

INTRODUCTION TO DATA SCIENCE

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

20/10, 27/10,
3/11 2020

WFAiS UJ, Informatyka Stosowana
I stopień studiów

Regression for predictions

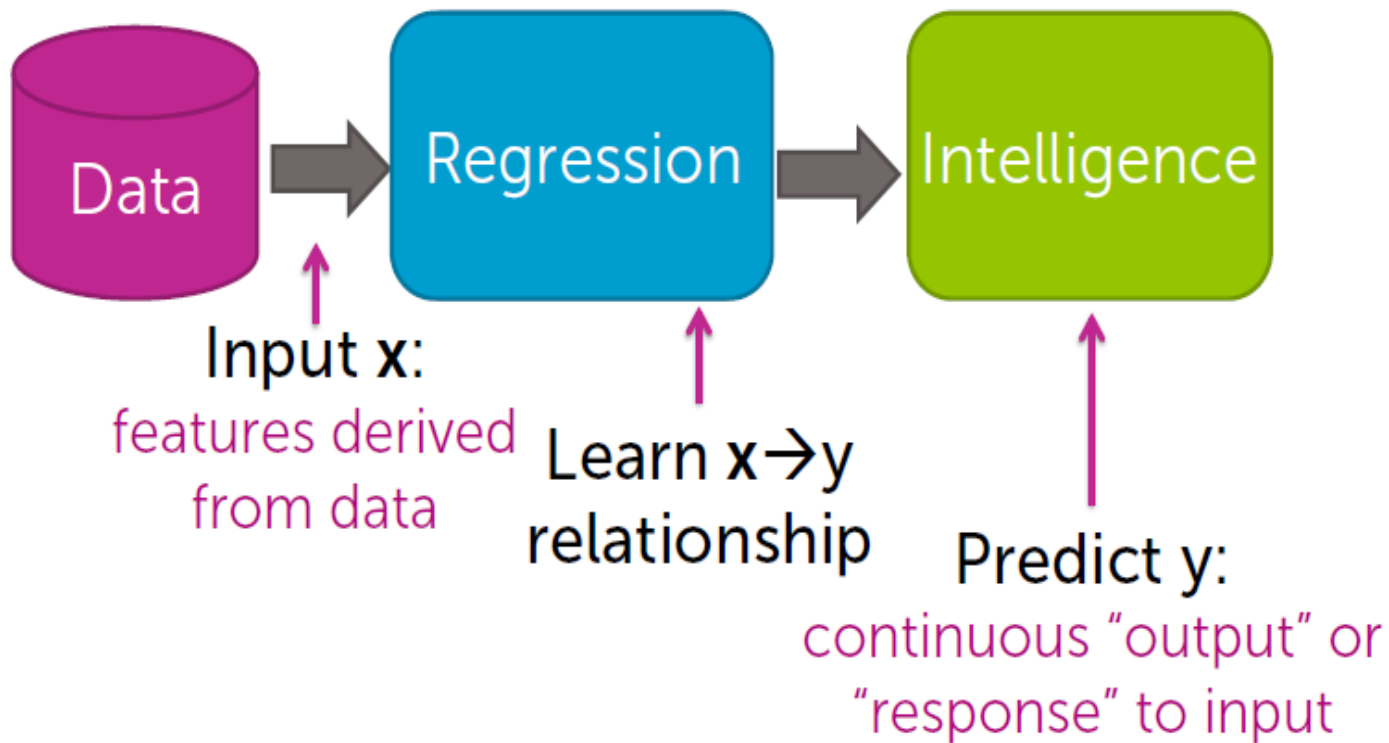
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- ❑ **Simple regression**
- ❑ **Multiple regression**
- ❑ **Assesing performance**
- ❑ **Ridge regression**
- ❑ **Feature selection and lasso regression**
- ❑ **Nearest neighbor and kernel regression**

What is regression?

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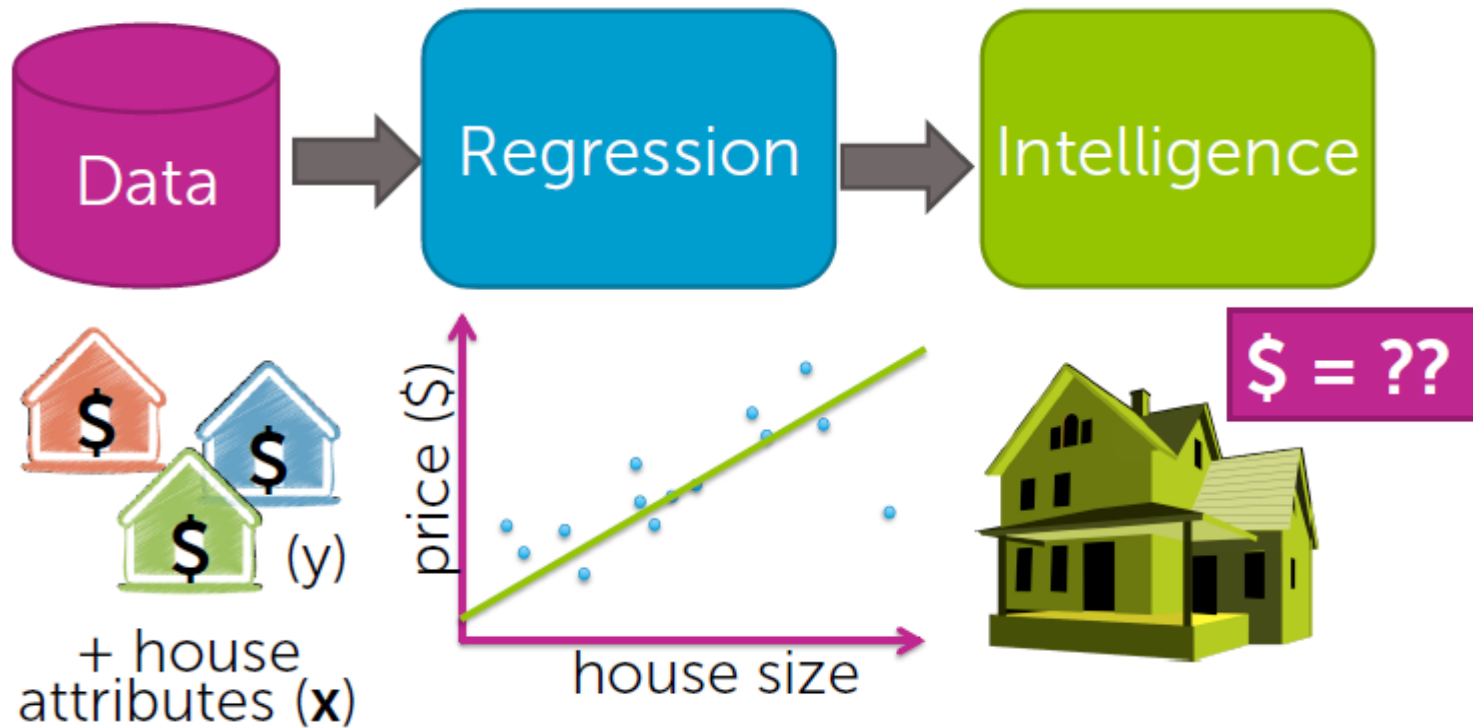
From features to predictions



Case study

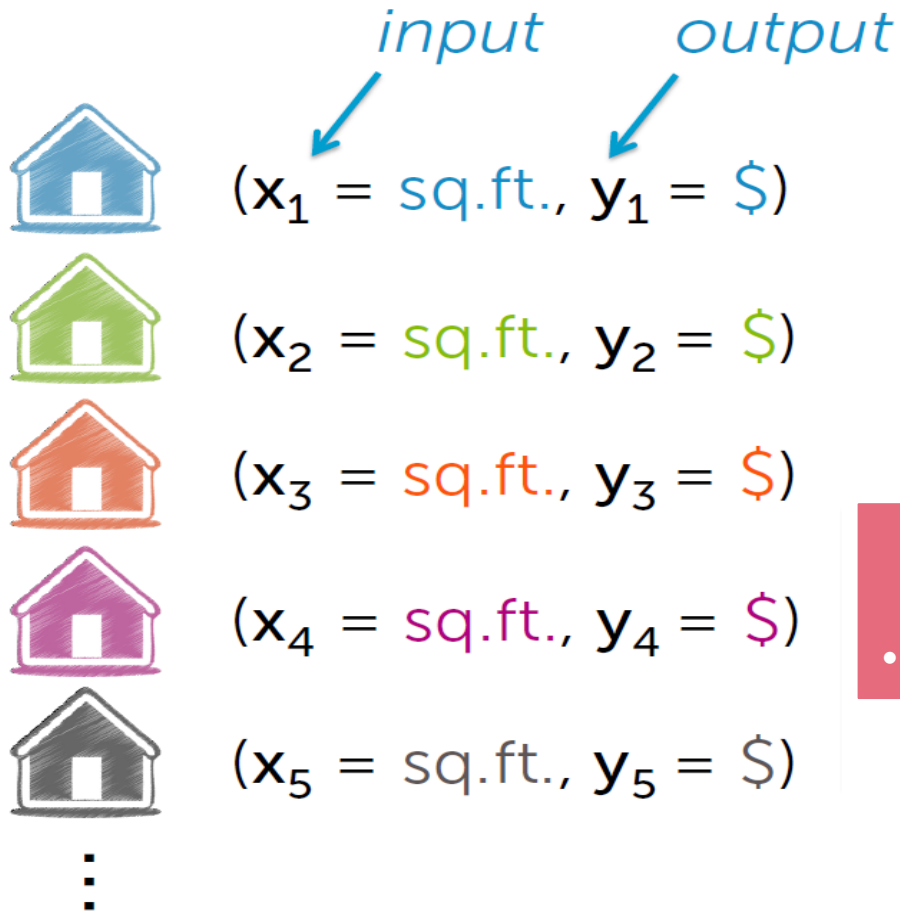
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Predicting house prices



Data

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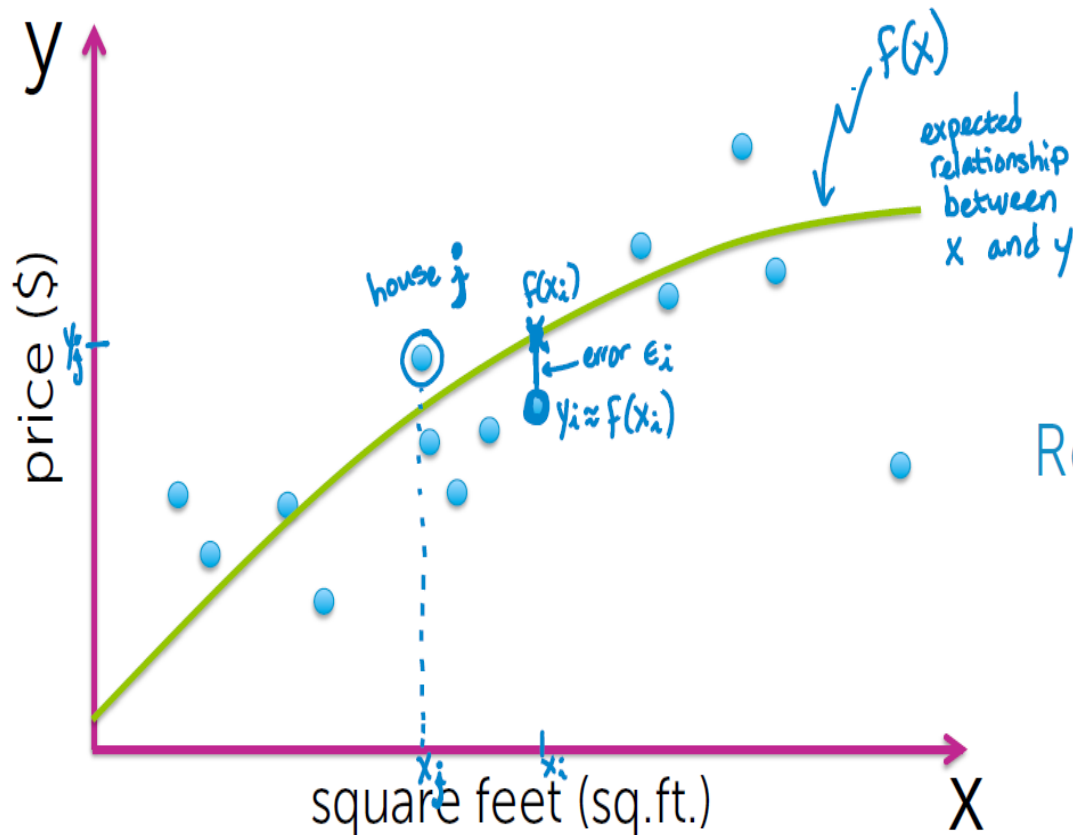


Input vs output

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

Model: assume functional relationship

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

Regression model:

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

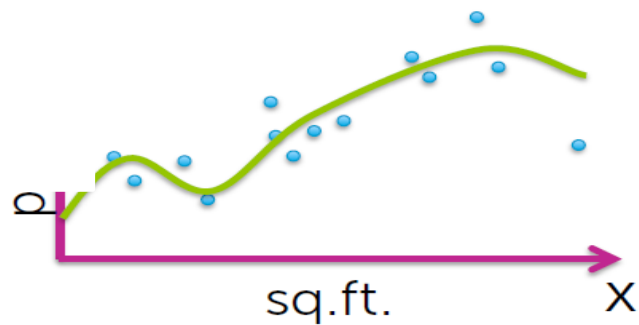
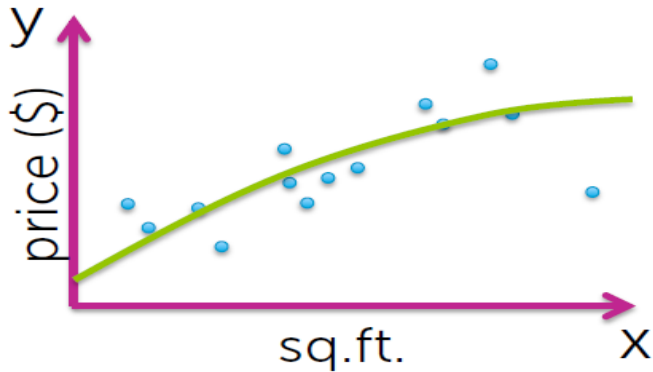
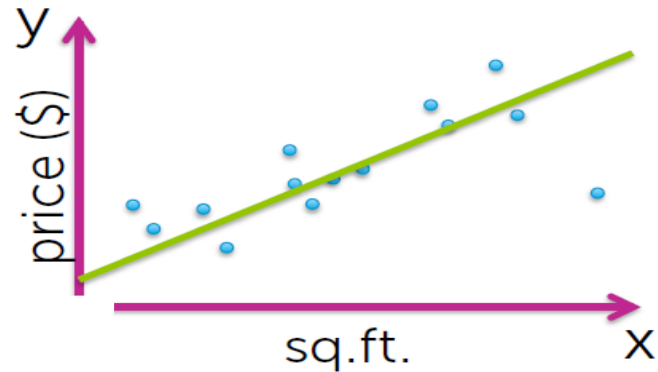
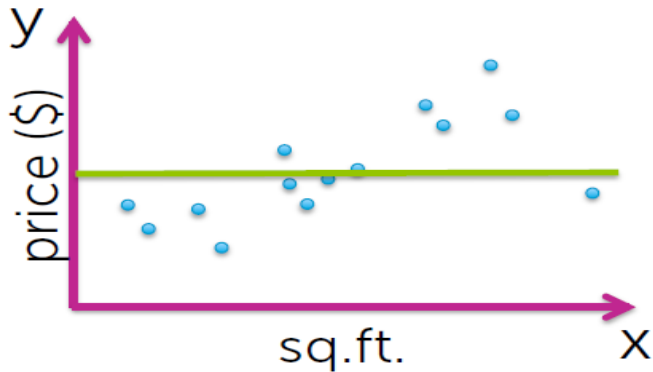
$E[\epsilon_i] = 0$ ← equally likely that error is + or -
↑ expected value

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

Task 1:

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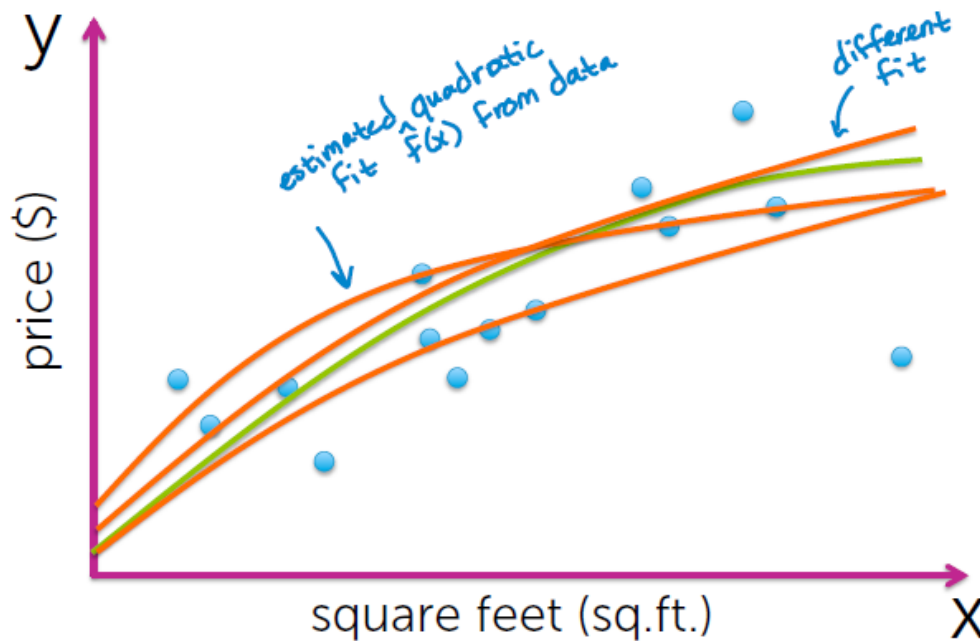
Which model to fit?



Task 2:

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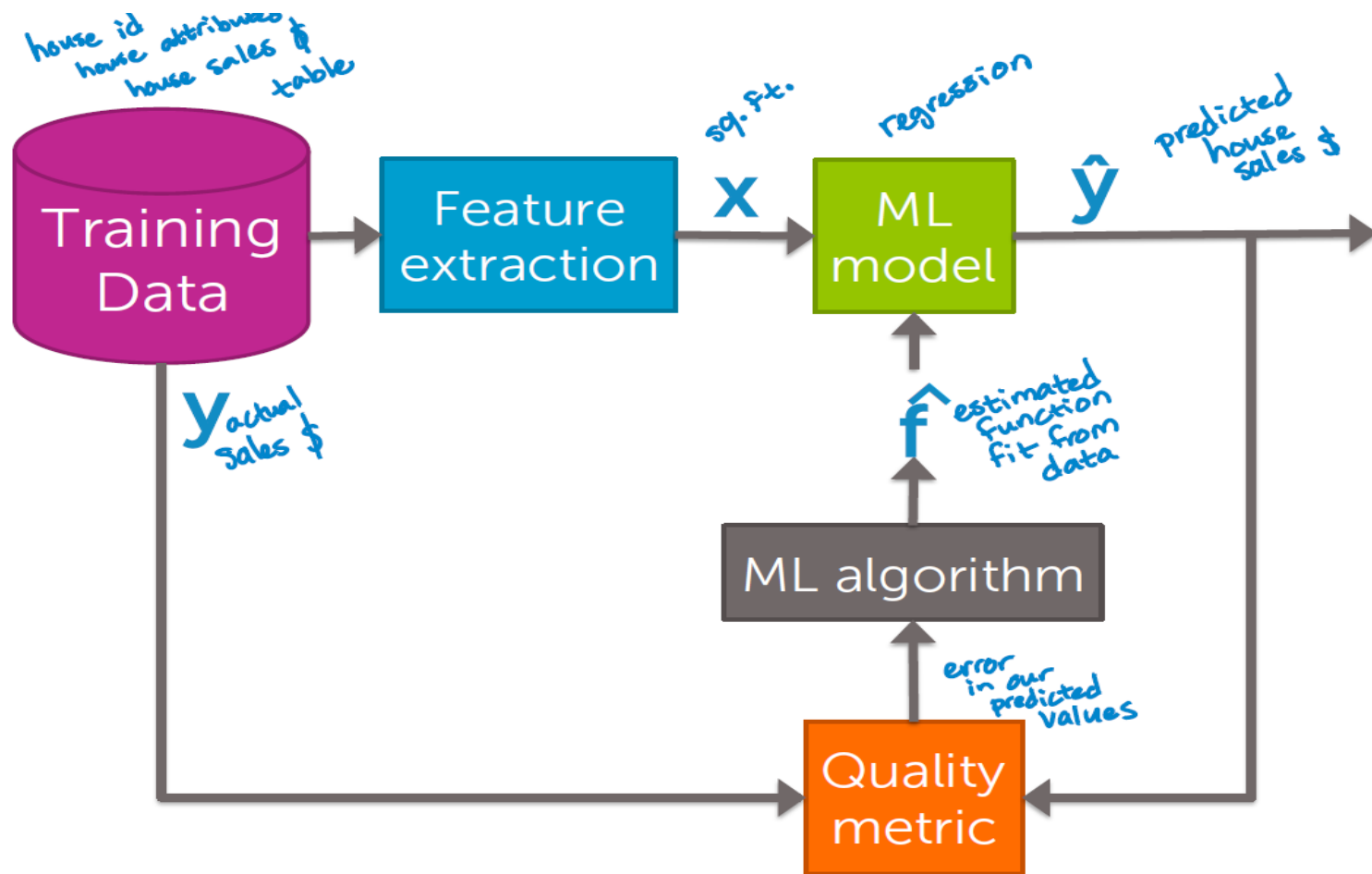
For a given model $f(x)$ estimate function $\hat{f}(x)$ from data



Assume model $f(x)$ is a quadratic function

How it works: baseline flow chart

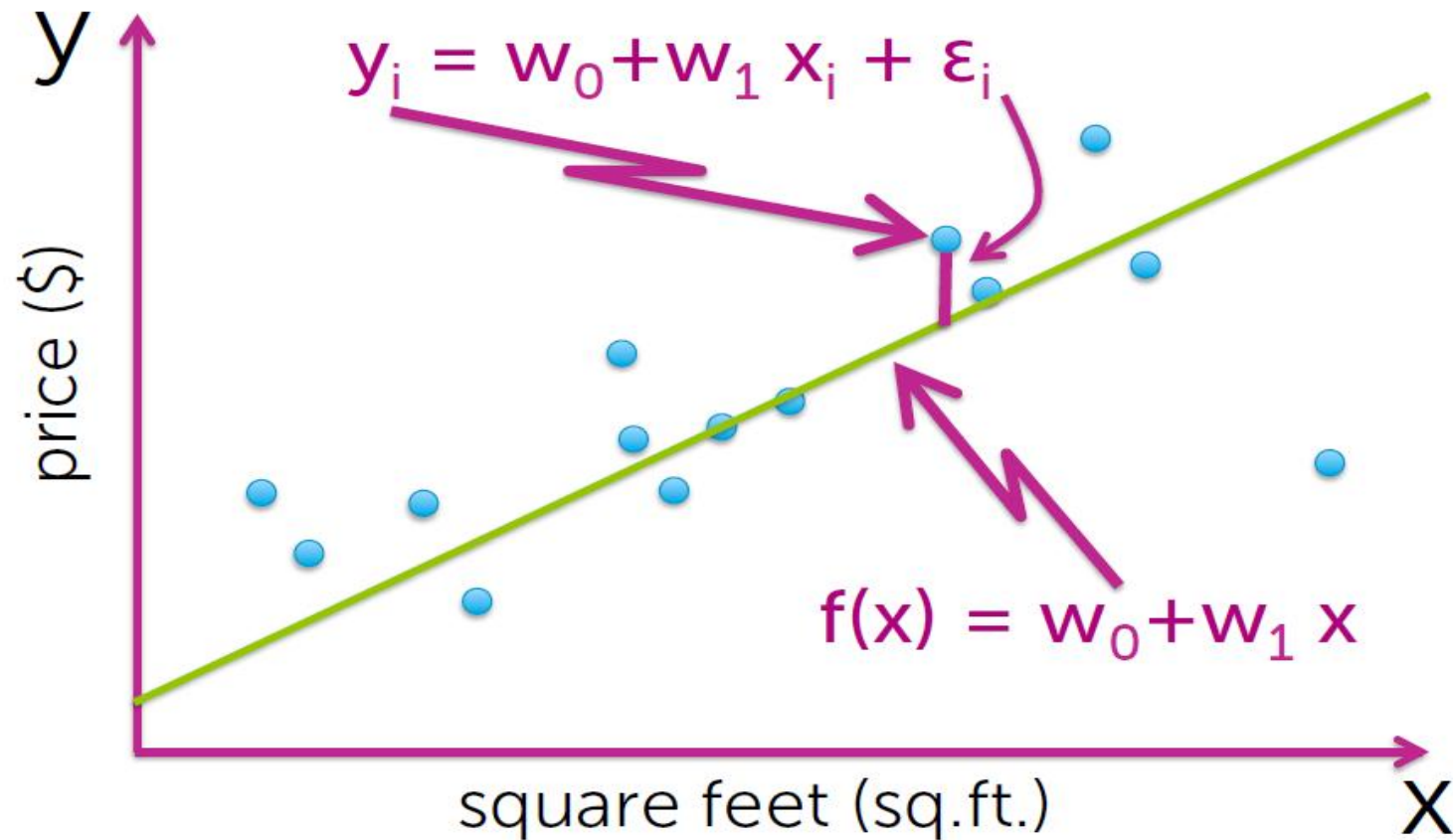
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SIMPLE LINEAR REGRESSION

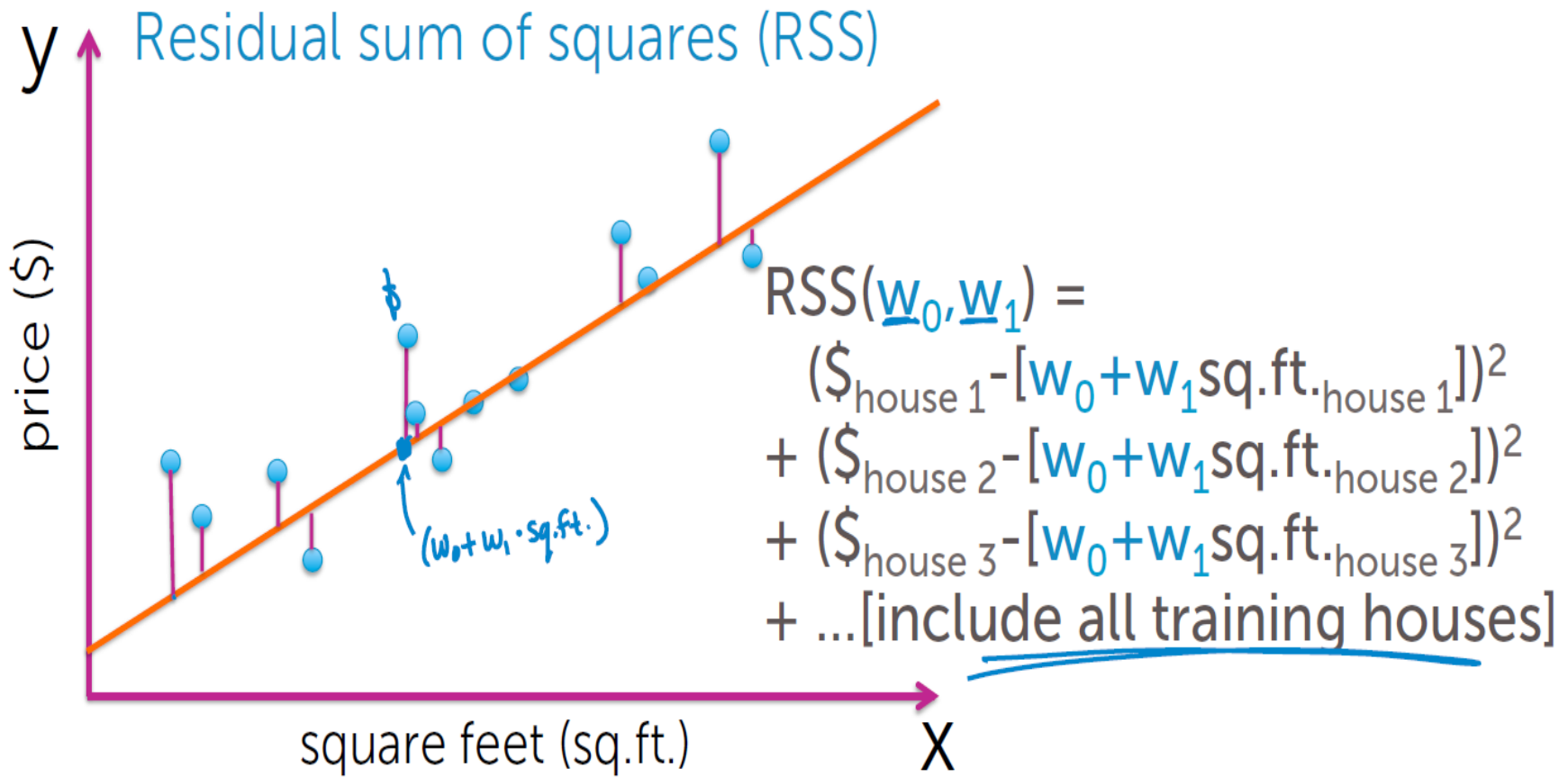
Simple linear regression model

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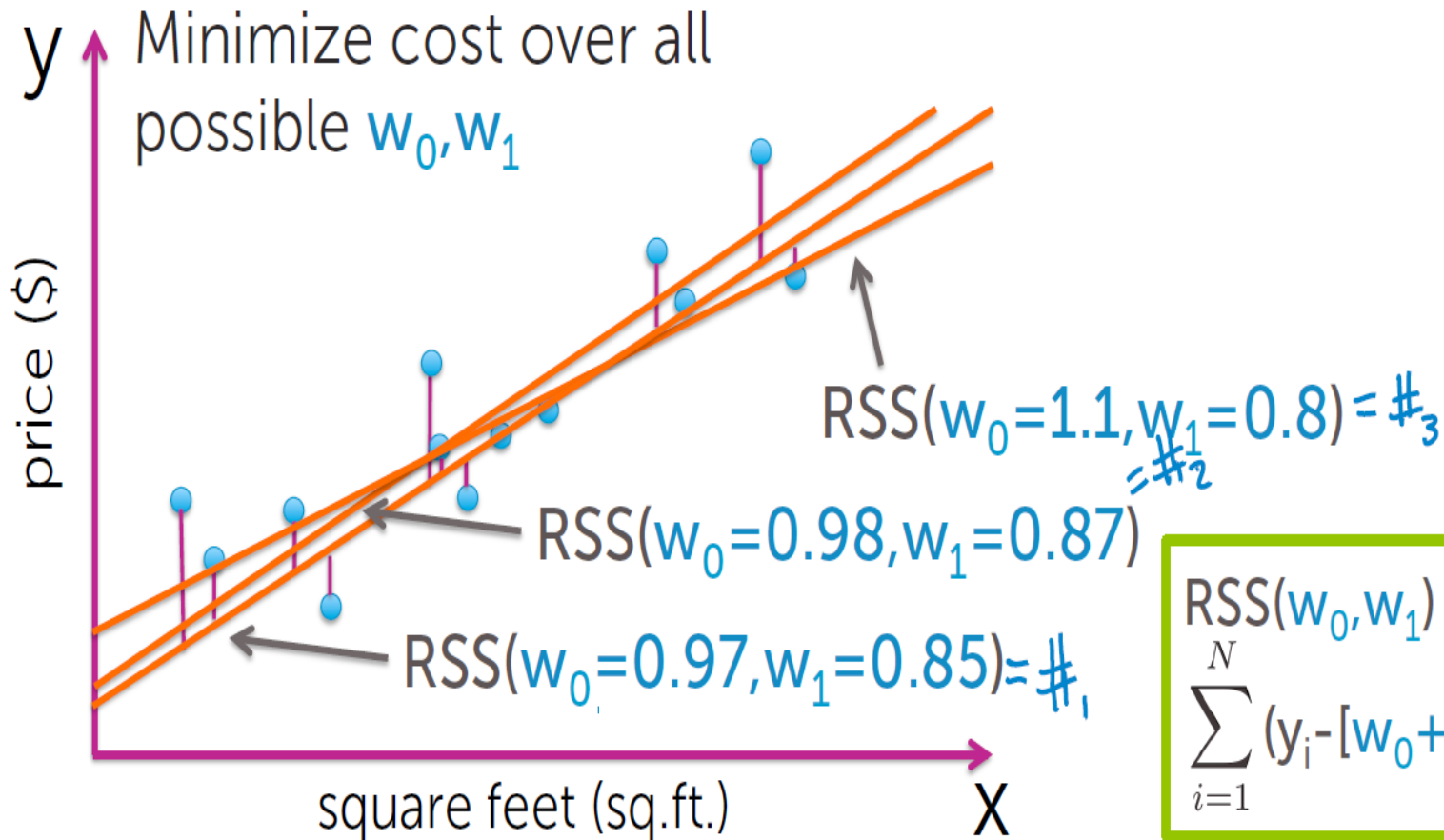
The cost of using a given line

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Find „best” line

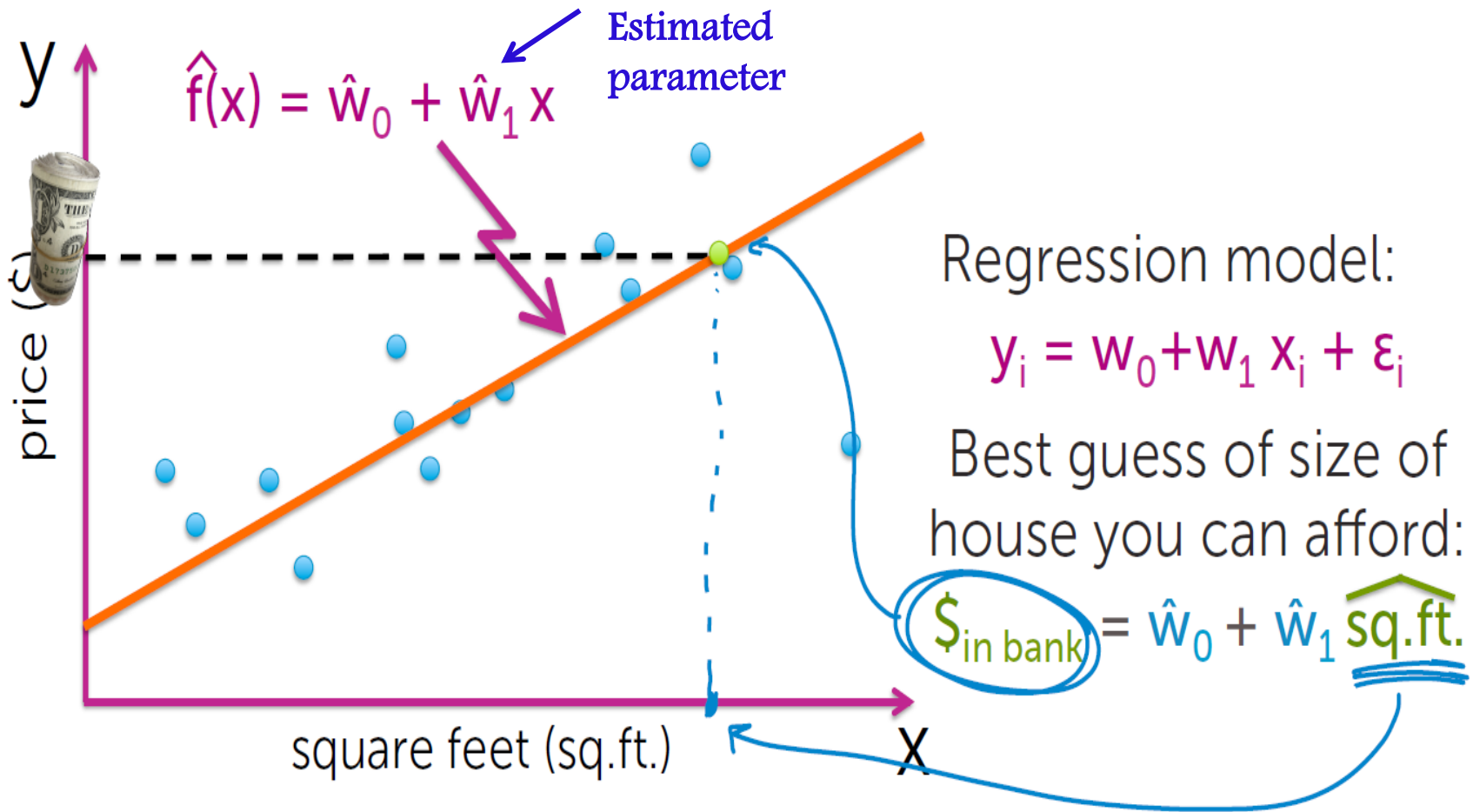
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$$RSS(w_0, w_1) = \sum_{i=1}^N (y_i - [w_0 + w_1 x_i])^2$$

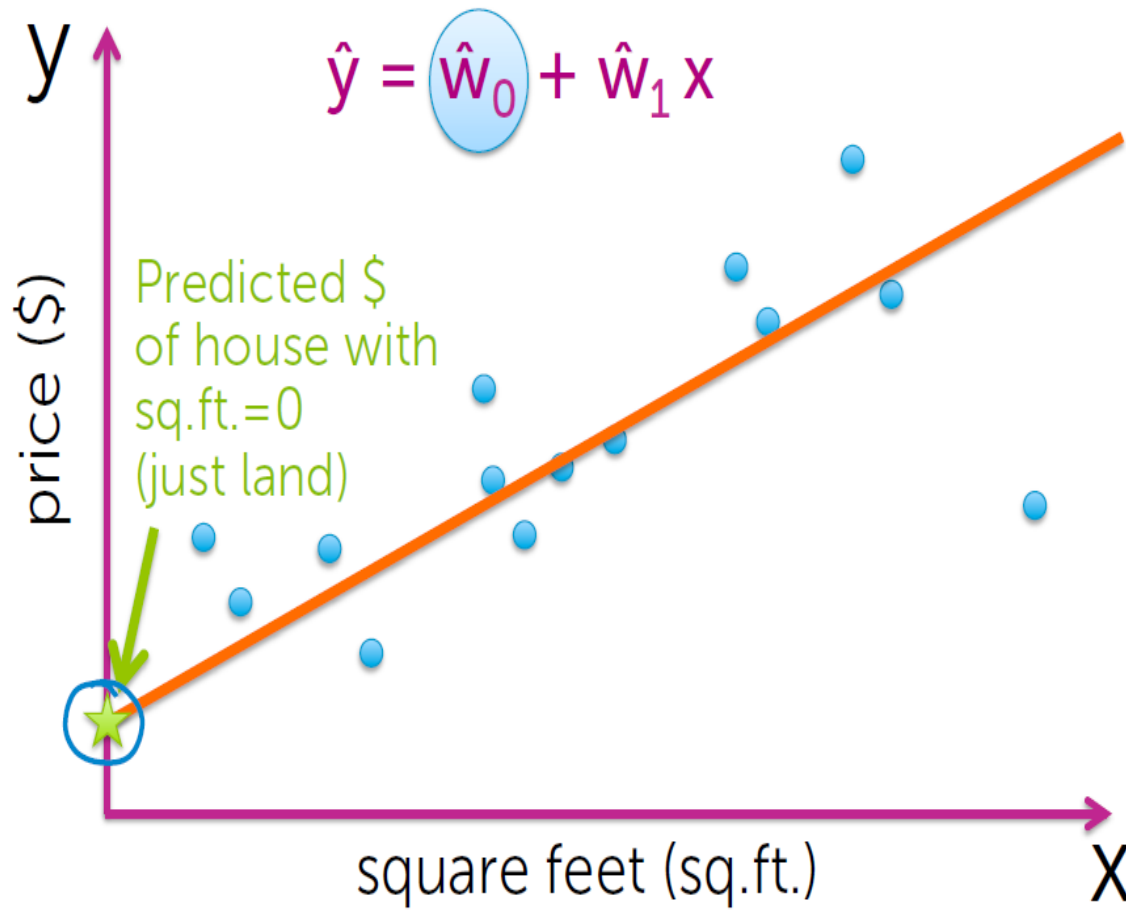
Predicting size of house you can afford

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Interpreting the coefficients

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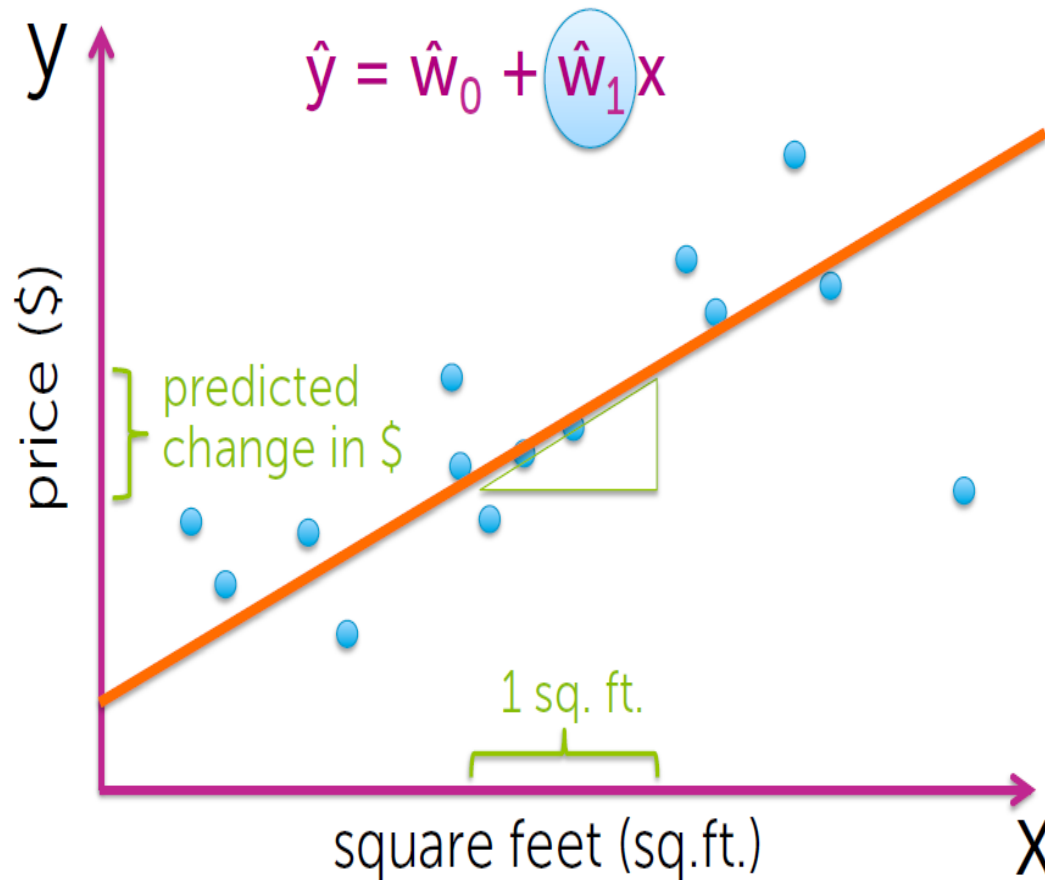


$$\hat{y} = \hat{w}_0 \text{ when } x=0$$

not very meaningful

Interpreting the coefficients

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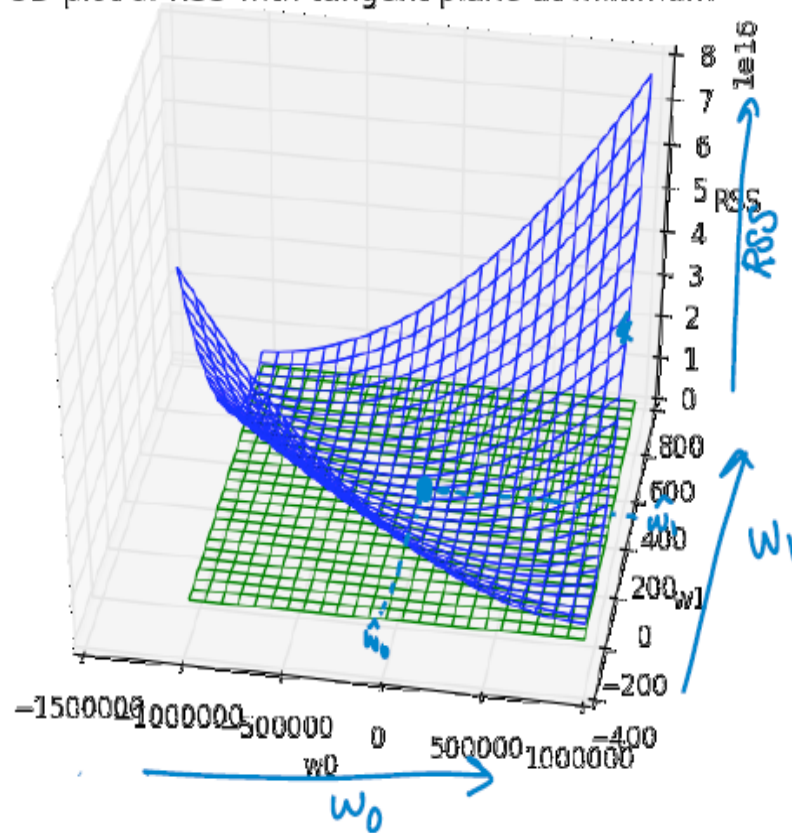
Magnitude of fit parameters depend on the units of both features and observations

$$\begin{aligned} & \hat{\$}_{1001 \text{ sq.ft.}} - \hat{\$}_{1000 \text{ sq.ft.}} \\ &= \hat{w}_0 + \hat{w}_1 \cdot 1001 \text{ sq.ft.} \\ &\quad - (\hat{w}_0 + \hat{w}_1 \cdot 1000 \text{ sq.ft.}) \\ &= \hat{w}_1 \\ &\text{predicted change in the output} \\ &\quad \text{per unit change in input} \end{aligned}$$

ML algorithm: minimising the cost

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3D plot of RSS with tangent plane at minimum



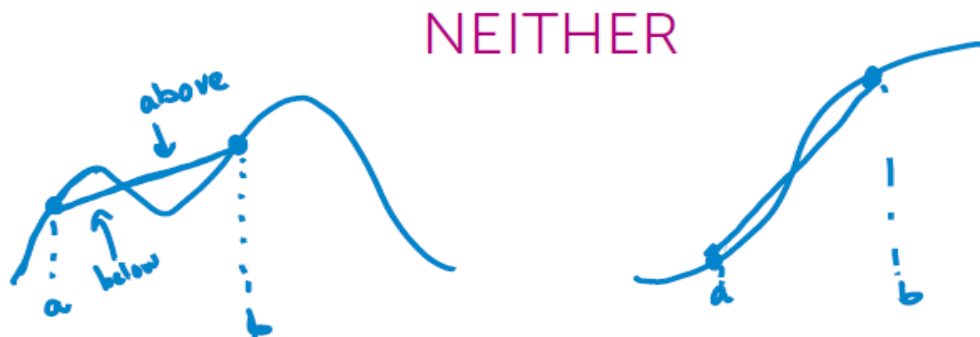
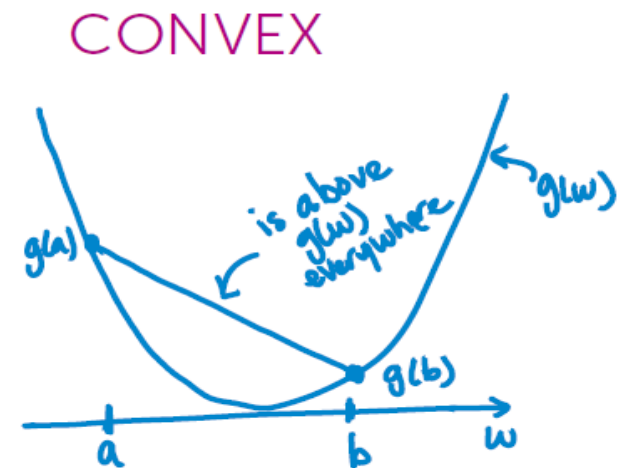
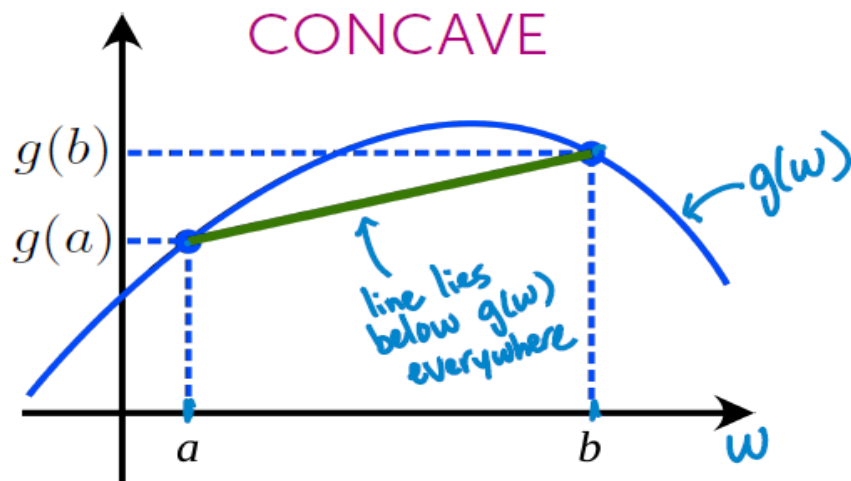
Minimize function
over all possible w_0, w_1

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

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

Convex/concave function

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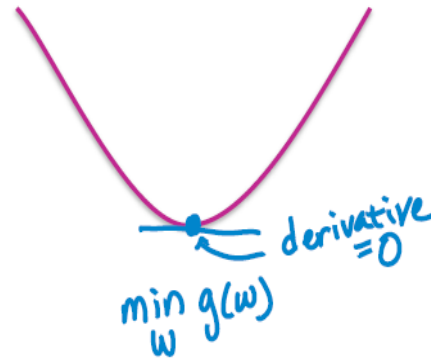
Finding max/min analytically

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CONCAVE



CONVEX



NEITHER



no solution to derivative = 0

A hand-drawn graph of a function that is neither concave nor convex, represented by a monotonically increasing S-shaped curve. An arrow points to the curve with the label "no solution to derivative = 0".

Example:

$$g(w) = 5 - (w - 10)^2$$

$$\begin{aligned}\frac{dg(w)}{dw} &= 0 - 2(w - 10)^1 \cdot 1 \\ &= -2w + 20\end{aligned}$$

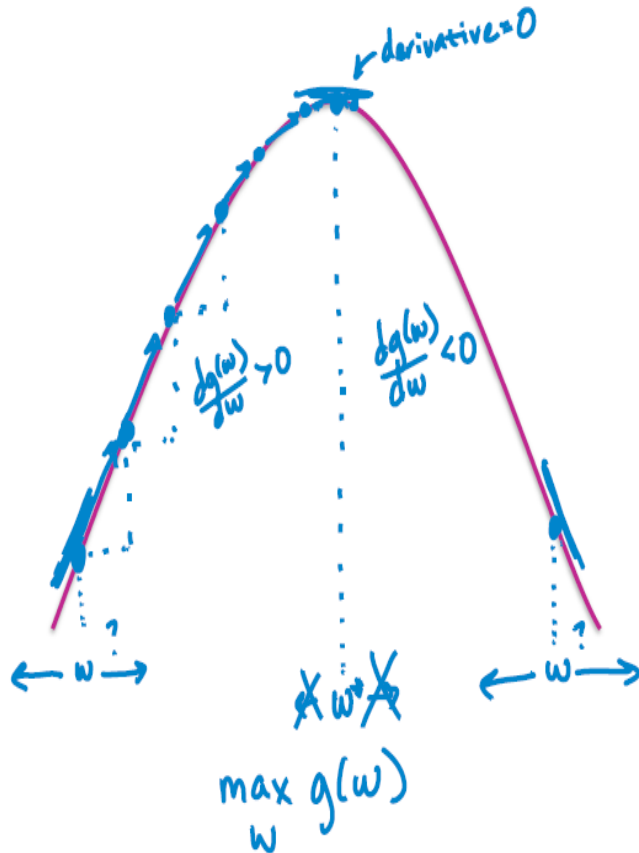
set derivate = 0:

$$\begin{aligned}-2w + 20 &= 0 \\ w &= 10\end{aligned}$$



Finding the max via hill climbing

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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 ?)

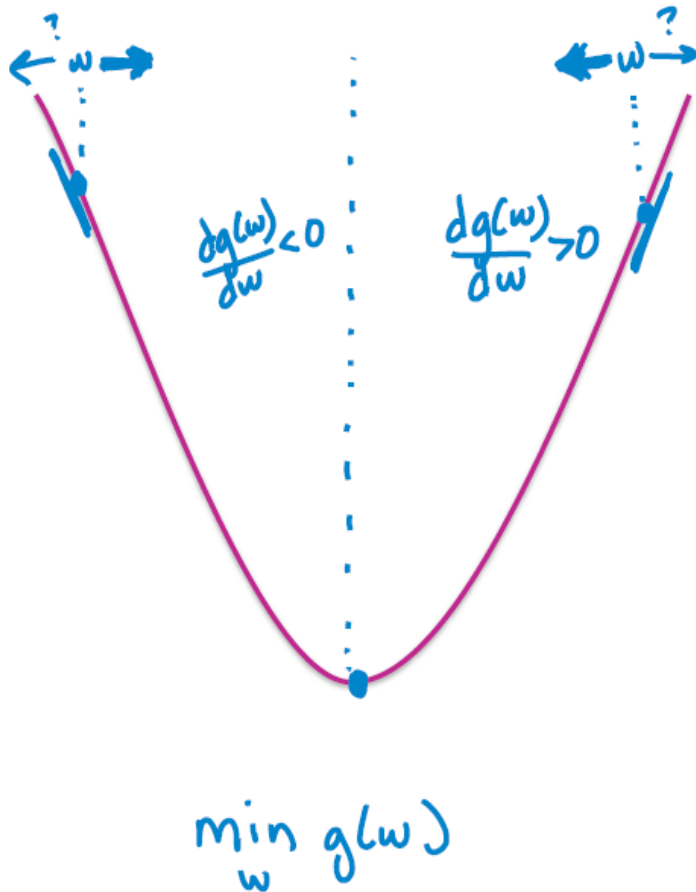
While not converged

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

iteration t stepsize

Finding the min via hill descent

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

Algorithm:

while not converged

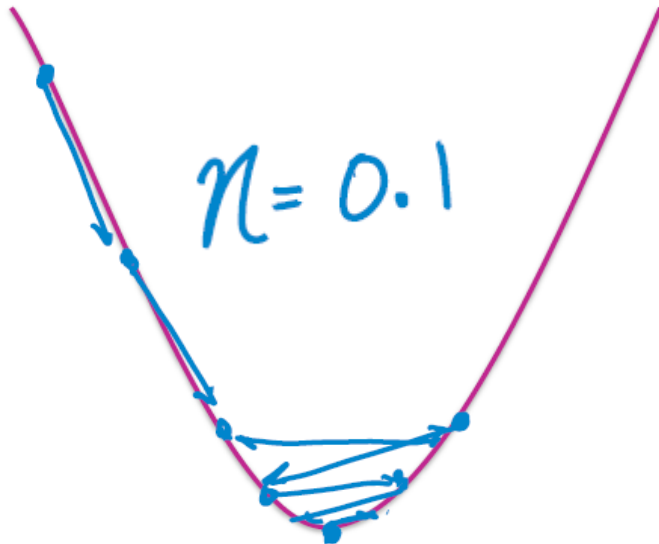
$$w^{(t+1)} \leftarrow w^{(t)} - \eta \left. \frac{dg}{dw} \right|_{w^{(t)}}$$

Choosing the step size (stepsize schedule)

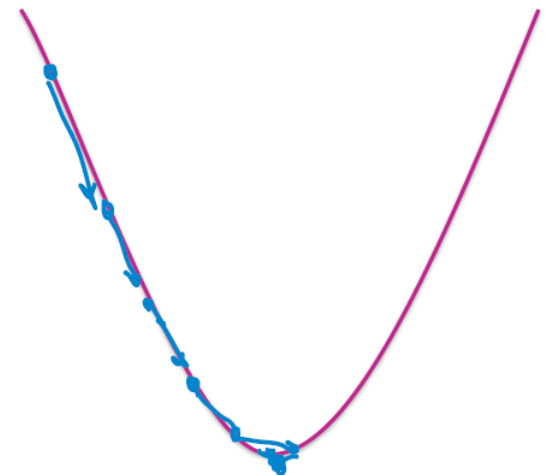
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Fixed

Works well for strongly convex functions

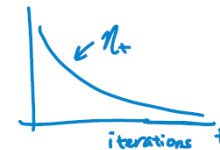


Varying



Common choices:

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



Try not to decrease η too fast

Convergence criteria

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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

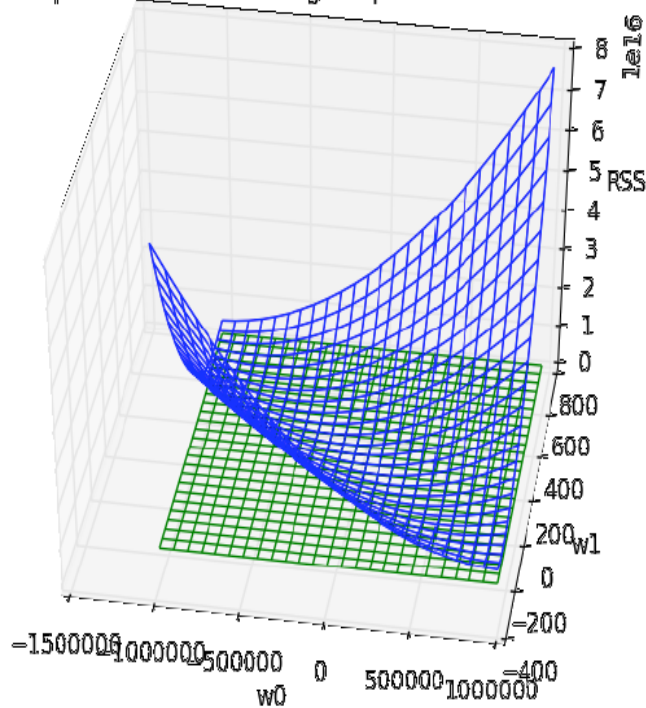
Algorithm:

while not converged
 $w^{(t+1)} \leftarrow w^{(t)} - \eta \left. \frac{dg}{dw} \right|_{w^{(t)}}$

Moving to multiple dimensions

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3D plot of RSS with tangent plane at minimum



$$\nabla g(\mathbf{w}) = \begin{bmatrix} \frac{\partial g}{\partial w_0} \\ \frac{\partial g}{\partial w_1} \\ \vdots \\ \frac{\partial g}{\partial w_p} \end{bmatrix}$$

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

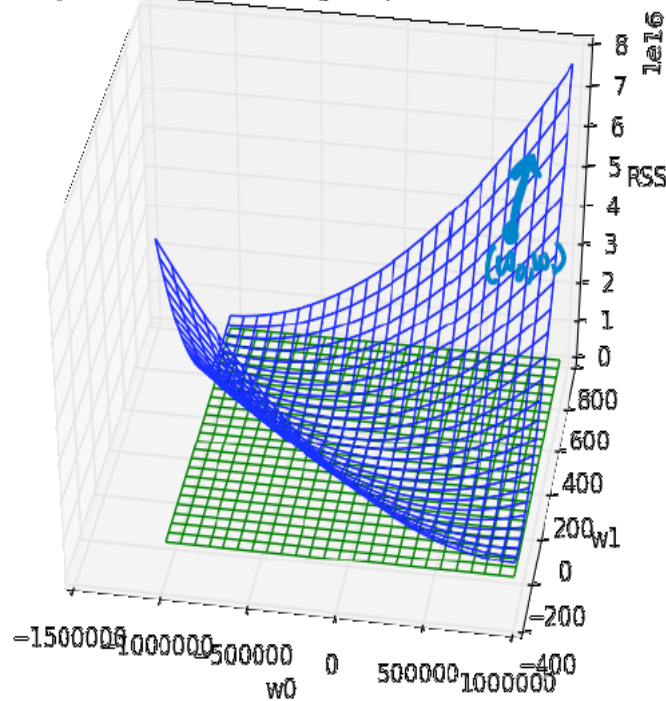
$(p+1)$ -dimensional vector

partial derivative is like a derivative with respect to w_i , treating all other variables as constants

Gradient example

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3D plot of RSS with tangent plane at minimum



$$g(\mathbf{w}) = 5w_0 + 10w_0w_1 + 2w_1^2$$

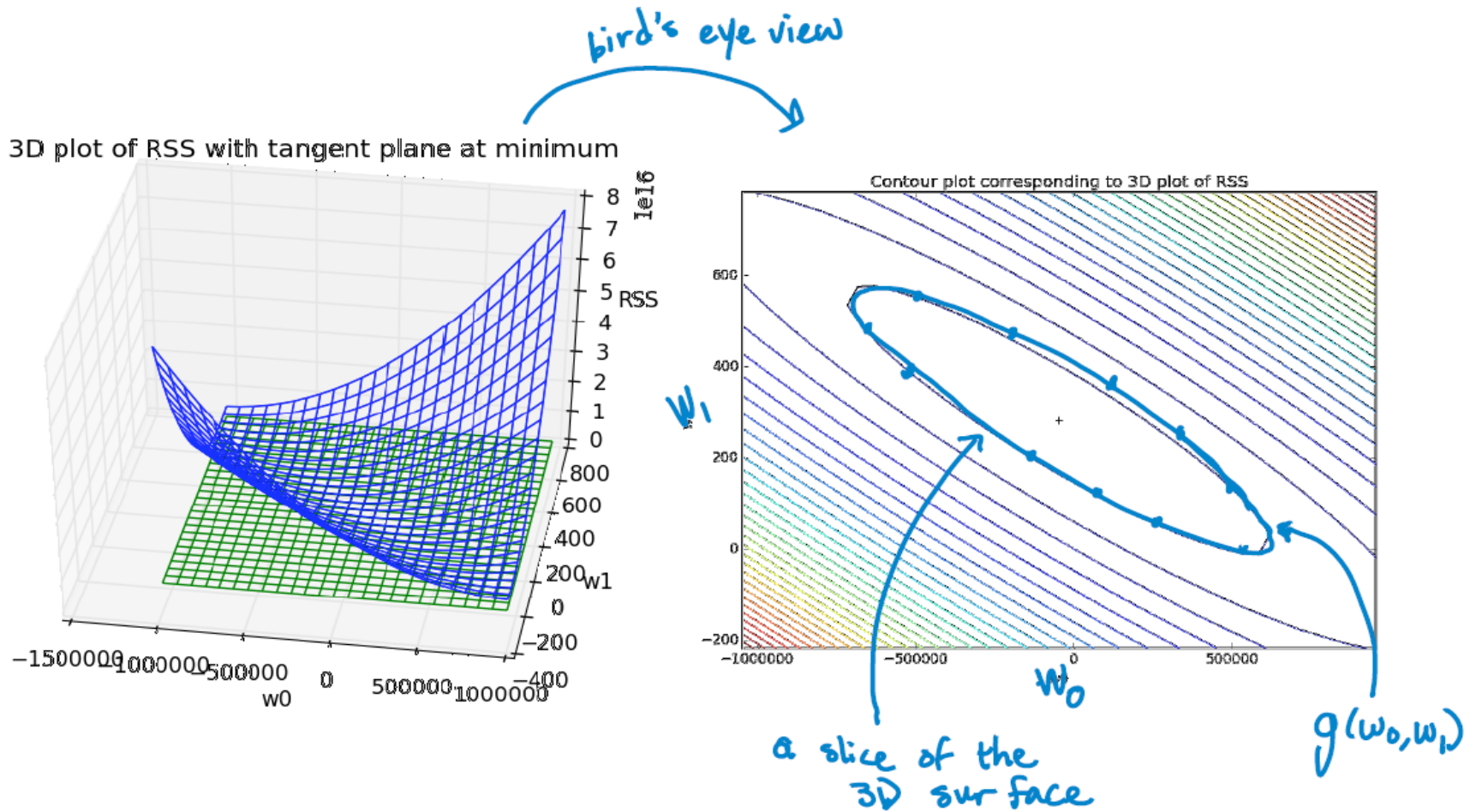
$$\frac{\partial g}{\partial w_0} = 5 + 10w_1$$

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

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

Contour plots

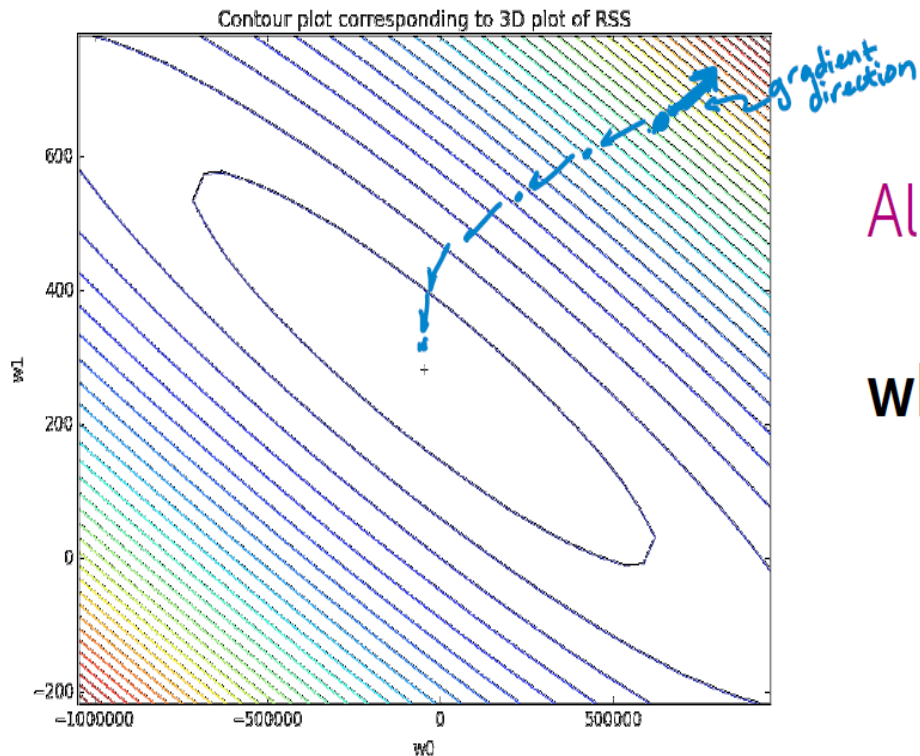
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Gradient descent

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Algorithm:

while not converged

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

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

Convergence:
 $\|\nabla g(w)\| < \epsilon$

Compute the gradient

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

Taking the derivative w.r.t. w_0

$$\begin{aligned} & \sum_{i=1}^N 2 (y_i - [w_0 + w_1 x_i])' \cdot (-1) \\ &= -2 \sum_{i=1}^N (y_i - [w_0 + w_1 x_i]) \end{aligned}$$

Putting it together:

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

Taking the derivative w.r.t. w_1

$$\begin{aligned} & \sum_{i=1}^N 2 \underline{(y_i - [w_0 + w_1 x_i])'} \cdot (-x_i) \\ &= -2 \sum_{i=1}^N (y_i - [w_0 + w_1 x_i]) \underline{x_i} \end{aligned}$$

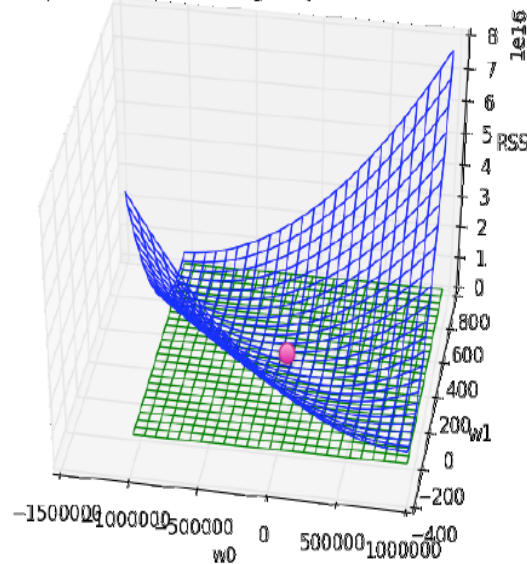
Approach 1: set gradient to 0

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

This method is called „Closed form solution“

3D plot of RSS with tangent plane at minimum



top term:

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

average house sales price
estimate of the slope
average sq. ft.

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:

$$\begin{aligned} &\sum_{i=1}^N y_i \\ &\sum_{i=1}^N x_i \\ &\sum_{i=1}^N y_i x_i \\ &\sum_{i=1}^N x_i^2 \end{aligned}$$

Approach 2: gradient descent

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Interpreting the gradient:

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

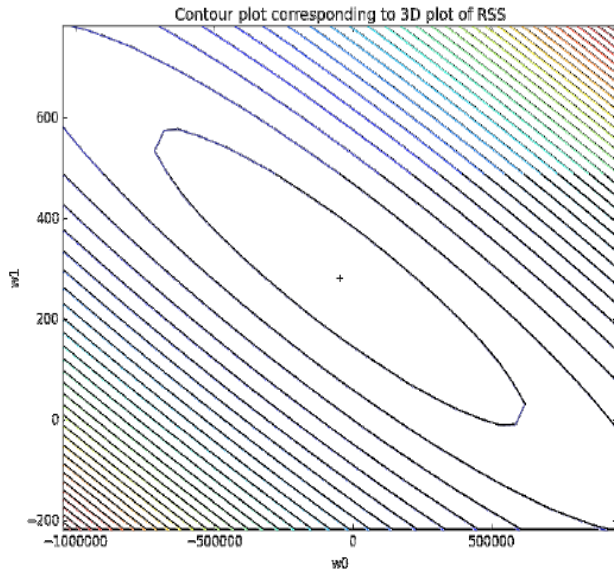
Handwritten annotations:

- y_i : actual house sales observation
- $\hat{y}_i(w_0, w_1)$: predicted value

Approach 2: gradient descent

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



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 $\sum [y_i - \hat{y}_i]$ is positive

→ w_0 is going to increase

similar intuition for w_1 , but multiply by x_i

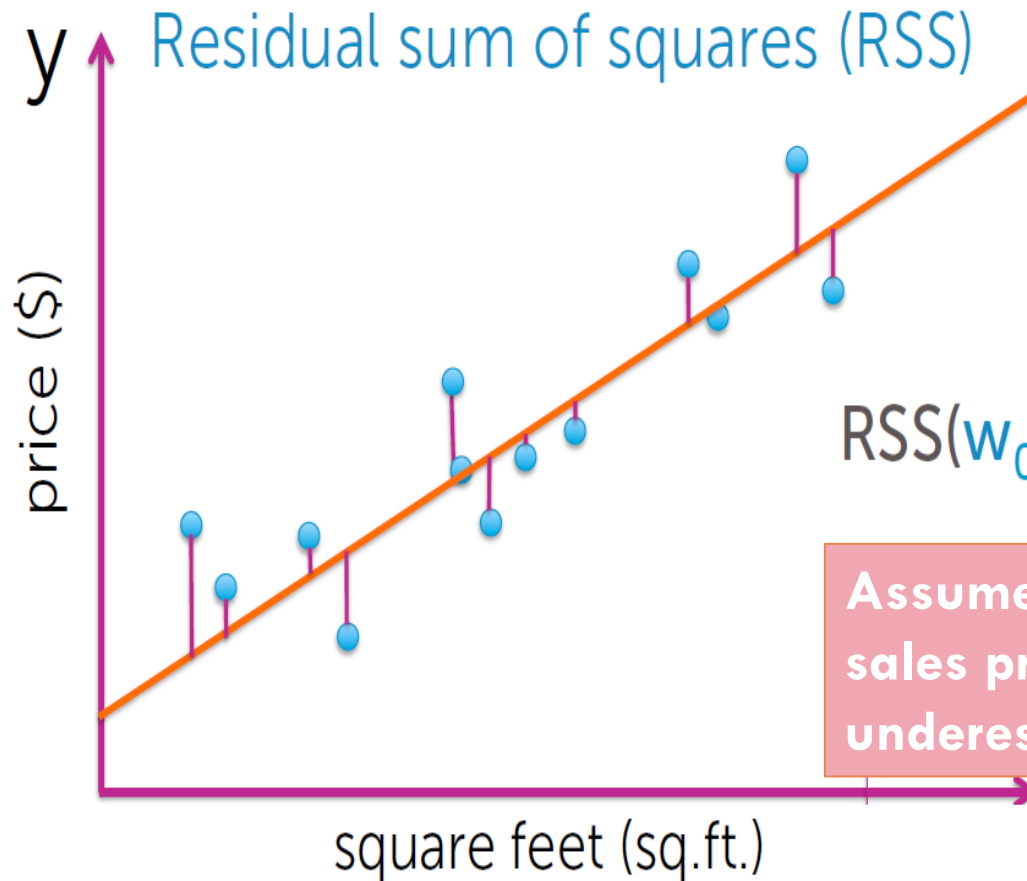
Comparing the approaches

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

Symmetric cost function

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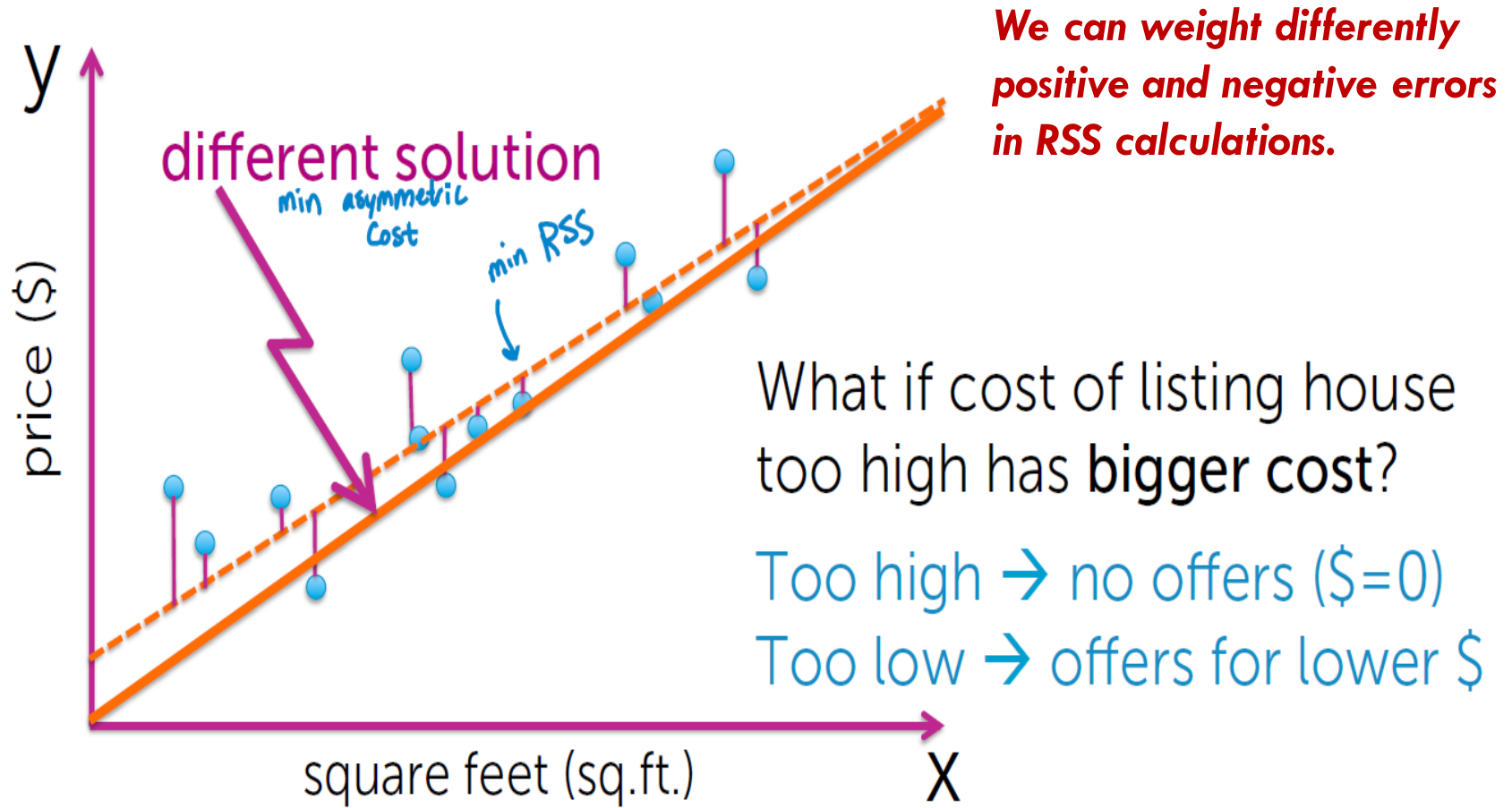


$$RSS(w_0, w_1) = \sum_{i=1}^N (y_i - [w_0 + w_1 x_i])^2$$

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

Asymmetric cost functions

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What you can do now

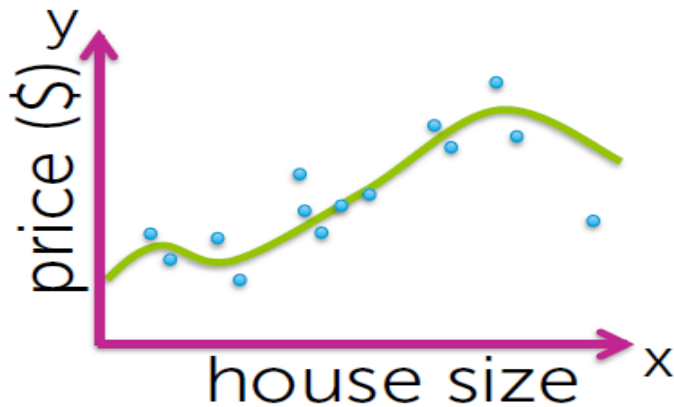
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- Describe the input (features) and output (real-valued predictions) of a regression model
- Calculate a goodness-of-fit metric (e.g., RSS)
- Estimate model parameters to minimize RSS using gradient descent
- Interpret estimated model parameters
- 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

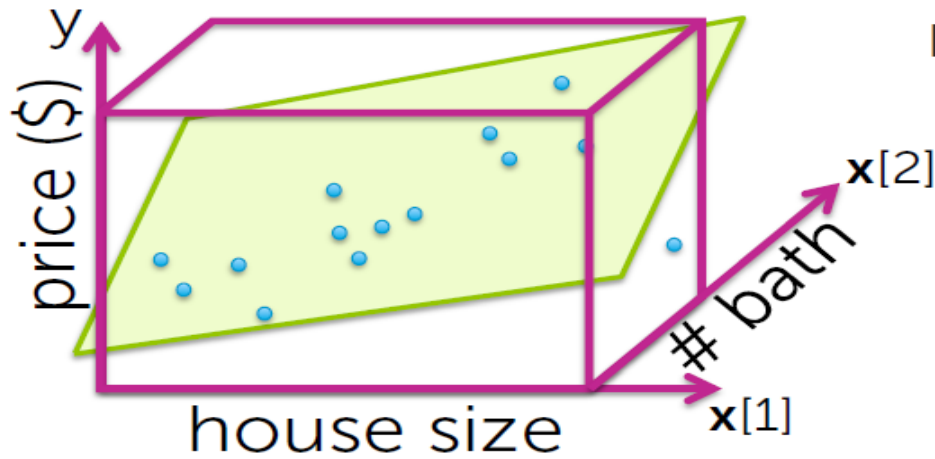
MULTIPLE REGRESSION

Multiple regression

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Fit **more complex relationships** than just a line



Incorporate more inputs

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

Polynomial regression

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Model:

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

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

...

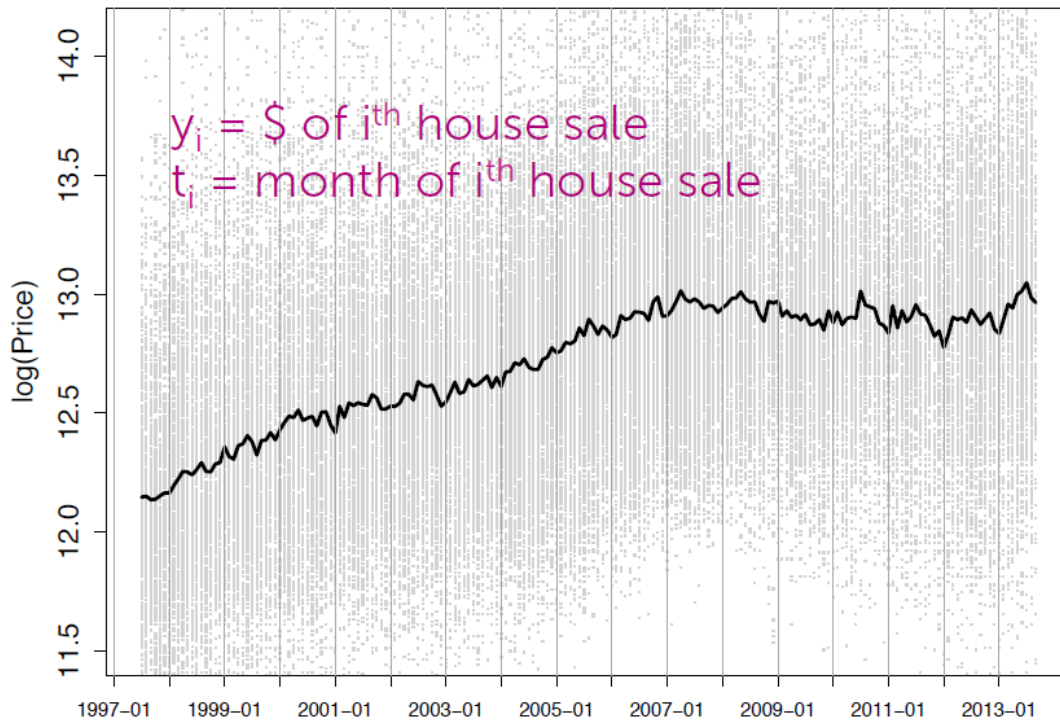
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feature $p+1 = x^p$ parameter $p+1 = w_p$

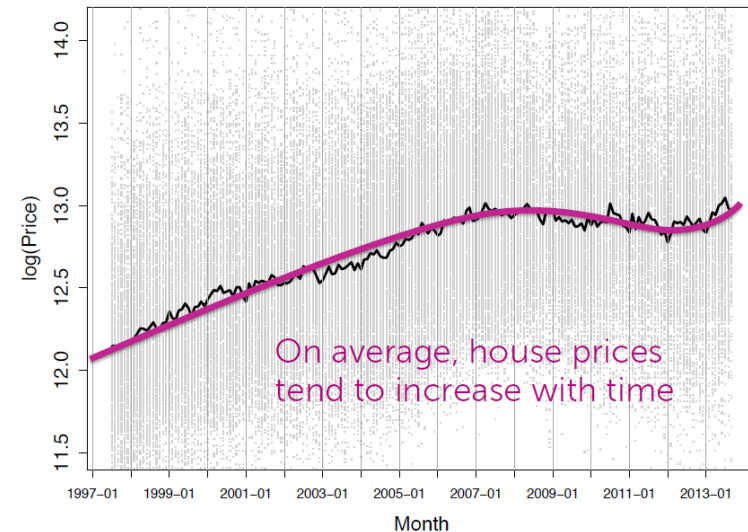
Other functional forms of one input

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□ Trends in time series



Month ← House sales recorded monthly

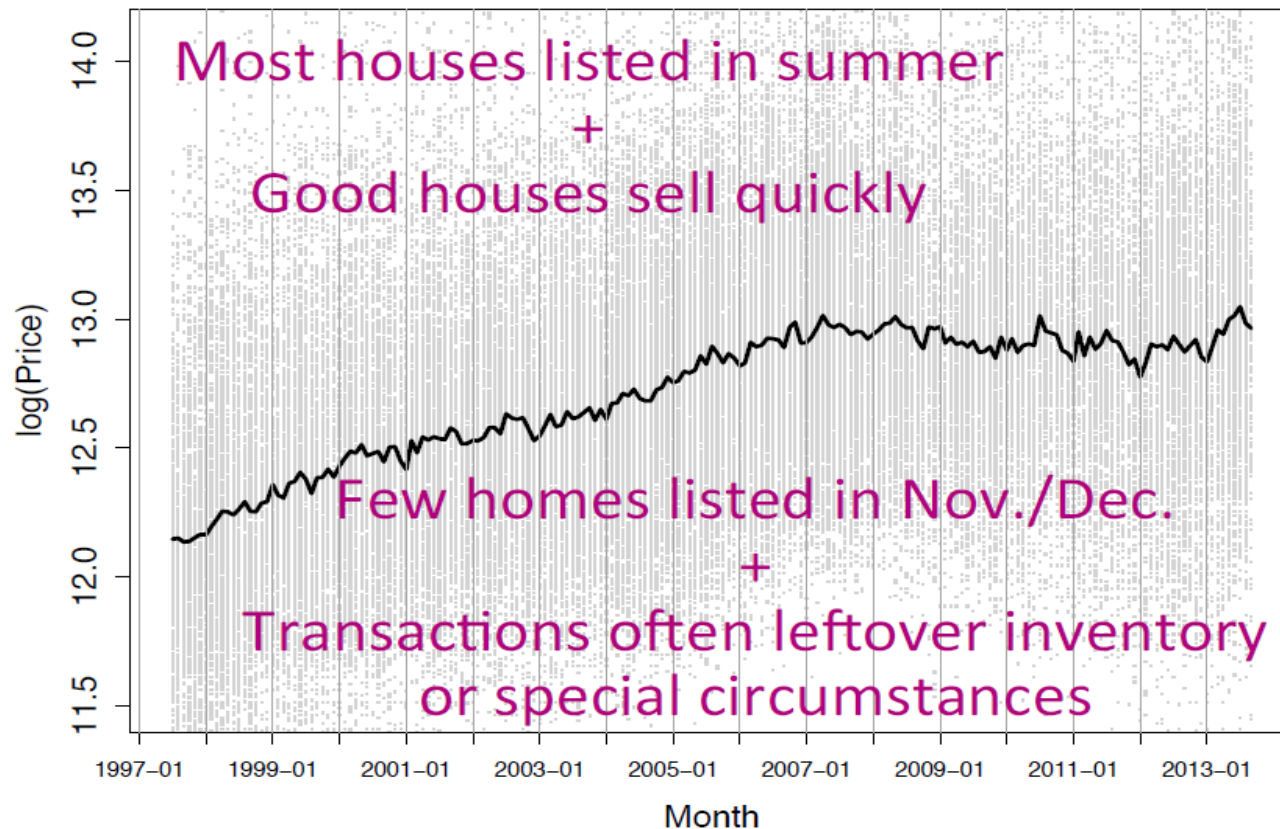


This trend can be modeled with polynomial function.

Other functional forms of one input

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□ Seasonality



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Example of detrending

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Model:

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

Linear trend

Unknown phase/shift

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

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Equivalently,

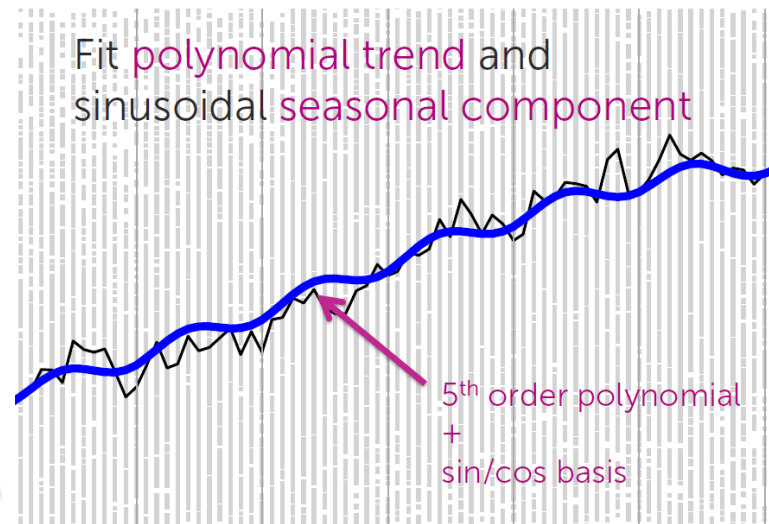
$$y_i = w_0 + w_1 t_i + w_2 \sin(2\pi t_i / 12) + w_3 \cos(2\pi t_i / 12) + \varepsilon_i$$

feature 1 = 1 (constant)

feature 2 = t

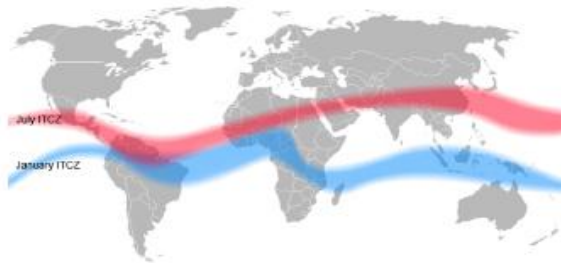
feature 3 = $\sin(2\pi t/12)$

feature 4 = $\cos(2\pi t/12)$

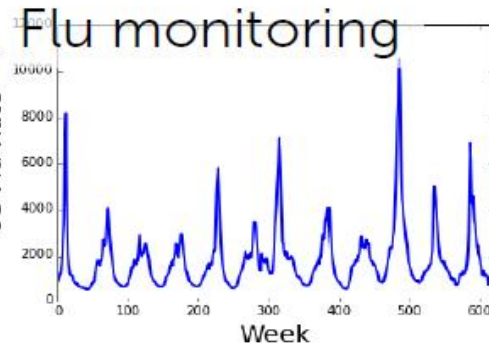


Other examples of seasonality

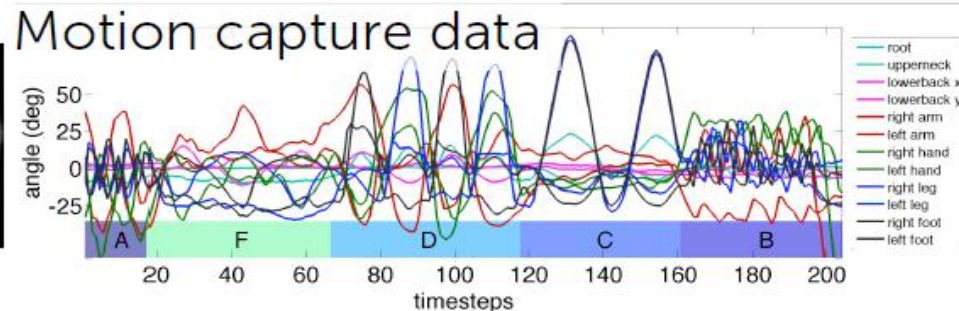
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Weather modeling
(e.g., temperature, rainfall)



Demand forecasting
(e.g., jacket purchases)



Generic basic expansion

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Model:

$$\begin{aligned} y_i &= w_0 h_0(x_i) + w_1 h_1(x_i) + \dots + w_D h_D(x_i) + \varepsilon_i \\ &= \sum_{j=0}^D w_j h_j(x_i) + \varepsilon_i \end{aligned}$$

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

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

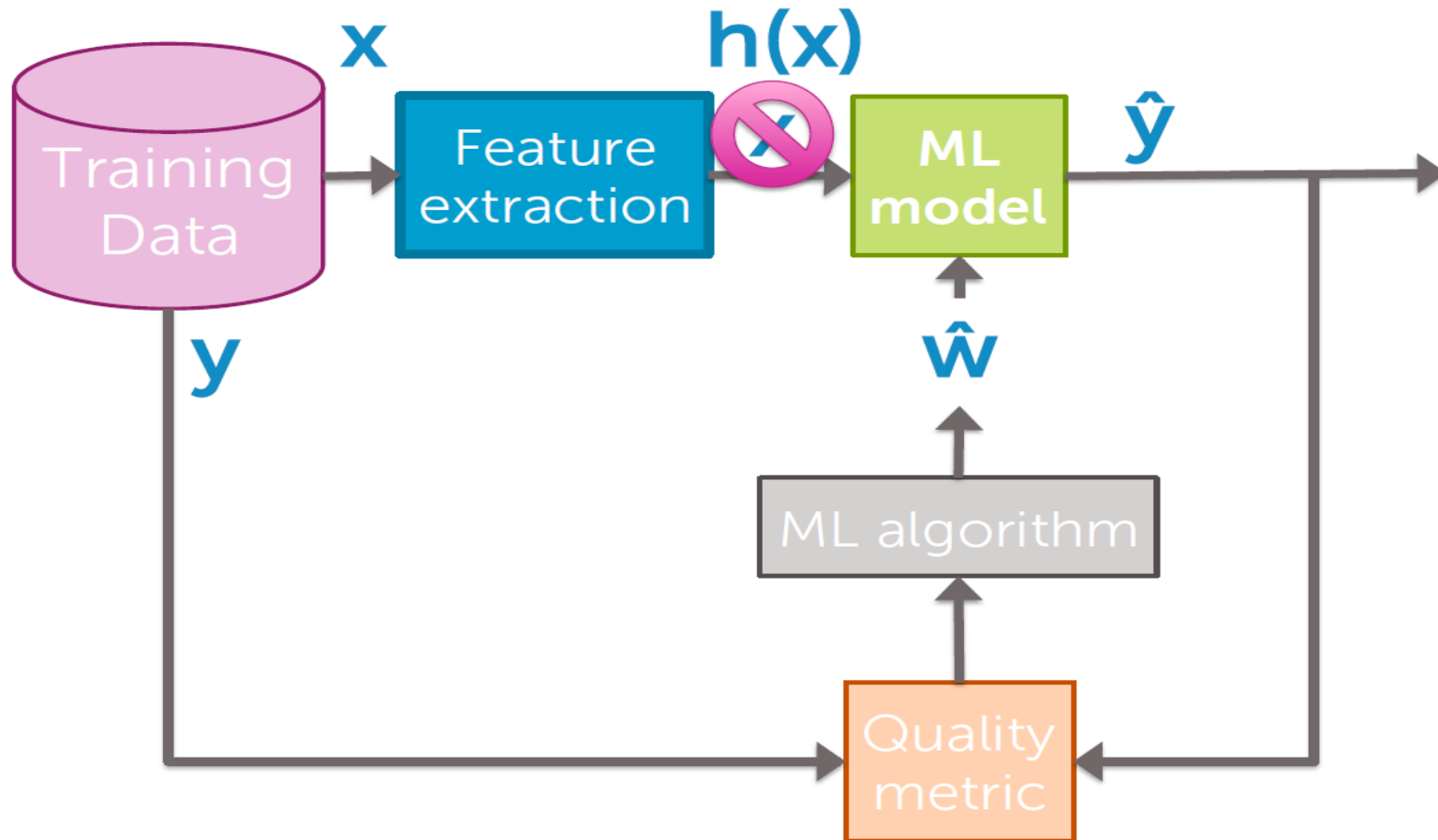
feature 3 = $h_2(x)$... e.g., x^2 or $\sin(2\pi x/12)$

...

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

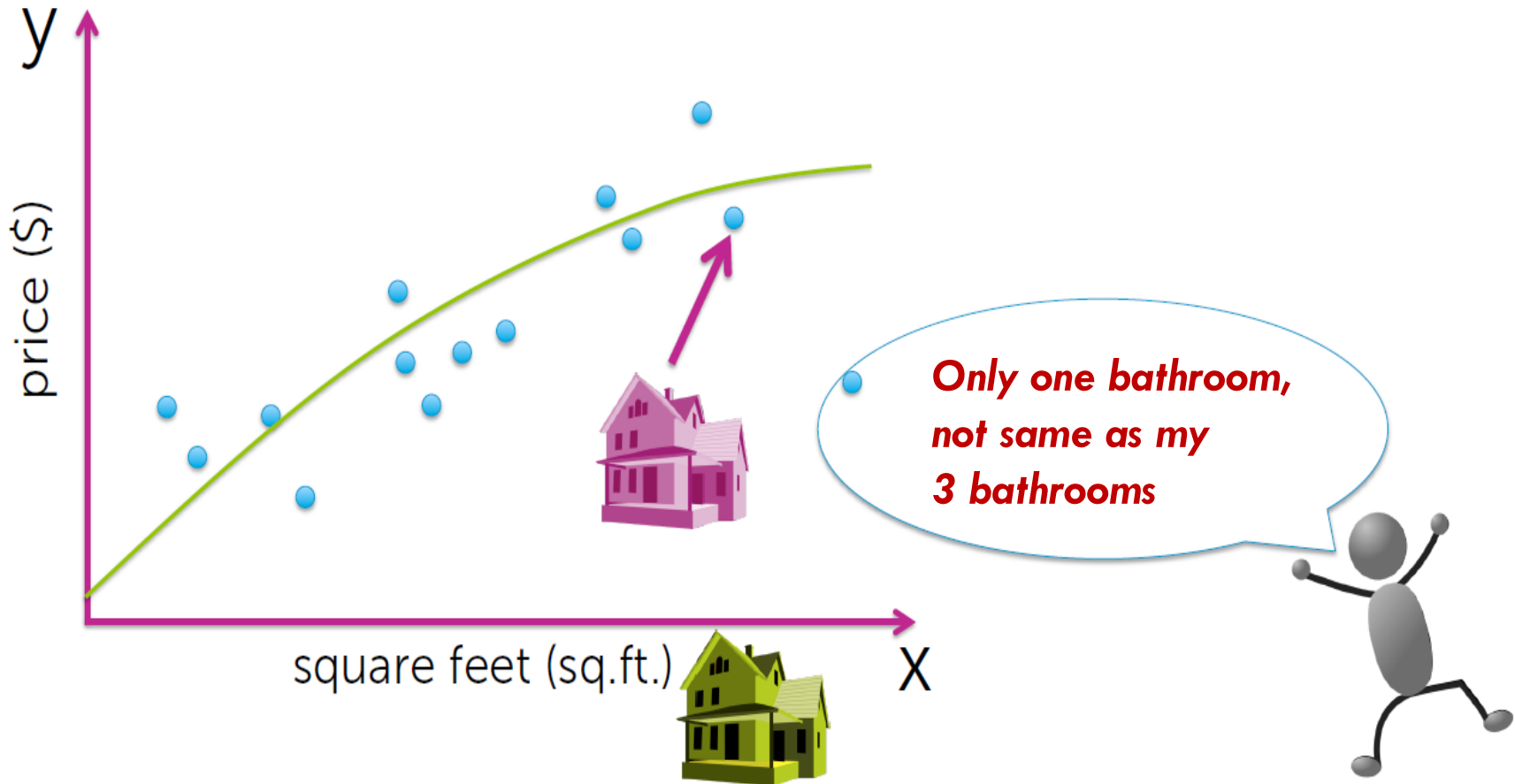
More realistic flow chart

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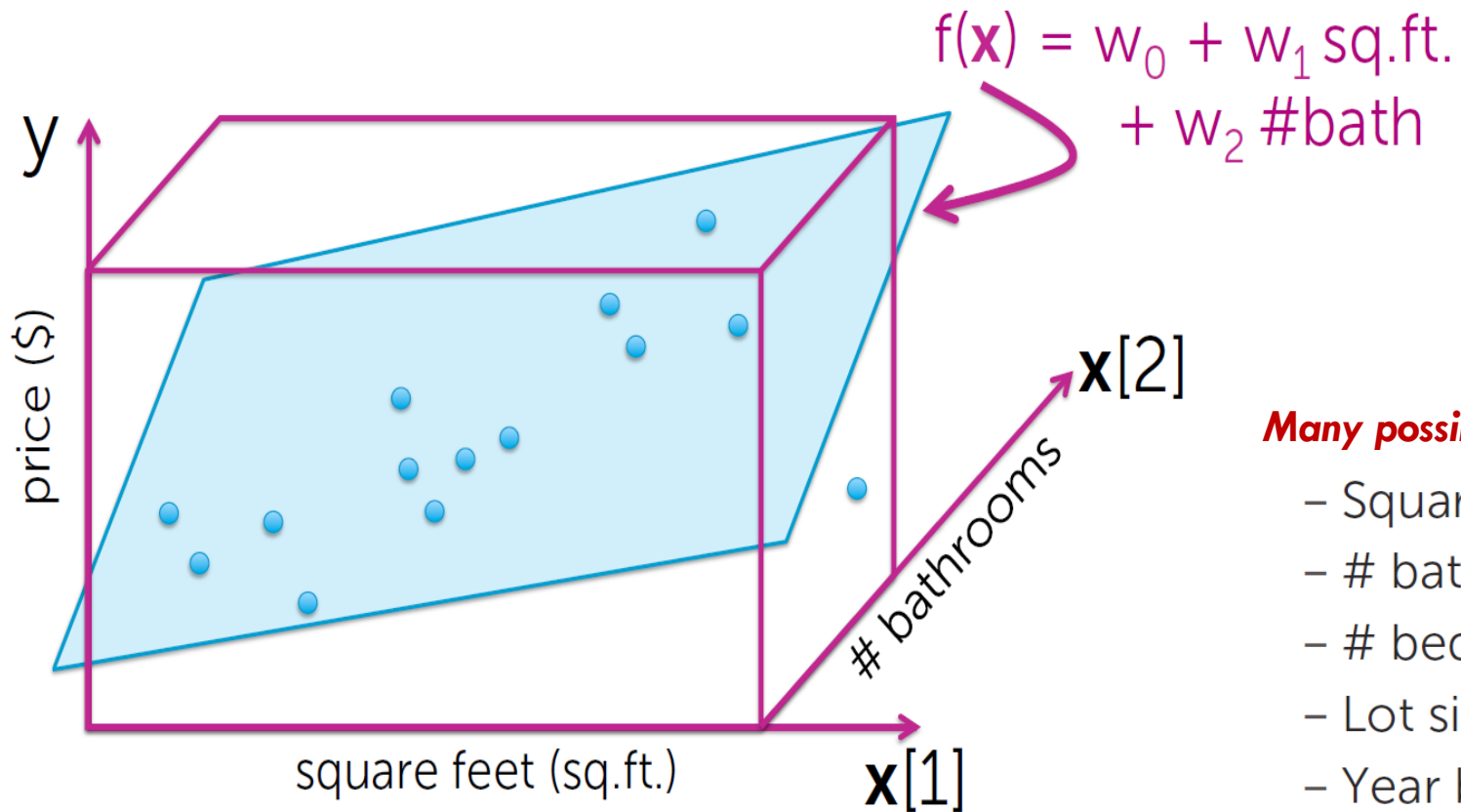
Incorporating multiple inputs

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Incorporating multiple inputs

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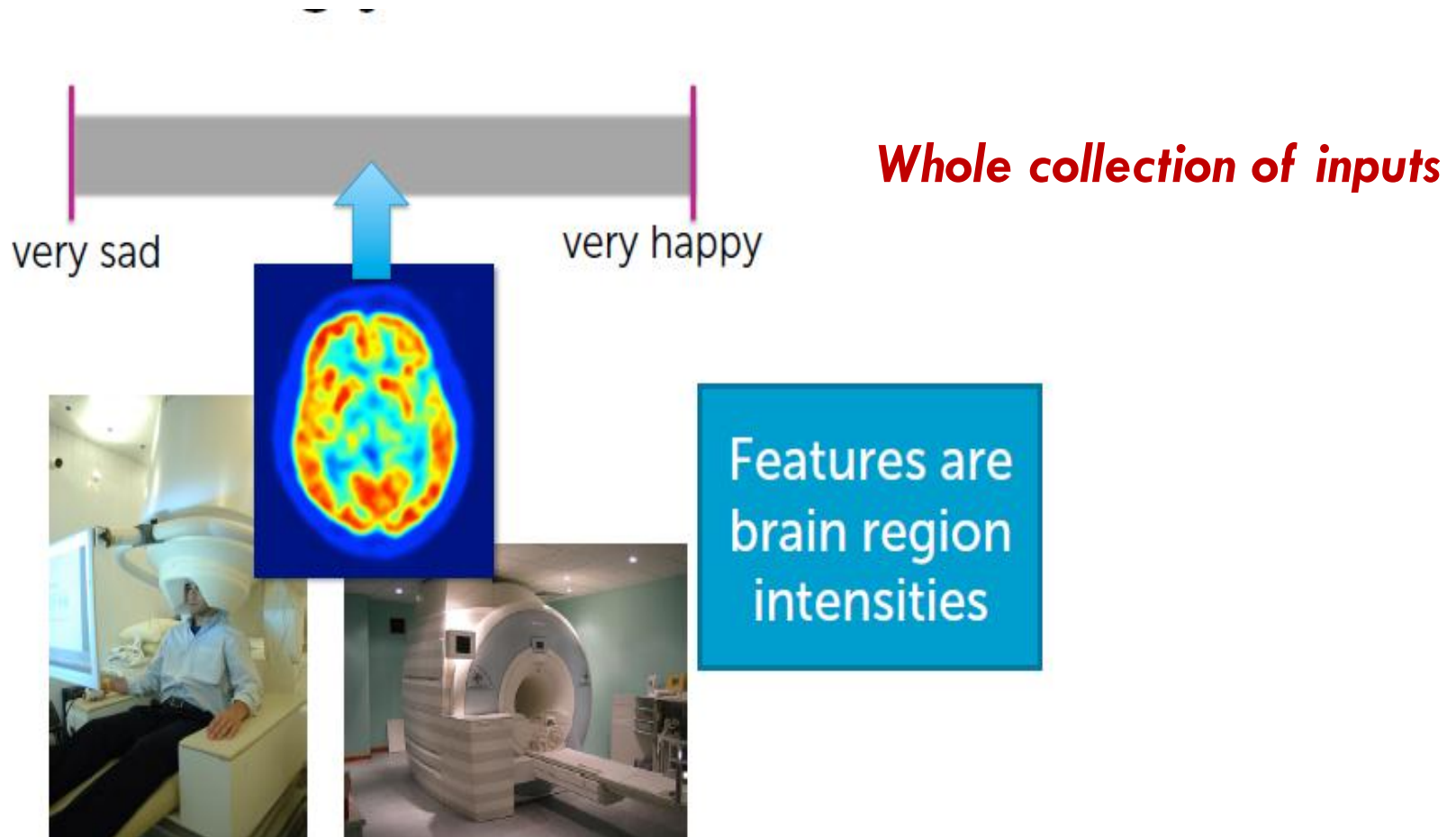
Many possible inputs

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

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Reading your brain

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General notation

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Output: y  scalar

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

 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

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Model:

Noise term



$$y_i = w_0 + w_1 \mathbf{x}_i[1] + \dots + w_d \mathbf{x}_i[d] + \epsilon_i$$

feature 1 = 1

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

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

...

feature $d+1$ = $\mathbf{x}[d]$... e.g., lot size

More generally: D-dimensional curve

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Model:

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

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

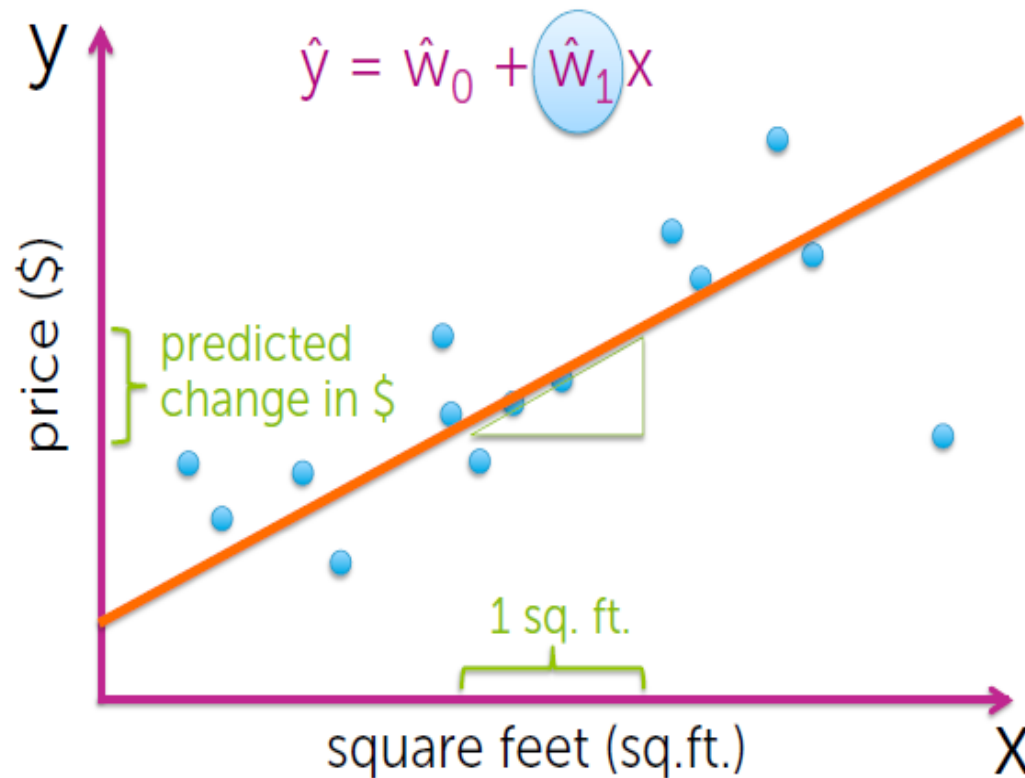
...

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

Interpreting coefficients

52

Simple linear regression



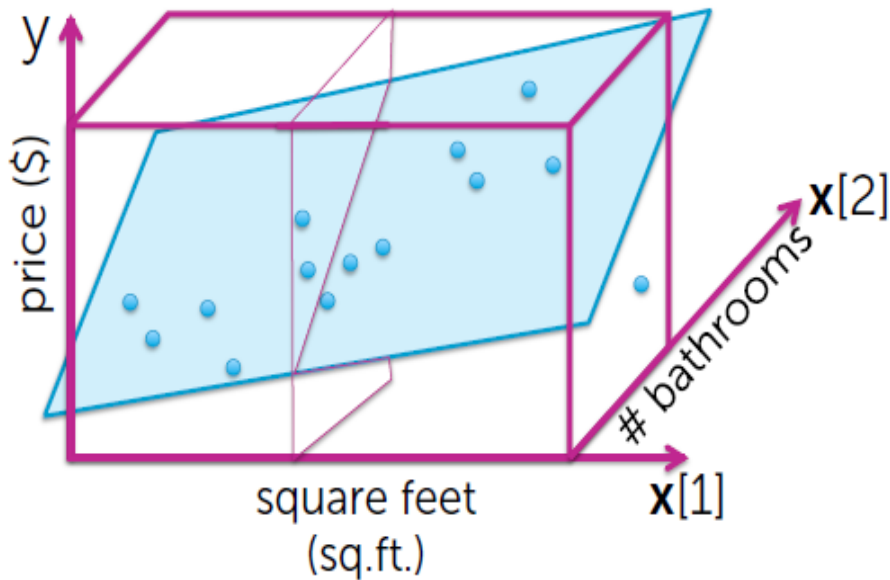
Interpreting coefficients

53

Two linear features

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

fix

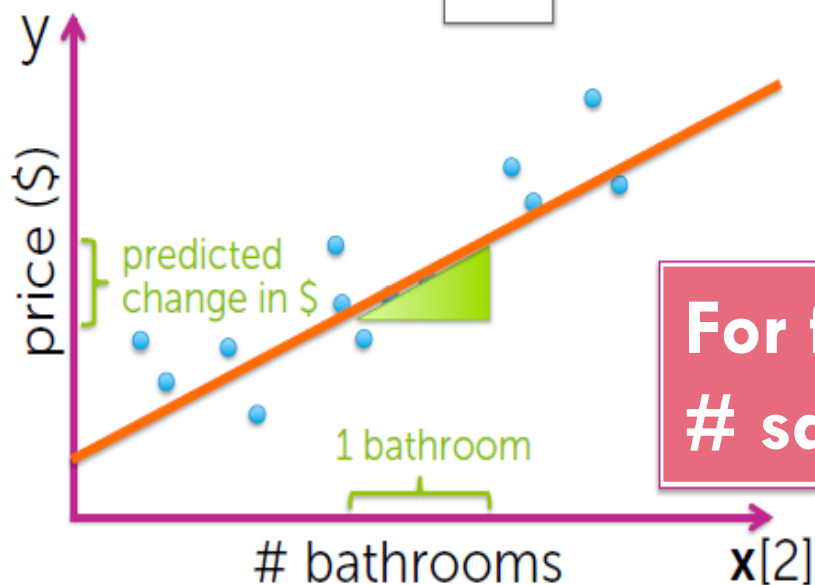


Interpreting coefficients

54

Two linear features

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



But...

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

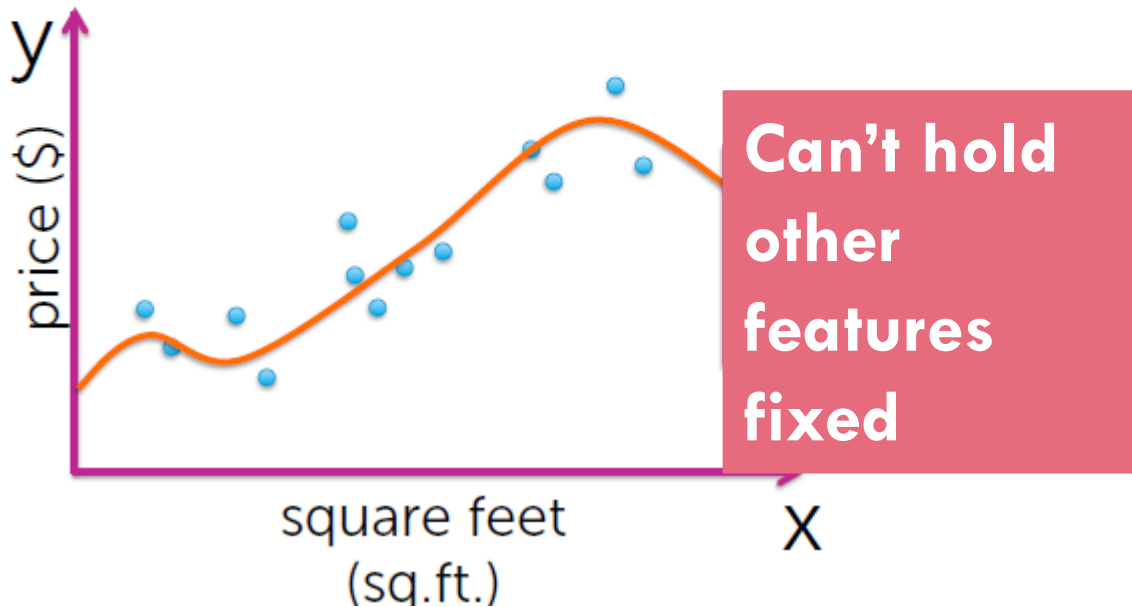
Think about interpretation.

Interpreting coefficients

55

Polynomial regression

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



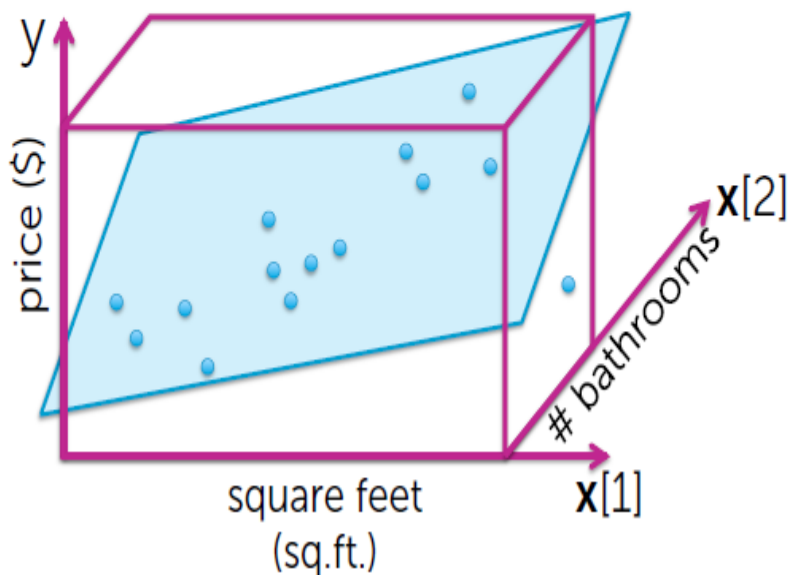
*Then ...
can't interpret
coefficients*

Interpreting coefficients

56

Multiple linear features

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



But...

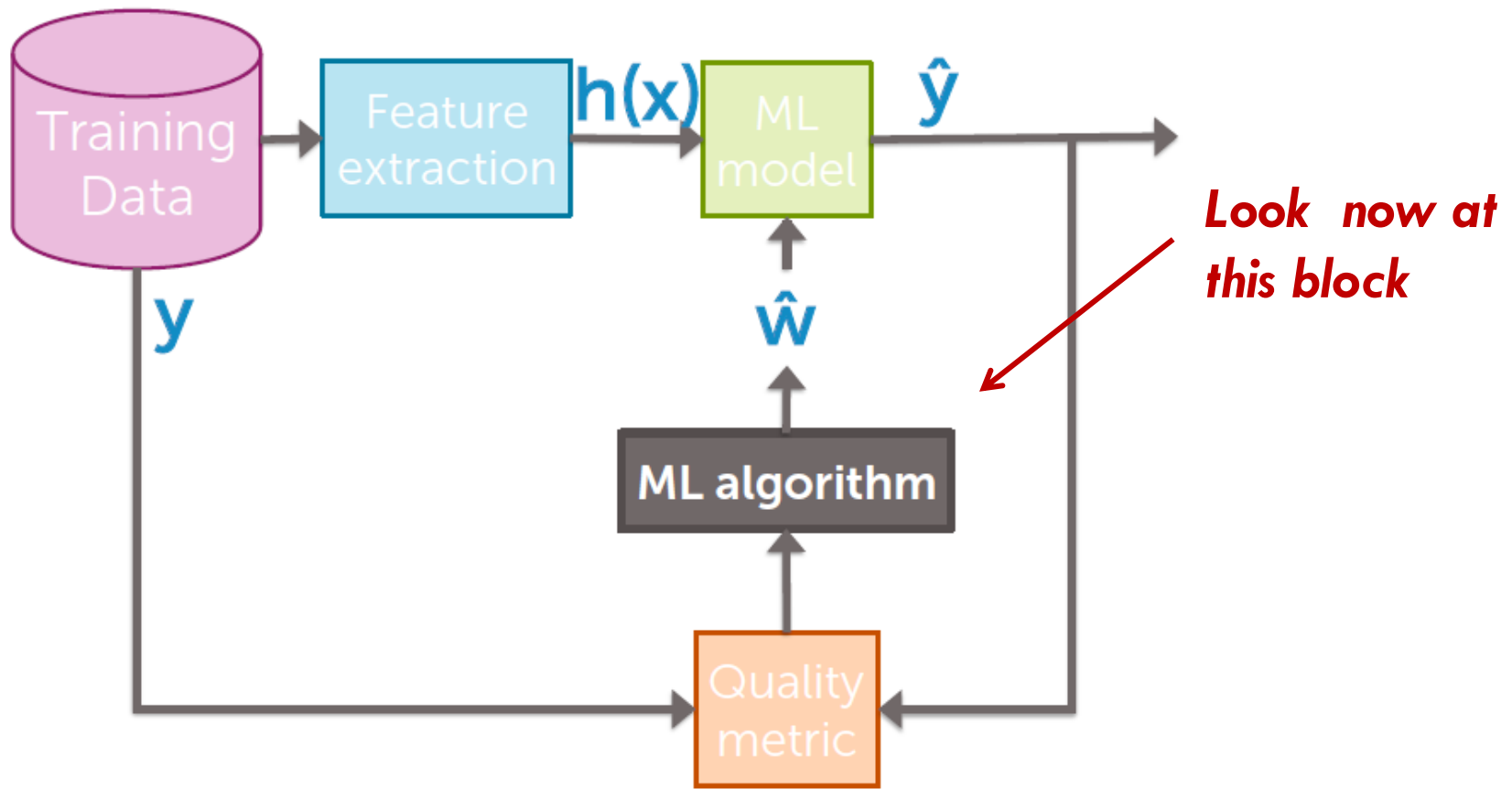
increasing #bedrooms for fixed #sq.ft will make your bedrooms smaller and smaller.

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-dimensions

57



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

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Rewriting in matrix notation

59

For all observations together

$Y = H W + \epsilon$

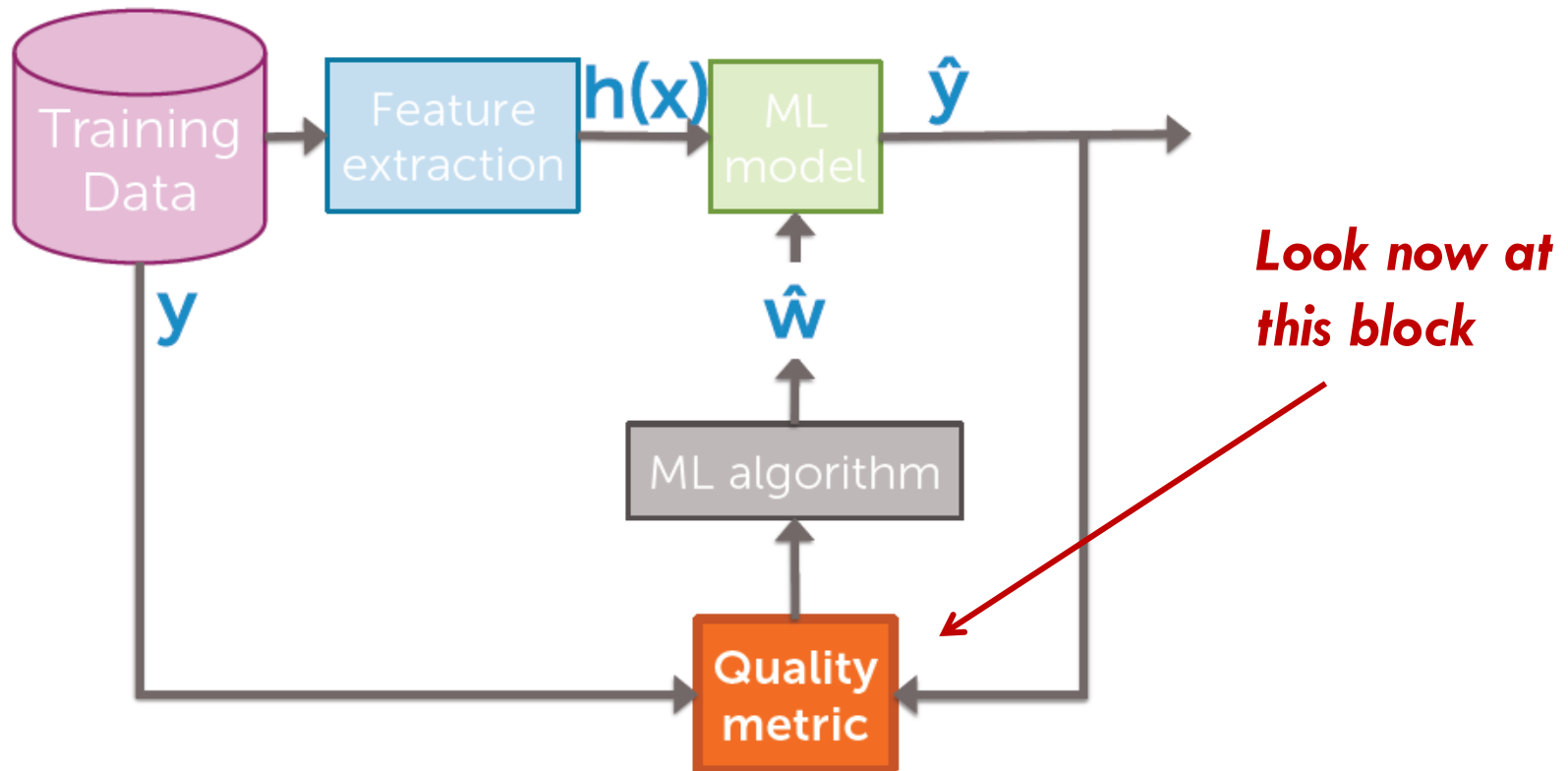
The diagram illustrates the matrix notation for a linear model across all observations. On the left, a pink vertical vector Y contains observations $y_1, y_2, y_3, \dots, y_N$. In the middle, a green grid H contains feature functions $h_0(x_1), h_1(x_1), h_2(x_1), \dots, h_D(x_1)$ for the first observation, and similar rows for subsequent observations up to $h_0(x_N), h_1(x_N), \dots, h_D(x_N)$. To the right of H is a blue vertical vector W containing weights $w_0, w_1, w_2, \dots, w_D$. Further right is a grey vertical vector ϵ containing error terms $\epsilon_1, \epsilon_2, \epsilon_3, \dots, \epsilon_N$. An equals sign is placed between Y and H , and a plus sign is placed between W and ϵ . A handwritten blue arrow points from $h_1(x_1)$ to the first row of the H matrix.

Here is our
ML algorithm

$\Rightarrow \boxed{Y = H W + \epsilon}$

Fitting in D-dimensions

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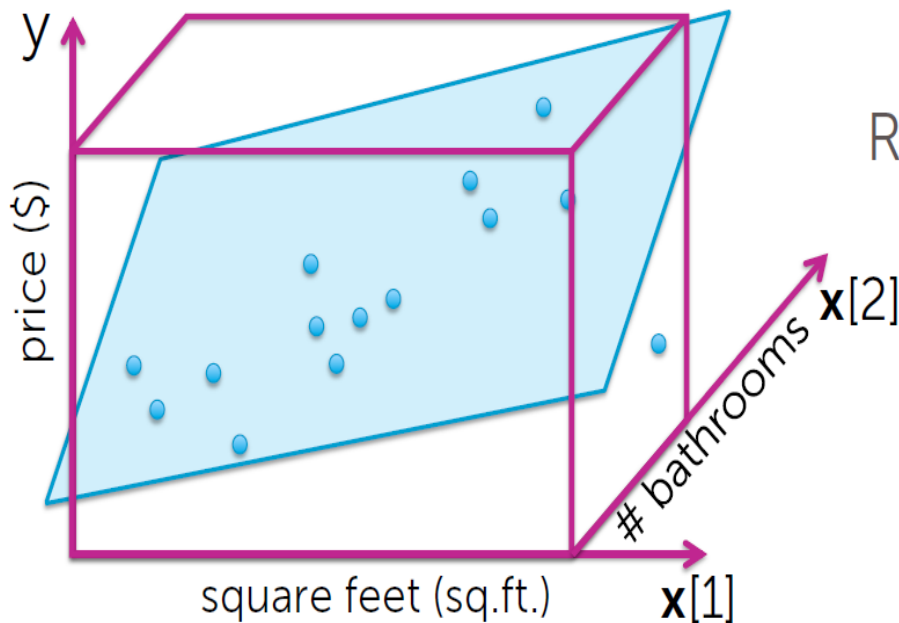
Machine Learning Specialization

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Cost function in D-dimension

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RSS in vector notation



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

Diagram illustrating the vector notation for the hypothesis function \hat{y}_i :

$\hat{y}_i =$ [$h_0(x_i)$ $h_1(x_i)$ \dots $h_D(x_i)$] \cdot w

The vector w is shown as a column vector with elements $w_0, w_1, w_2, \dots, w_D$.

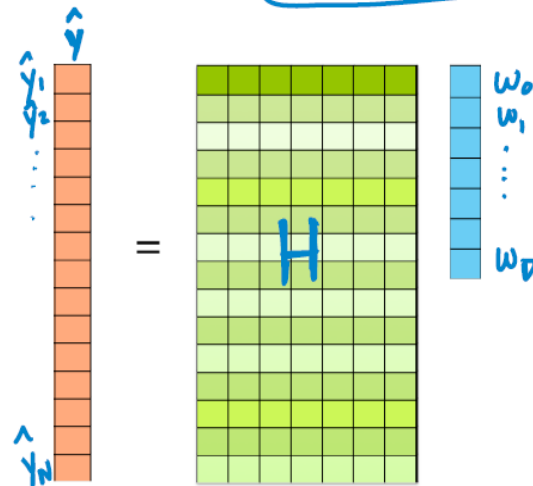
Cost function in D-dimension

62

RSS in matrix notation

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

Why? (part 1)



$$\hat{\mathbf{y}} = \mathbf{H}\mathbf{w}$$


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

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

Regression model for D-dimension

63

RSS in matrix notation

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


Why? (part 2)

residual ₁	residual ₂	residual ₃	...	residual _N
residual ₁	residual ₂	residual ₃	...	residual _N

$$\begin{aligned} &= (\text{residual}_1^2 + \text{residual}_2^2 + \dots + \text{residual}_N^2) \\ &= \sum_{i=1}^N \text{residual}_i^2 \\ &\triangleq \text{RSS}(\mathbf{w}) \end{aligned}$$

Regression model for D-dimension

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Gradient of RSS

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

Why? By analogy to 1D case:

$$\begin{aligned}\frac{d}{dw} (y-hw)(y-hw) &= \frac{d}{dw} (y-hw)^2 = 2 \cdot (y-hw)' (-h) \\ &= -2h(y-hw)\end{aligned}$$

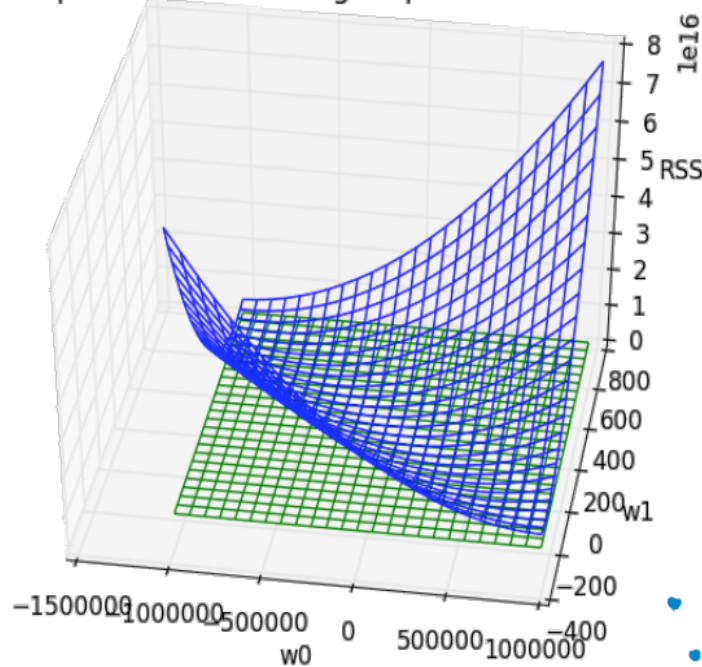
Scalars

Regression model for D-dimension

65

Approach 1: set gradient to zero

3D plot of RSS with tangent plane at minimum



Closed form solution

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

Solve for \mathbf{w} :

$$-\cancel{2}\mathbf{H}^T\mathbf{y} + \cancel{2}\mathbf{H}^T\mathbf{H}\hat{\mathbf{w}} = 0$$

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

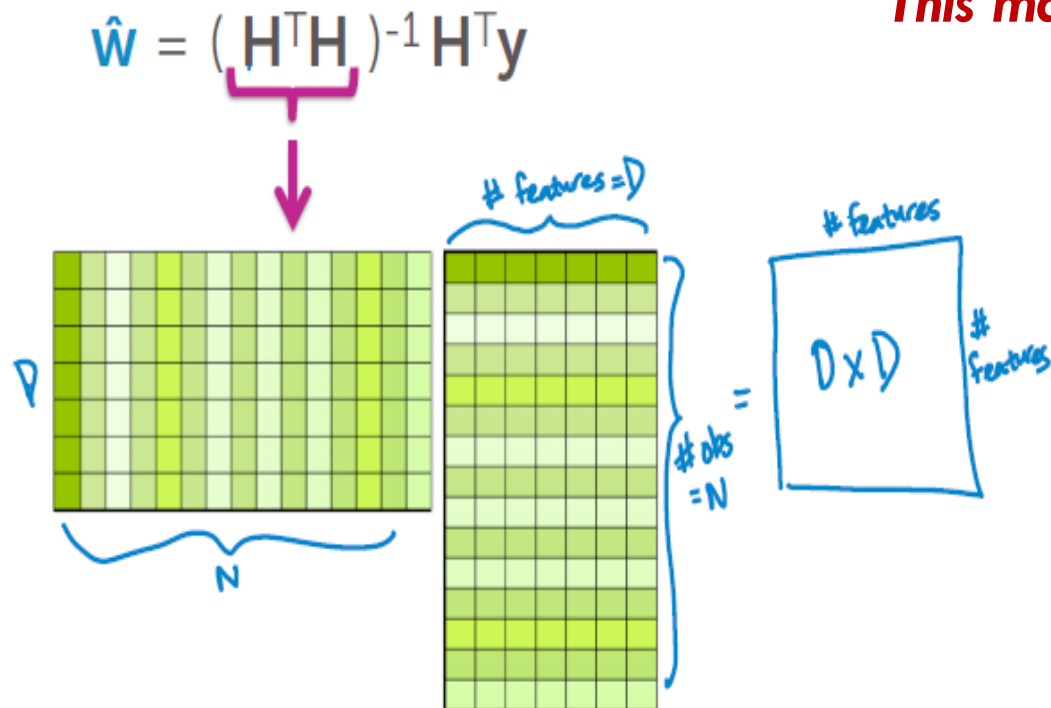
$$\underbrace{(\mathbf{H}^T\mathbf{H})^{-1}}_{\mathbf{I}} \mathbf{H}^T\mathbf{H}\hat{\mathbf{w}} = (\mathbf{H}^T\mathbf{H})^{-1}\mathbf{H}^T\mathbf{y}$$

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

$$\begin{aligned} \bullet \mathbf{A}^{-1}\mathbf{A} &= \mathbf{I} \\ \bullet \mathbf{I}\mathbf{v} &= \mathbf{v} \\ \bullet \mathbf{I}\mathbf{v} &= \mathbf{v} \end{aligned}$$

Closed-form solution

66



This matrix might not be invertible.

Invertible if:
In most cases is $N > D$

really,
of linearly
ind. observations
↓

Complexity of inverse:

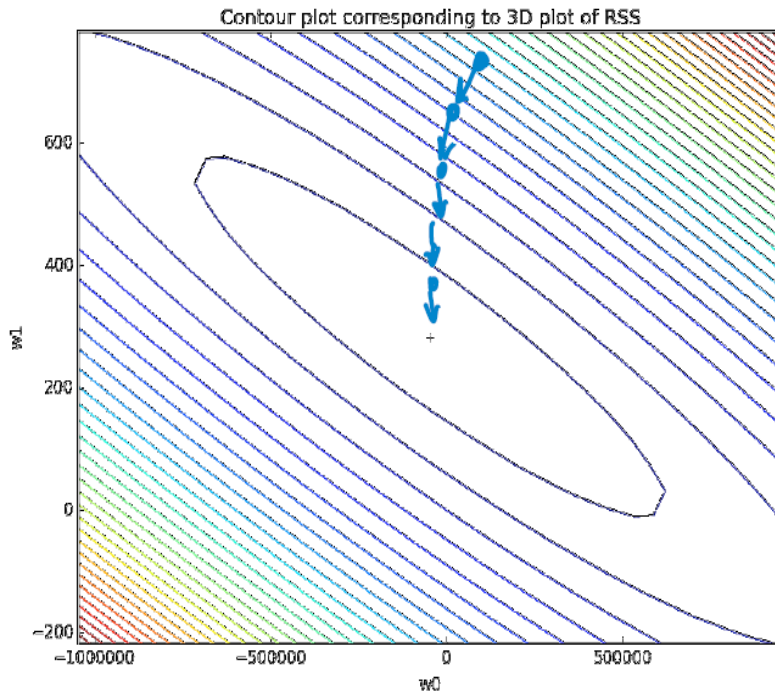
$$O(D^3)$$

This might not be CPU feasible.

Regression model for D-dimension

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Approach 2: gradient descent



We initialise our solution somewhere and then ...

while not converged

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

Gradient descent

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

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

Partial with respect to w_j

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

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

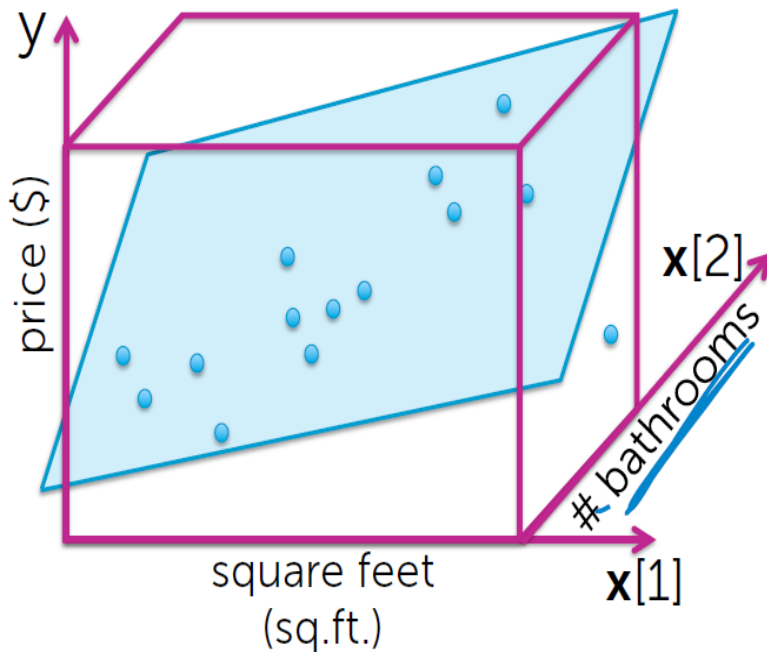
Update to j^{th} feature weight:

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

Regression model for D-dimension

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Interpreting elementwise



Update to ^{# bathrooms} j^{th} feature weight:

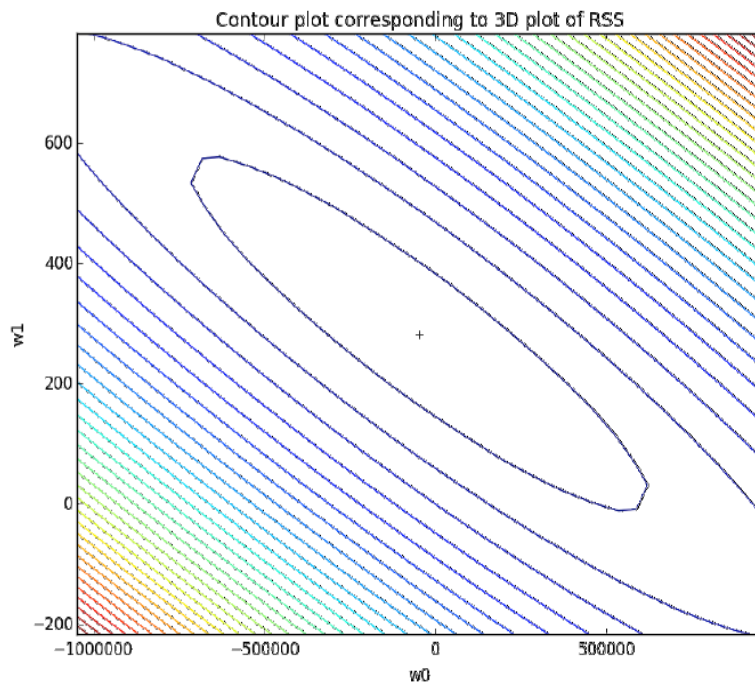
$$w_j^{(t+1)} \leftarrow w_j^{(t)} + 2\eta \sum_{i=1}^N \underbrace{h_j(\mathbf{x}_i)}_{\substack{\# \text{ bath for} \\ \text{house } i}} (y_i - \hat{y}_i(\mathbf{w}^{(t)}))$$

If underestimating impact of # bath ($\hat{w}_j^{(t)}$ is too small)
then $(y_i - \hat{y}_i(\mathbf{w}^{(t)}))$ on average
weighted by # bath will be positive
 $\Rightarrow w_j^{(t+1)} > w_j^{(t)}$ (increase)

Summary of gradient descent

70

Extremely useful algorithm in several applications



```
init  $\mathbf{w}^{(1)} = \mathbf{0}$  (or randomly, or smartly),  $t = 1$   
while  $\|\nabla \text{RSS}(\mathbf{w}^{(t)})\| > \epsilon$   
    for  $j = 0, \dots, D$   
         $\text{partial}[j] = -2 \sum_{i=1}^N h_j(\mathbf{x}_i)(y_i - \hat{y}_i(\mathbf{w}^{(t)}))$   
         $\mathbf{w}_j^{(t+1)} \leftarrow \mathbf{w}_j^{(t)} - \eta \text{partial}[j]$   
     $t \leftarrow t + 1$ 
```

Handwritten notes:
- A blue arrow points from the ϵ in the while loop to the word "tolerance".
- A blue arrow points from the norm symbol $\|\cdot\|$ to the expression $\sqrt{\text{partial}[0]^2 + \dots + \text{partial}[D]^2}$.

What you can do now

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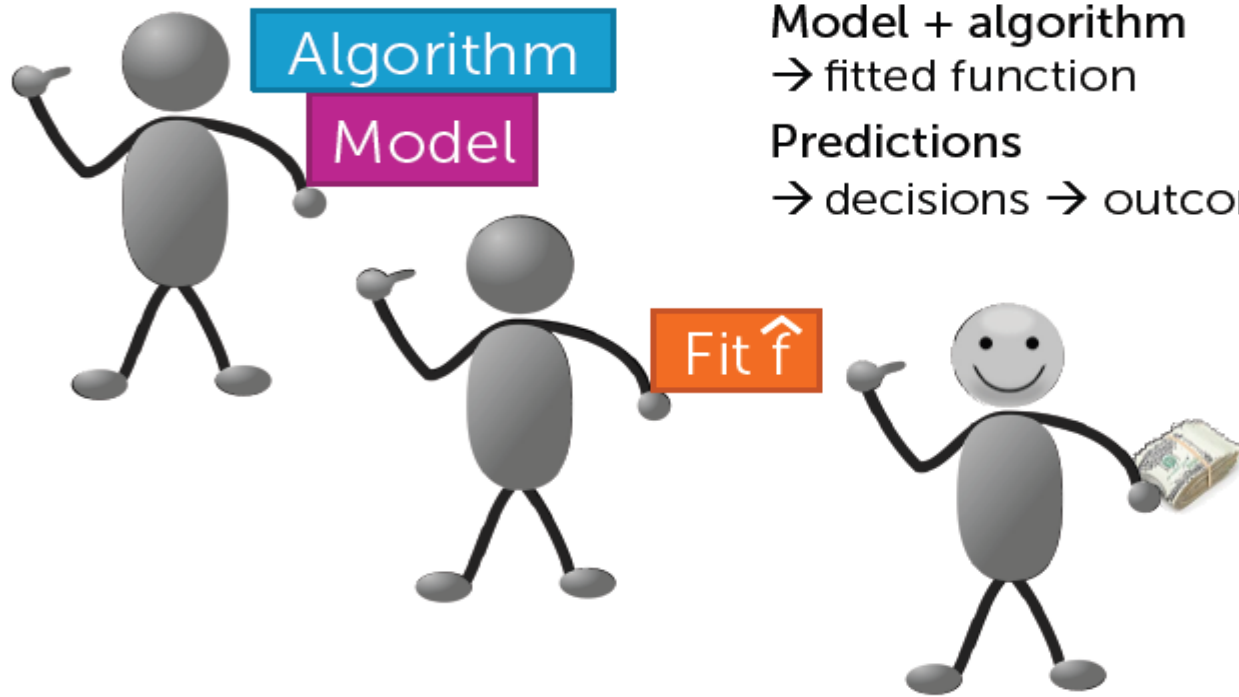
- Describe polynomial regression
- Detrend a time series using trend and seasonal components
- Write a regression model using multiple inputs or features thereof
- Cast both polynomial regression and regression with multiple inputs as regression with multiple features
- Calculate a goodness-of-fit metric (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

73

Make predictions, get \$, right??



Assessing performance

74

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: $\text{Loss} = 0$

My predictions: $\text{Loss} = ???$

Measuring loss

75

“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:

Cost of using \hat{w} at x
when y is true

$L(y, f_{\hat{w}}(\mathbf{x}))$

actual value $\hat{f}(\mathbf{x}) = \text{predicted value } \hat{y}$

Examples:

(assuming loss for underpredicting = overpredicting)

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

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

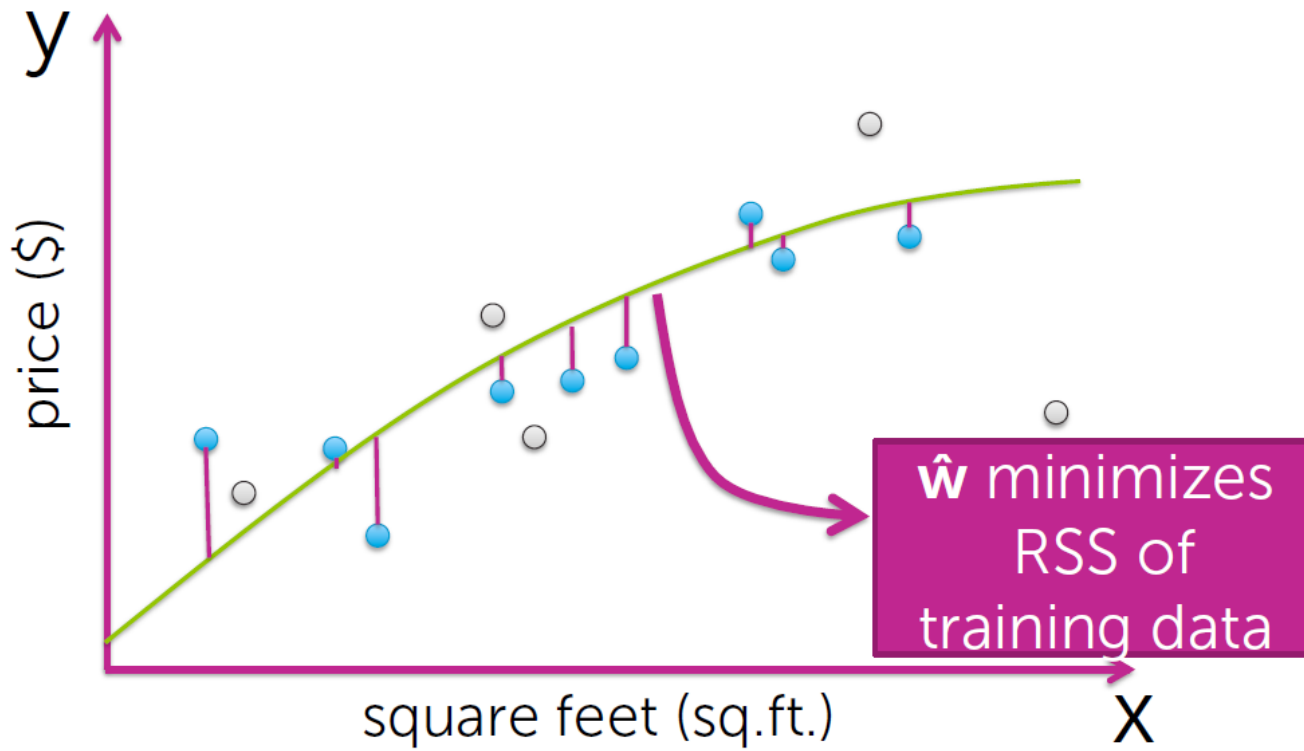
Symmetric loss functions



Accessing the loss

76

Use training data



Compute training error

77

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

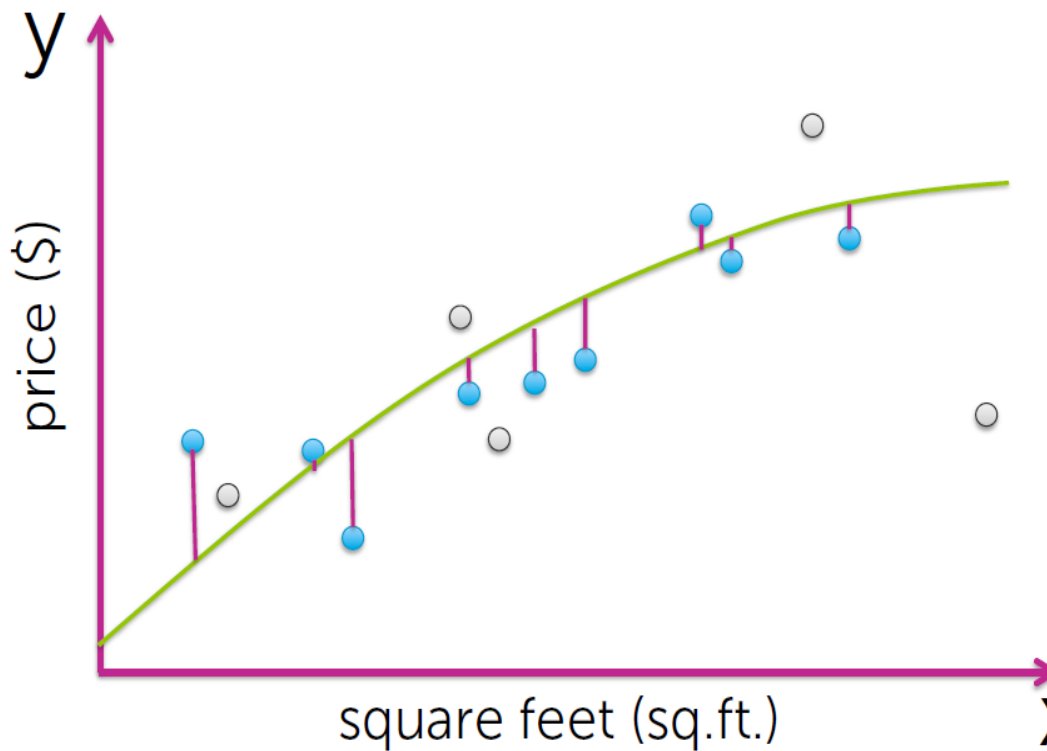
$$= \frac{1}{N} \sum_{i=1}^N L(y_i, f_{\hat{\mathbf{w}}}(\mathbf{x}_i))$$

 fit using training data

Training error

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



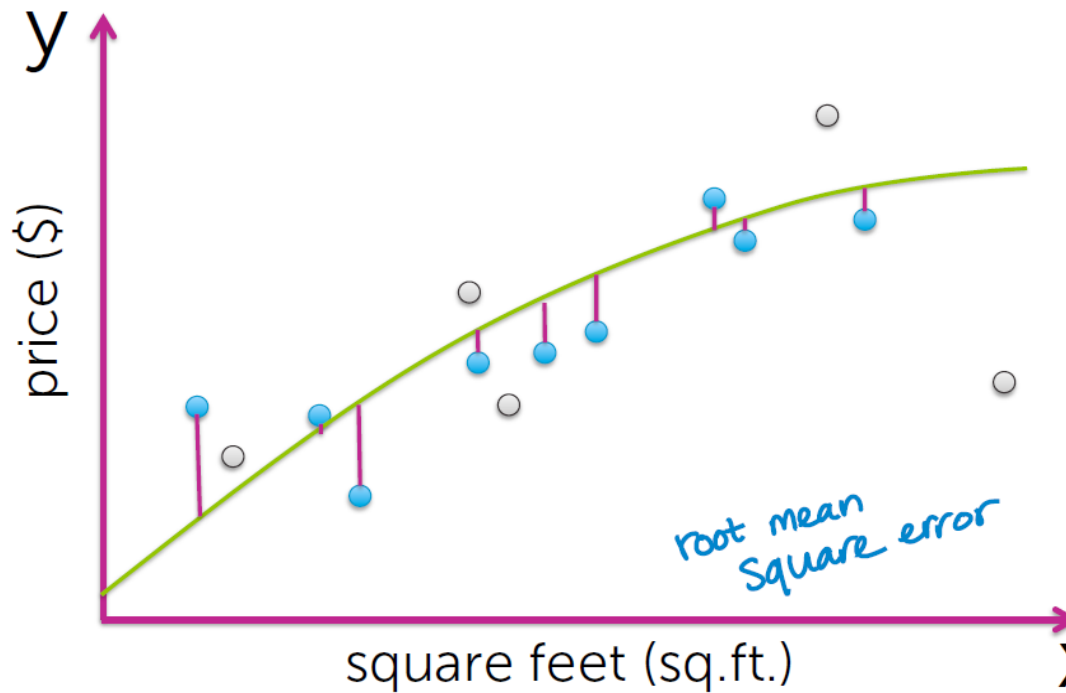
Convention is to take average here

Training error ($\hat{\mathbf{w}}$) = $1/N * [(\$_{\text{train } 1} - f_{\hat{\mathbf{w}}}(\text{sq.ft.}_{\text{train } 1}))^2 + (\$_{\text{train } 2} - f_{\hat{\mathbf{w}}}(\text{sq.ft.}_{\text{train } 2}))^2 + (\$_{\text{train } 3} - f_{\hat{\mathbf{w}}}(\text{sq.ft.}_{\text{train } 3}))^2 + \dots \text{include all training houses}]$

Training error

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More intuitive is to take RMSE, same units as y



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

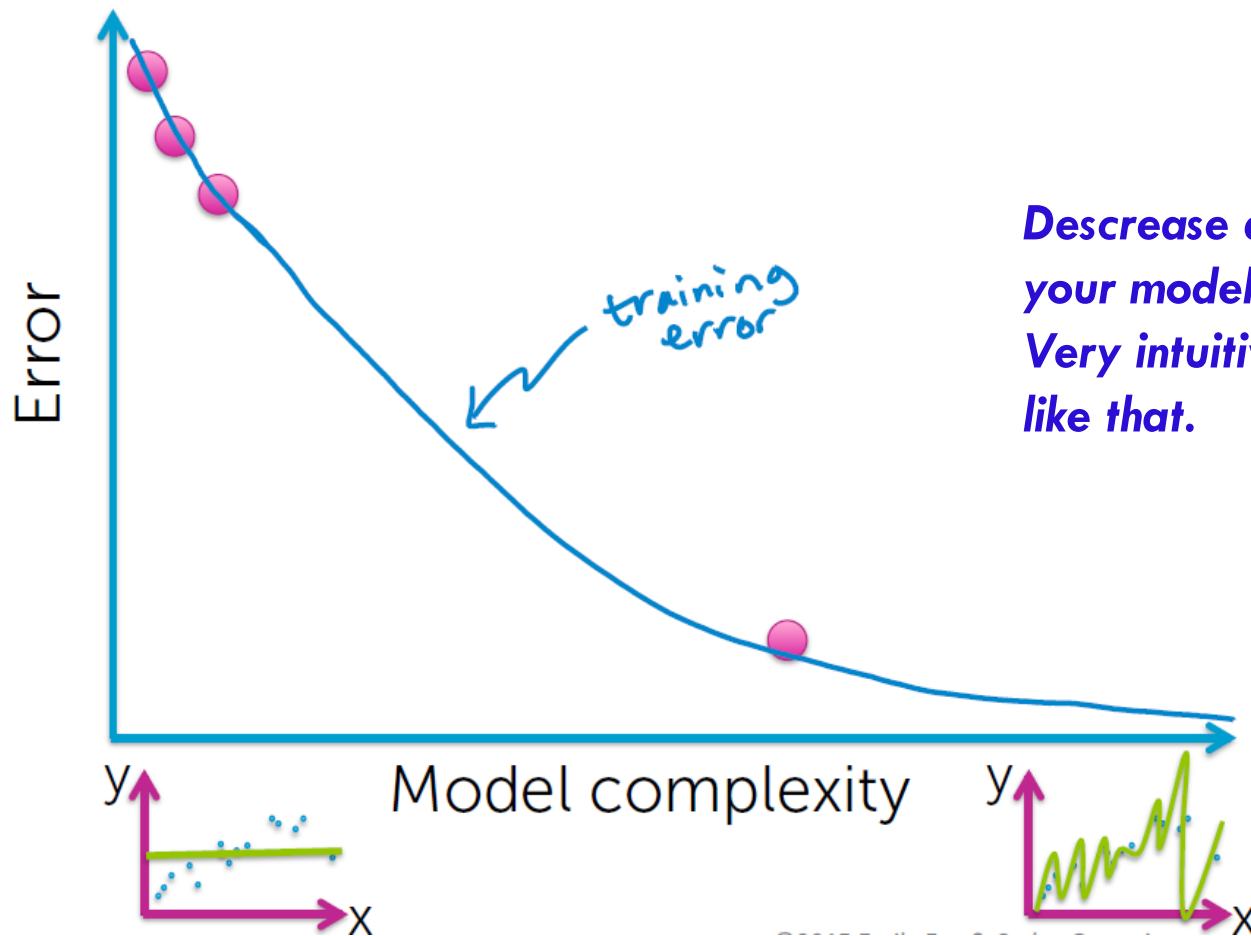
$$\frac{1}{N} \sum_{i=1}^N (y_i - f_{\hat{\mathbf{w}}}(\mathbf{x}_i))^2$$

RMSE =

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

Training error vs. model complexity

80

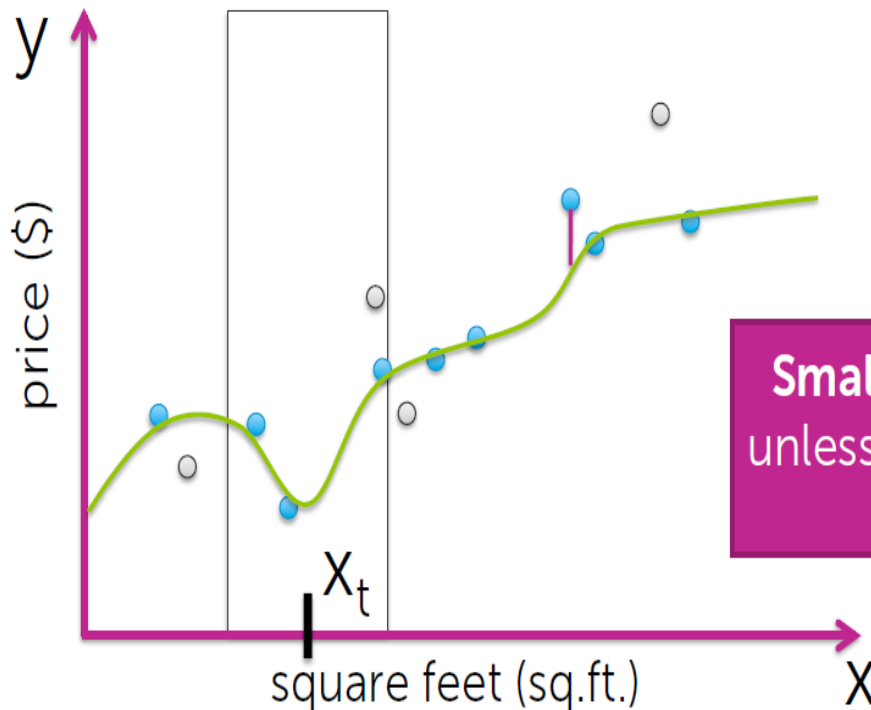


*Decrease as you increase
your model complexity.
Very intuitive why it is
like that.*

Is training error a good measure?

81

Issue: Training error is overly optimistic
because \hat{w} was fit to training data





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

Small training error \neq good predictions
unless training data includes everything you might ever see

Generalisation (true) error

82

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

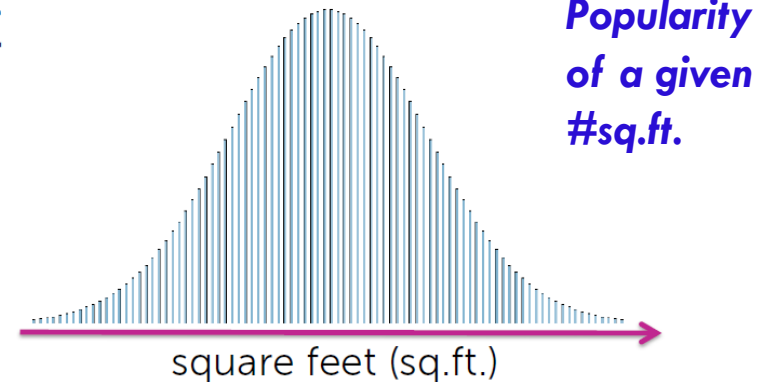


Lots of houses
in neighborhood,
but not in dataset

Distribution over house

83

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



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



Generalisation error definition

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

Formally:

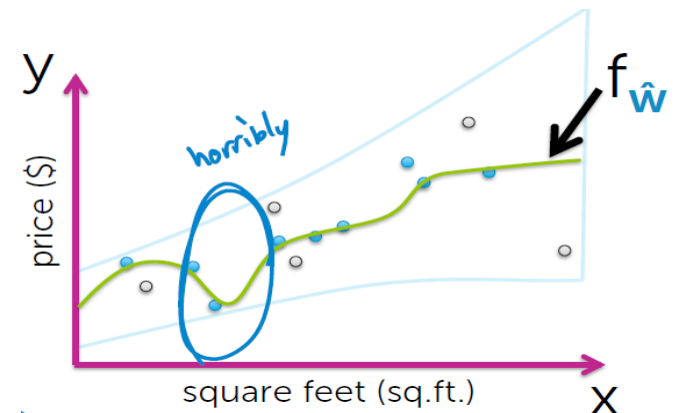
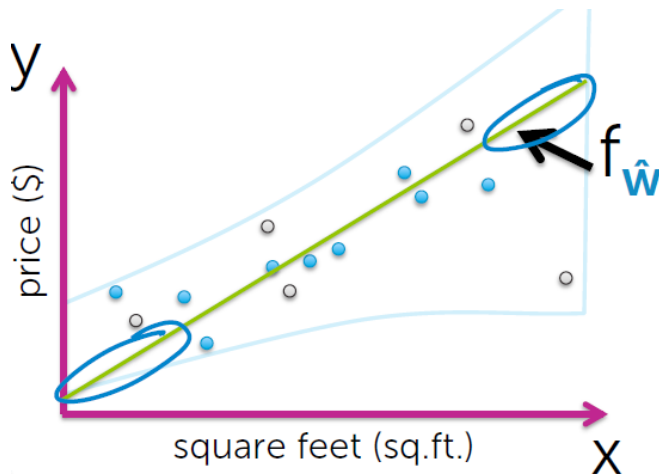
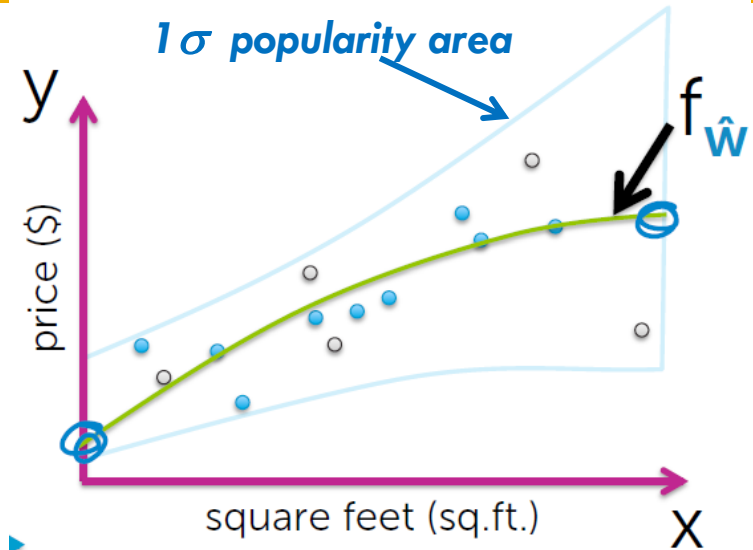
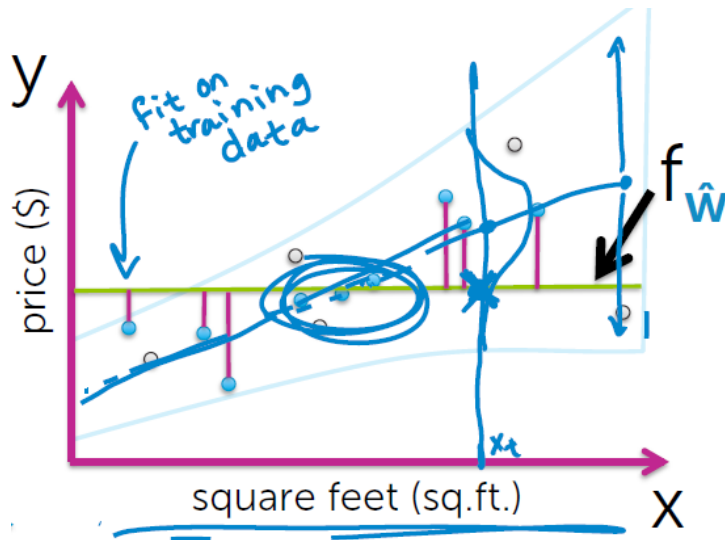
average over all possible
(\mathbf{x}, y) pairs weighted by
how likely each is

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

fit using training data

Generalisation error (weighted with popularity) vs model complexity

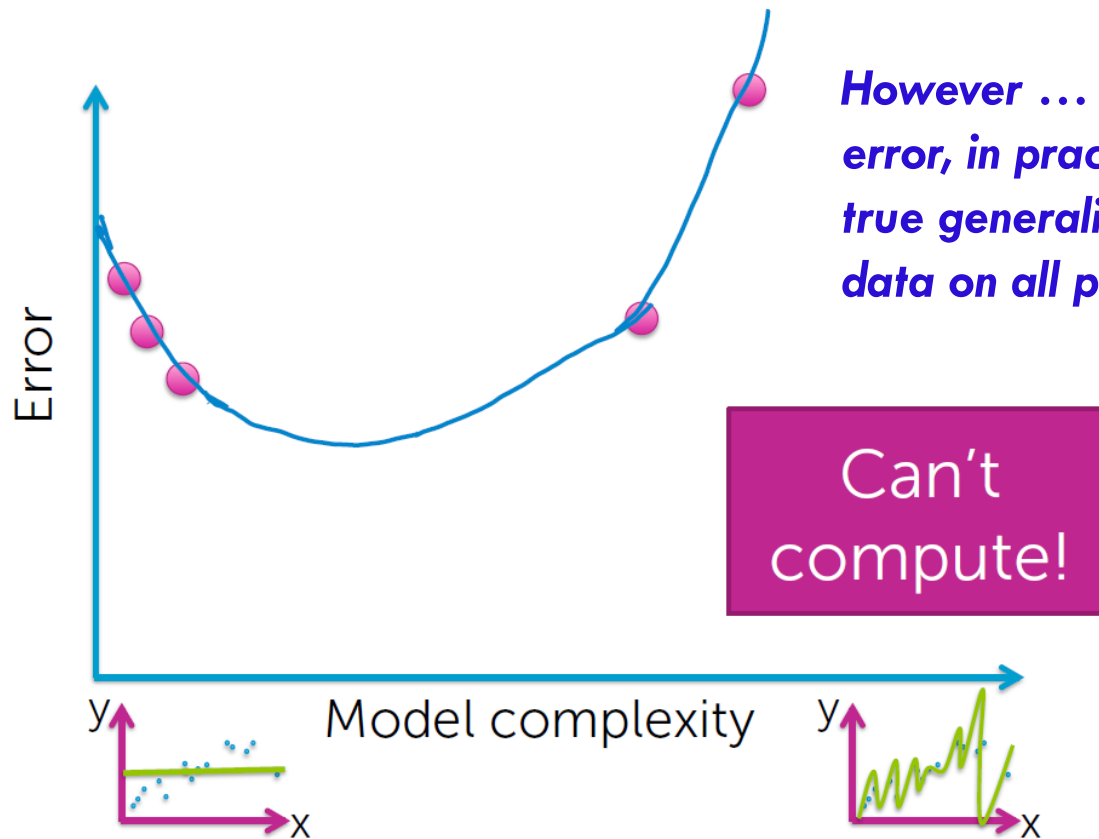
85



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Generalisation error vs model complexity

86



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.

Can't
compute!

Forming a test set

87

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

88

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

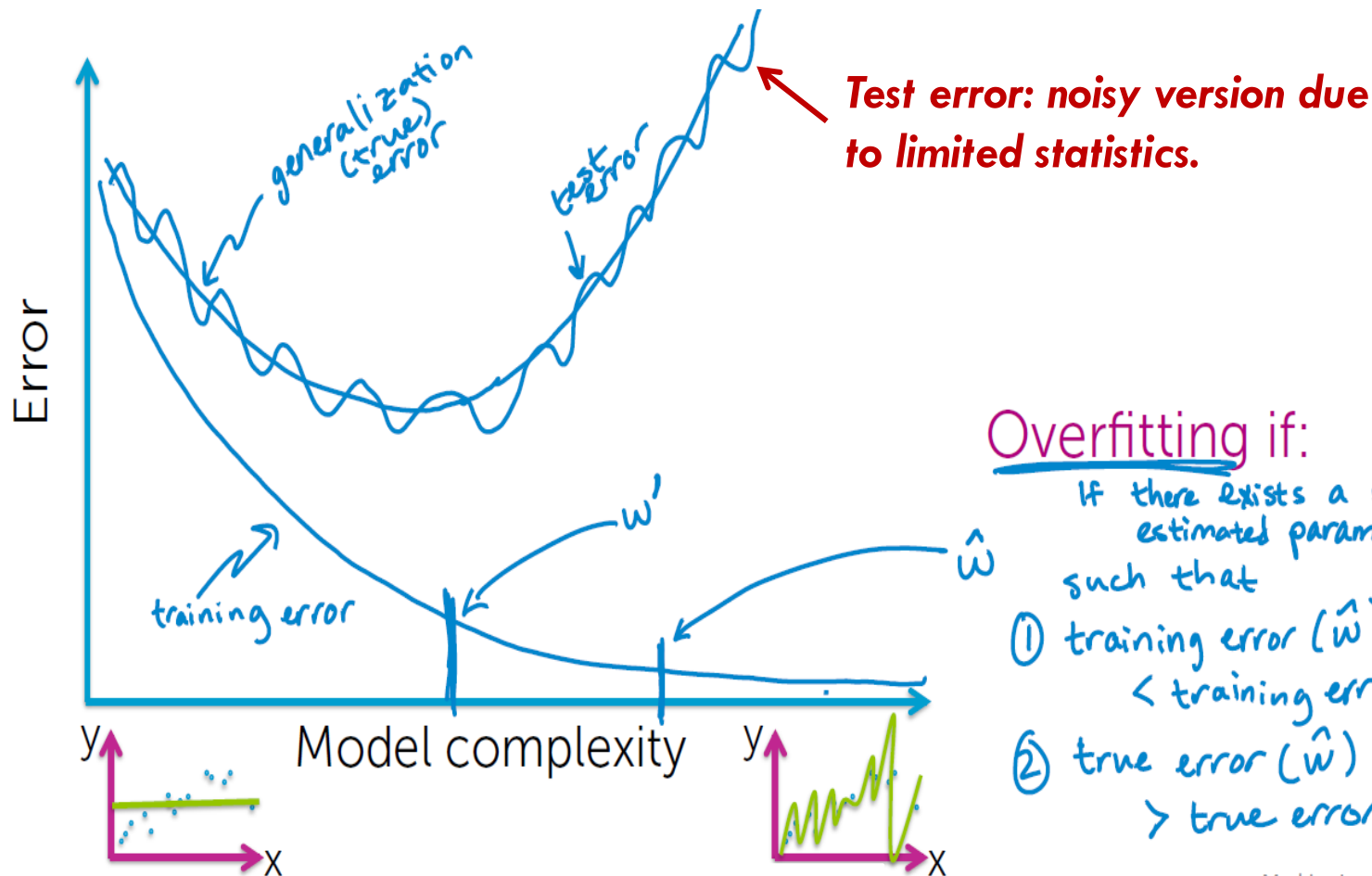


fit using training data

**has never seen
test data!**

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

89



Training/test splits

90



↑
Too few $\rightarrow \hat{w}$ poorly estimated



↑
Too few \rightarrow 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

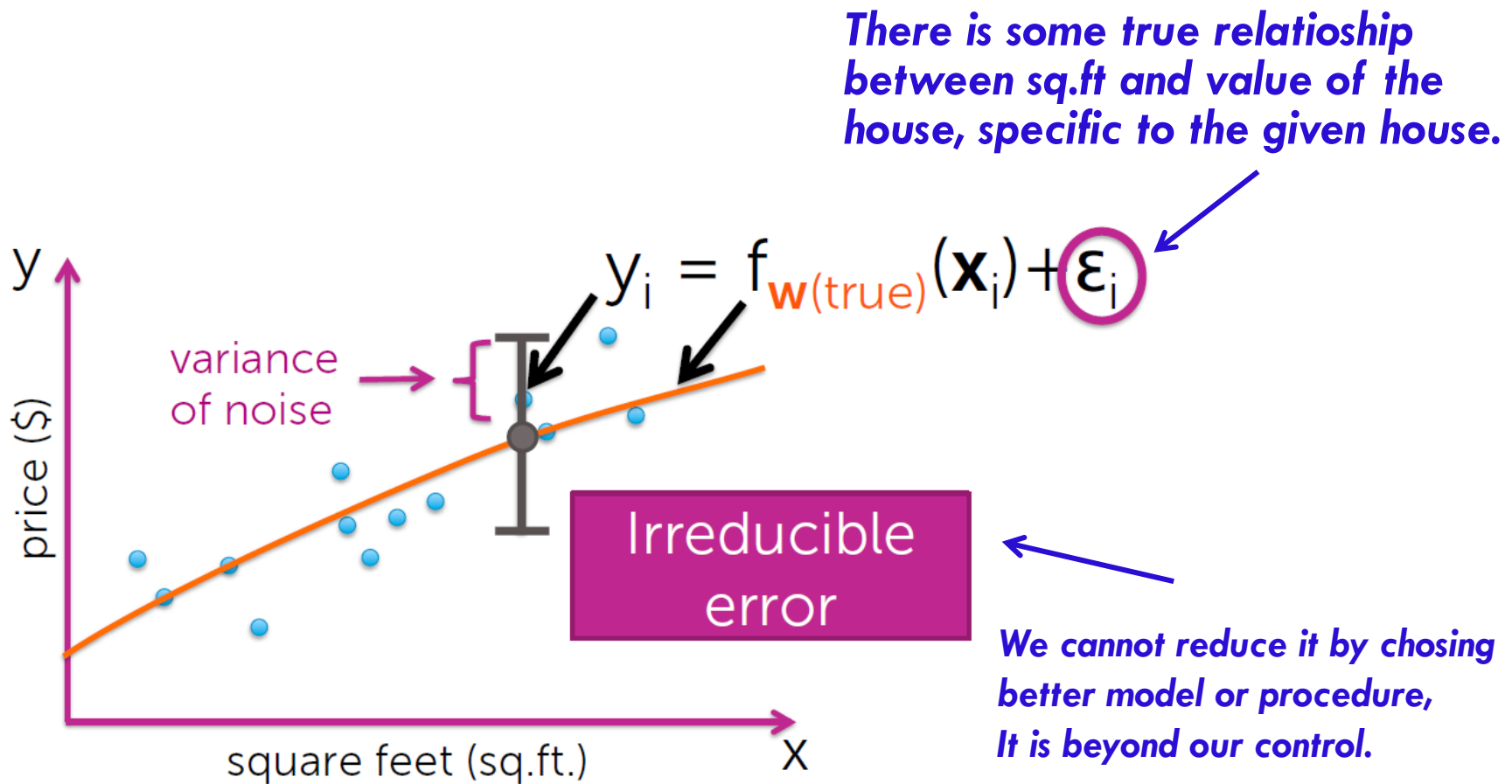
91

In forming predictions, there are 3 sources of error:

1. Noise
2. Bias
3. Variance

Data are inherently noisy

92

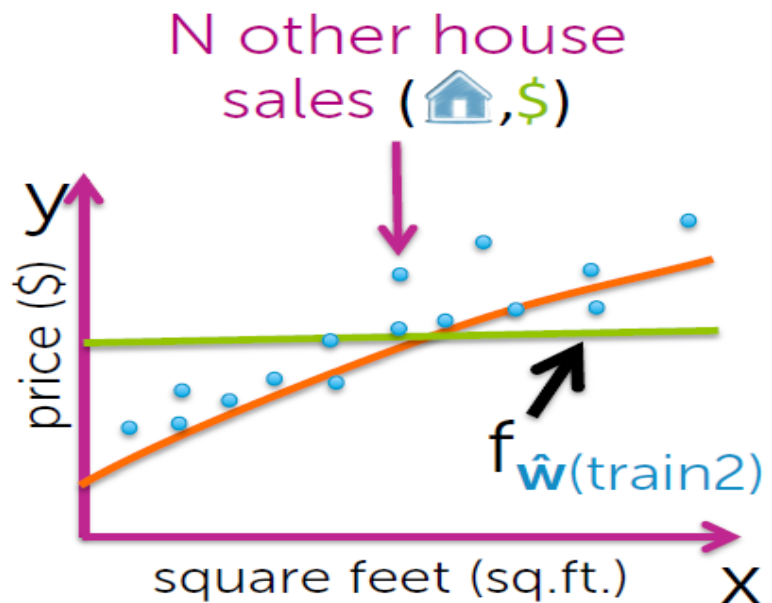
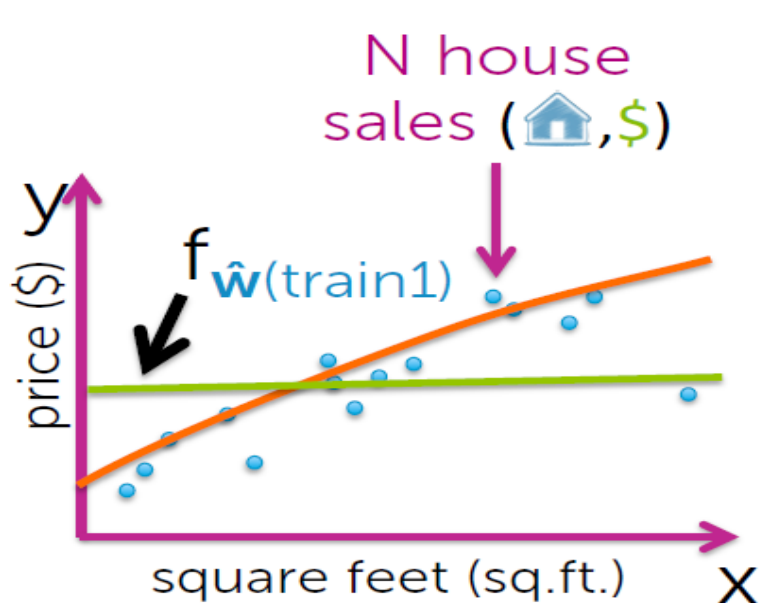


Bias contribution

93

This contribution we can control.

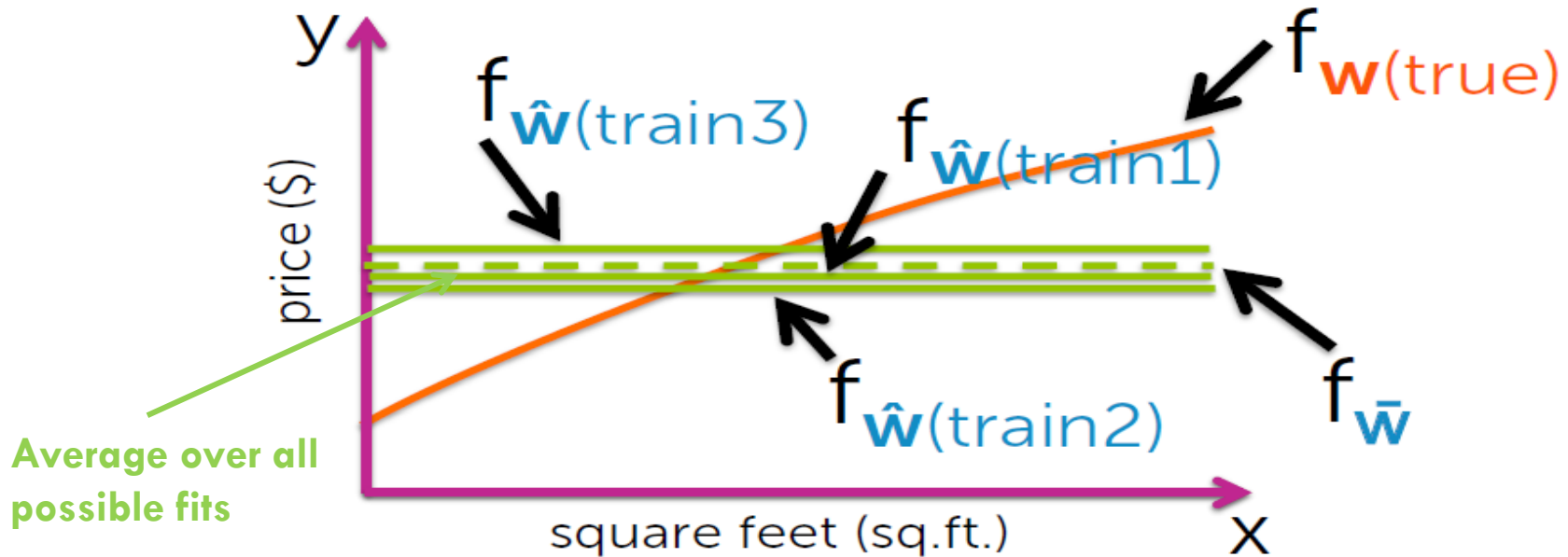
Assume we fit a constant function



Bias contribution

94

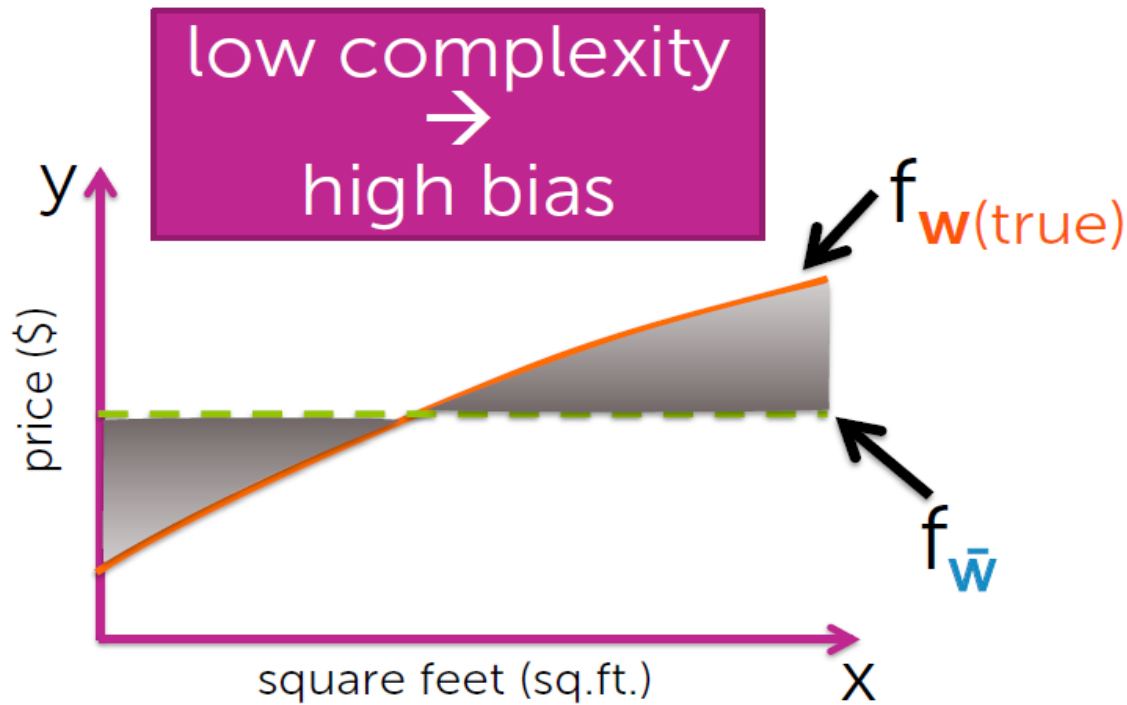
Over all possible size N training sets, what do I expect my fit to be?



Bias contribution

95

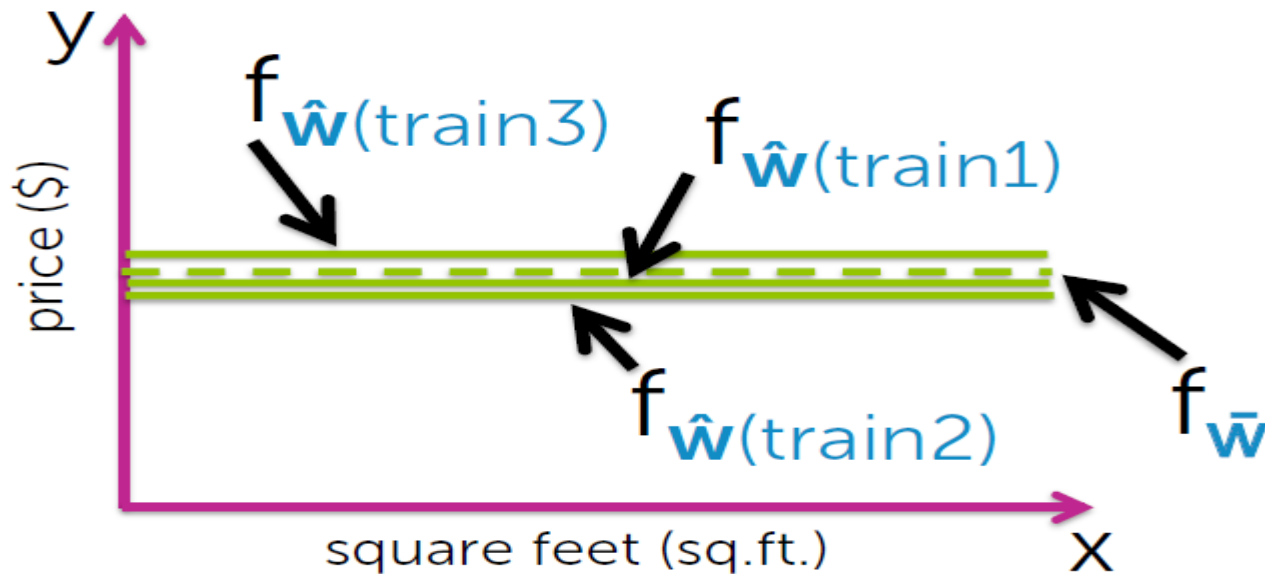
$\text{Bias}(\mathbf{x}) = f_{\mathbf{w}(\text{true})}(\mathbf{x}) - f_{\bar{\mathbf{w}}}(\mathbf{x})$ ← Is our approach flexible enough to capture $f_{\mathbf{w}(\text{true})}$?
If not, error in predictions.



Variance contribution

96

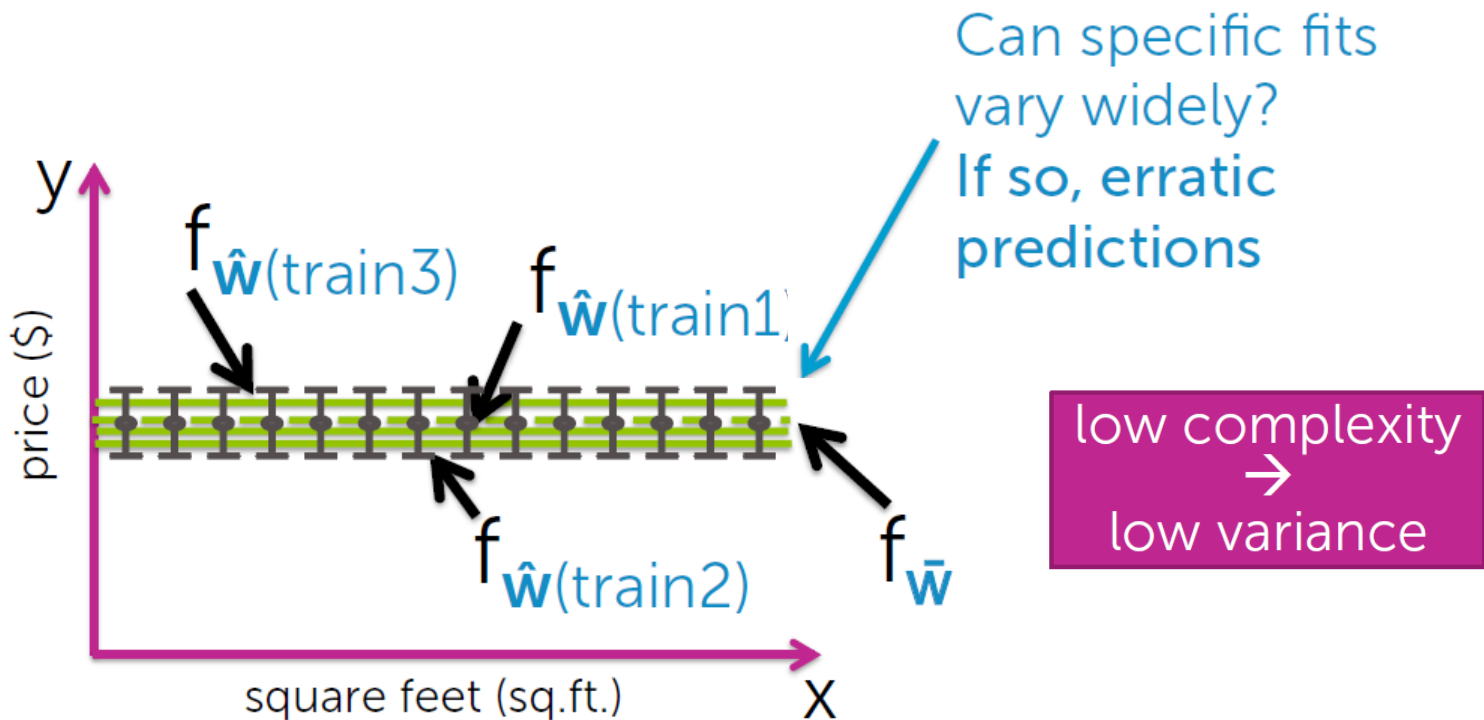
How much do specific fits vary from the expected fit?



Variance contribution

97

How much do specific fits vary from the expected fit?

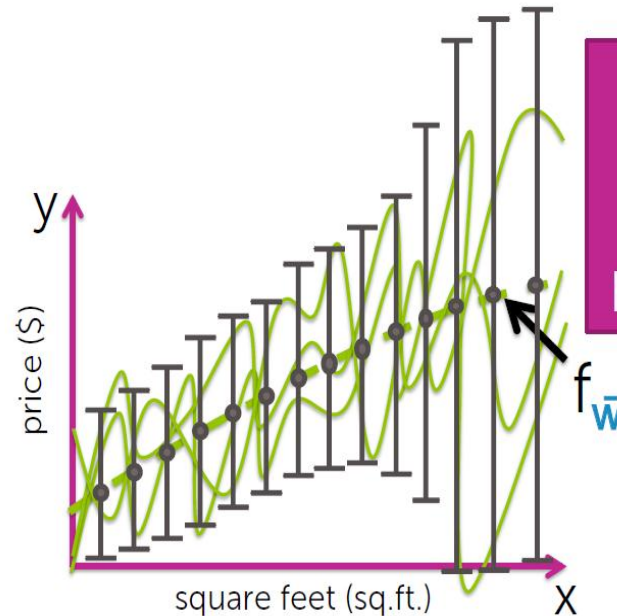
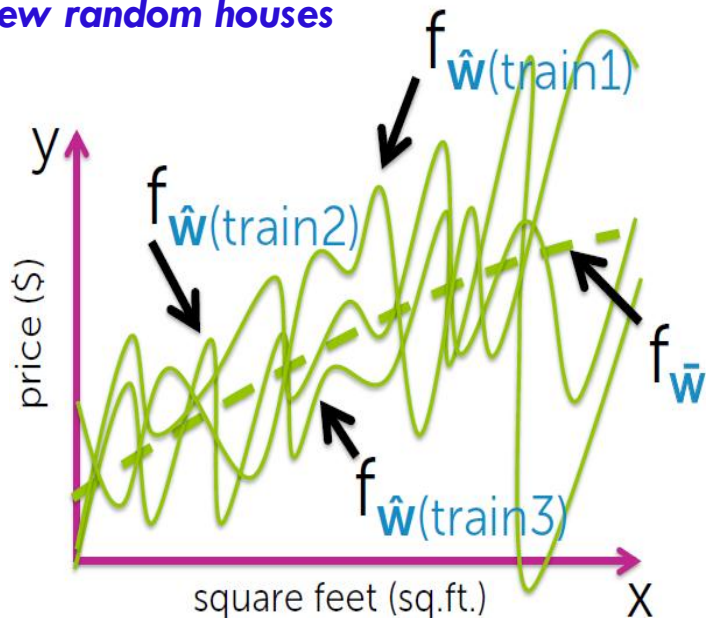


Variance of high complexity models

98

Assume we fit a high-order polynomial

*For each train remove
few random houses*



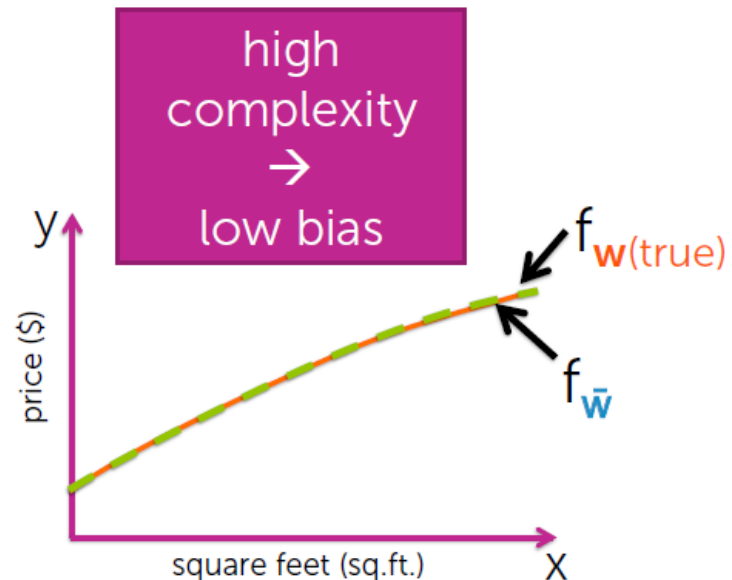
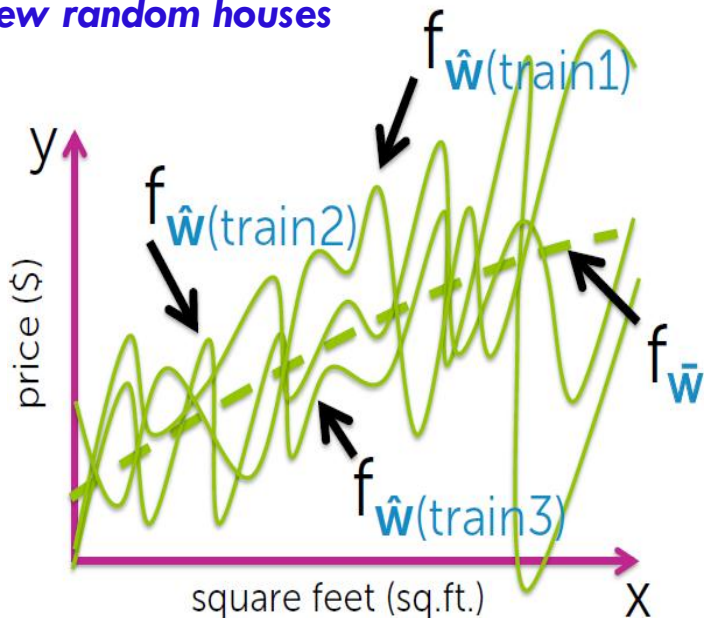
high
complexity
→
high variance

Bias of high complexity models

99

Assume we fit a high-order polynomial

*For each train remove
few random houses*

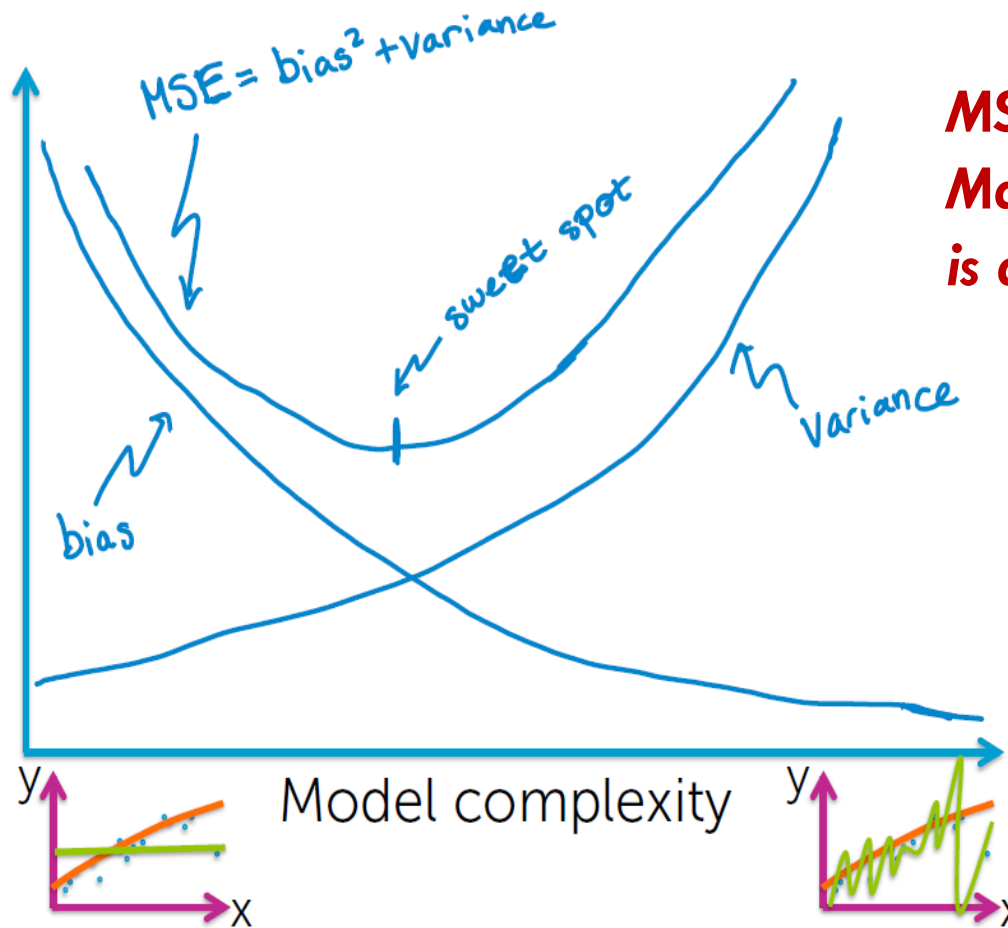


*High complexity models are very flexible,
pick better average trends.*

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Bias –variance tradeoff

100



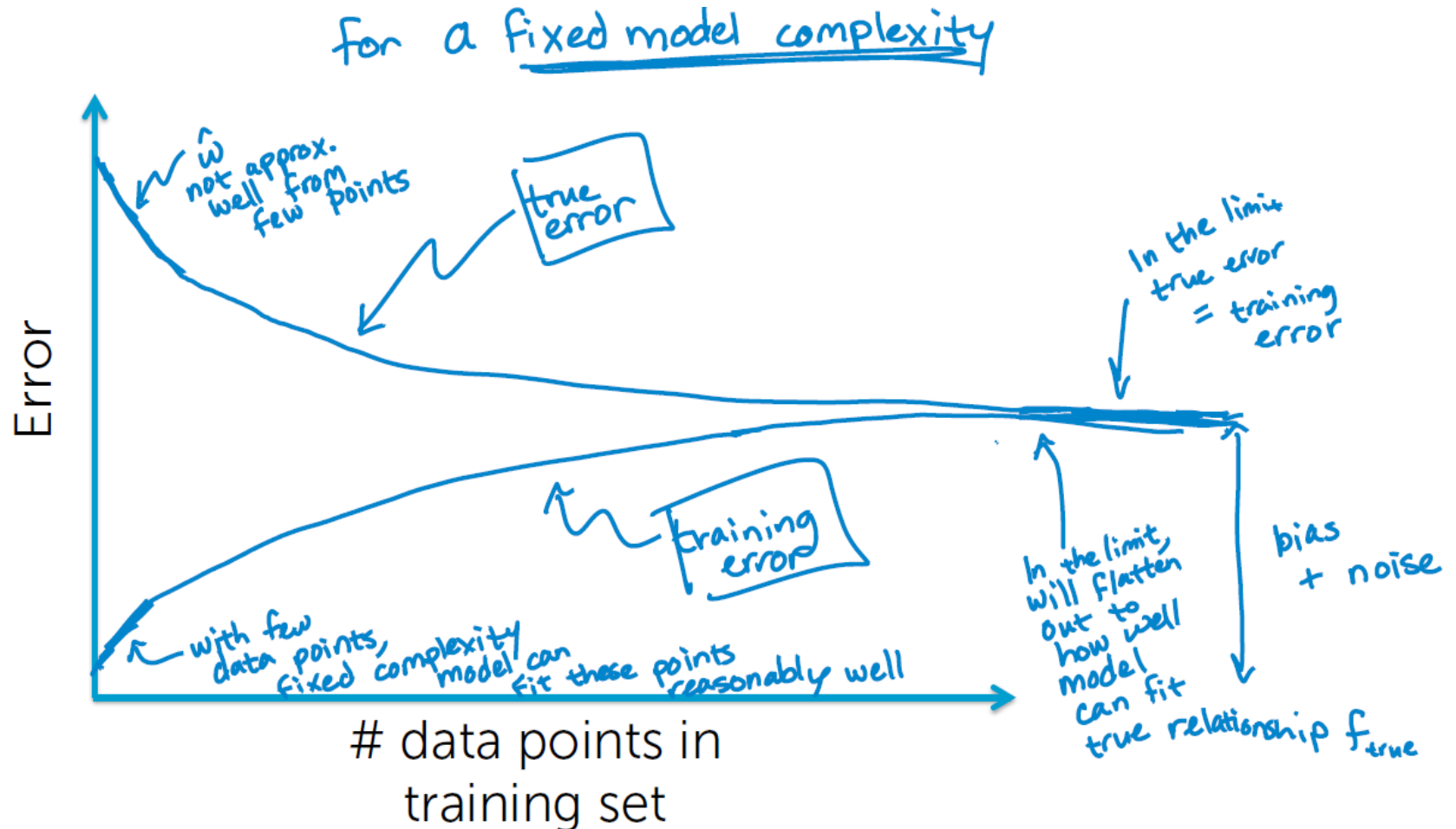
MSE = mean square error
Machine Learning
is all about this tradeoff

But....

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

Errors vs amount of data

101



The regression/ML workflow

102

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

103

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

104

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

Overly optimistic!

Hypothetical implementation

105

Training set

Test set

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

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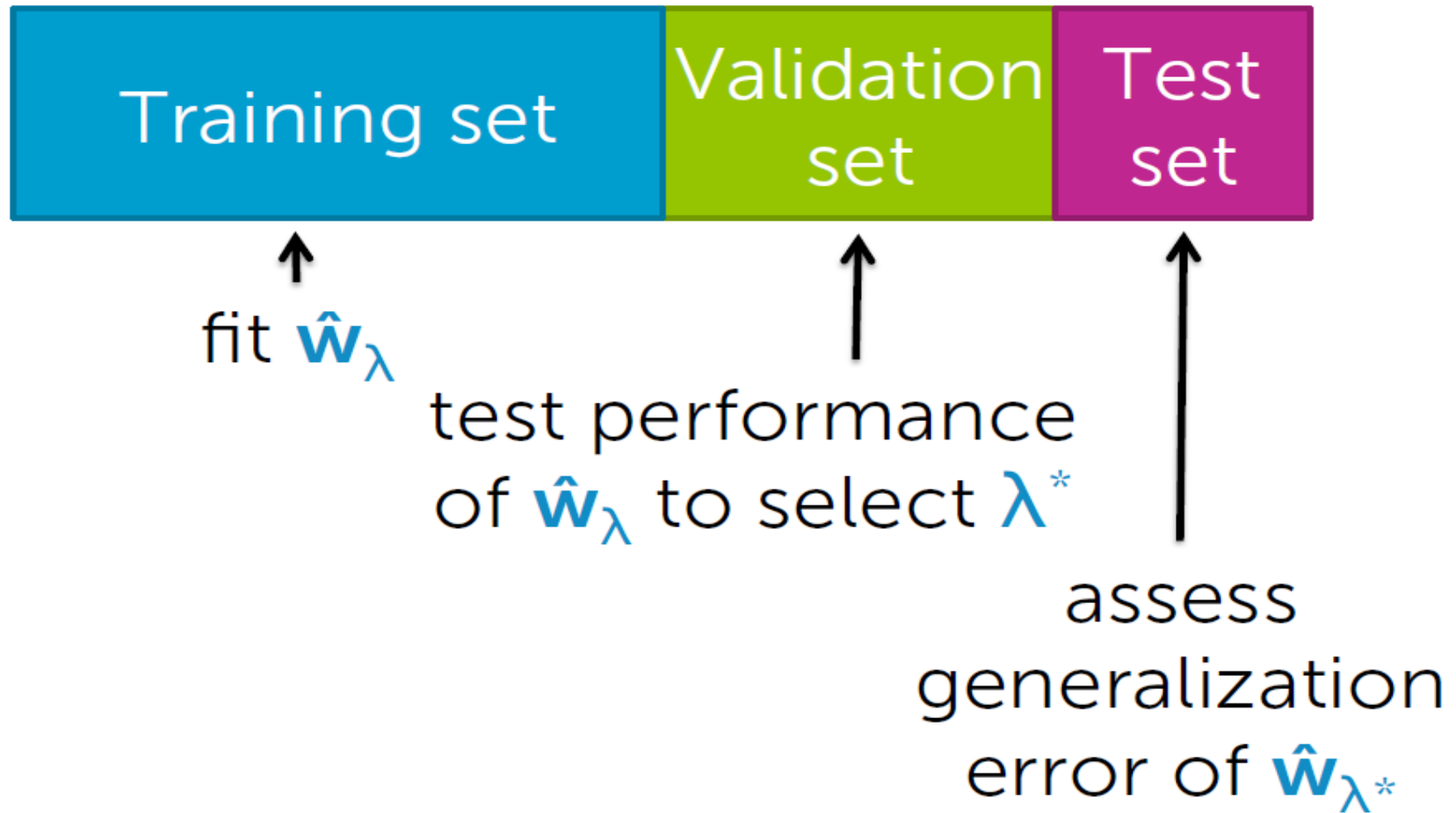


Solution: Create two “test” sets!

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

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Typical splits

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80%

10%

10%

50%

25%

25%

What you can do now

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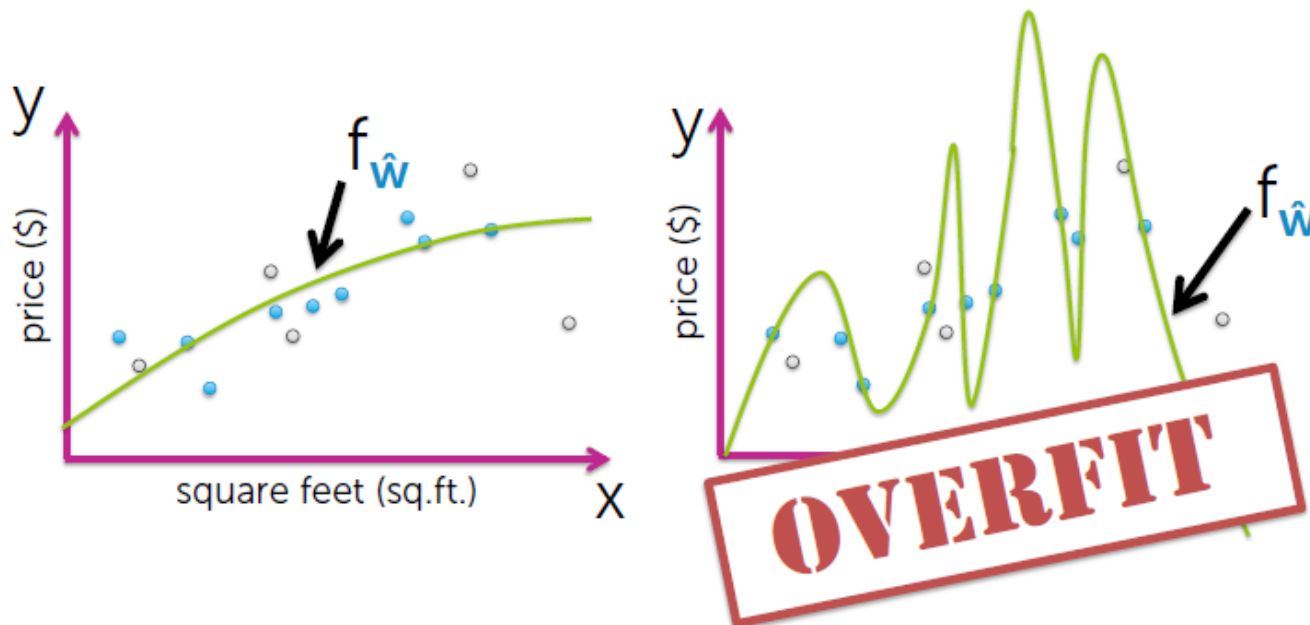
- Describe what a loss function is and give examples
- Contrast training, generalization, and test error
- Compute training and test error given a loss function
- Discuss issue of assessing performance on training set
- Describe tradeoffs in forming training/test splits
- List and interpret the 3 sources 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

111

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



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

Overfitting with many features

112

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?

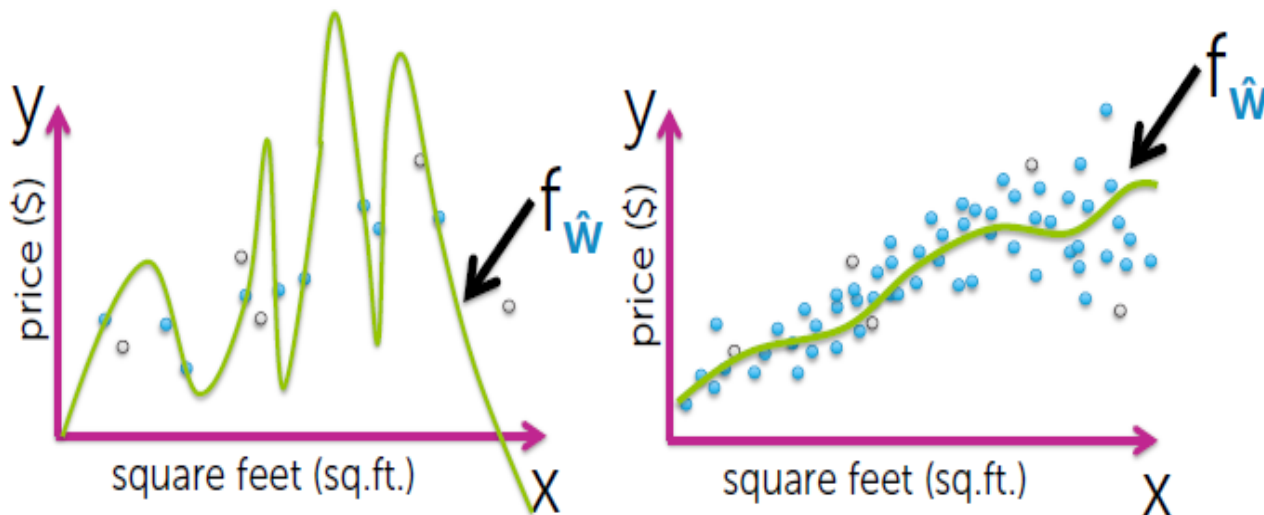
113

Few observations (N small)

→ rapidly overfit as model complexity increases

Many observations (N very large)

→ harder to overfit



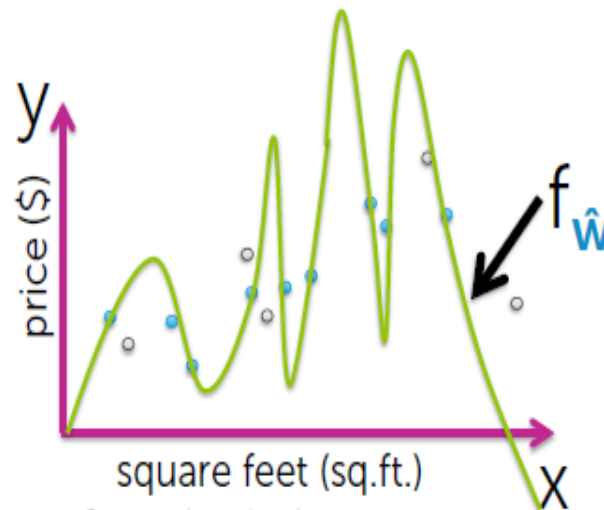
How does # of inputs influence overfitting?

114

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

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

HARD

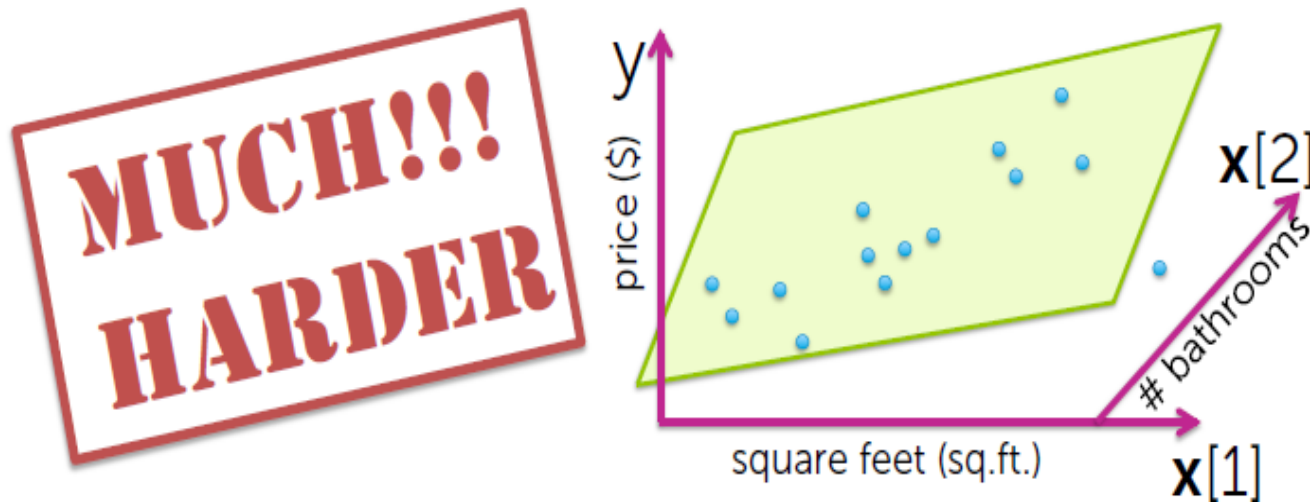


How does # of inputs influence overfitting?

115

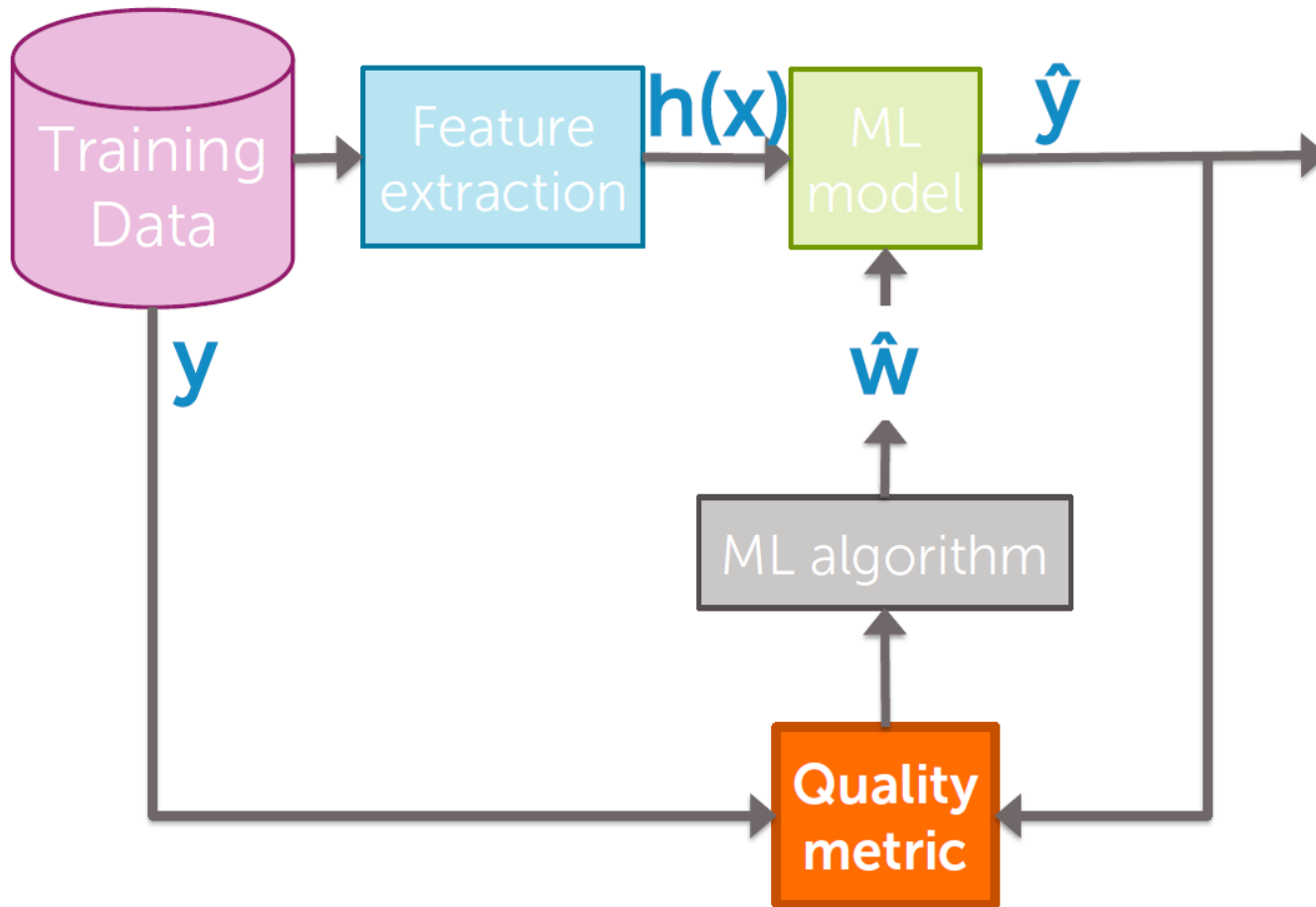
d inputs (e.g., sq.ft., #bath, #bed, lot size, year,...):

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



Lets improve quality metric blok

116

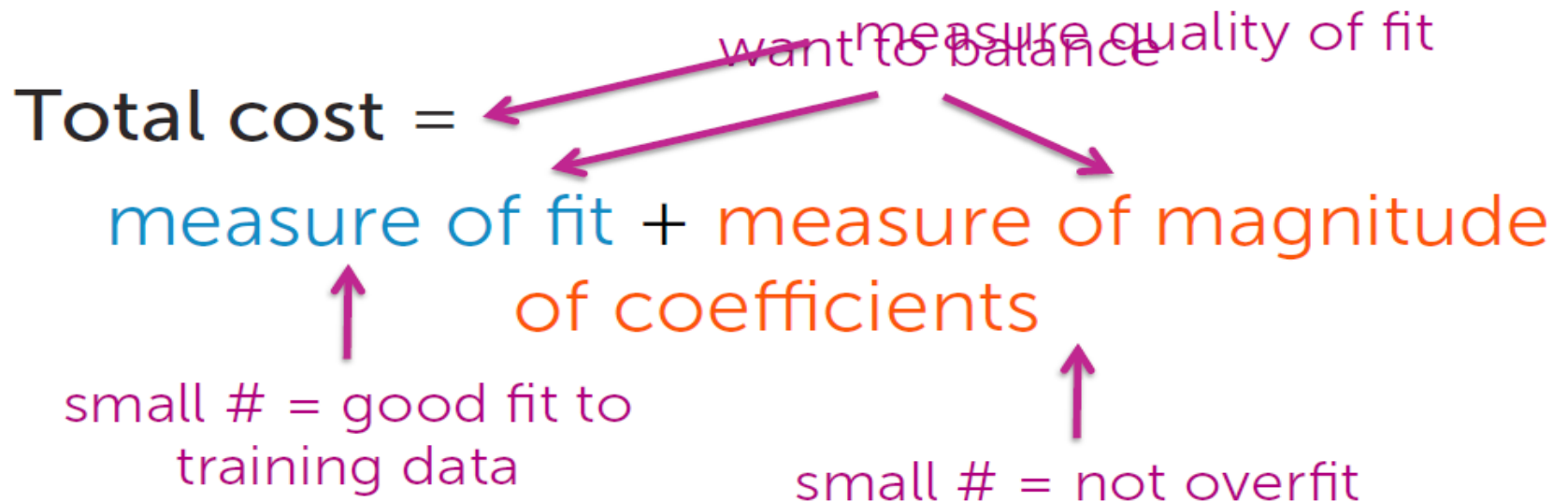


Desire total cost format

117

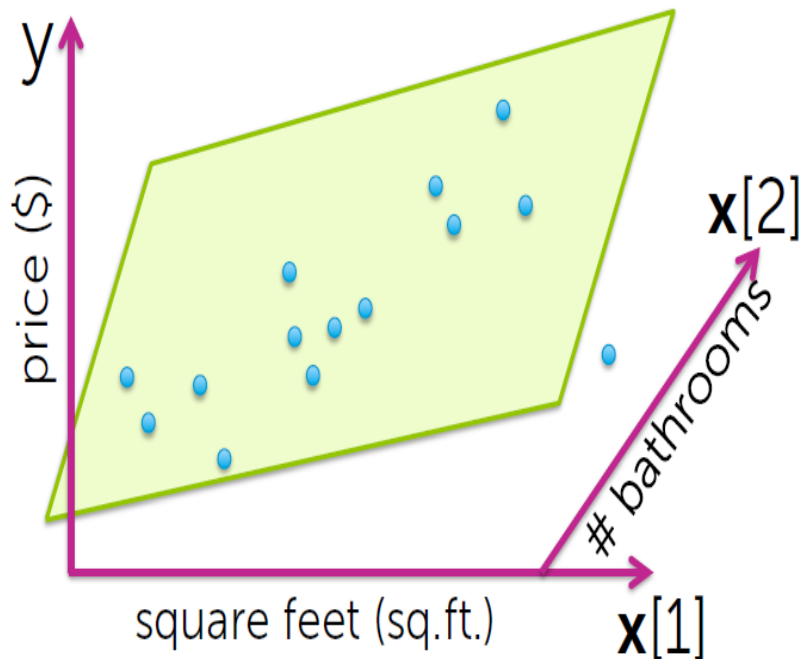
Want to balance:

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



Measure of fit to training data

118



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

pred. value using \mathbf{w}

small RSS \rightarrow model fitting training data well

Measure of magnitude of regression coefficients

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What summary # is indicative of size of regression coefficients?

- Sum? $w_0 = 1,527,301$ $w_1 = -1,605,253$
 $w_0 + w_1 = \text{small \#}$

← But ... the coefficients are very large

- Sum of absolute value?
 $|w_0| + |w_1| + \dots + |w_D| = \sum_{j=0}^D |w_j| \triangleq \|w\|_1$ L_1 norm ... discuss more in next module
- Sum of squares (L_2 norm)
 $w_0^2 + w_1^2 + \dots + w_D^2 = \sum_{j=0}^D w_j^2 \triangleq \|w\|_2^2$ L_2 norm ... focus of this module

Consider specific total cost

120

Total cost =

The diagram illustrates the components of the total cost function. It shows the equation: $\text{measure of fit} + \text{measure of magnitude of coefficients}$. A purple bracket under the first term points to $\text{RSS}(\mathbf{w})$. Another purple bracket under the second term points to $\|\mathbf{w}\|_2^2$.

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

Consider resulting objectives

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

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

 tuning parameter = balance of fit and magnitude

Ridge regression
(a.k.a L_2 regularization)

If $\lambda=0$:

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

If $\lambda=\infty$:

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

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

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

Ridge regression: bias-variance tradeoff

122

Large λ :

high bias, low variance

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

In essence, λ
controls model
complexity

Small λ :

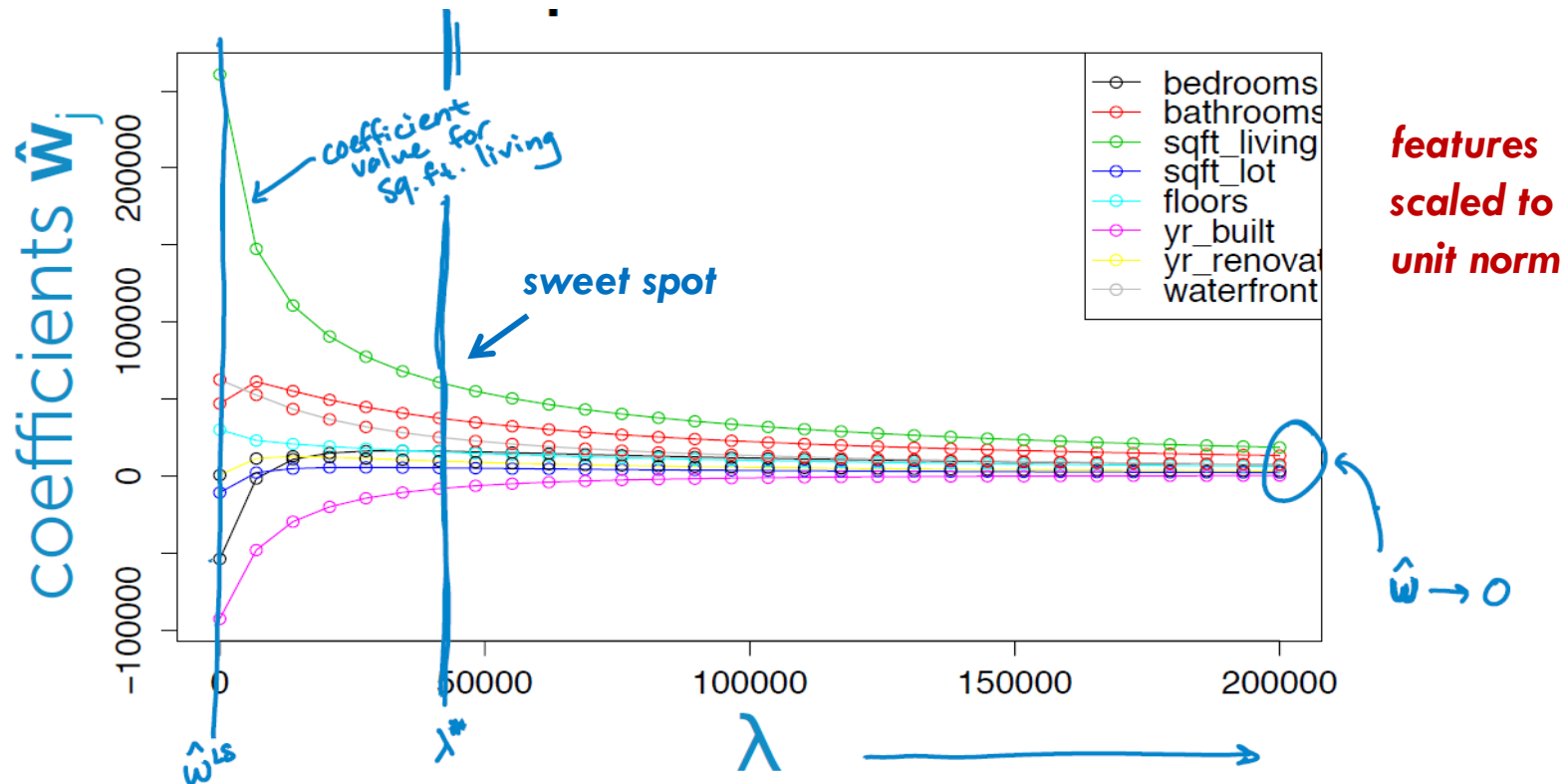
low bias, high variance

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

Ridge regression: coefficients path

123

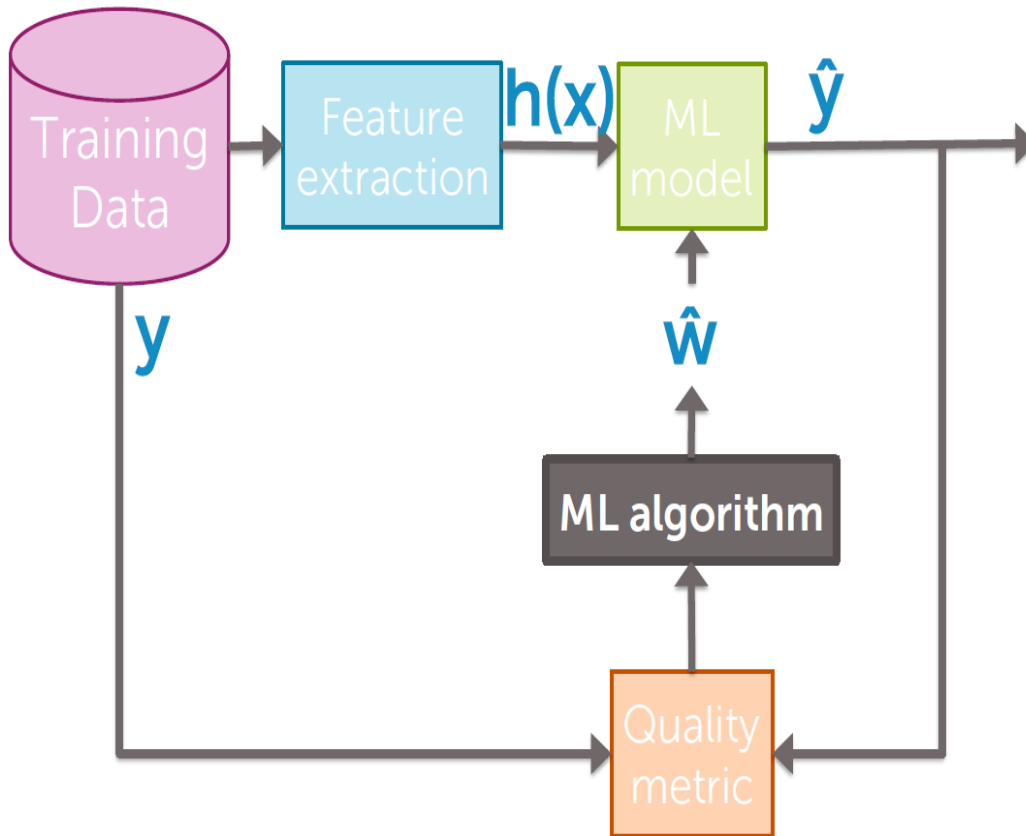
What happens if we refit our high-order polynomial, but now using **ridge regression**?



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Flow chart

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Model for all N observations together

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

The equation is represented using matrices and vectors. \mathbf{y} is a vertical vector of 10 pink squares. \mathbf{H} is a 10x10 grid of squares, mostly green and grey, with a bright yellow-green horizontal band in the middle. \mathbf{w} is a vertical vector of 10 blue squares. $\boldsymbol{\varepsilon}$ is a vertical vector of 10 grey squares.

Ridge regression: cost in matrix notation

125

In matrix form, ridge regression cost is:

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

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

$$= \begin{bmatrix} \boxed{} & \boxed{} & \boxed{} & \boxed{} & \boxed{} \end{bmatrix} \begin{bmatrix} \boxed{} \\ \boxed{} \\ \boxed{} \\ \boxed{} \\ \boxed{} \end{bmatrix}$$

$w_0 \quad w_1 \quad w_2 \quad \dots \quad w_D$ w_0
 w_1
 w_2
 \vdots
 w_D

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

Gradient of ridge regression cost

126

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

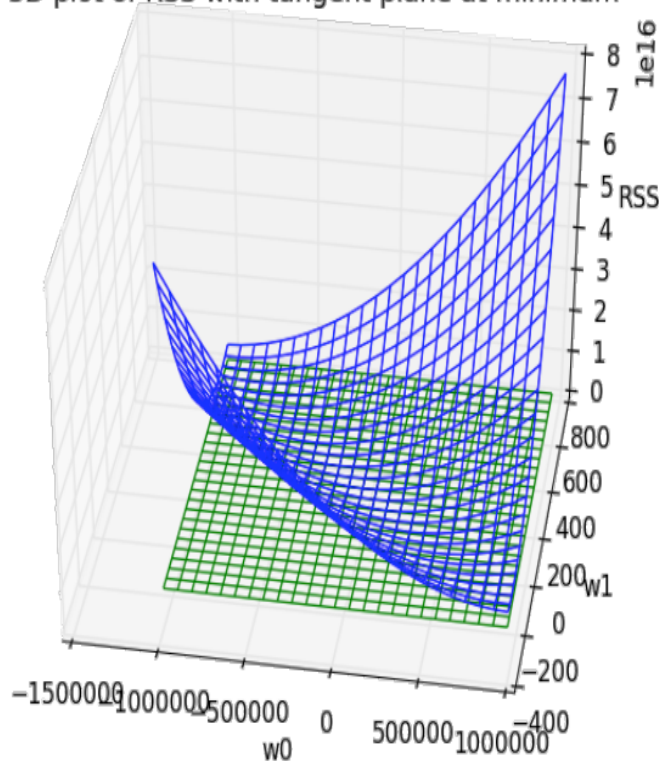
Why? By analogy to 1d case...

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

Ridge regression: closed-form solution

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3D plot of RSS with tangent plane at minimum



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

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

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

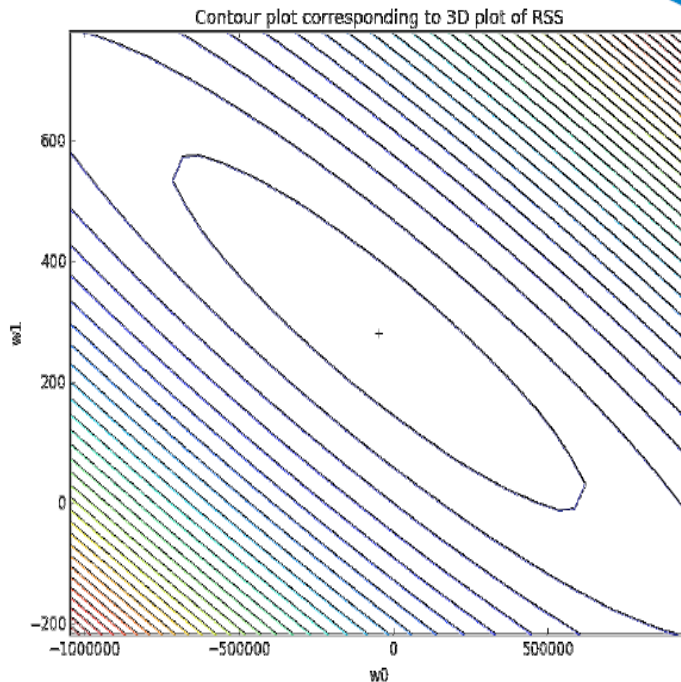
$$(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I})\hat{\mathbf{w}} = \mathbf{H}^T\mathbf{y}$$

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

Ridge regression: gradient descent

128

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



Update to j^{th} feature weight:

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

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

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

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

Summary of ridge regression algorithm

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

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

for $j = 0, \dots, D$

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

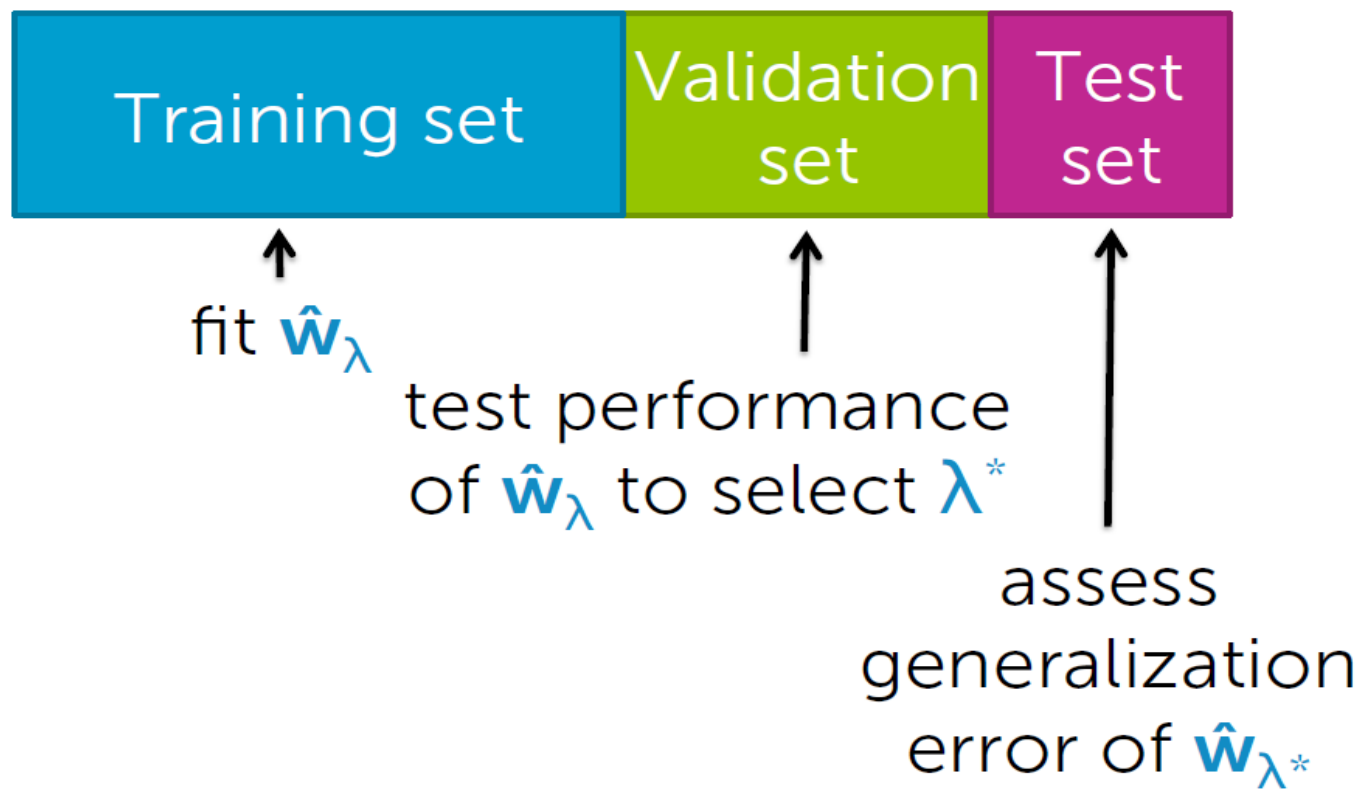
$w_j^{(t+1)} \leftarrow (1 - 2\eta\lambda) w_j^{(t)} - \eta \text{partial}[j]$

$t \leftarrow t + 1$

How to choose λ

130

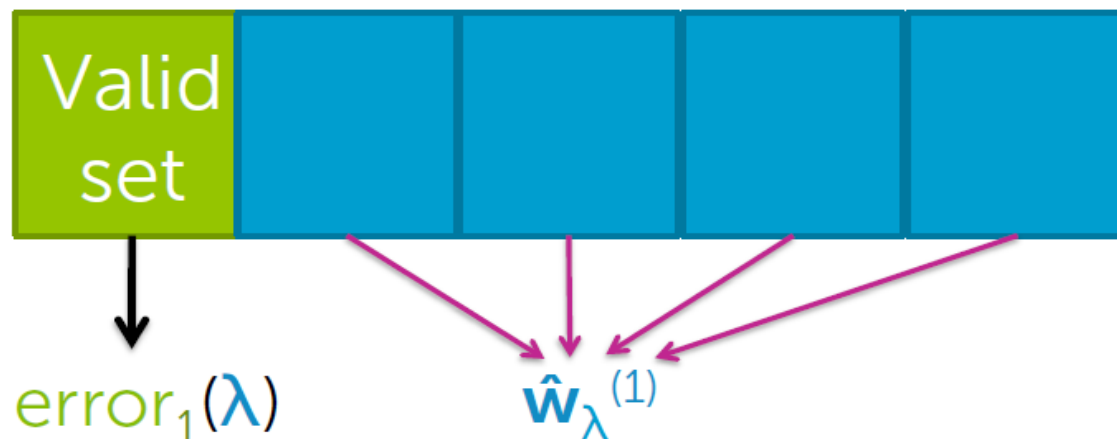
If sufficient amount of data...



How to choose λ

131

K-fold cross validation



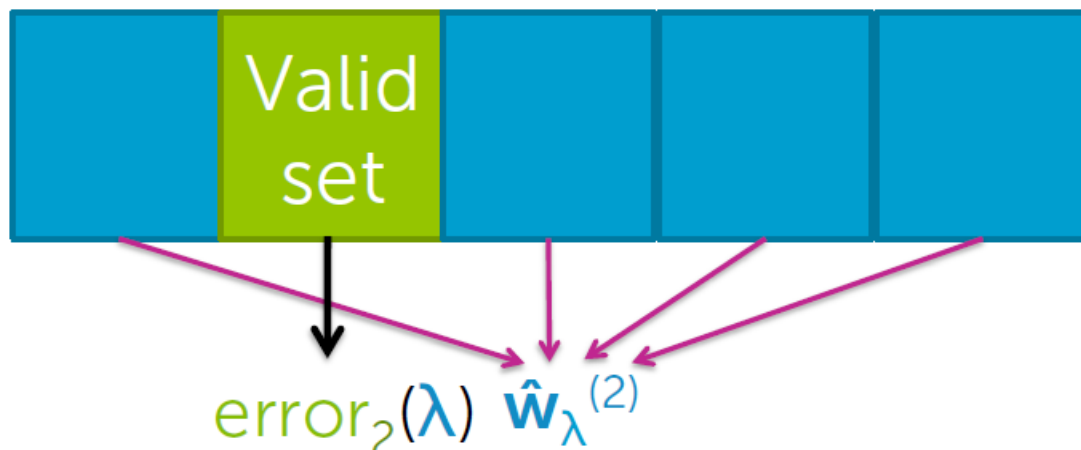
For $k=1, \dots, K$

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

How to choose λ

132

K-fold cross validation



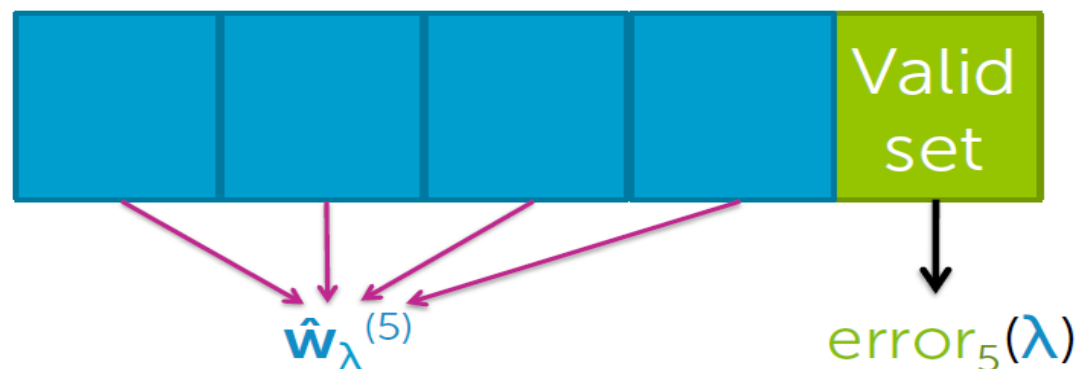
For $k=1, \dots, K$

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

How to choose λ

133

K-fold cross validation



For $k=1, \dots, K$

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

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

How to choose λ

134

K-fold cross validation



Repeat procedure for each choice of λ

Choose λ^* to minimize $CV(\lambda)$

What value of K

135

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

136

Recall multiple regression model

Model:

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

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?

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Standard ridge regression cost:

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

 strength of penalty

Encourages intercept w_0 to also be small

Do we want a small intercept?

Conceptually, not indicative of overfitting...

Do we penalize intercept?

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

Modified ridge regression cost:

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

□ **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

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- 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?

141

Efficiency:

- If $\text{size}(\mathbf{w}) = 100\text{B}$, 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?

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

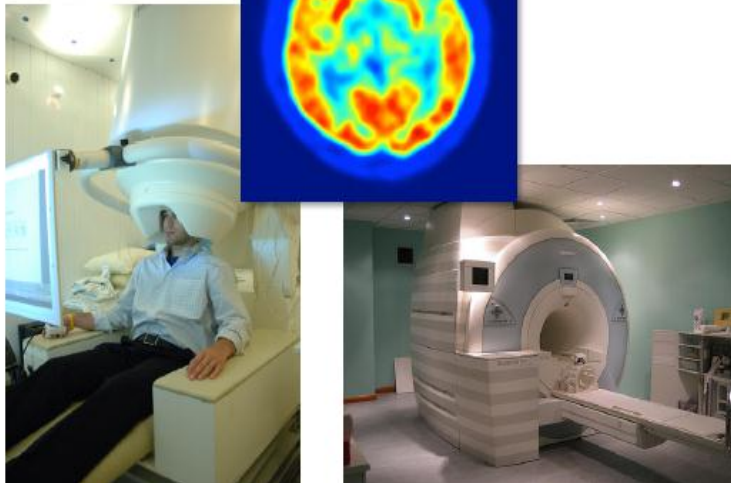
Sprinkler System

⋮

Sparcity

143

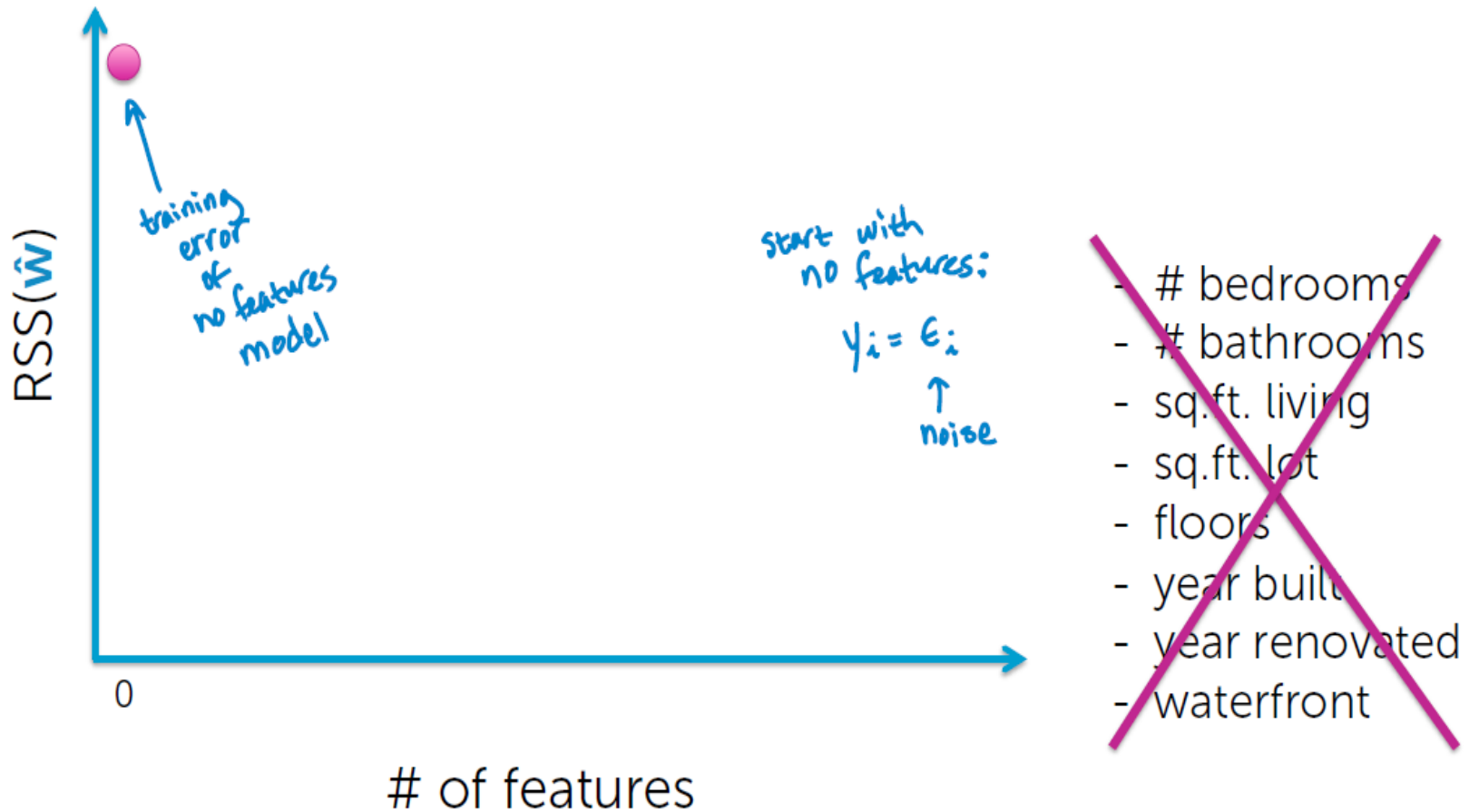
Reading your mind



Activity in which
brain regions
can predict
happiness?

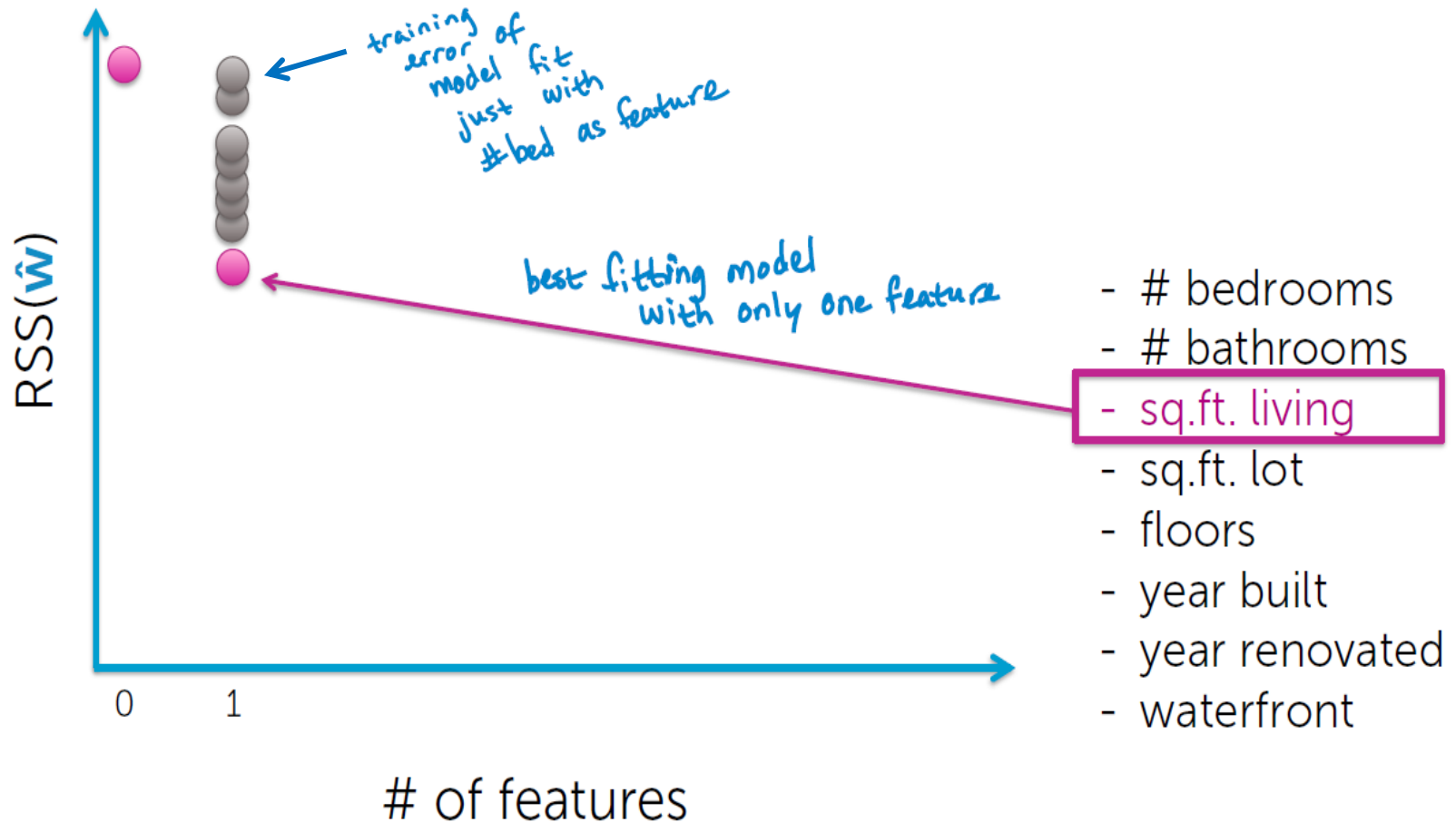
Find best model of size: 0

144



Find best model of size: 1

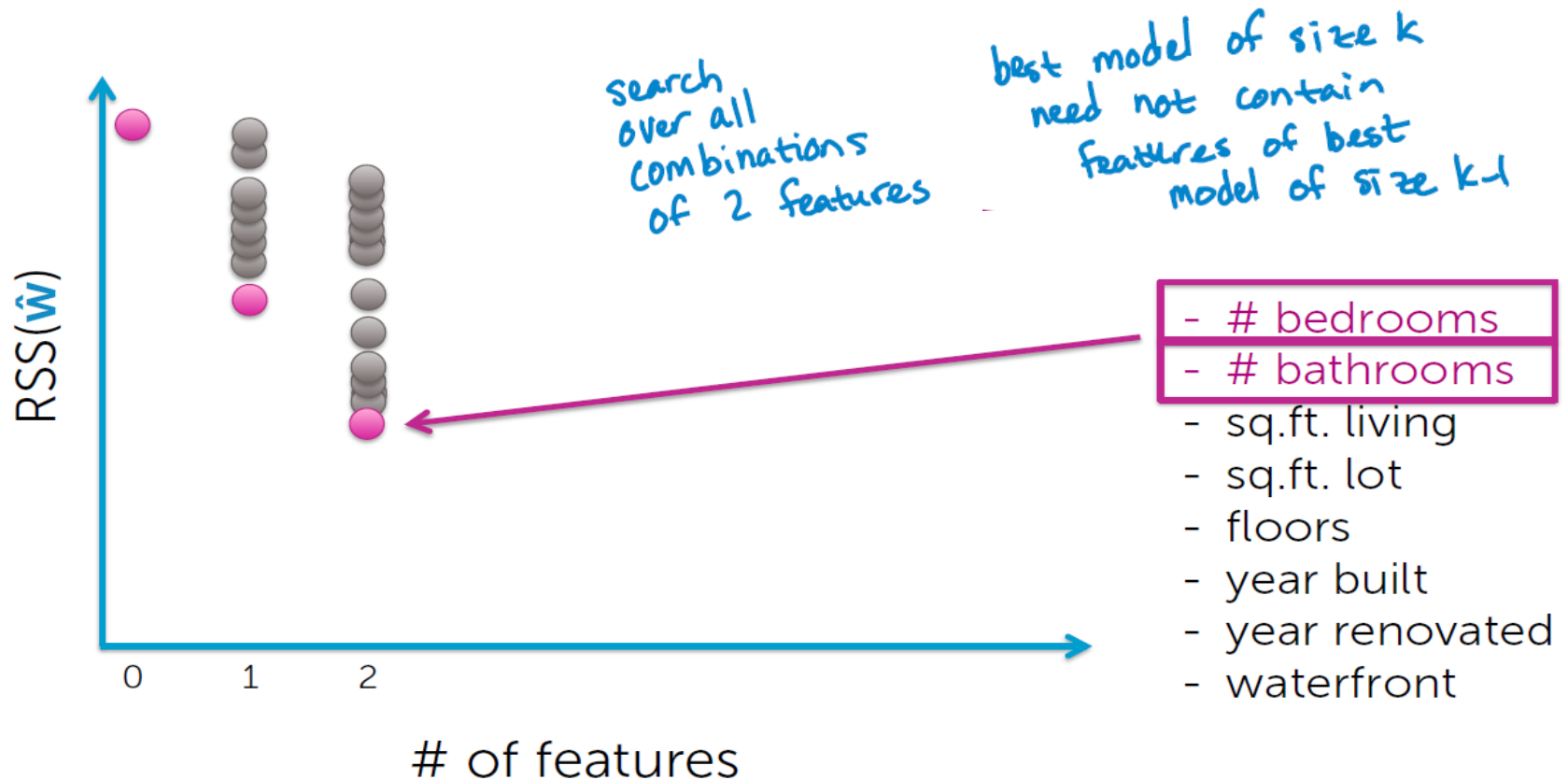
145



Find best model of size: 2

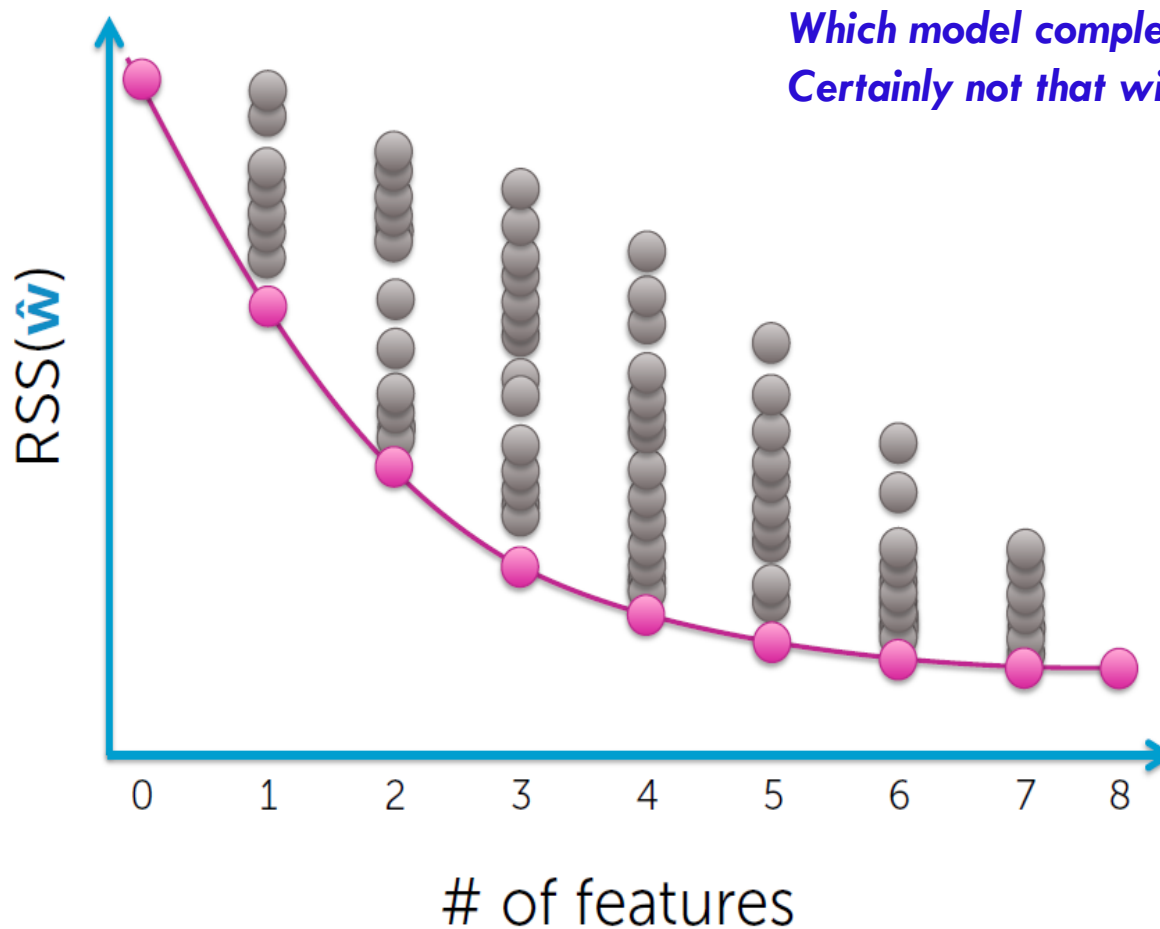
146

Note: not necessarily nested!



Find best model of size: N

147



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

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

Choosing model complexity

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Option 1: Assess on validation set

Option 2: Cross validation

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

Complexity of „all subsets”

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How many models were evaluated?

- each indexed by features included

$$y_i = \varepsilon_i$$

$$y_i = w_0 h_0(\mathbf{x}_i) + \varepsilon_i$$

$$y_i = w_1 h_1(\mathbf{x}_i) + \varepsilon_i$$

⋮

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

⋮

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

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

[0 0 0 ... 0 0 0]

[1 0 0 ... 0 0 0]

[0 1 0 ... 0 0 0]

⋮

[1 1 0 ... 0 0 0]

⋮

[1 1 1 ... 1 1 1]

2 2 2 · · · 2

2^{D+1}

$$2^8 = 256$$

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

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

$$2^{100B} = \text{HUGE!!!!!!}$$

Typically,
computationally
infeasible

Greedy algorithm

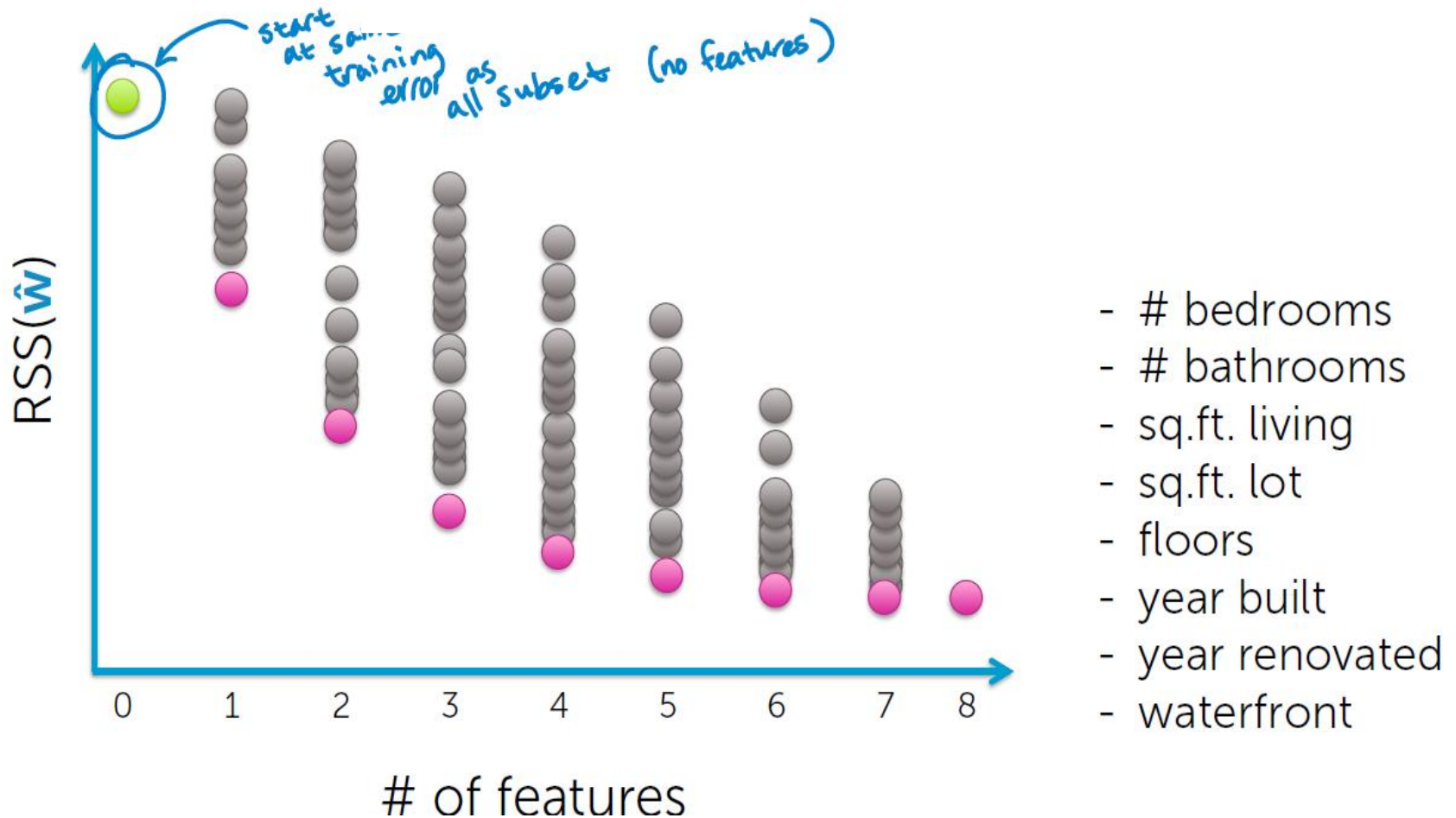
150

Forward stepwise algorithm

1. Pick a dictionary of features $\{h_0(\mathbf{x}), \dots, h_D(\mathbf{x})\}$
 - e.g., polynomials for linear regression
2. Greedy heuristic:
 - i. Start with empty set of features $F_0 = \emptyset$
(or simple set, like just $h_0(\mathbf{x})=1 \rightarrow y_i = w_0 + \epsilon_i$)
 - 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

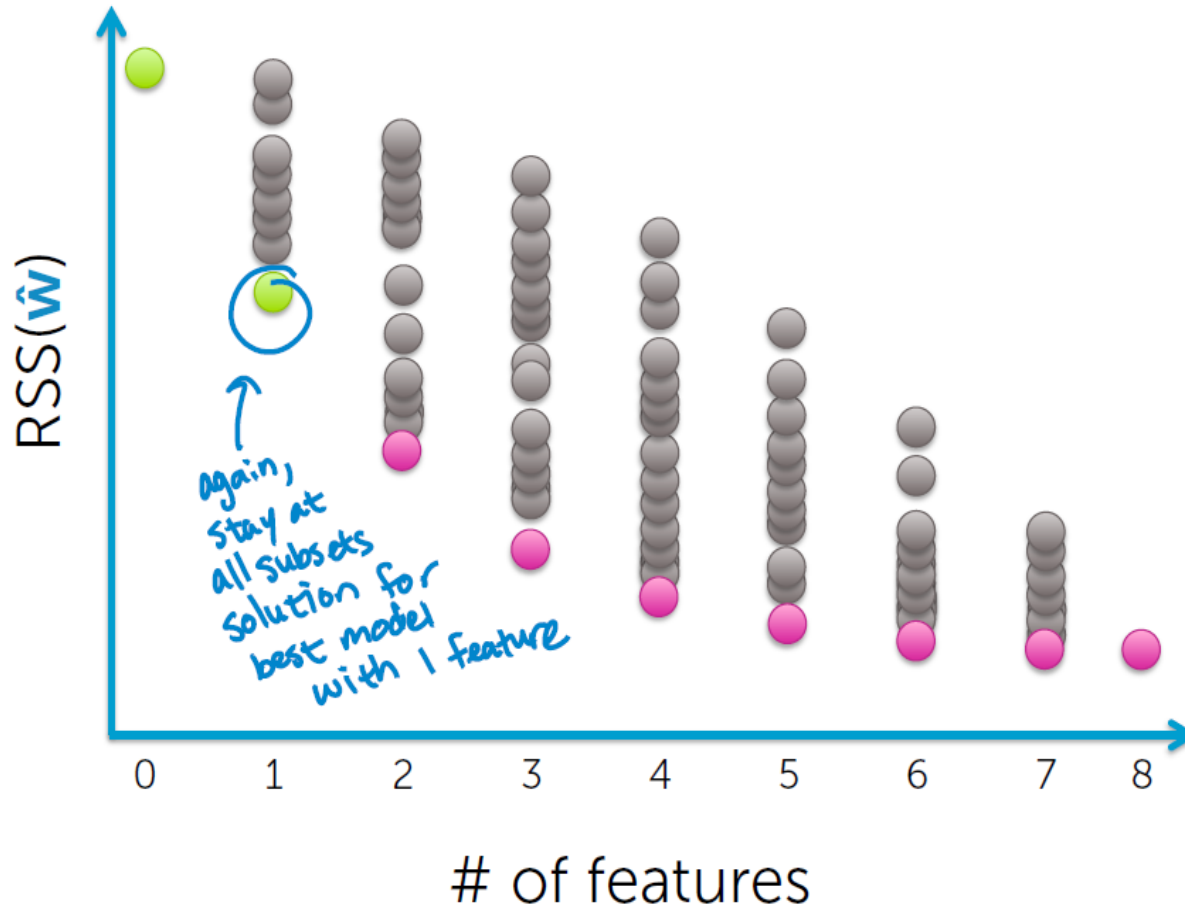
Visualizing greedy algorithm

151



Visualizing greedy algorithm

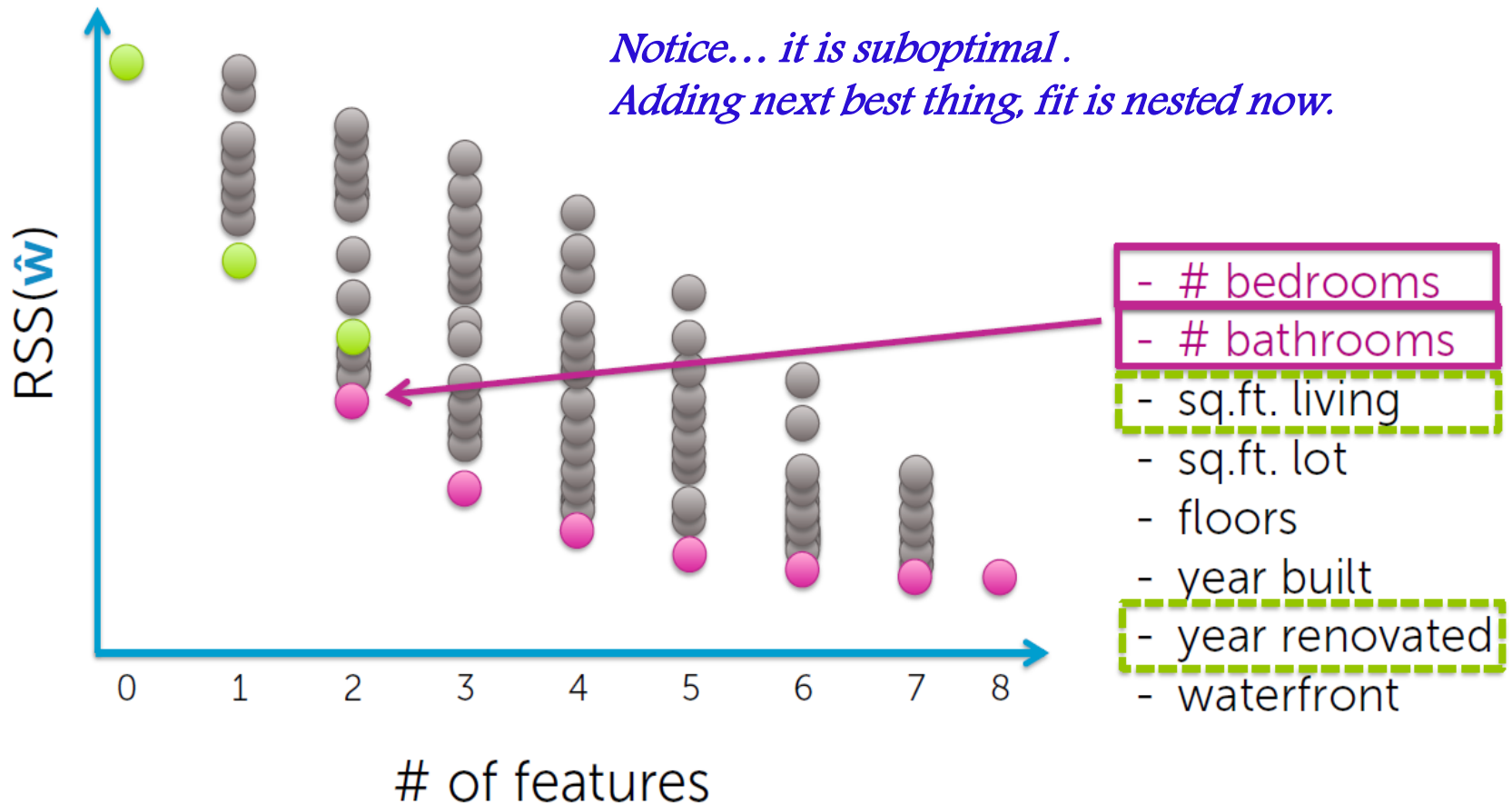
152



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

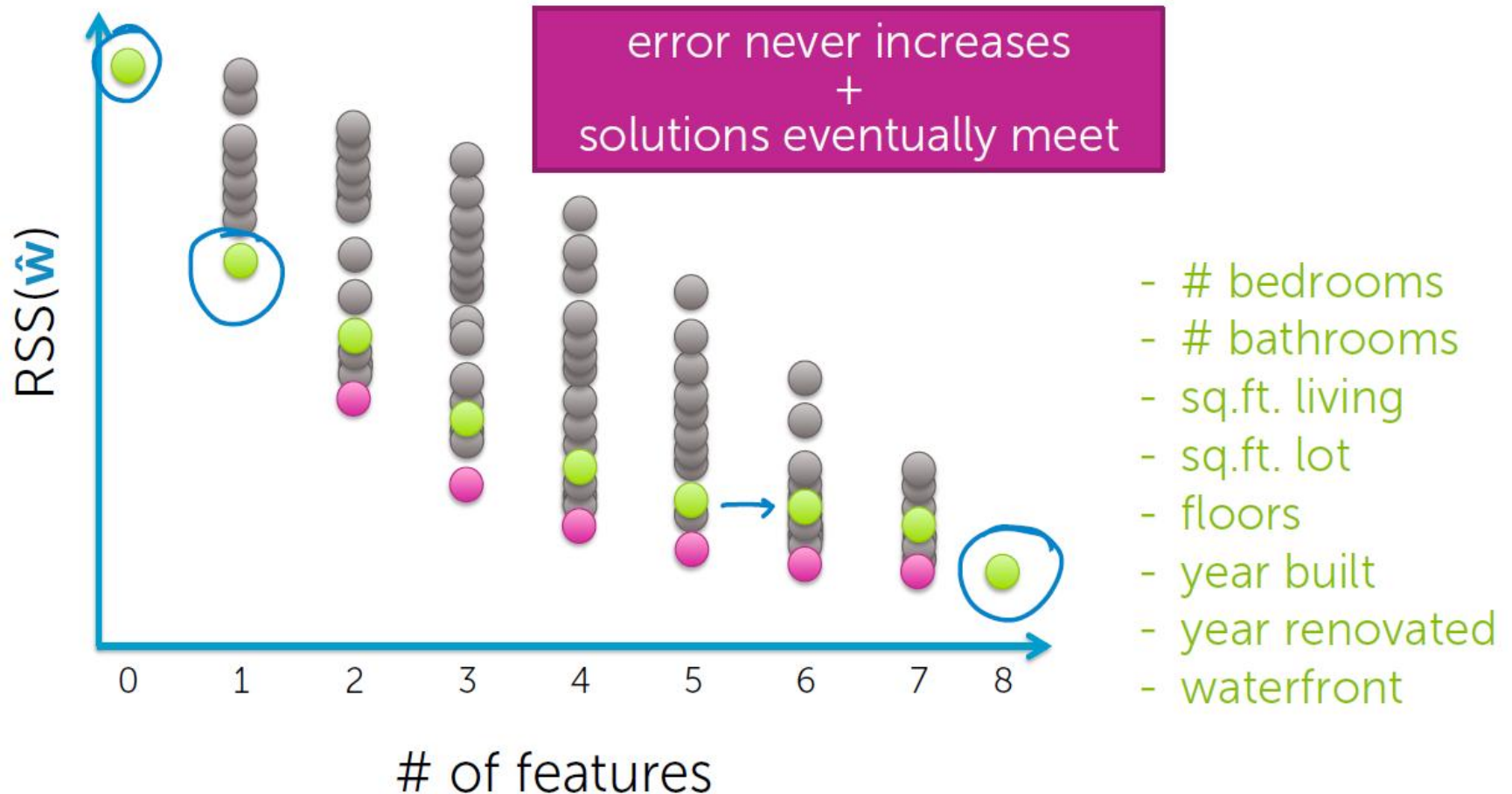
Visualizing greedy algorithm

153



Visualizing greedy algorithm

154



When do we stop?

155

When training error is low enough?

No!

When test error is low enough?

No!

Use *validation set* or *cross validation*!

Complexity of forward stepwise

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How many models were evaluated?

- 1st step, D models
- 2nd step, $D-1$ models (add 1 feature out of $D-1$ possible)
- 3rd 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

157

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

158

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?

159

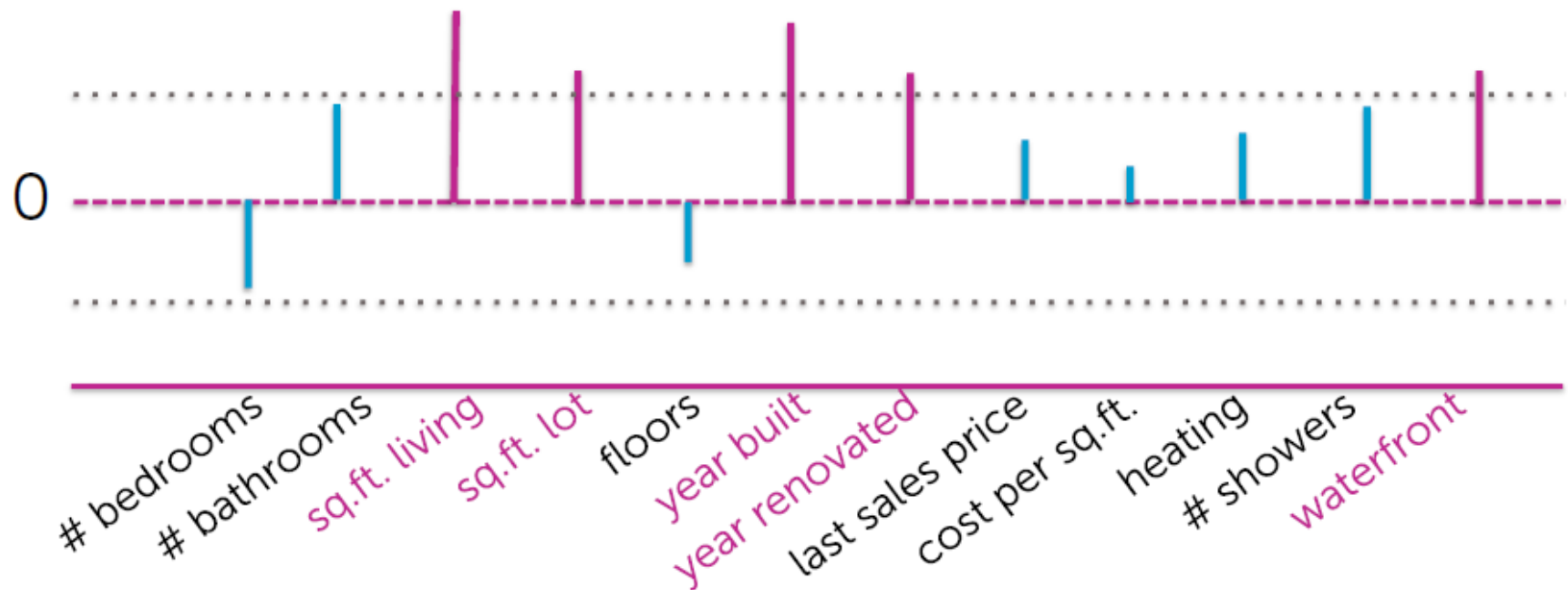
Why don't we just set small ridge coefficients to 0?



Thresholding ridge coefficients?

160

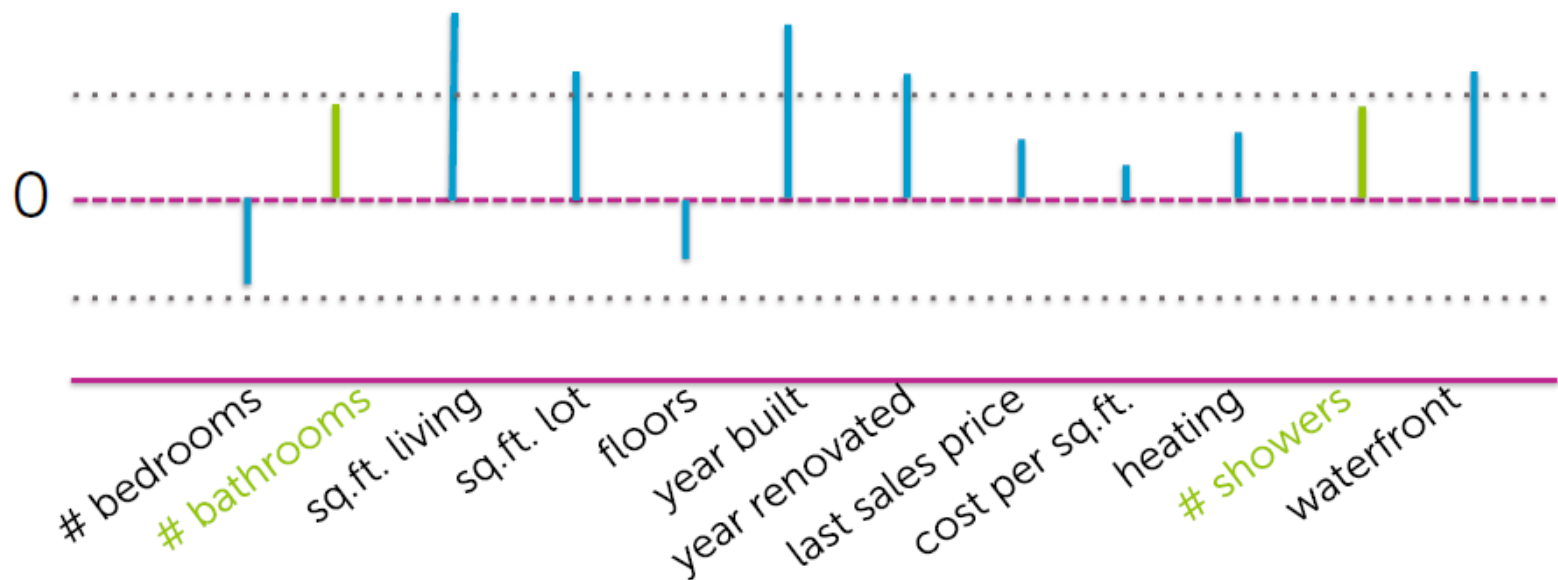
Selected features for a given threshold value



Thresholding ridge coefficients?

161

Let's look at two related features...

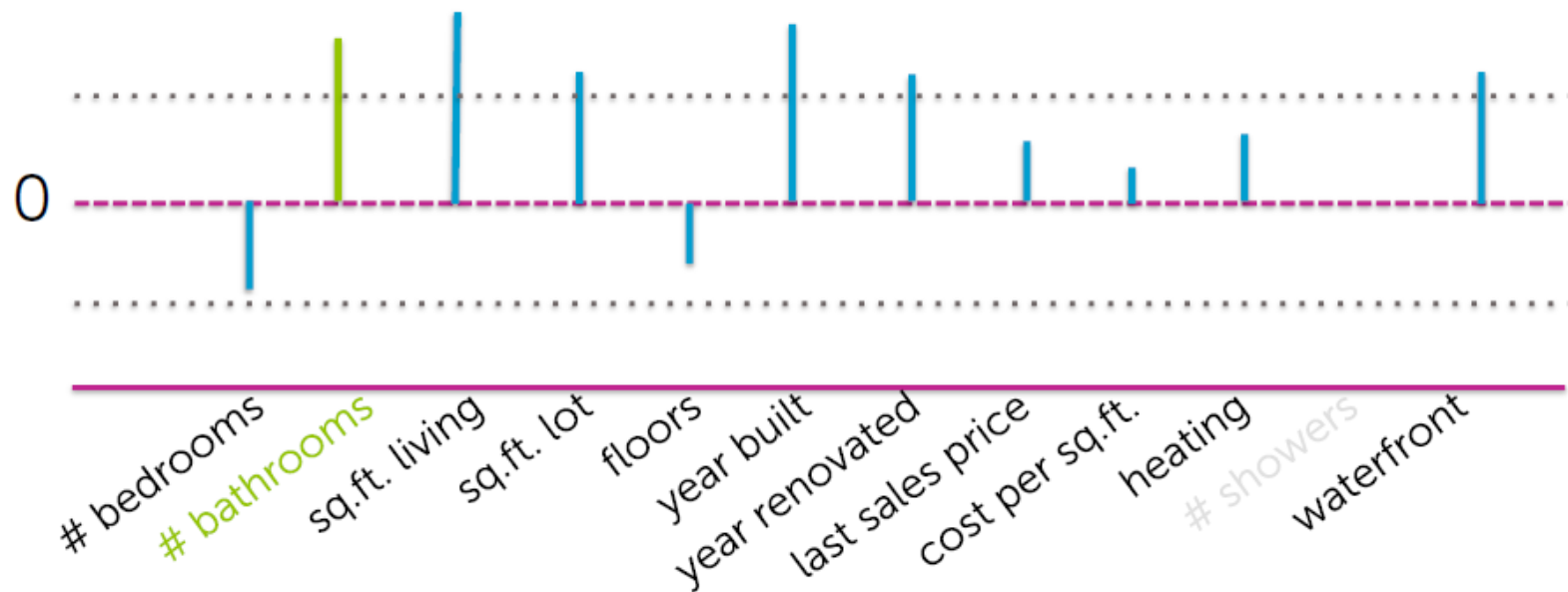


Nothing measuring bathrooms was included!

Thresholding ridge coefficients?

162

If only one of the features had been included...



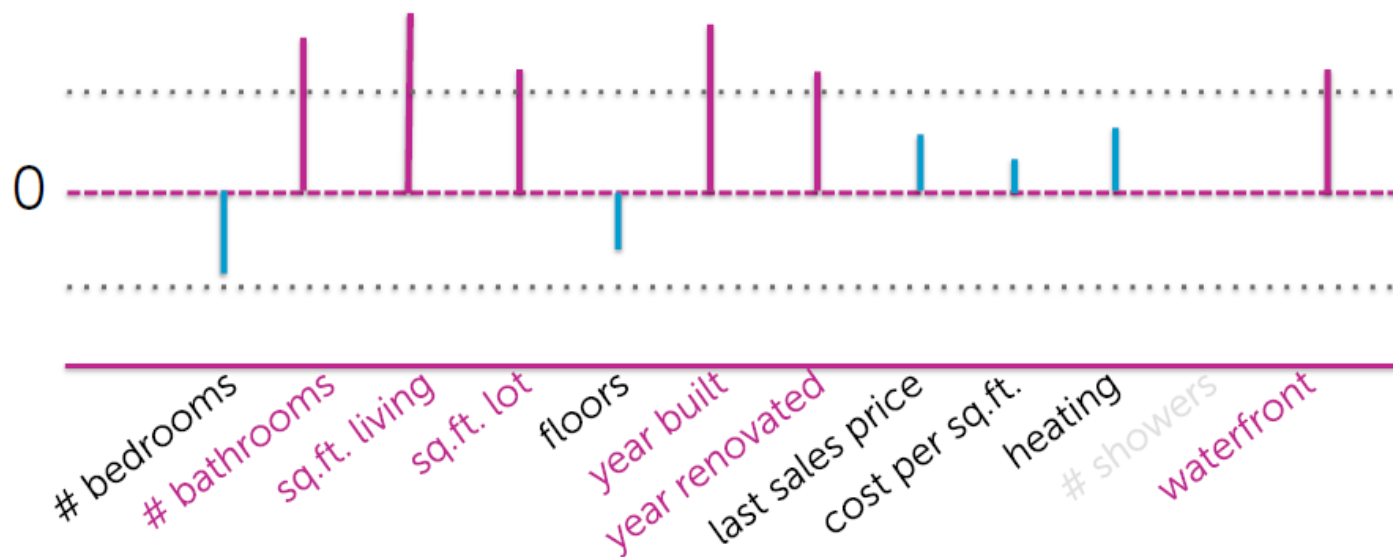
Remember:

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?

163

Would have included bathrooms in selected model



Can regularization lead directly to sparsity?

Try this cost instead of ridge ...

164

Total cost =

measure of fit + λ measure of magnitude of coefficients
RSS(\mathbf{w})

$$\|\mathbf{w}\|_1 = |w_0| + \dots + |w_D|$$

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

Leads to
sparse
solutions!

Lasso regression

165

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

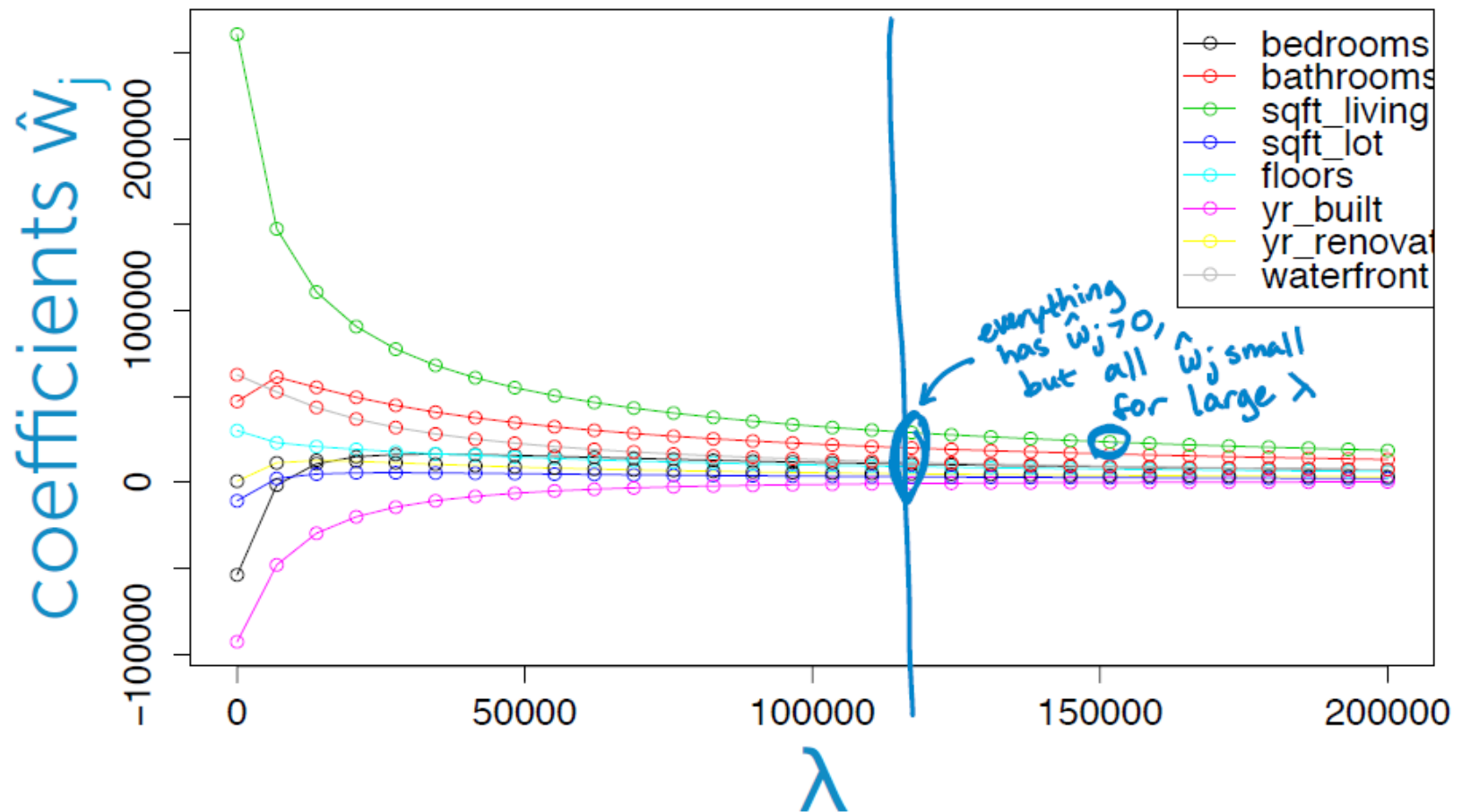
If $\lambda=0$: $\hat{\mathbf{w}}^{\text{lasso}} = \hat{\mathbf{w}}^{\text{LS}}$ (unregularized solution)

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

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

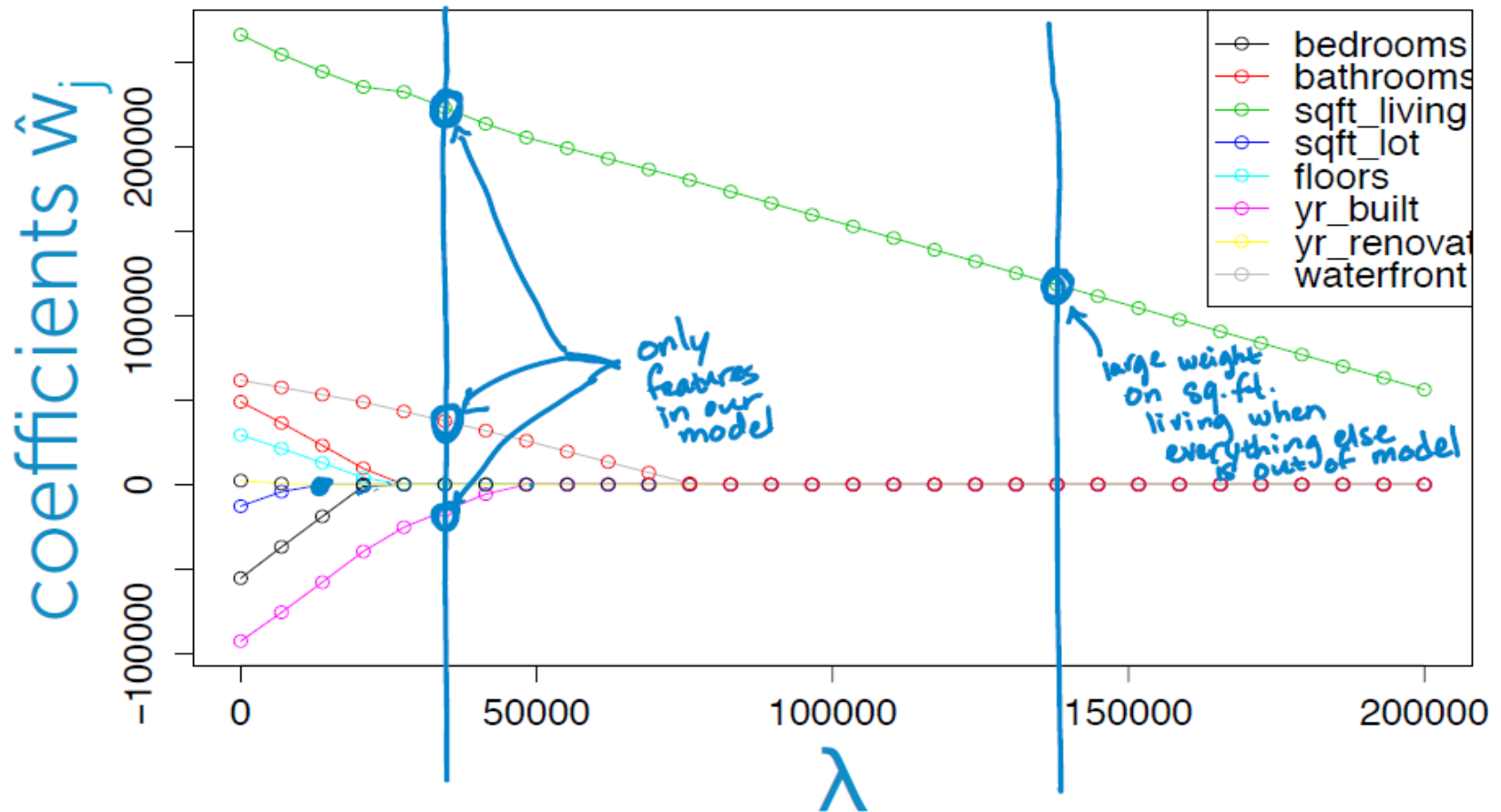
Coefficient path: ridge

166



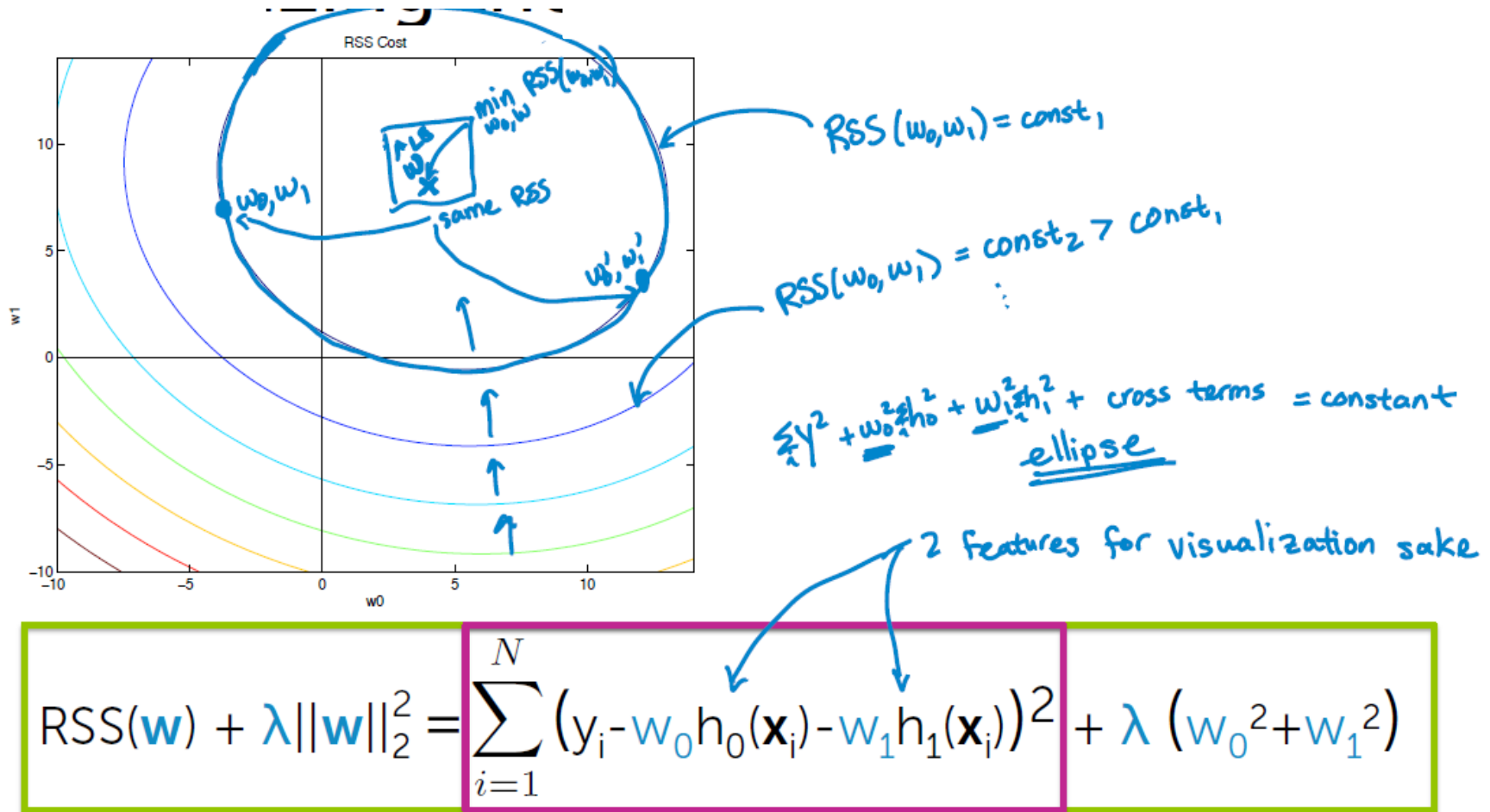
Coefficient path: lasso

167



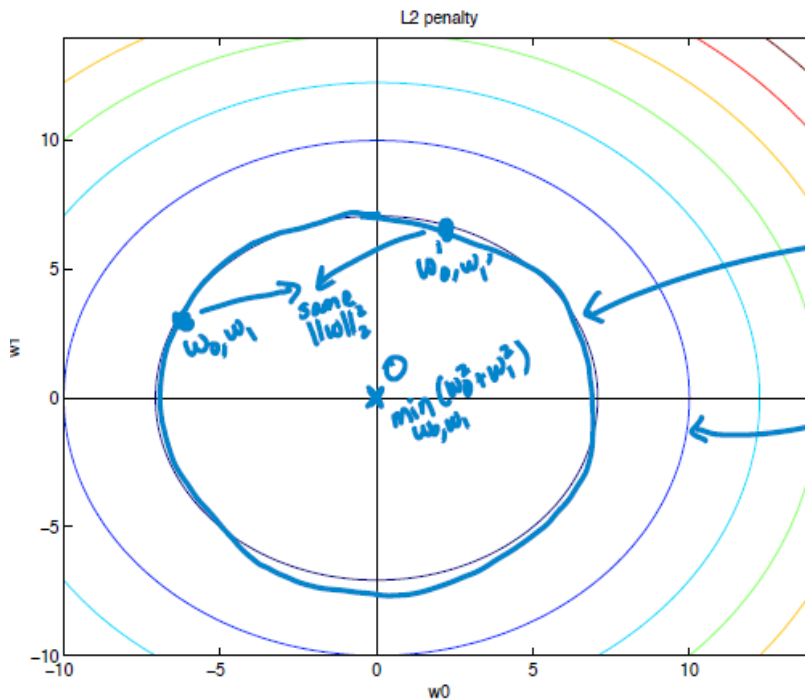
Visualising ridge cost in 2D

168



Visualising ridge cost in 2D

169



$$\|w\|_2^2 = \text{const}_1$$

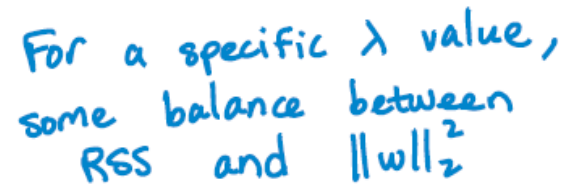
$$\|w\|_2^2 = \text{const}_2 > \text{const}_1$$

$$w_0^2 + w_1^2 = \text{constant}$$

circle

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

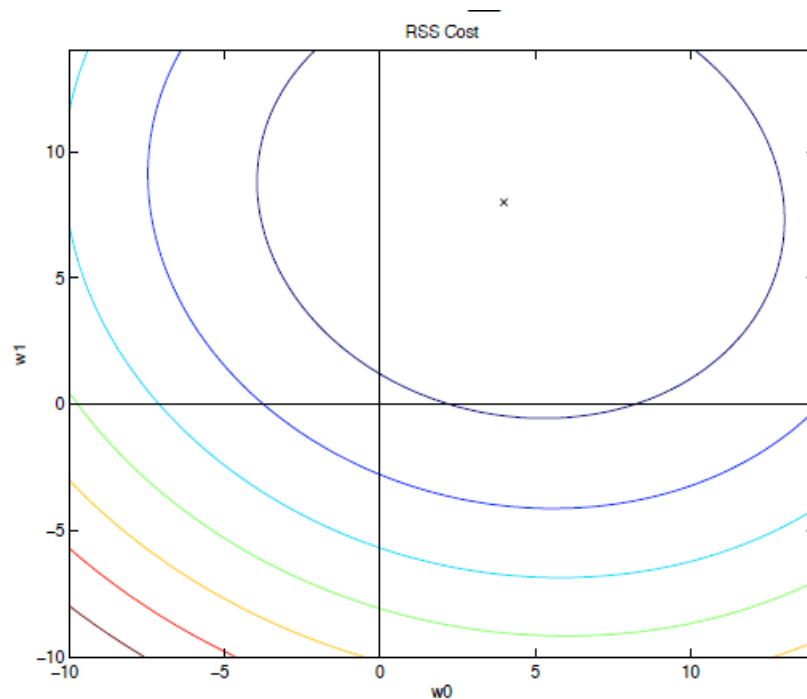
170



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Visualising lasso cost in 2D

171

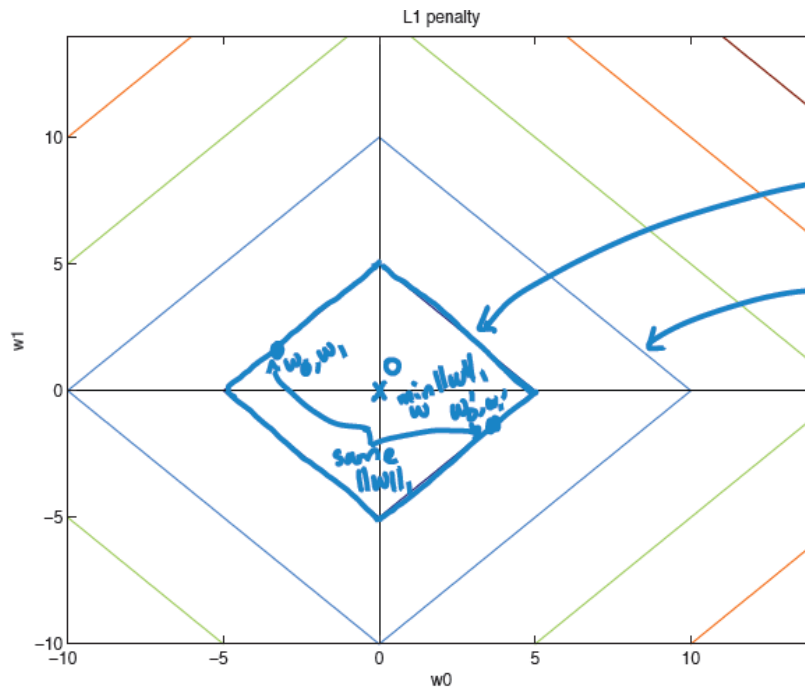


RSS contours for lasso are exactly the same as those for ridge!

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

Visualising lasso cost in 2D

172



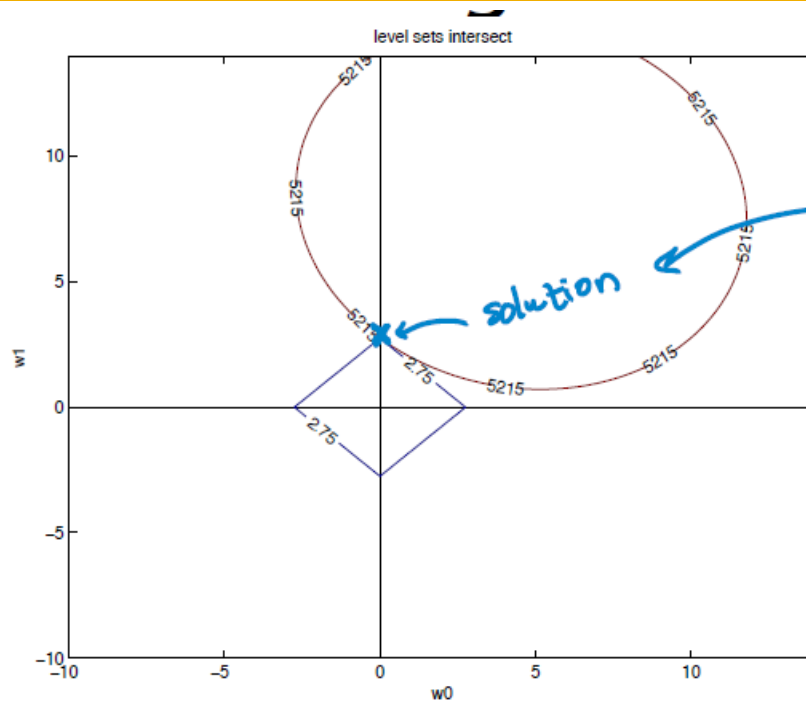
$\|w\|_1 = \text{const}_1$
 $\|w\|_1 = \text{const}_2 > \text{const}_1$
 \vdots

$|w_0| + |w_1| = \text{constant}$
diamond

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

Visualising lasso cost in 2D

173



For a specific value of λ ,

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

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

How we optimise for objective

174

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

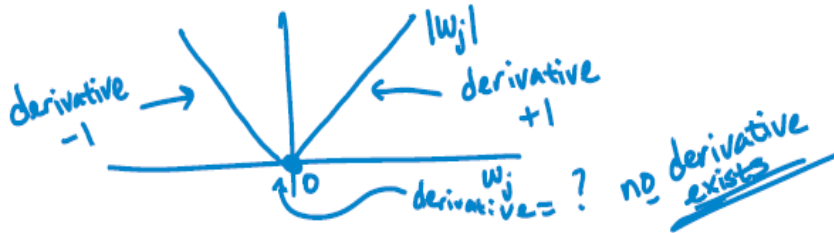
175

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

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

Issues:

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



gradients \rightarrow subgradients

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

can use subgradient descent

Coordinate descent

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Goal: Minimize some function g

$$\min_{\mathbf{w}} g(\mathbf{w})$$

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

when keeping others fixed

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

Coordinate descent:

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

while not converged

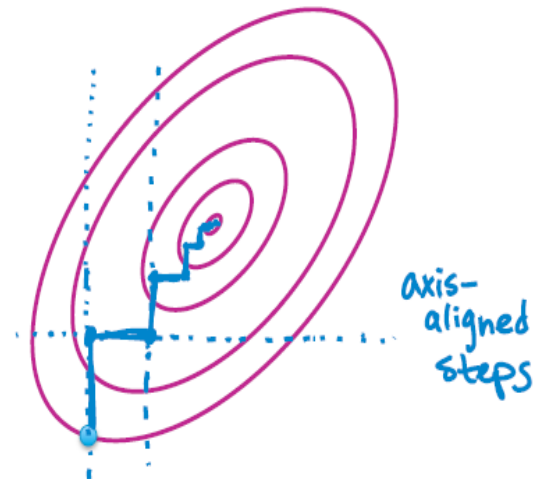
pick a coordinate j

$$\hat{w}_j \leftarrow$$

values from previous iterations

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

just min over j th coordinate



Comments on coordinate descent

177

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

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Normalizing features

Scale training columns (not rows!)
as:

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

Normalizer: z_j

Apply same training scale factors
to test data:

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

apply to test point

Normalizer: z_j

summing over training points



Optimising least squares objective

179

One coordinate at a time

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

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

$$\begin{aligned} \frac{\partial}{\partial w_j} \text{RSS}(\mathbf{w}) &= -2 \sum_{i=1}^N \underline{h}_j(\mathbf{x}_i) \left(y_i - \sum_{j=0}^D w_j \underline{h}_j(\mathbf{x}_i) \right) \\ &= -2 \sum_{i=1}^N \underline{h}_j(\mathbf{x}_i) \left(y_i - \sum_{k \neq j} w_k \underline{h}_k(\mathbf{x}_i) - w_j \underline{h}_j(\mathbf{x}_i) \right) \\ &= -2 \sum_{i=1}^N \underline{h}_j(\mathbf{x}_i) \left(y_i - \sum_{k \neq j} w_k \underline{h}_k(\mathbf{x}_i) \right) + 2 w_j \sum_{i=1}^N \underline{h}_j(\mathbf{x}_i)^2 \\ &\quad \underbrace{\hspace{10em}}_{\triangleq p_j} \\ &= -2 p_j + 2 w_j \end{aligned}$$

by definition of normalized features, = 1

Optimising least squares objective

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$$\text{RSS}(\mathbf{w}) = \sum_{i=1}^N \left(y_i - \sum_{j=0}^D w_j h_j(\mathbf{x}_i) \right)^2$$

Set partial = 0 and solve

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

$\hat{w}_j = \rho_j$

Coordinate descent for least squares regression

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

while not converged

for $j=0,1,\dots,D$

compute:

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

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

↑
prediction
without feature j

↑
Measure of the correlation between \mathbf{w}_j
and the residual without this feature.

How to access convergence

182

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

while not converged

for $j=0,1,\dots,D$

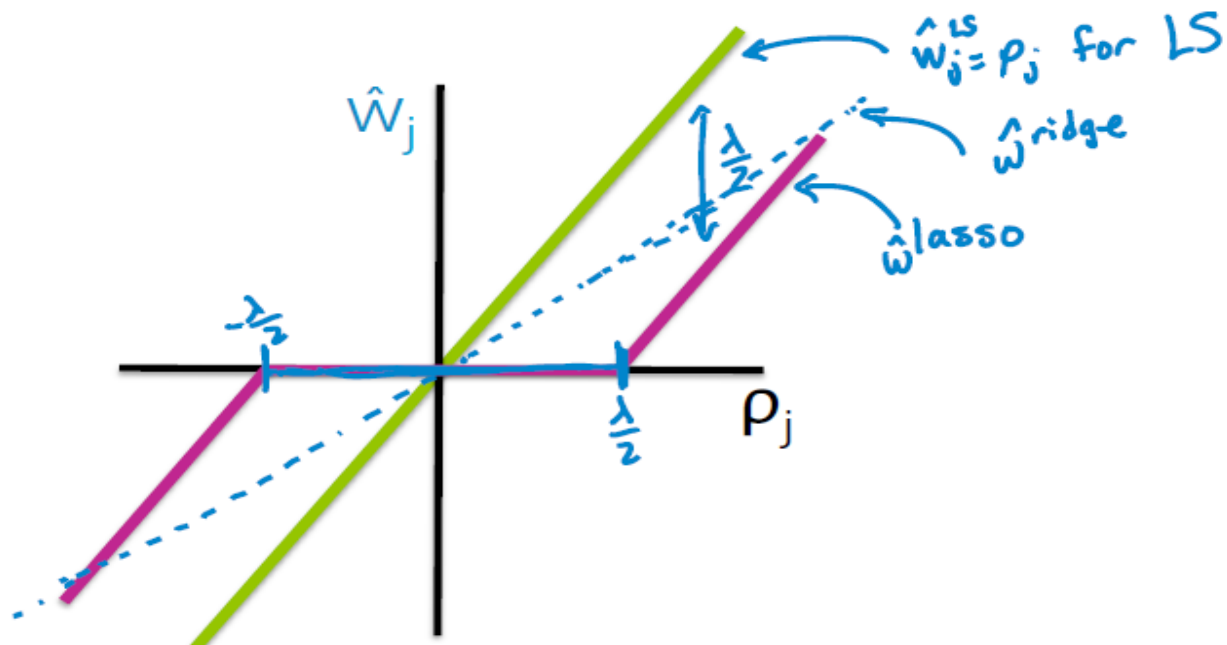
compute: $\rho_j = \sum_{i=1}^N \underline{h}_j(\mathbf{x}_i)(y_i - \hat{y}_i(\hat{\mathbf{w}}_{-j}))$

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

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



Convergence criteria

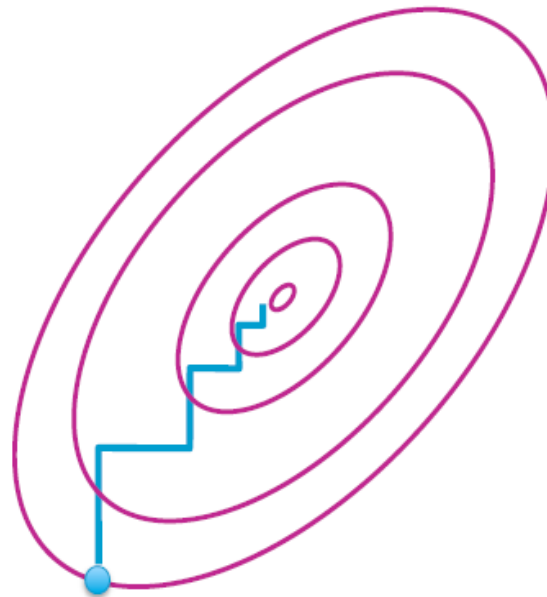
184

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 **$\max \text{ step} < \epsilon$**



Other lasso solvers

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

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

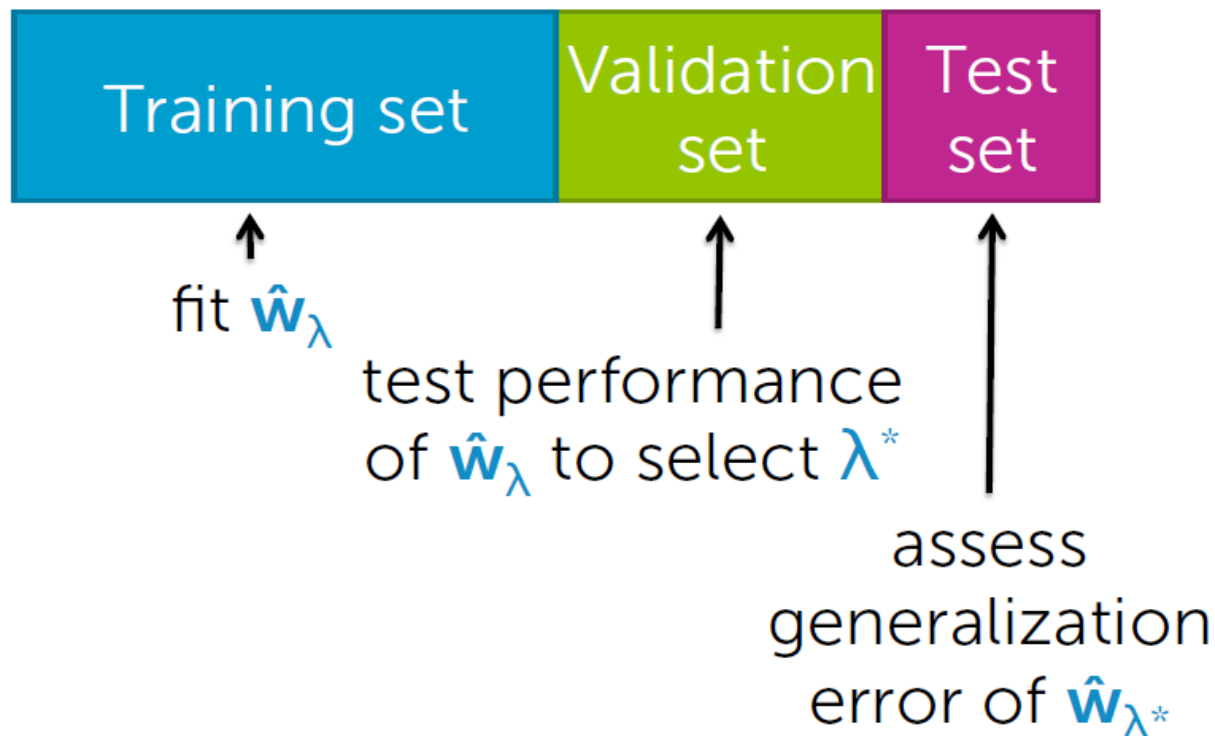
Now:

- **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 choose λ

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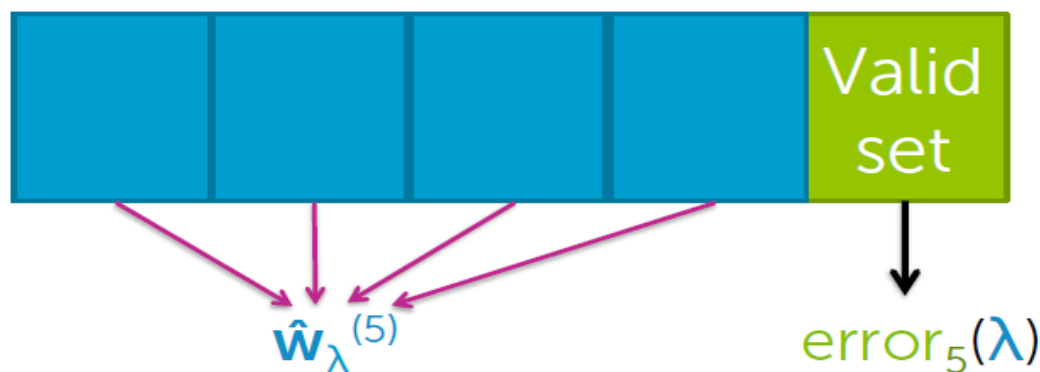
If sufficient amount of data...



How do we choose λ

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K-fold cross validation



For $k=1, \dots, K$

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

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

How do we chose λ

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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

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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

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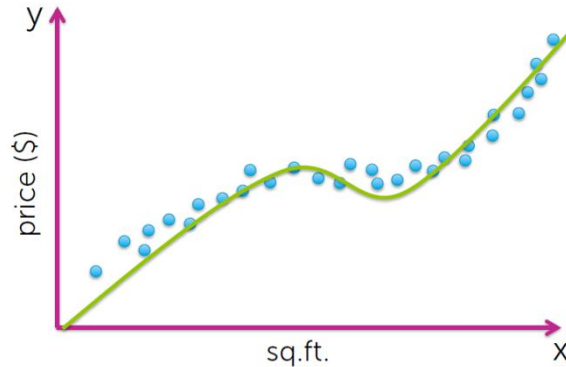
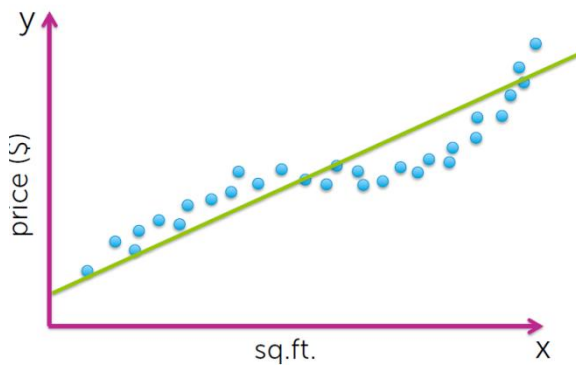
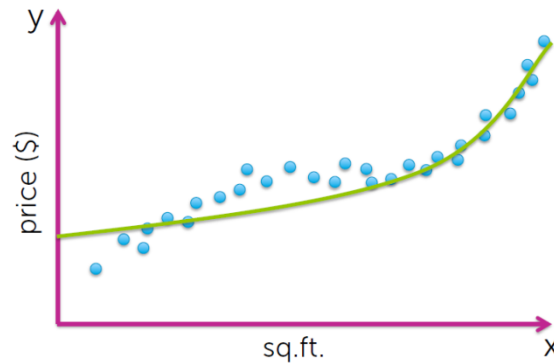
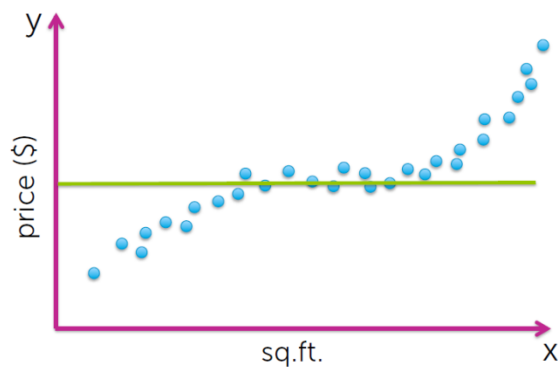
- Perform feature selection using “all subsets” and “forward stepwise” algorithms
- Analyze computational costs of these algorithms
- Contrast greedy and optimal algorithms
- Formulate lasso objective
- Describe what happens to estimated lasso coefficients as tuning parameter λ is varied
- Interpret 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

Fit globaly vs fit locally

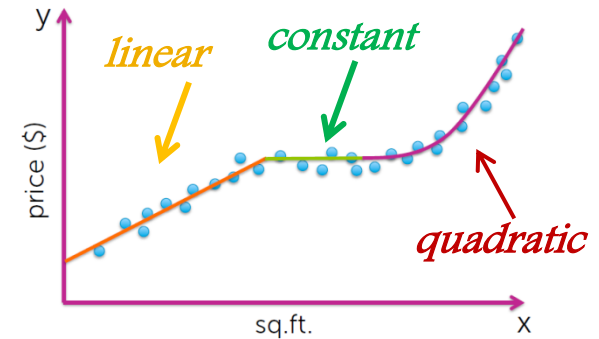
192

Parametric models



Below ...

*$f(x)$ is not really
a polynomial function*



What alternative do we have?

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If we:

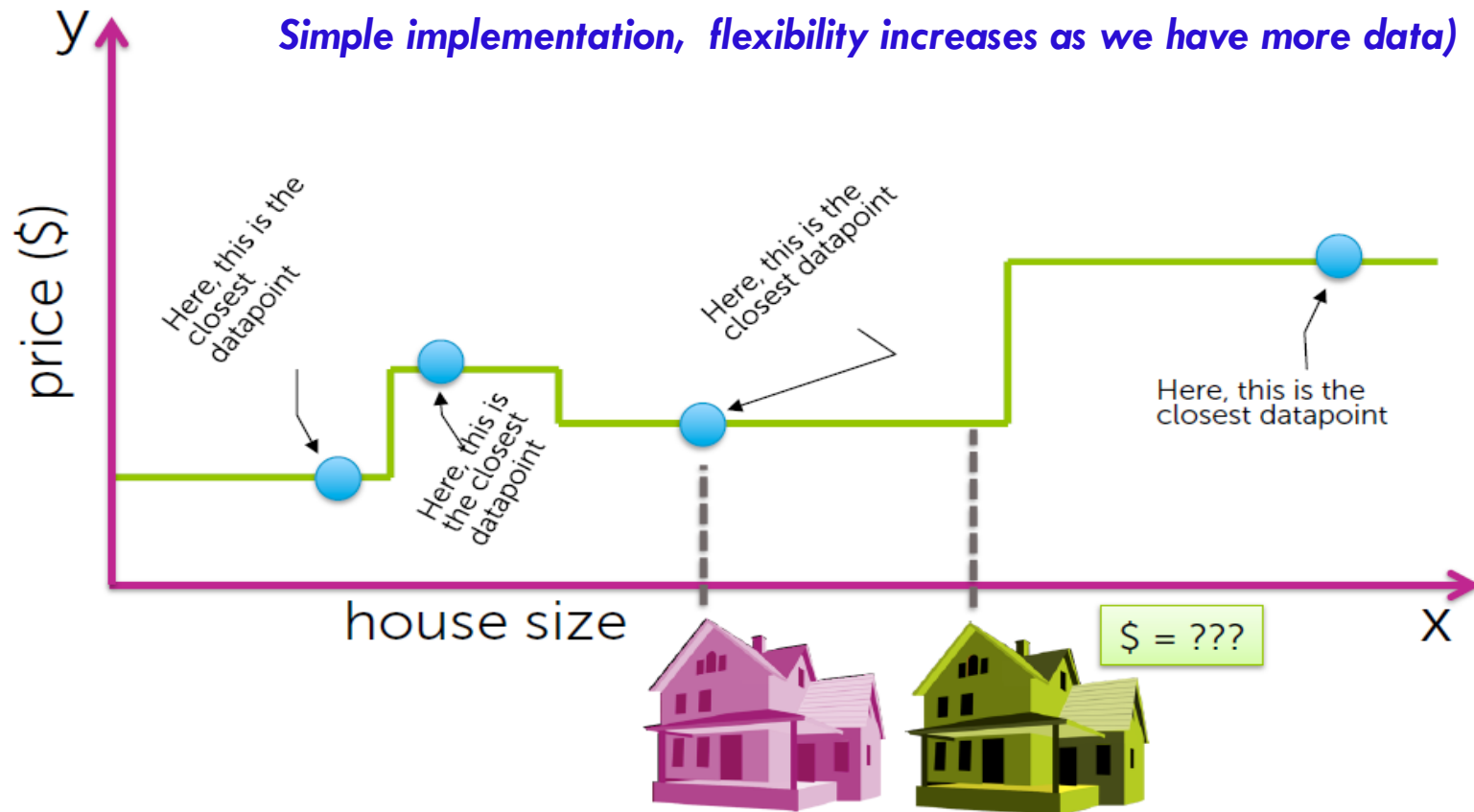
- Want to allow flexibility in $f(\mathbf{x})$ having local structure
- Don't want to infer “structural breaks”

What's a simple option we have?

- Assuming we have plenty of data...

Nearest Neighbor & Kernel Regression (nonparametric approach)

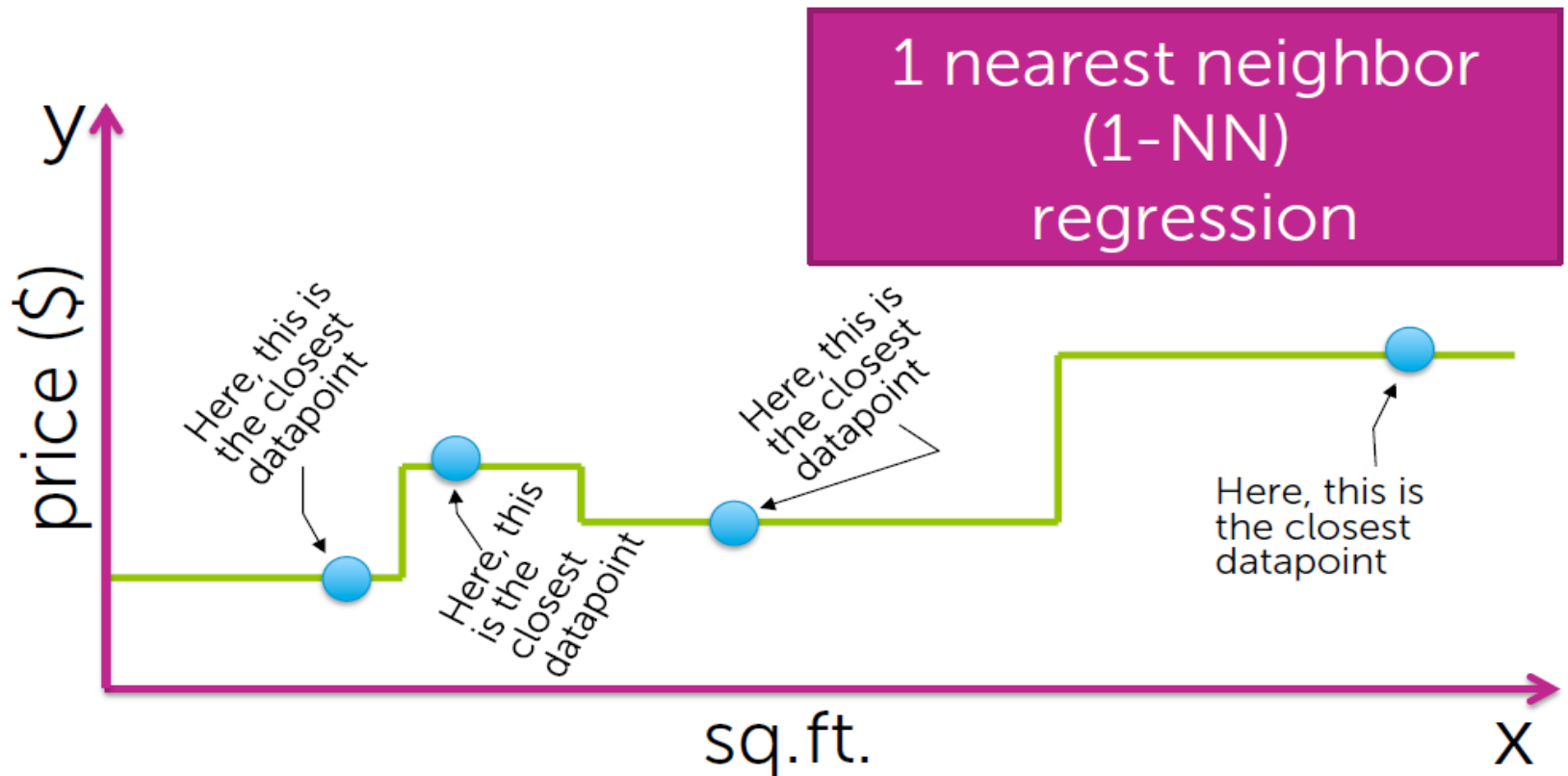
194



Fit locally to each data point

195

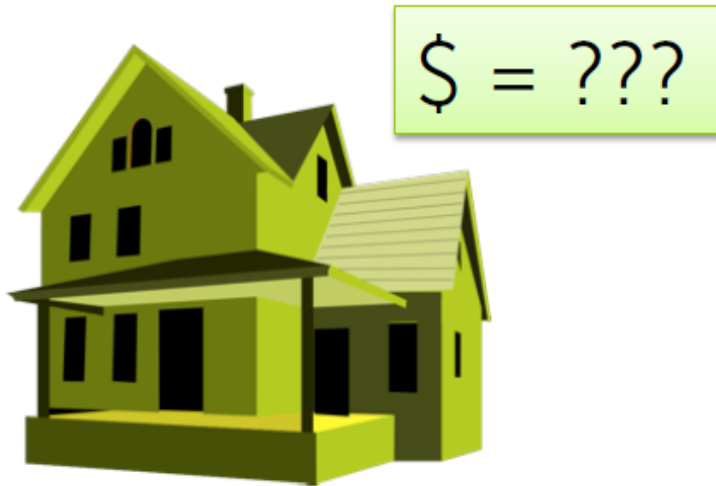
Predicted value = "closest" y_i



What people do naturally...

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



1-NN regression more formally

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

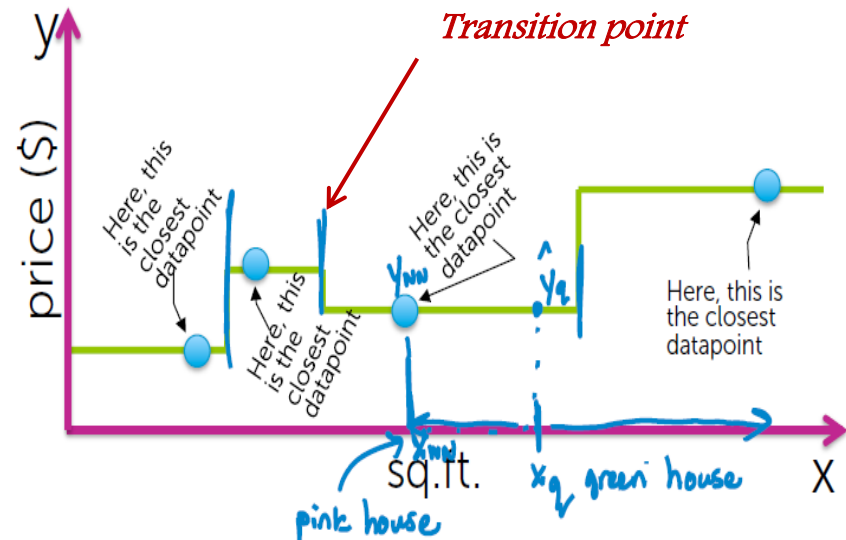
Query point: \mathbf{x}_q ← 🏠 \$?
big lime green house

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

$x_{NN} \leftarrow \min_i \text{distance}(x_i, x_q)$
big pink house

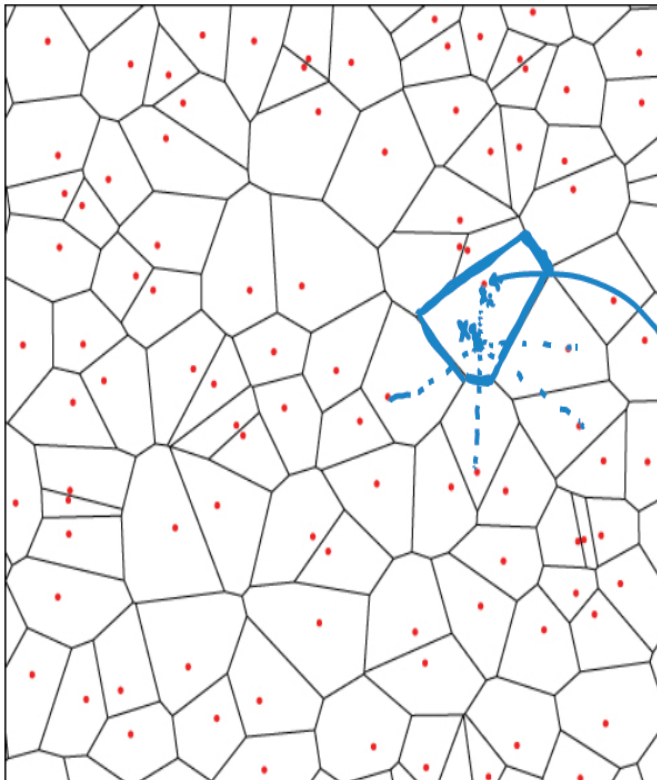
2. Predict

$\hat{y}_q = y_{NN}$
sales price of big pink house



Visualizing 1-NN in multiple dimensions

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Voronoi tessellation (or diagram):

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

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

Don't explicitly form!

Distance metrics: Notion of „closest”

199

In 1D, just Euclidean distance:

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

In multiple dimensions:

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

Weighting housing inputs

200

Some inputs are more relevant than others



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



Scaled Euclidan distance

201

Formally, this is achieved via

$$\text{distance}(\mathbf{x}_j, \mathbf{x}_q) =$$

$$\sqrt{a_1(\mathbf{x}_j[1] - \mathbf{x}_q[1])^2 + \dots + a_d(\mathbf{x}_j[d] - \mathbf{x}_q[d])^2}$$

weight on each input
(defining relative importance)

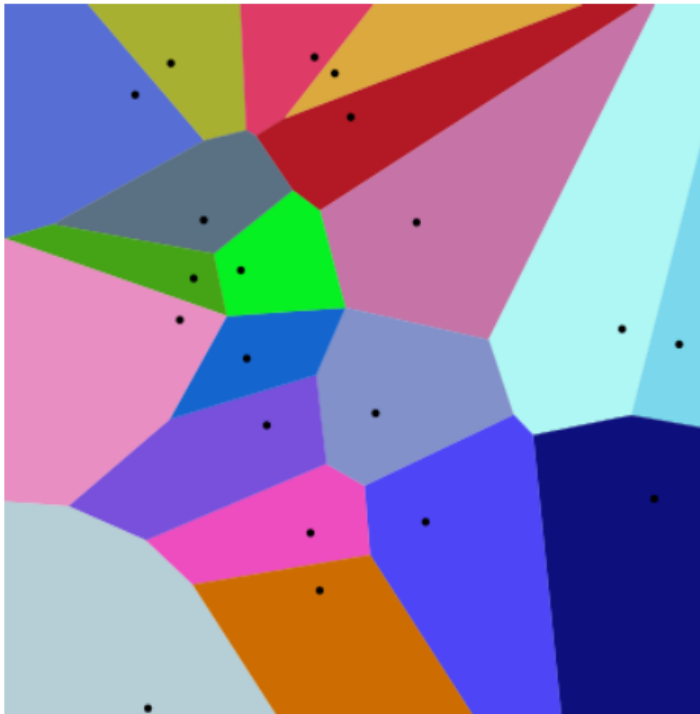
Other example distance metrics:

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

Different distance metrics

202

Euclidean distance



Manhattan distance



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Performing 1-NN search

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- Query house:



- Dataset:




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




1-NN algorithm



204

Initialize **Dist2NN** = ∞ ,  = \emptyset ← closest house



For $i=1,2,\dots,N$

 Compute: $\delta = \text{distance}(\text{img alt="house icon" data-bbox="535 445 590 515"}, \text{img alt="house icon" data-bbox="620 445 675 515"}_q)$ ← query house 

 If $\delta < \text{Dist2NN}$

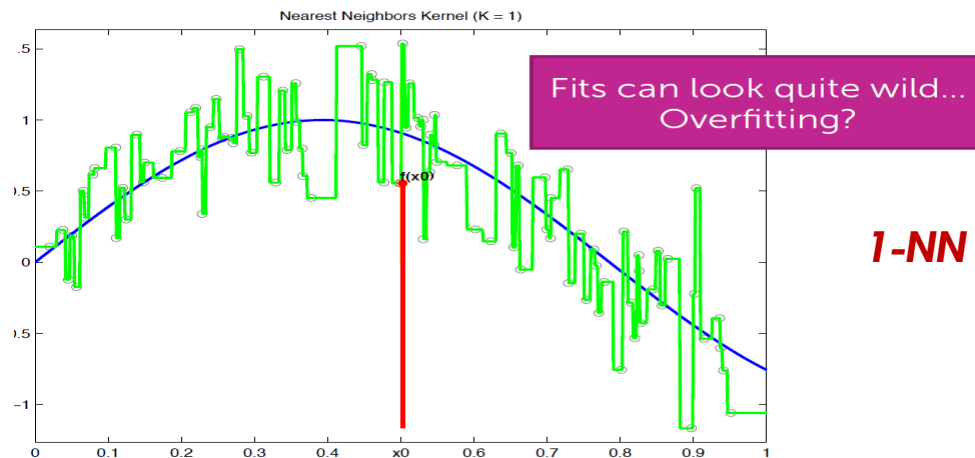
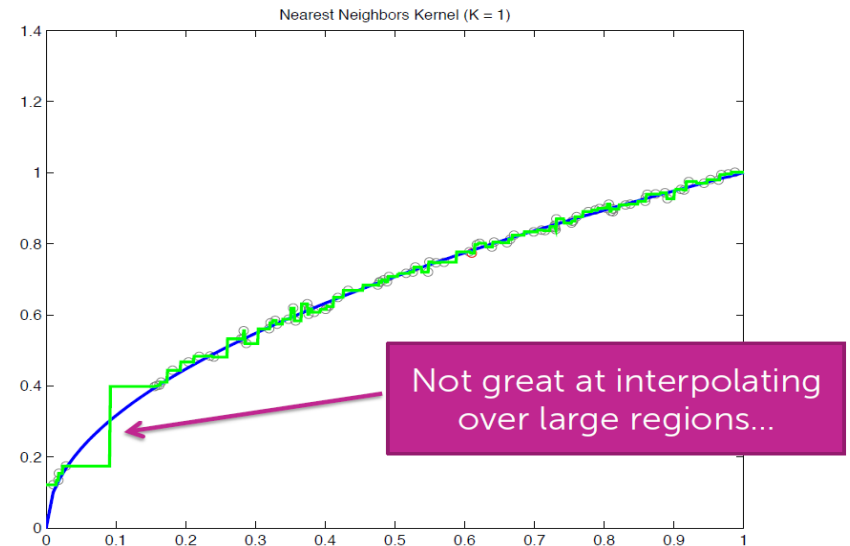
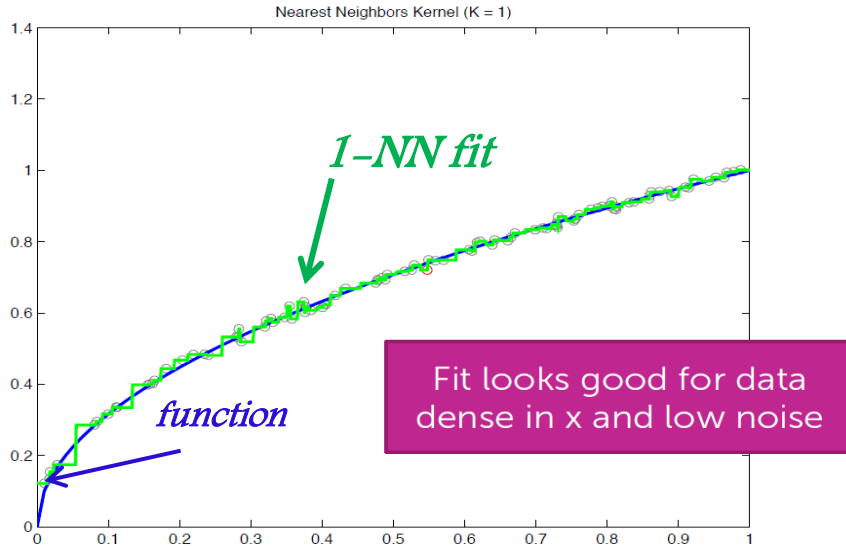
 set   _{i}

 set **Dist2NN** = δ

Return most similar house  ← closest house to query house 

1-NN in practice

205



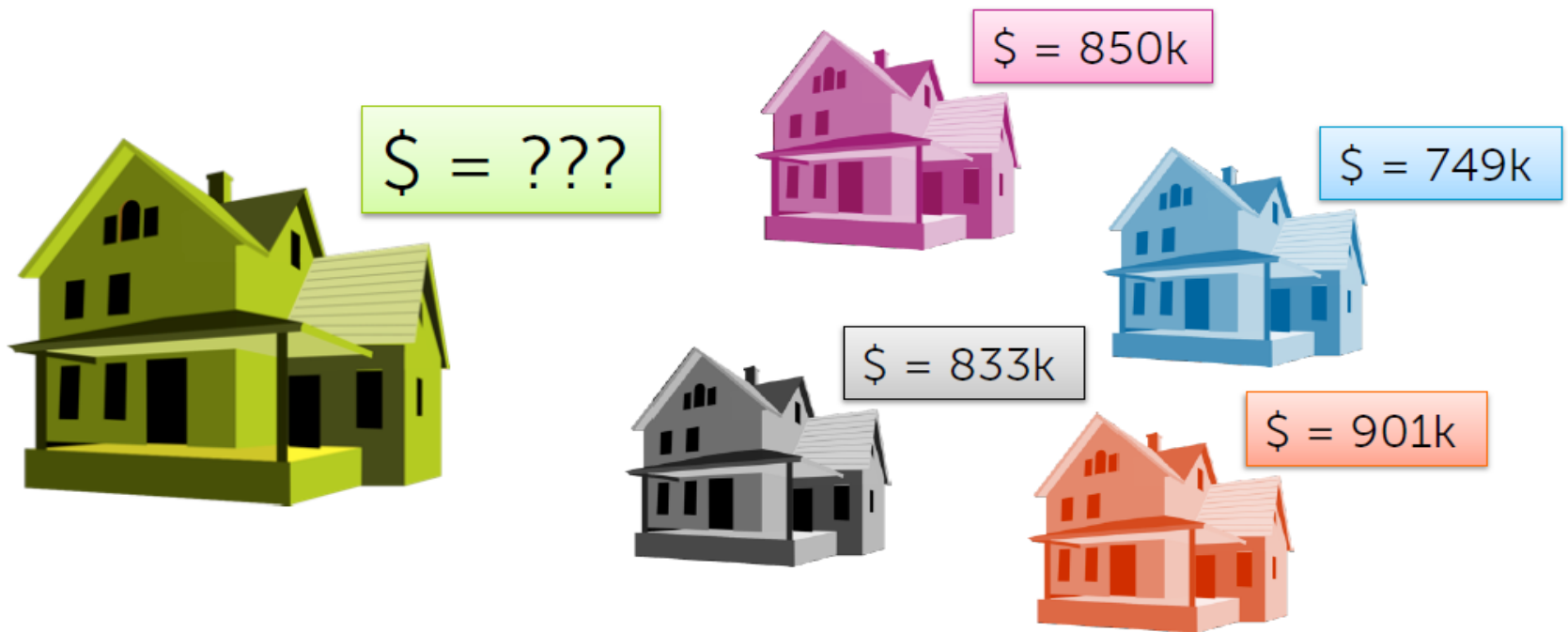
1-NN sensitive to noise in the data

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Get more „comps”

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



K-NN regression more formally

207

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

Query point: \mathbf{x}_q

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

$(x_{NN1}, x_{NN2}, \dots, x_{NNk})$ such that for any x_i not in nearest neighbor set,
 $\text{distance}(x_i, x_q) \geq \text{distance}(x_{NNk}, x_q)$

2. Predict

$$\begin{aligned}\hat{y}_q &= \frac{1}{k} (y_{NN1} + y_{NN2} + \dots + y_{NNk}) \\ &= \frac{1}{k} \sum_{j=1}^k y_{NNj}\end{aligned}$$

K-NN more formally

208

- Query house:



- Dataset:



- **Specify:** Distance metric
- **Output:** Most similar houses



K-NN algorithm

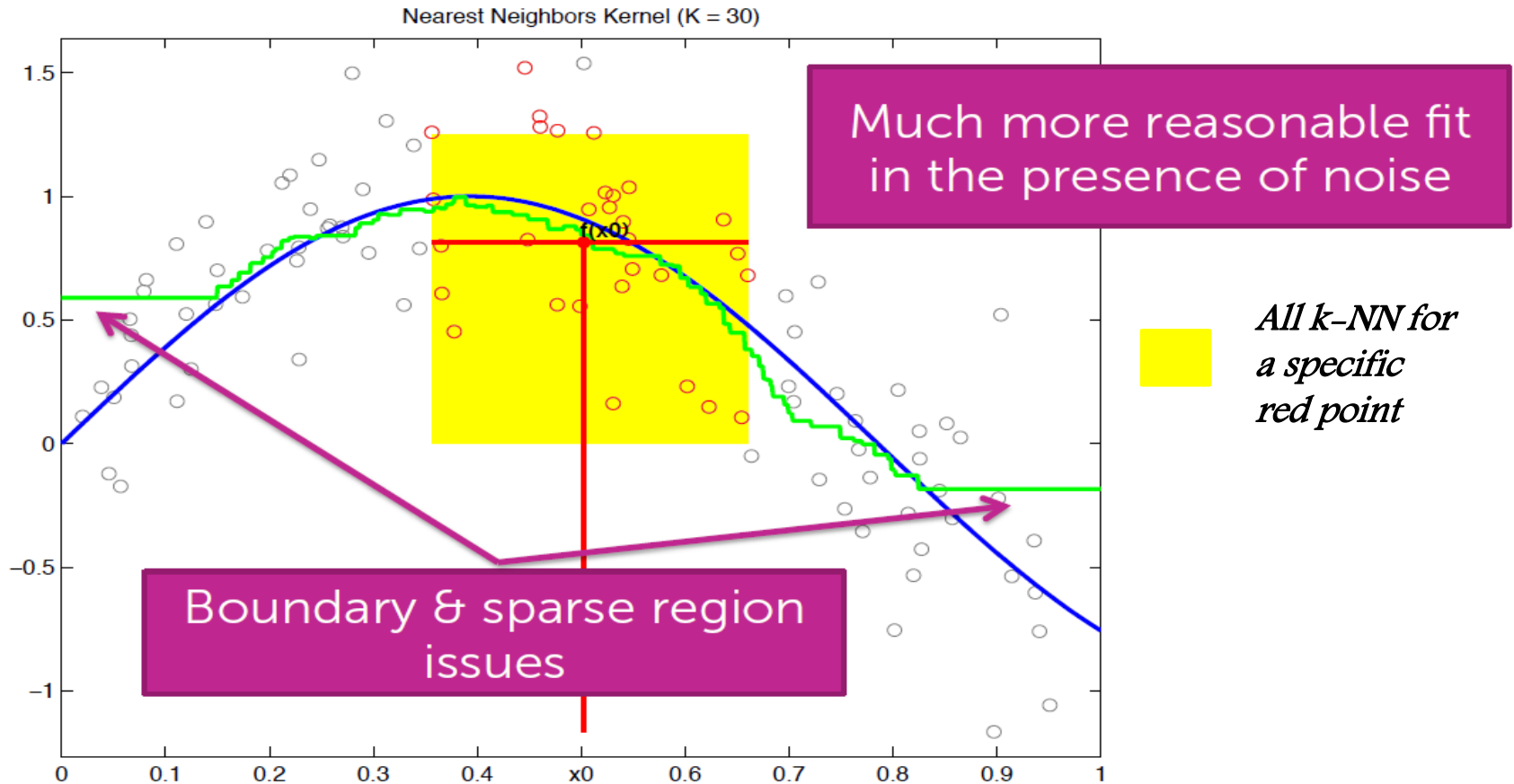
209

Initialize **Dist2kNN** = $\text{sort}(\delta_1, \dots, \delta_k)$ ← list of sorted distances
 $= \text{sort}(\text{house}_1, \dots, \text{house}_k)$ ← list of sorted houses

For $i = k+1, \dots, N$
 Compute: $\delta = \text{distance}(\text{house}_i, \text{house}_q)$ ← query house
 If $\delta < \text{Dist2kNN}[k]$
 find j such that $\delta > \text{Dist2kNN}[j-1]$ but $\delta < \text{Dist2kNN}[j]$
 remove furthest house and shift queue:
 $[j+1:k] = [j:k]$
 $\text{Dist2kNN}[j+1:k] = \text{Dist2kNN}[j:k-1]$
insert new NN $\text{set } \text{Dist2kNN}[j] = \delta$ and $\text{house}_j = \text{house}_i$
 Return k most similar houses ← closest houses to query house

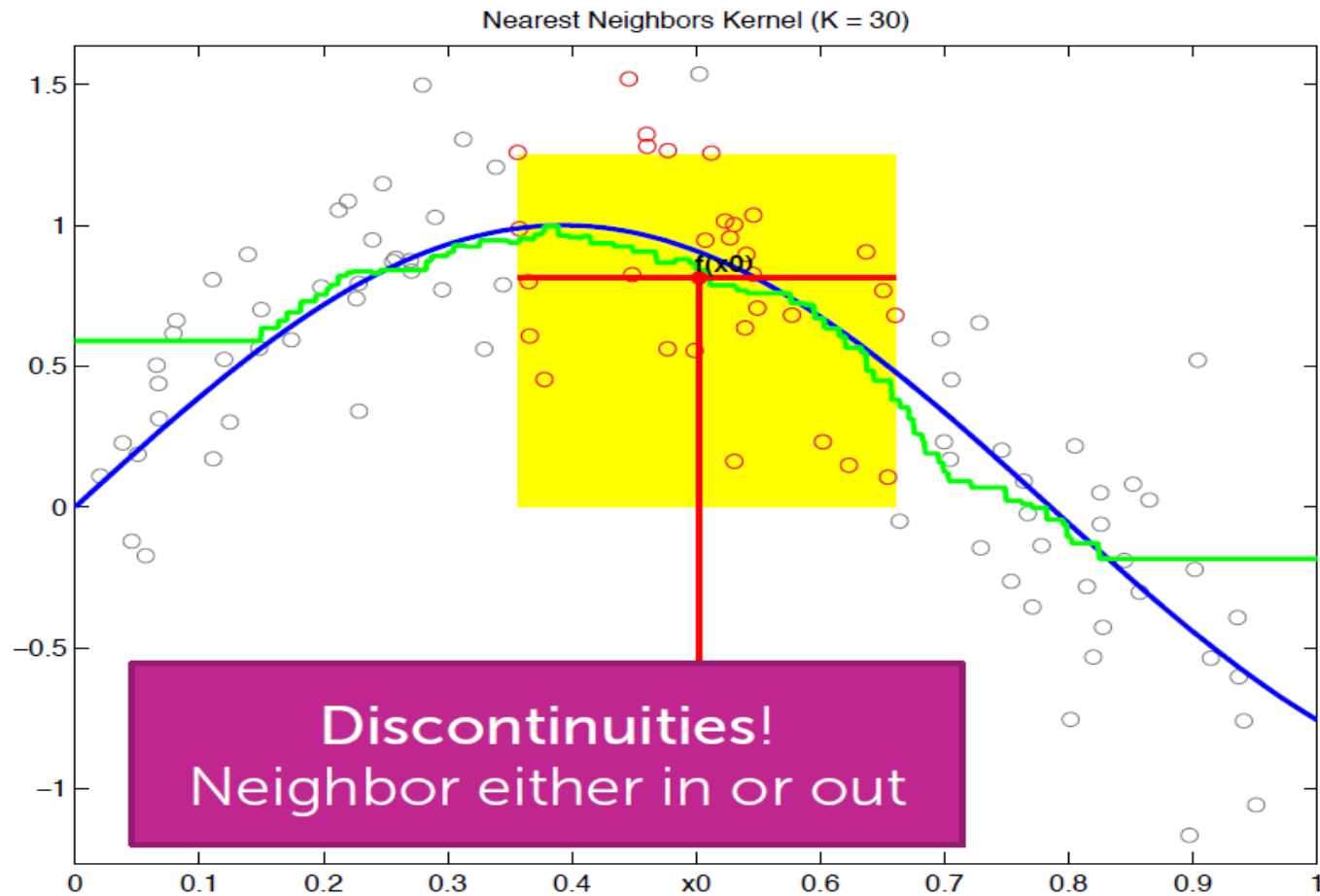
K-NN in practice

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K-NN in practice

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Issues with discontinuities

212

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

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

Predict:

weights on NN


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

How to define weights

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Want weight c_{qNNj} to be small when
 $\text{distance}(\mathbf{x}_{NNj}, \mathbf{x}_q)$ large

and c_{qNNj} to be large when
 $\text{distance}(\mathbf{x}_{NNj}, \mathbf{x}_q)$ small

Simple method :

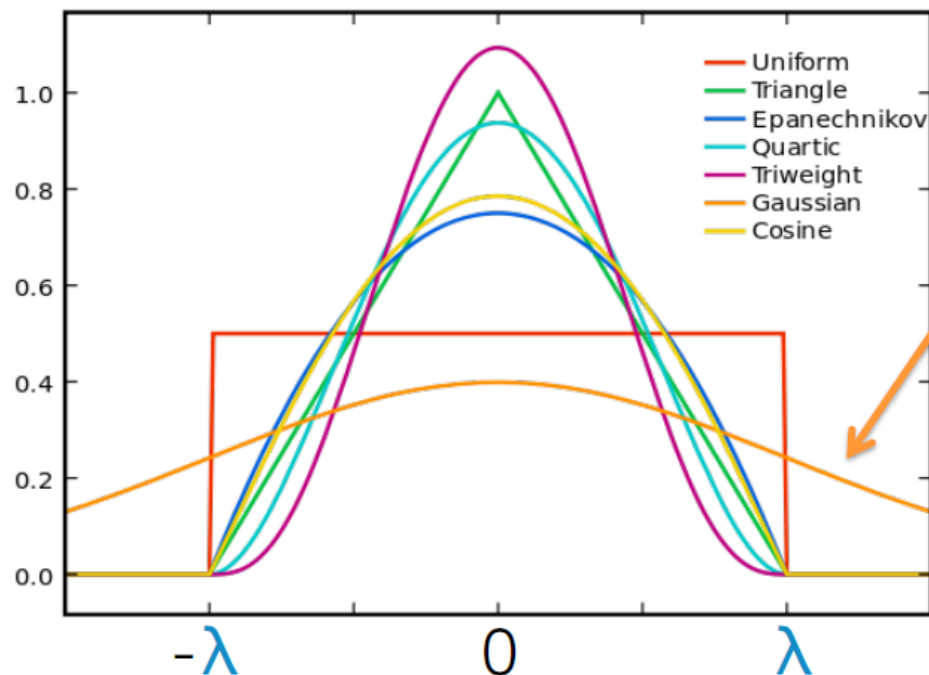
$$c_{qNNj} = \frac{1}{\text{distance}(\mathbf{x}_j, \mathbf{x}_q)}$$

Kernel weights for $d=1$

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

simple
isotropic case



Gaussian kernel:

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

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

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Instead of just weighting NN, weight *all* points

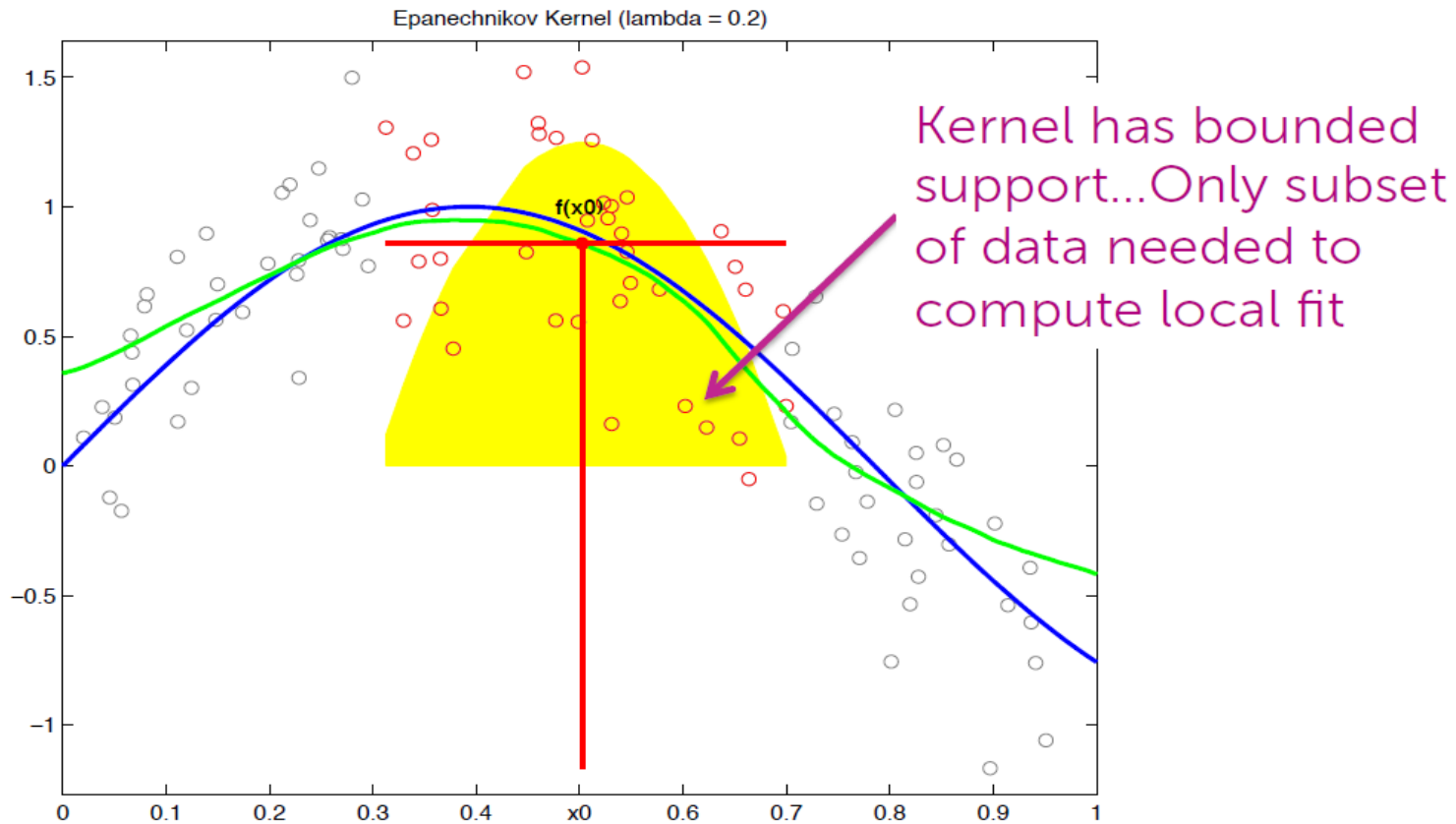
Predict:

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

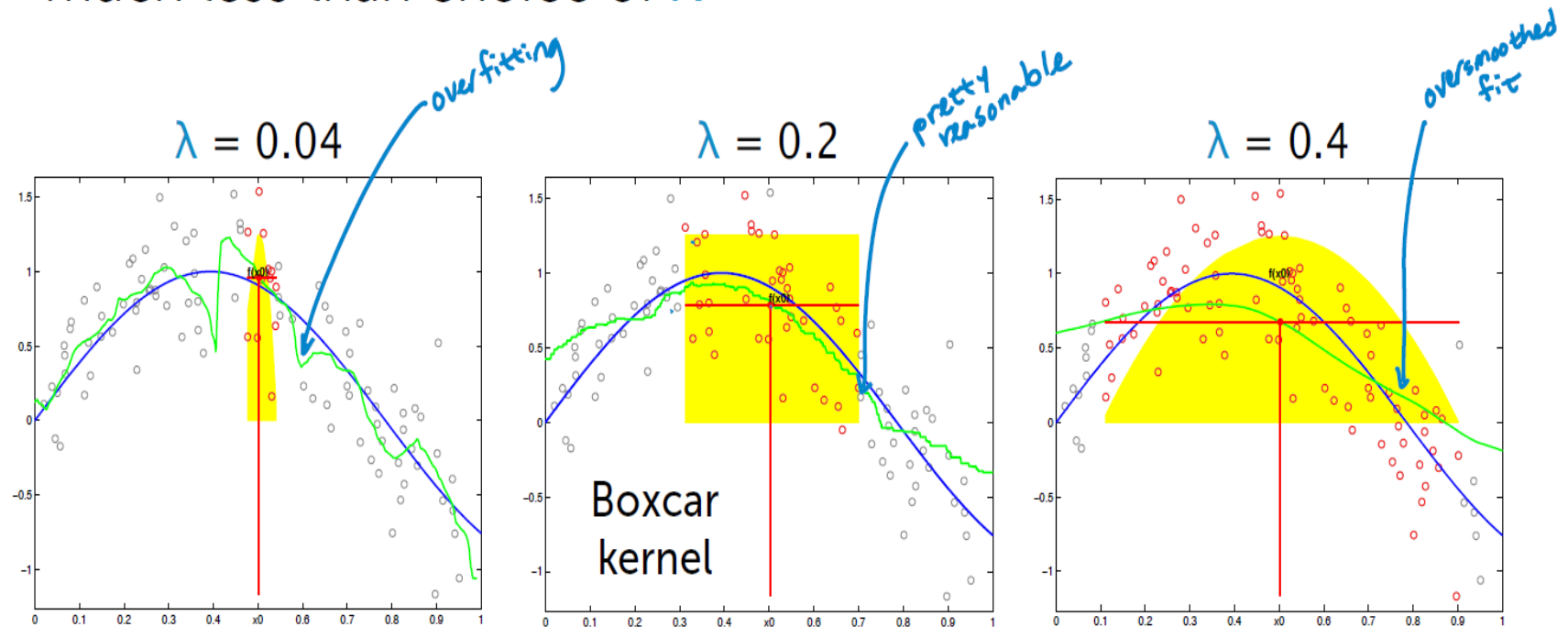
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Choice of bandwidth λ

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



Choosing λ (or k on k-NN)

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How to choose? Same story as always...

Cross Validation

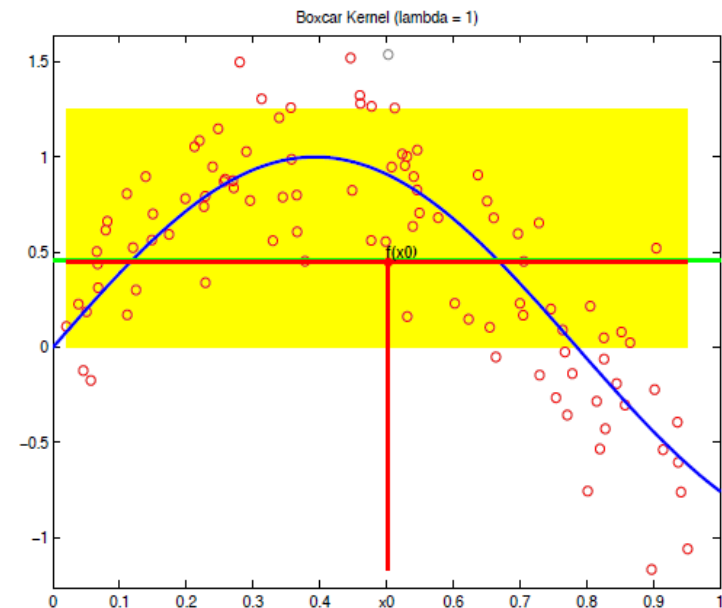
Contrasting with global average

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A globally constant fit weights all points equally

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

equal weight on each datapoint



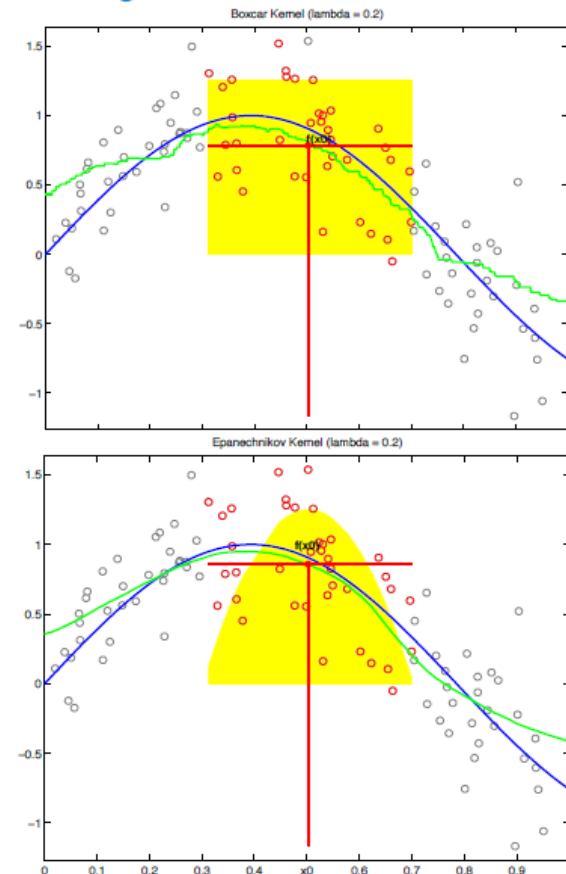
Contrasting with global average

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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

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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

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- 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

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k-NN and kernel regression are examples of **nonparametric** regression

General goals of nonparametrics:

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

Lots of other choices:

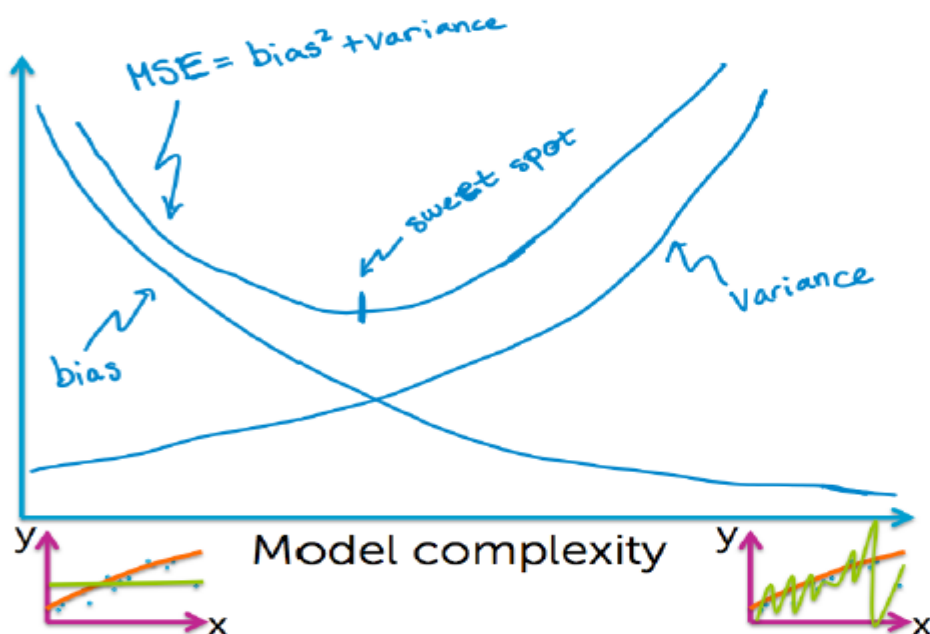
- Splines, trees, locally weighted structured regression models...

Limiting behaviour of NN

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Noiseless setting ($\epsilon_i=0$)

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

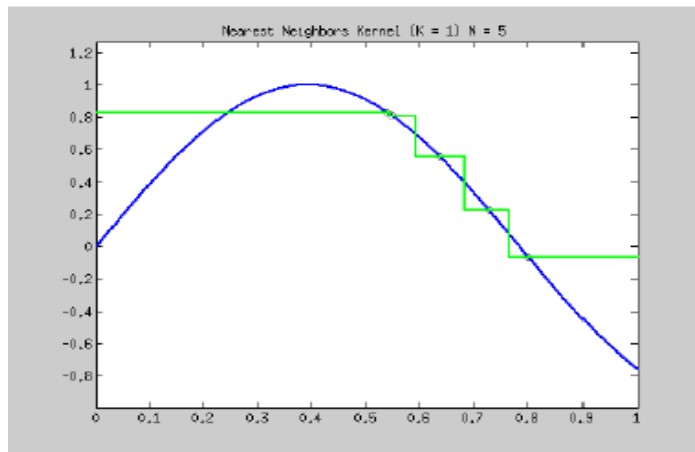


Limiting behaviour of NN

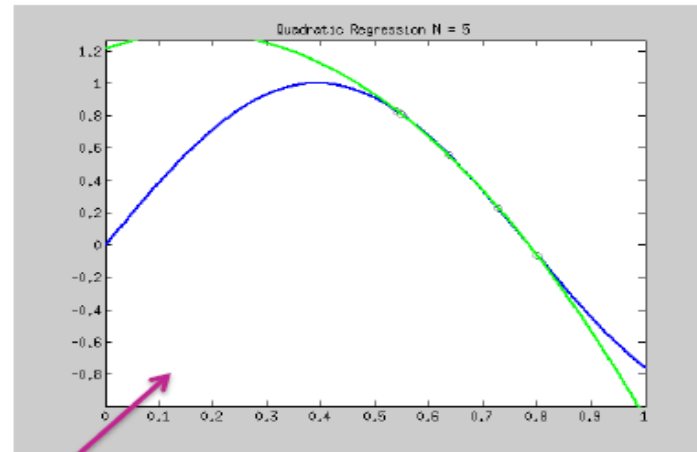
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Noiseless setting ($\epsilon_i=0$)

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



1-NN fit

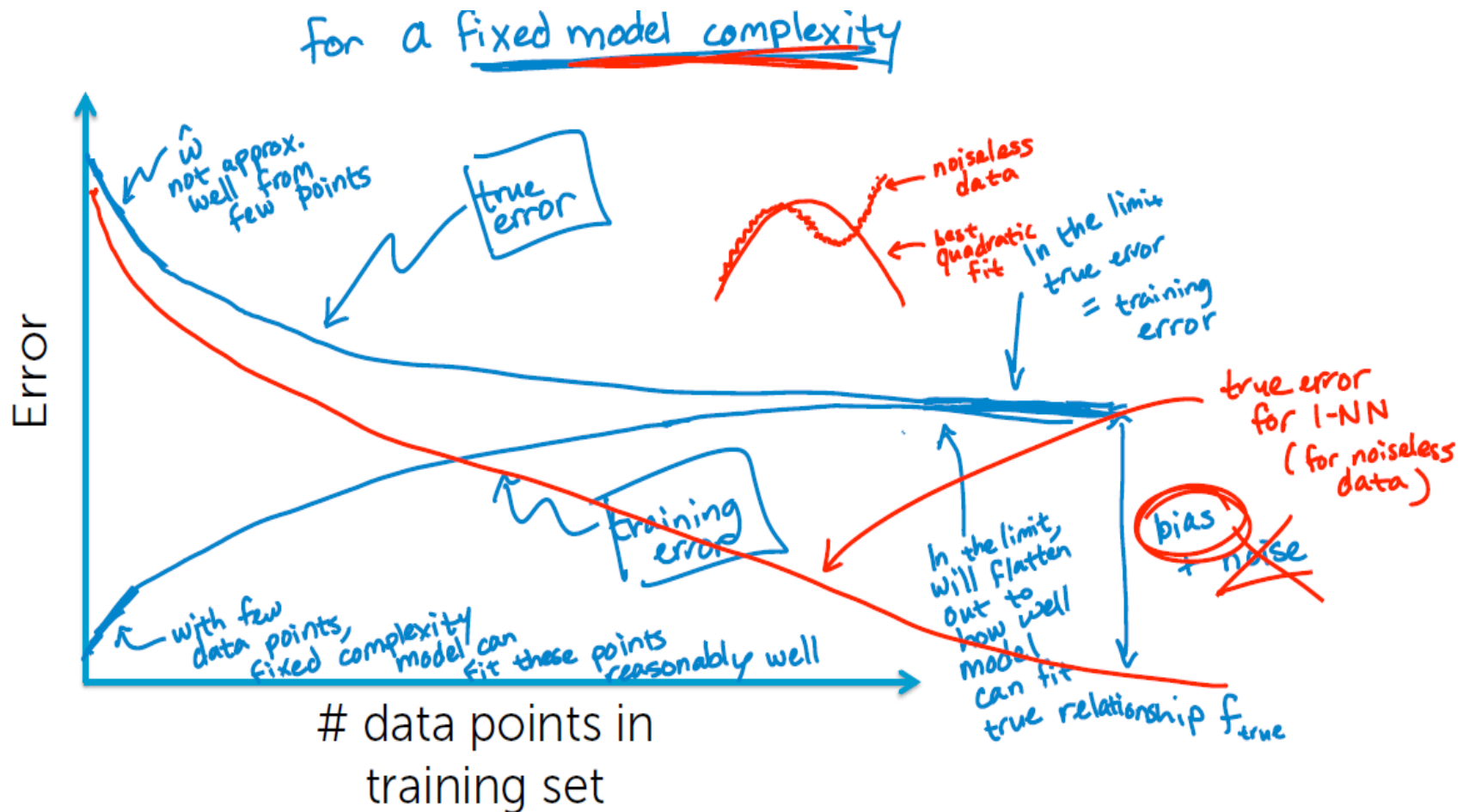


Quadratic fit

Not true for parametric models!

Error vs amount of data

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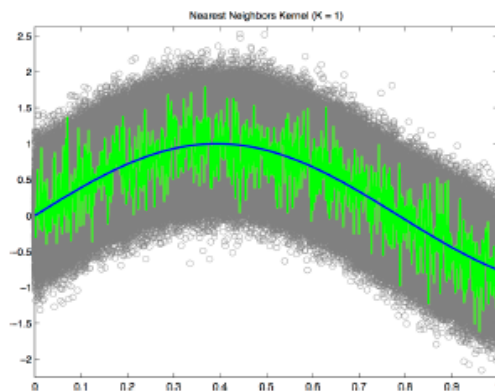


Limiting behaviour of NN

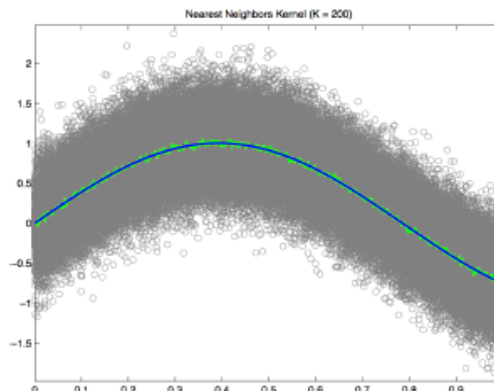
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Noisy data setting

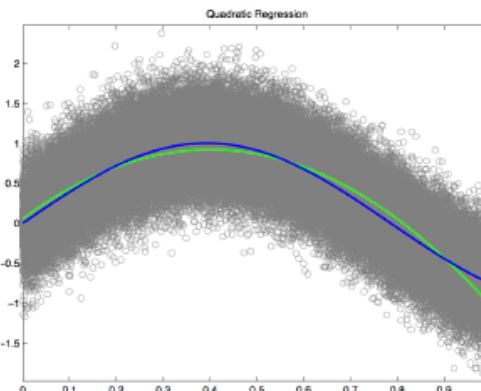
In the limit of getting an infinite amount of data, the **MSE of NN fit goes to 0** if **k grows, too**



1-NN fit



200-NN fit



Quadratic fit

Issues: NN and kernel methods

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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...

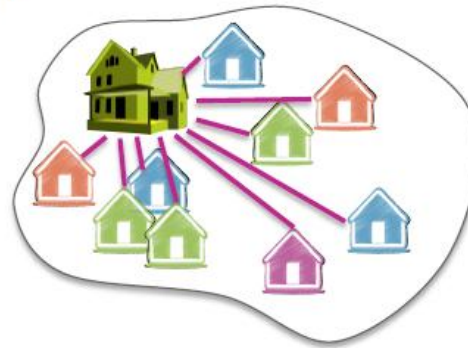
Issues: Complexity of NN search

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Naïve approach: **Brute force search**

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

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



Will talk more about efficient methods in
Clustering & Retrieval course

We discussed how to

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- 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

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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