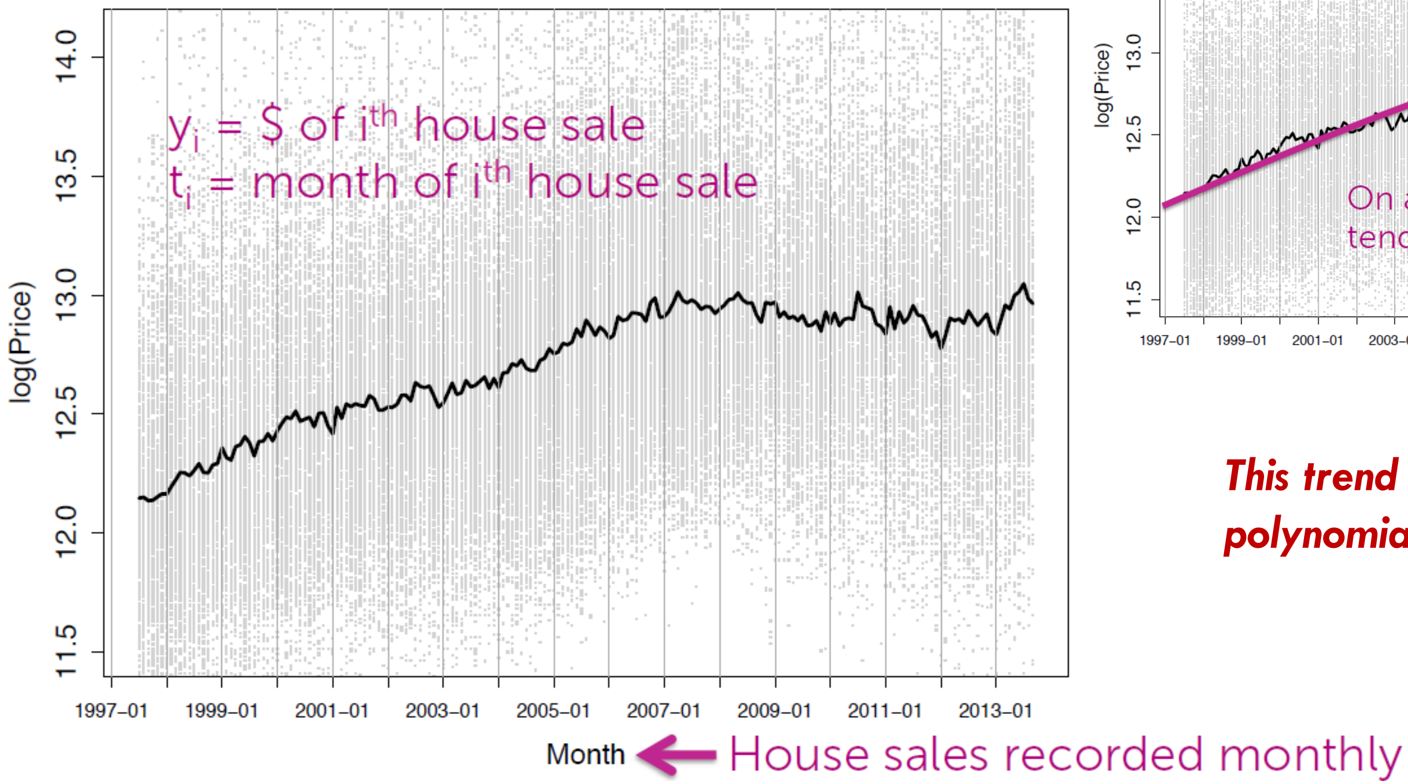
$$y_i = w_0 + w_1 x_i + w_2 x_i^2 + \ldots + w_p x_i^p + \varepsilon_i$$

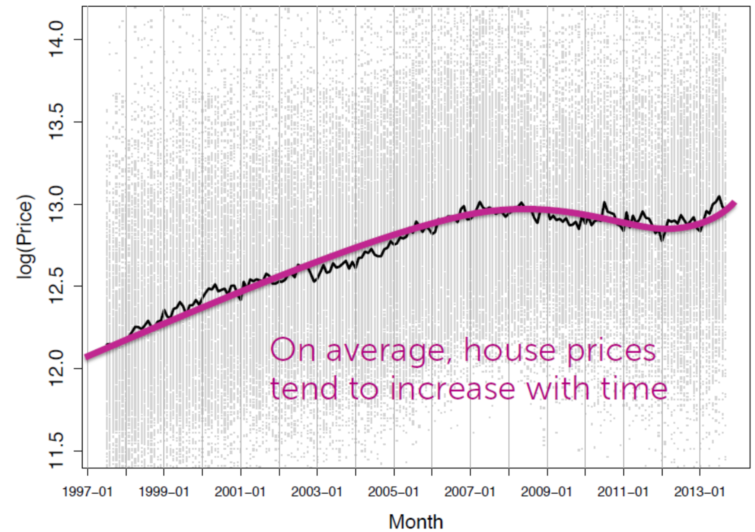
treat as different **features**

feature 1 = 1 (constant)	*parameter* 1 = w_0
feature 2 = x	*parameter* 2 = w_1
feature 3 = x^2	*parameter* 3 = w_2
…	…
feature p+1 = x^p	*parameter* p+1 = w_p

Other functional forms of one input

- **Trends in time series**

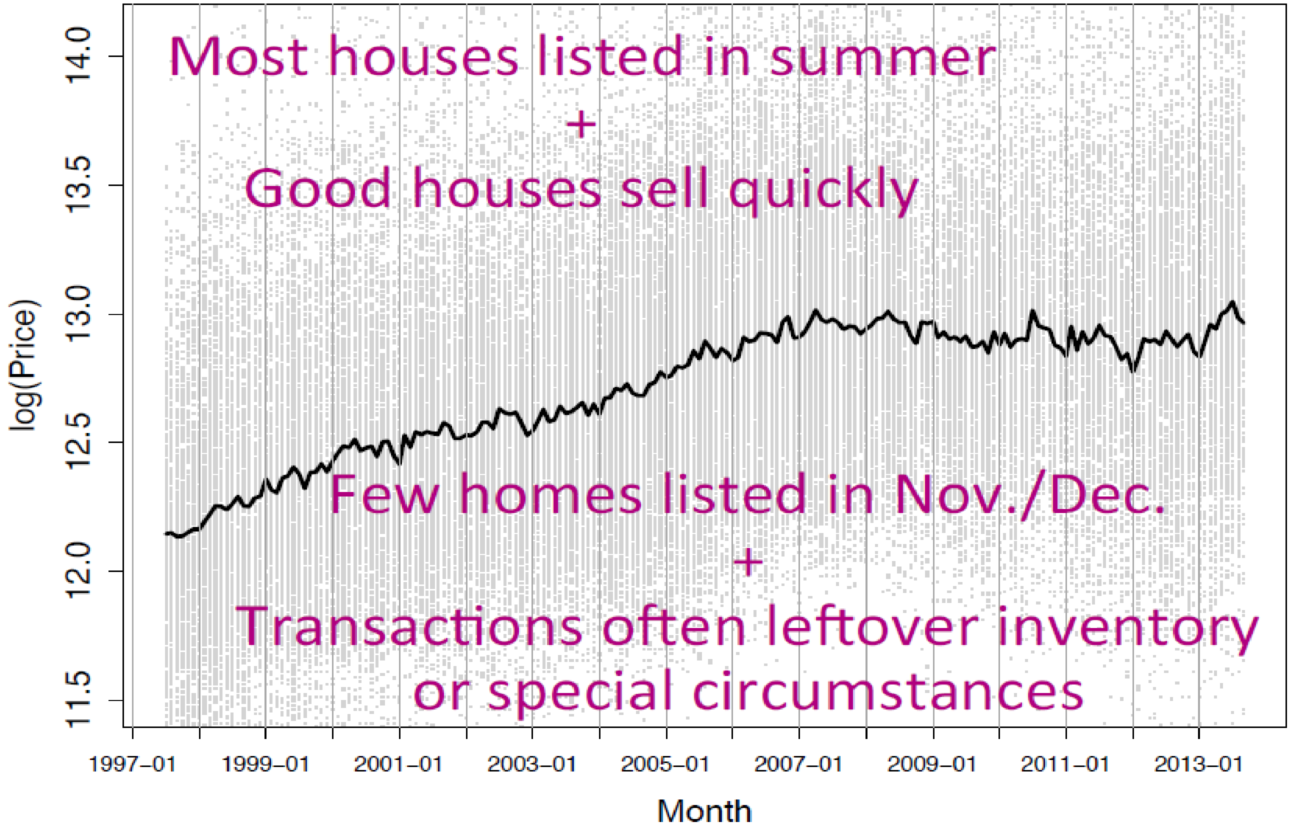




This trend can be modeled with polynomial function.

Other functional forms of one input

- **Seasonality**



Example of detrending

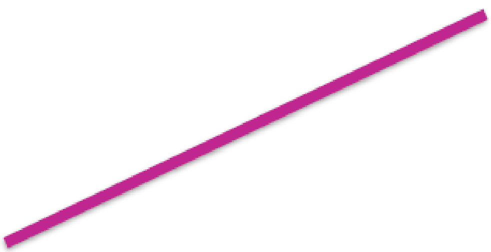
Model:

$$y_i = w_0 + w_1 t_i + w_2 \sin(2\pi t_i / 12 - \Phi) + \varepsilon_i$$

Unknown phase/shift

Linear trend

Seasonal component =
Sinusoid with period 12
(resets annually)



Trigonometric identity: sin(a-b)=sin(a)cos(b)-cos(a)sin(b)

$\rightarrow \sin(2\pi t_i / 12 - \Phi) = \sin(2\pi t_i / 12)\cos(\Phi) - \cos(2\pi t_i / 12)\sin(\Phi)$

Example of detrending

Equivalently,

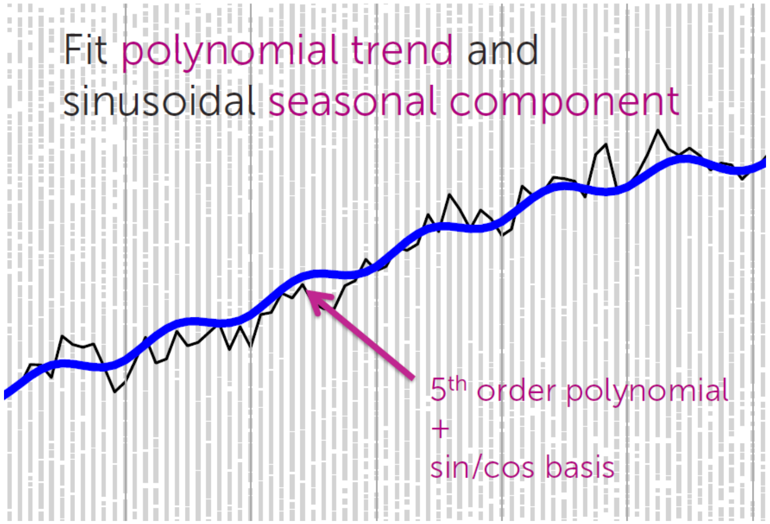
$$y_i = w_0 + w_1 t_i + w_2 \sin(2\pi t_i / 12) + w_3 \cos(2\pi t_i / 12) + \varepsilon_i$$

feature 1 = 1 (constant)

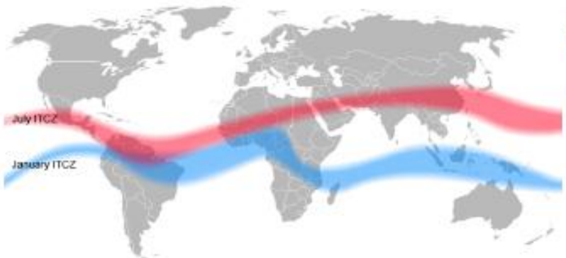
feature 2 = t

feature 3 = sin(2πt/12)

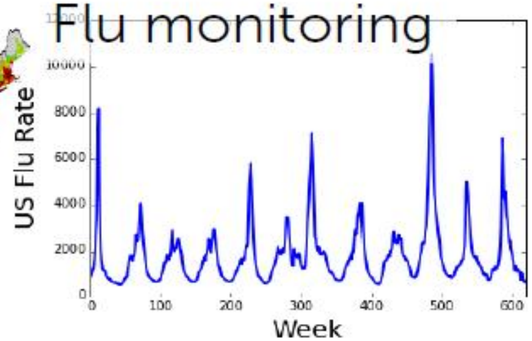
feature 4 = cos(2πt/12)

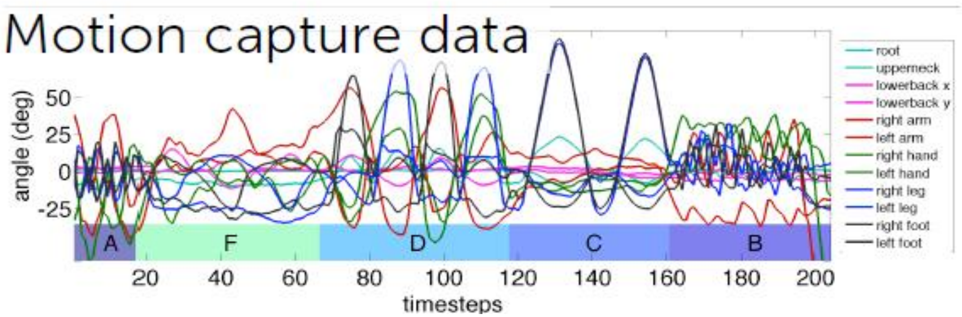


Other examples of seasonality



Weather modeling
(e.g., temperature, rainfall)





Generic basic expansion

Model:

$$y_i = w_0 h_0(x_i) + w_1 h_1(x_i) + \ldots + w_D h_D(x_i) + \varepsilon_i$$

$$= \sum_{j=0}^{D} w_j h_j(x_i) + \varepsilon_i$$

feature 1 = $h_0(x)$...often 1 (constant)

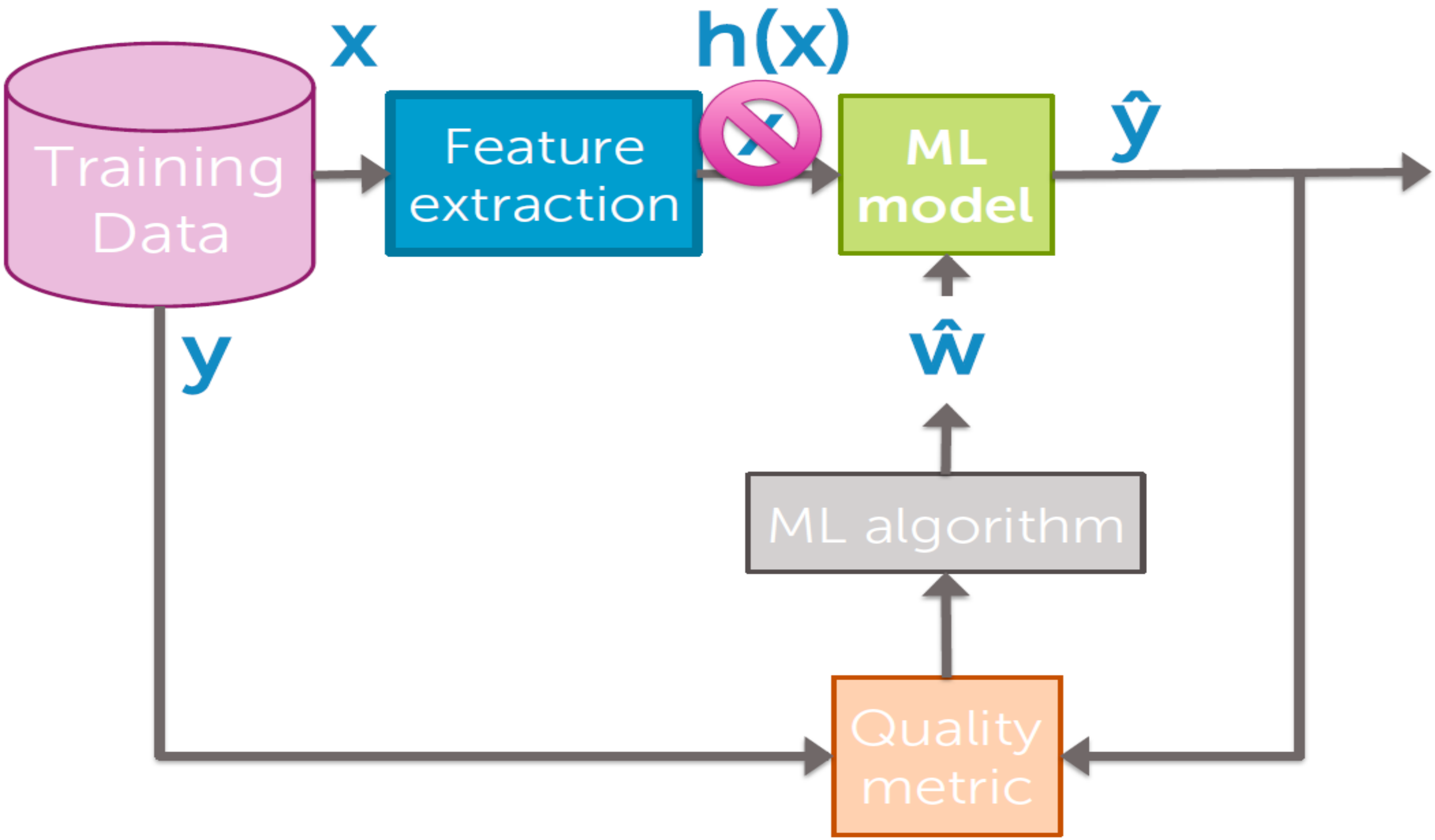
feature 2 = $h_1(x)$... e.g., x

feature 3 = $h_2(x)$... e.g., x^2 or $\sin(2\pi x/12)$

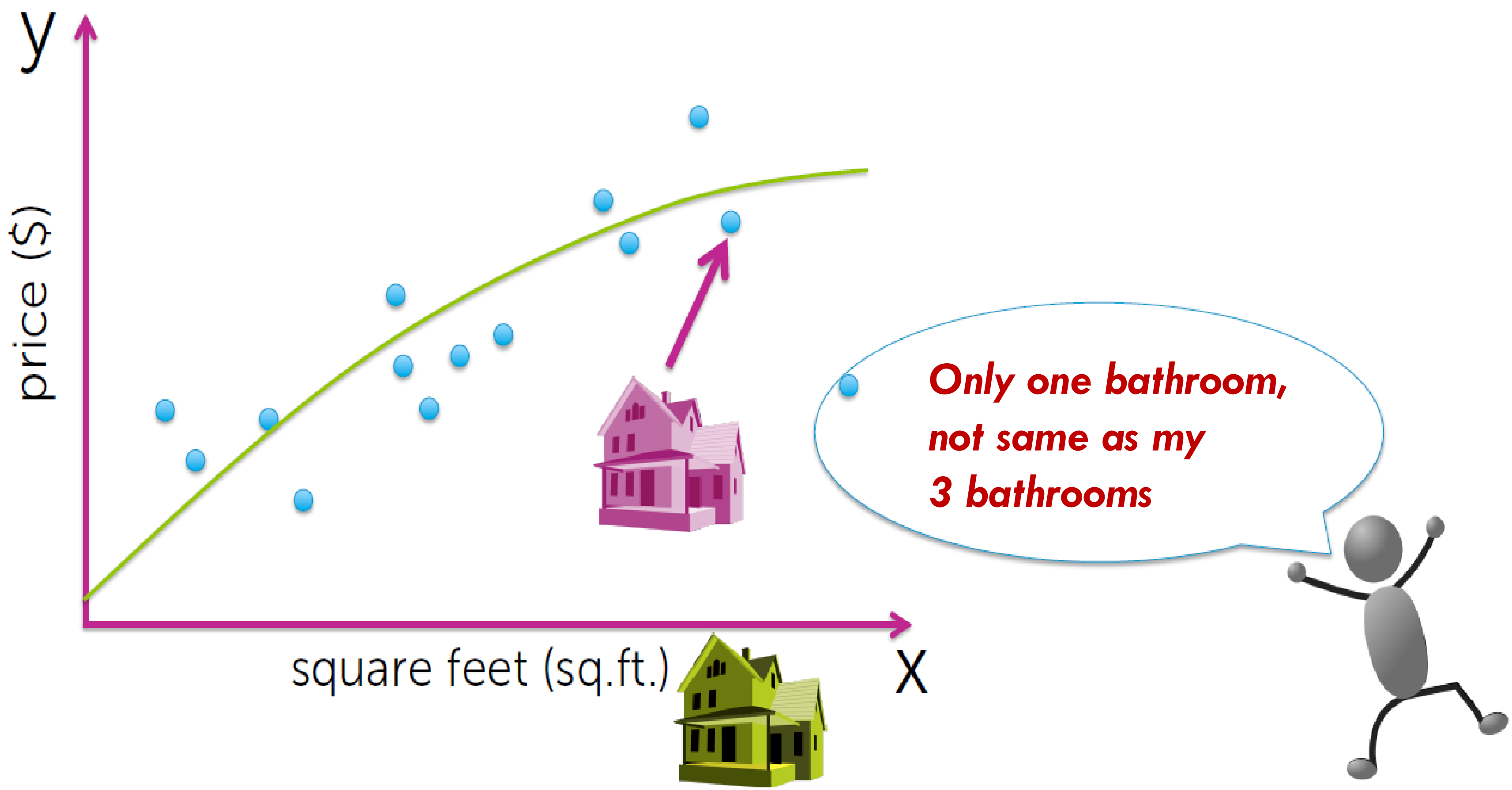
...

feature D+1 = $h_D(x)$... e.g., x^p

More realistic flow chart

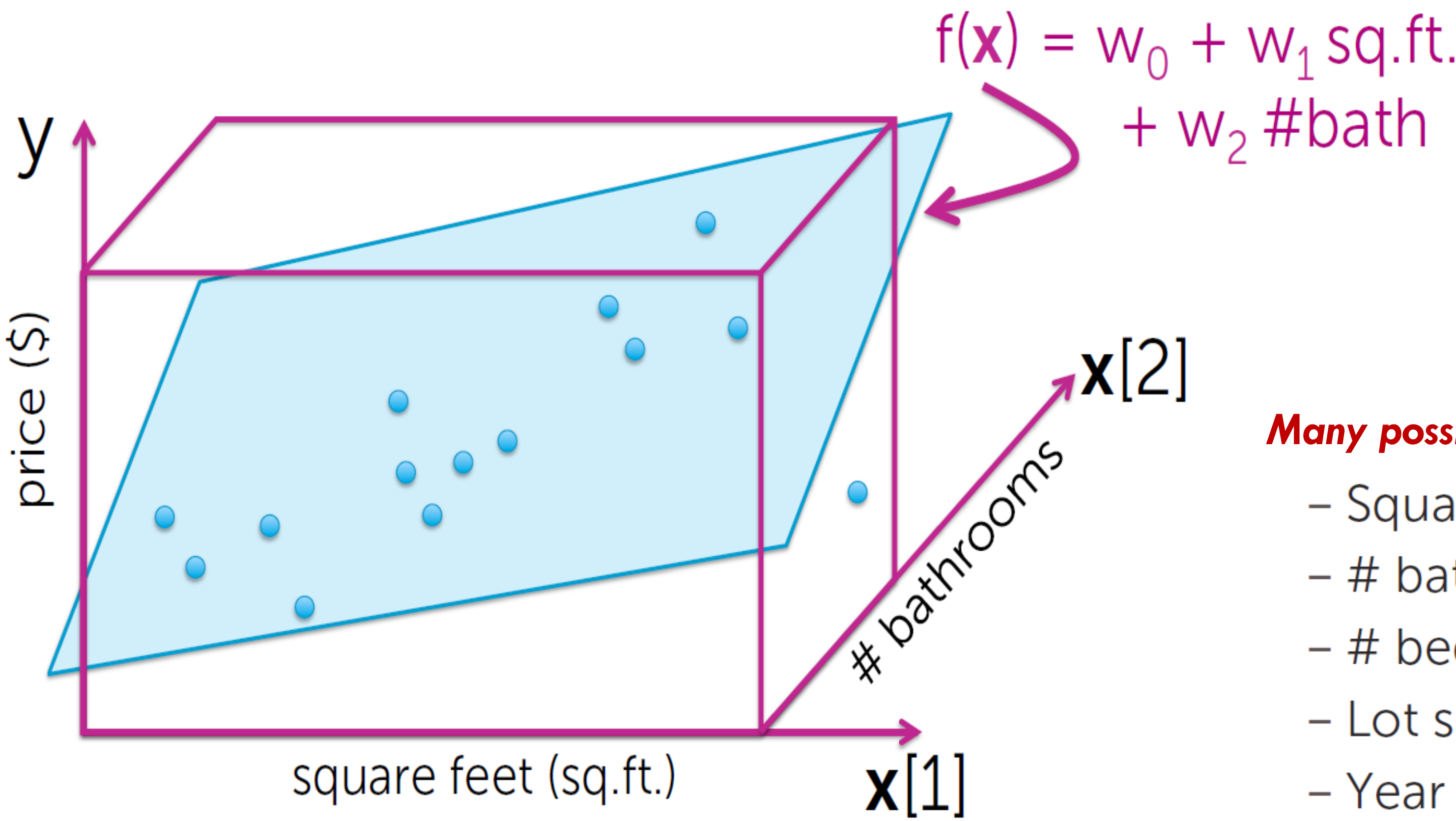


Incorporating multiple inputs



– ...

Incorporating multiple inputs



Many possible inputs

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

General notation

Output: y scalar

Inputs: $\mathbf{x} = (\mathbf{x}[1], \mathbf{x}[2], \ldots, \mathbf{x}[d])$

d-dim vector

Notational conventions:

- $\mathbf{x}[j]$ = j^{th} input (*scalar*)
- $h_j(\mathbf{x})$ = j^{th} feature (*scalar*)
- $\mathbf{x}_i$ = input of i^{th} data point (*vector*)
- $\mathbf{x}_i[j]$ = j^{th} input of i^{th} data point (*scalar*)

Simple hyperplane

Model:

Noise term

$$y_i = w_0 + w_1\, \mathbf{x}_i[1] + \ldots + w_d\, \mathbf{x}_i[d] + \varepsilon_i$$

feature 1 = 1

feature 2 = **x**[1] … e.g., sq. ft.

feature 3 = **x**[2] … e.g., #bath

…

feature d+1 = **x**[d] … e.g., lot size

More generally: D-dimensional curve

Model:

$$y_i = w_0\, h_0(\mathbf{x}_i) + w_1\, h_1(\mathbf{x}_i) + \ldots + w_D\, h_D(\mathbf{x}_i) + \varepsilon_i$$

$$= \sum_{j=0}^{D} w_j\, h_j(\mathbf{x}_i) + \varepsilon_i$$

More on notation

\# observations $(\mathbf{x}_i, y_i)$: N

\# inputs $\mathbf{x}[j]$: d

\# features $h_j(\mathbf{x})$: D

feature 1 = $h_0(\mathbf{x})$ … e.g., 1

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

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

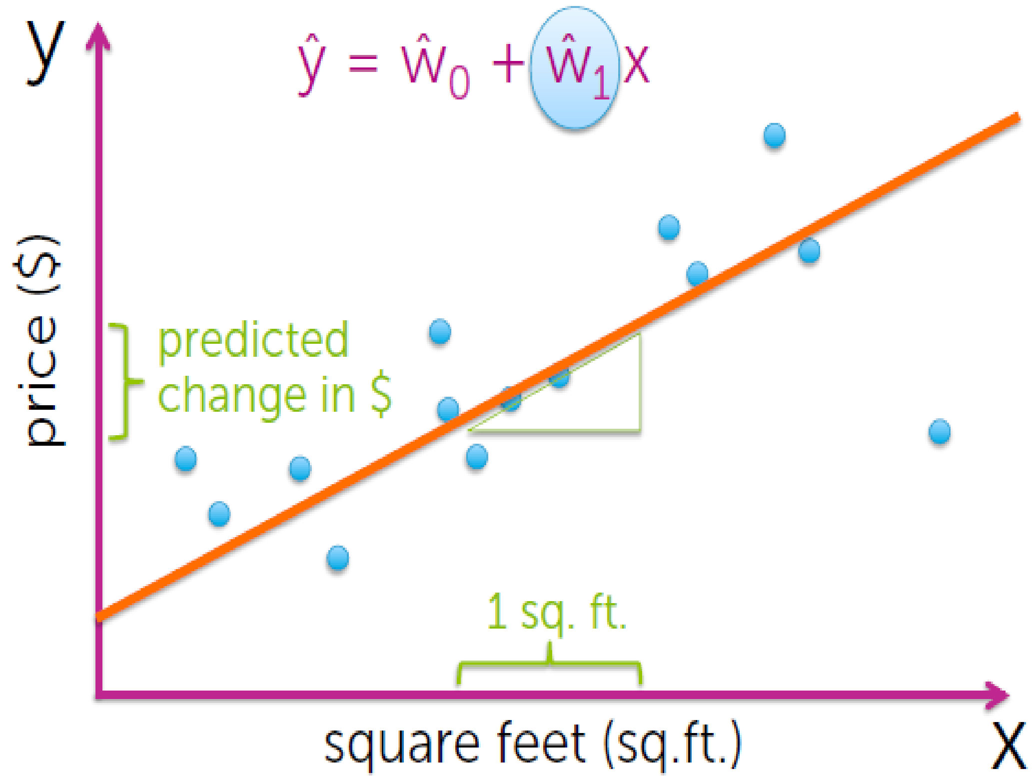
or, $\log(\mathbf{x}[7])\, \mathbf{x}[2]$ = log(#bed) x #bath

…

feature D+1 = $h_D(\mathbf{x})$ … some other function of $\mathbf{x}[1]$,…, $\mathbf{x}[d]$

Interpreting coefficients

Simple linear regression

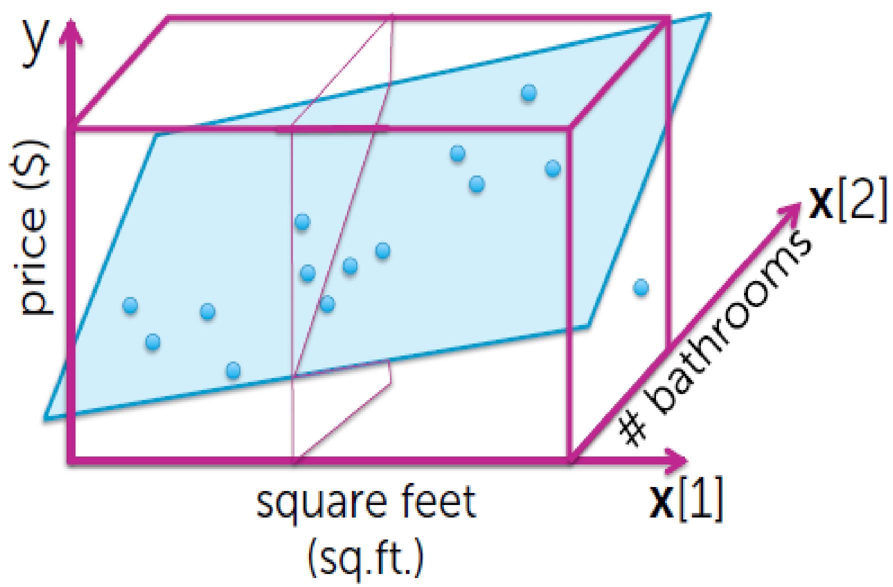


Interpreting coefficients

Two linear features

$$\hat{y} = \hat{w}_0 + \hat{w}_1 \boxed{\mathbf{x}[1]} + \hat{w}_2\,\mathbf{x}[2]$$

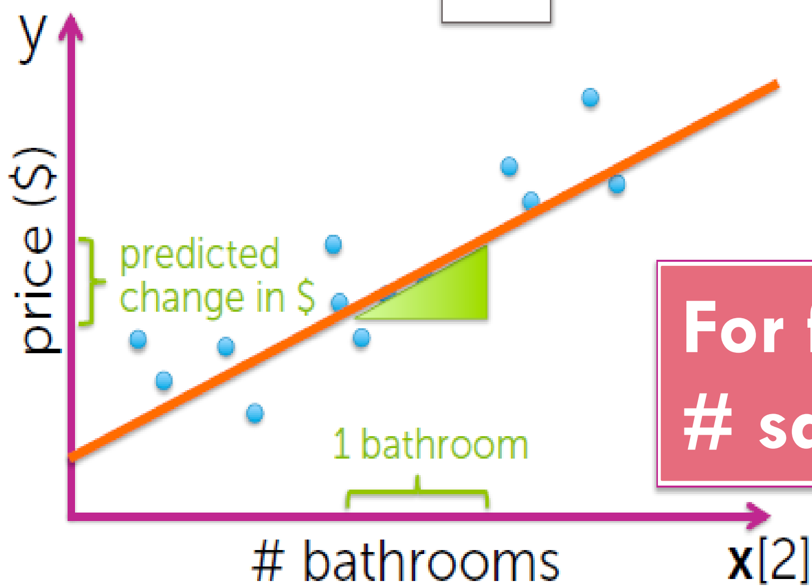
fix



Interpreting coefficients

Two linear features

$$\hat{y} = \hat{w}_0 + \hat{w}_1 \underbrace{\boxed{\mathbf{x}[1]}}_{\text{fix}} + \hat{w}_2 \mathbf{x}[2]$$



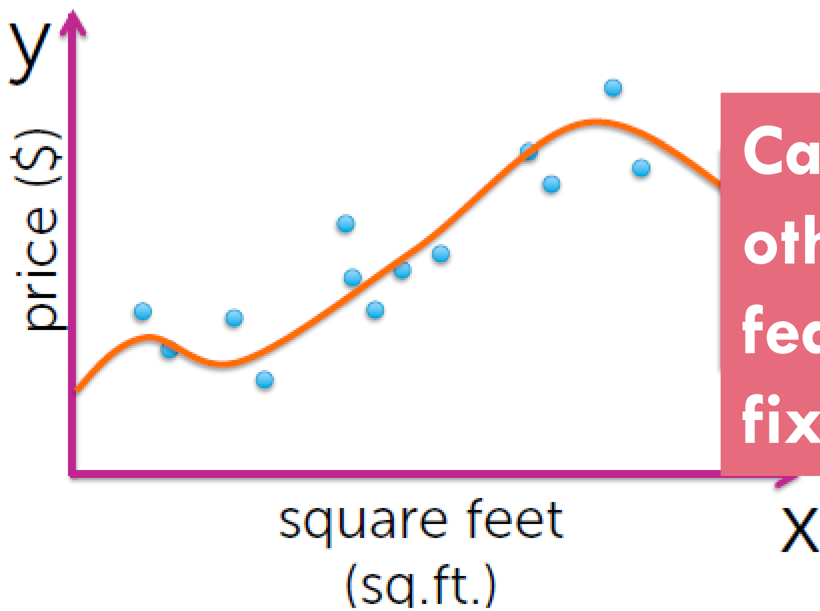
For fixed # sq.ft.!

But…
increasing #bathrooms for fixed #sq.ft will make your bedrooms smaller and smaller.
Think about interpretation.

Interpreting coefficients

Polynomial regression

$$\hat{y} = \hat{w}_0 + \hat{w}_1 x + \ldots + \hat{w}_j x^j + \ldots + \hat{w}_p x^p$$



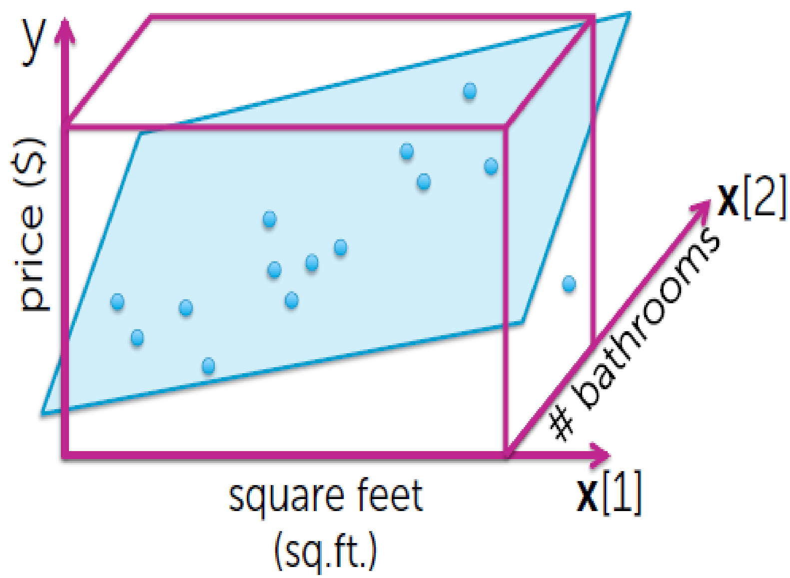
Can't hold other features fixed

Then … can't interpret coefficients

Interpreting coefficients

Multiple linear features

$$\hat{y} = \hat{w}_0 + \hat{w}_1 \underset{\text{fix}}{\boxed{\mathbf{x}[1]}} \underset{\text{fix}}{\boxed{+ \ldots}} + \hat{w}_j \mathbf{x}[j] \underset{\text{fix}}{\boxed{+ \ldots}} + \hat{w}_d \underset{\text{fix}}{\boxed{\mathbf{x}[d]}}$$



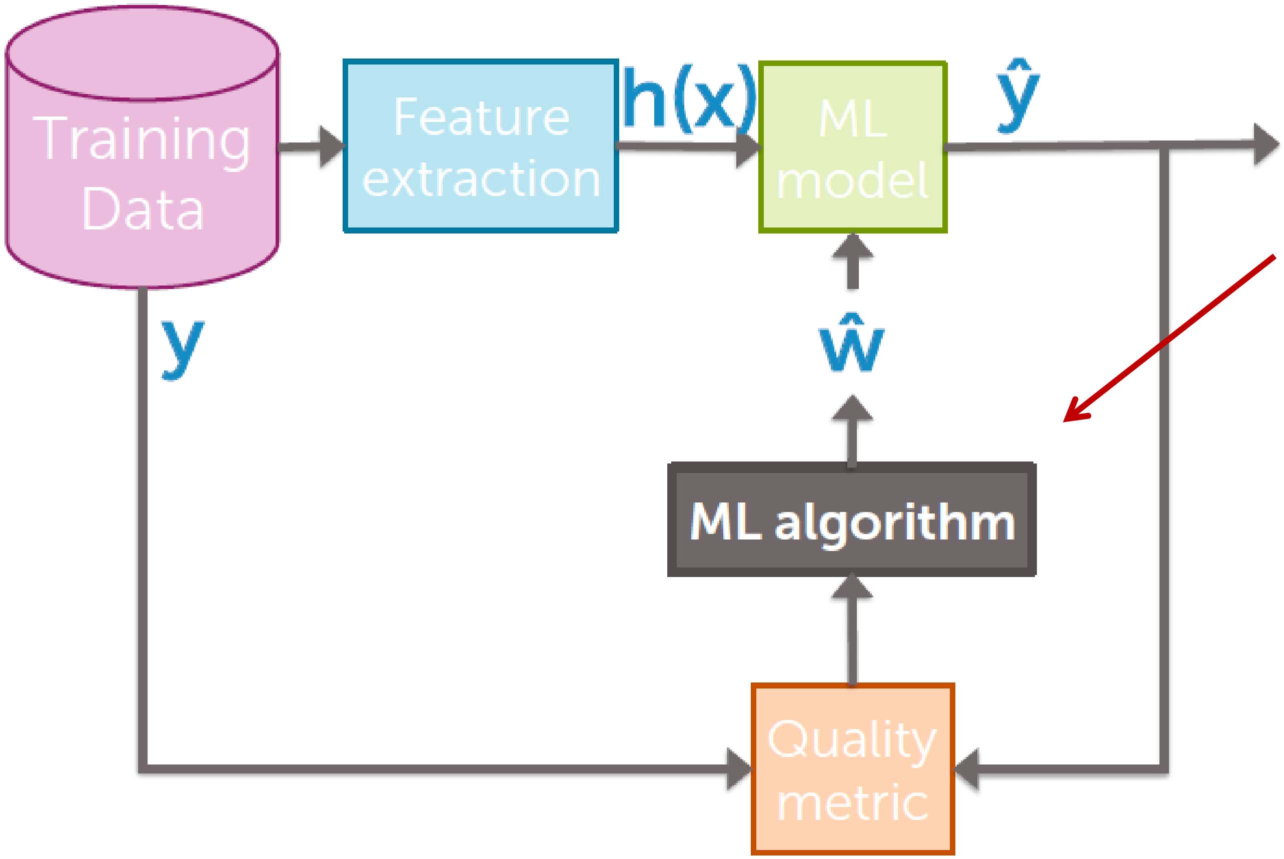
But…

increasing #bedrooms for fixed #sq.ft will make your bedrooms smaller and smaller.

You can end with negative coefficient. Might not be so if you removed #sq.ft from the model.

Think about interpretation in context of the model you put in.

Fitting in D-dimmensions

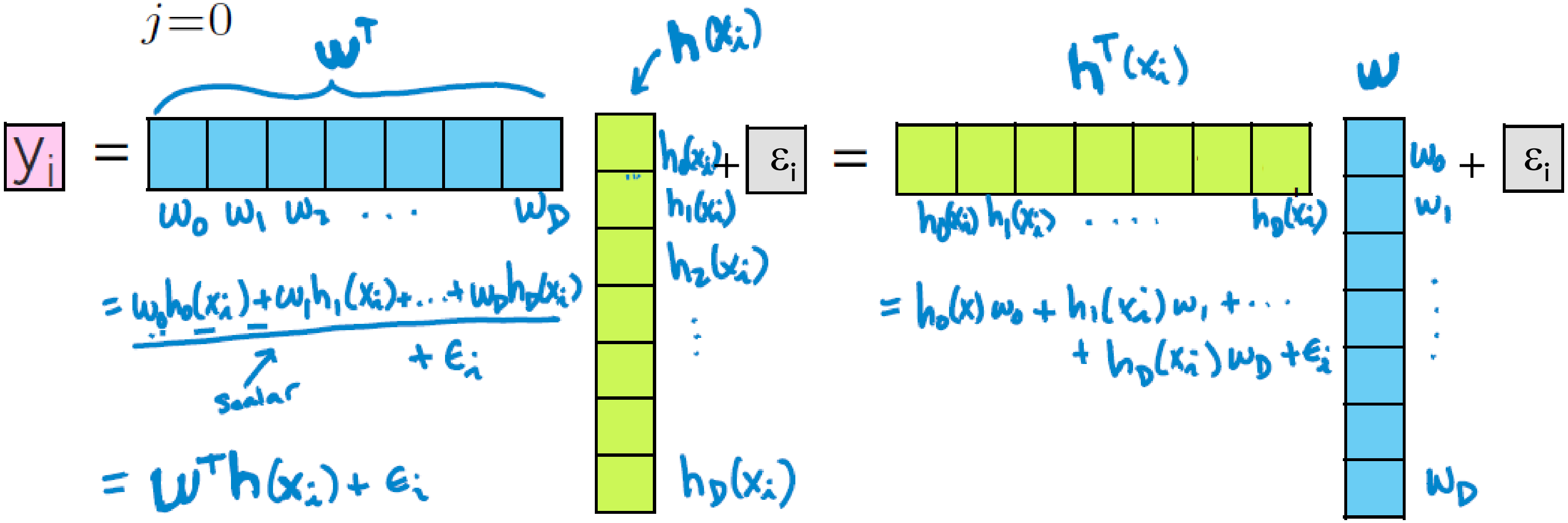


Look now at this block

Rewriting in vector notation

For observation i

$$y_i = \sum_{j=0}^{D} w_j h_j(\mathbf{x}_i) + \varepsilon_i$$



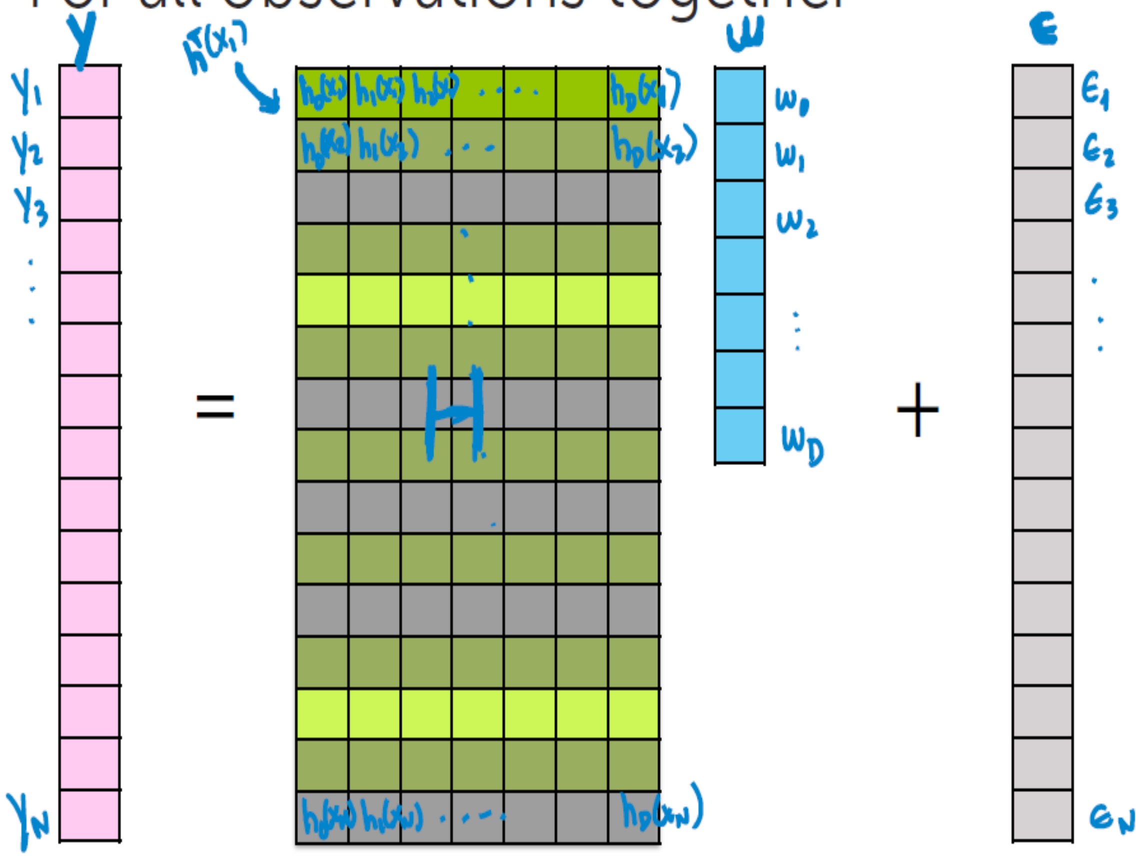
$= \underline{w_0 h_0(x_i) + w_1 h_1(x_i) + \dots + w_D h_D(x_i)} + \varepsilon_i$

$= w^T h(x_i) + \varepsilon_i$

$= h_0(x) w_0 + h_1(x_i) w_1 + \dots + h_D(x_i) w_D + \varepsilon_i$

Rewriting in matrix notation

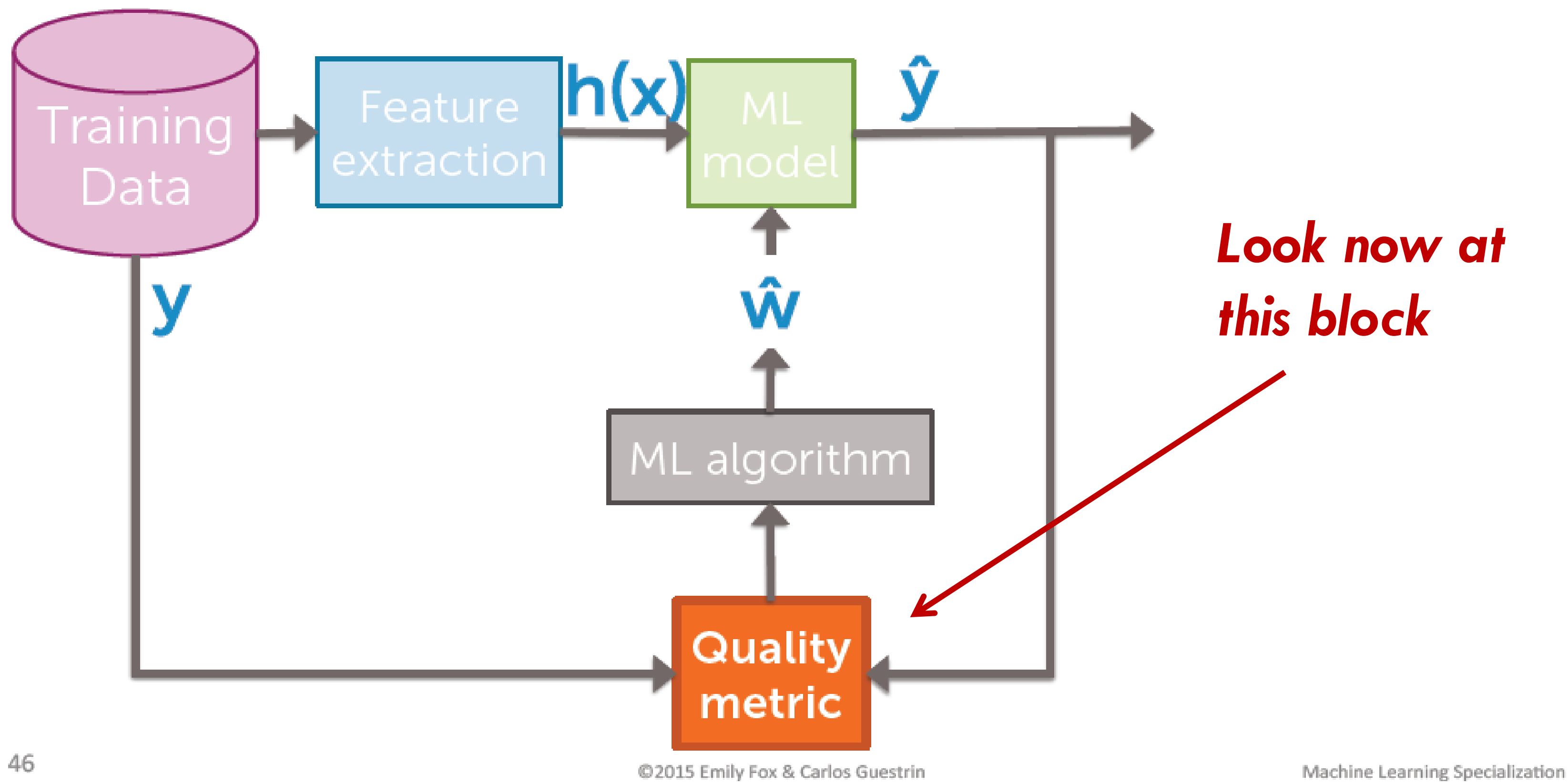
For all observations together



Here is our ML algorithm

$$\Rightarrow \boxed{y = Hw + \epsilon}$$

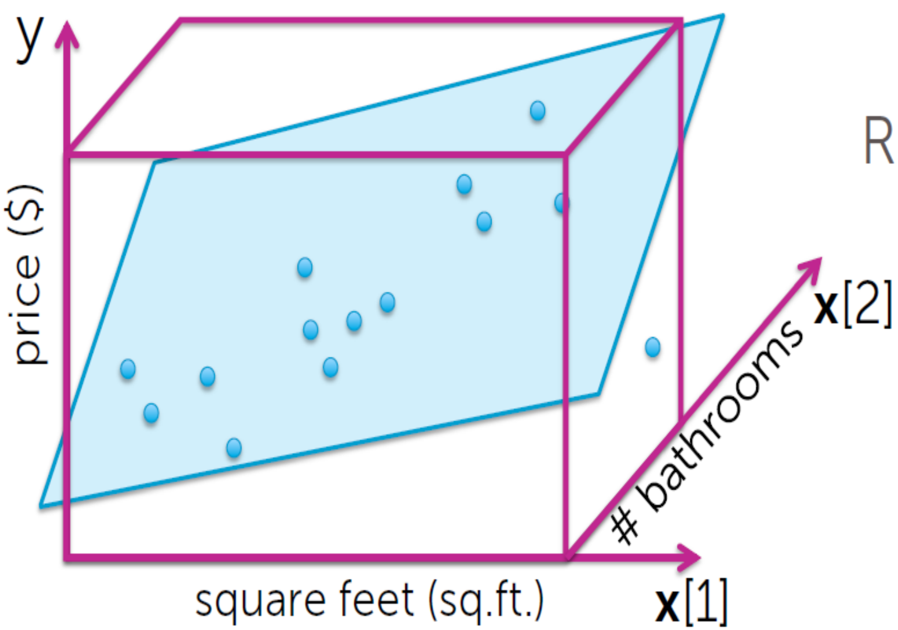
Fitting in D-dimmensions



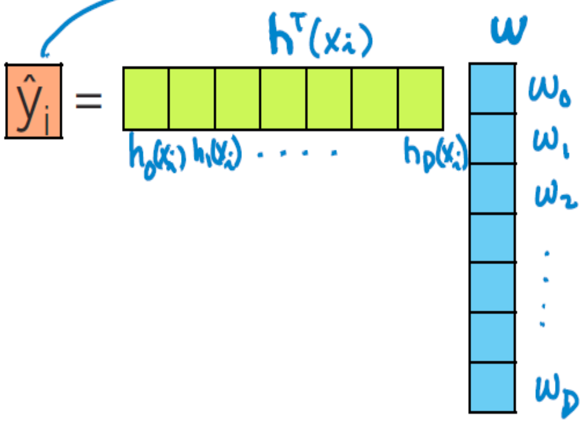
Look now at this block

Cost function in D-dimmension

RSS in vector notation



$$RSS(\mathbf{w}) = \sum_{i=1}^{N} (y_i - \underbrace{h^T(x_i)\, w}_{\hat{y}_i(w)})^2$$



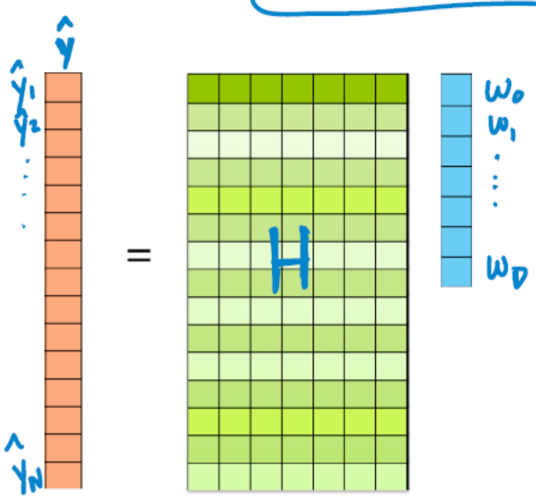
Cost function in D-dimmension

RSS in matrix notation

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

$$= (y-Hw)^T(y-Hw)$$

Why? (part 1)



$$\hat{y} = Hw$$

$$(y-Hw) = (y-\hat{y}) = \begin{bmatrix} \text{residual}_1 \\ \text{residual}_2 \\ \vdots \\ \text{residual}_N \end{bmatrix}$$

$$\text{residual}_i = y_i - \hat{y}_i$$

Regression model for D-dimmension

RSS in matrix notation

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

$$= (\mathbf{y} - \mathbf{H}\mathbf{w})^T \underbrace{(\mathbf{y} - \mathbf{H}\mathbf{w})}$$

Why? (part 2)

$$\begin{bmatrix} \text{residual}_1 & \text{residual}_2 & \text{residual}_3 & \cdots & \text{residual}_N \end{bmatrix} \begin{bmatrix} \text{residual}_1 \\ \text{residual}_2 \\ \text{residual}_3 \\ \cdots \\ \text{residual}_N \end{bmatrix} = \begin{aligned} &(\text{residual}_1^2 + \text{residual}_2^2 + \cdots \\ &\quad + \text{residual}_N^2) \\ &= \sum_{i=1}^{N} \text{residual}_i^2 \\ &\triangleq \mathrm{RSS}(w) \end{aligned}$$

Regression model for D-dimmension

Gradient of RSS

$$\nabla \text{RSS}(\mathbf{w}) = \nabla[(\mathbf{y}-\mathbf{H}\mathbf{w})^T(\mathbf{y}-\mathbf{H}\mathbf{w})]$$
$$= -2\mathbf{H}^T(\mathbf{y}-\mathbf{H}\mathbf{w})$$

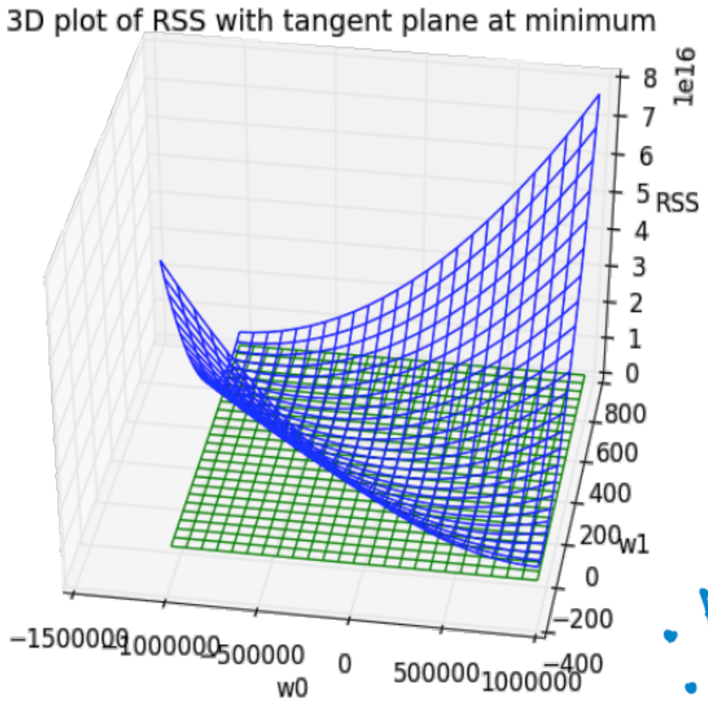
Why? By analogy to 1D case:

$$\frac{d}{dw}(y-hw)(y-hw) = \frac{d}{dw}(y-hw)^2 = 2\cdot(y-hw)^1(-h)$$
$$= -2h(y-hw)$$

scalars

Regression model for D-dimmension

Approach 1: set gradient to zero



Closed form solution

$\nabla \text{RSS}(\mathbf{w}) = -2\mathbf{H}^T(\mathbf{y}-\mathbf{H}\mathbf{w}) = 0$

Solve for **w**:

$-\cancel{2}H^Ty + \cancel{2}H^TH\hat{w} = 0$

$H^TH\hat{w} = H^Ty$

$\underbrace{(H^TH)^{-1}H^TH}_{I}\hat{w} = (H^TH)^{-1}H^Ty$

$\hat{w} = (H^TH)^{-1}H^Ty$

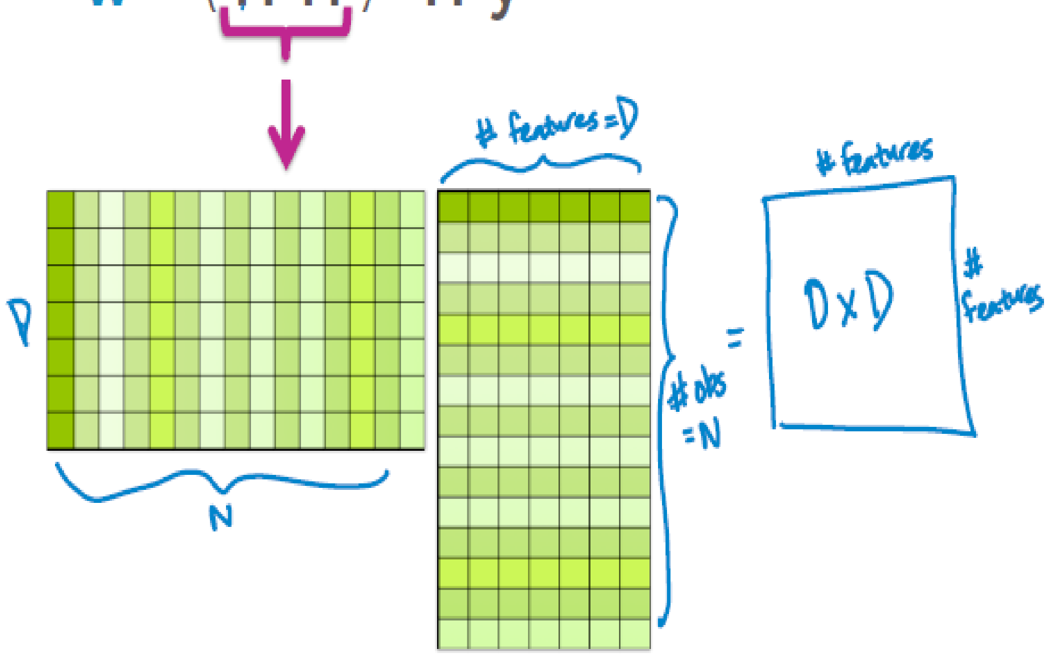
- $A^{-1}A = I$
- $Iv = v$

$IV = V$

Closed-form solution

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

This matrix might not be invertible.



really, # of linearly ind. observations

Invertible if:

In most cases is $N > D$

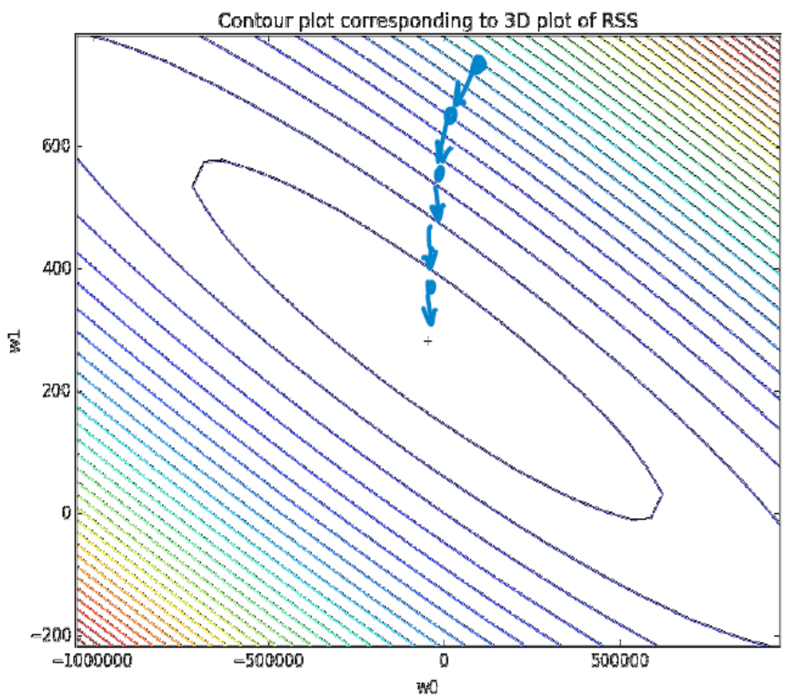
Complexity of inverse:

$O(D^3)$

This might not be CPU feasible.

Regression model for D-dimmension

Approach 2: gradient descent



We initialise our solution somewhere and then …

while not converged

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \eta \underbrace{\nabla \mathrm{RSS}(\mathbf{w}^{(t)})}_{-2\mathbf{H}^T(\mathbf{y}-\mathbf{H}\mathbf{w})}$$

$$\leftarrow w^{(t)} + 2\eta H^T(y - \underbrace{Hw^{(t)}}_{\hat{y}(w^{(t)})})$$

Gradient descent

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

$$= \sum_{i=1}^{N} (y_i - w_0 h_0(x_i) - w_1 h_1(x_i) - \ldots - w_D h_D(x_i))^2$$

Partial with respect to w_j

$$\sum_{i=1}^{N} 2(y_i - w_0 h_0(x_i) - w_1 h_1(x_i) \ldots - w_D h_D(x_i))^1 \cdot (-h_j(x_i))$$

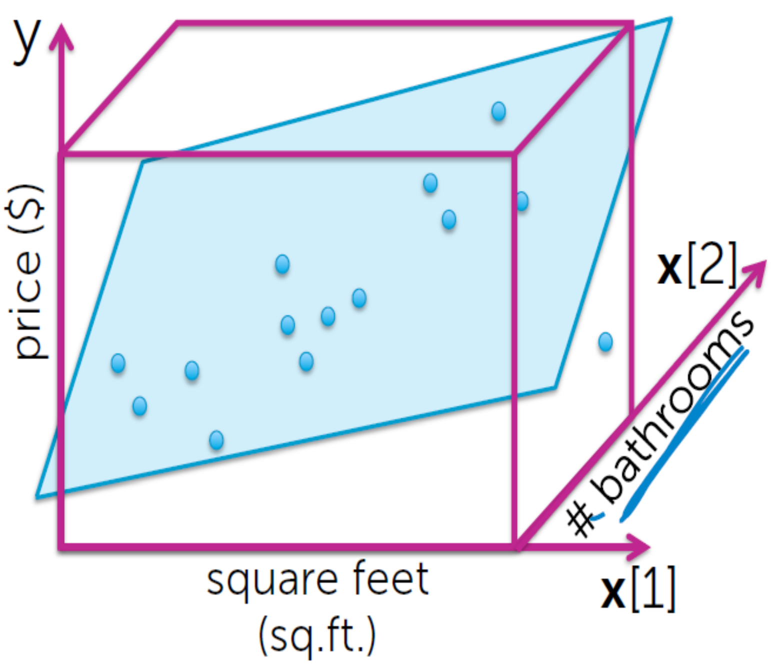
$$= -2 \sum_{i=1}^{N} h_j(x_i)(y_i - h(x_i)^T w)$$

Update to j^{th} feature weight:

$$w_j^{(t+1)} \leftarrow w_j^{(t)} - \eta\Big(-2\sum_{i=1}^{N} h_j(x_i)(y_i - \underbrace{h^T(x_i)\, w^{(t)}}_{\hat{y}_i(w^{(t)})})\Big)$$

Regression model for D-dimmension

Interpreting elementwise



bathrooms

Update to jth feature weight:

bath for house i

$$w_j^{(t+1)} \leftarrow w_j^{(t)} + 2\eta \sum_{i=1}^{N} h_j(\mathbf{x}_i)(y_i - \hat{y}_i(\mathbf{w}^{(t)}))$$

If underestimating impact of # bath ($\hat{w}_j^{(t)}$ is too small)

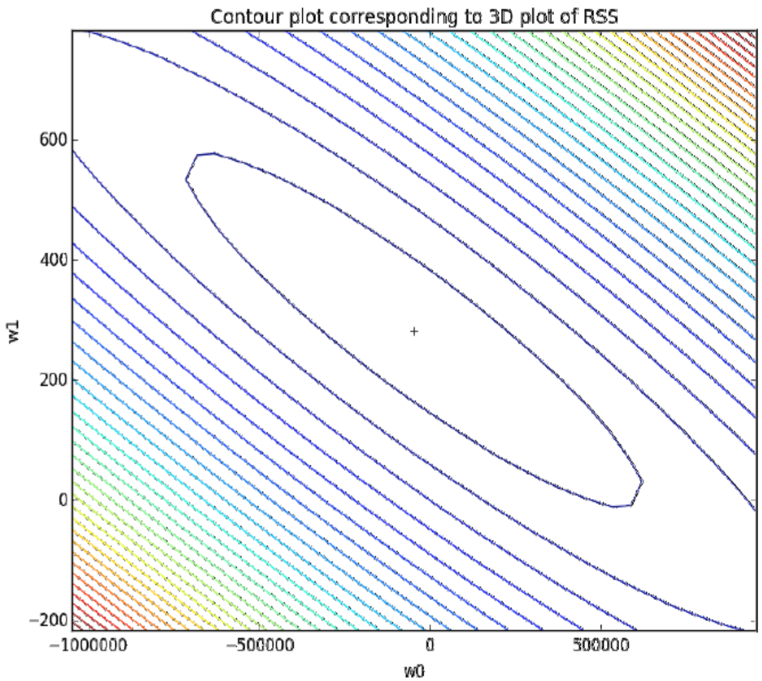
then $(y_i - \hat{y}_i(w^{(t)}))$ on average

weighted by # bath will be positive

$\Rightarrow w_j^{(t+1)} > w_j^{(t)}$ (increase)

Summary of gradient descent

Extremely useful algorithm in several applications



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

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

$\sqrt{\text{partial}[0]^2 + \ldots + \text{partial}[D]^2}$

for $j=0,\ldots,D$

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

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

$t \leftarrow t+1$

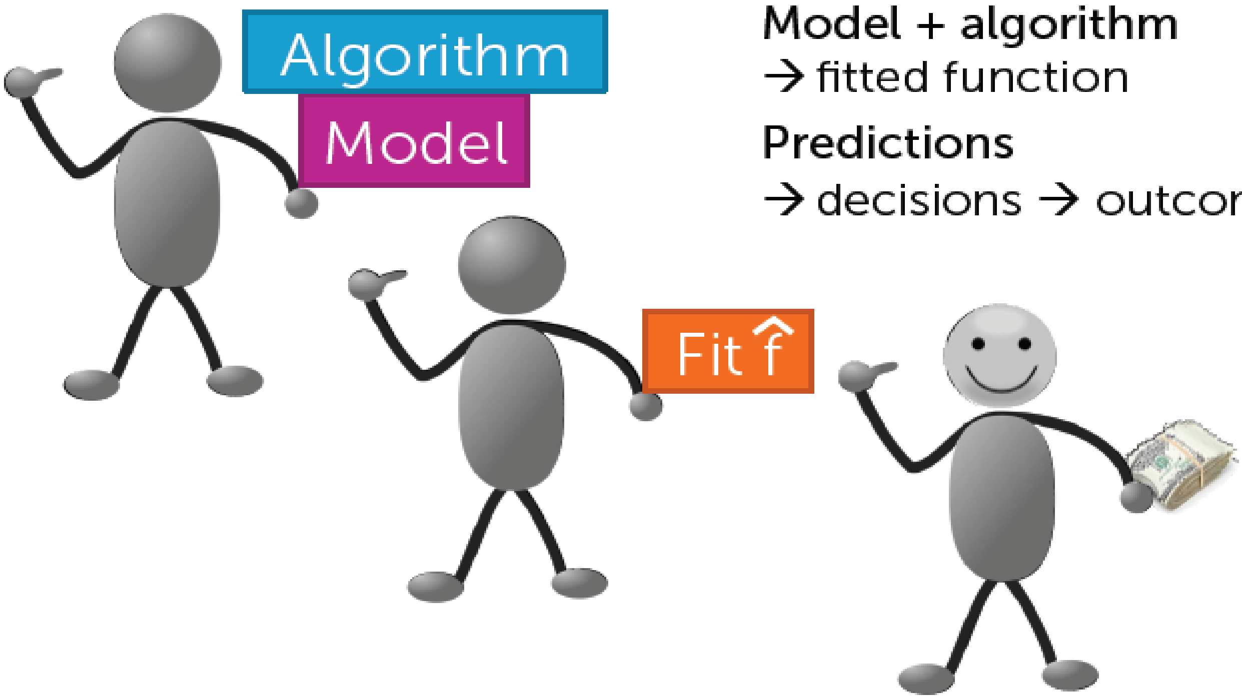
What you can do now

- Describe polynomial regression
- Detrend a time series using trend and seasonal components
- Write a regression model using multiple inputs or features thereof
- Cast both polynomial regression and regression with multiple inputs as regression with multiple features
- Calculate a goodness-of-fit metric (e.g., RSS)
- Estimate model parameters of a general multiple regression model to minimize RSS:
  - In closed form
  - Using an iterative gradient descent algorithm
- Interpret the coefficients of a non-featurized multiple regression fit
- Exploit the estimated model to form predictions
- Explain applications of multiple regression beyond house price modeling

ACCESSING PERFORMANCE

Assessing performance

Make predictions, get $, right??



Model + algorithm
→ fitted function

Predictions
→ decisions → outcome

Assessing performance

Or, how much am I losing?

Example: Lost $ due to inaccurate listing price

- Too low → low offers
- Too high → few lookers + no/low offers

How much am I losing compared to perfection?

Perfect predictions: Loss = 0

My predictions: Loss = ???

Measuring loss

"Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful." George Box, 1987.

Loss function:

$L(y, \underbrace{f_{\hat{w}}(\mathbf{x})}_{\hat{f}(\mathbf{x}) = \text{predicted value } \hat{y}})$

actual value

Cost of using ŵ at x when y is true

Examples:
(assuming loss for underpredicting = overpredicting)

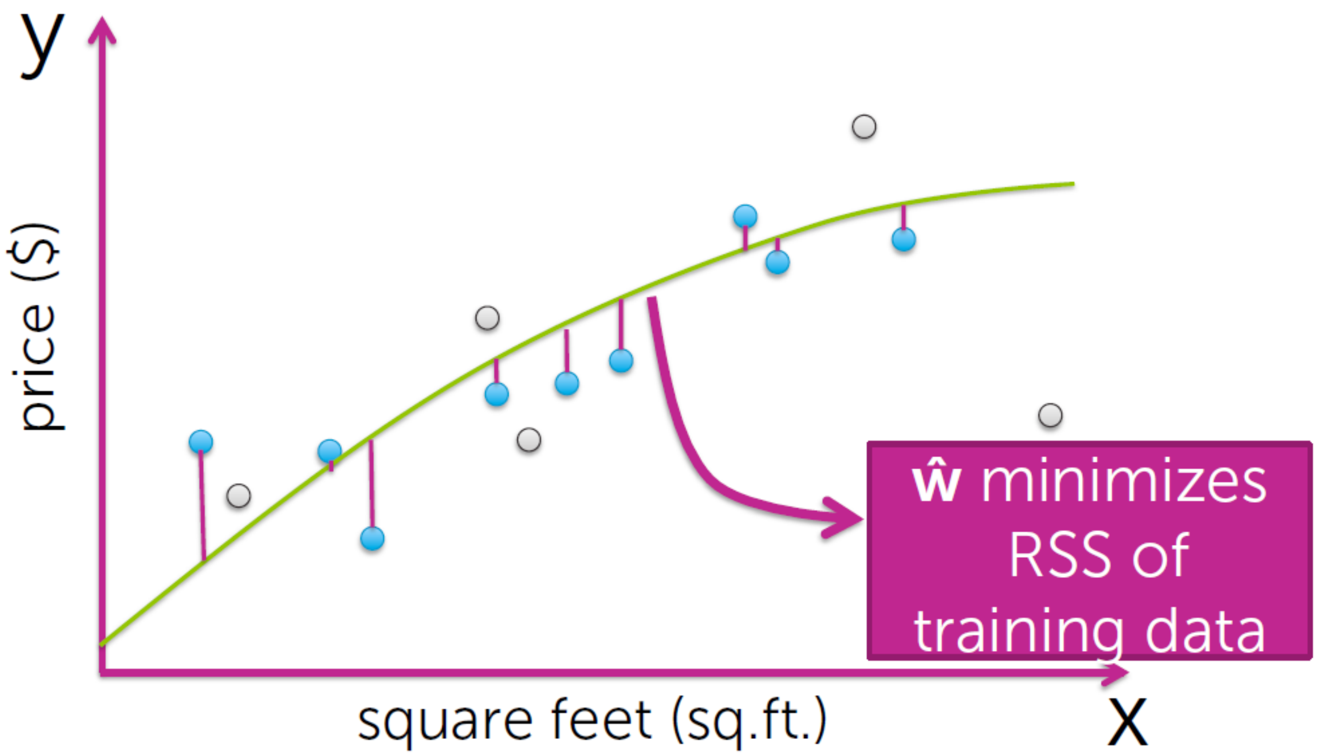
Absolute error: $L(y, f_{\hat{w}}(\mathbf{x})) = |y - f_{\hat{w}}(\mathbf{x})|$

Squared error: $L(y, f_{\hat{w}}(\mathbf{x})) = (y - f_{\hat{w}}(\mathbf{x}))^2$

Symmetric loss functions

Accessing the loss

Use training data



Compute training error

1. Define a loss function $L(y, f_{\hat{\mathbf{w}}}(\mathbf{x}))$
   – E.g., squared error, absolute error,...

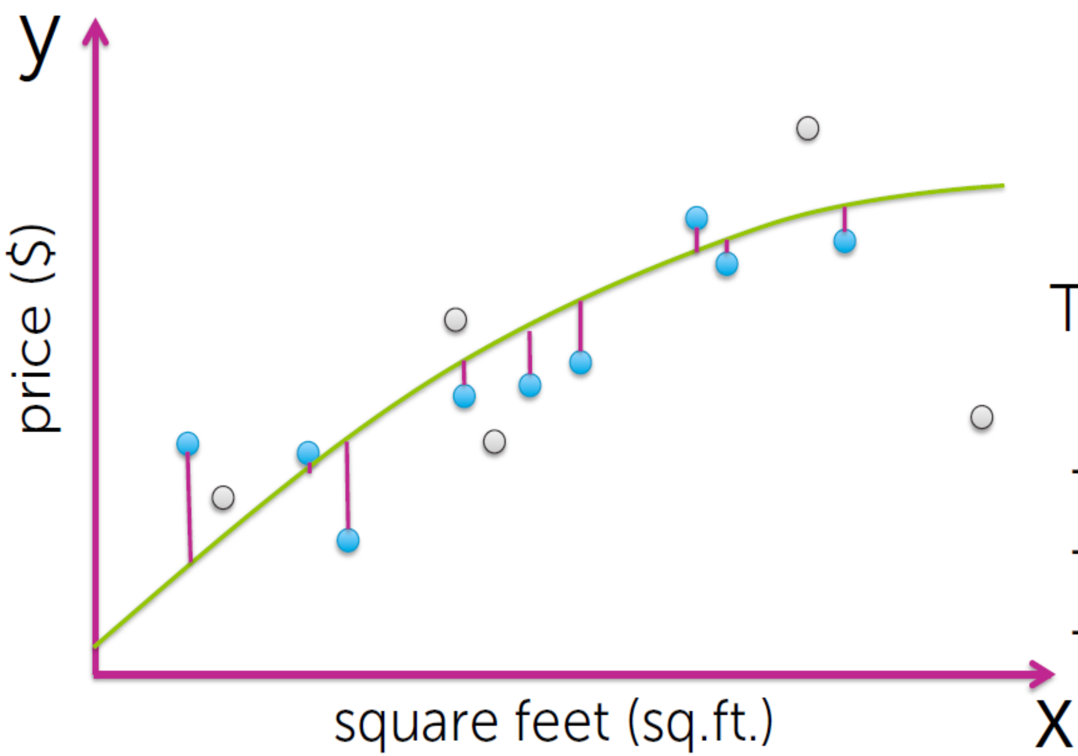
2. Training error
   = avg. loss on houses in training set

$$= \frac{1}{N} \sum_{i=1}^{N} L(y_i, f_{\hat{\mathbf{w}}}(\mathbf{x}_i))$$

fit using training data

Training error

Use squared error loss $(y-f_{\hat{w}}(x))^2$



Convention is to take average here

Training error ($\hat{w}$) = 1/N *

$[(\$_{train\ 1}-f_{\hat{w}}(sq.ft._{train\ 1}))^2$

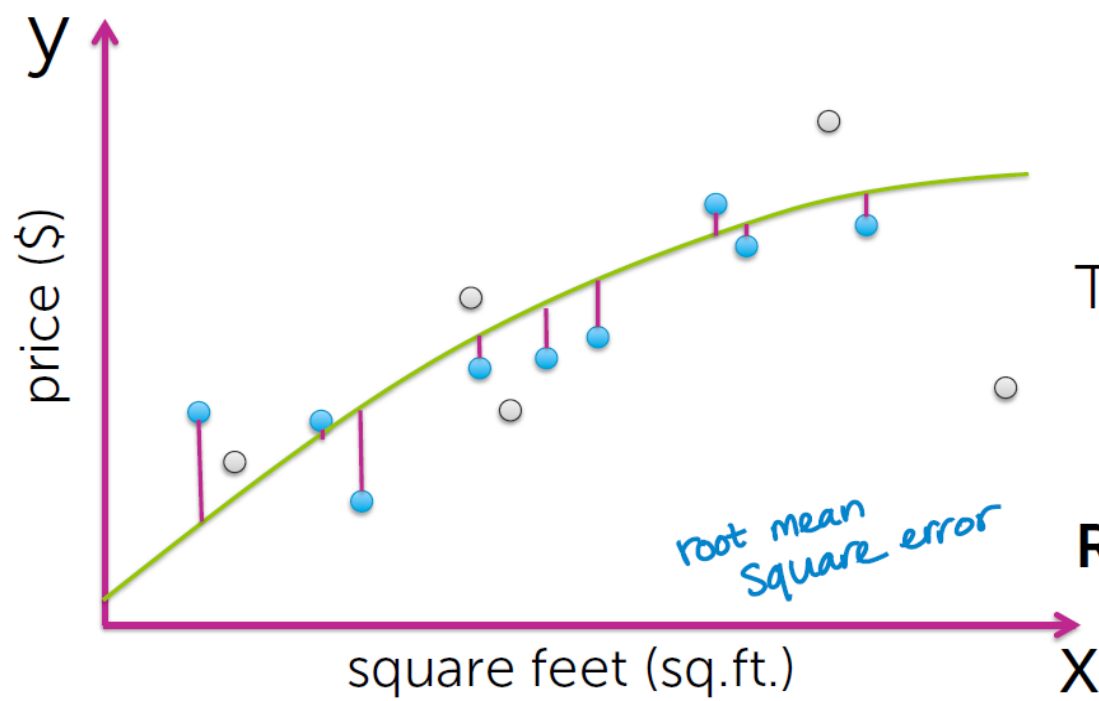
$+ (\$_{train\ 2}-f_{\hat{w}}(sq.ft._{train\ 2}))^2$

$+ (\$_{train\ 3}-f_{\hat{w}}(sq.ft._{train\ 3}))^2$

+ ... include all training houses]

Training error

More intuitive is to take RMSE, same units as y



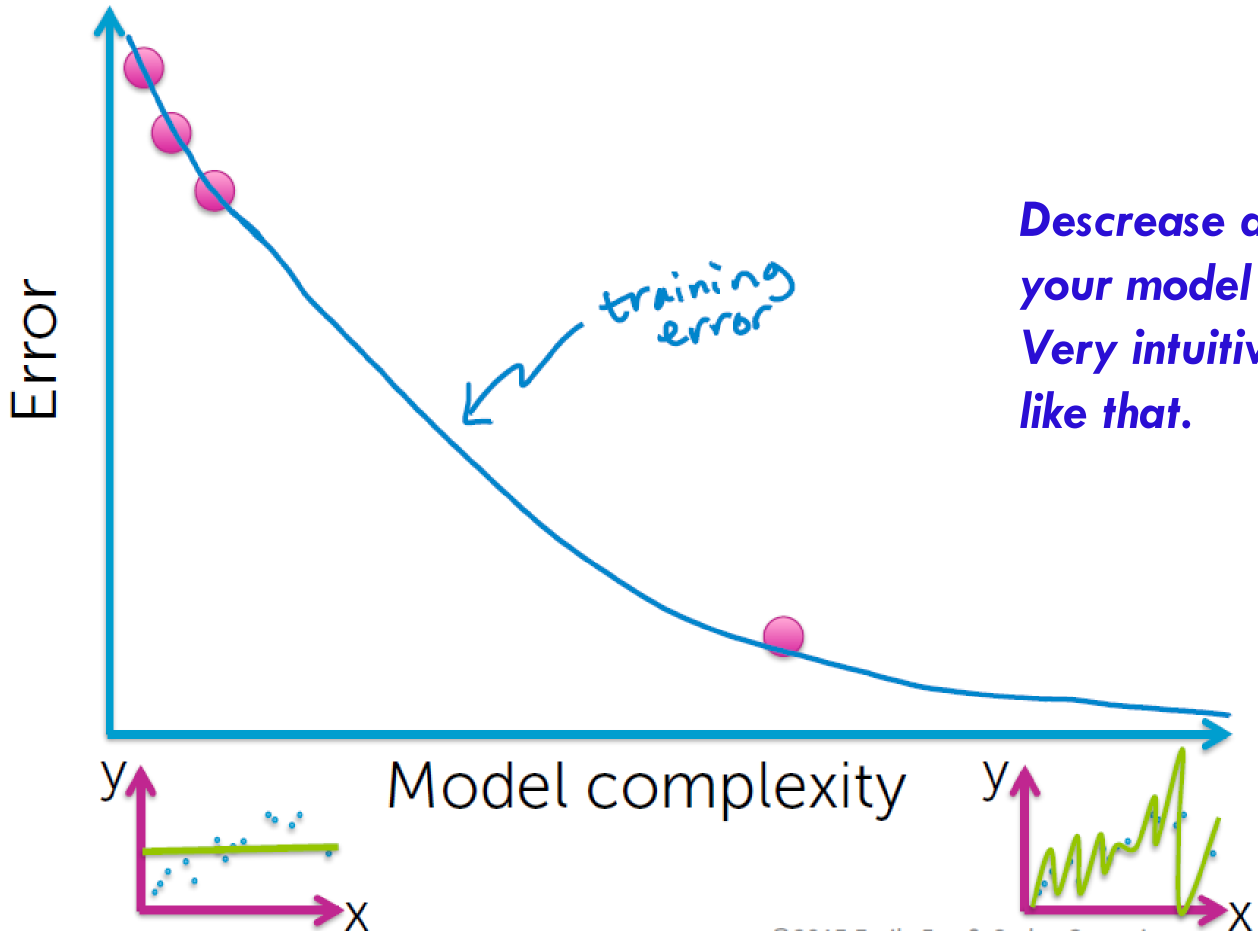
Training error ($\hat{\mathbf{w}}$) =

$$\frac{1}{N}\sum_{i=1}^{N}(y_i - f_{\hat{\mathbf{w}}}(\mathbf{x}_i))^2$$

RMSE =

$$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - f_{\hat{\mathbf{w}}}(\mathbf{x}_i))^2}$$

Training error vs. model complexity

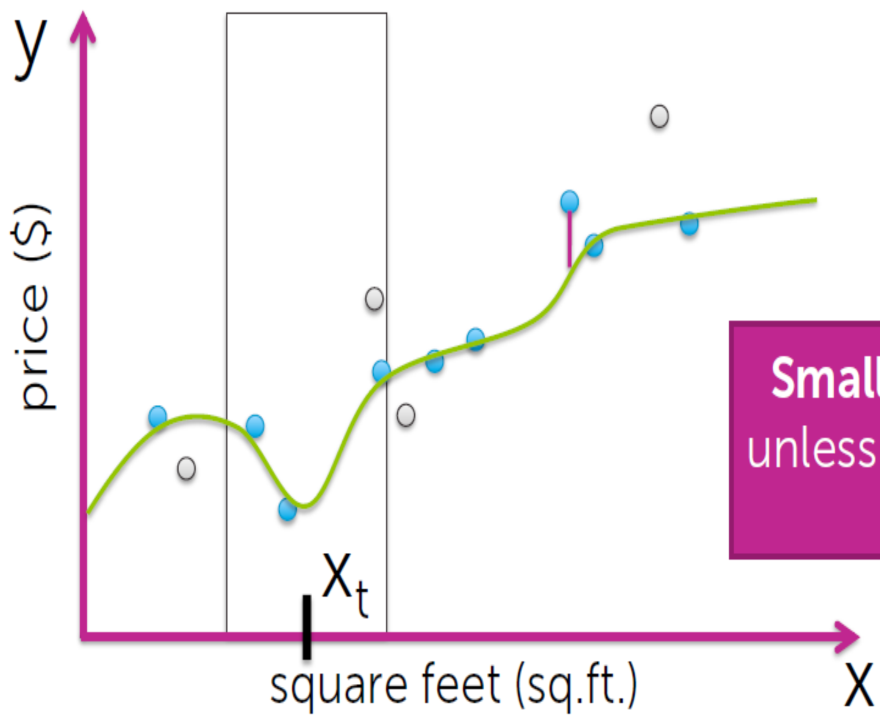


Descrease as you increase your model complexity. Very intuitive why it is like that.

Is training error a good measure?

Issue: Training error is overly optimistic

because $\hat{\mathbf{w}}$ was fit to training data

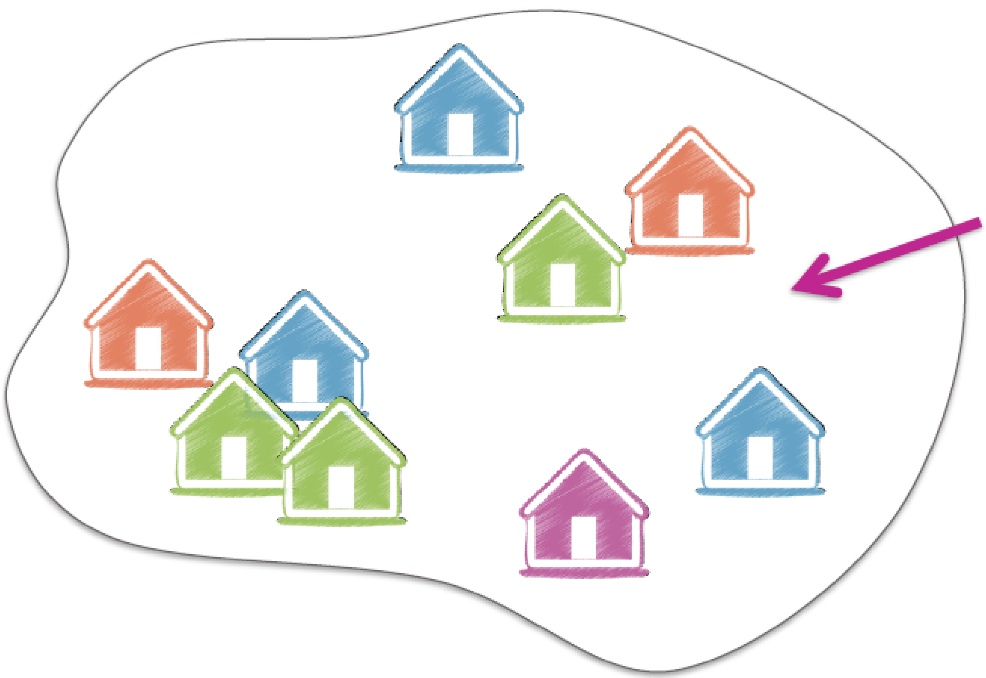


Is there something particularly wrong about having x_t square feet ???

Small training error ≠> good predictions
unless training data includes everything you might ever see

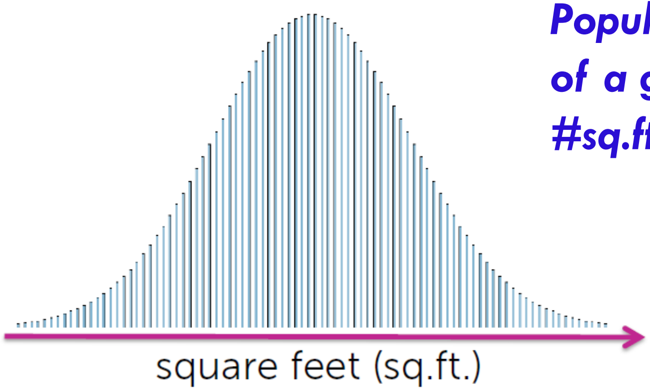
Generalisation (true) error

Really want estimate of loss over all possible (,$) pairs



Distribution over house

In our neighborhood, houses of what # sq.ft. ( ) are we likely to see?



Popularity of a given #sq.ft.

For houses with a given # sq.ft. ( ), what house prices $ are we likely to see?

For fixed # sq.ft.

Generalisation error definition

Really want estimate of loss over all possible (, $) pairs

Formally:

average over all possible ($\mathbf{x}$,y) pairs weighted by how likely each is

$$\text{generalization error} = E_{\mathbf{x},y}\left[L(y, f_{\hat{\mathbf{w}}}(\mathbf{x}))\right]$$

fit using training data

Generalisation error definition

Really want estimate of loss over all possible (,$) pairs

discrete r.v.

$E[x] = \sum_i x_i \, p(x_i)$

cont. r.v.

$E[x] = \int x \, p(x) \, dx$

$E[f(x)] = \int f(x) \, p(x) \, dx$

Formally:

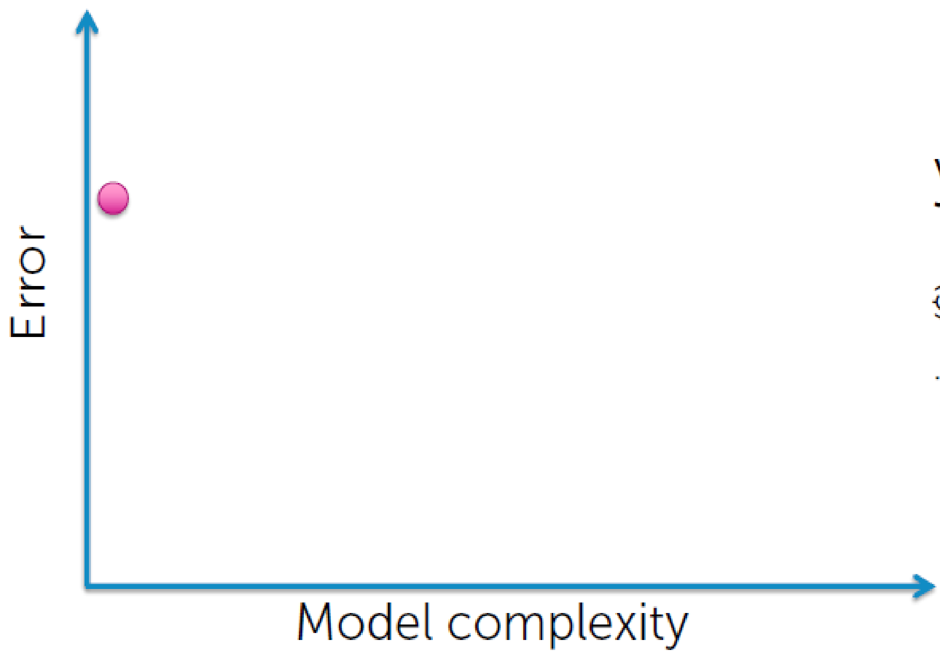
average over all possible ($\mathbf{x}$,y) pairs weighted by how likely each is

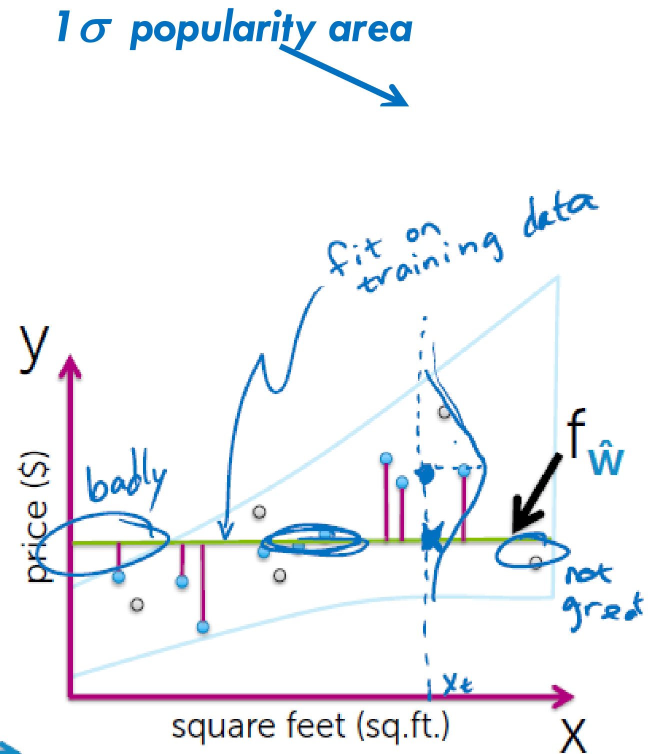
$$\text{generalization error} = E_{\mathbf{x},y}\left[L(y, f_{\hat{w}}(\mathbf{x}))\right]$$

$$= \int L(y, f_{\hat{w}}(\mathbf{x})) \underbrace{p(\mathbf{x}, y)}_{p(x)\,p(y|x)} \, dx \, dy$$

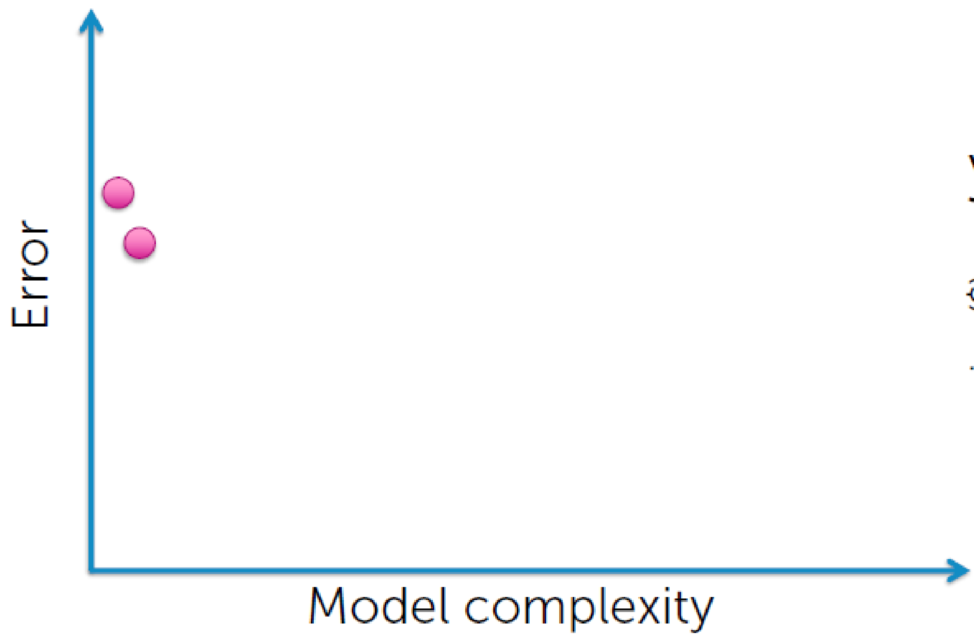
fit using training data

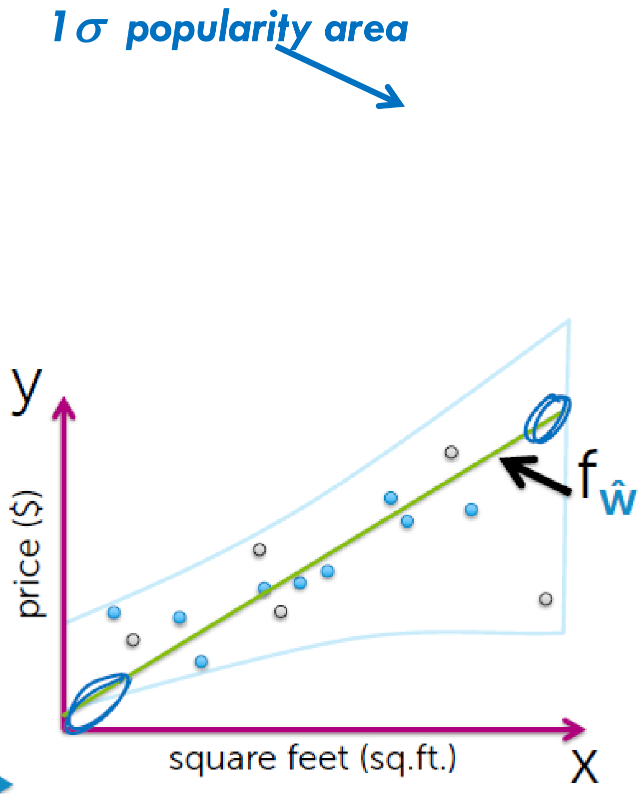
Generalisation error vs model complexity



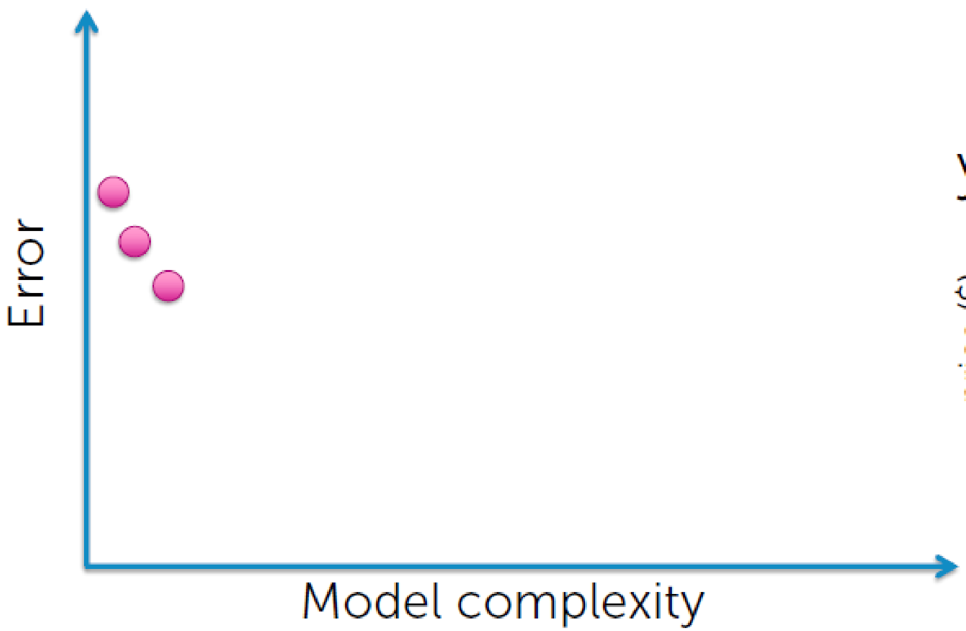


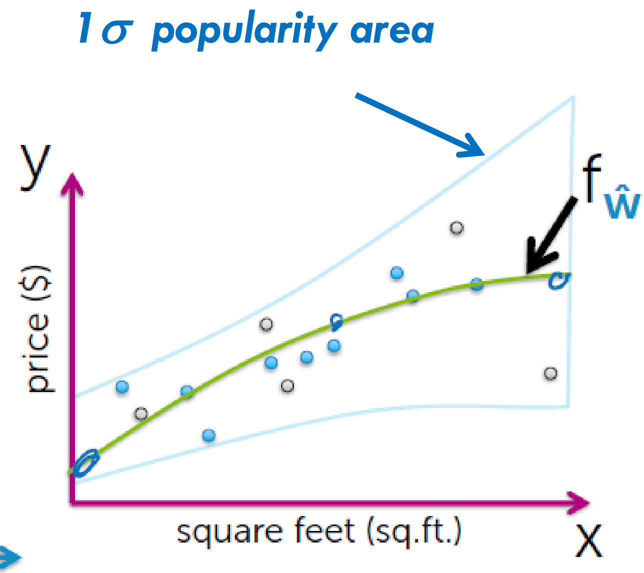
Generalisation error vs model complexity



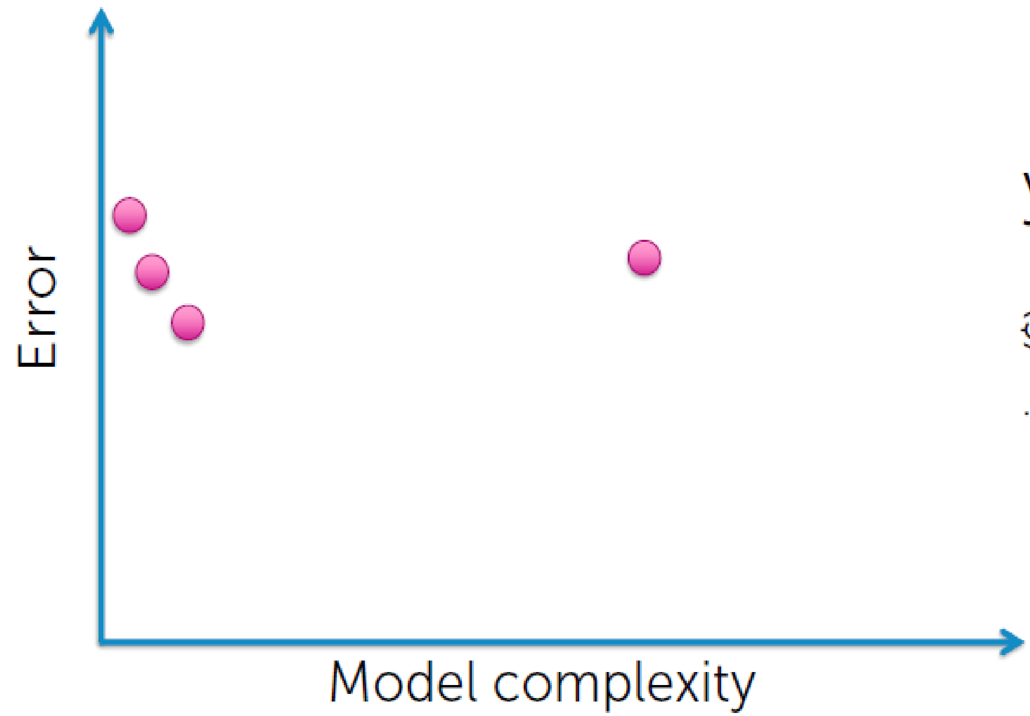


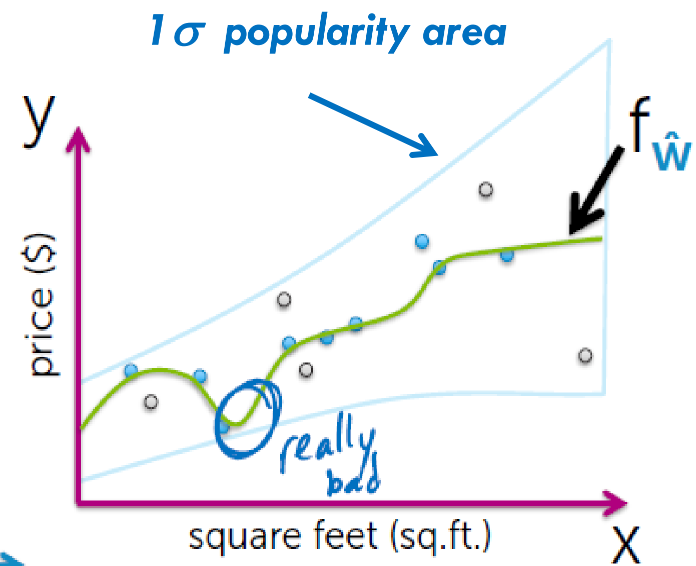
Generalisation error vs model complexity



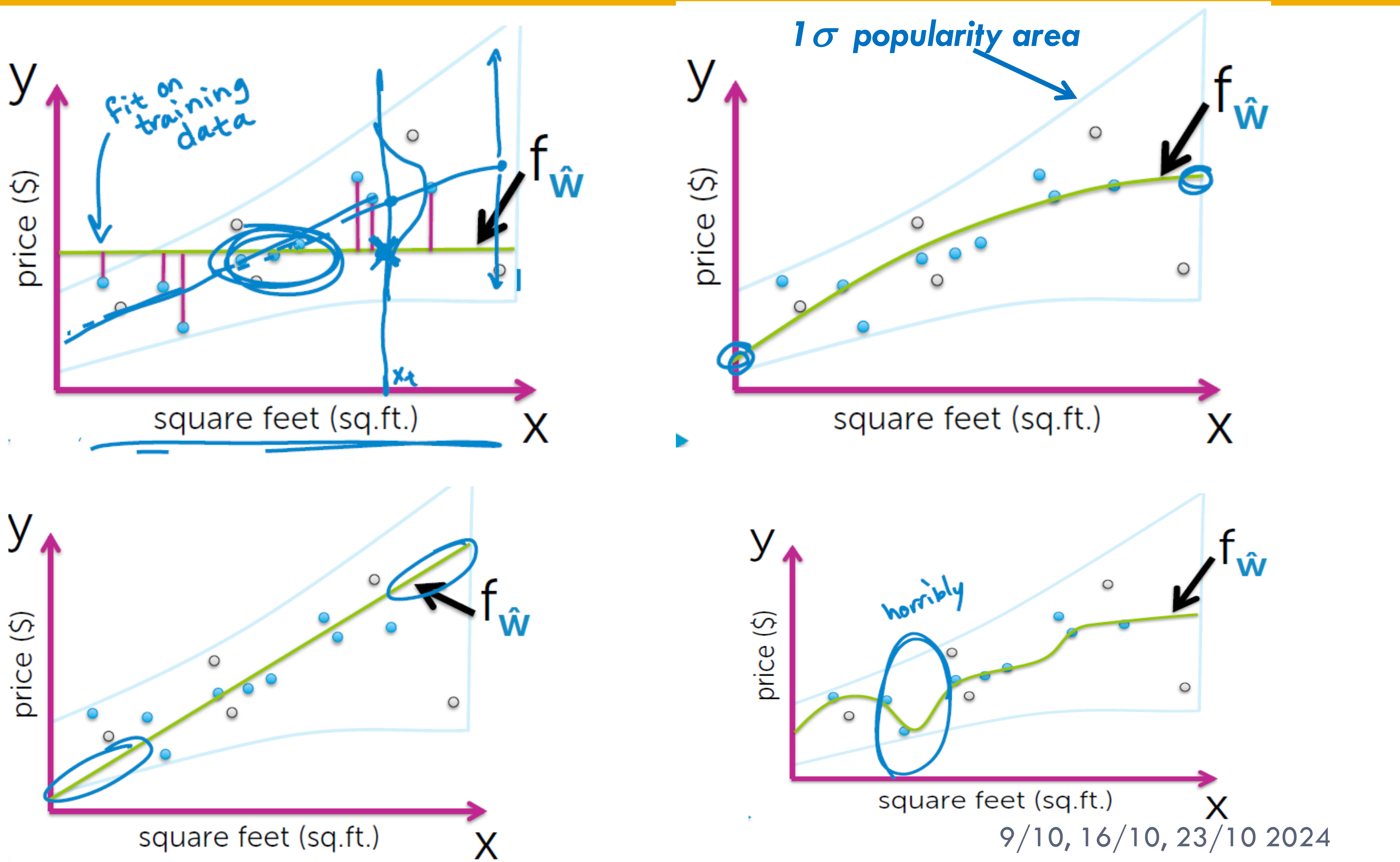


Generalisation error vs model complexity

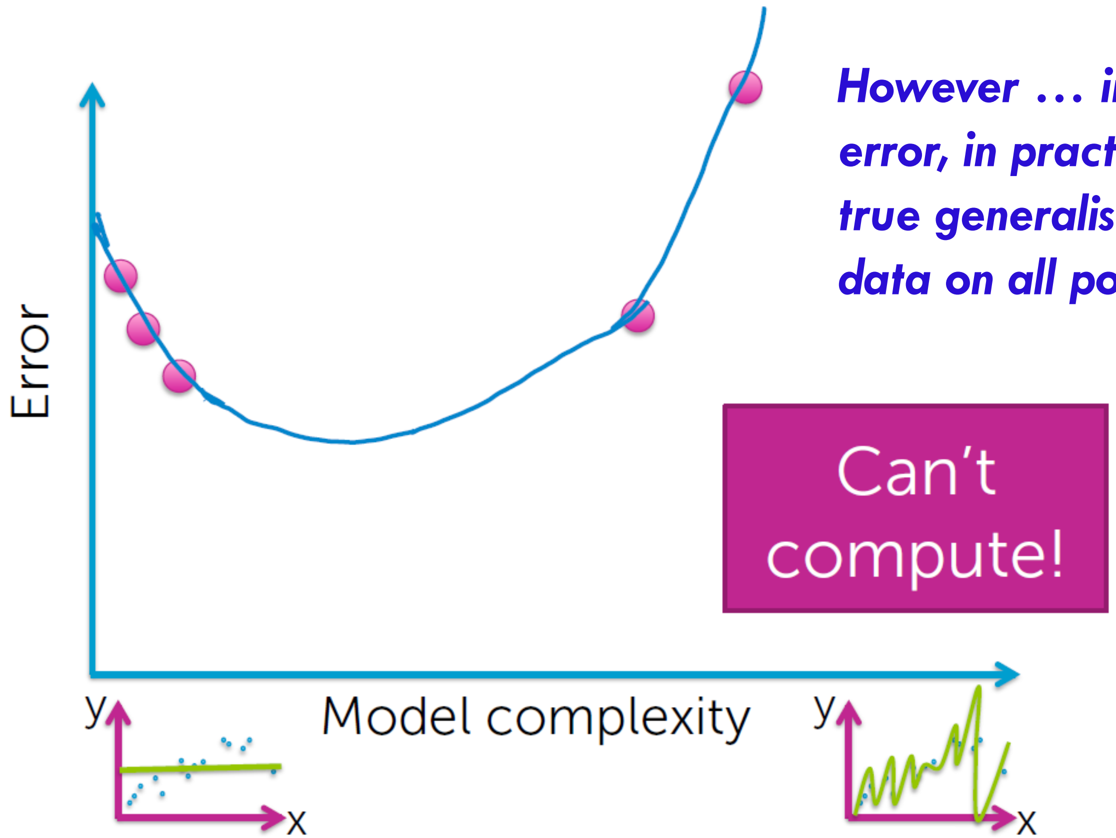




Generalisation error (weighted with popularity) vs model complexity



Generalisation error vs model complexity



However … in contrast to the training error, in practice we cannot really compute true generalisation error. We don't have data on all possible houses in the area.

Forming a test set

Hold out some (,$) that are *not* used for fitting the model

We want to approximate generalisation error.

Test set: proxy for „everything you might see"

Training set

Test set

Compute test error

Test error

= avg. loss on houses in test set

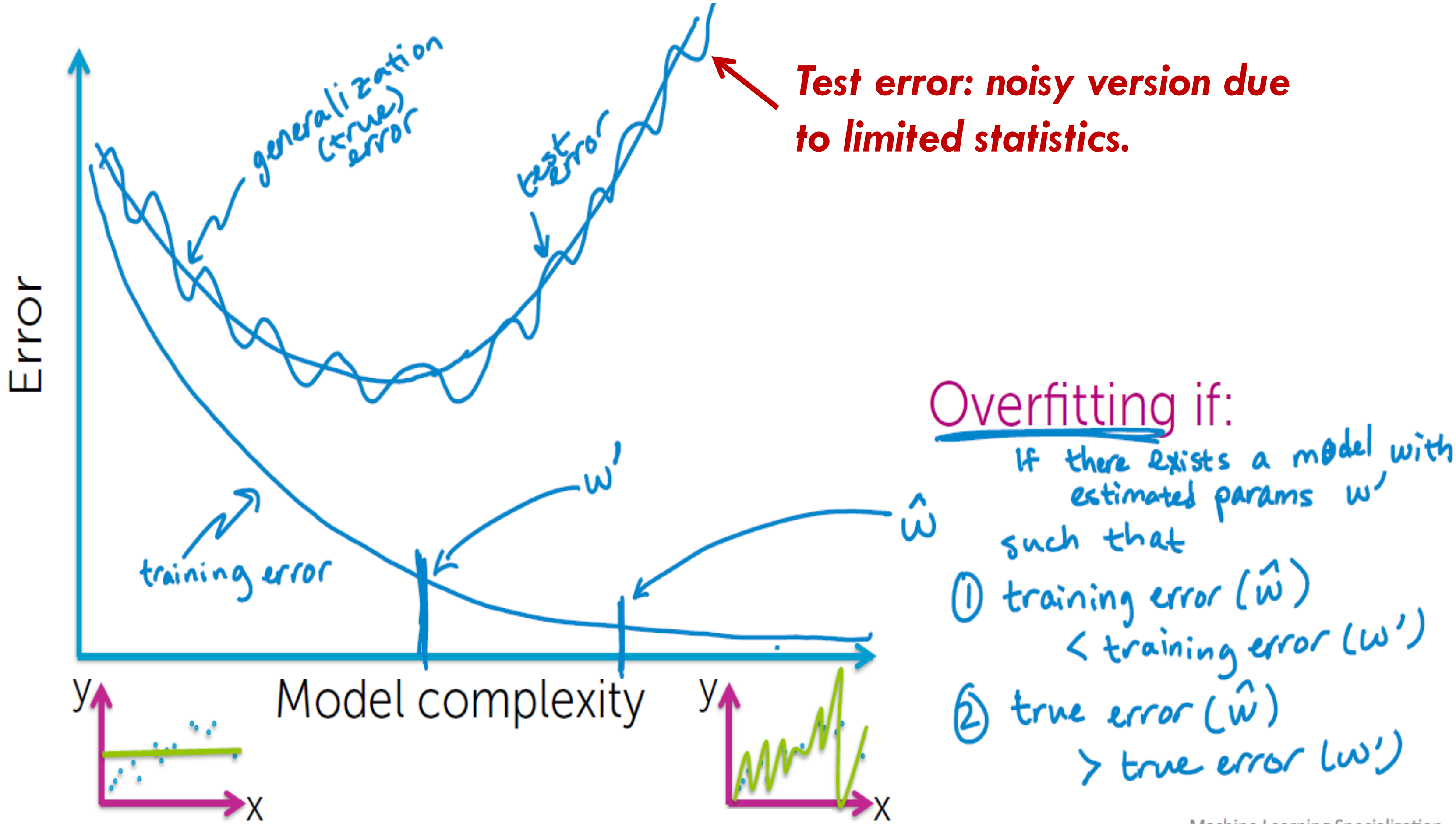
$$= \frac{1}{N_{test}} \sum_{i \text{ in test set}} L(y_i, f_{\hat{\mathbf{w}}}(\mathbf{x}_i))$$

test points

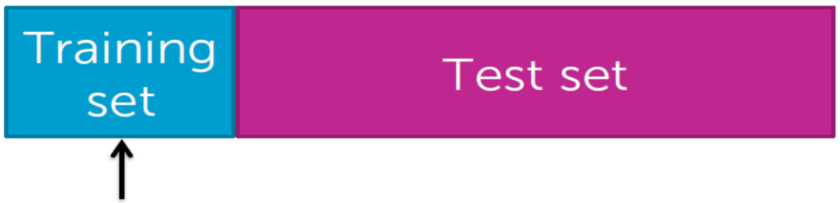
fit using training data

has never seen test data!

Training, true and test error vs. model complexity. Notion of overfitting.



Training/test splits



Too few → $\hat{\mathbf{w}}$ poorly estimated

Too few → test error bad approximation of generalization error

Typically, just enough test points to form a reasonable estimate of generalization error

If this leaves too few for training, other methods like **cross validation** (will see later…)

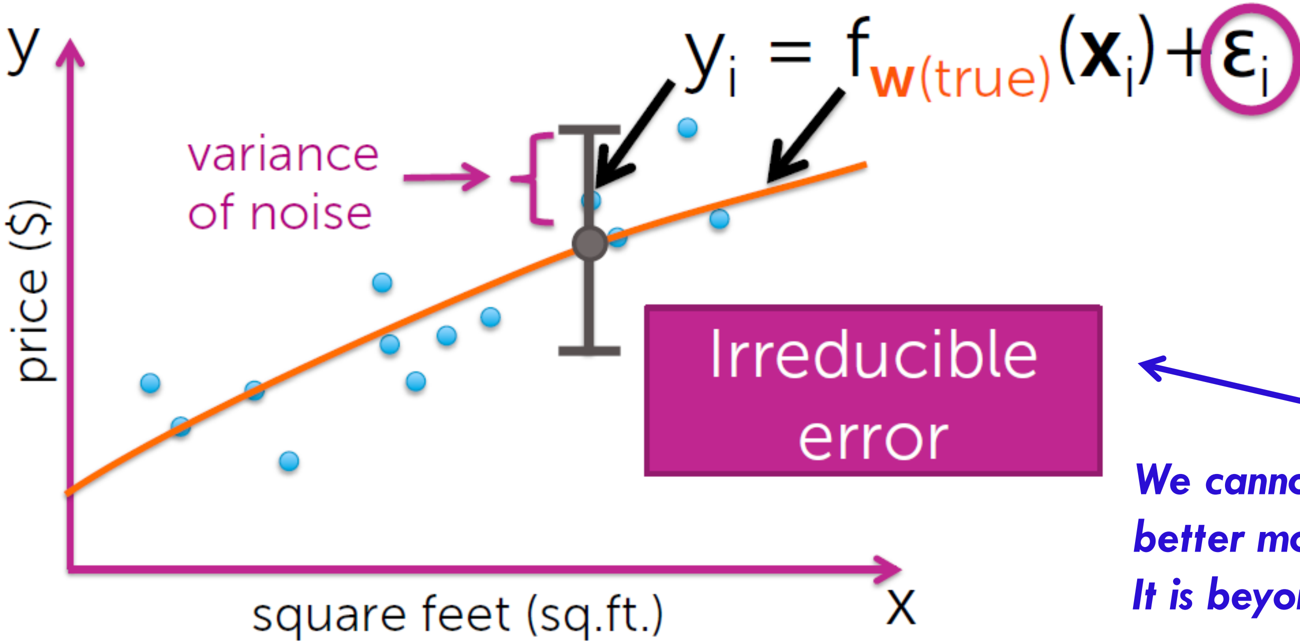
Three sources of errors

In forming predictions, there are 3 sources of error:

1. Noise
2. Bias
3. Variance

Data are inherently noisy

There is some true relatioship between sq.ft and value of the house, specific to the given house.

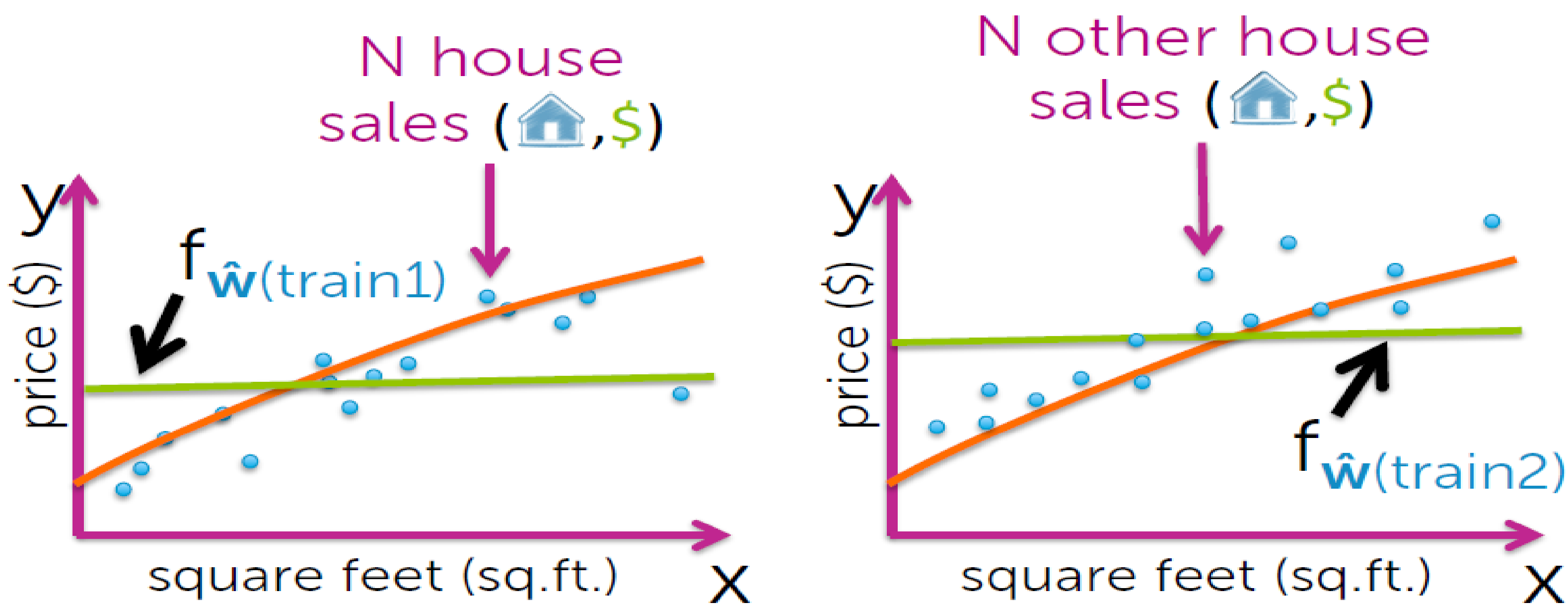


We cannot reduce it by chosing better model or procedure,
It is beyond our control.

Bias contribution

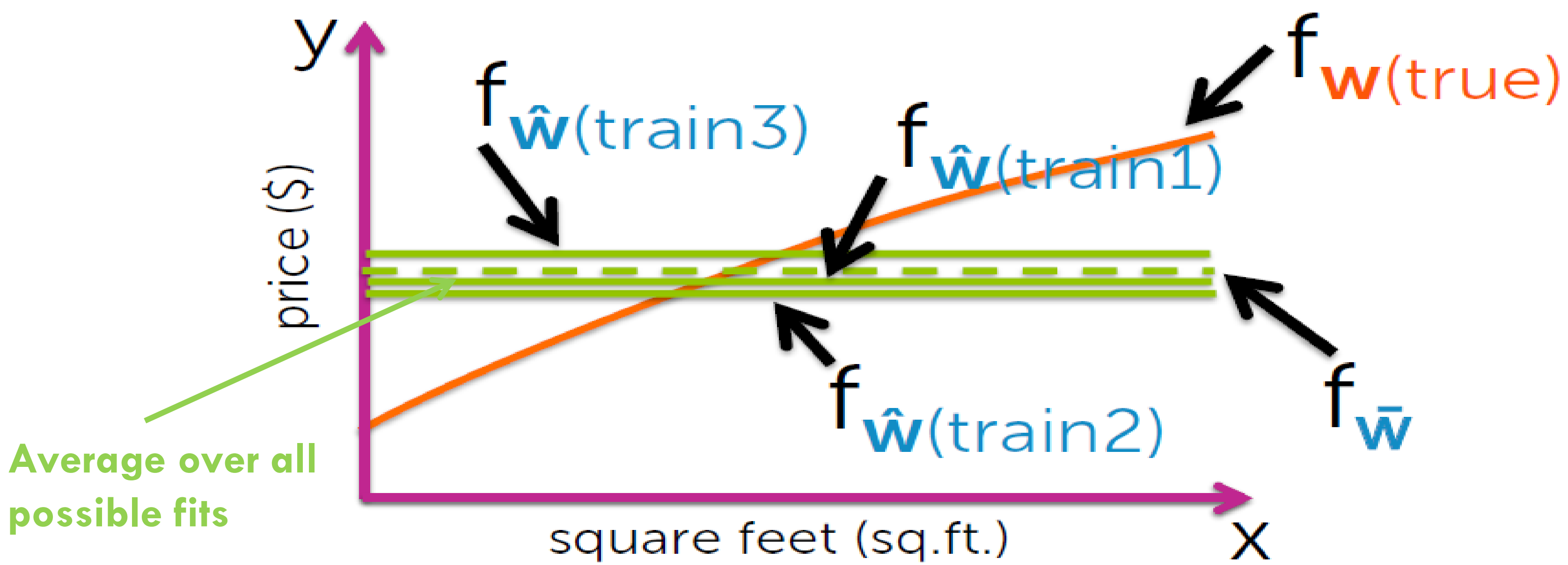
This contribution we can control.

Assume we fit a constant function



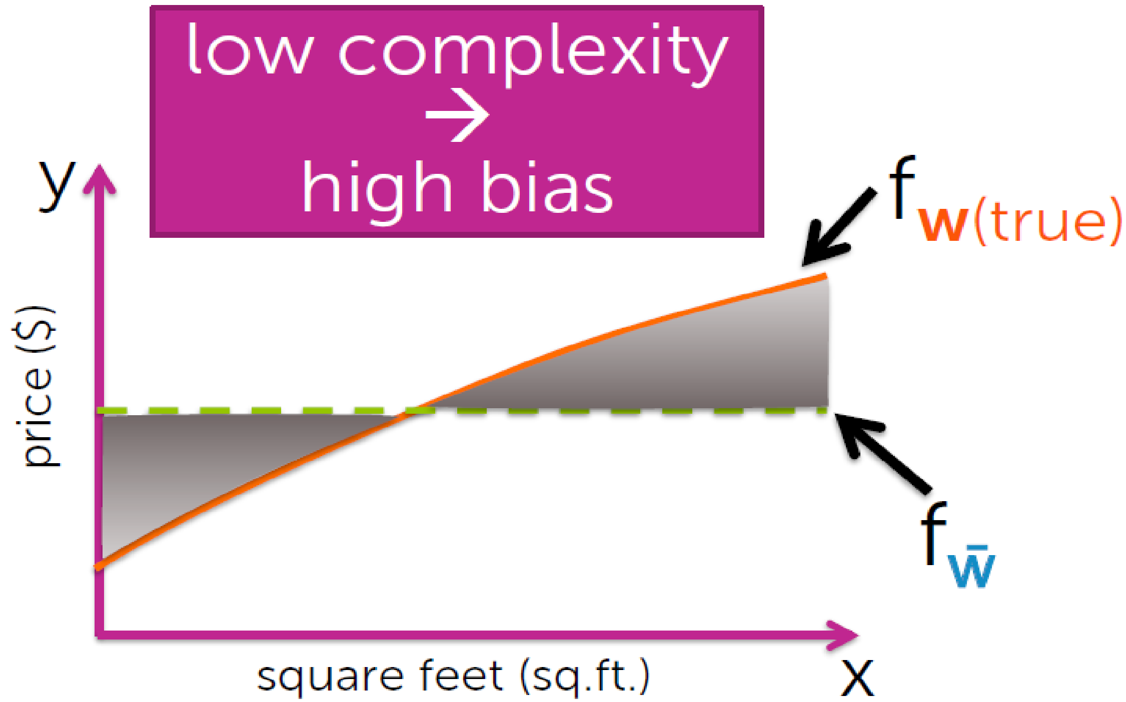
Bias contribution

Over all possible size N training sets, what do I expect my fit to be?



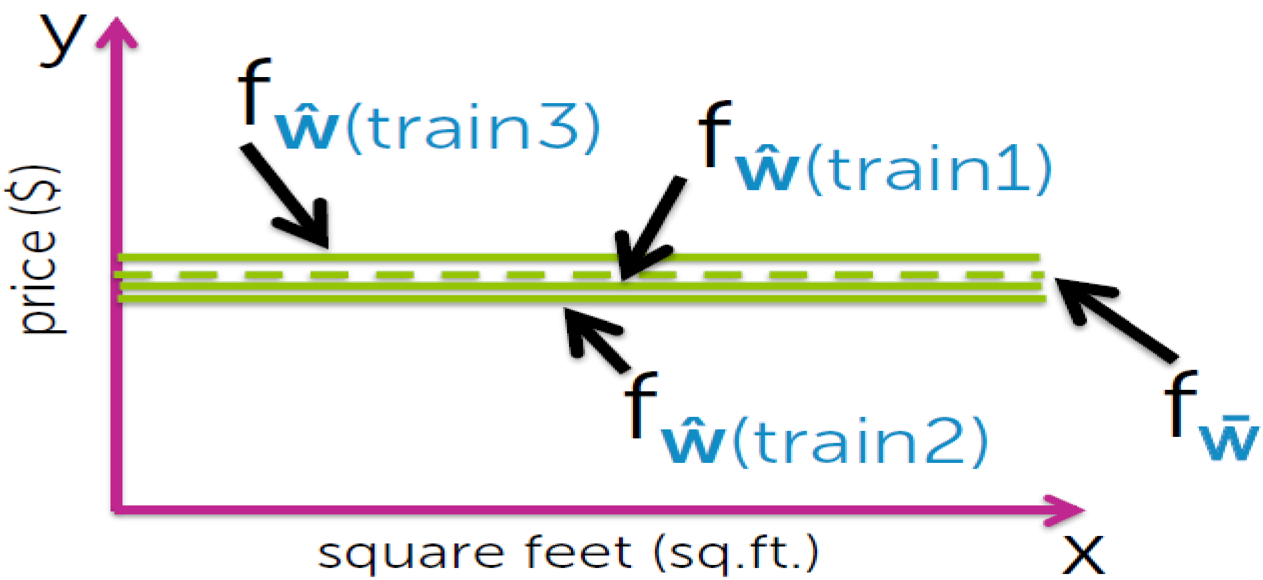
Bias contribution

$\text{Bias}(\mathbf{x}) = f_{\mathbf{w}(\text{true})}(\mathbf{x}) - f_{\bar{\mathbf{w}}}(\mathbf{x})$ ← Is our approach flexible enough to capture $f_{\mathbf{w}(\text{true})}$? **If not, error in predictions.**



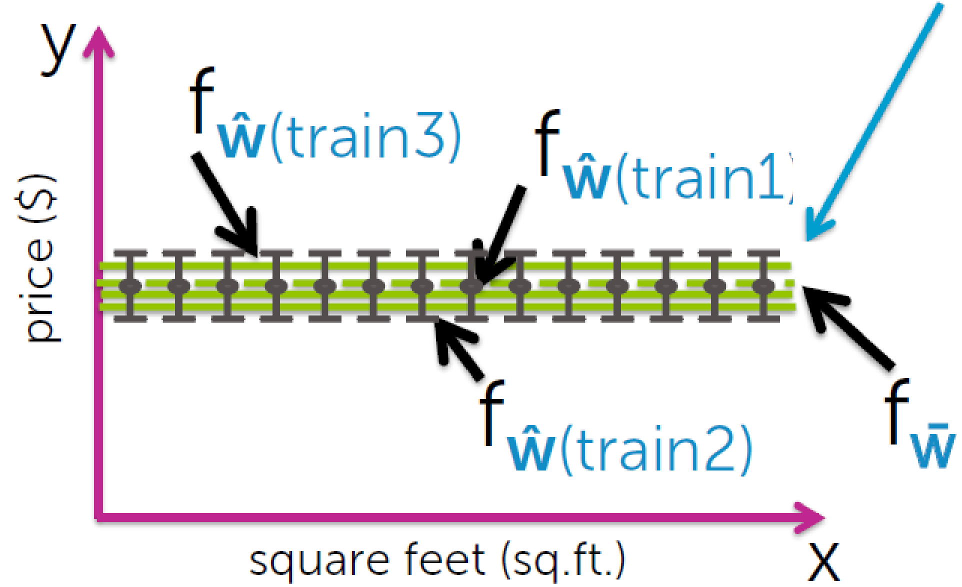
Variance contribution

How much do specific fits vary from the expected fit?



Variance contribution

How much do specific fits vary from the expected fit?



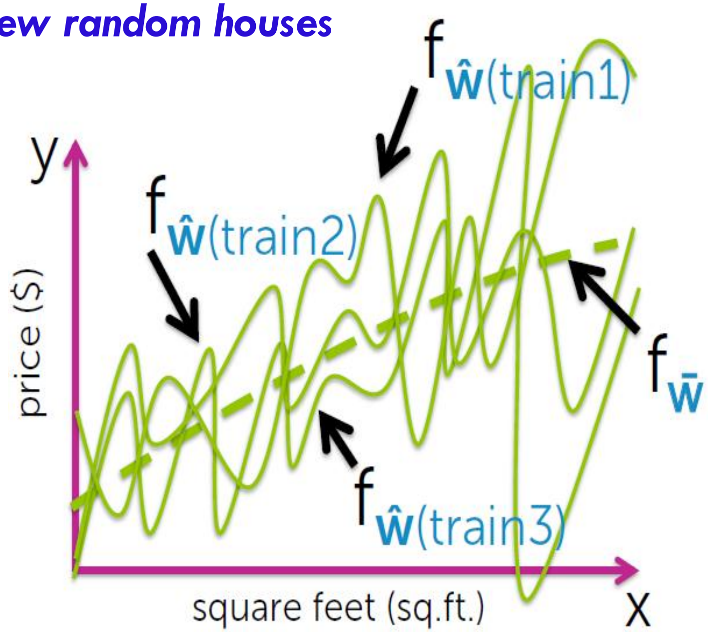
Can specific fits vary widely?
If so, erratic predictions

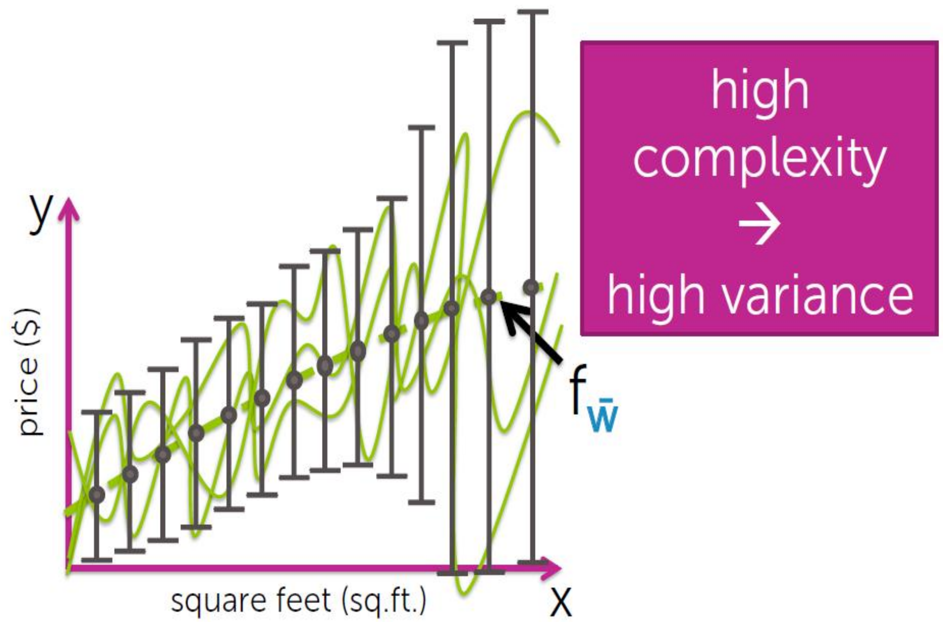
low complexity → low variance

Variance of high complexity models

Assume we fit a high-order polynomial

For each train remove few random houses

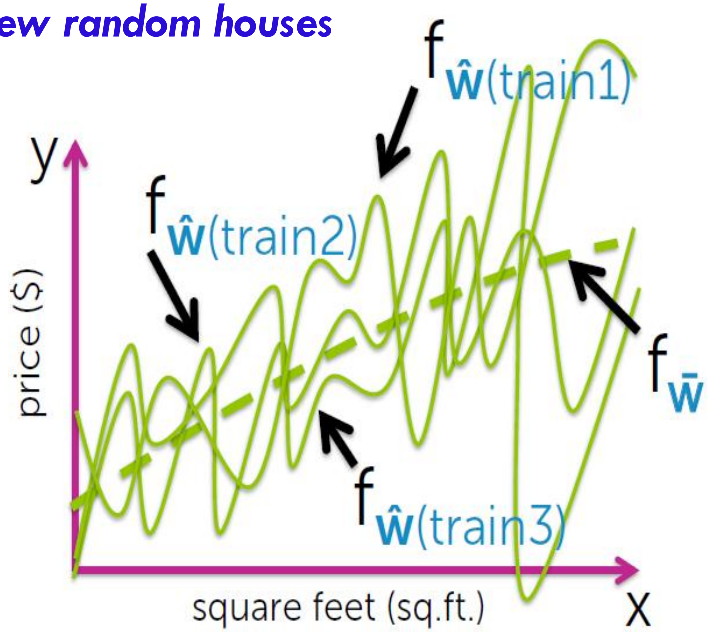


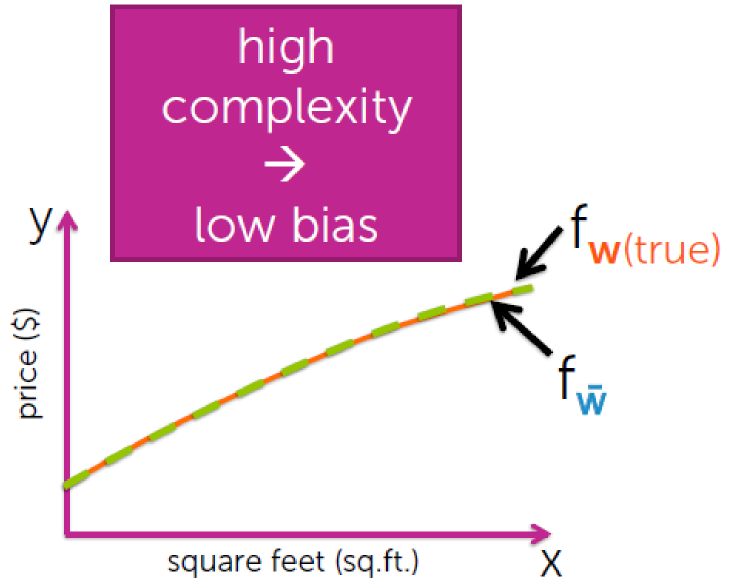


Bias of high complexity models

Assume we fit a high-order polynomial

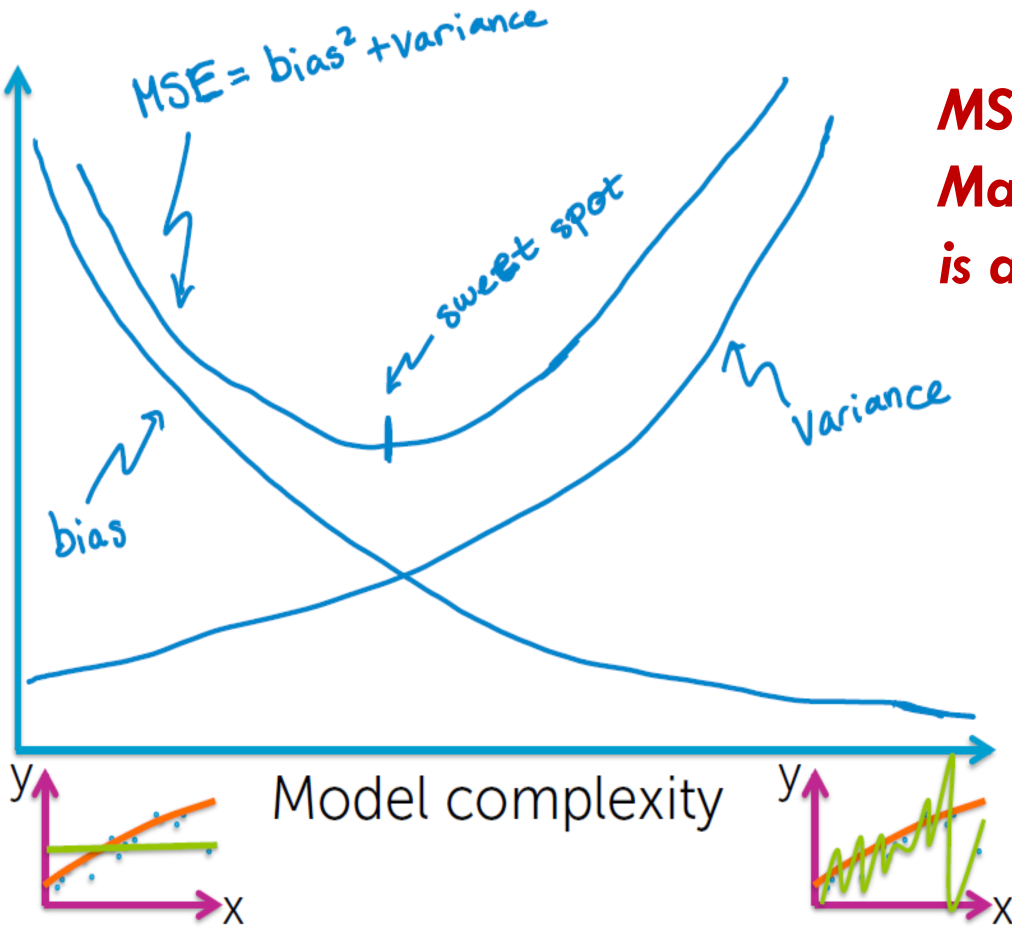
For each train remove few random houses





High complexity models are very flexible, pick better average trends.

Bias –variance tradeoff

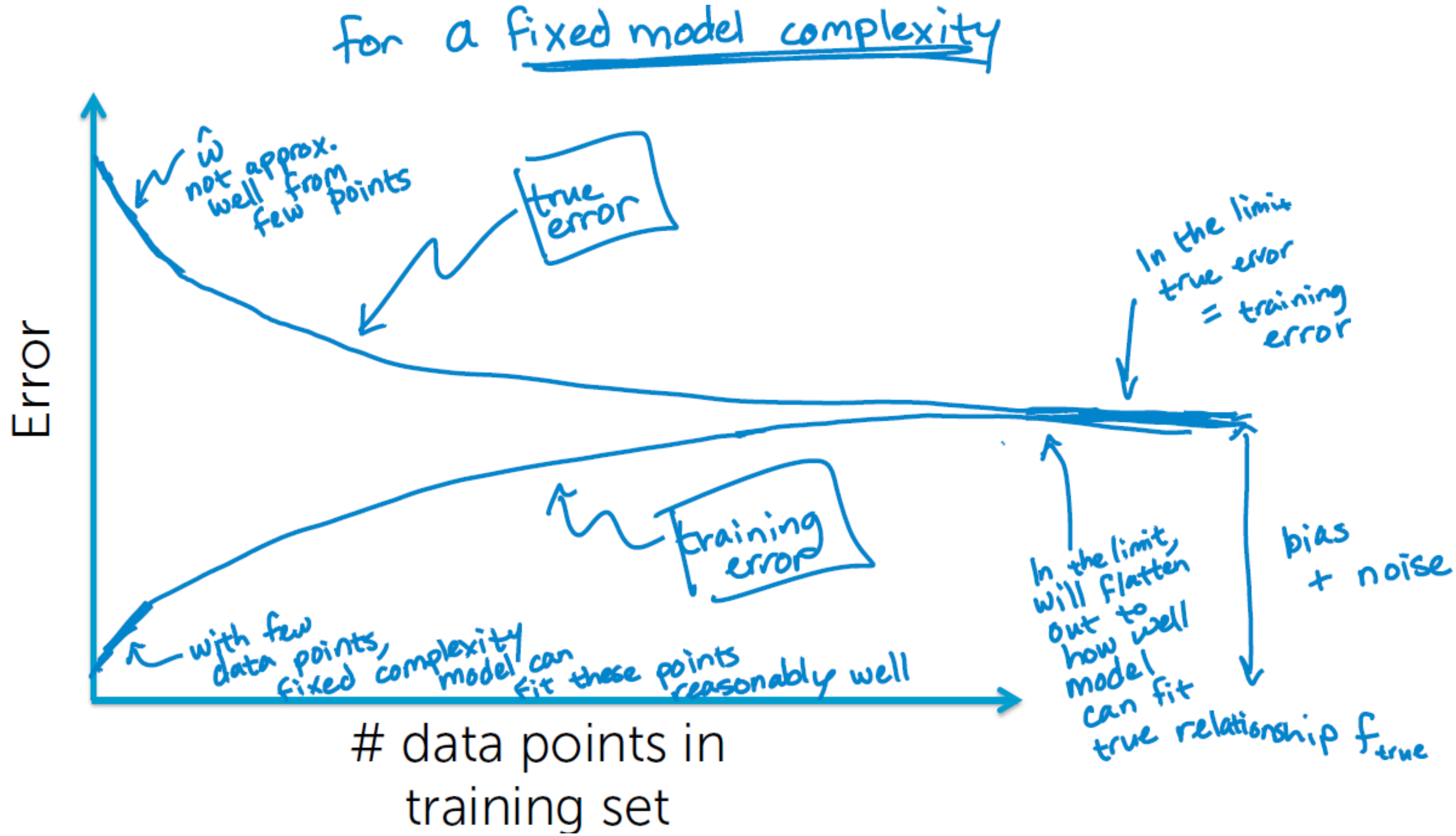


MSE = mean square error
Machine Learing
is all about this tradeoff

But….

Just like with generalization error, we cannot compute bias and variance

Errors vs amount of data



The regression/ML workflow

1. **Model selection**
   Often, need to choose tuning parameters λ controlling model complexity (e.g. degree of polynomial)

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

Hypothetical implementation

Training set	Test set

1. **Model selection**

For each considered model complexity λ :

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

2. **Model assessment**

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

Hypothetical implementation

Training set	Test set

1. **Model selection**

For each considered model complexity λ :

i. Estimate parameters $\hat{\mathbf{w}}_\lambda$ on **training data**

ii. Assess performance of $\hat{\mathbf{w}}_\lambda$ on **test data**

iii. Choose λ^* to be λ with lowest test error

Overly optimistic!

2. **Model assessment**

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

Hypothetical implementation

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

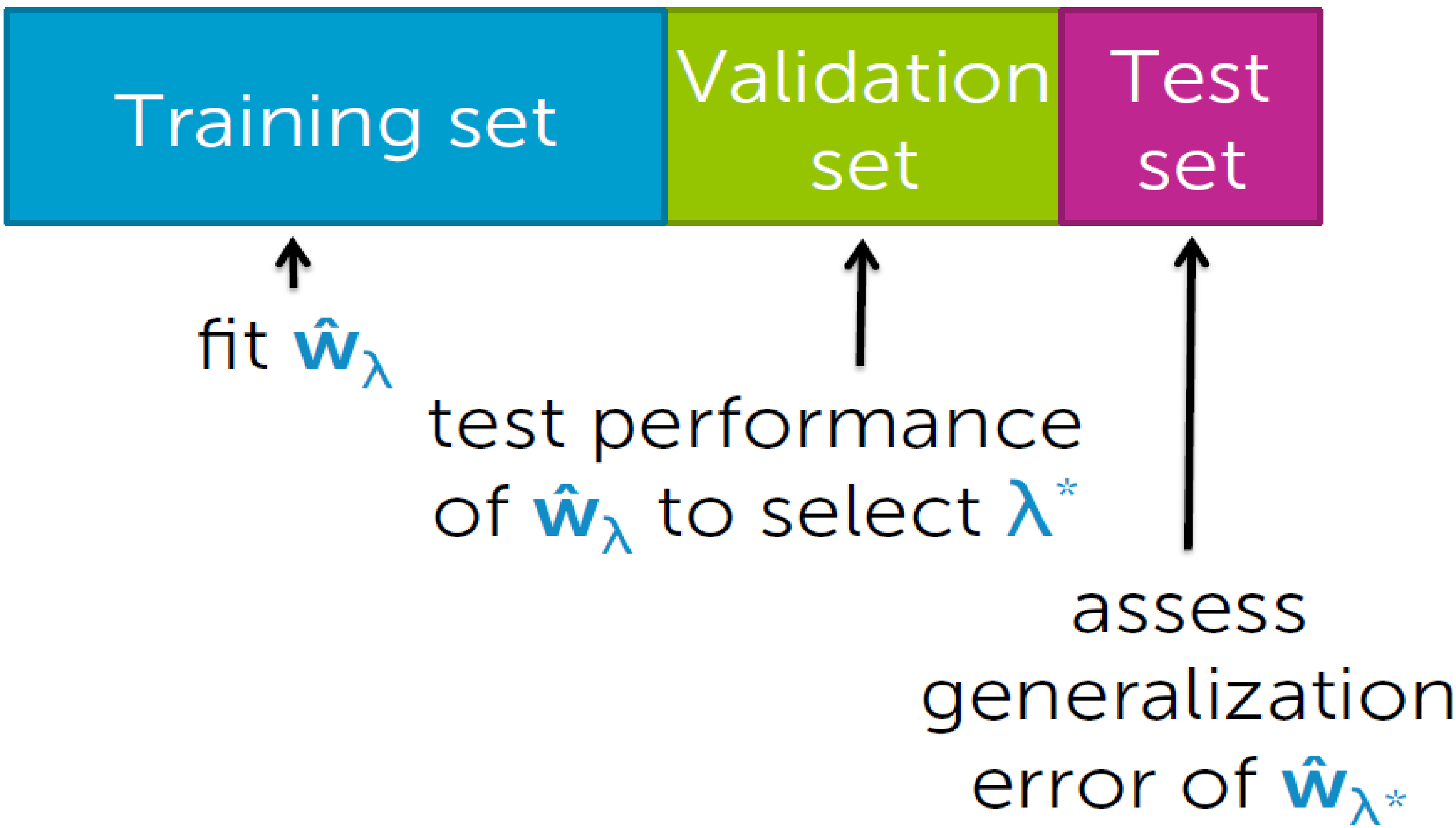
- λ^* was selected to minimize test error (i.e., λ^* was fit on test data)
- If test data is not representative of the whole world, then $\hat{\mathbf{w}}_{\lambda^*}$ will typically perform worse than test error indicates

Practical implementation

Solution: Create two "test" sets!

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

Practical implementation



Typical splits

Training set	Validation set	Test set
80%	10%	10%
50%	25%	25%

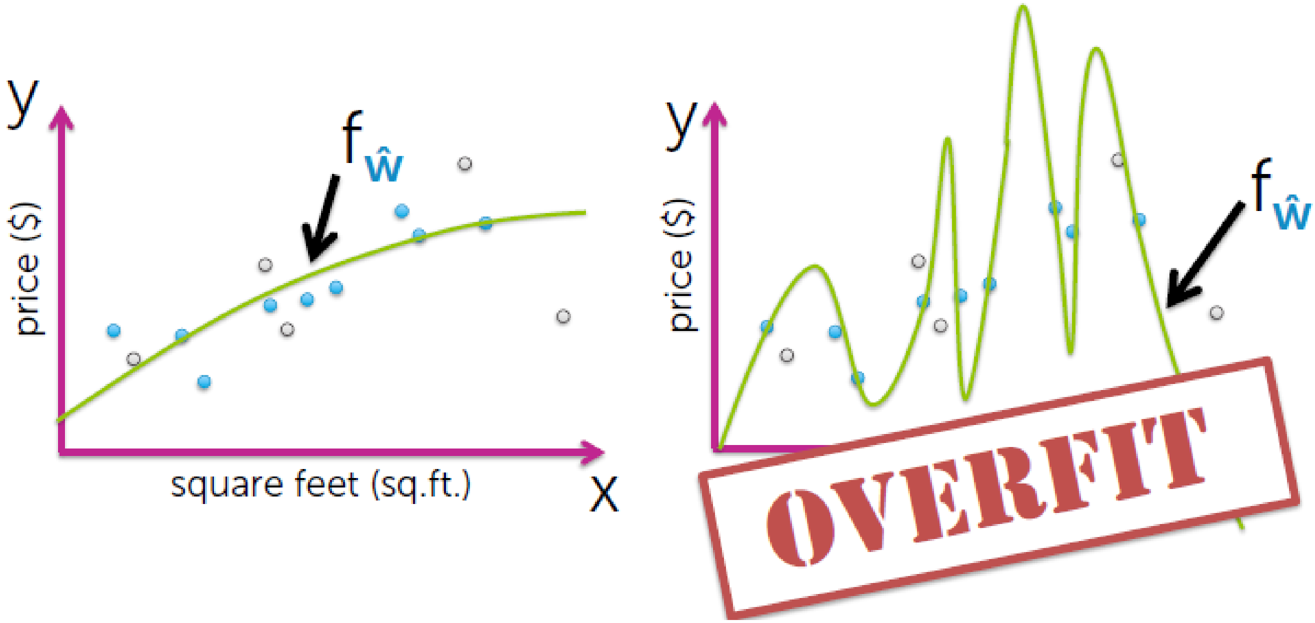
What you can do now

- Describe what a loss function is and give examples
- Contrast training, generalization, and test error
- Compute training and test error given a loss function
- Discuss issue of assessing performance on training set
- Describe tradeoffs in forming training/test splits
- List and interpret the 3 sources of avg. prediction error
  - Irreducible error, bias, and variance
- Discuss issue of selecting model complexity on test data and then using test error to assess generalization error
- Motivate use of a validation set for selecting tuning parameters (e.g., model complexity)
- Describe overall regression workflow

RIDGE REGRESSION

Flexibility of high-order polynomials

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



Symptoms for overfitting: often associated with very large value of estimated parameters $\hat{w}$

Overfitting with many features

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

Or, generically,
lots of features (D large)

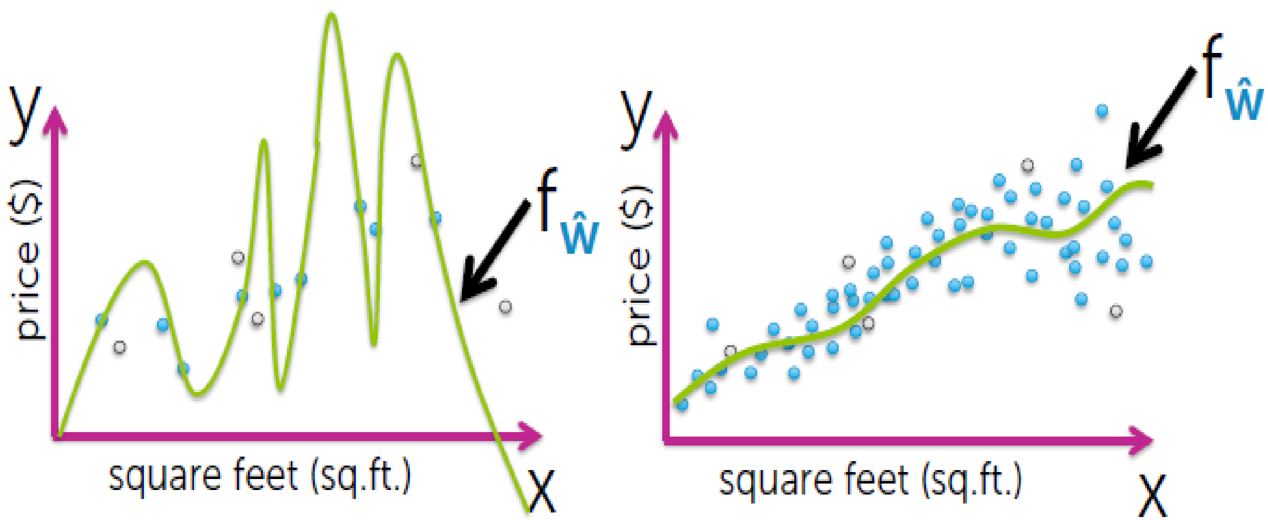
$$y_i = \sum_{j=0}^{D} w_j h_j(\mathbf{x}_i) + \varepsilon_i$$

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

How does # of observations influence overfitting?

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

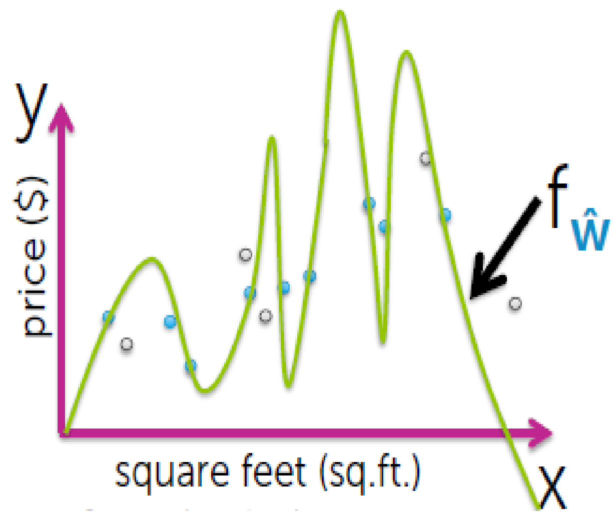
Many observations (N very large)
→ harder to overfit



How does # of inputs influence overfitting?

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

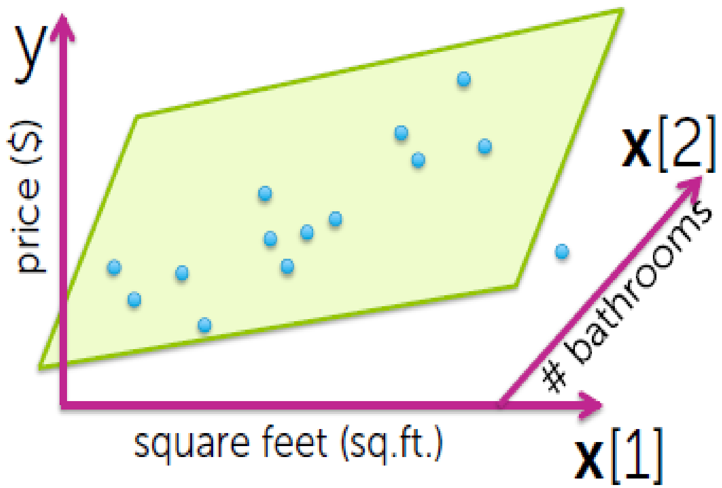
Data must include representative examples of all possible (sq.ft., $) pairs to avoid overfitting



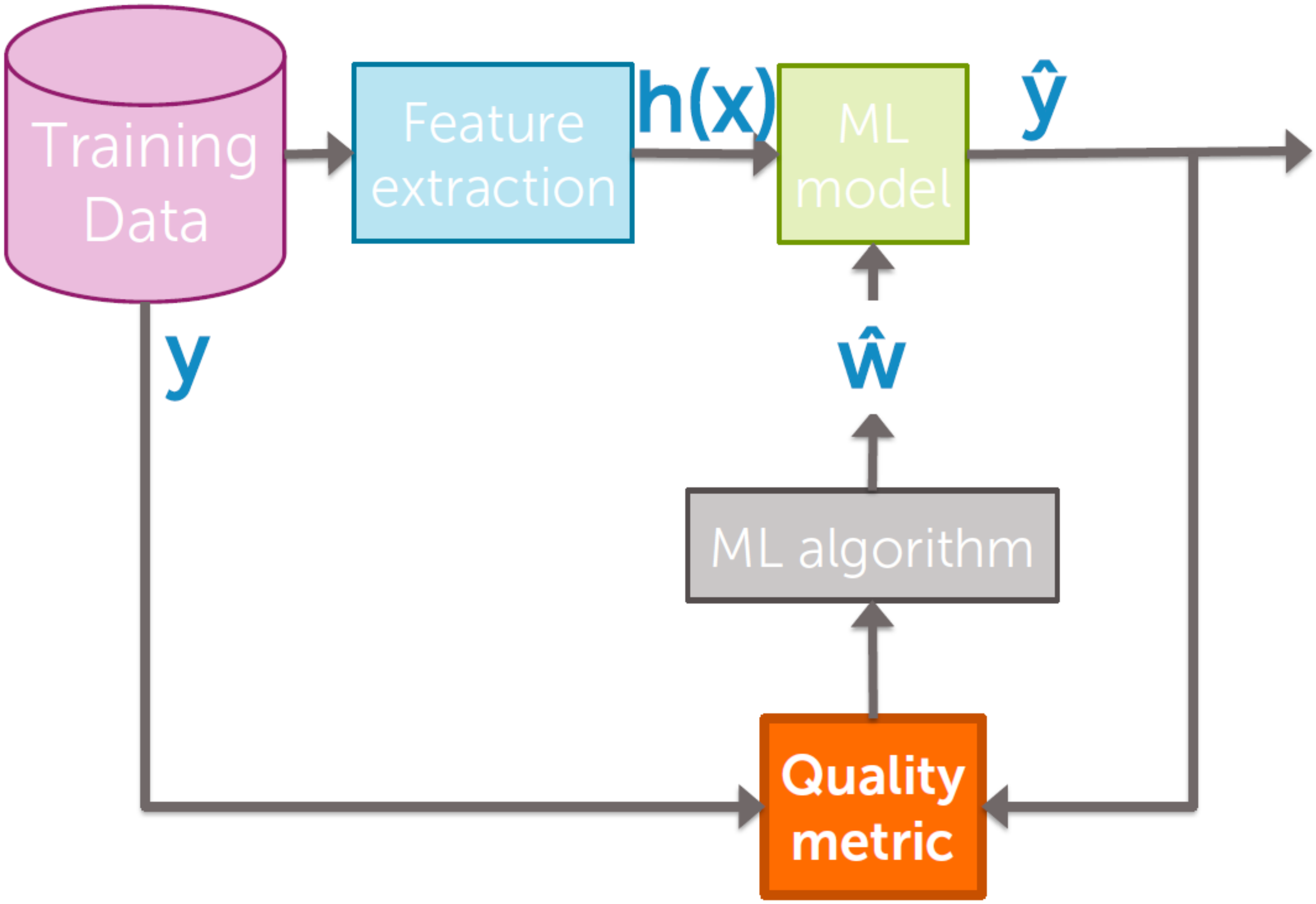
How does # of inputs influence overfitting?

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



Lets improve quality metric blok



Desire total cost format

Want to balance:

i. How well function fits data

ii. Magnitude of coefficients

want to balance

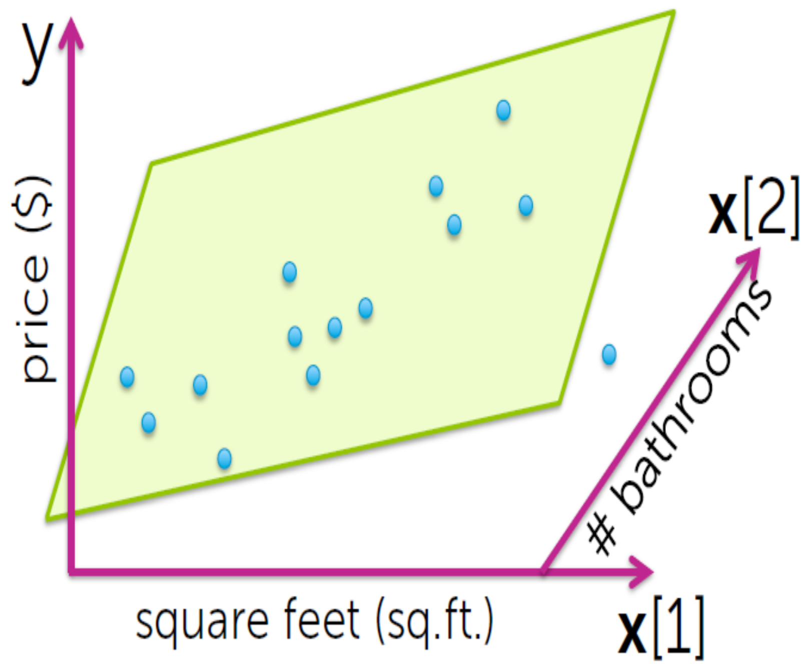
Total cost =

measure of fit + measure of magnitude of coefficients

small # = good fit to training data

small # = not overfit

Measure of fit to training data



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

$$= \sum_{i=1}^{N} (y_i - \hat{y}_i(\mathbf{w}))^2$$

pred. value using w

small RSS → model fitting training data well

Measure of magnitude of regression coefficients

What summary # is indicative of size of regression coefficients?

- Sum? $w_0 = 1{,}527{,}301 \quad w_1 = -1{,}605{,}253$

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

  But … the coefficients are very large

- Sum of absolute value?

  $|w_0| + |w_1| + \ldots + |w_D| = \sum_{j=0}^{D} |w_j| \triangleq \|w\|_1$ L_1 norm … discuss more in next module

- Sum of squares (L_2 norm)

  $w_0^2 + w_1^2 + \ldots + w_D^2 = \sum_{j=0}^{D} w_j^2 \triangleq \|w\|_2^2$ L_2 norm … focus of this module

Consider specific total cost

Total cost =

$$\underbrace{\text{measure of fit}}_{\text{RSS}(\mathbf{w})} + \underbrace{\text{measure of magnitude of coefficients}}_{||\mathbf{w}||_2^2}$$

Consider resulting objectives

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

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

Ridge regression
(a.k.a L_2 regularization)

tuning parameter = balance of fit and magnitude

If λ=0:

reduces to minimizing RSS(w), as before (old solution) → $\hat{w}^{LS}$ ← least squares

If λ=∞:

For solutions where $\hat{w} \neq 0$, then total cost is ∞

If $\hat{w}=0$, then total cost = RSS(0) → solution is $\hat{w}=0$

If λ in between: Then $0 \leq \|\hat{w}\|_2^2 \leq \|\hat{w}^{LS}\|_2^2$

Ridge regression: bias-variance tradeoff

Large λ:

high bias, low variance

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

In essence, λ controls model complexity

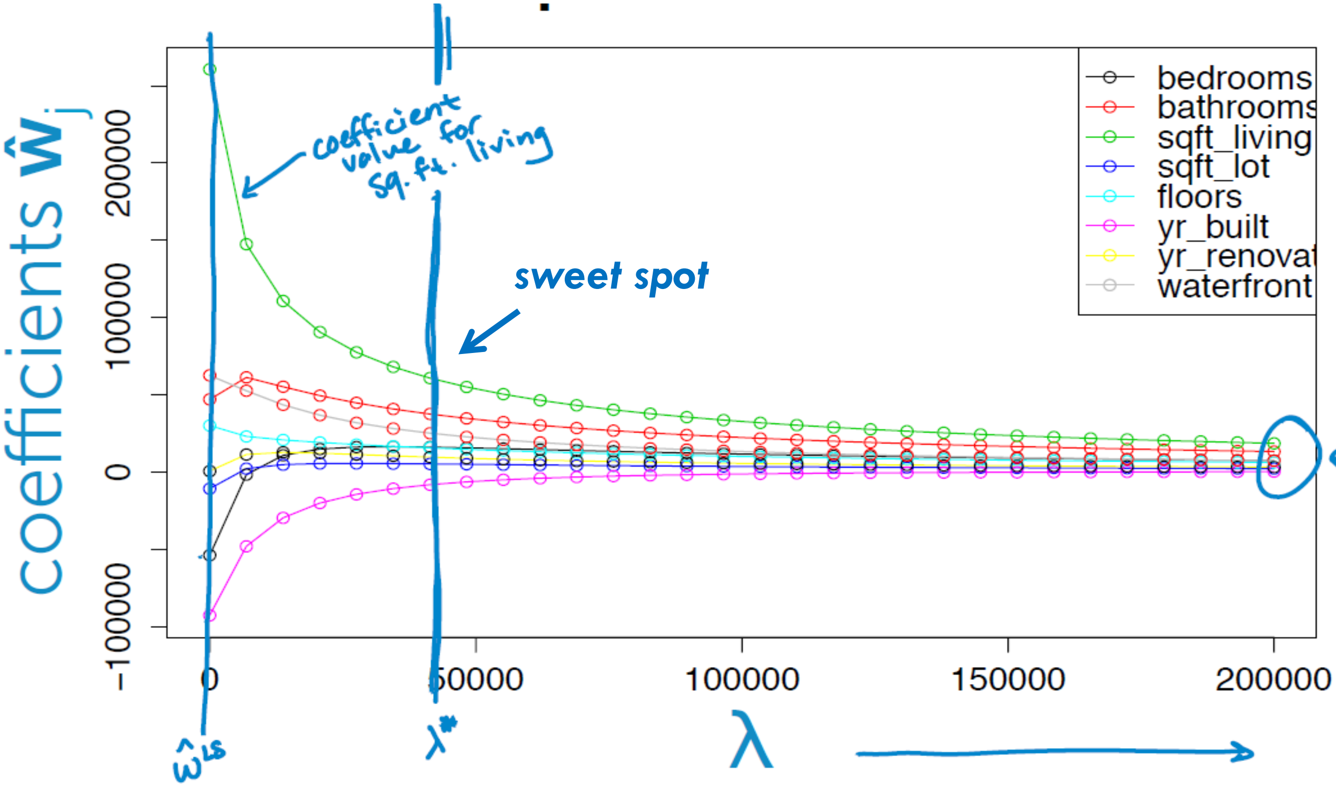
Small λ:

low bias, high variance

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

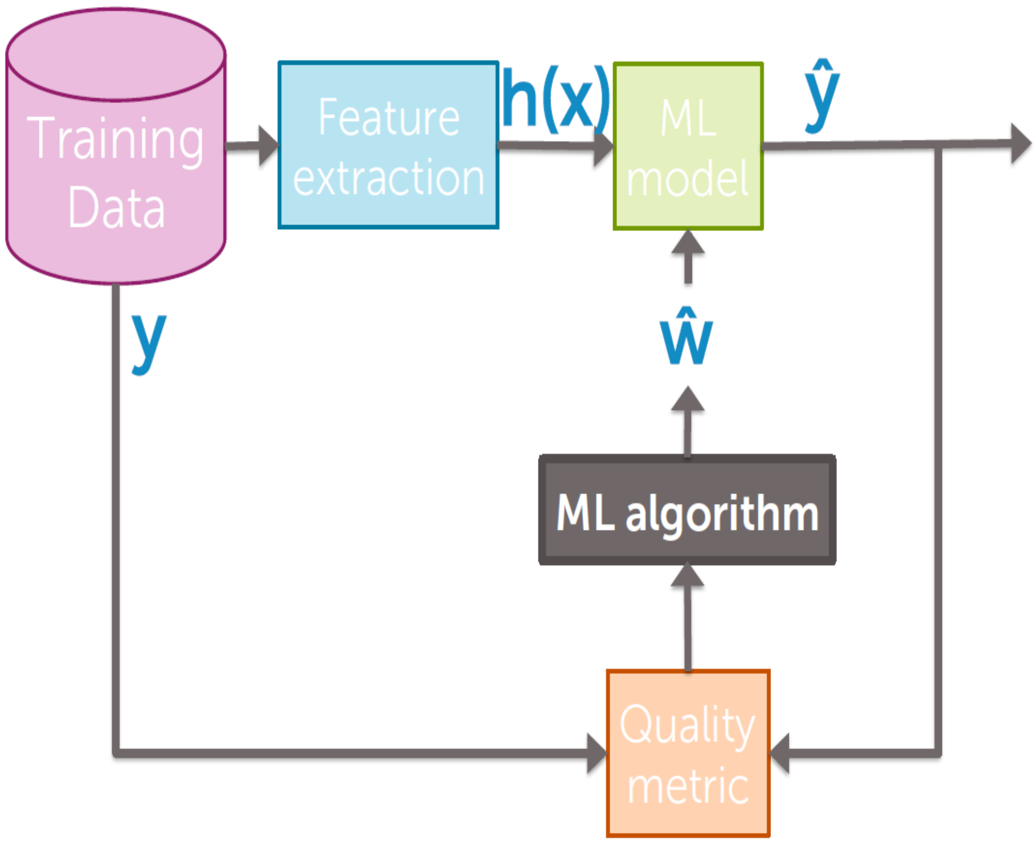
Ridge regression: coefficients path

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

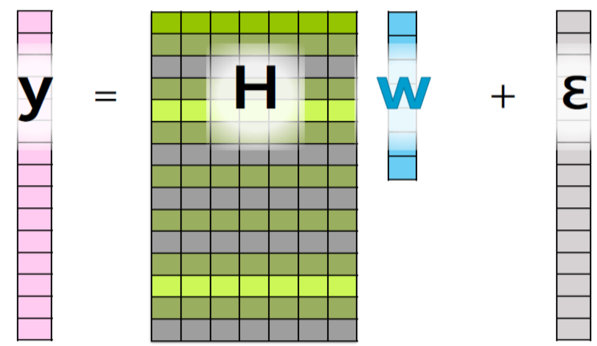


features scaled to unit norm

Flow chart



Model for all N observations together



Ridge regression: cost in matrix notation

In matrix form, ridge regression cost is:

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

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

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

$$= \begin{bmatrix} w_0 & w_1 & w_2 & \cdots & w_D \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix}$$

$$= w^T w$$

Gradient of ridge regresion cost

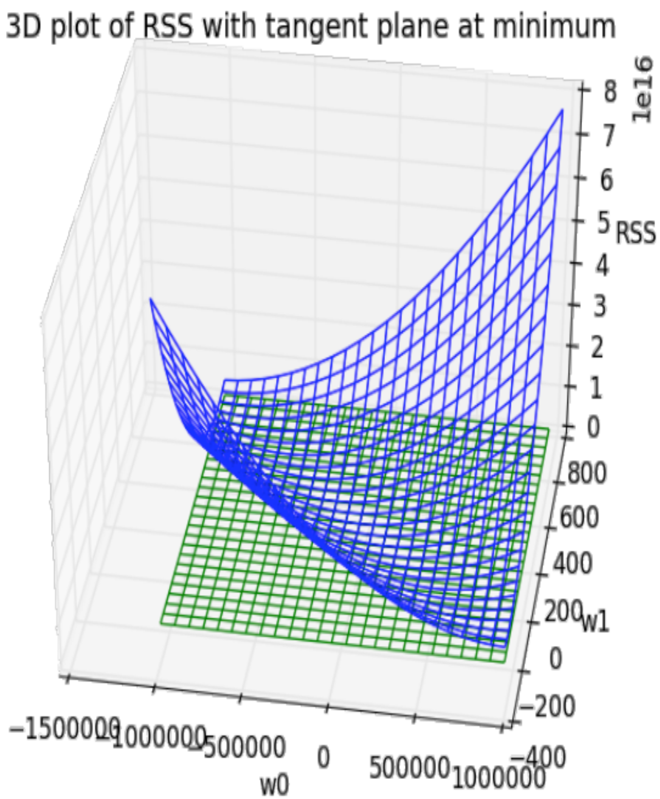
$$\nabla[RSS(\mathbf{w}) + \lambda||\mathbf{w}||_2^2] = \nabla[(\mathbf{y}-\mathbf{H}\mathbf{w})^T(\mathbf{y}-\mathbf{H}\mathbf{w}) + \lambda\mathbf{w}^T\mathbf{w}]$$

$$= \underbrace{\nabla[(\mathbf{y}-\mathbf{H}\mathbf{w})^T(\mathbf{y}-\mathbf{H}\mathbf{w})]}_{-2\mathbf{H}^T(\mathbf{y}-\mathbf{H}\mathbf{w})} + \lambda \underbrace{\nabla[\mathbf{w}^T\mathbf{w}]}_{2\mathbf{w}}$$

Why? By analogy to 1d case…

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

Ridge regression: closed-form solution



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

Solve for **w**:

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

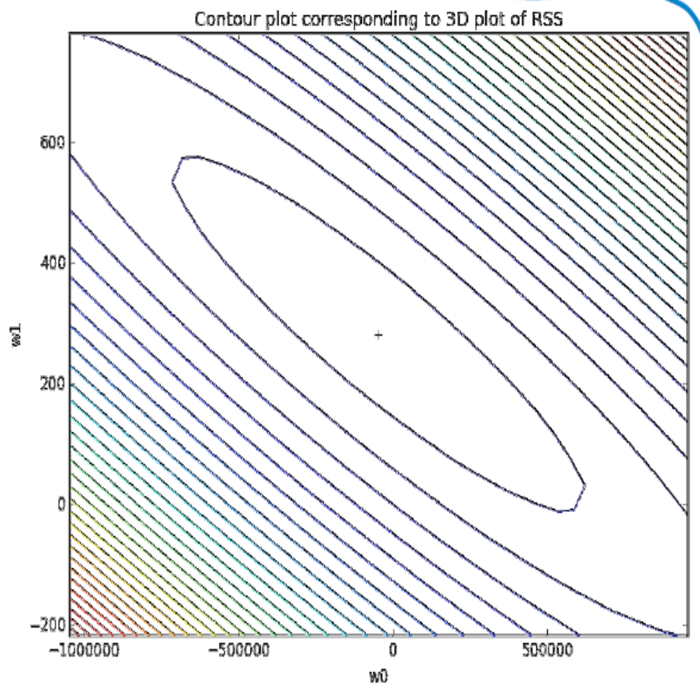
$$H^T H \hat{w} + \lambda I \hat{w} = H^T y$$

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

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

Ridge regression: gradient descent

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



Update to j^{th} feature weight:

$$w_j^{(t+1)} \leftarrow w_j^{(t)} - \eta * \left[-2 \sum_{i=1}^{N} h_j(\mathbf{x}_i)(y_i - \hat{y}_i(\mathbf{w}^{(t)})) + 2\lambda w_j^{(t)} \right]$$

Same as before (from RSS term)

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

Summary of ridge regression algorithm

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

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

for $j=0,\ldots,D$

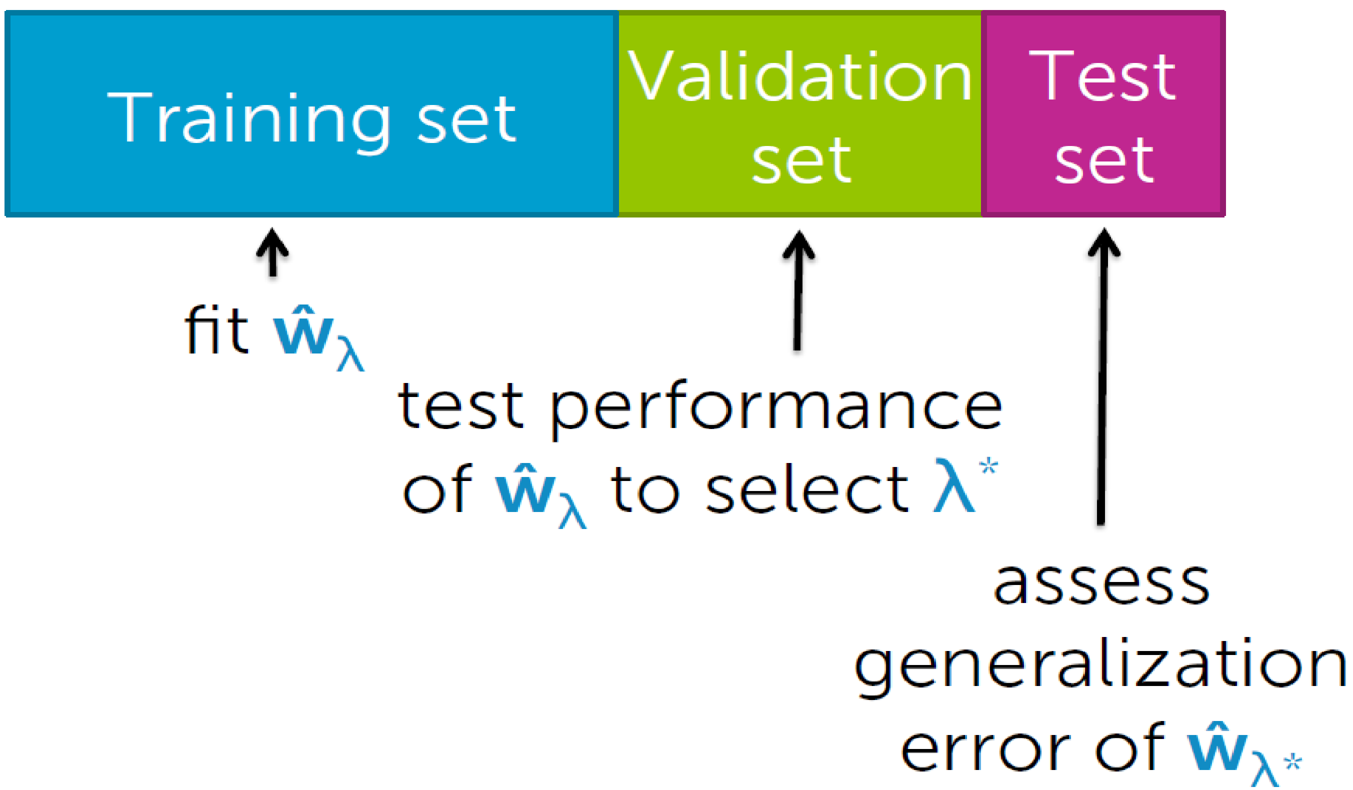
partial[j] $= -2\, h_j \sum_{i=1}^{N} h_j(\mathbf{x}_i)(y_i-\hat{y}_i(\mathbf{w}^{(t)}))$

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

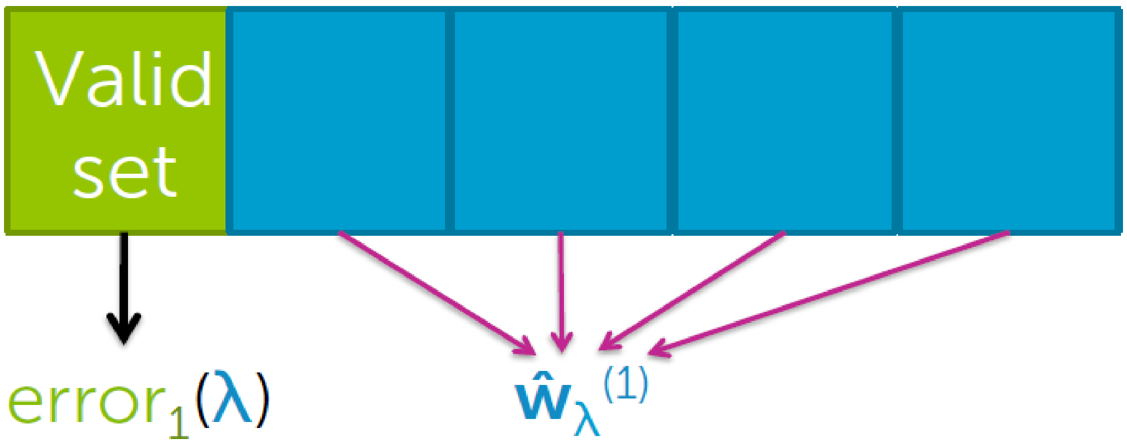
$t \leftarrow t + 1$

How to choose λ

If sufficient amount of data...



K-fold cross validation

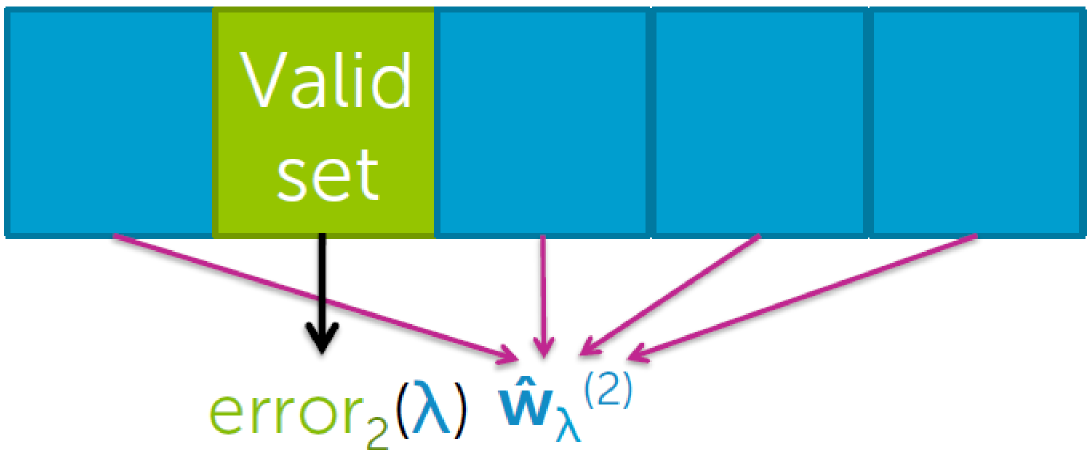


For k=1,...,K

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

How to choose λ

K-fold cross validation

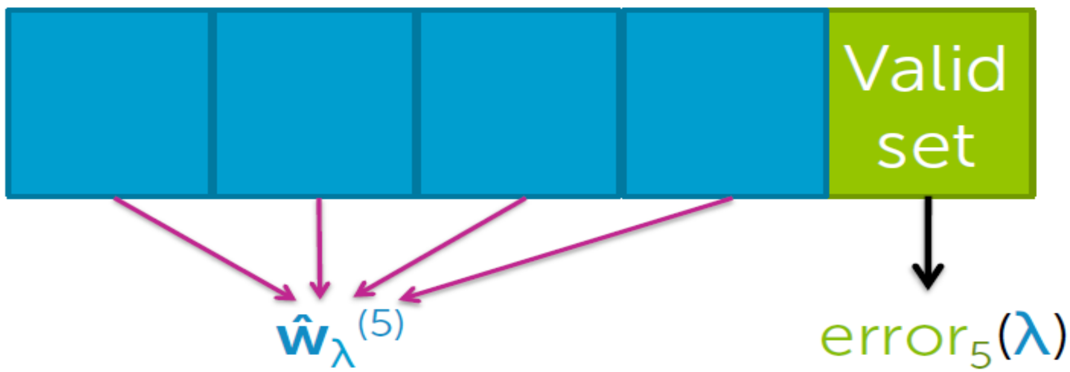


For k=1,…,K

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

How to choose λ

K-fold cross validation



For k=1,…,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: $CV(\lambda) = \frac{1}{K}\sum_{k=1}^{K} \text{error}_k(\lambda)$

How to choose λ

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:

$$y_i = w_0 h_0(\mathbf{x}_i) + w_1 h_1(\mathbf{x}_i) + \ldots + w_D h_D(\mathbf{x}_i) + \varepsilon_i$$

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

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., $\mathbf{x}[d]$

Do we penalize intercept?

Standard ridge regression cost:

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

strength of penalty

Encourages intercept w_0 to also be small

Do we want a small intercept?

Conceptually, not indicative of overfitting…

Do we penalize intercept?

- **Option 1: don't penalize intercept**

  Modified ridge regression cost:

  $$\mathrm{RSS}(w_{0,}\mathbf{w}_{rest}) + \lambda \|\mathbf{w}_{rest}\|_2^2$$

- **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)

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

FEATURES SELECTION

&

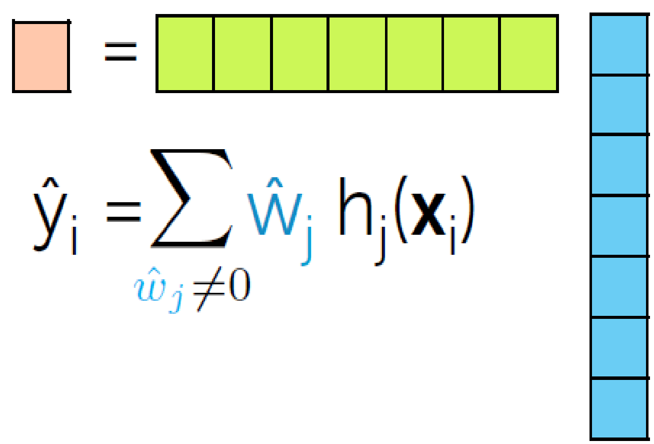
LASSO REGRESSION

Why features selection?

Efficiency:

- If size(**w**) = 100B, each prediction is expensive
- If $\hat{\mathbf{w}}$ sparse, computation only depends on # of non-zeros

many zeros



$$\hat{y}_i = \sum_{\hat{w}_j \neq 0} \hat{w}_j \, h_j(\mathbf{x}_i)$$

Interpretability:

- Which features are relevant for prediction?

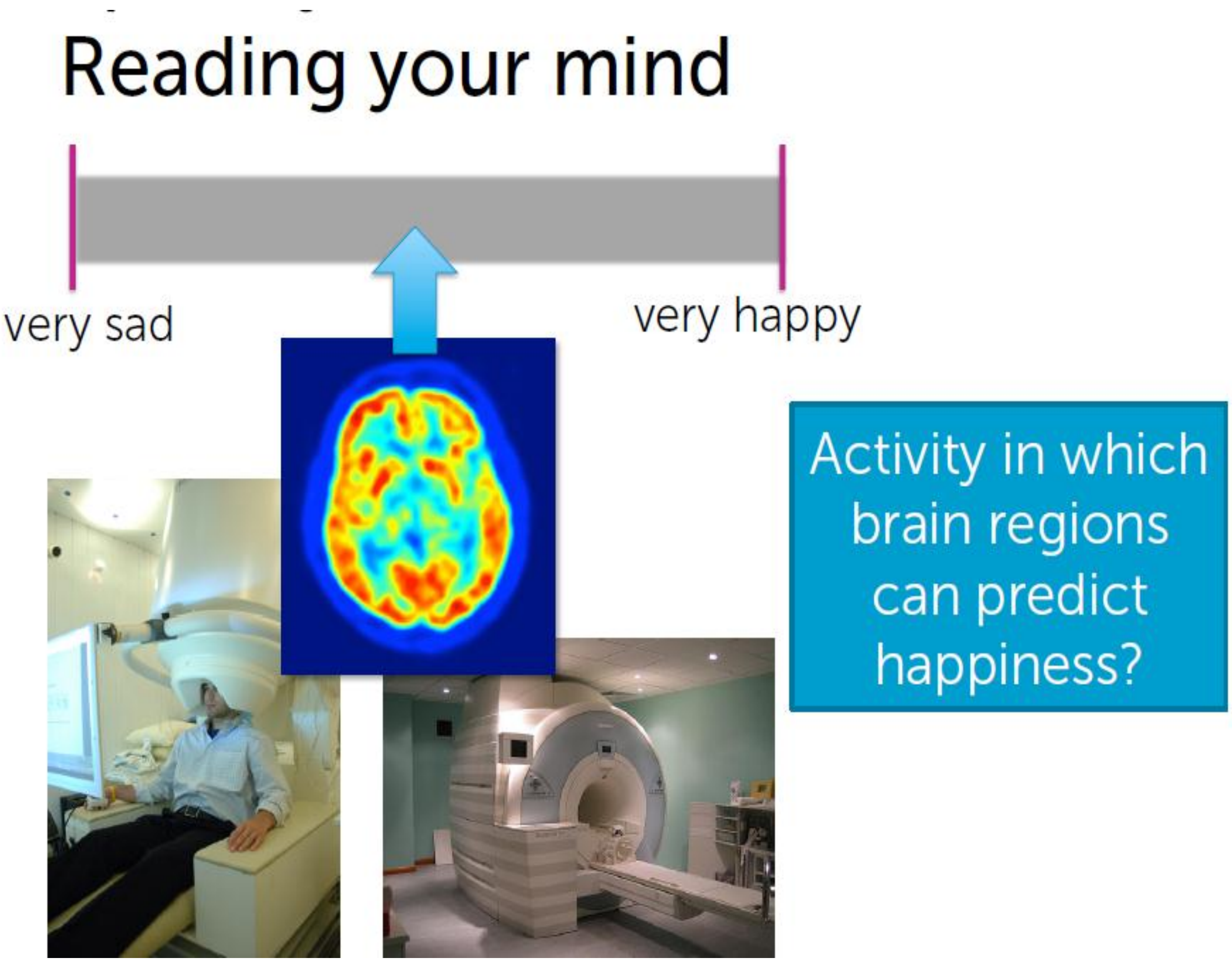
Sparcity

Housing application

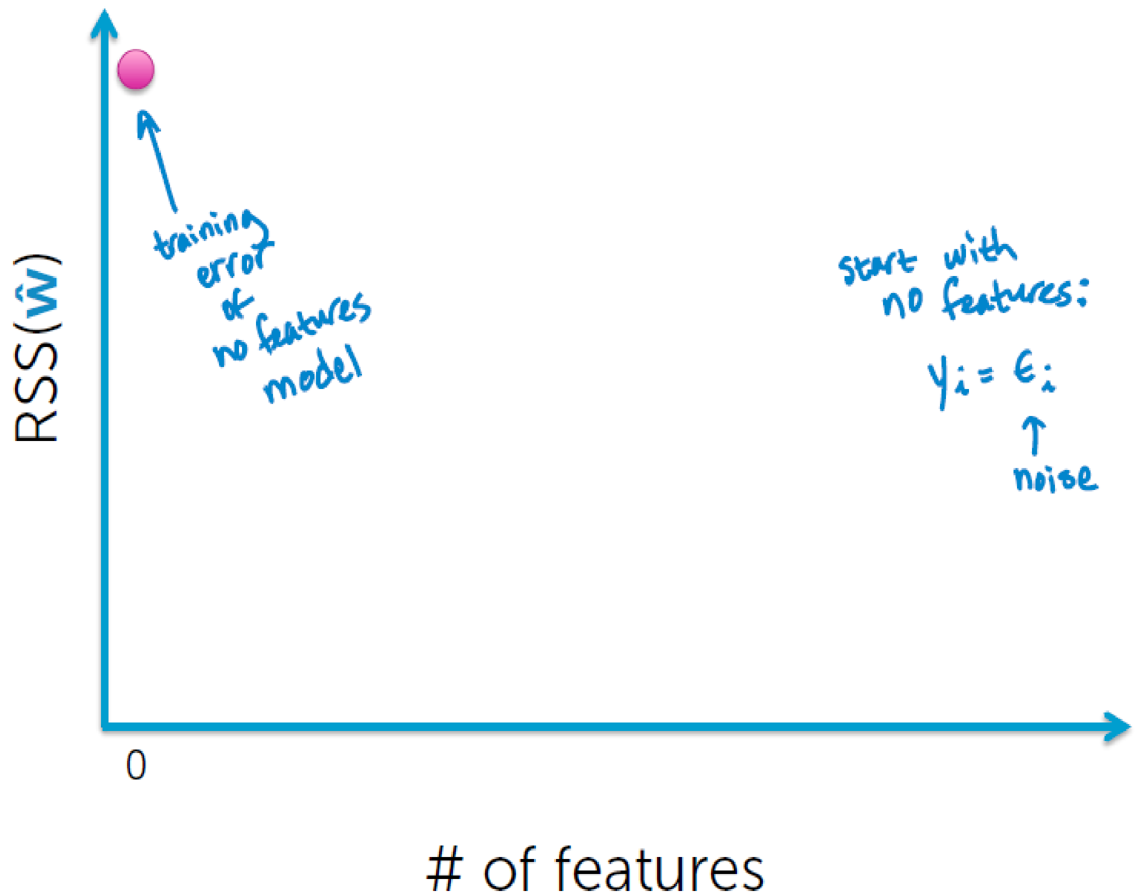
Lot size
Single Family
Year built
Last sold price
Last sale price/sqft
Finished sqft
Unfinished sqft
Finished basement sqft
floors
Flooring types
Parking type
Parking amount
Cooling
Heating
Exterior materials
Roof type
Structure style

Dishwasher
Garbage disposal
Microwave
Range / Oven
Refrigerator
Washer
Dryer
Laundry location
Heating type
Jetted Tub
Deck
Fenced Yard
Lawn
Garden
Sprinkler System
⋮

Sparcity

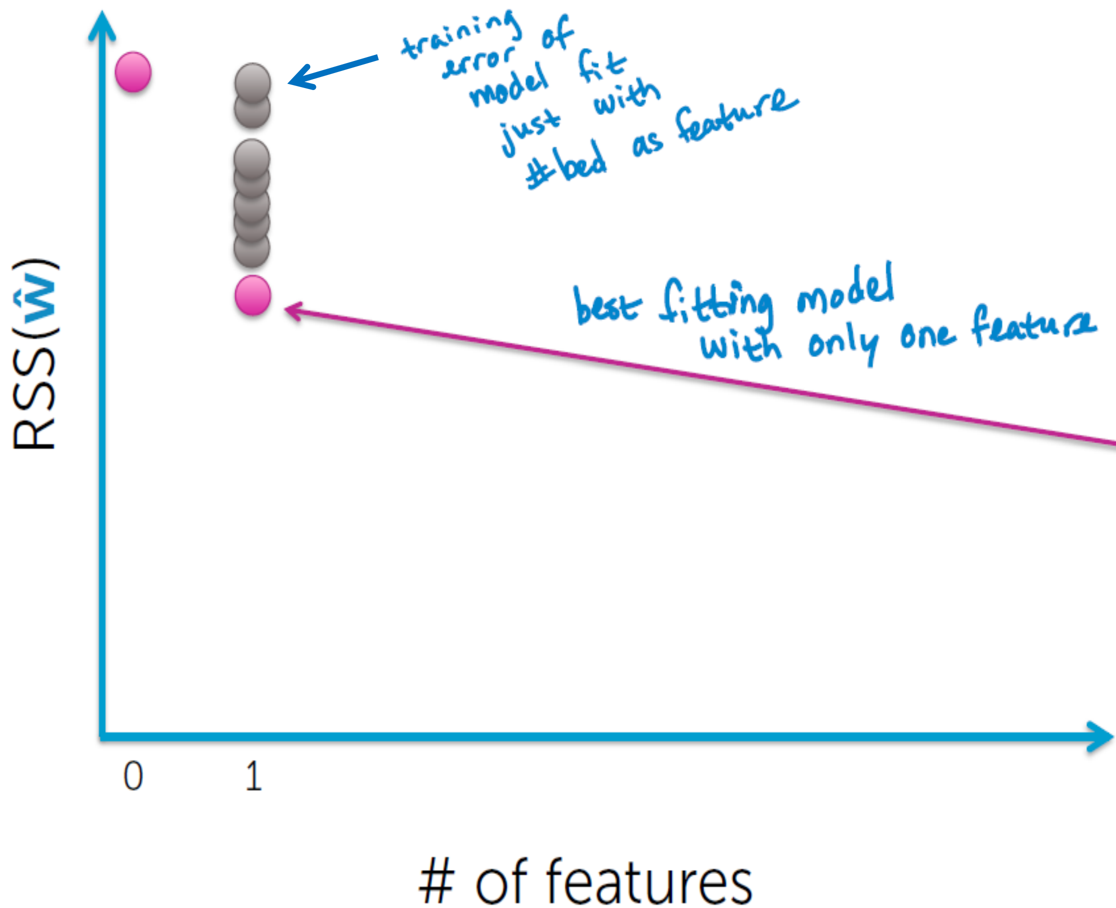

Reading your mind
very sad
very happy
Activity in which brain regions can predict happiness?

Find best model of size: 0



- ~~# bedrooms~~
- ~~# bathrooms~~
- ~~sq.ft. living~~
- ~~sq.ft. lot~~
- ~~floors~~
- ~~year built~~
- ~~year renovated~~
- ~~waterfront~~

Find best model of size: 1



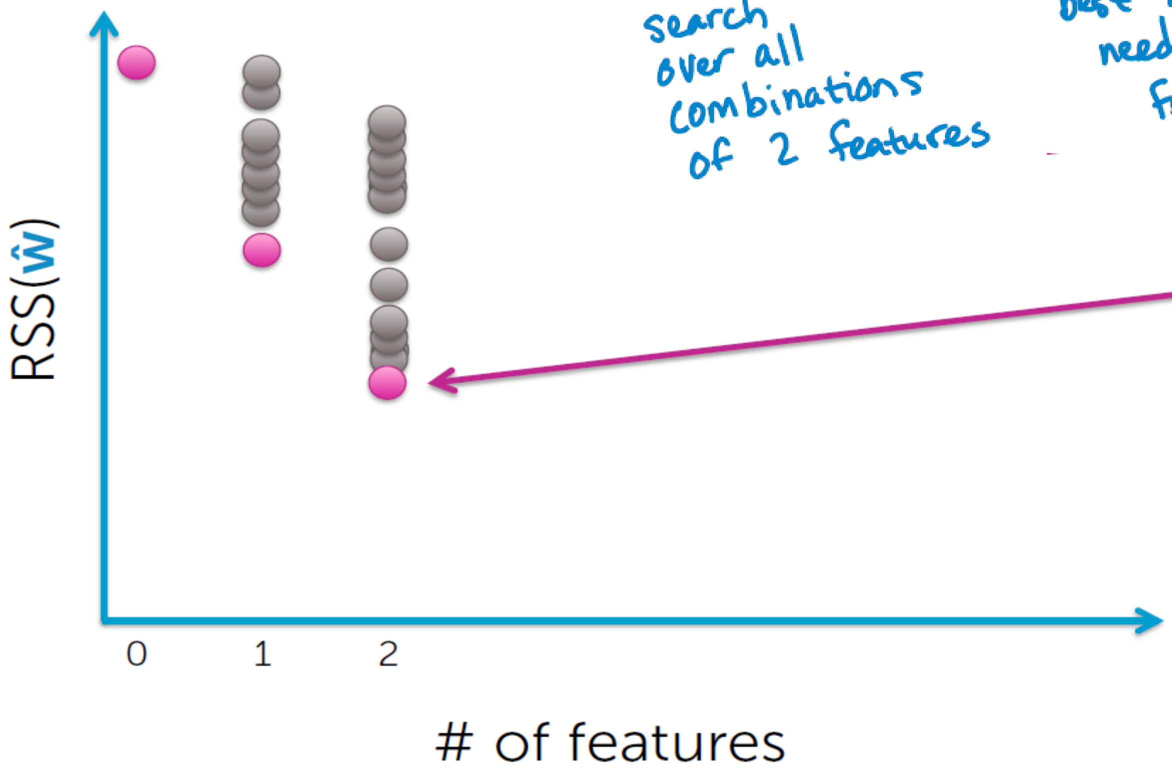
- # bedrooms
- # bathrooms
- sq.ft. living
- sq.ft. lot
- floors
- year built
- year renovated
- waterfront

Find best model of size: 2

Note: not necessarily nested!

search over all combinations of 2 features

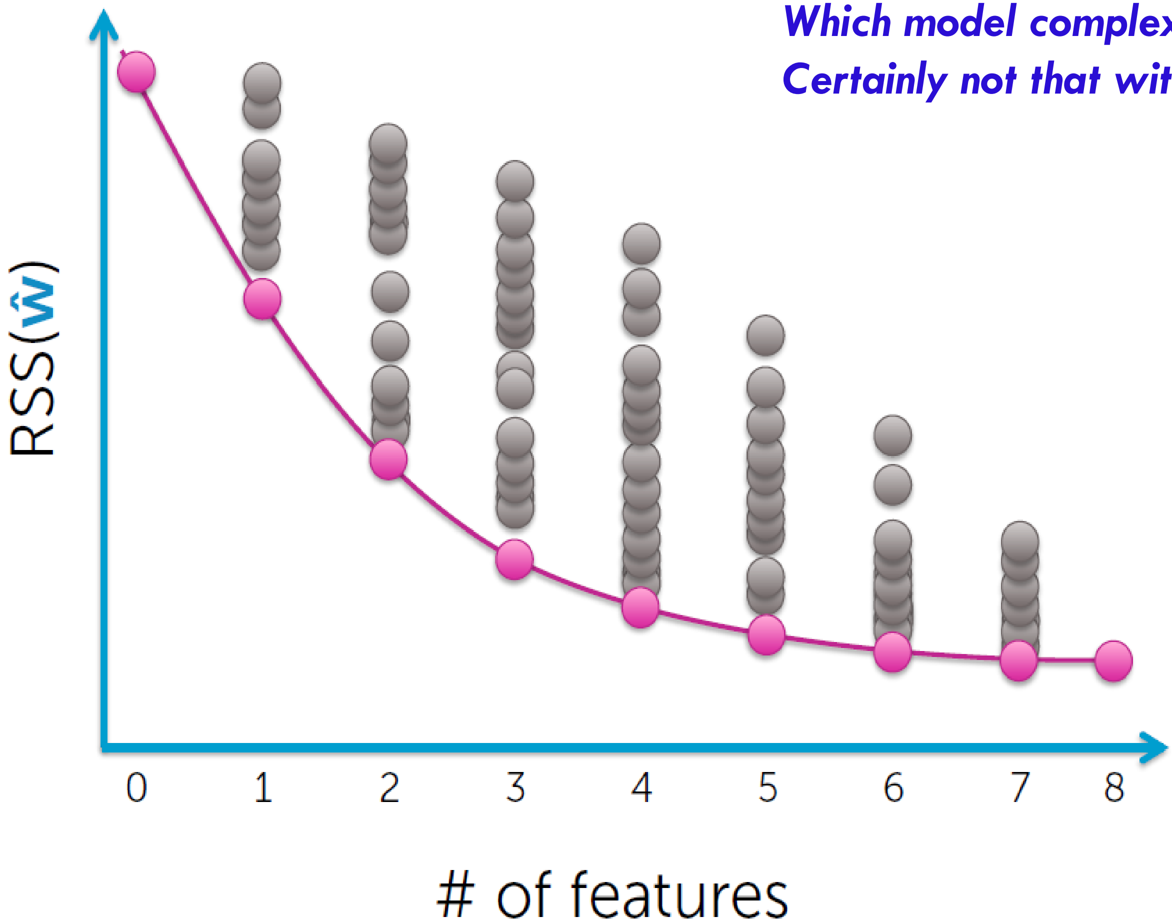
best model of size k need not contain features of best model of size k-1



- $\boxed{\text{\# bedrooms}}$
- $\boxed{\text{\# bathrooms}}$
- sq.ft. living
- sq.ft. lot
- floors
- year built
- year renovated
- waterfront

Find best model of size: N

Which model complexity to choose?
Certainly not that with the smalest training error!



- # bedrooms
- # bathrooms
- sq.ft. living
- sq.ft. lot
- floors
- year built
- year renovated
- waterfront

Choosing model complexity

Option 1: Assess on validation set

Option 2: Cross validation

Option 3+: Other metrics for penalizing model complexity like BIC…

Complexity of „all subsets"

How many models were evaluated?

- each indexed by features included

feature 0 ← 0 if "no", 1 if "yes"
feature 1 ... feature D

$$\left.\begin{array}{ll}
y_i = \varepsilon_i & [0\ 0\ 0\ \dots\ 0\ 0\ 0] \\
y_i = w_0 h_0(\mathbf{x}_i) + \varepsilon_i & [1\ 0\ 0\ \dots\ 0\ 0\ 0] \\
y_i = w_1 h_1(\mathbf{x}_i) + \varepsilon_i & [0\ 1\ 0\ \dots\ 0\ 0\ 0] \\
\vdots & \vdots \\
y_i = w_0 h_0(\mathbf{x}_i) + w_1 h_1(\mathbf{x}_i) + \varepsilon_i & [1\ 1\ 0\ \dots\ 0\ 0\ 0] \\
\vdots & \vdots \\
y_i = w_0 h_0(\mathbf{x}_i) + w_1 h_1(\mathbf{x}_i) + \dots + w_D h_D(\mathbf{x}_i) + \varepsilon_i & [1\ 1\ 1\ \dots\ 1\ 1\ 1] \\
 & \ \ 2\ \ 2\ \ 2\ \dots\ 2
\end{array}\right\} 2^{D+1}$$

$2^8 = 256$

$2^{30} = 1{,}073{,}741{,}824$

$2^{1000} = 1.071509 \times 10^{301}$

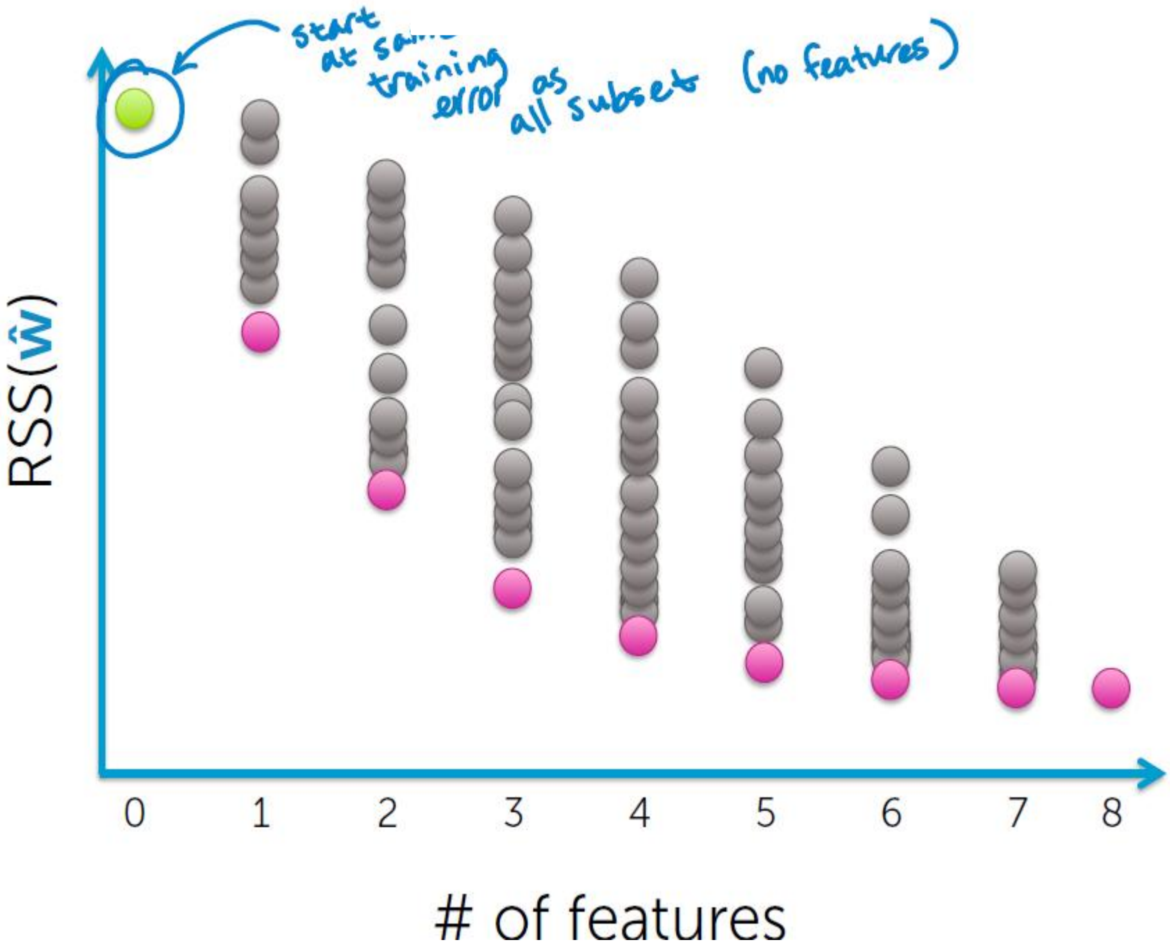
2^{100B} = HUGE!!!!!!

Typically, computationally infeasible

Forward stepwise algorithm

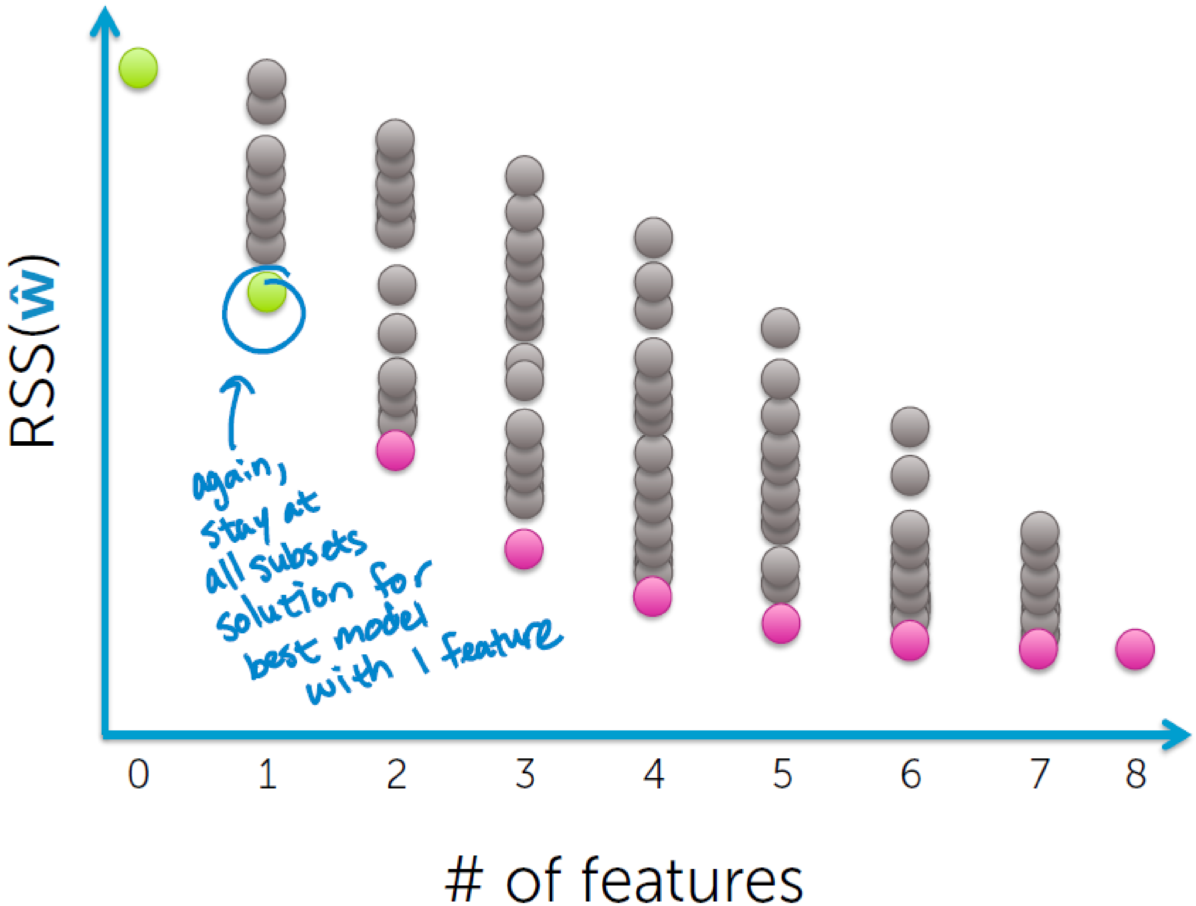
1. Pick a dictionary of features $\{h_0(\mathbf{x}),\ldots,h_D(\mathbf{x})\}$
   – e.g., polynomials for linear regression
2. Greedy heuristic:
   i. Start with empty set of features $F_0 = \varnothing$
      (or simple set, like just $h_0(\mathbf{x})=1 \rightarrow y_i = w_0 + \varepsilon_i$)
   ii. Fit model using current feature set F_t to get $\hat{\mathbf{w}}^{(t)}$
   iii. Select next best feature $h_{j*}(\mathbf{x})$
      – e.g., $h_j(\mathbf{x})$ resulting in lowest training error when learning with $F_t + \{h_j(\mathbf{x})\}$
   iv. Set $F_{t+1} \leftarrow F_t + \{h_{j*}(\mathbf{x})\}$
   v. Recurse

Visualizing greedy algorithm



- # bedrooms
- # bathrooms
- sq.ft. living
- sq.ft. lot
- floors
- year built
- year renovated
- waterfront

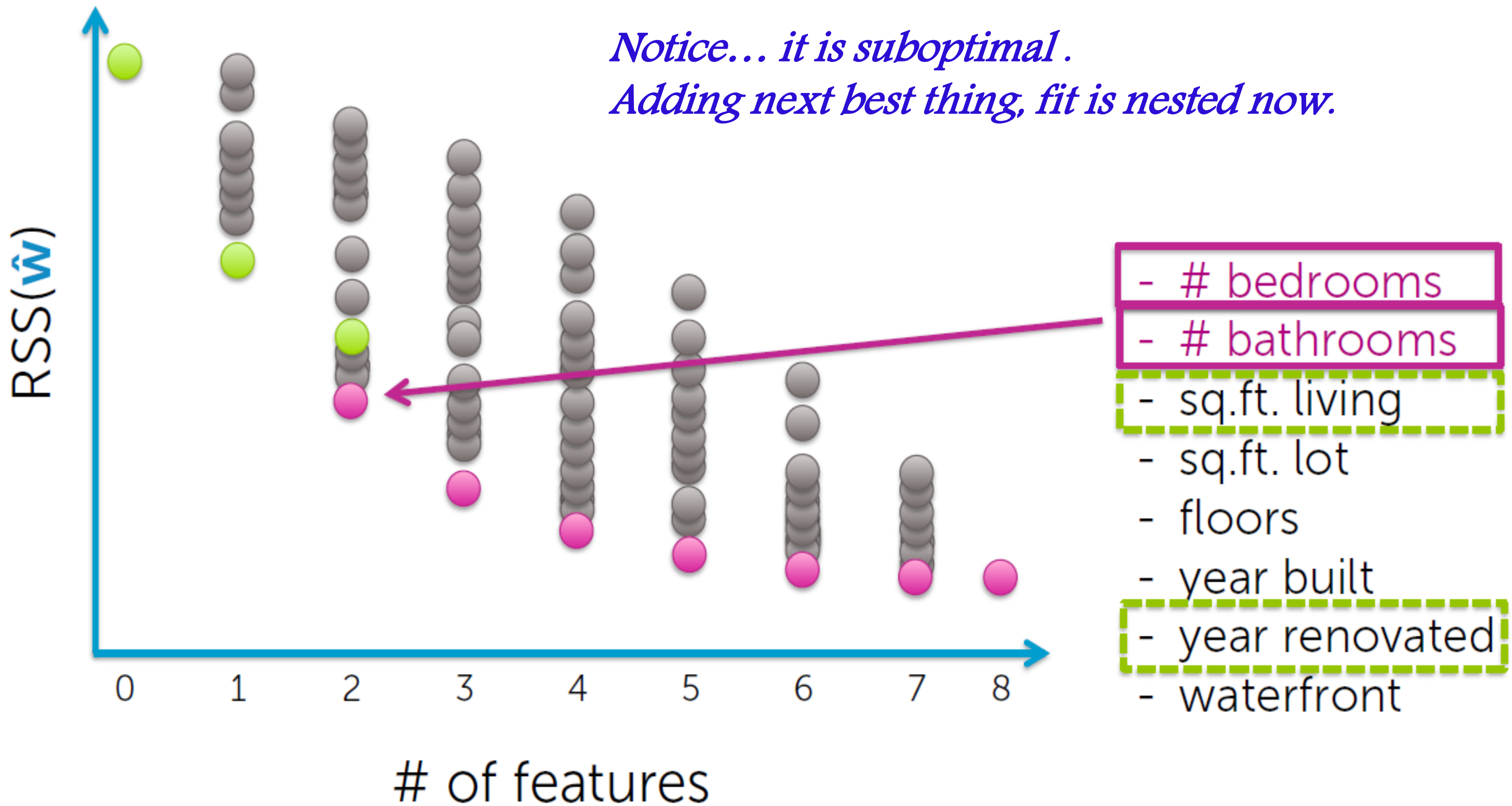
Visualizing greedy algorithm



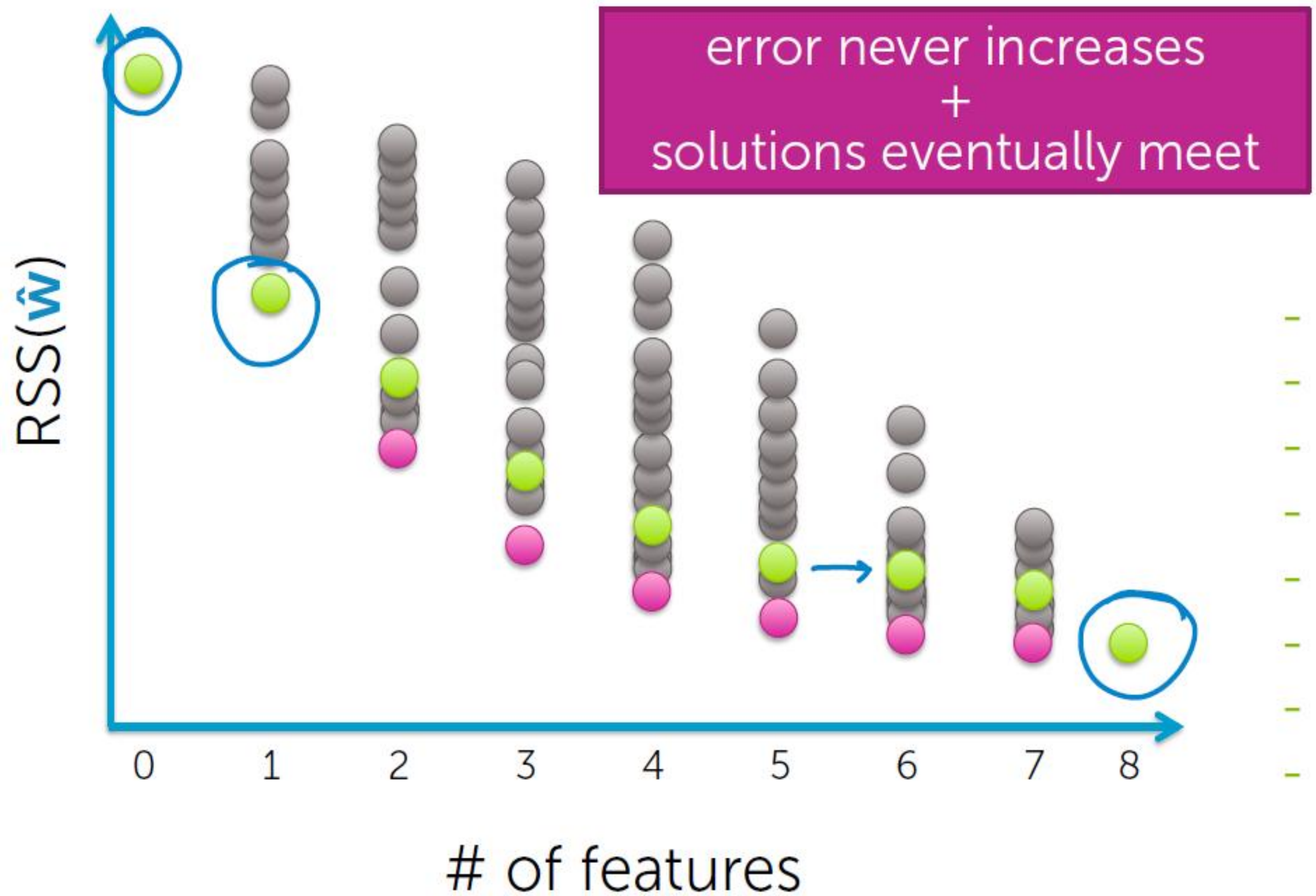
- # bedrooms
- # bathrooms
- sq.ft. living
- sq.ft. lot
- floors
- year built
- year renovated
- waterfront

Visualizing greedy algorithm

Notice… it is suboptimal .
Adding next best thing, fit is nested now.



Visualizing greedy algorithm



- # bedrooms
- # bathrooms
- sq.ft. living
- sq.ft. lot
- floors
- year built
- year renovated
- waterfront

When do we stop?

When **training error** is low enough?

No!

When **test error** is low enough?

No!

Use ***validation set*** ***or*** ***cross validation!***

Complexity of forward stepwise

How many models were evaluated?

- 1^{st} step, D models
- 2^{nd} step, D-1 models (add 1 feature out of D-1 possible)
- 3^{rd} step, D-2 models (add 1 feature out of D-2 possible)
- ...

How many steps?

- Depends
- At most D steps (to full model)

$O(D^2) \ll 2^D$

for large D

Other greedy algorithms

Instead of starting from simple model
and always growing…

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.

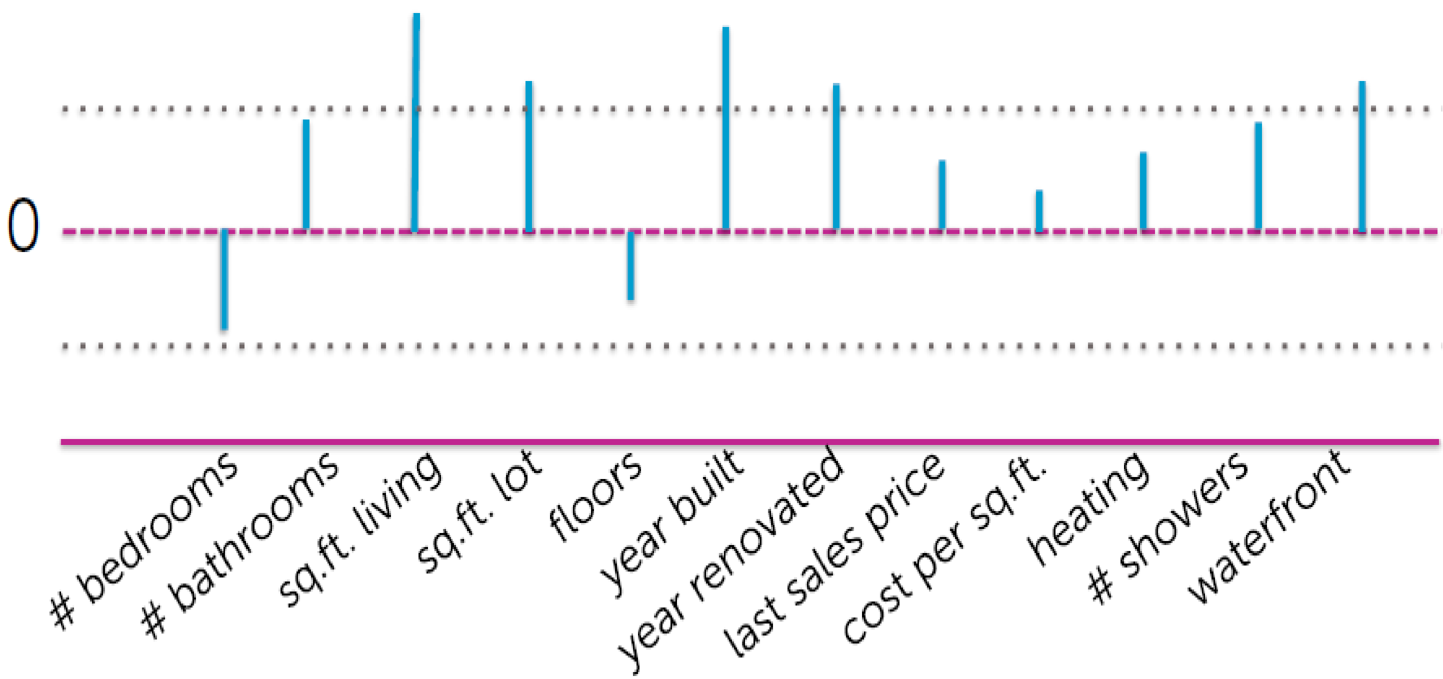
Using regularisation for features selection

Instead of searching over a **discrete** set of solutions, can we use regularization?

- Start with full model (all possible features)
- "Shrink" some coefficients *exactly* to 0
  - i.e., knock out certain features
- Non-zero coefficients indicate "selected" features

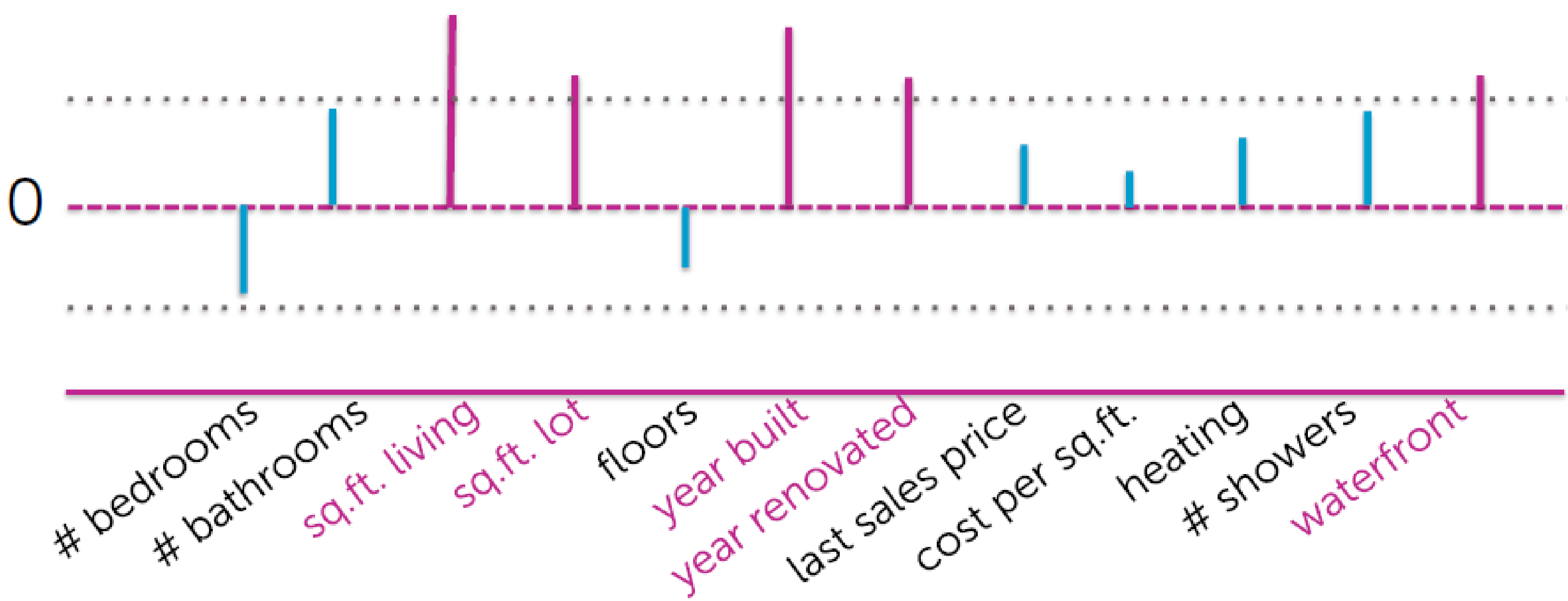
Thresholding ridge coefficients?

Why don't we just set small ridge coefficients to 0?



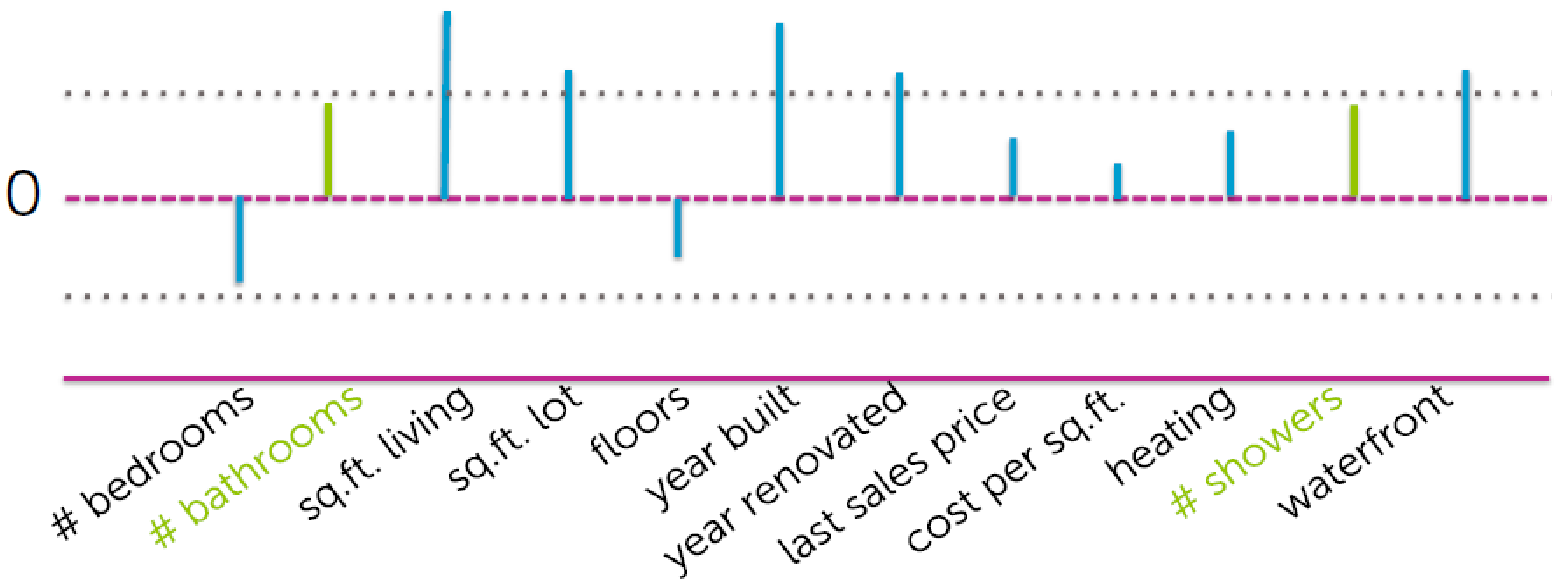
Thresholding ridge coefficients?

Selected features for a given threshold value



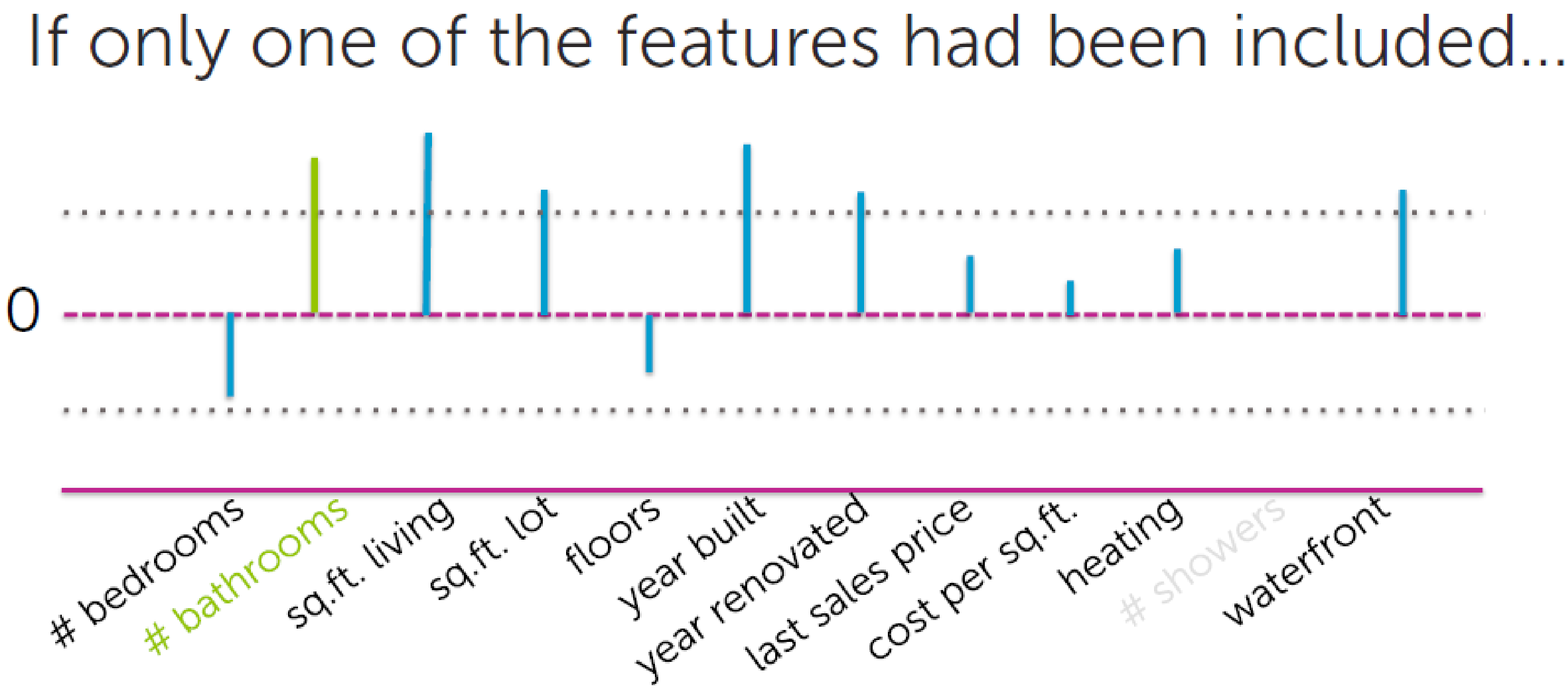
Thresholding ridge coefficients?

Let's look at two related features…



Nothing measuring bathrooms was included!

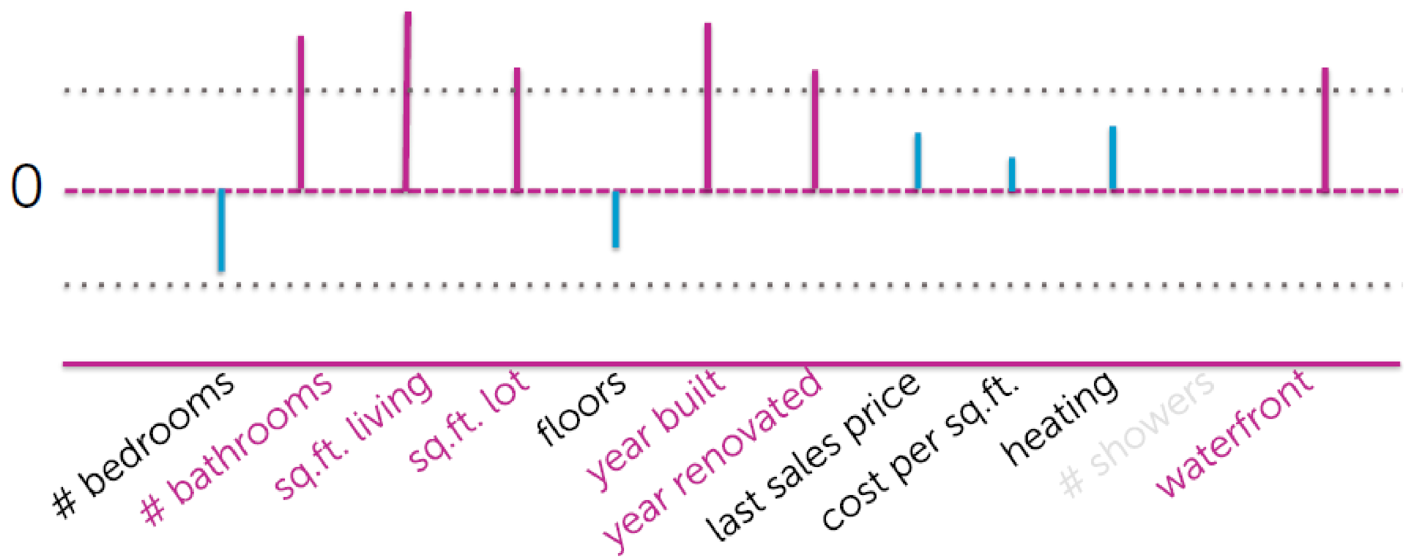
Thresholding ridge coefficients?



Remember:
this is linear model. If we assume that #showers = #bathrooms and remove one of them from the model, coefficients will sum up.

Thresholding ridge coefficients?

Would have included bathrooms in selected model



Can regularization lead directly to sparsity?

Try this cost instead of ridge ...

Total cost =

$$\underbrace{\text{measure of fit}}_{\text{RSS}(\mathbf{w})} + \lambda \underbrace{\text{measure of magnitude of coefficients}}_{||\mathbf{w}||_1 = |w_0| + \ldots + |w_D|}$$

Lasso regression
(a.k.a. L_1 regularized regression)

Leads to **sparse** solutions!

Lasso regression

Just like ridge regression, solution is governed by a continuous parameter λ

$$\text{RSS}(\mathbf{w}) + \lambda\|\mathbf{w}\|_1$$

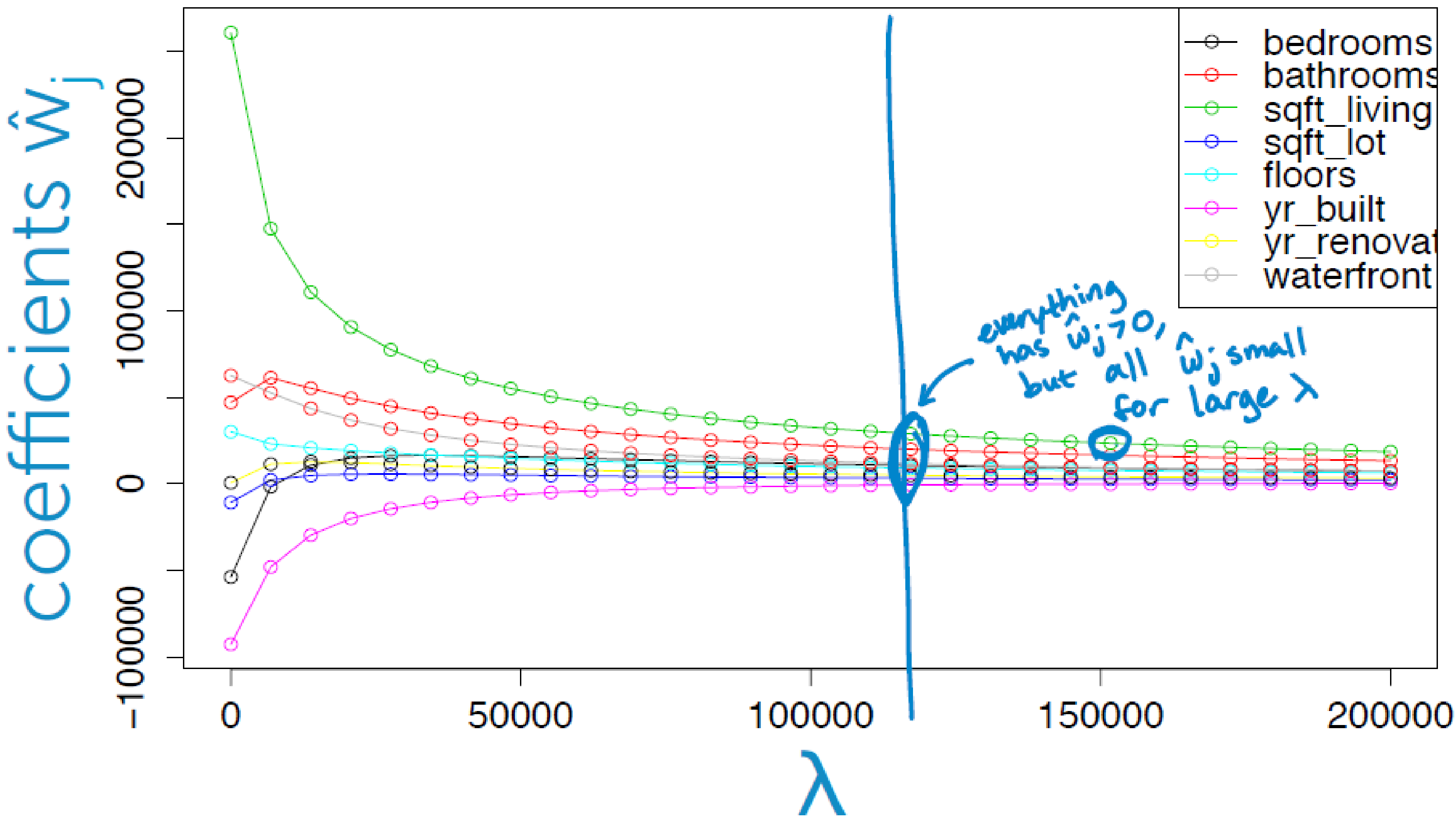
tuning parameter = balance of fit and sparsity

If $\lambda=0$: $\hat{w}^{lasso} = \hat{w}^{LS}$ (unregularized solution)

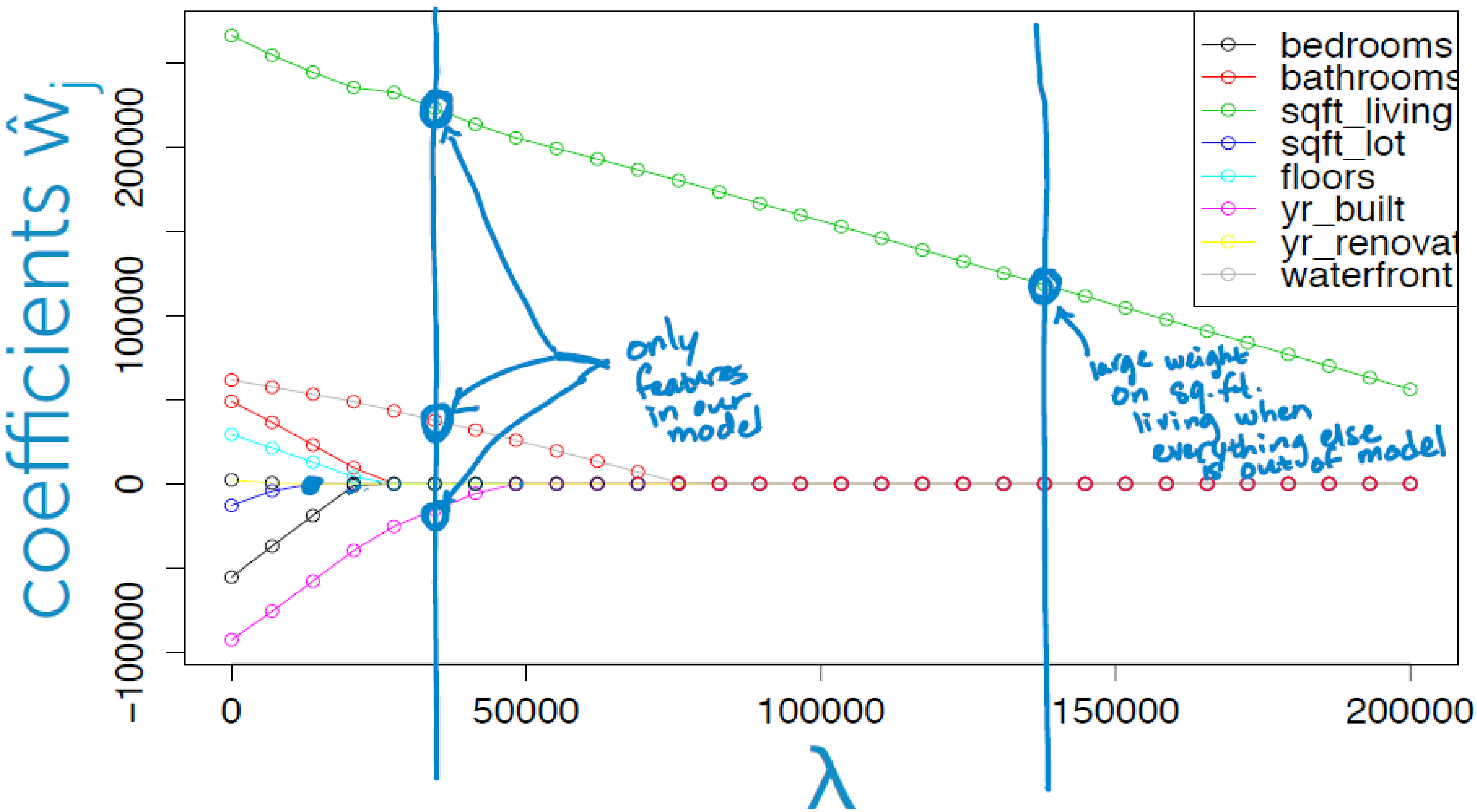
If $\lambda=\infty$: $\hat{w}^{lasso} = 0$

If λ in between: $0 \leq \|\hat{w}^{lasso}\|_1 \leq \|\hat{w}^{LS}\|_1$

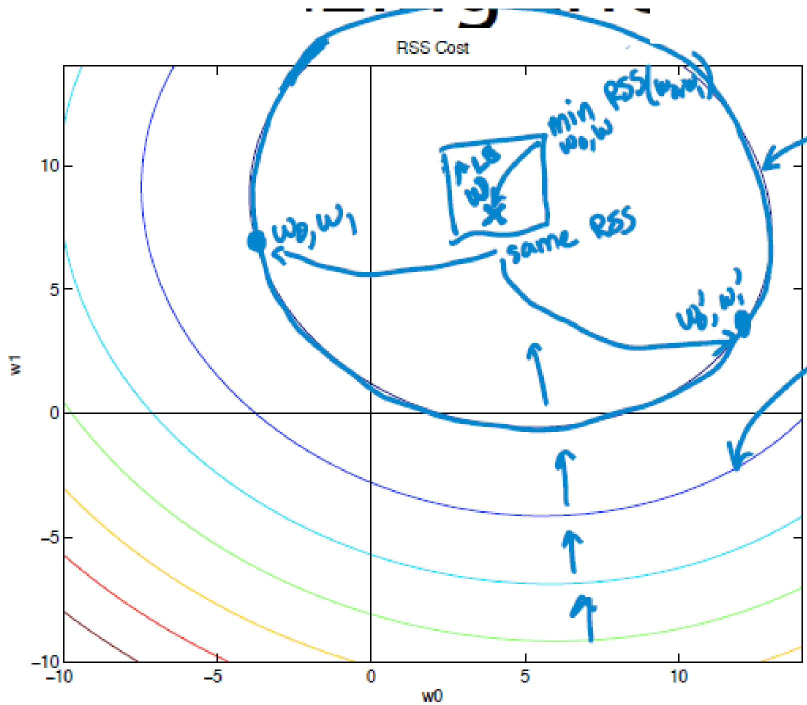
Coefficient path: ridge



Coefficient path: lasso



Visualising ridge cost in 2D



$RSS(w_0,w_1) = const_1$

$RSS(w_0,w_1) = const_2 > const_1$

⋮

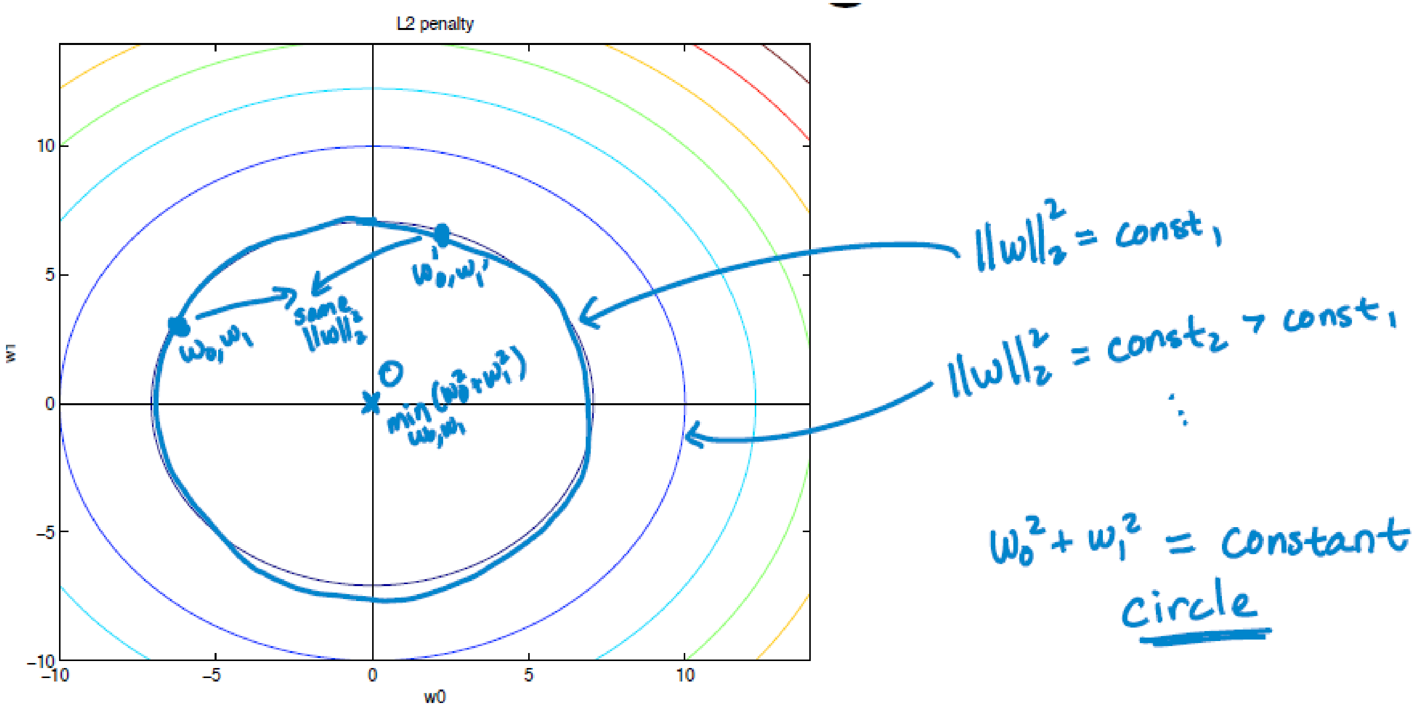
$\sum_i y_i^2 + w_0^2 \sum_i h_0^2 + w_1^2 \sum_i h_1^2$ + cross terms = constant

ellipse

2 features for visualization sake

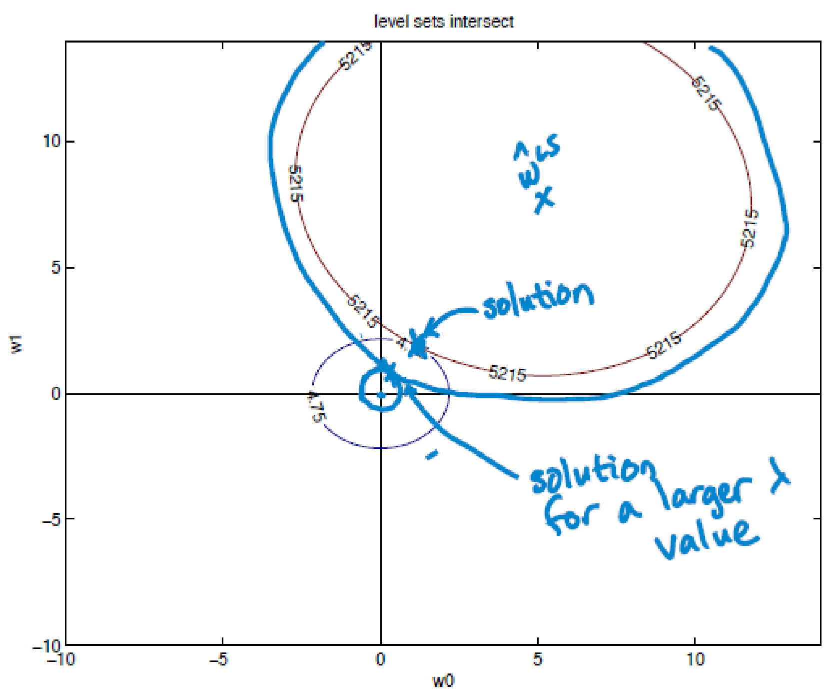
$$\mathrm{RSS}(\mathbf{w}) + \lambda \|\mathbf{w}\|_2^2 = \sum_{i=1}^{N} \left(y_i - w_0 h_0(\mathbf{x}_i) - w_1 h_1(\mathbf{x}_i)\right)^2 + \lambda \left(w_0^2 + w_1^2\right)$$

Visualising ridge cost in 2D



$$\mathrm{RSS}(\mathbf{w}) + \lambda\|\mathbf{w}\|_2^2 = \sum_{i=1}^{N}\left(y_i - w_0 h_0(\mathbf{x}_i) - w_1 h_1(\mathbf{x}_i)\right)^2 + \lambda\,\boxed{(w_0^2 + w_1^2)}$$

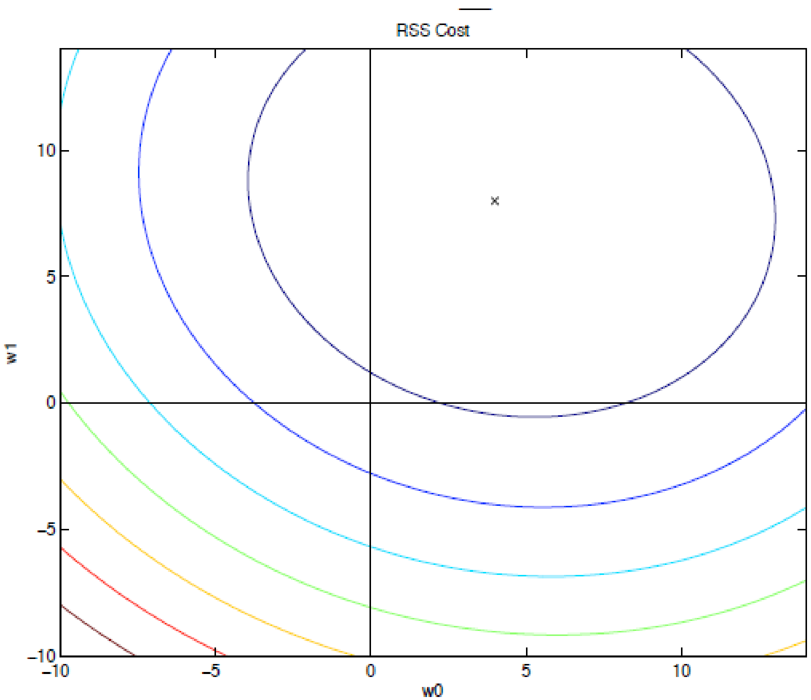
Visualising ridge cost in 2D



For a specific λ value, some balance between RSS and $\|w\|_2^2$

$$\text{RSS}(\mathbf{w}) + \lambda\|\mathbf{w}\|_2^2 = \sum_{i=1}^{N}(y_i - w_0 h_0(\mathbf{x}_i) - w_1 h_1(\mathbf{x}_i))^2 + \lambda\,(w_0^2 + w_1^2)$$

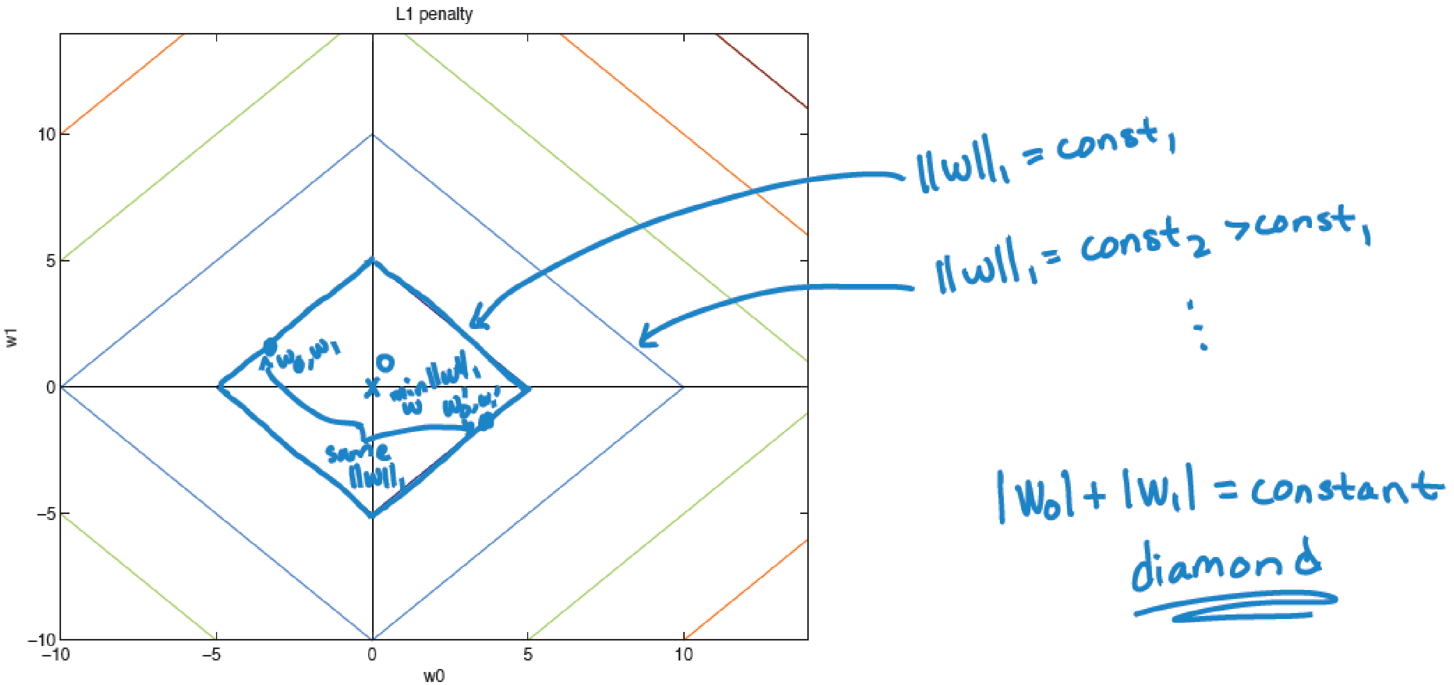
Visualising lasso cost in 2D



RSS contours for lasso are exactly the same as those for ridge!

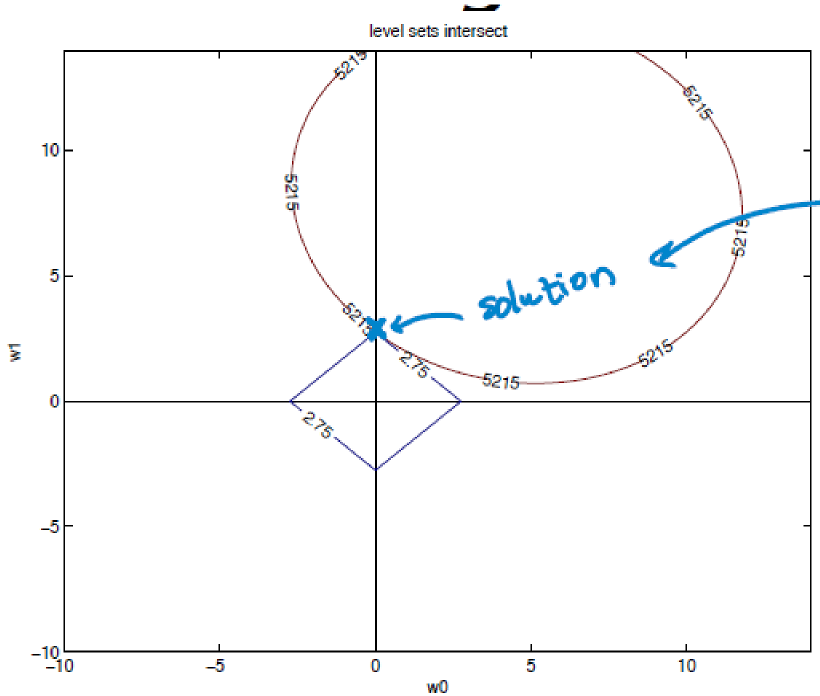
$$\mathrm{RSS}(\mathbf{w}) + \lambda\|\mathbf{w}\|_1 = \boxed{\sum_{i=1}^{N}(y_i - w_0 h_0(\mathbf{x}_i) - w_1 h_1(\mathbf{x}_i))^2} + \lambda\,(|w_0|+|w_1|)$$

Visualising lasso cost in 2D



$$\text{RSS}(\mathbf{w}) + \lambda||\mathbf{w}||_1 = \sum_{i=1}^{N}(y_i - w_0 h_0(\mathbf{x}_i) - w_1 h_1(\mathbf{x}_i))^2 + \lambda \boxed{(|w_0|+|w_1|)}$$

Visualising lasso cost in 2D



For a specific value of λ,

We are getting sparce solution, the $w_0 = 0$

$$\mathrm{RSS}(\mathbf{w}) + \lambda \|\mathbf{w}\|_1 = \sum_{i=1}^{N} (y_i - w_0 h_0(\mathbf{x}_i) - w_1 h_1(\mathbf{x}_i))^2 + \lambda\,(|w_0| + |w_1|)$$

How we optimise for objective

To solve for $\hat{\mathbf{w}}$, previously took gradient of total cost objective and either:

1) Derived closed-form solution
2) Used in gradient descent algorithm

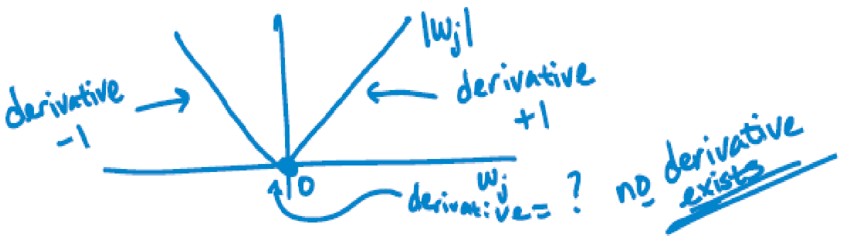
Optimise for lasso objective

Lasso total cost: $\text{RSS}(\mathbf{w}) + \lambda \|\mathbf{w}\|_1$

$\sum_{j=0}^{D} |w_j|$

Issues:

1) What's the derivative of $|w_j|$?



gradients → subgradients

2) Even if we could compute derivative, no closed-form solution

can use subgradient descent

Coordinate descent

Goal: Minimize some function g $\min_{w} g(w)$

$g(w) = g(w_0, w_1, \dots, w_D)$

when keeping others fixed

Often, hard to find minimum for all coordinates, but easy for each coordinate

Coordinate descent:

Initialize $\hat{w} = 0$ (or smartly…)

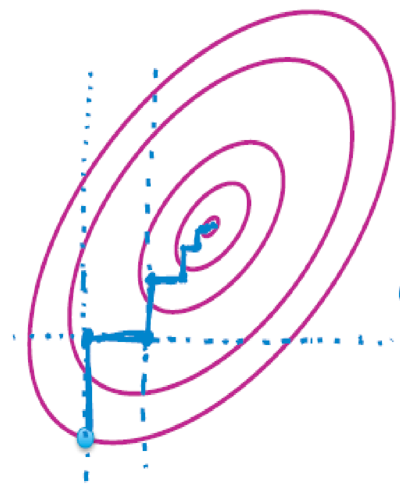
while not converged

pick a coordinate j

$\hat{w}_j \leftarrow \min_{\omega} g(\hat{w}_0, \dots, \hat{w}_{j-1}, \omega, \hat{w}_{j+1}, \dots, \hat{w}_D)$

values from previous iterations

just min over j^{th} coordinate



axis-aligned steps

Comments on coordinate descent

How do we pick next coordinate?

- At random ("random" or "stochastic" coordinate descent), round robin, …

No stepsize to choose!

Super useful approach for *many* problems

- Converges to optimum in some cases (e.g., "strongly convex")
- Converges for lasso objective

Normalizing features

Normalizing features

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

$$\underline{h}_j(\mathbf{x}_k) = \frac{h_j(\mathbf{x}_k)}{\boxed{\sqrt{\sum_{i=1}^{N} h_j(\mathbf{x}_i)^2}}}$$

Normalizer: z_j

Apply same training scale factors to test data:

$$\underline{h}_j(\mathbf{x}_k) = \frac{h_j(\mathbf{x}_k)}{\boxed{\sqrt{\sum_{i=1}^{N} h_j(\mathbf{x}_i)^2}}}$$

apply to test point

Normalizer: z_j

summing over training points

Optimising least squares objective

One coordinate at a time

$$\boxed{\mathrm{RSS}(\mathbf{w}) = \sum_{i=1}^{N}\Big(y_i - \sum_{j=0}^{D} w_j \underline{h}_j(\mathbf{x}_i)\Big)^2}$$

normalized features

Fix all coordinates $\mathbf{w}_{-j}$ and take partial w.r.t. w_j

all w_k for $k \neq j$

1d optimization coordinate by coordinate

$$\frac{\partial}{\partial w_j}\mathrm{RSS}(\mathbf{w}) = -2\sum_{i=1}^{N}\underline{h}_j(\mathbf{x}_i)\Big(y_i - \sum_{j=0}^{D} w_j \underline{h}_j(\mathbf{x}_i)\Big)$$

$$= -2\sum_{i=1}^{N} \underline{h}_j(x_i)\Big(y_i - \sum_{k\neq j} w_k \underline{h}_k(x_i) - w_j \underline{h}_j(x_i)\Big)$$

$$= \underbrace{-2\sum_{i=1}^{N} \underline{h}_j(x_i)\Big(y_i - \overbrace{\sum_{k\neq j} w_k \underline{h}_k(x_i)}\Big)}_{\triangleq\, \rho_j} + 2w_j \boxed{\sum_{i=1}^{N} \underline{h}_j(x_i)^2}$$

by definition of normalized features, $=1$

$$= -2\rho_j + 2w_j$$

Optimising least squares objective

$$\boxed{RSS(\mathbf{w}) = \sum_{i=1}^{N} (y_i - \sum_{j=0}^{D} w_j \underline{h}_j(\mathbf{x}_i))^2}$$

Set partial = 0 and solve

$$\frac{\partial}{\partial w_j} RSS(\mathbf{w}) = -\cancel{2}\rho_j + \cancel{2}w_j = 0$$

$$\hat{w}_j = \rho_j$$

Coordinate descent for least squares regression

Initialize $\hat{\mathbf{w}} = 0$ (or smartly...)

while not converged

for j=0,1,...,D

compute: $$\rho_j = \sum_{i=1}^{N} \underline{h}_j(\mathbf{x}_i)\overbrace{(y_i - \hat{y}_i(\hat{\mathbf{w}}_{-j}))}^{\text{residual } \textit{without} \text{ feature j}}$$

prediction *without* feature j

set: $\hat{w}_j = \rho_j$

Measure of the correlation between w_j and the residual without this feature.

How to access convergence

Initialize $\hat{\mathbf{w}} = 0$ (or smartly...)

$\boxed{\text{while not converged}}$

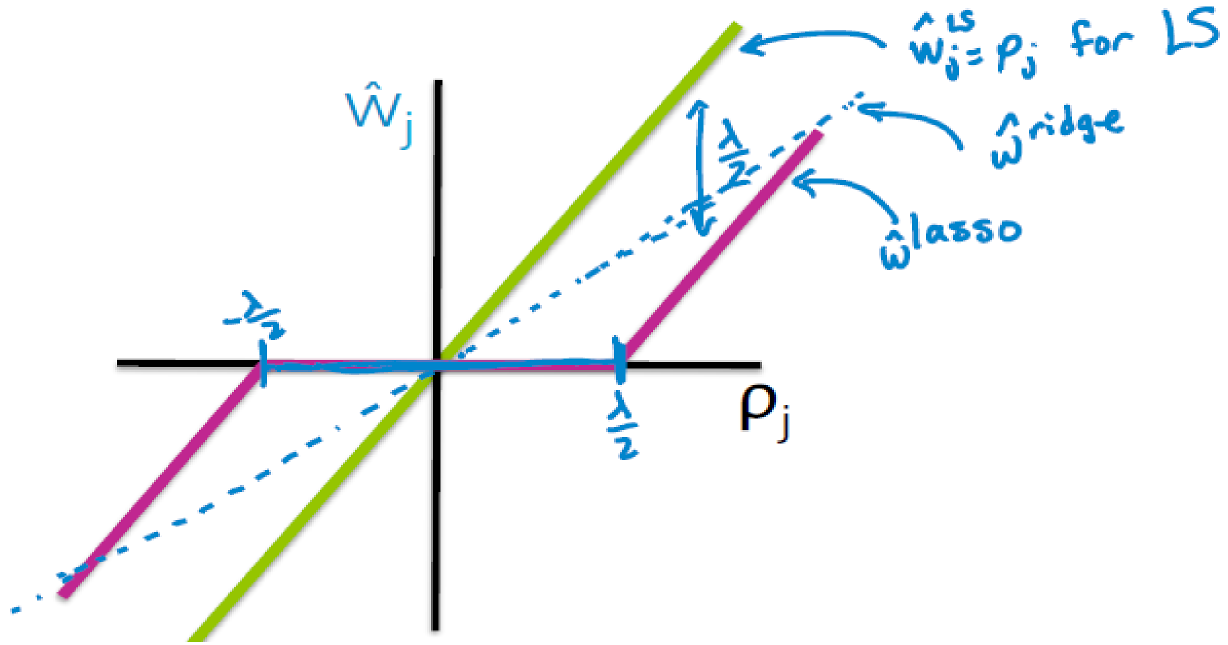
for j=0,1,...,D

compute: $$\rho_j = \sum_{i=1}^{N} \underline{h}_j(\mathbf{x}_i)(y_i - \hat{y}_i(\hat{\mathbf{w}}_{-j}))$$

set: $$\hat{w}_j = \begin{cases} \rho_j + \lambda/2 & \text{if } \rho_j < -\lambda/2 \\ 0 & \text{if } \rho_j \text{ in } [-\lambda/2, \lambda/2] \\ \rho_j - \lambda/2 & \text{if } \rho_j > \lambda/2 \end{cases}$$

Soft thresholding

$$\hat{w}_j = \begin{cases} \rho_j + \lambda/2 & \text{if } \rho_j < -\lambda/2 \\ 0 & \text{if } \rho_j \text{ in } [-\lambda/2, \lambda/2] \\ \rho_j - \lambda/2 & \text{if } \rho_j > \lambda/2 \end{cases}$$



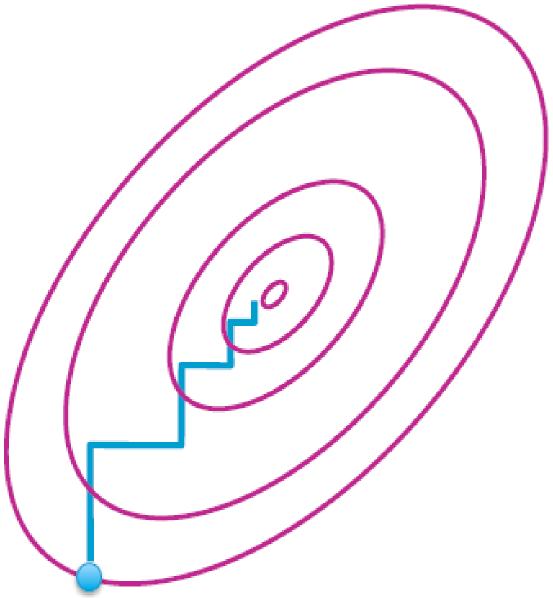
Convergence criteria

When to stop?

For convex problems, will start to take smaller and smaller steps

Measure size of steps taken in a full loop over all features

– stop when max step < ε



Other lasso solvers

Classically: Least angle regression (LARS) [Efron et al. '04]

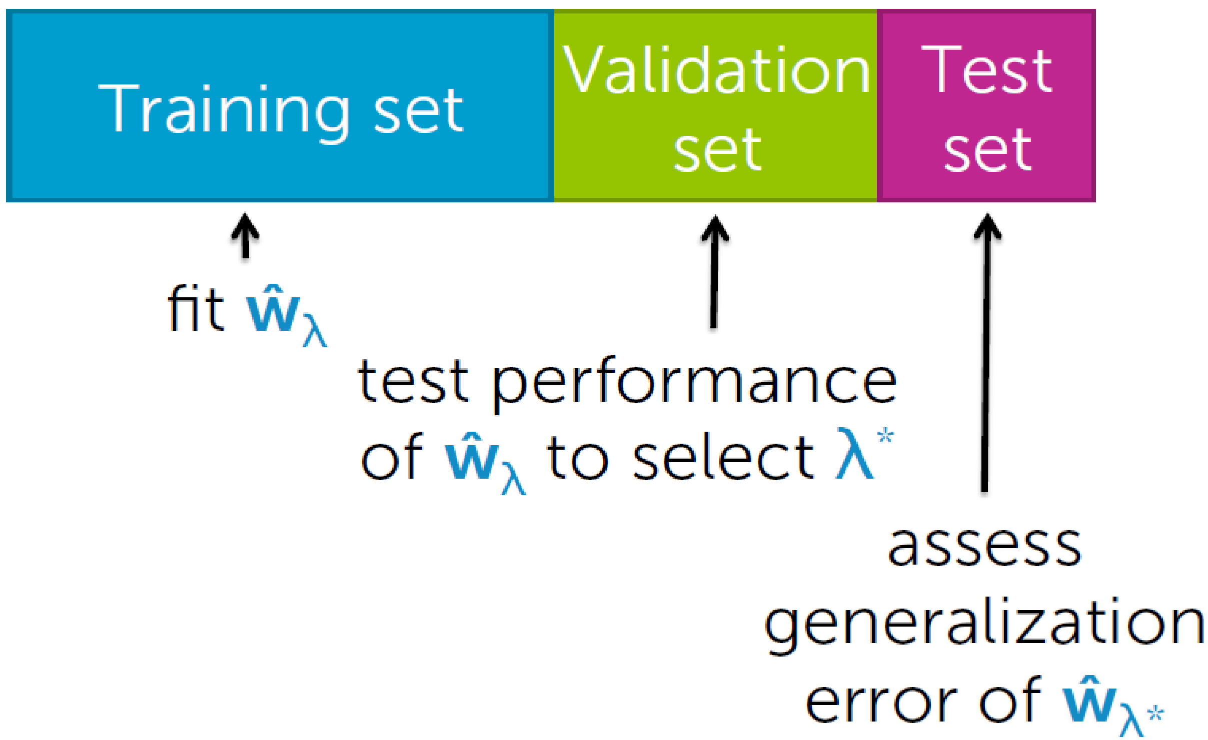
Then: Coordinate descent algorithm
[Fu '98, Friedman, Hastie, & Tibshirani '08]

Now:

- Parallel CD (e.g., Shotgun, [Bradley et al. '11])
- Other parallel learning approaches for linear models
  - Parallel stochastic gradient descent (SGD) (e.g., Hogwild! [Niu et al. '11])
  - Parallel independent solutions then averaging [Zhang et al. '12]
- Alternating directions method of multipliers (ADMM) [Boyd et al. '11]

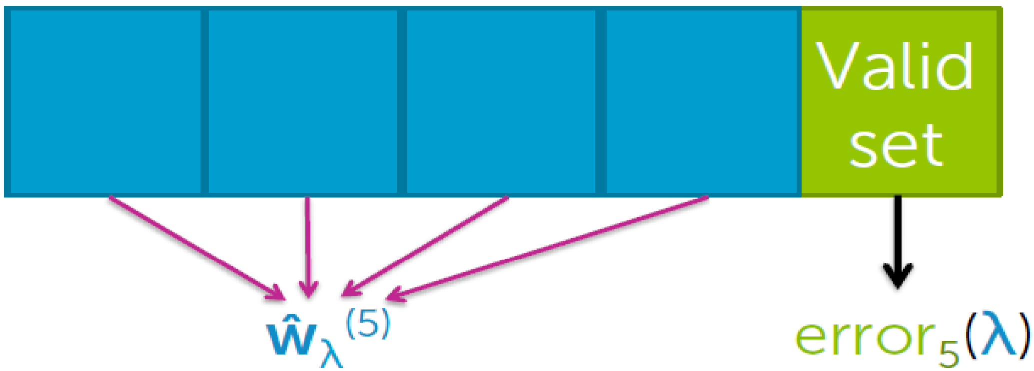
How do we chose λ

If sufficient amount of data…



How do we chose λ

K-fold cross validation



For k=1,…,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: $CV(\lambda) = \frac{1}{K}\sum_{k=1}^{K} \text{error}_k(\lambda)$

Choosing λ via cross validation

Cross validation is choosing the λ that provides best predictive accuracy

Tends to favor less sparse solutions, and thus smaller λ, than optimal choice for feature selection

c.f., "Machine Learning: A Probabilistic Perspective", Murphy, 2012 for further discussion

Impact of feature selection and lasso

Lasso has changed machine learning, statistics, & electrical engineering

But, for feature selection in general, be careful about interpreting selected features

- selection only considers features included
- sensitive to correlations between features
- result depends on algorithm used
- there are theoretical guarantees for lasso under certain conditions

What you can do now

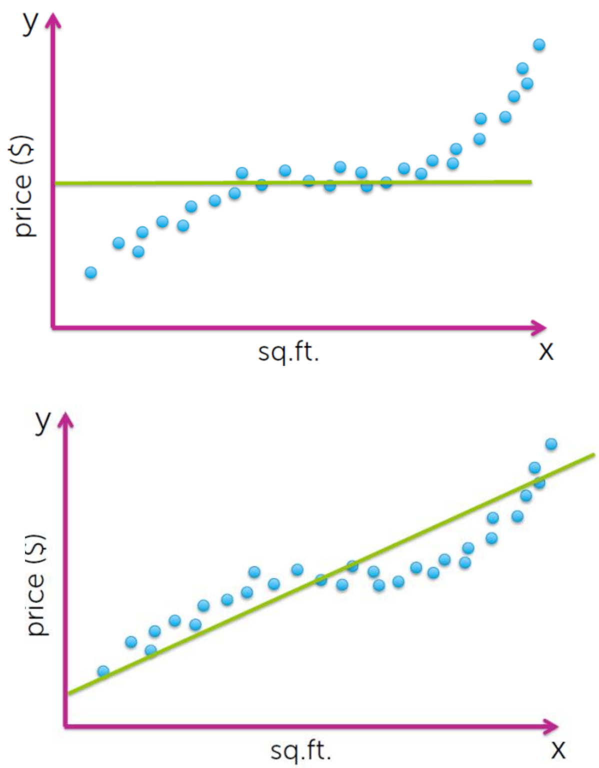
- Perform feature selection using "all subsets" and "forward stepwise" algorithms
- Analyze computational costs of these algorithms
- Contrast greedy and optimal algorithms
- Formulate lasso objective
- Describe what happens to estimated lasso coefficients as tuning parameter λ is varied
- Interpret lasso coefficient path plot
- Contrast ridge and lasso regression
- Describe geometrically why L1 penalty leads to sparsity
- Estimate lasso regression parameters using an iterative coordinate descent algorithm
- Implement K-fold cross validation to select lasso tuning parameter λ

NONPARAMETRIC REGRESSION

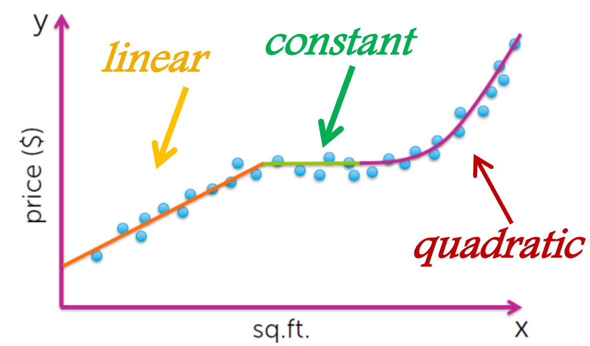
9/10, 16/10, 23/10 2024

Fit globaly vs fit locally

Parametric models



Below …
f(x) is not really
a polynomial function



What alternative do we have?

If we:

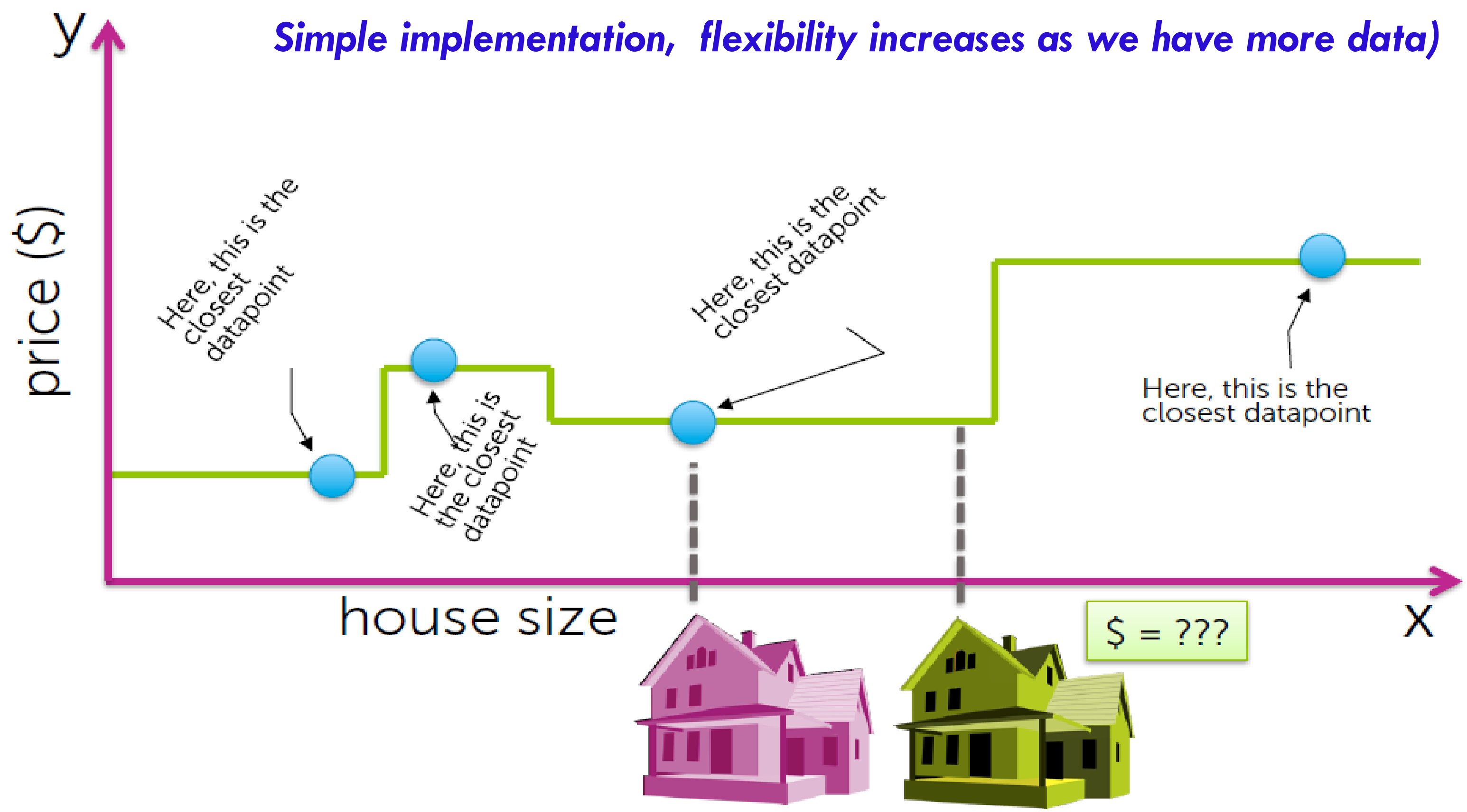
– Want to allow flexibility in f(**x**) having local structure

– Don't want to infer "structural breaks"

What's a simple option we have?

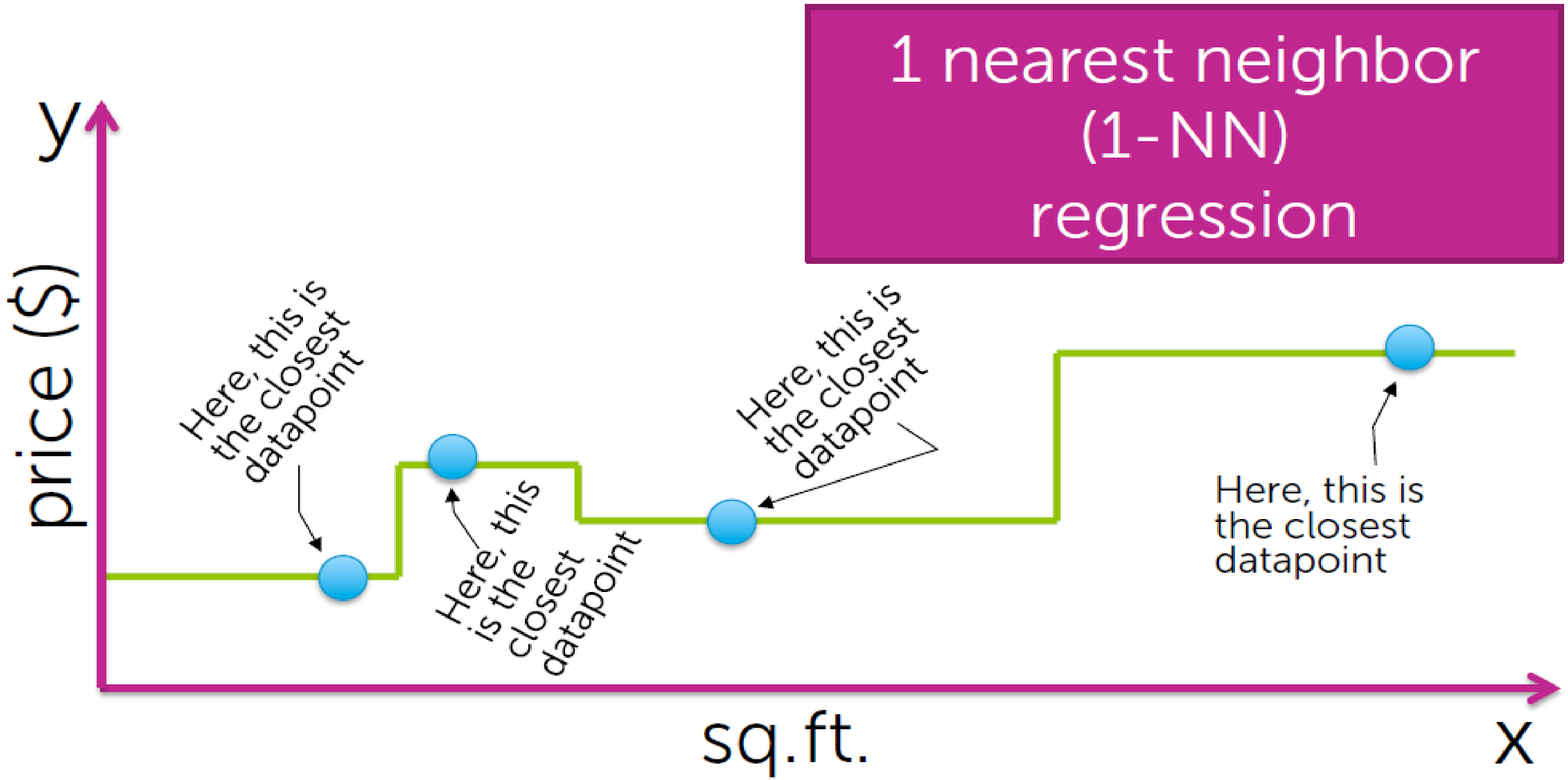
– Assuming we have plenty of data…

Nearest Neighbor & Kernel Regression (nonparametric approach)



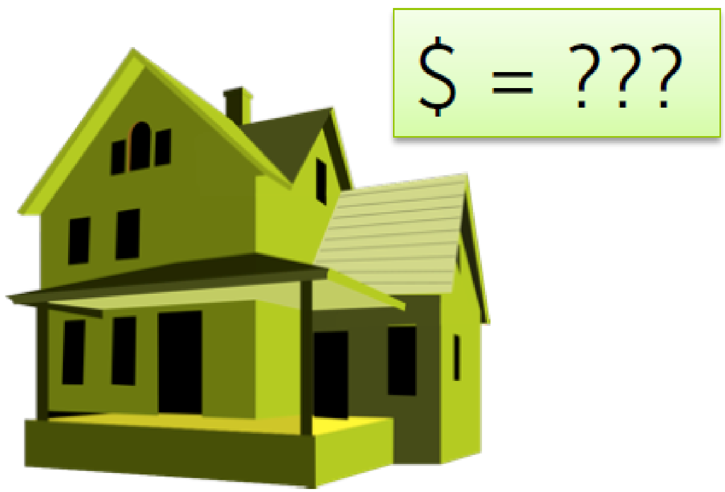
Fit locally to each data point

Predicted value = "closest" y_i



What people do naturally…

Real estate agent assesses value by finding sale of most similar house



1-NN regression more formally

Dataset of (🏠,$) pairs: $(\mathbf{x}_1,y_1), (\mathbf{x}_2,y_2),\ldots,(\mathbf{x}_N,y_N)$

Query point: $\mathbf{x}_q$ ← $?

big lime green house

1. Find "closest" $\mathbf{x}_i$ in dataset

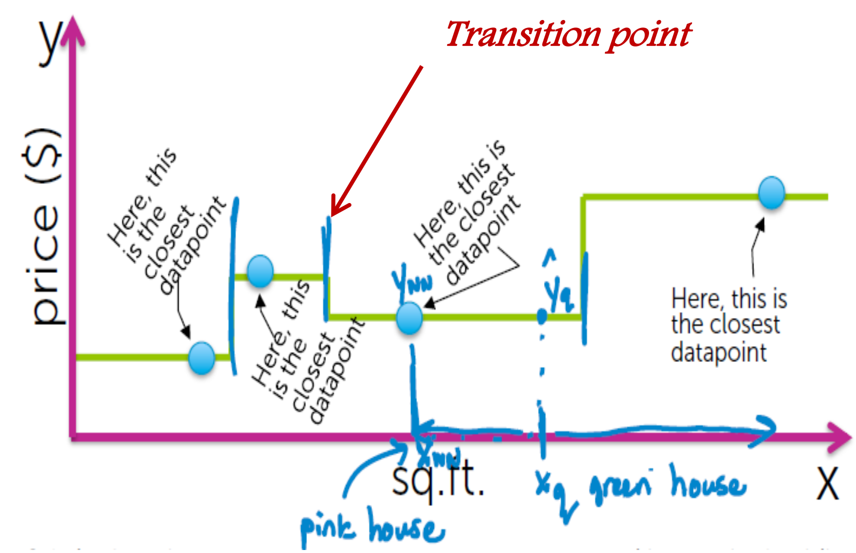
$$X_{NN} \leftarrow \min_i \text{distance}(x_i, x_q)$$

big pink house

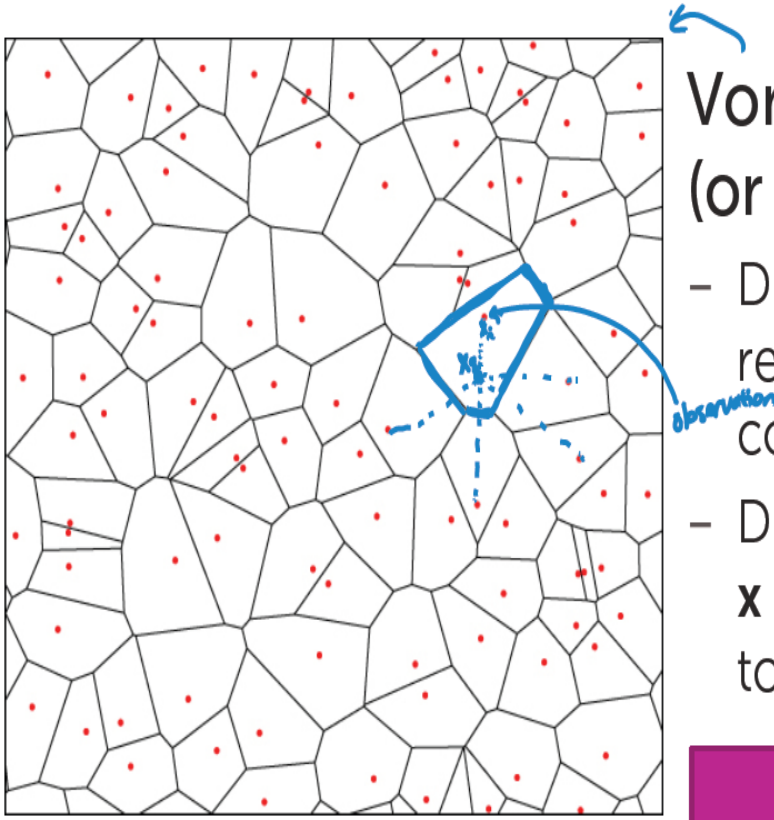
2. Predict

$$\hat{y}_q = y_{NN}$$

sales price of big pink house



Visualizing 1-NN in multiple dimensions



Voronoi tesselation (or diagram):

- Divide space into N regions, each containing 1 datapoint
- Defined such that any **x** in region is "closest" to region's datapoint

x_q closer to x_i than any other x_j for $j \neq i$.

Don't explicitly form!

Distance metrics: Notion of „closest”

In 1D, just Euclidean distance:

$$\boxed{\text{distance}(x_j, x_q) = |x_j - x_q|}$$

In multiple dimensions:

- can define many interesting distance functions
- most straightforwardly, might want to weight different dimensions differently

Weighting housing inputs

Some inputs are more relevant than others

 # bedrooms
 # bathrooms
sq.ft. living
sq.ft. lot
floors
year built
year renovated
waterfront

Scaled Euclidan distance

Formally, this is achieved via

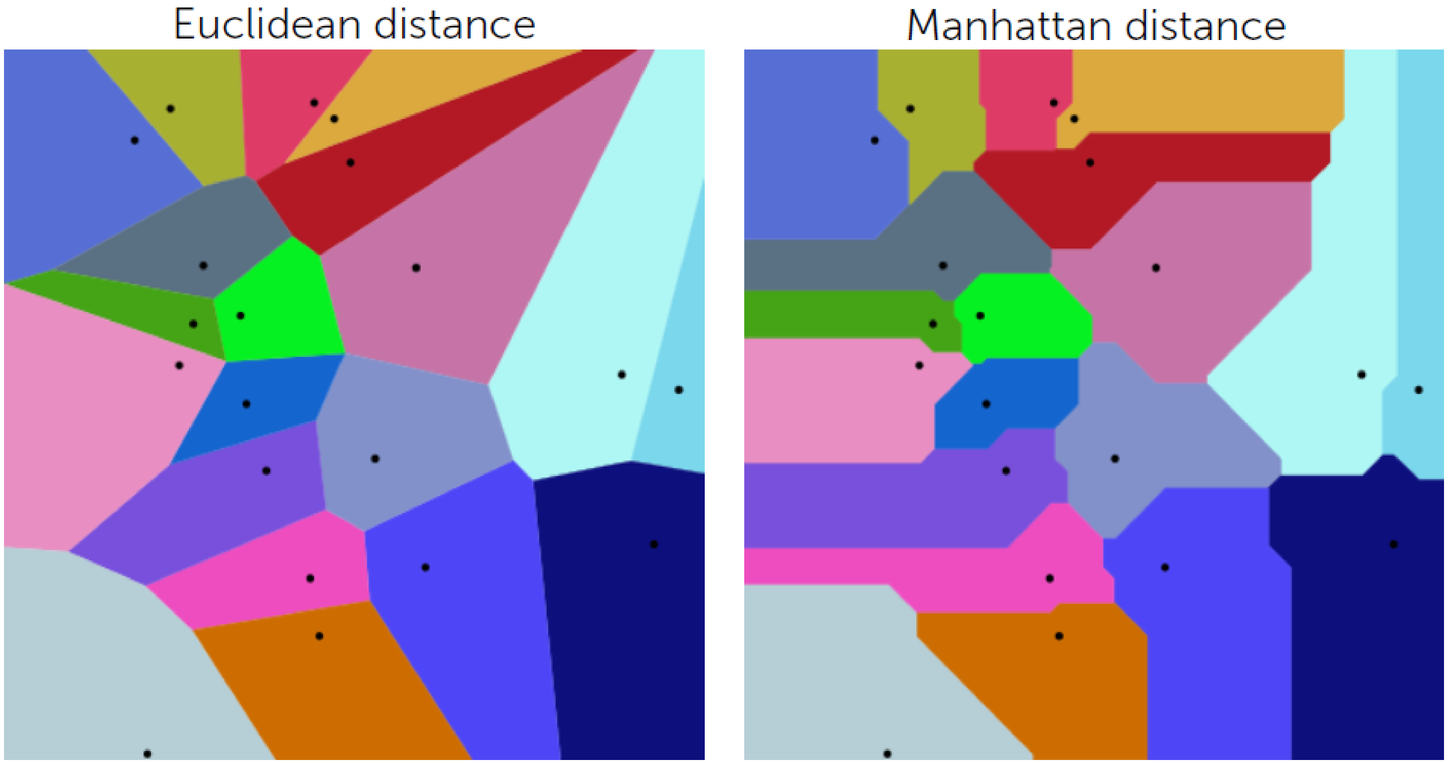
$$\text{distance}(\mathbf{x}_j, \mathbf{x}_q) = \sqrt{a_1(\mathbf{x}_j[1]-\mathbf{x}_q[1])^2 + \ldots + a_d(\mathbf{x}_j[d]-\mathbf{x}_q[d])^2}$$

weight on each input
(defining relative importance)

Other example distance metrics:

– Mahalanobis, rank-based, correlation-based, cosine similarity, Manhattan, Hamming, ...

Different distance metrics



Performing 1-NN search

- Query house: 
- Dataset: 
- **Specify:** Distance metric
- **Output:** Most similar house 

1-NN algorithm

closest house

Initialize **Dist2NN** = ∞,  = ∅

For i=1,2,…,N

query house

Compute: **δ = distance(**$_i$ **,** $_q$**)**

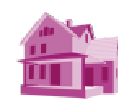
If **δ < Dist2NN**

set  $_i$

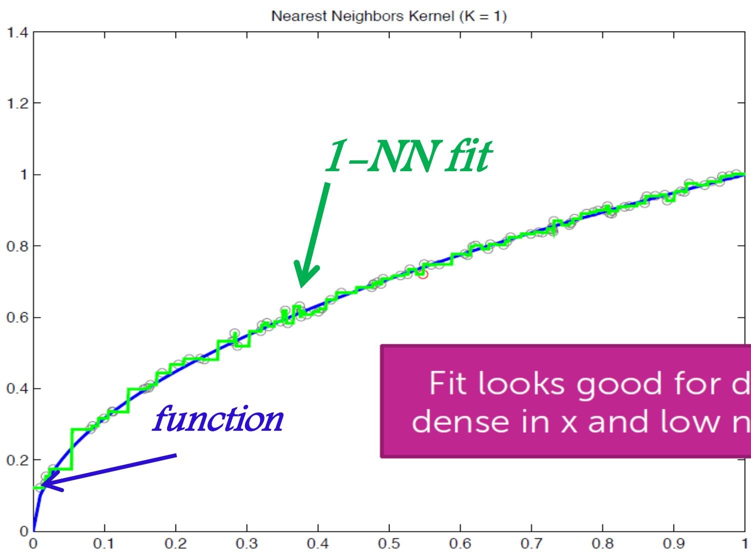
set **Dist2NN = δ**

Return most similar house 

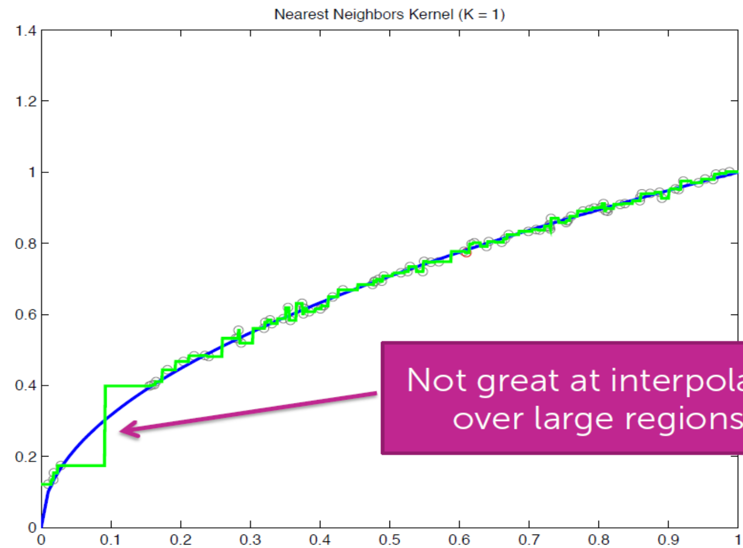
closest house
to query house



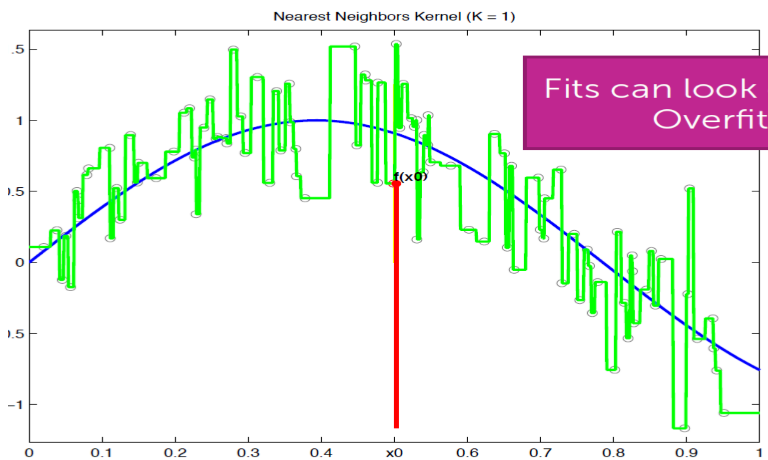
1-NN in practice



Fit looks good for data dense in x and low noise



Not great at interpolating over large regions...

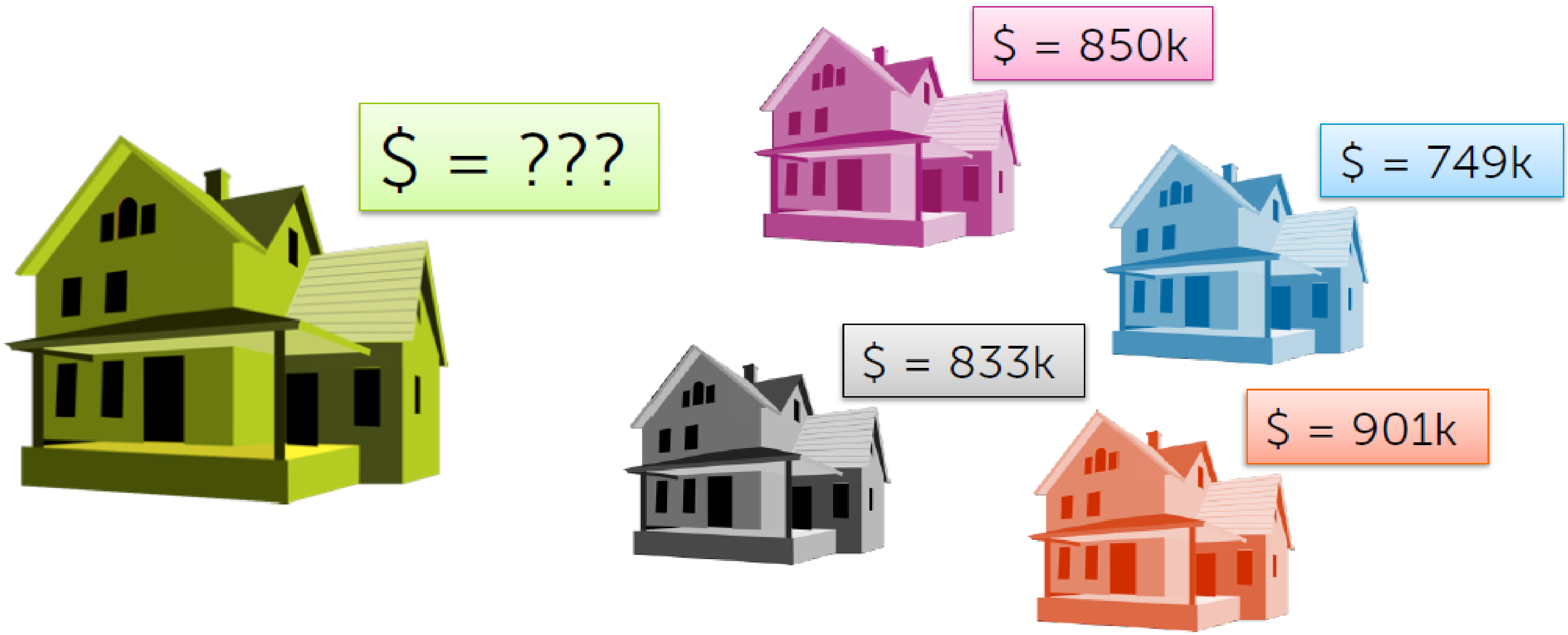


Fits can look quite wild... Overfitting?

1-NN sensitive to noise in the data

Get more „comps"

More reliable estimate if you base estimate off of a larger set of comparable homes



K-NN regression more formally

Dataset of (,$) pairs: $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)$

Query point: $\mathbf{x}_q$

1. Find k closest $\mathbf{x}_i$ in dataset

   $(x_{NN_1}, x_{NN_2}, \ldots, x_{NN_k})$ such that for any x_i not in nearest neighbor set,

   $\text{distance}(x_i, x_q) \geq \text{distance}(x_{NN_k}, x_q)$

2. Predict

$$\hat{y}_q = \frac{1}{k}\left(y_{NN_1} + y_{NN_2} + \ldots + y_{NN_k}\right)$$

$$= \frac{1}{k}\sum_{j=1}^{k} y_{NN_j}$$

K-NN more formally

- Query house: 
- Dataset: 
- **Specify:** Distance metric
- **Output:** Most similar houses

K-NN algorithm

sort first **k houses**
by distance to query house

Initialize **Dist2kNN** = sort($\delta_1,\ldots,\delta_k$) ← list of sorted distances

= so ,…, $_1$ $_k$ ← list of sorted houses

For i=k+1,…,N

Compute: δ = **distance(** $_i$ **,** $_q$ **)** ← query house

If δ < **Dist2kNN**[k]

find j such that δ > **Dist2kNN**[j-1] but δ < **Dist2kNN**[j]

remove furthest house and shift queue:

[j+1 = [j:k

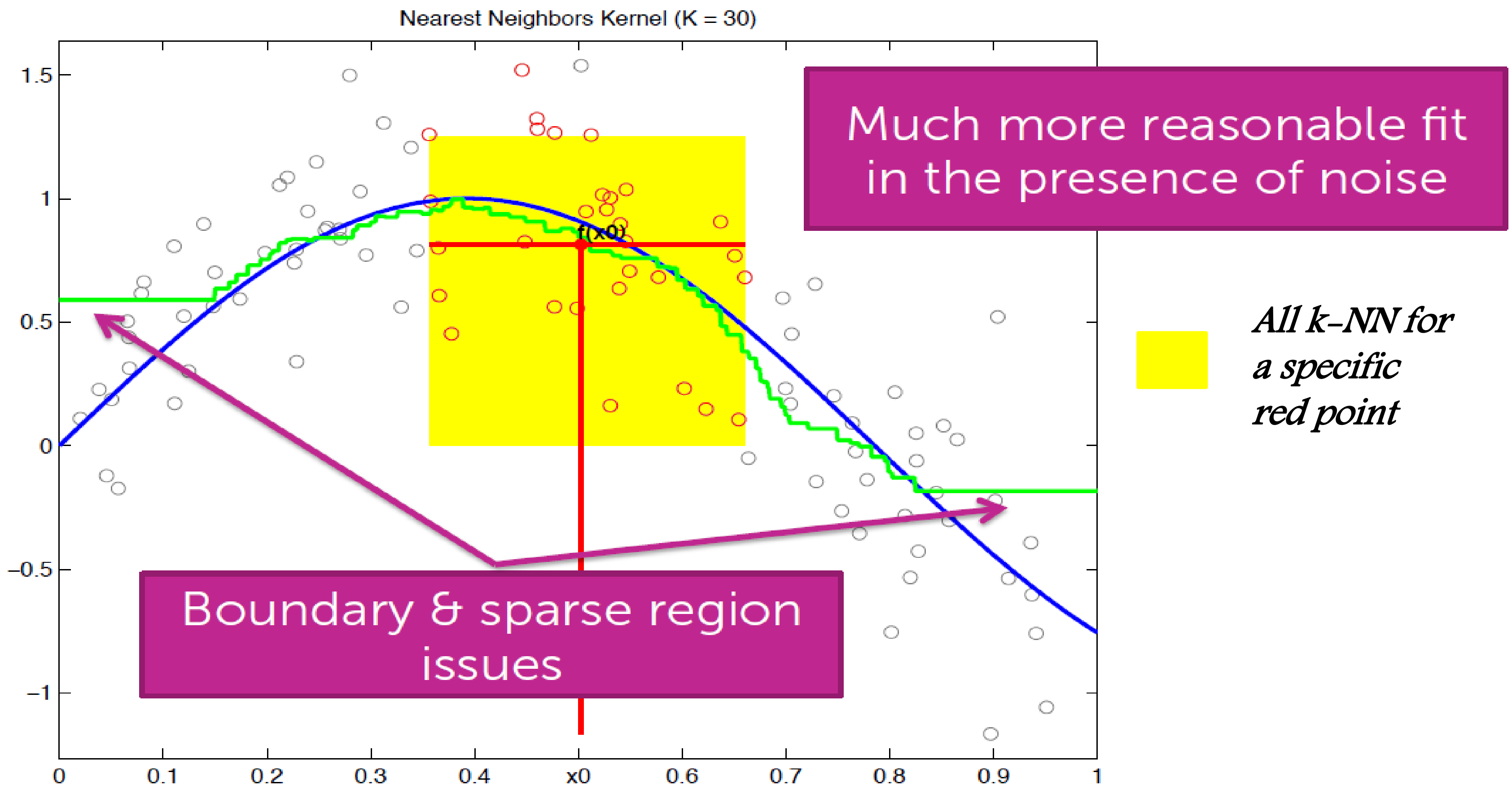
Dist2kNN[j+1:k] = **Dist2kNN**[j:k-1]

insert new NN

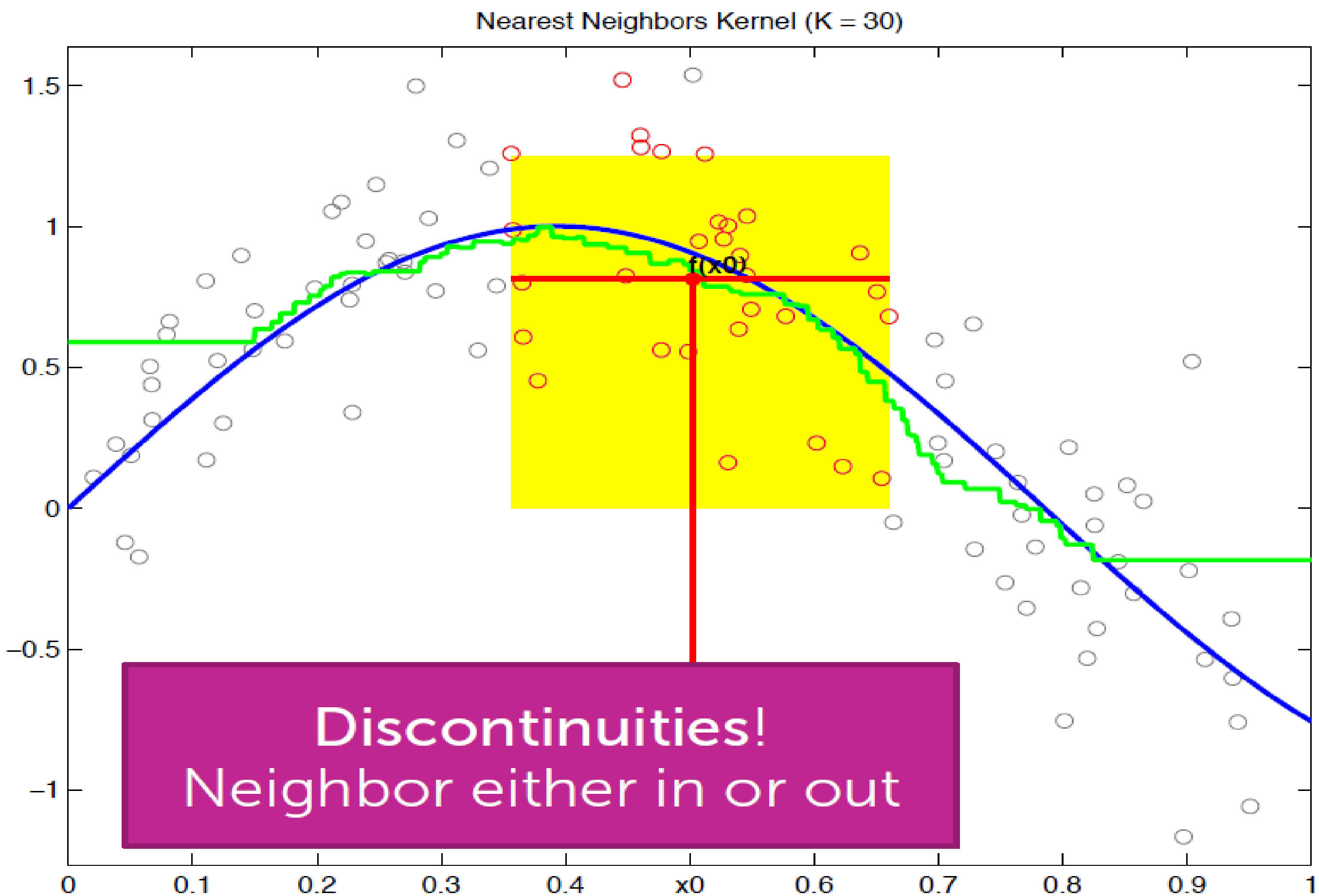
set **Dist2kNN**[j] = δ and = $_i$

Return k most similar houses ← closest houses to query house

K-NN in practice



K-NN in practice



Issues with discontinuities

Overall predictive accuracy might be okay, but...

For example, in housing application:

- If you are a buyer or seller, this matters
- Can be a jump in estimated value of house going just from 2640 sq.ft. to 2641 sq.ft.
- Don't really believe this type of fit

Weighted k-NN

Weigh more similar houses more than those less similar in list of k-NN

Predict:

weights on NN

$$\hat{y}_q = \frac{c_{qNN1}y_{NN1} + c_{qNN2}y_{NN2} + c_{qNN3}y_{NN3} + \ldots + c_{qNNk}y_{NNk}}{\sum_{j=1}^{k} c_{qNNj}}$$

How to define weights

Want weight c_{qNNj} to be small when

distance($\mathbf{x}_{NNj}$,$\mathbf{x}_q$) large

and c_{qNNj} to be large when

distance($\mathbf{x}_{NNj}$,$\mathbf{x}_q$) small

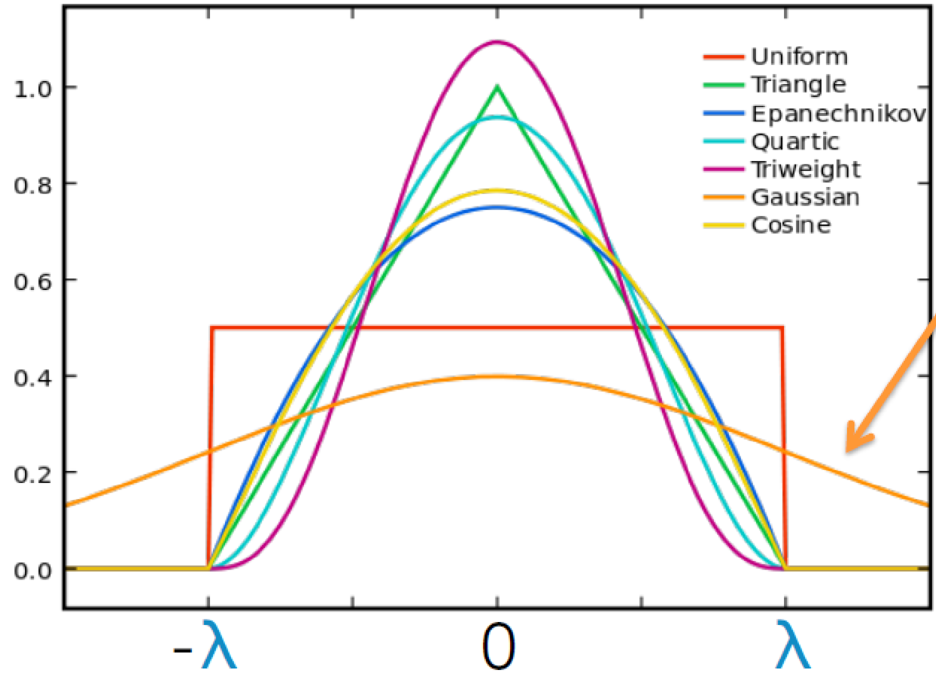
Simple method :

$$c_{qNN_j} = \frac{1}{\text{distance}(x_j, x_q)}$$

Kernel weights for d=1

Define: $c_{qNNj} = \mathrm{Kernel}_{\lambda}(|x_{NNj} - x_q|)$

simple isotropic case



Gaussian kernel:

$\mathrm{Kernel}_{\lambda}(|x_i - x_q|) = \exp(-(x_i - x_q)^2/\lambda)$

Note: never exactly 0!

Kernel drives how the weights will decay, if at all, as a function of the distance.

Kernel regression

Nadaraya-Watson
kernel weighted average

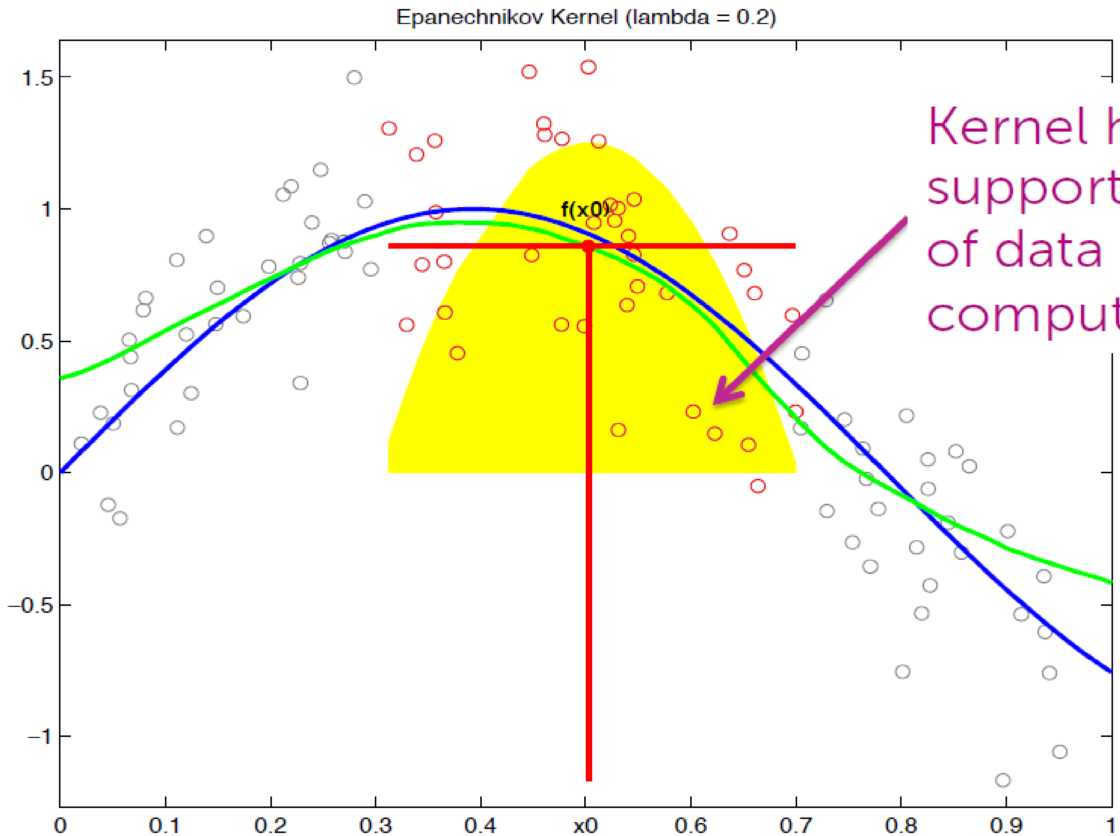
Instead of just weighting NN, weight *all* points

Predict:

weight on each datapoint

$$\hat{y}_q = \frac{\sum_{i=1}^{N} c_{qi} y_i}{\sum_{i=1}^{N} c_{qi}} = \frac{\sum_{i=1}^{N} \text{Kernel}_\lambda(\text{distance}(\mathbf{x}_i, \mathbf{x}_q)) * y_i}{\sum_{i=1}^{N} \text{Kernel}_\lambda(\text{distance}(\mathbf{x}_i, \mathbf{x}_q))}$$

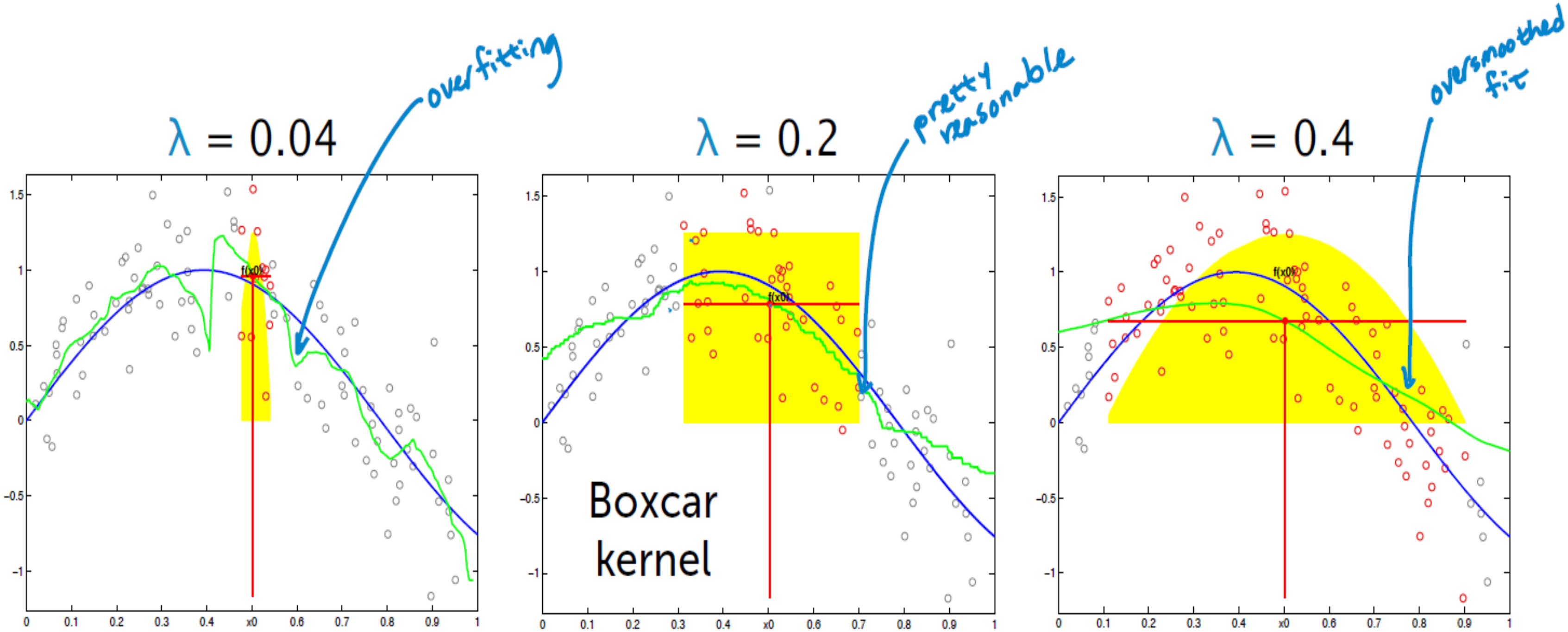
Kernel regression in practice



Kernel has bounded support…Only subset of data needed to compute local fit

Choice of bandwith λ

Often, choice of kernel matters much less than choice of λ



Choosing λ (or k on k-NN)

How to choose? Same story as always…

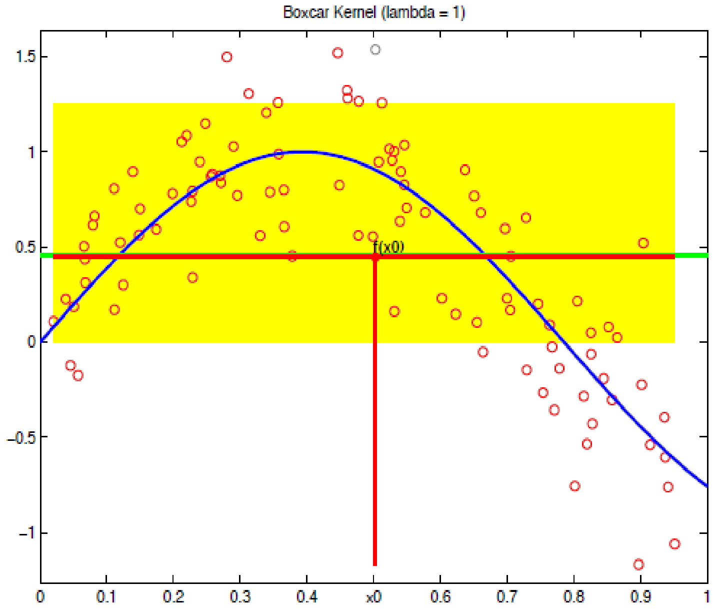
Cross Validation

Contrasting with global average

A globally constant fit weights all points equally

equal weight on each datapoint

$$\hat{y}_q = \frac{1}{N}\sum_{i=1}^{N} y_i = \frac{\sum_{i=1}^{N} c\, y_i}{\sum_{i=1}^{N} c}$$

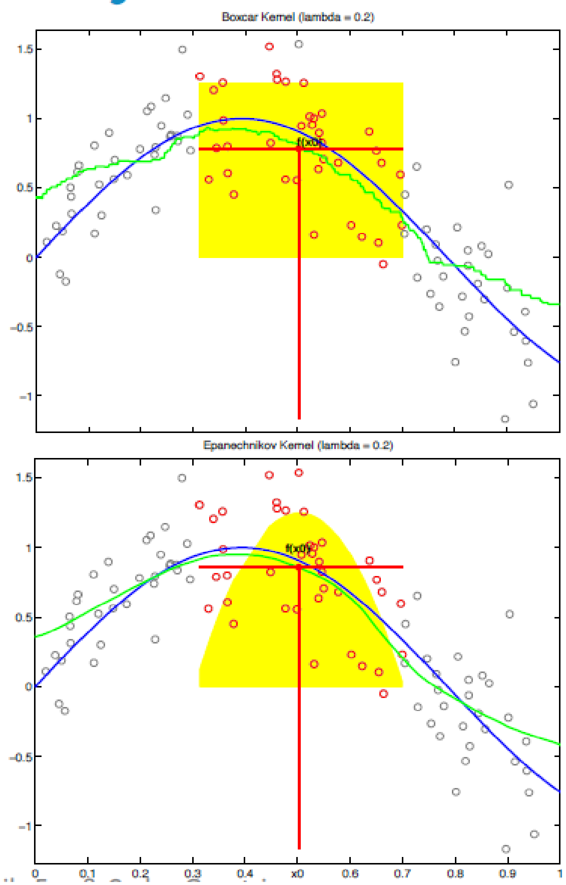


Contrasting with global average

Kernel regression leads to locally constant fit

– slowly add in some points and and let others gradually die off

$$\hat{y}_q = \frac{\sum_{i=1}^{N} \text{Kernel}_\lambda(\text{distance}(\mathbf{x}_i,\mathbf{x}_q)) * y_i}{\sum_{i=1}^{N} \text{Kernel}_\lambda(\text{distance}(\mathbf{x}_i,\mathbf{x}_q))}$$



Local linear regression

So far, discussed fitting constant function locally at each point

→ "locally weighted averages"

Can instead fit a line or polynomial locally at each point

→ "locally weighted linear regression"

Local regression rules of thumb

- Local linear fit reduces bias at boundaries with minimum increase in variance
- Local quadratic fit doesn't help at boundaries and increases variance, but does help capture curvature in the interior
- With sufficient data, local polynomials of odd degree dominate those of even degree

Recommended default choice:

local linear regression

Nonparametric approaches

k-NN and kernel regression are examples of nonparametric regression

General goals of nonparametrics:

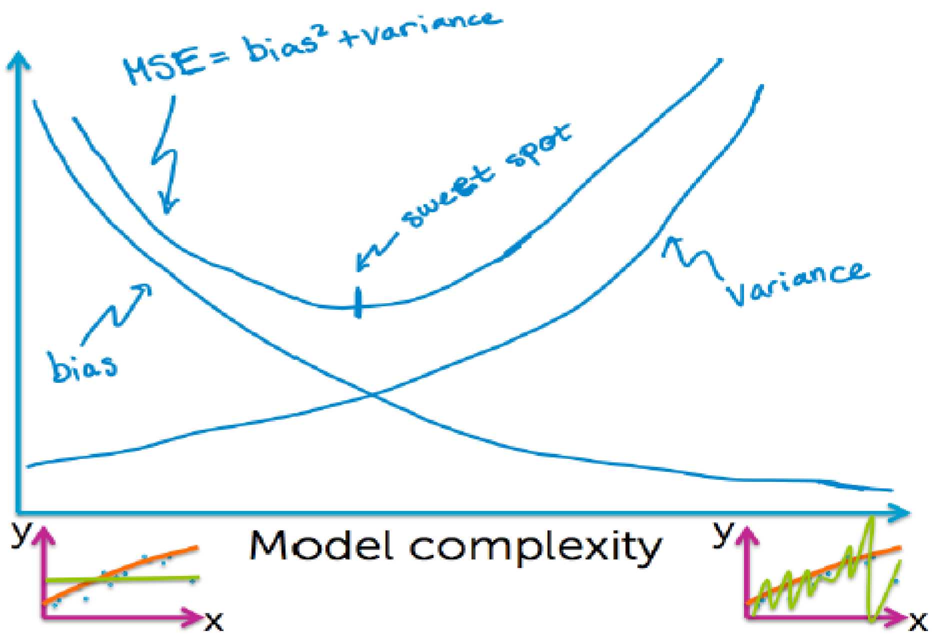
- Flexibility
- Make few assumptions about f(**x**)
- Complexity can grow with the number of observations N

Lots of other choices:

- Splines, trees, locally weighted structured regression models…

Noiseless setting ($\varepsilon_i = 0$)

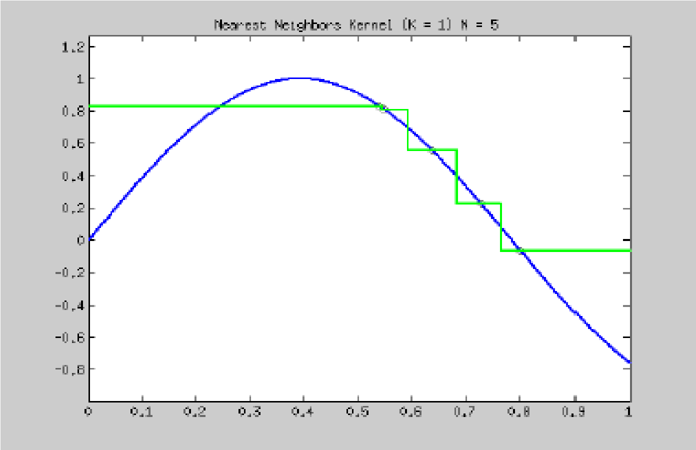
In the limit of getting an infinite amount of noiseless data, the MSE of 1-NN fit goes to 0



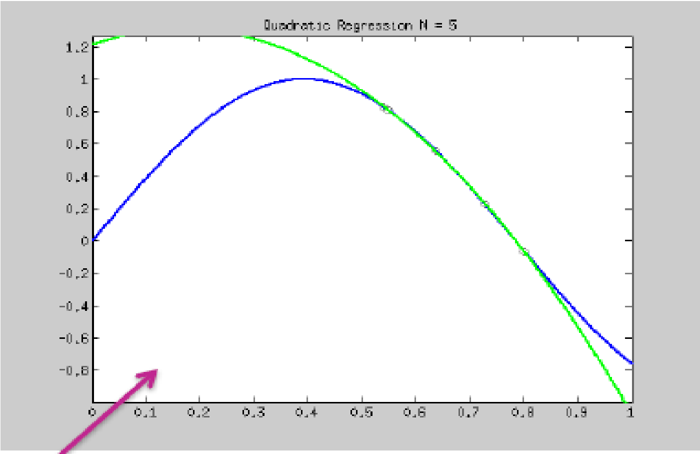
Limiting behaviour of NN

Noiseless setting ($\varepsilon_i = 0$)

In the limit of getting an infinite amount of noiseless data, the MSE of 1-NN fit goes to 0



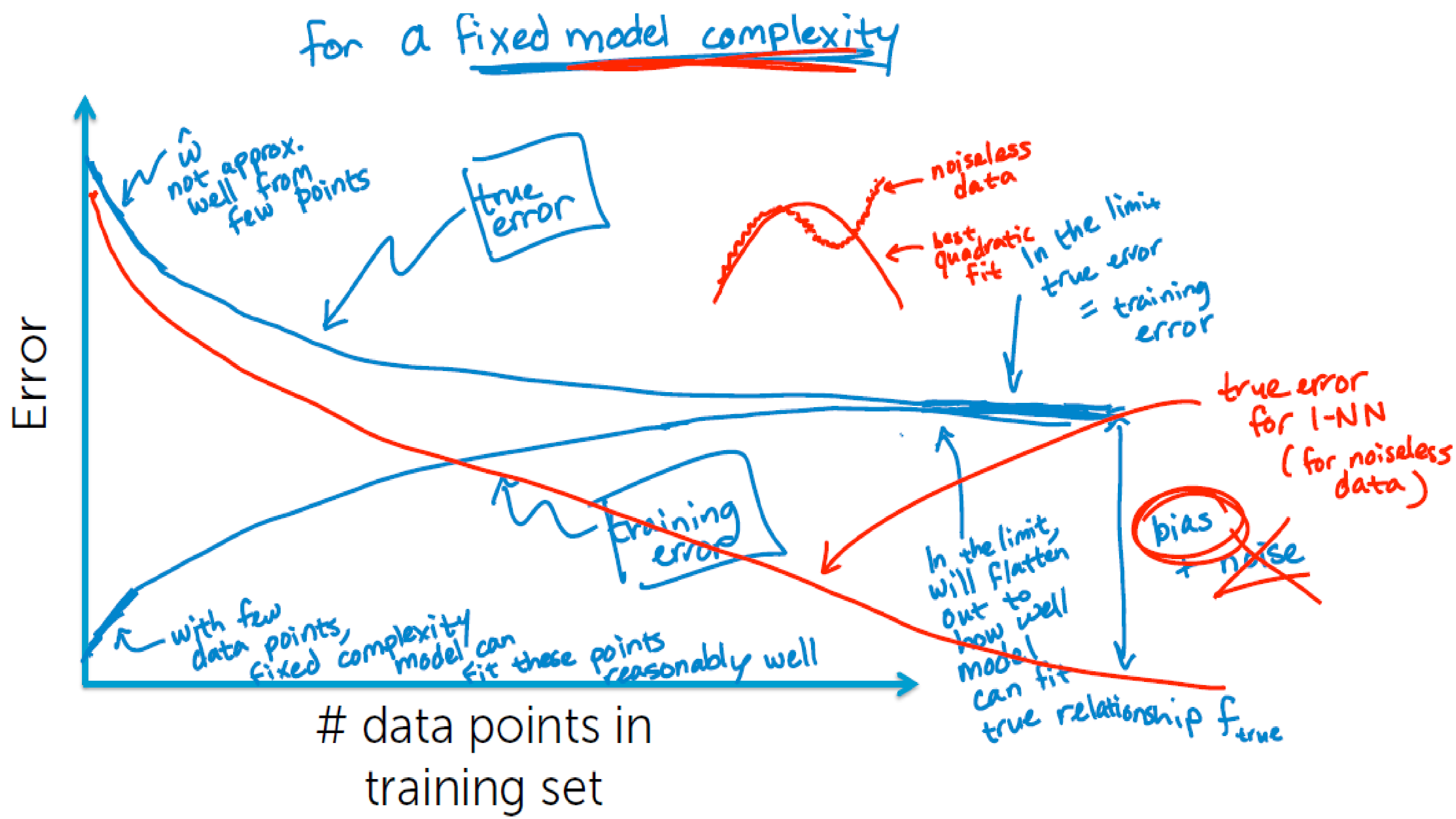
1-NN fit



Quadratic fit

Not true for parametric models!

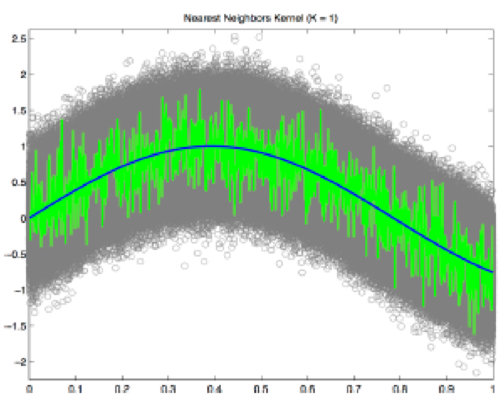
Error vs amount of data



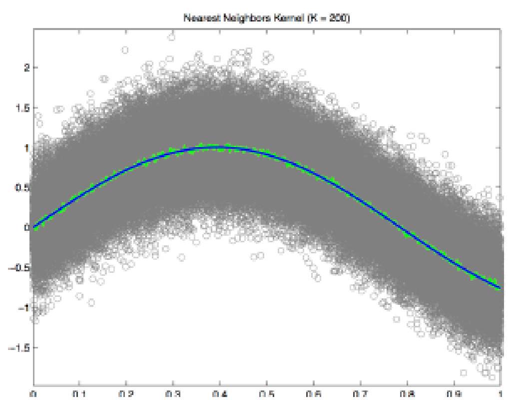
Limiting behaviour of NN

Noisy data setting

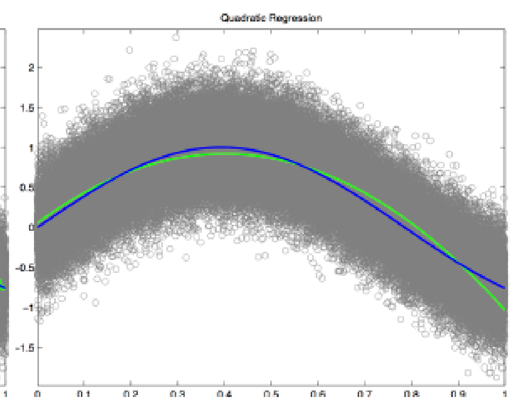
In the limit of getting an infinite amount of data, the MSE of NN fit goes to 0 if k grows, too



1-NN fit



200-NN fit



Quadratic fit

Issues: NN and kernel methods

NN and kernel methods work well when the data cover the space, but…

- the more dimensions d you have, the more points N you need to cover the space
- need $N = O(\exp(d))$ data points for good performance

This is where parametric models become useful…

Issues: Complexity of NN search

Naïve approach: **Brute force search**

- Given a query point $\mathbf{x}_q$
- Scan through each point $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$
- O(N) distance computations per 1-NN query!
- O(Nlogk) per k-NN query!

What if N is huge???
(and many queries)

Will talk more about efficient methods in Clustering & Retrieval course

We have discussed how to

- Motivate the use of nearest neighbor (NN) regression
- Define distance metrics in 1D and multiple dimensions
- Perform NN and k-NN regression
- Analyze computational costs of these algorithms
- Discuss sensitivity of NN to lack of data, dimensionality, and noise
- Perform weighted k-NN and define weights using a kernel
- Define and implement kernel regression
- Describe the effect of varying the kernel bandwidth λ or # of nearest neighbors k
- Select λ or k using cross validation
- Compare and contrast kernel regression with a global average fit
- Define what makes an approach nonparametric and why NN and kernel regression are considered nonparametric methods
- Analyze the limiting behavior of NN regression

Summarising

Models

- Linear regression
- Regularization: Ridge (L2), Lasso (L1)
- Nearest neighbor and kernel regression

Algorithms

- Gradient descent
- Coordinate descent

Concepts

- Loss functions, bias-variance tradeoff, cross-validation, sparsity, overfitting, model selection, feature selection