

Simple Regression:

Linear regression with one input

Emily Fox & Carlos Guestrin

Machine Learning Specialization

University of Washington

Recall Task: Predicting house prices

How much is my house worth?



How much is my house worth?



Look at recent sales in my neighborhood

- How much did they sell for?



Regression fundamentals: data, model, task

Data

input output



($x_1 = \text{sq.ft.}$, $y_1 = \$$)



($x_2 = \text{sq.ft.}$, $y_2 = \$$)



($x_3 = \text{sq.ft.}$, $y_3 = \$$)



($x_4 = \text{sq.ft.}$, $y_4 = \$$)



($x_5 = \text{sq.ft.}$, $y_5 = \$$)

:

Data



input *output*
 $(x_1 = \text{sq.ft.}, y_1 = \$)$



$(x_2 = \text{sq.ft.}, y_2 = \$)$



$(x_3 = \text{sq.ft.}, y_3 = \$)$



$(x_4 = \text{sq.ft.}, y_4 = \$)$



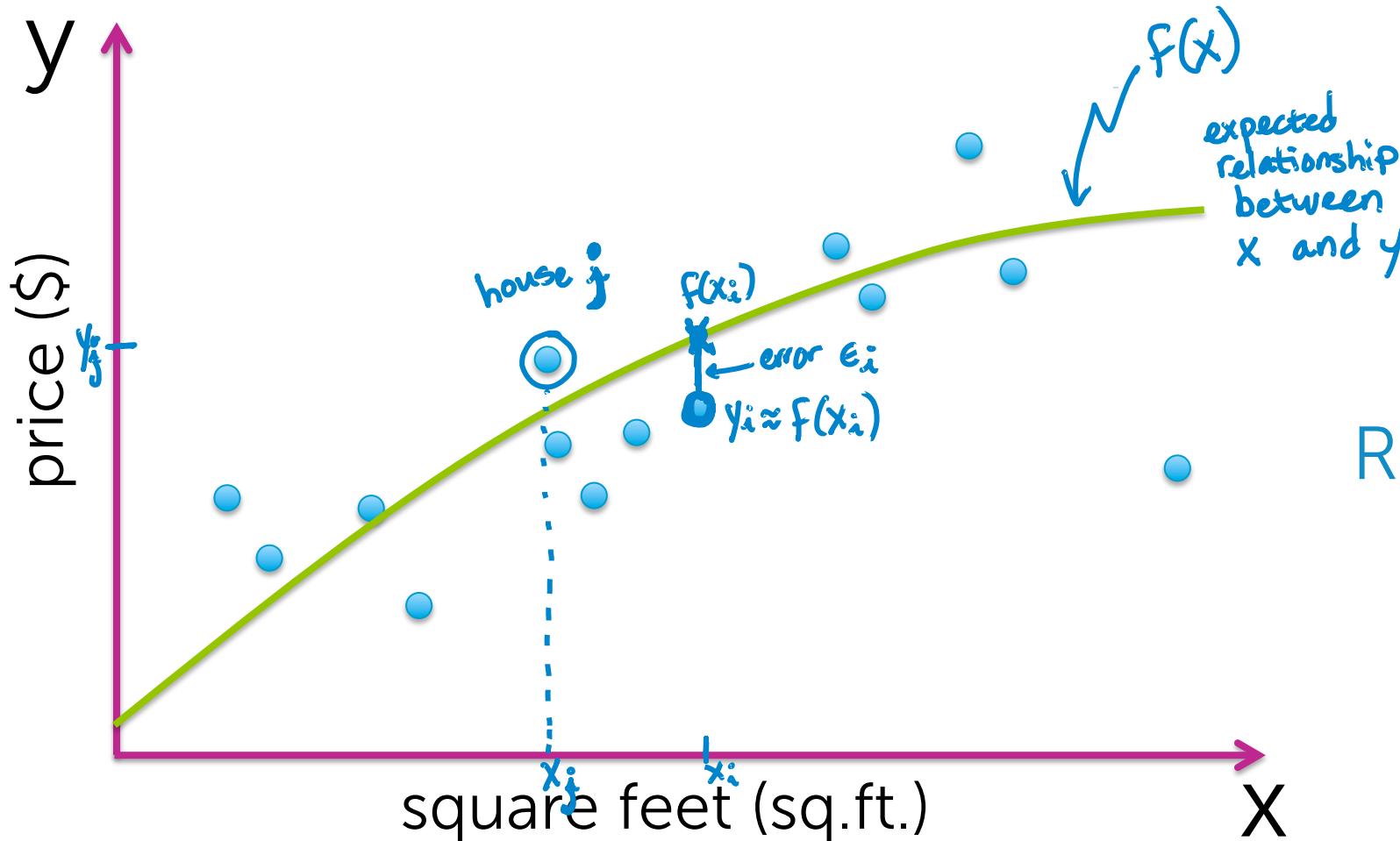
$(x_5 = \text{sq.ft.}, y_5 = \$)$

⋮

Input vs. Output:

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

Model – How we assume the world works



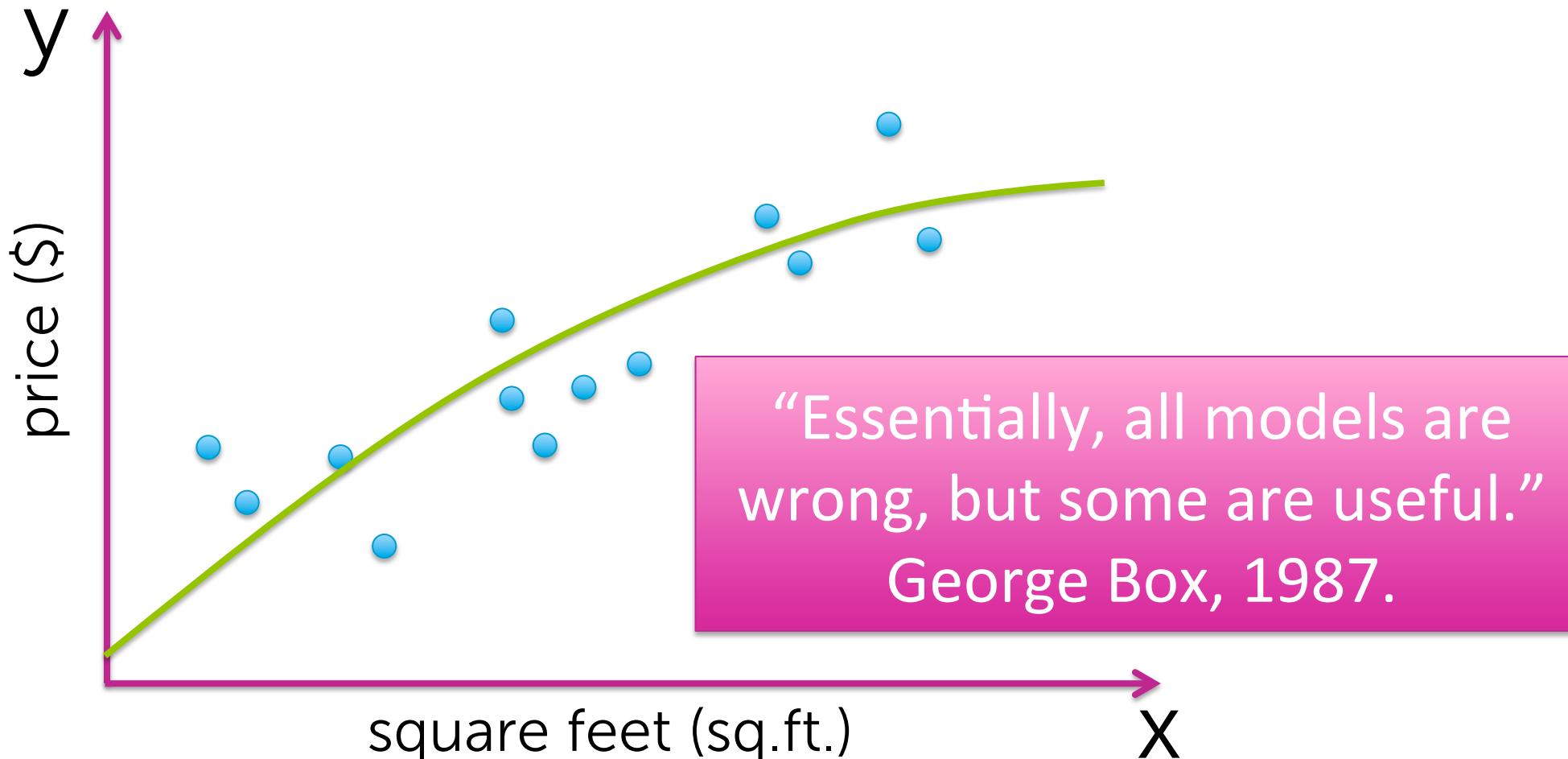
Regression model:

$$y_i = f(x_i) + e_i$$

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

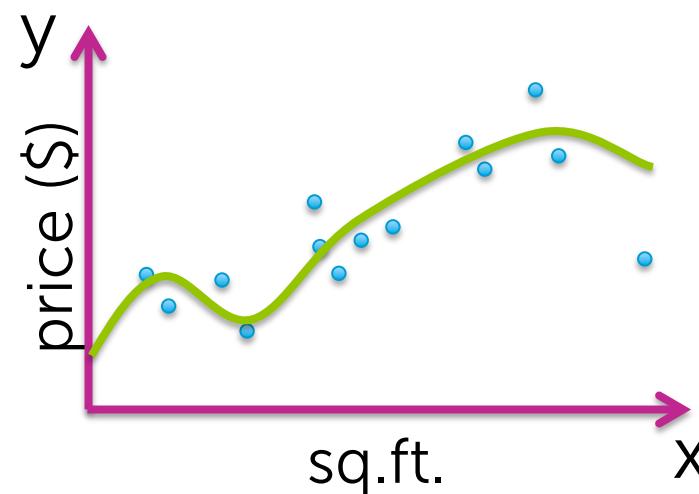
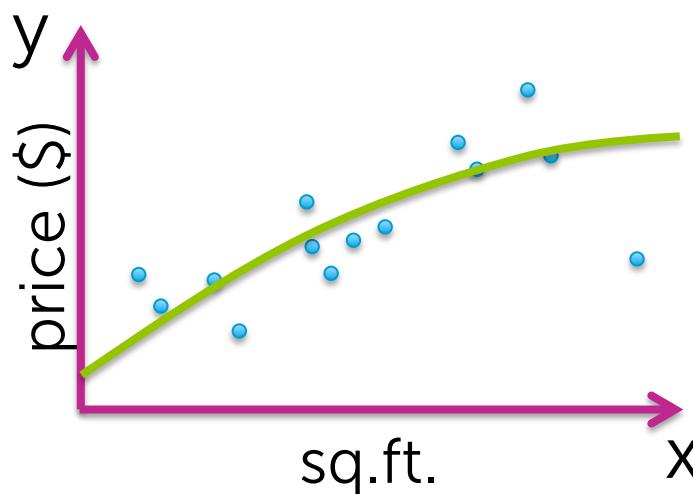
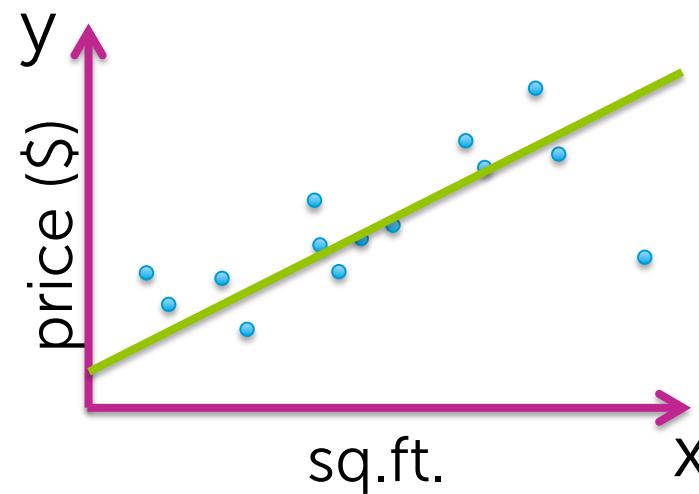
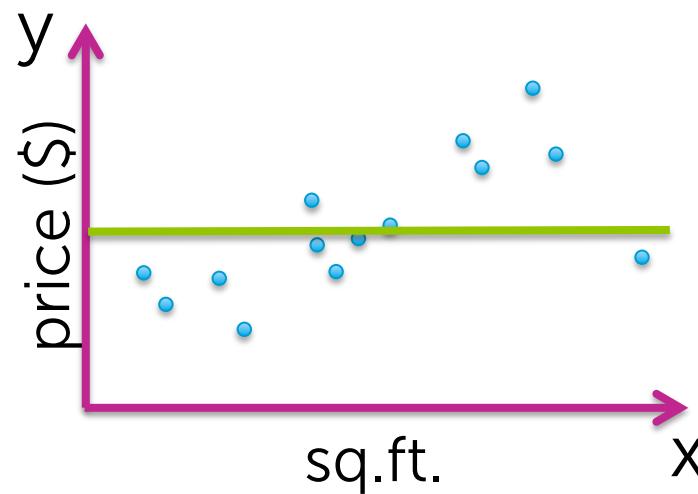
y_i is equally likely to be above or below $f(x_i)$

Model – How we *assume* the world works

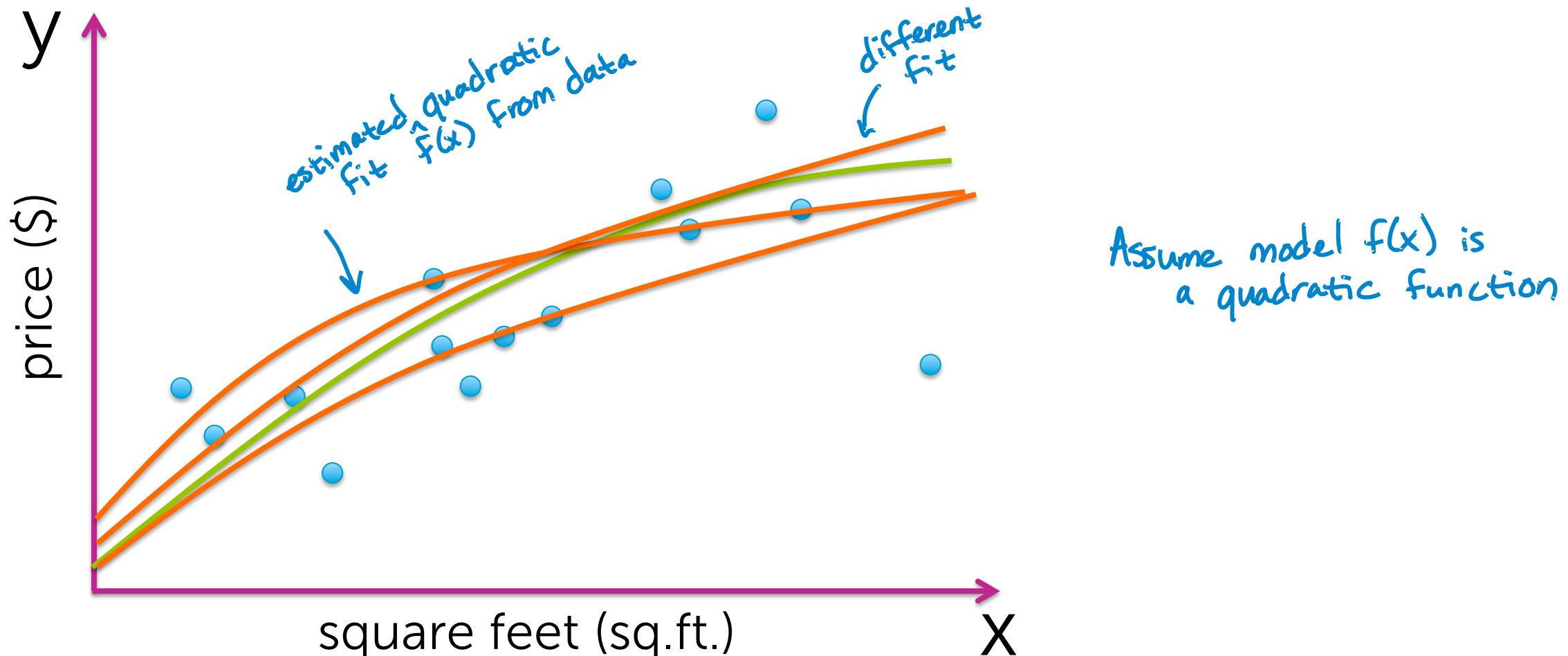


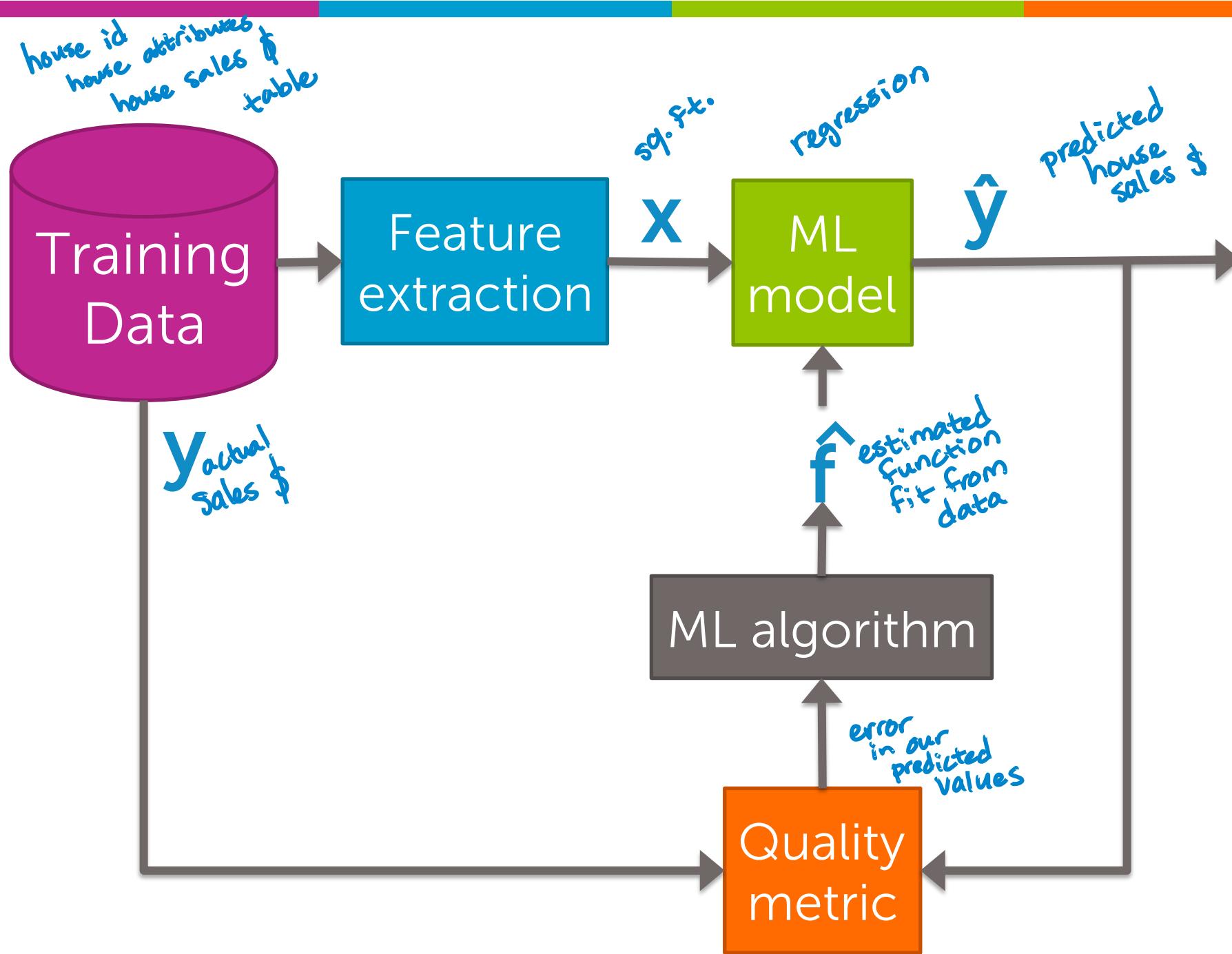
Task 1–

Which model $f(x)$?

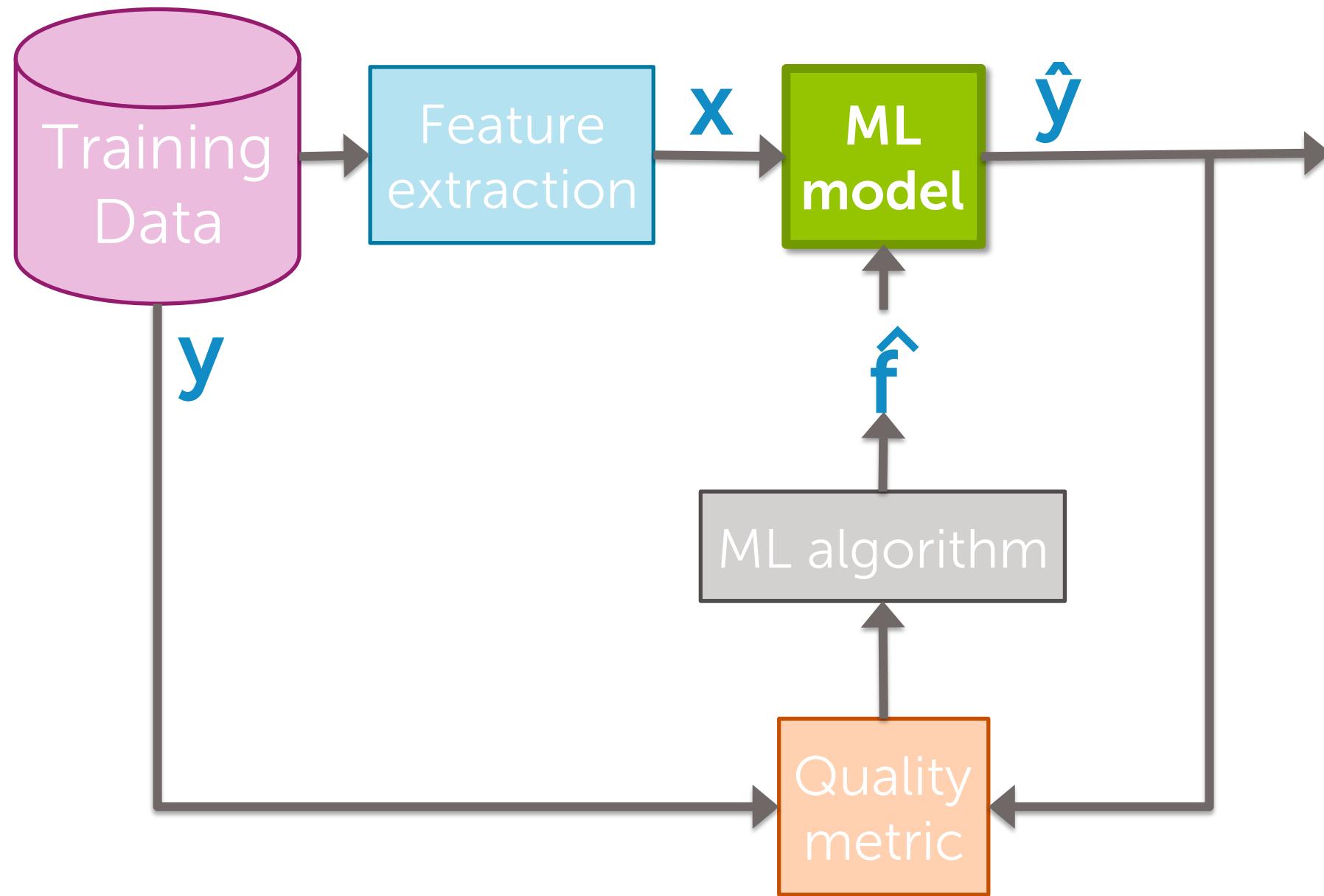


Task 2 – For a given model $f(x)$, estimate function $\hat{f}(x)$ from data

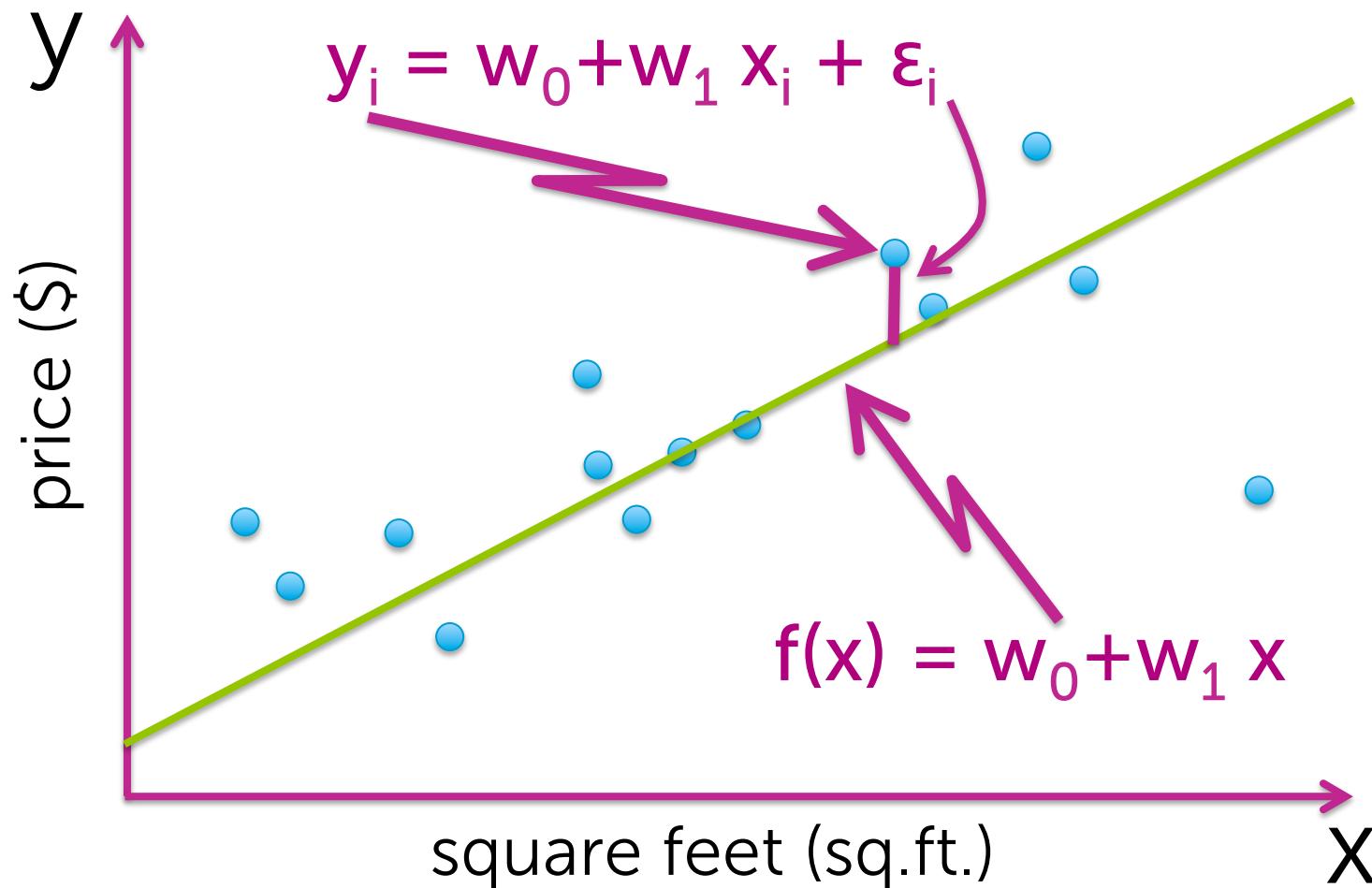




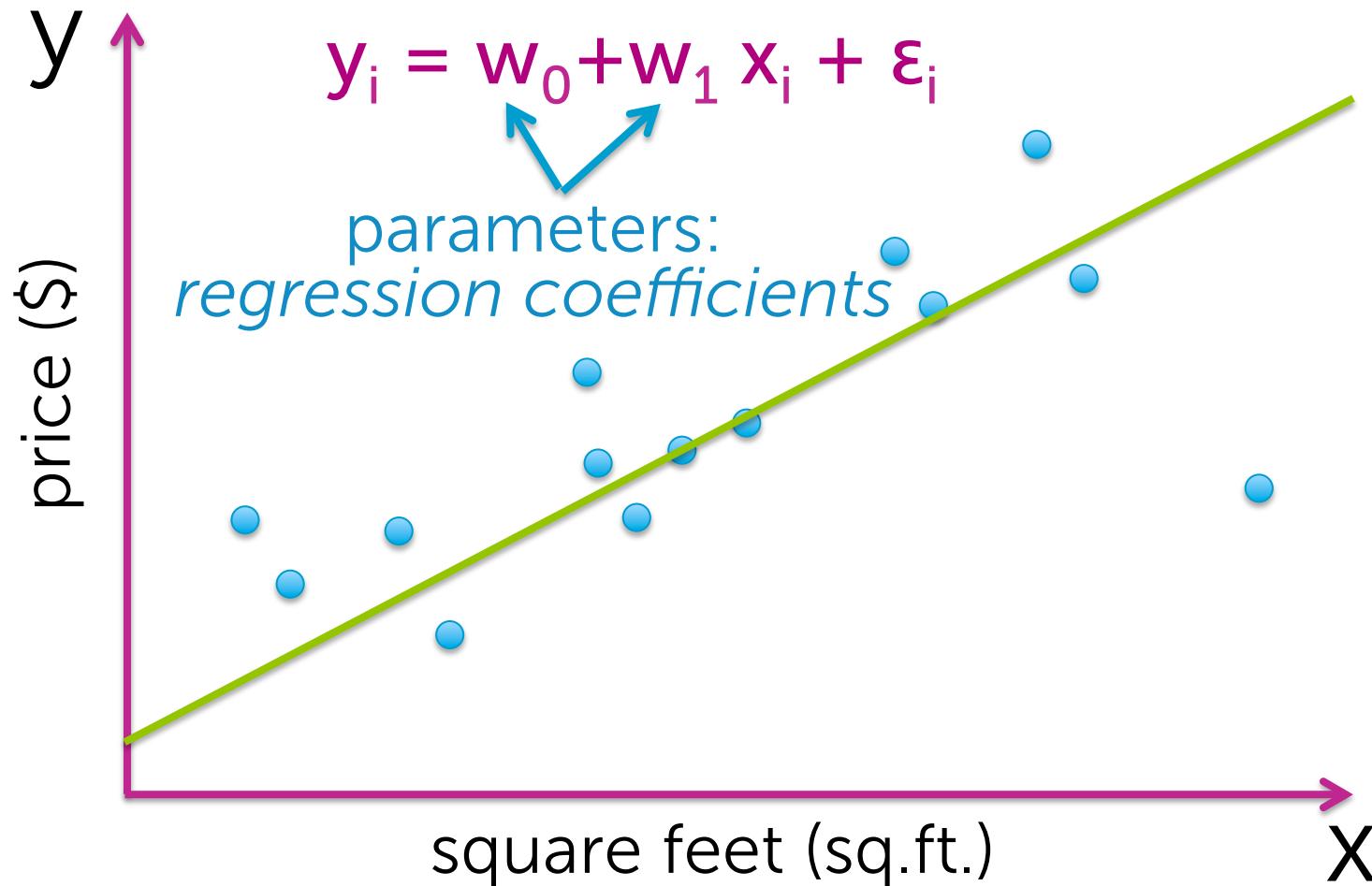
Simple linear regression



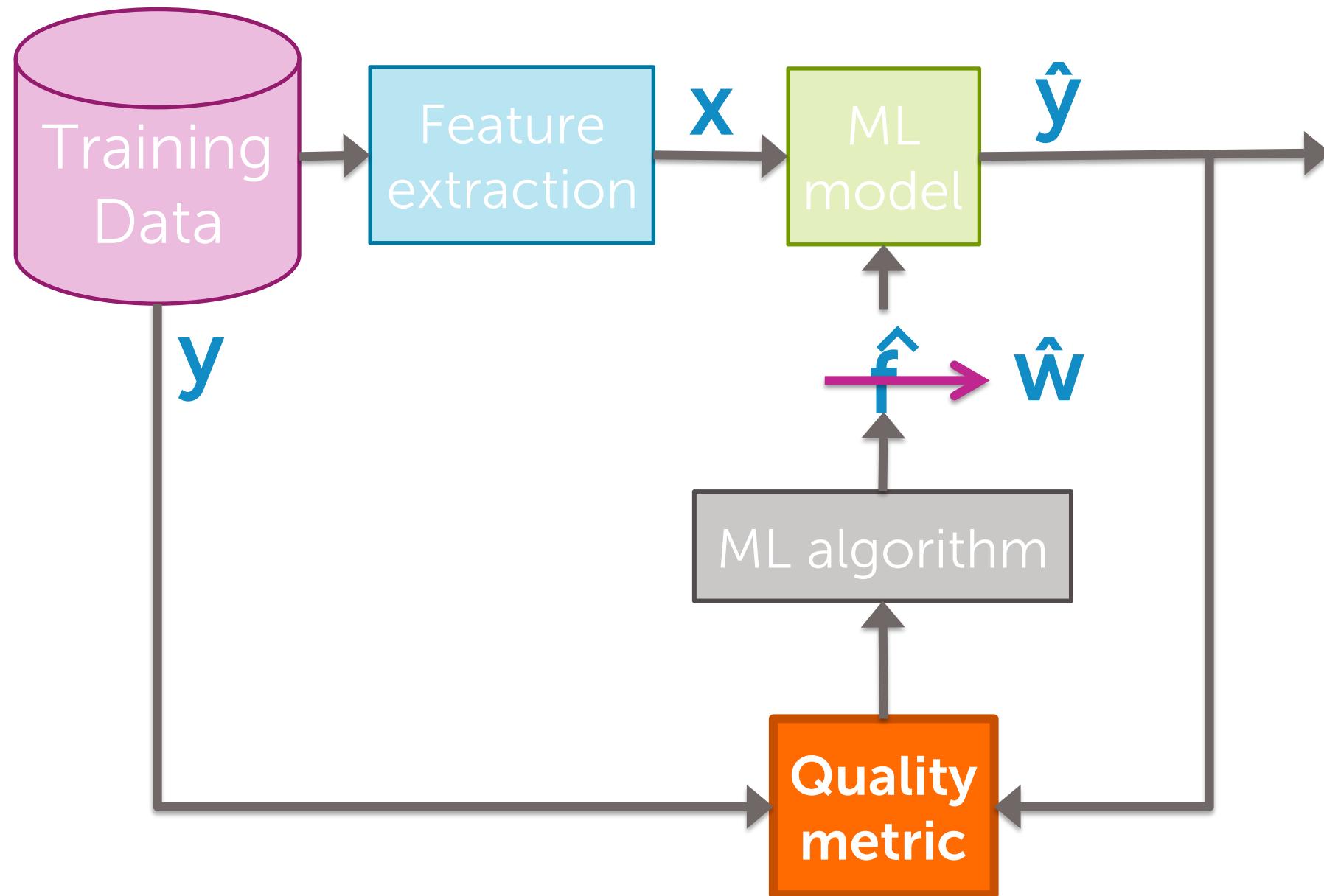
Simple linear regression model



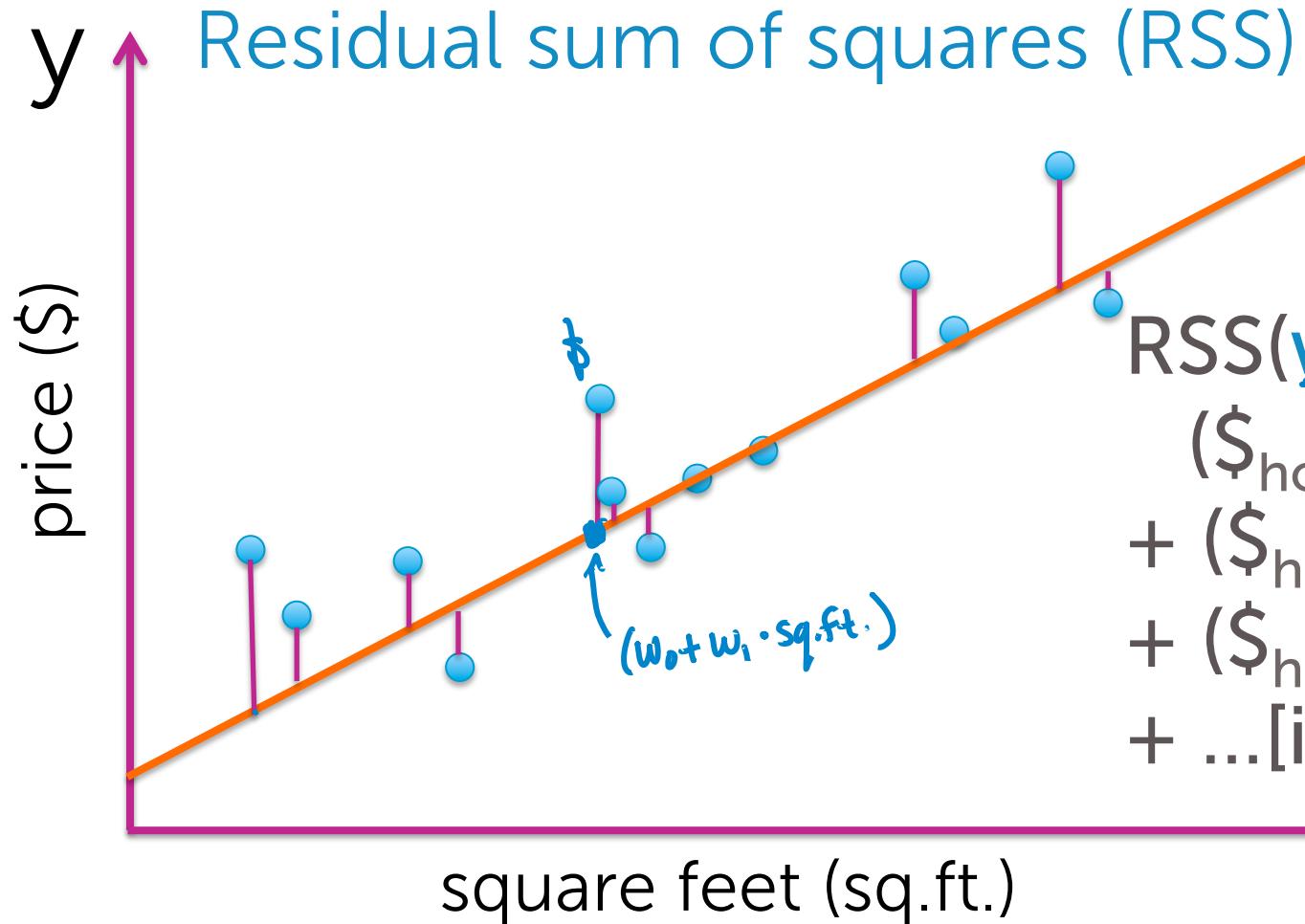
Simple linear regression model



Fitting a line to data

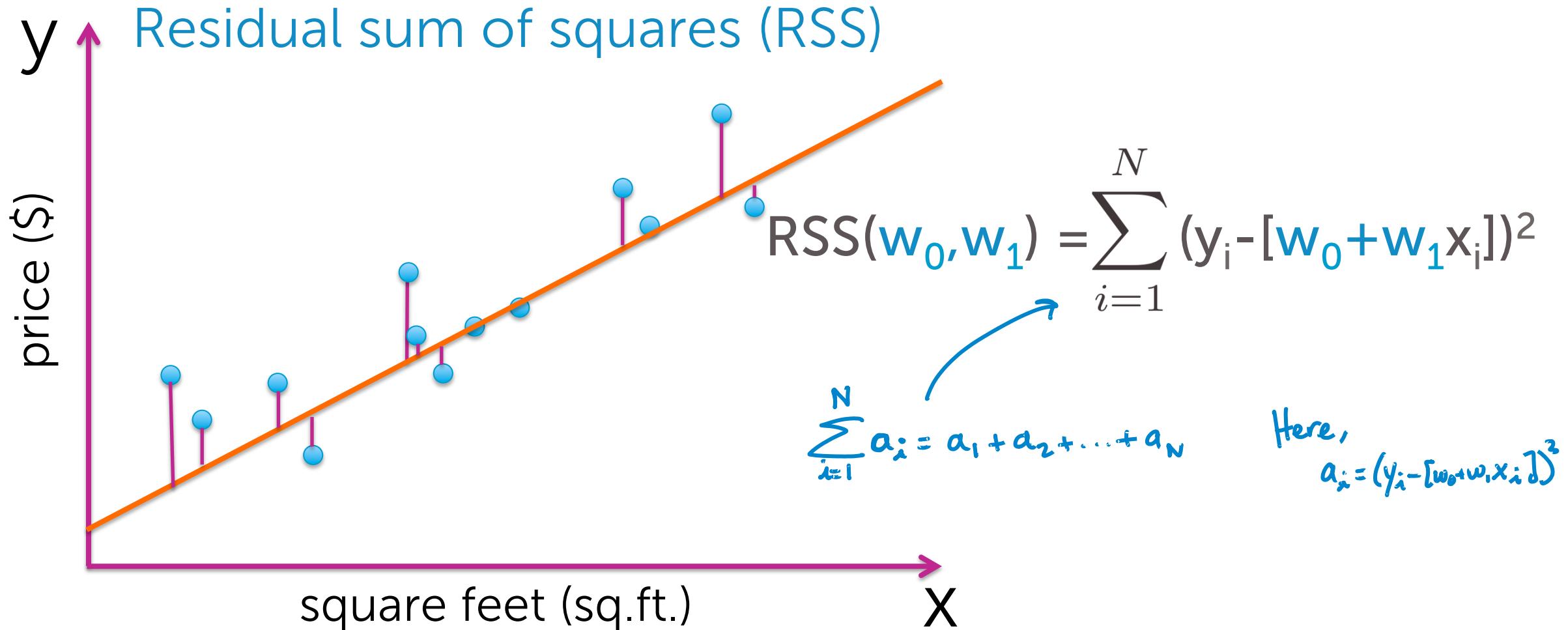


"Cost" of using a given line

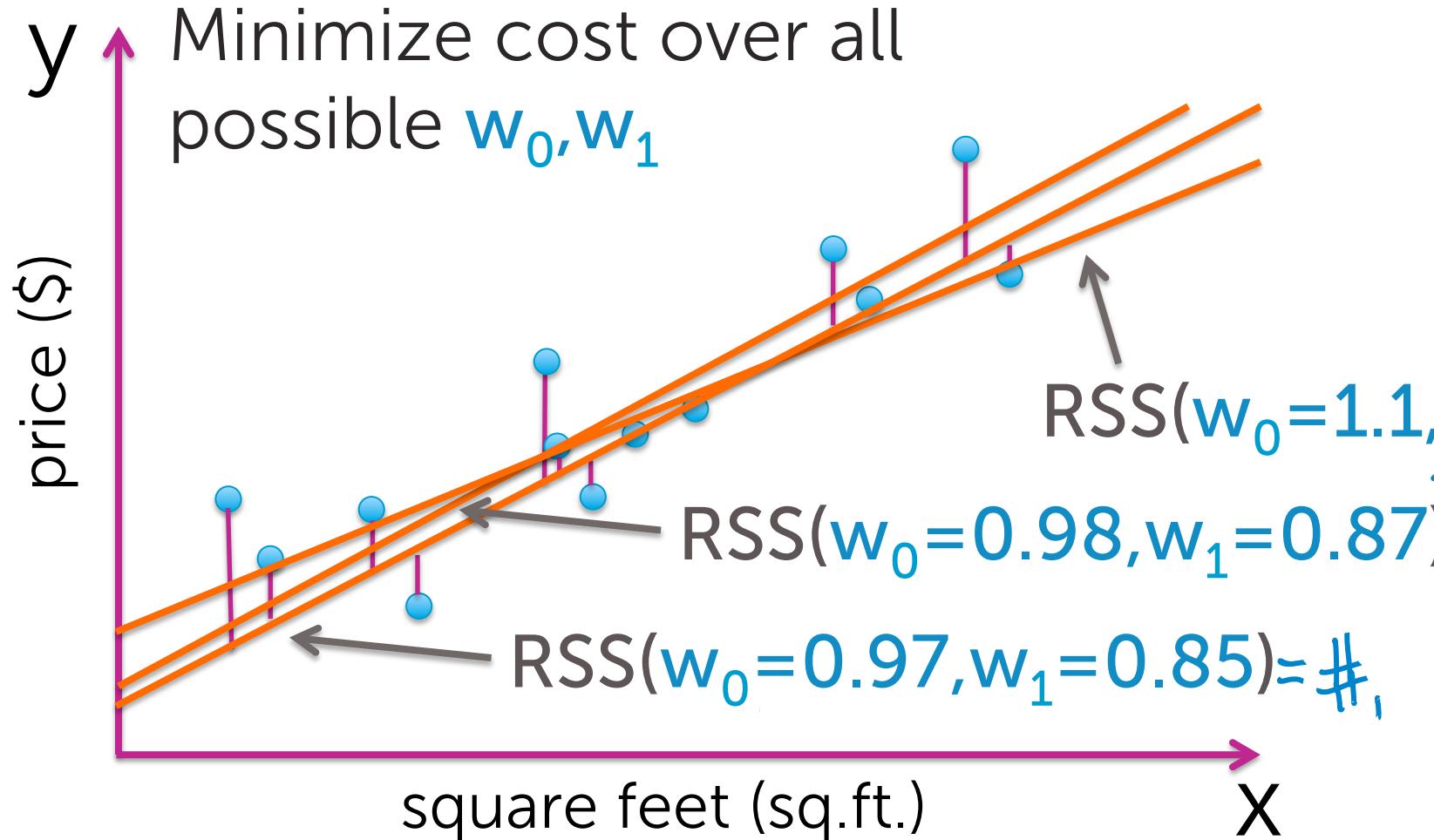


$$\begin{aligned} \text{RSS}(\underline{w}_0, \underline{w}_1) = & (\$_{\text{house 1}} - [\underline{w}_0 + \underline{w}_1 \cdot \text{sq.ft.}_{\text{house 1}}])^2 \\ & + (\$_{\text{house 2}} - [\underline{w}_0 + \underline{w}_1 \cdot \text{sq.ft.}_{\text{house 2}}])^2 \\ & + (\$_{\text{house 3}} - [\underline{w}_0 + \underline{w}_1 \cdot \text{sq.ft.}_{\text{house 3}}])^2 \\ & + \dots \text{[include all training houses]} \end{aligned}$$

"Cost" of using a given line



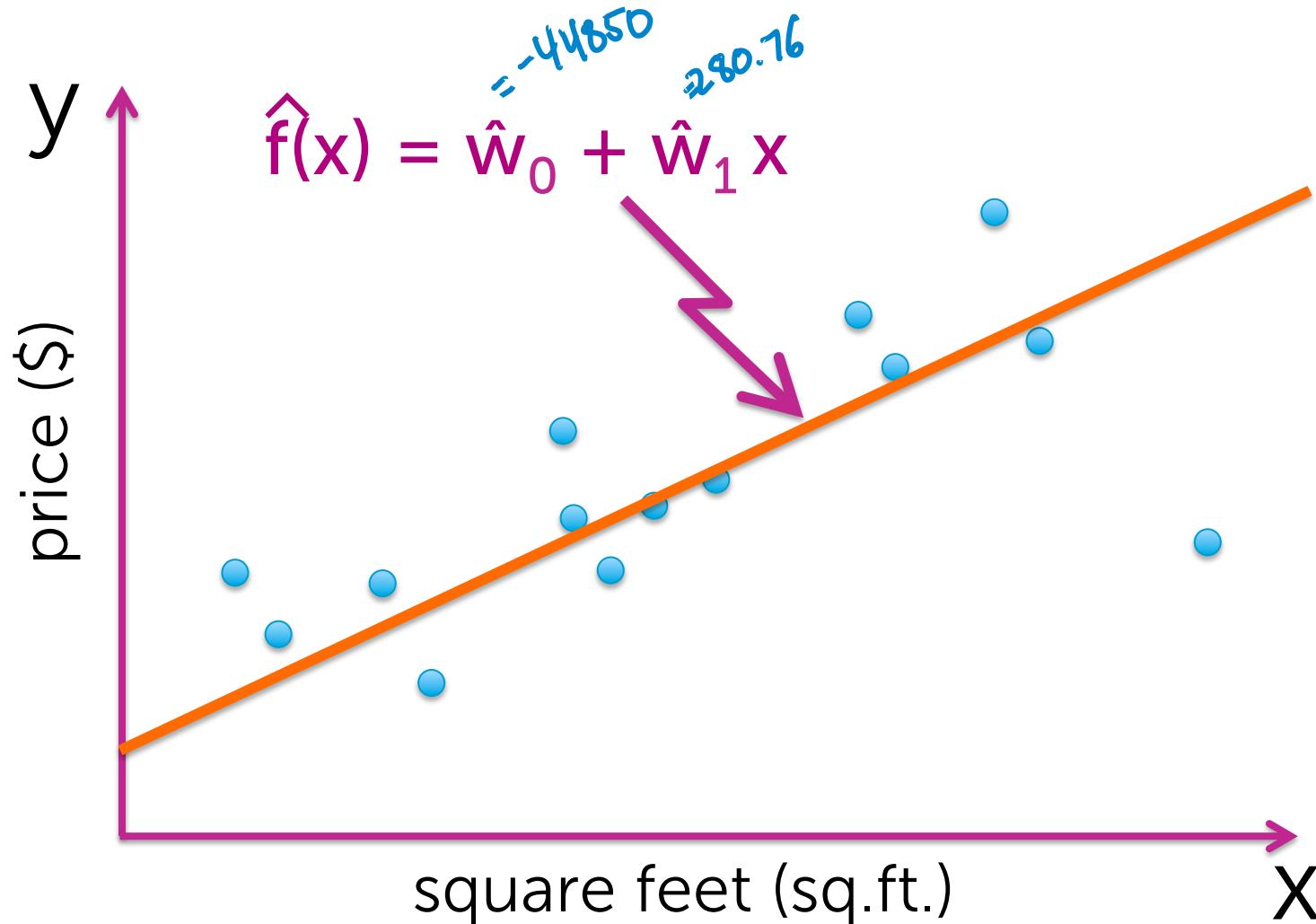
Find “best” line



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

The fitted line: use + interpretation

Model vs. fitted line



Regression model:

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

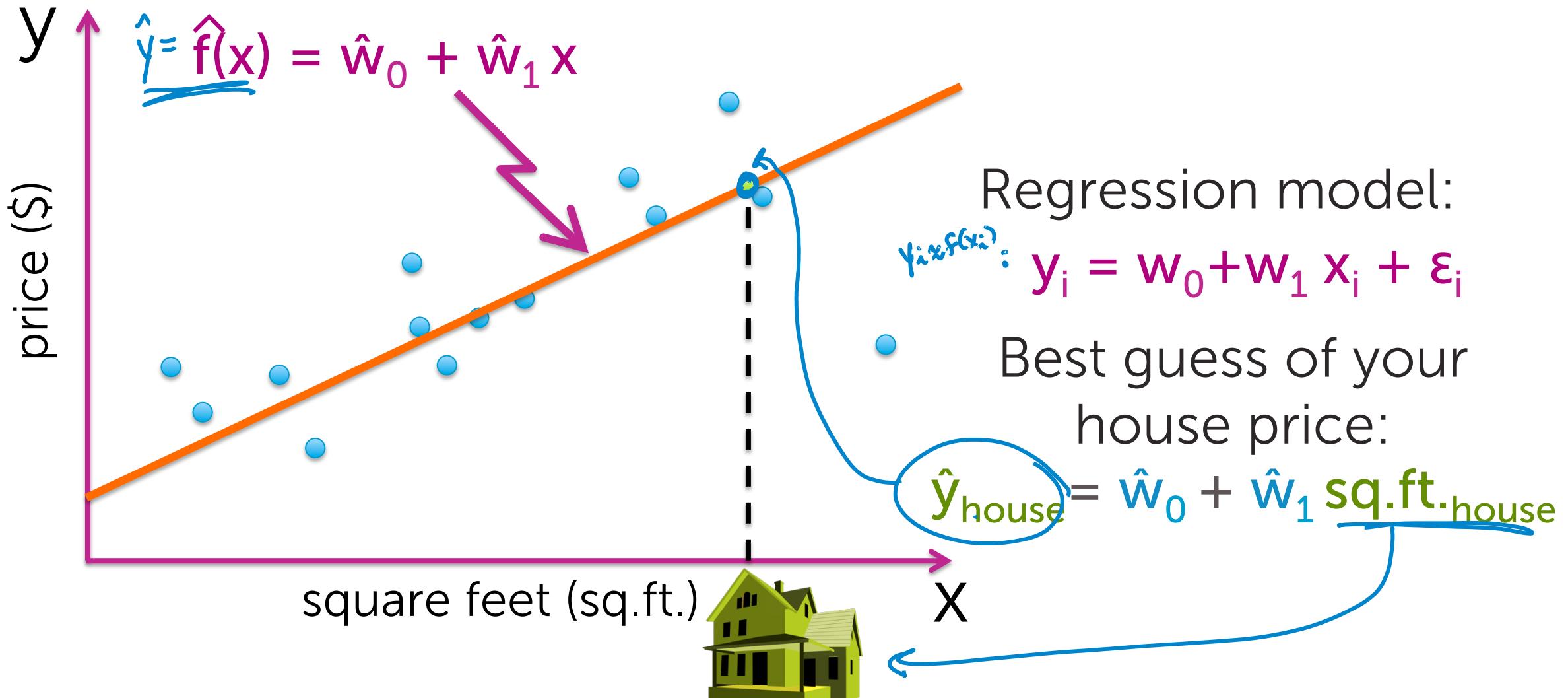
parameters (unknown variables)

Estimated parameters:

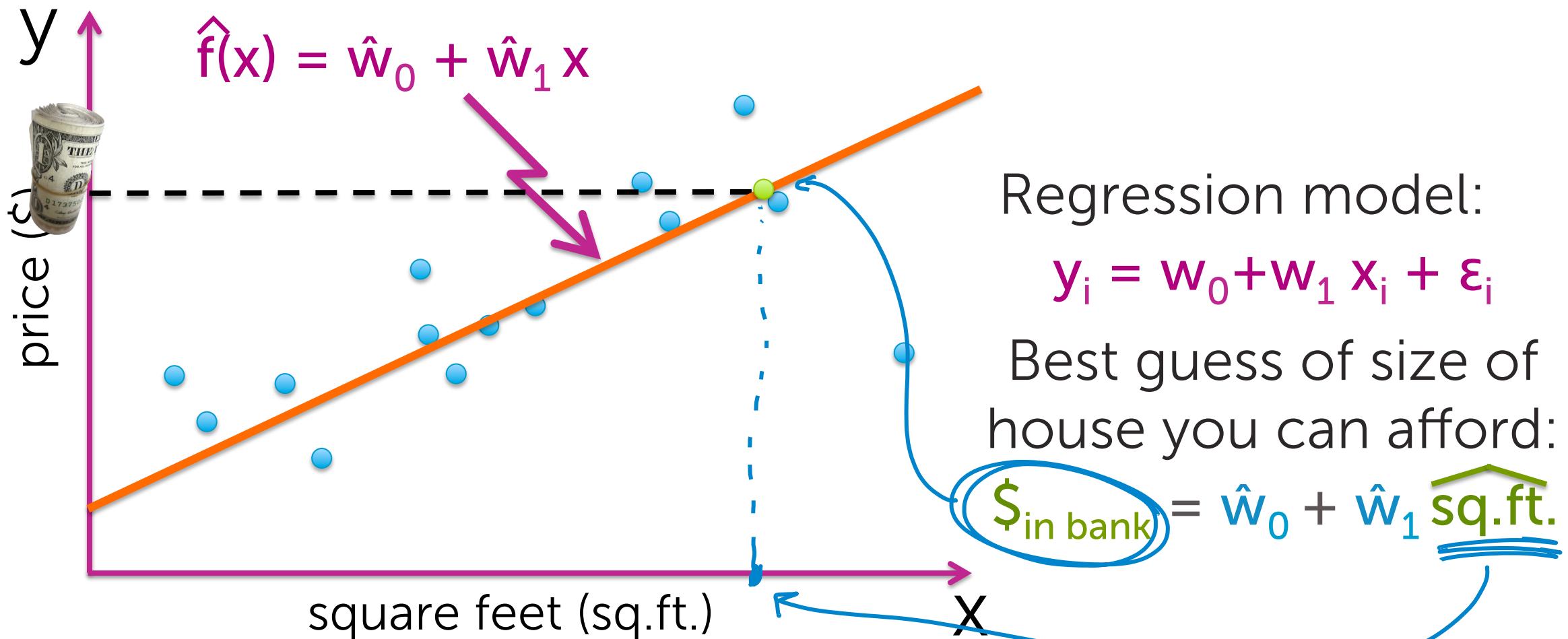
$$\hat{w}_0 = -44950, \hat{w}_1 = 280.76$$

take actual values

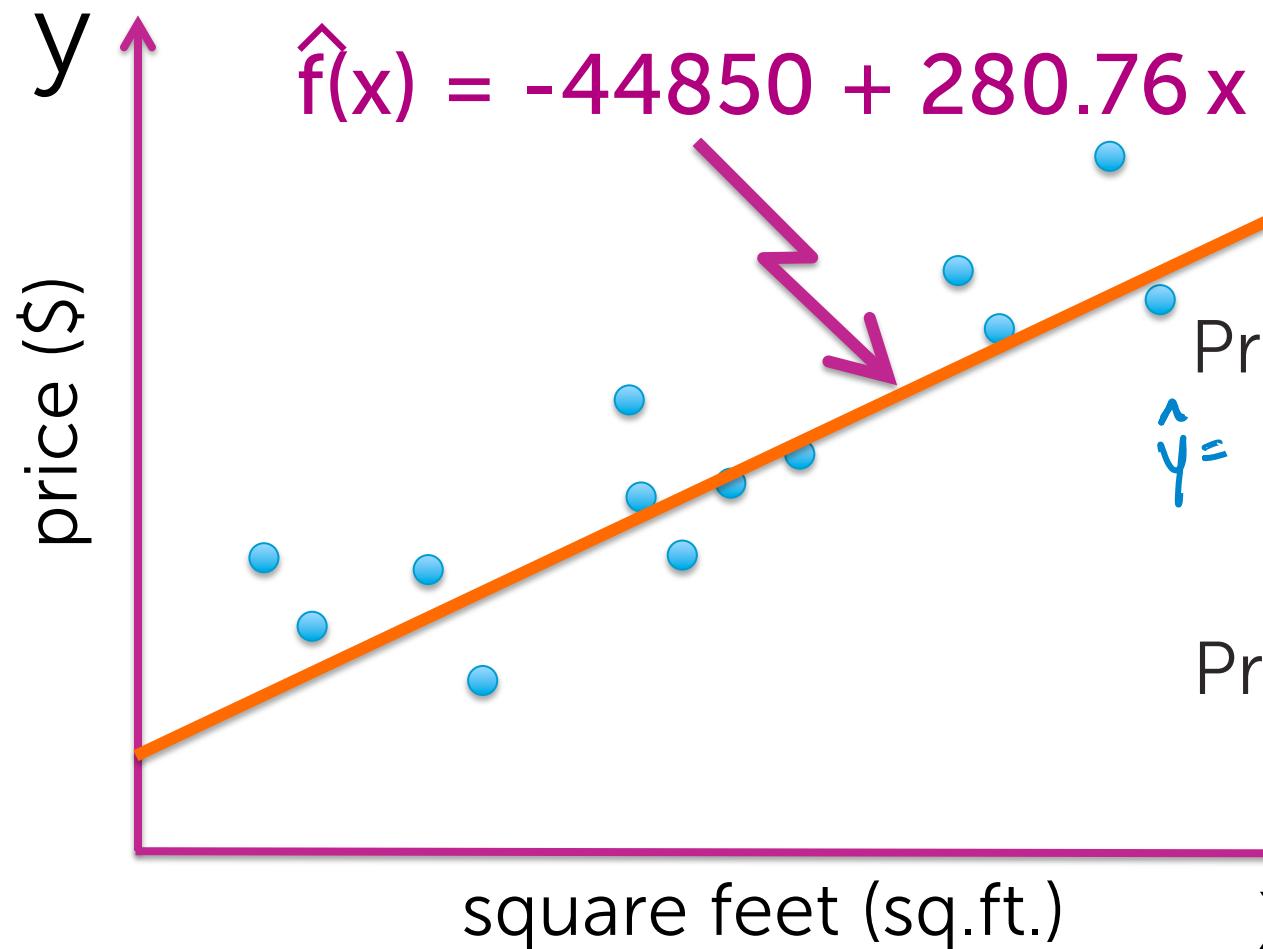
Seller: Predicting your house price



Buyer: Predicting size of house



A concrete example



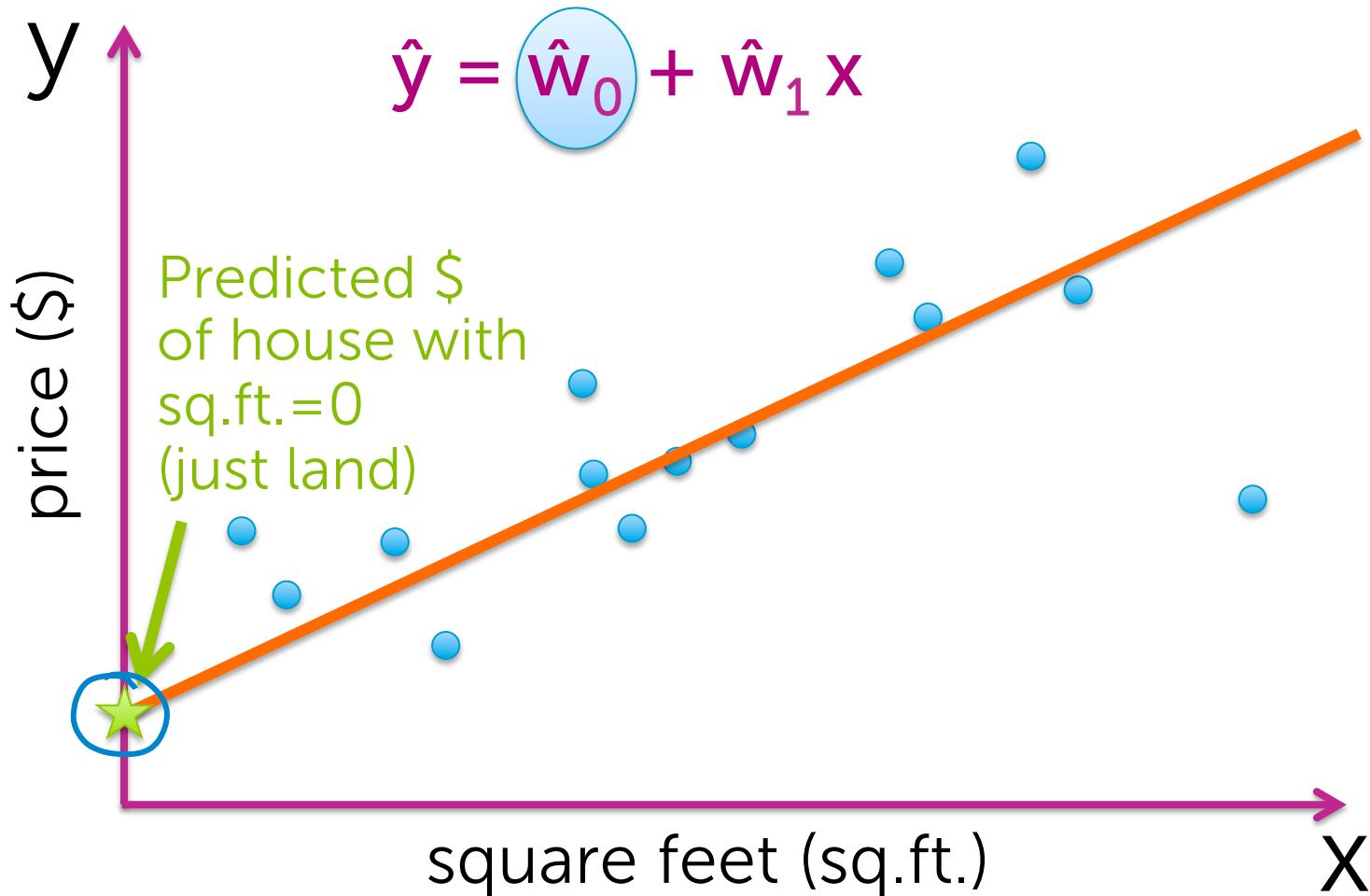
Predict \$ of 2,640 sq.ft. house:

$$\begin{aligned}\hat{y} &= -44850 + 280.76 * \underline{2,640} \\ &= \$696,356\end{aligned}$$

Predict sq.ft. of \$859,000 sale:

$$\begin{aligned}(859000 + 44850) / 280.76 \\ &= 3,219 \text{ sq.ft.}\end{aligned}$$

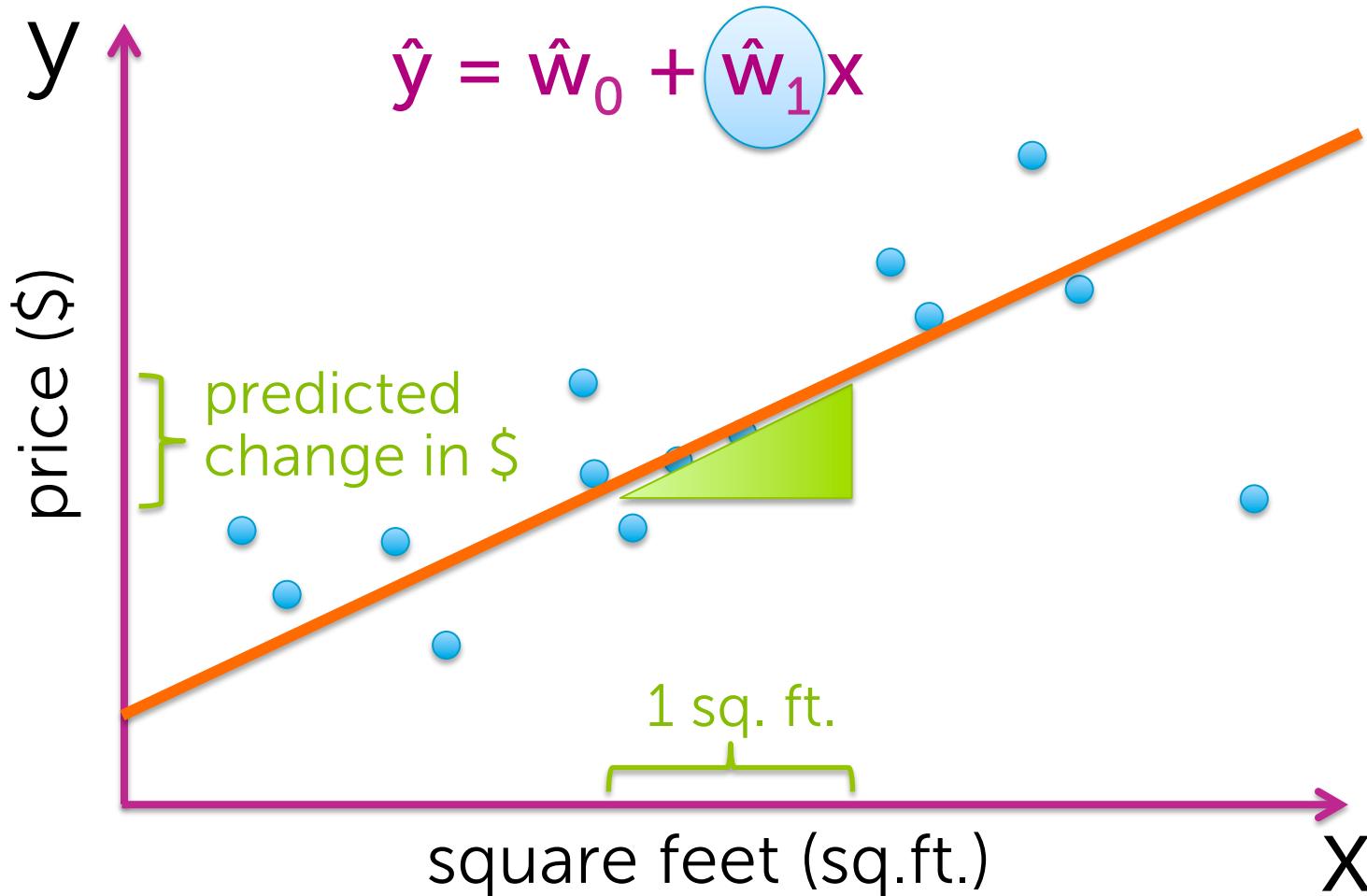
Interpreting the coefficients



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

not very meaningful

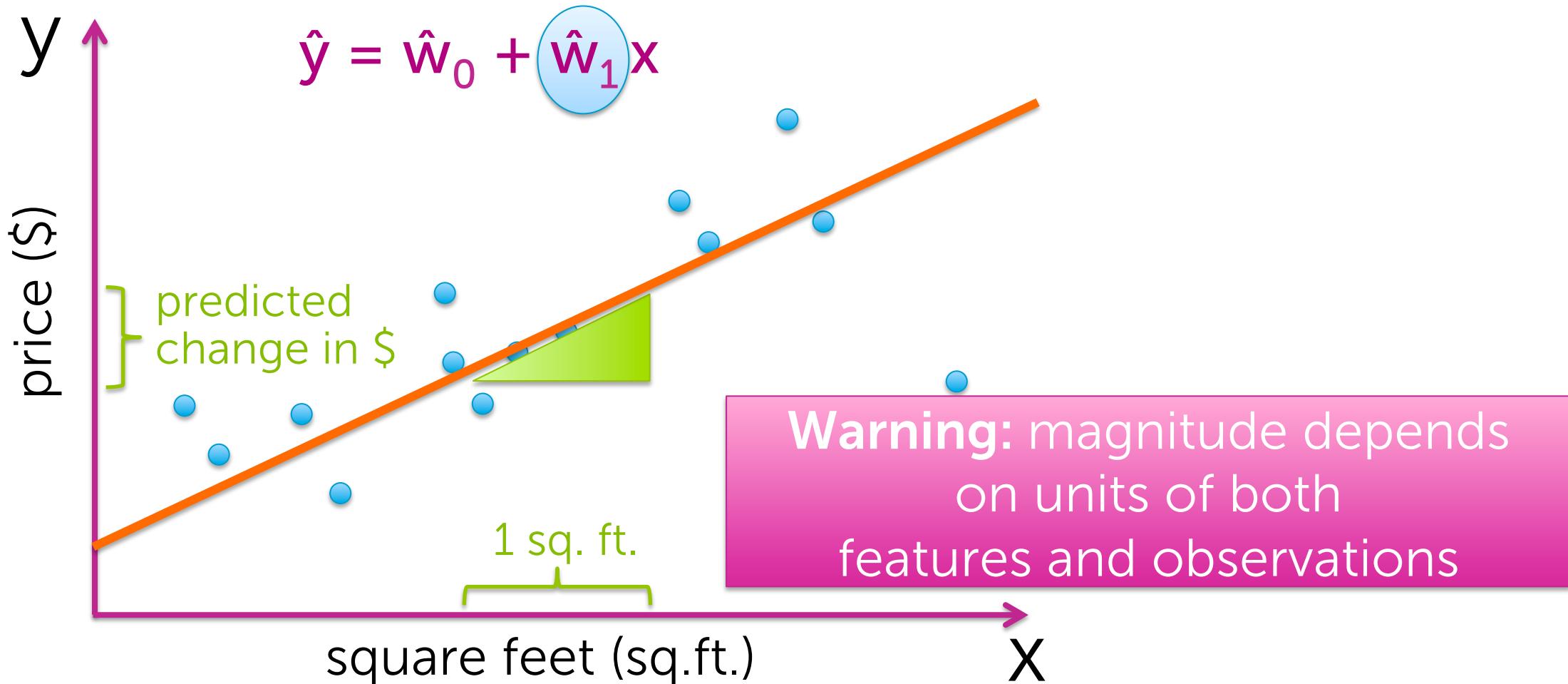
Interpreting the coefficients



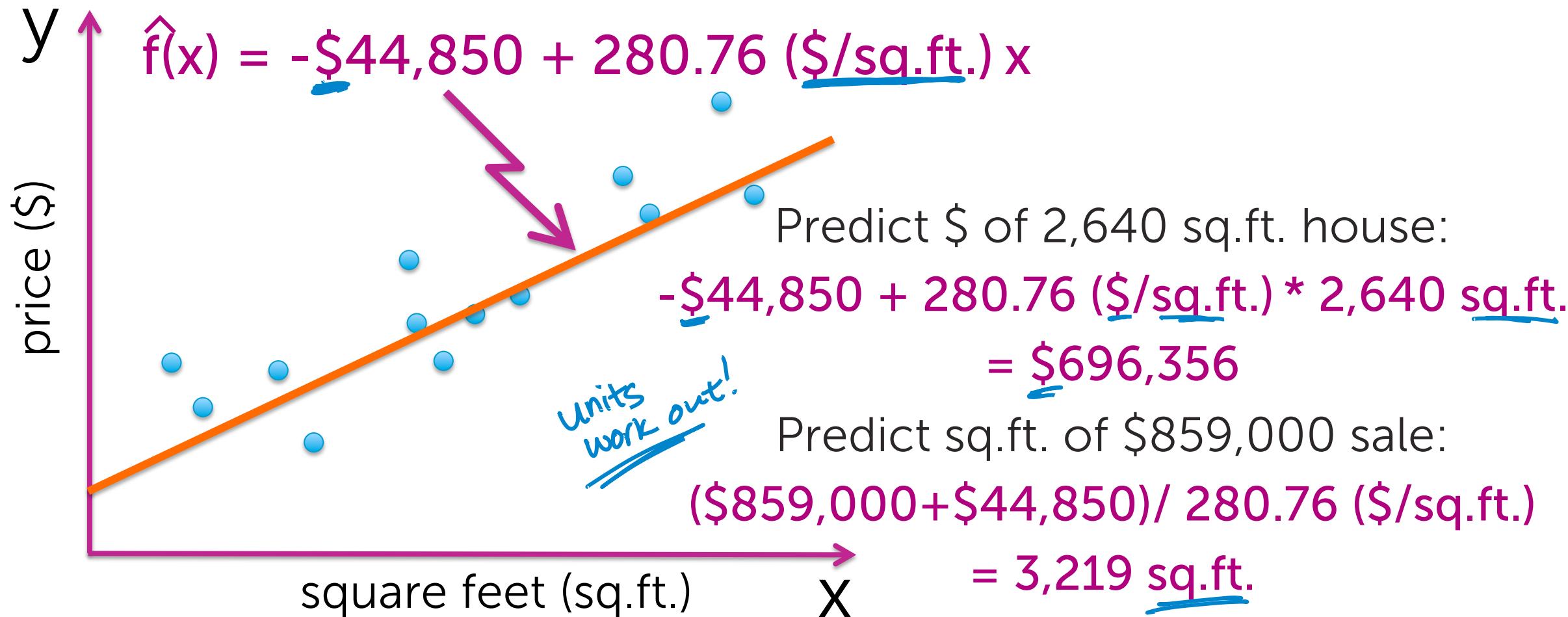
$$\begin{aligned}\hat{y}_{1001 \text{ sq.ft.}} - \hat{y}_{1000 \text{ sq.ft.}} &= \hat{w}_0 + \hat{w}_1 \cdot 1001 \text{ sq.ft.} \\ &\quad - (\hat{w}_0 + \hat{w}_1 \cdot 1000 \text{ sq.ft.}) \\ &= \hat{w}_1\end{aligned}$$

predicted change in the output
per unit change in input

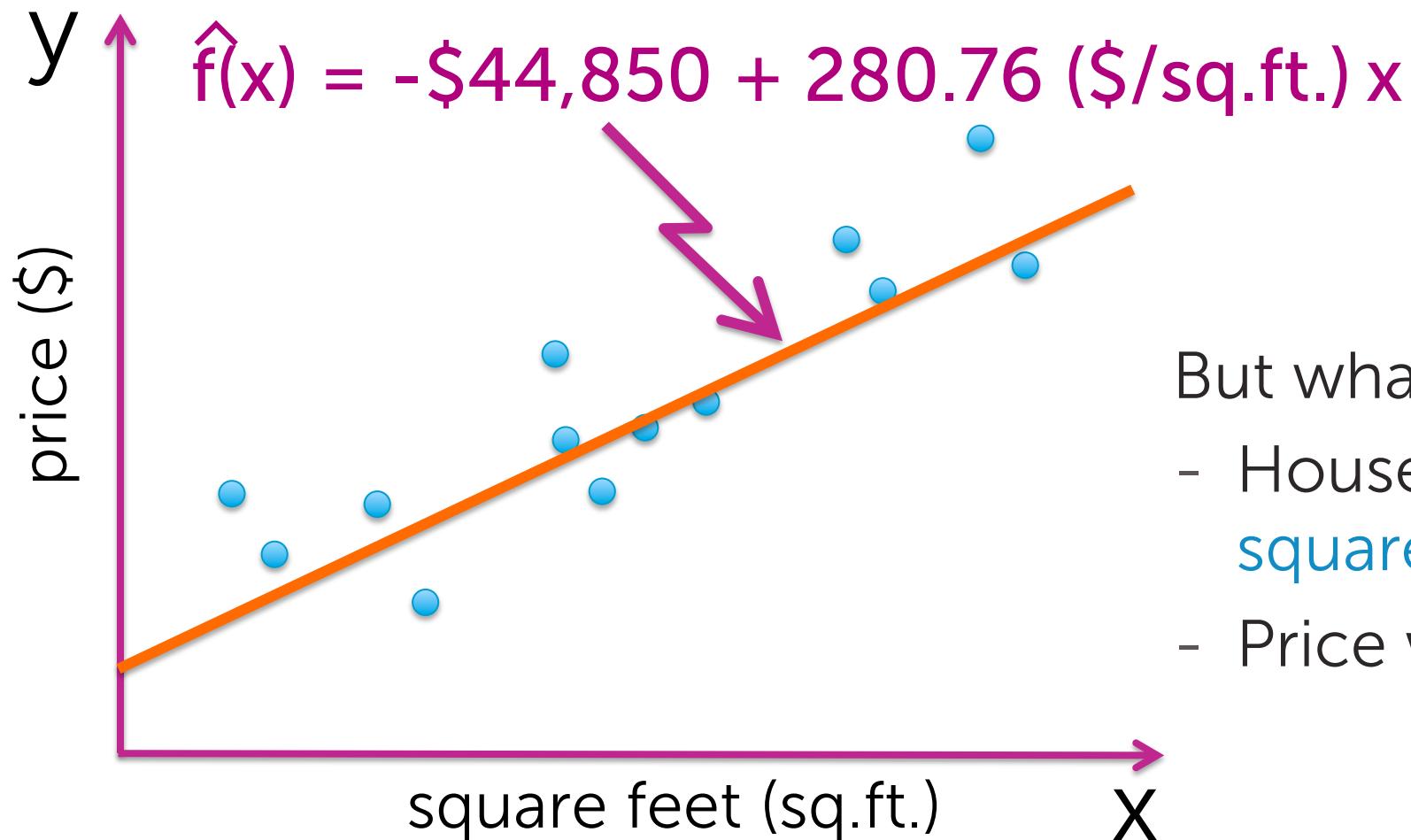
Interpreting the coefficients



A concrete example



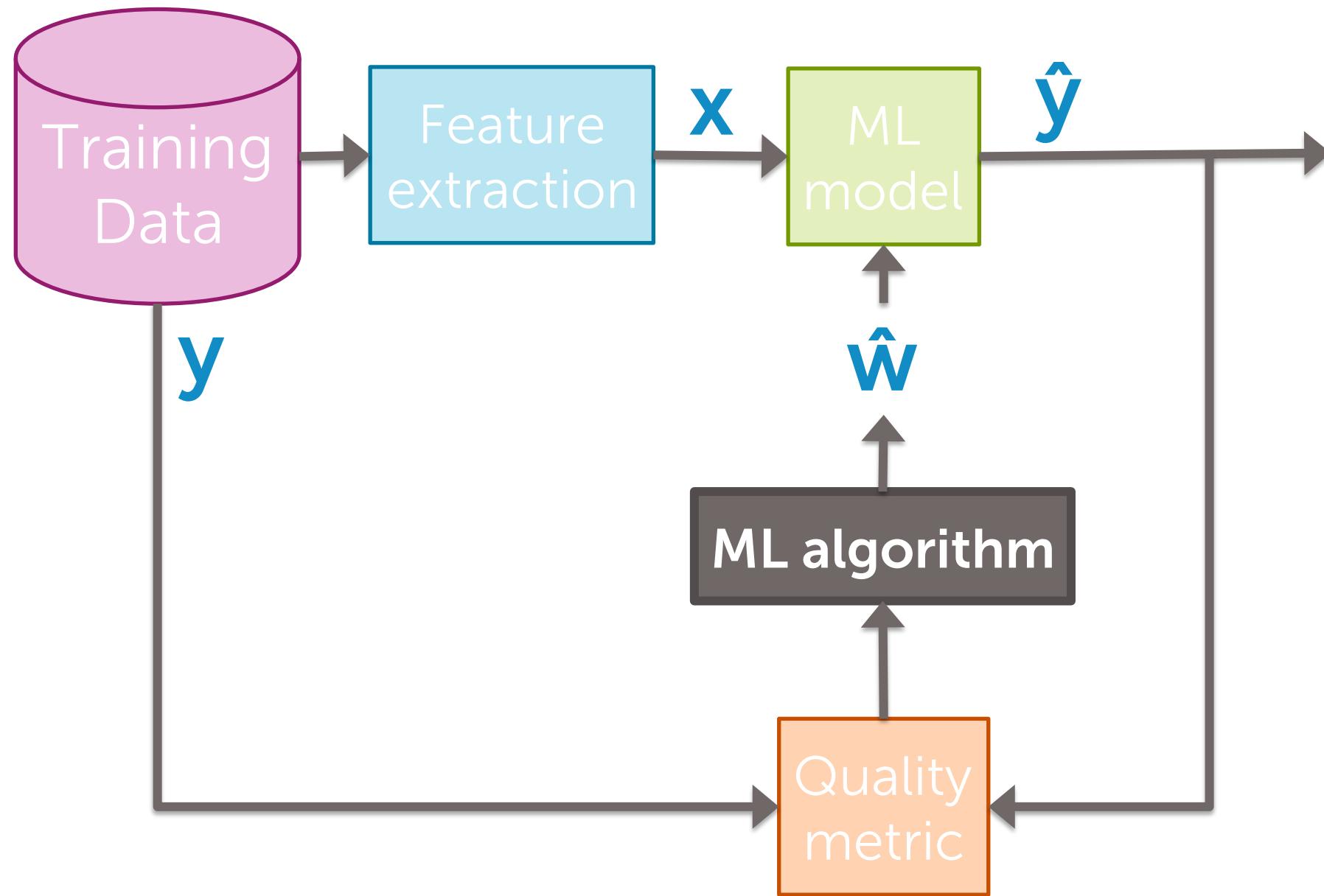
A concrete example



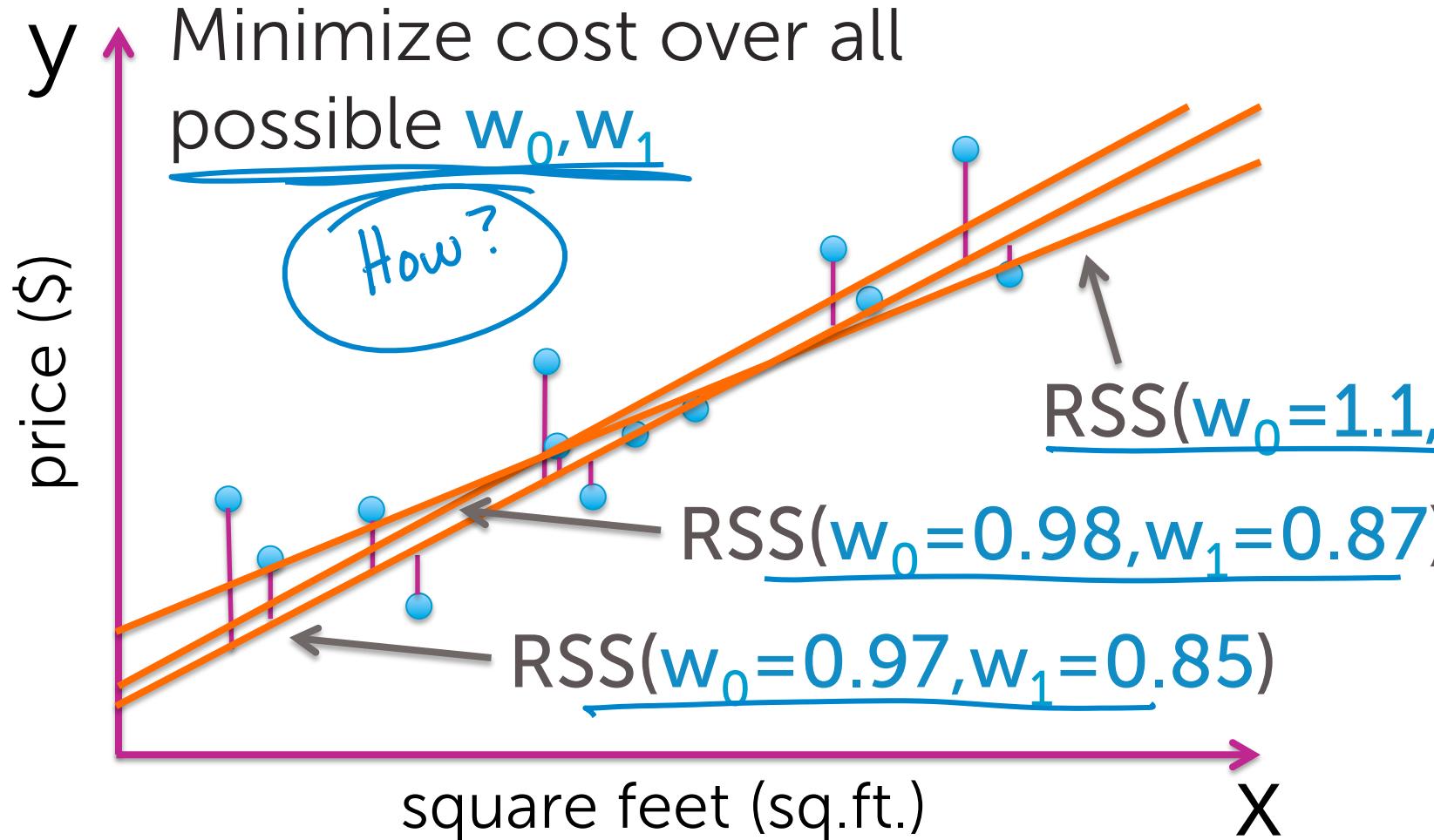
But what if:

- House was measured in square meters?
- Price was measured in RMB?

Algorithms for fitting the model



Find “best” line

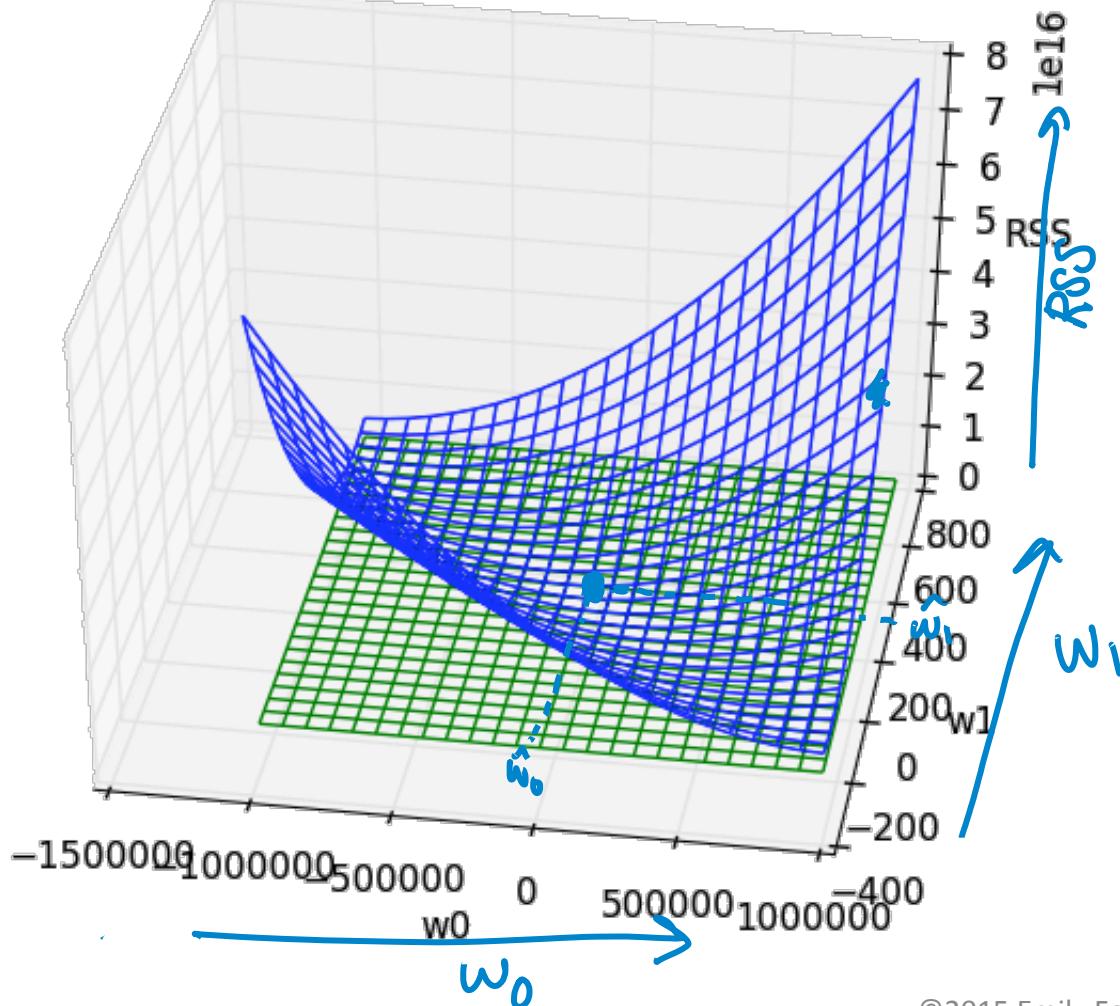


Recall:

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

Minimizing the cost

3D plot of RSS with tangent plane at minimum



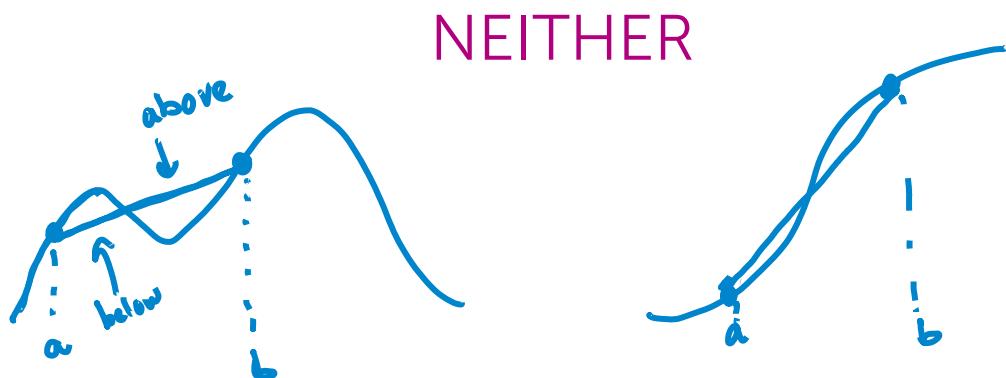
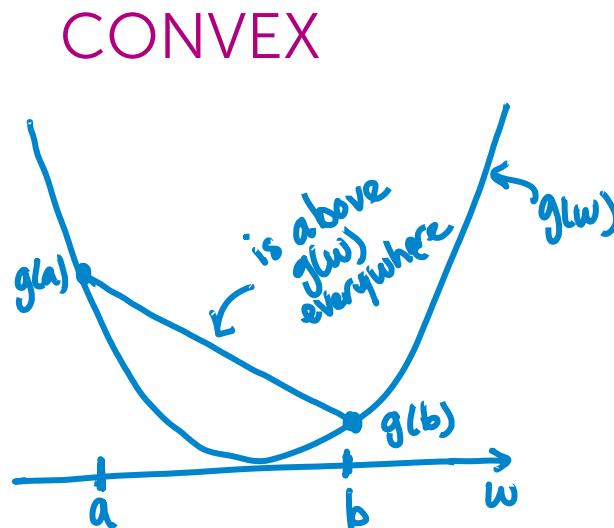
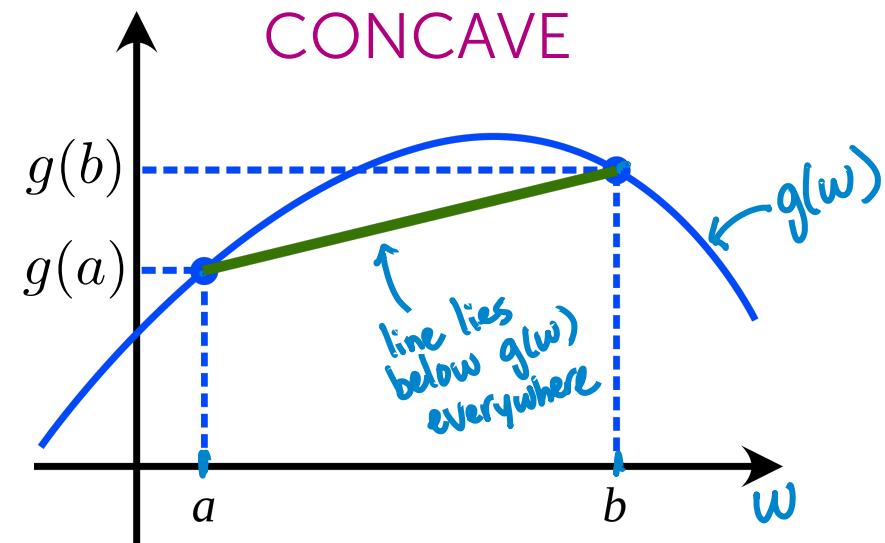
Minimize function
over all possible w_0, w_1

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

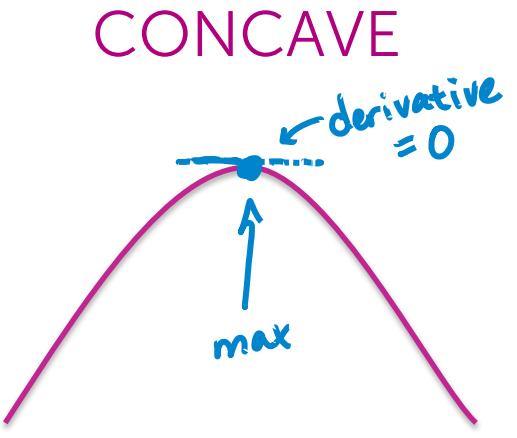
RSS(w_0, w_1) is a function
of 2 variables = $g(w_0, w_1)$

An aside on optimization

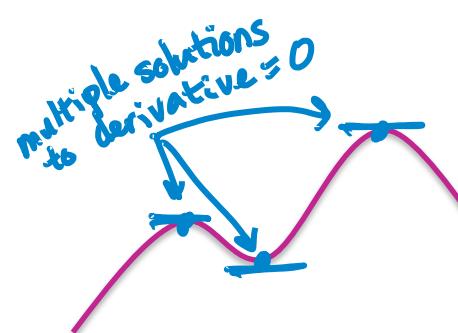
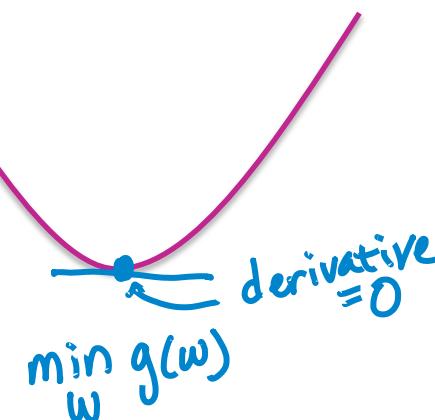
Convex/concave functions



Finding the max or min analytically



CONVEX



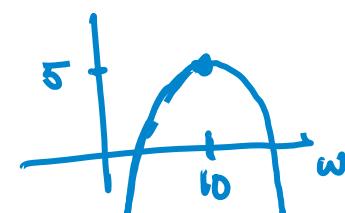
no solution to derivative = 0

Example:

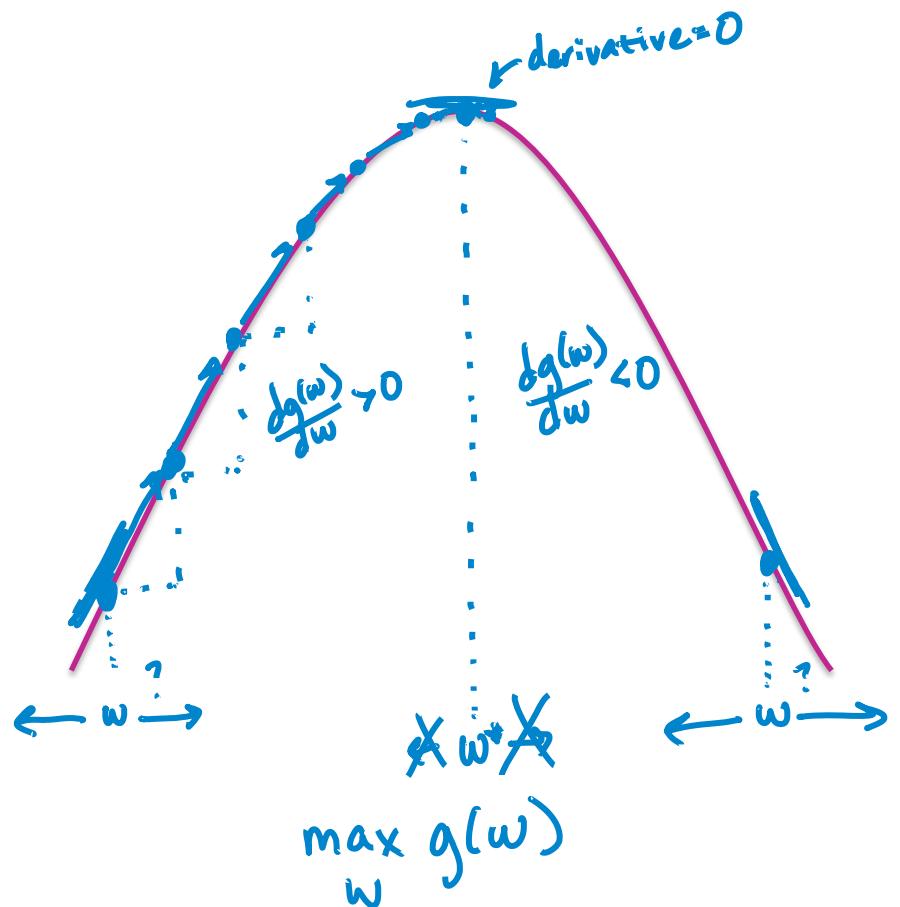
$$g(w) = 5 - (w-10)^2$$

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

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



Finding the max via hill climbing



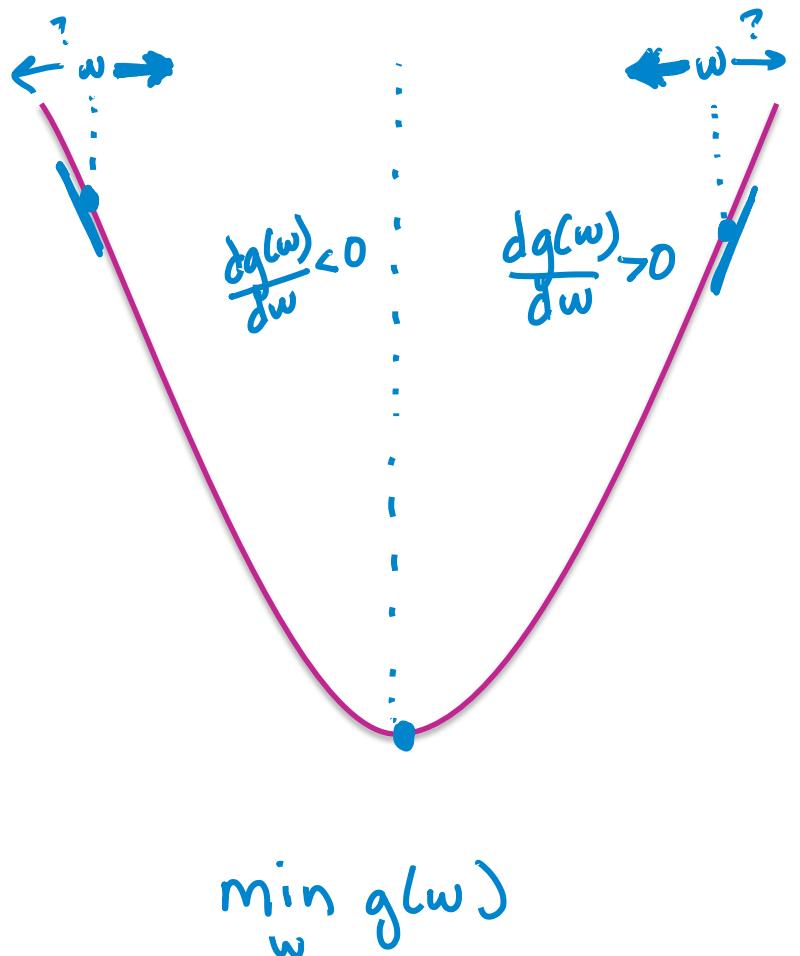
How do we know whether to move w to right or left?
(Inc. or dec. the value of w ?)

while not converged

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

iteration t stepsize

Finding the min via hill descent



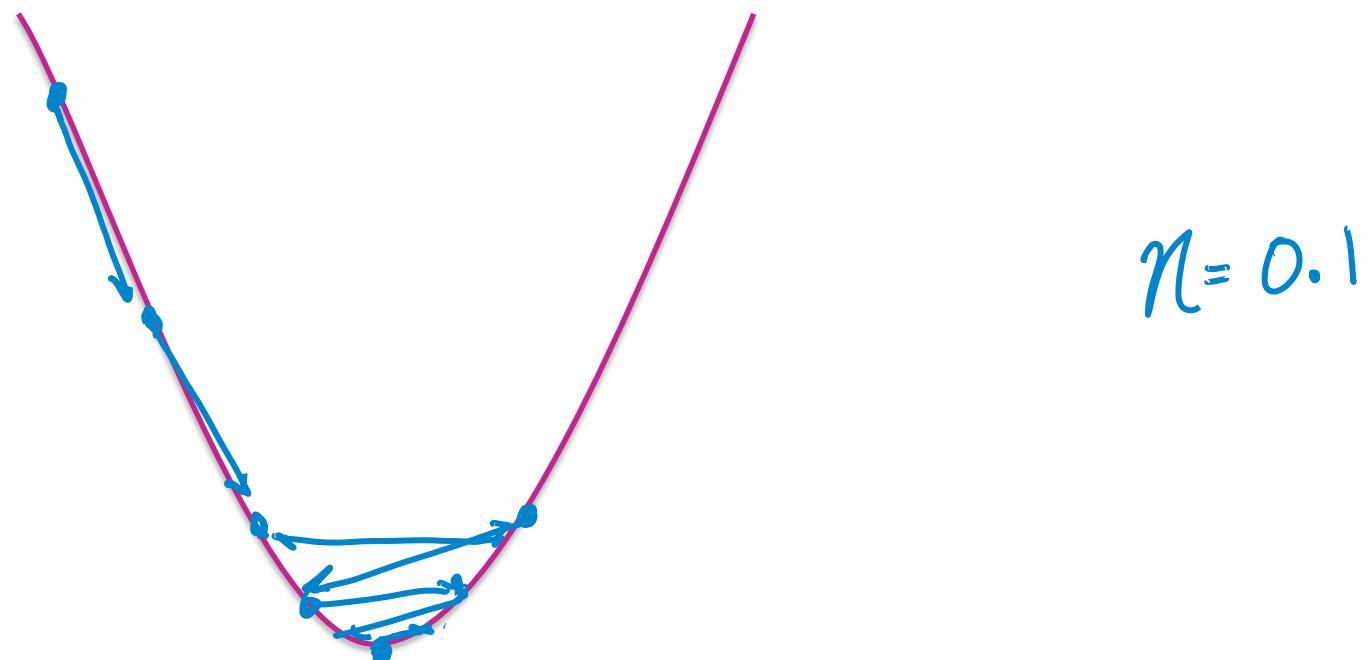
when derivative is positive, we want to decrease w
and when derivative is negative, we want to increase w

Algorithm:

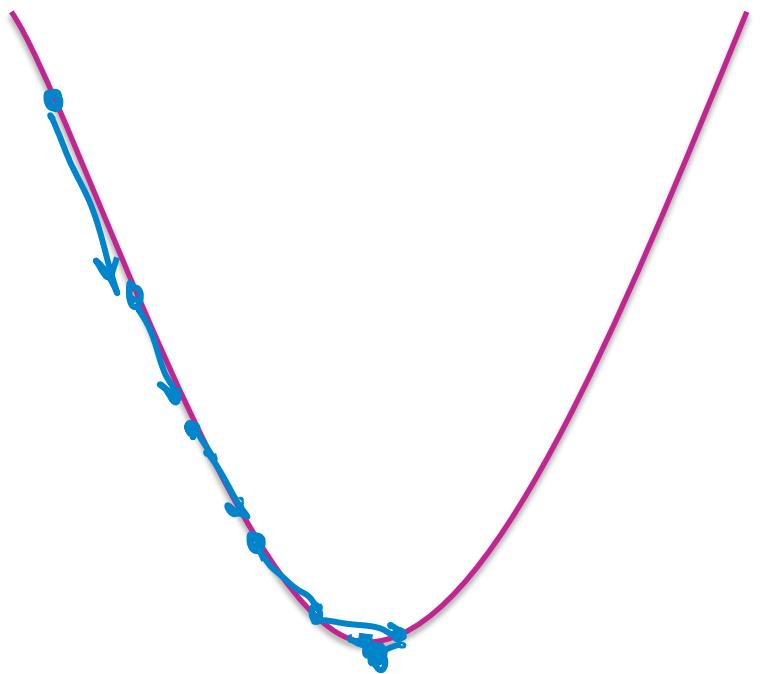
while not converged
 $w^{(t+1)} \leftarrow w^{(t)} - \eta \left. \frac{dg}{dw} \right|_{w^{(t)}}$

Choosing the stepsize—

Fixed stepsize



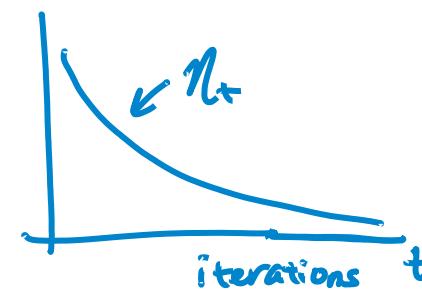
Choosing the stepsize— Decreasing stepsize or stepsize schedule



Common choices:

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

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



Convergence criteria

For convex functions,
optimum occurs when

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

In practice, stop when

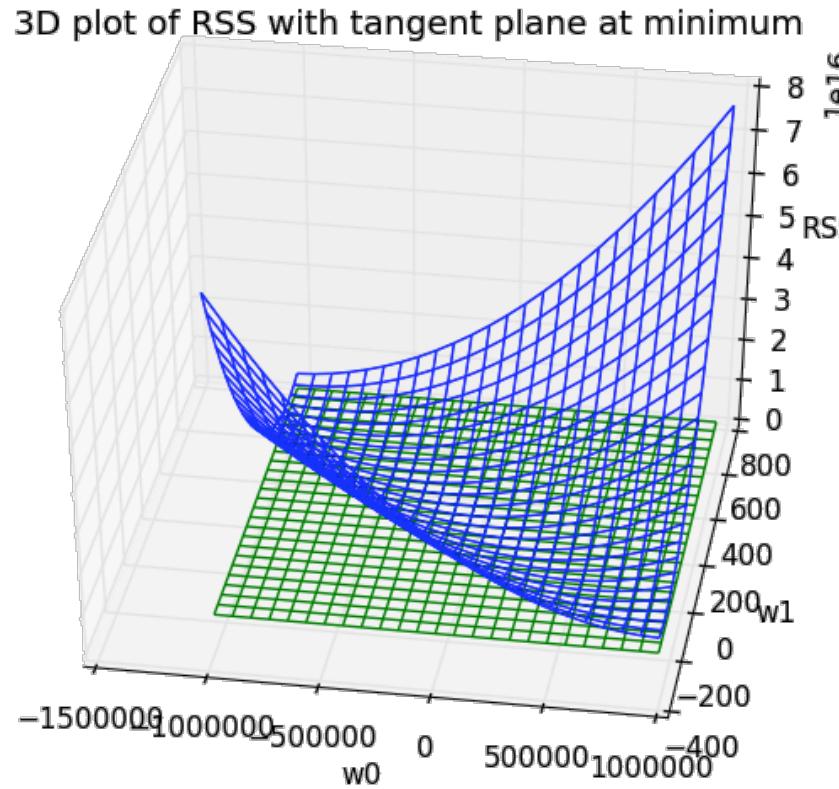
$$\left| \frac{dg(w)}{dw} \right| < \epsilon$$

*threshold
to be set*

Algorithm:

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

Moving to multiple dimensions: Gradients



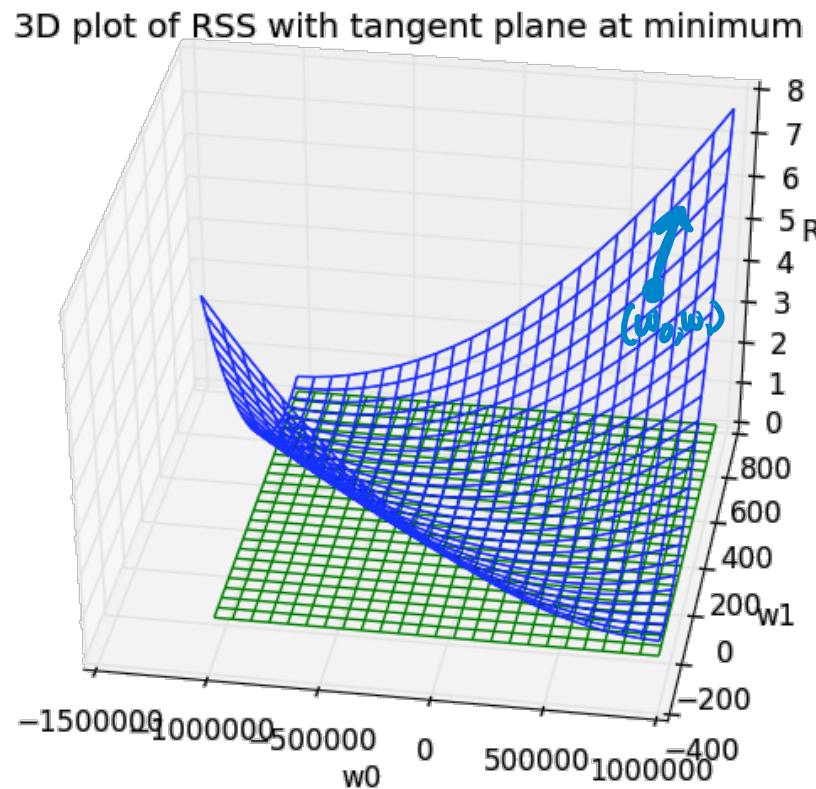
$$\nabla g(\mathbf{w}) = \begin{bmatrix} \frac{\partial g}{\partial w_0} \\ \frac{\partial g}{\partial w_1} \\ \vdots \\ \frac{\partial g}{\partial w_p} \end{bmatrix}$$

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

($p+1$) -dimensional vector

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

Gradient example



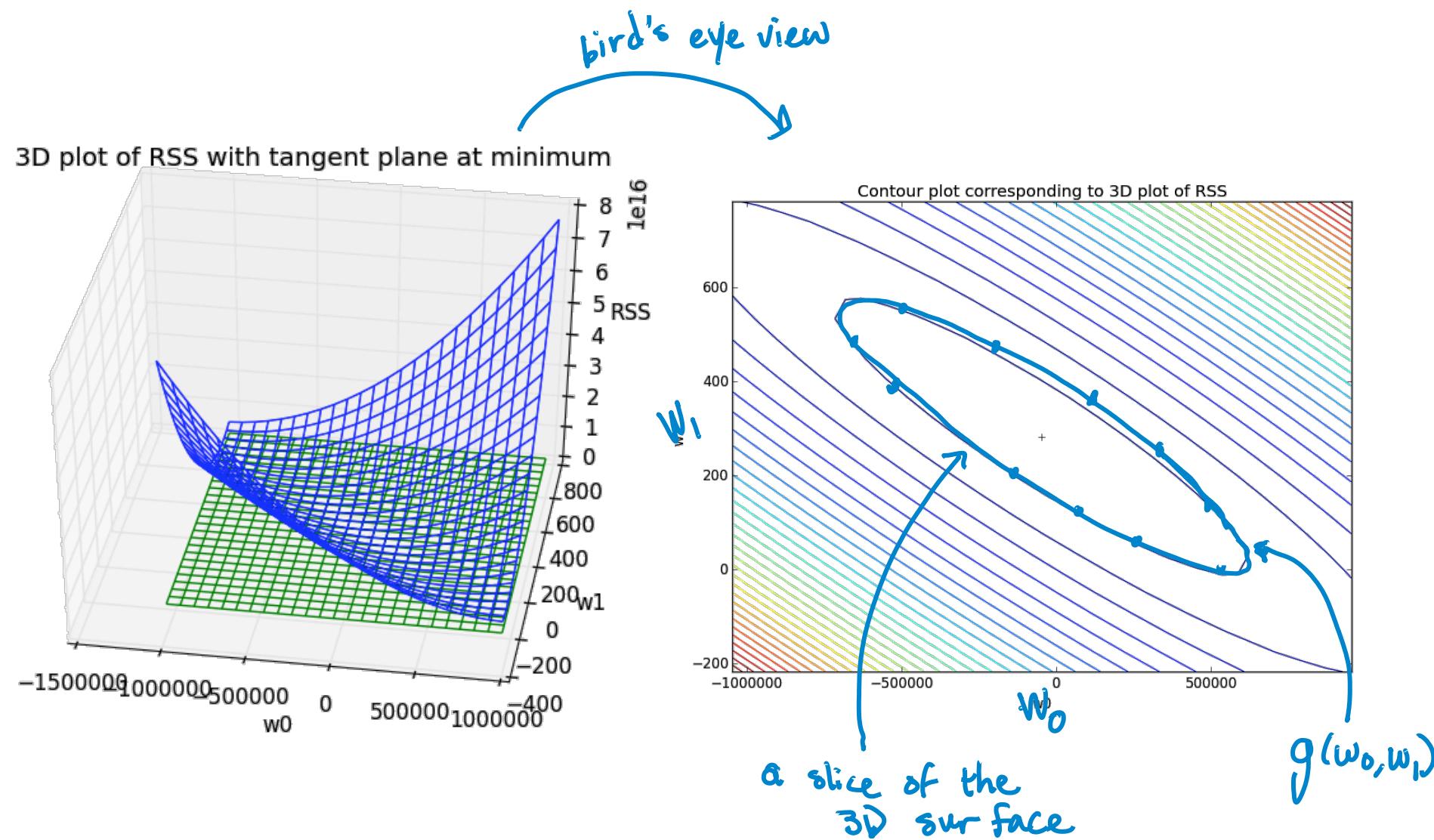
$$g(\mathbf{w}) = 5w_0 + 10w_0w_1 + 2w_1^2$$

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

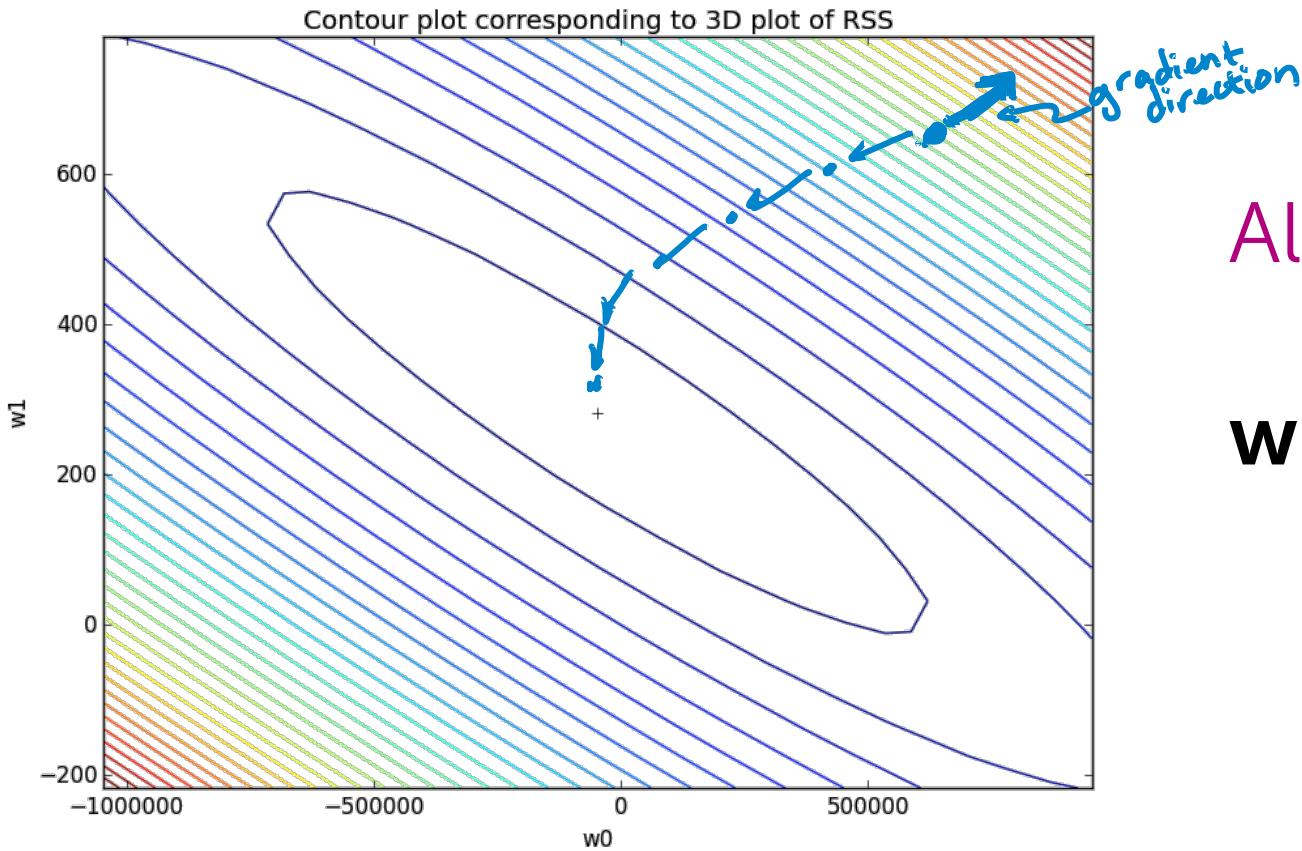
$$\frac{\partial g}{\partial w_1} = 10w_0 + 4w_1$$

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

Contour plots



Gradient descent



Algorithm:

while not converged
 $w^{(t+1)} \leftarrow w^{(t)} - \eta \nabla g(w^{(t)})$

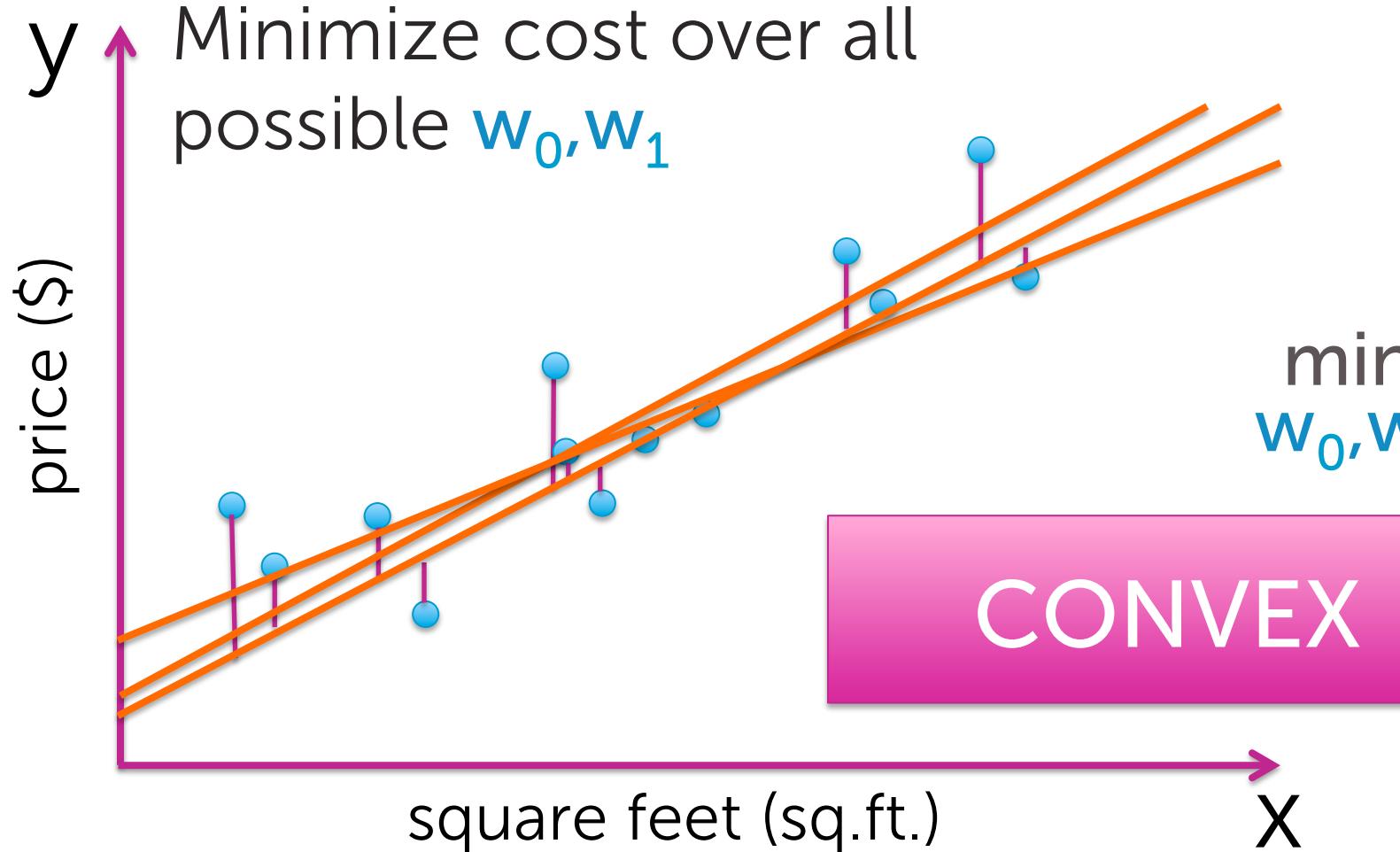
$\begin{bmatrix} \cdot \\ \vdots \\ \cdot \end{bmatrix} \leftarrow \begin{bmatrix} \cdot \\ \vdots \\ \cdot \end{bmatrix} - \eta \begin{bmatrix} \cdot \\ \vdots \\ \cdot \end{bmatrix}$

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

Finding the least squares line

Find “best” line

Minimize cost over all possible w_0, w_1



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

⇒ solution is unique
+ gradient descent alg. will converge to minimum

Compute the gradient

$$\text{RSS}(\mathbf{w}_0, \mathbf{w}_1) = \sum_{i=1}^N (y_i - [\mathbf{w}_0 + \mathbf{w}_1 x_i])^2$$

Aside:

$$\begin{aligned}\frac{d}{dw} \sum_{i=1}^N g_i(w) &= \frac{d}{dw} \underbrace{(g_1(w) + g_2(w) + \dots + g_N(w))}_{\cdot \cdot \cdot} \\ &= \frac{d}{dw} g_1(w) + \frac{d}{dw} g_2(w) + \dots + \frac{d}{dw} g_N(w) \\ &= \sum_{i=1}^N \frac{d}{dw} g_i(w)\end{aligned}$$

In our case

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

same for w_1

Compute the gradient

$$\text{RSS}(\mathbf{w}_0, \mathbf{w}_1) = \sum_{i=1}^N (y_i - [\mathbf{w}_0 + \mathbf{w}_1 x_i])^2$$

Taking the derivative w.r.t. \mathbf{w}_0

$$\sum_{i=1}^N 2(y_i - [\mathbf{w}_0 + \mathbf{w}_1 x_i])^1 \cdot (-1)$$

$$= -2 \sum_{i=1}^N (y_i - [\mathbf{w}_0 + \mathbf{w}_1 x_i])$$

Compute the gradient

$$\text{RSS}(\mathbf{w}_0, \mathbf{w}_1) = \sum_{i=1}^N (y_i - [\mathbf{w}_0 + \mathbf{w}_1 x_i])^2$$

Taking the derivative w.r.t. \mathbf{w}_1

$$\sum_{i=1}^N 2(y_i - [\mathbf{w}_0 + \mathbf{w}_1 x_i]) \cdot (-x_i)$$

$$= -2 \sum_{i=1}^N (y_i - [\mathbf{w}_0 + \mathbf{w}_1 x_i]) \underline{x_i}$$

Compute the gradient

$$\text{RSS}(\mathbf{w}_0, \mathbf{w}_1) = \sum_{i=1}^N (y_i - (\mathbf{w}_0 + \mathbf{w}_1 x_i))^2$$

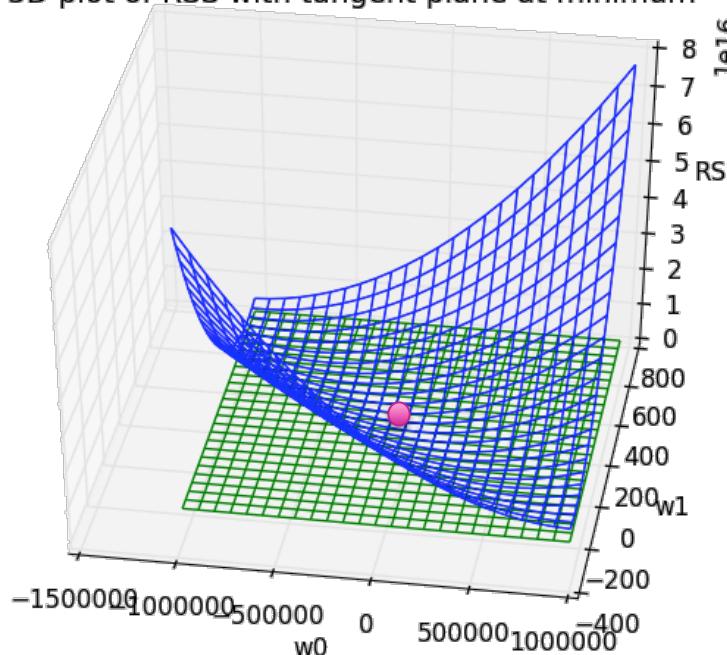
Putting it together:

$$\nabla \text{RSS}(\mathbf{w}_0, \mathbf{w}_1) = \begin{bmatrix} -2 \sum_{i=1}^N [y_i - (\mathbf{w}_0 + \mathbf{w}_1 x_i)] \\ -2 \sum_{i=1}^N [y_i - (\mathbf{w}_0 + \mathbf{w}_1 x_i)] x_i \end{bmatrix}$$

Approach 1: Set gradient = 0

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

3D plot of RSS with tangent plane at minimum



Plug in:

top term: $\hat{w}_0 = \frac{\sum y_i}{N} - \hat{w}_1 \frac{\sum x_i}{N}$

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

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

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

Note:

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

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

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

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

Approach 2: Gradient descent

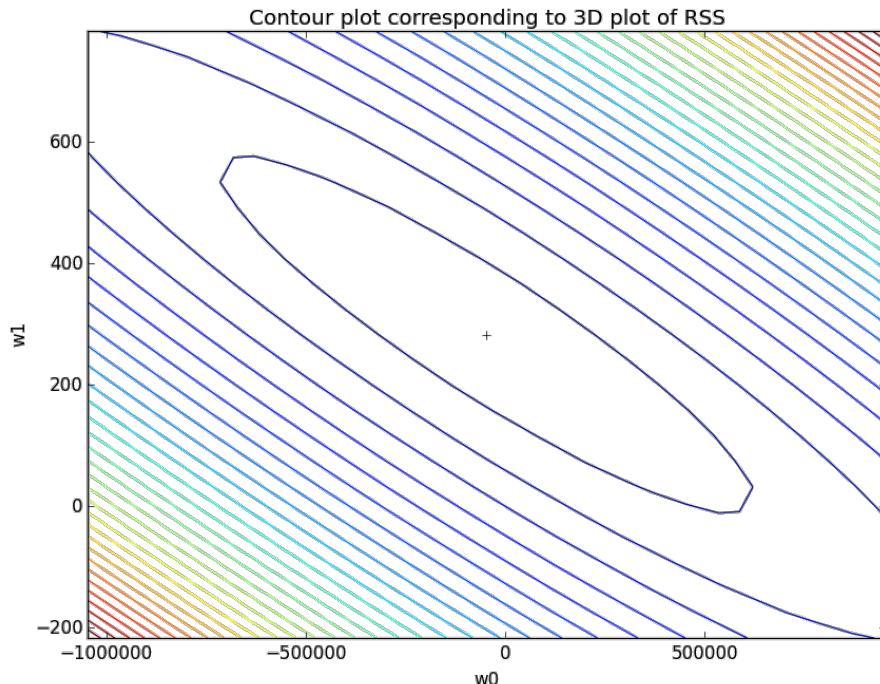
Interpreting the gradient:

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

Annotations for the first term:
actual house sales observation
 y_i predicted value
 $\hat{y}_i(w_0, w_1)$

Approach 2: Gradient descent

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



while not converged

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

If overall, underpredicting \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

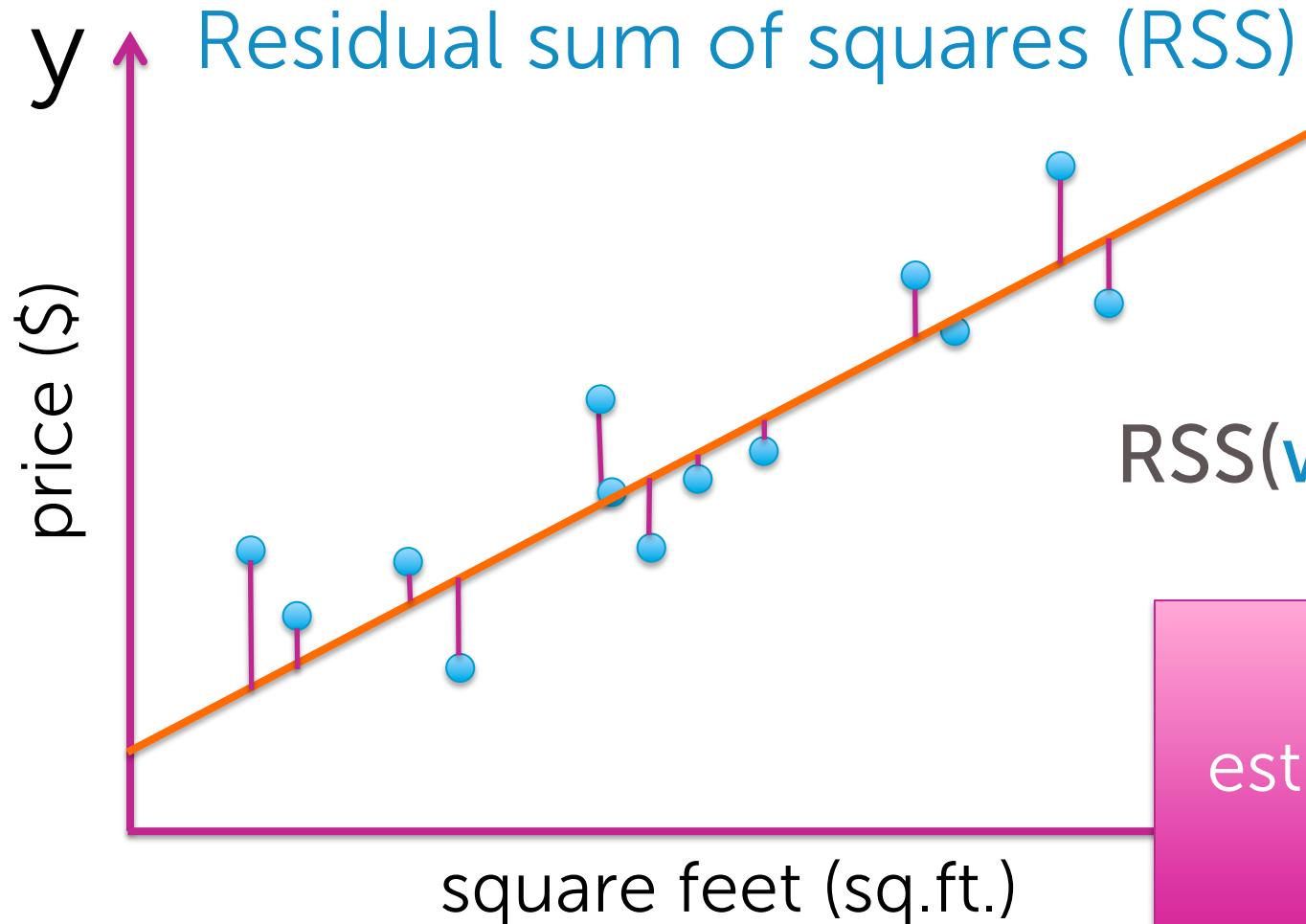
Comparing the approaches

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

Influence of high leverage points

Asymmetric errors

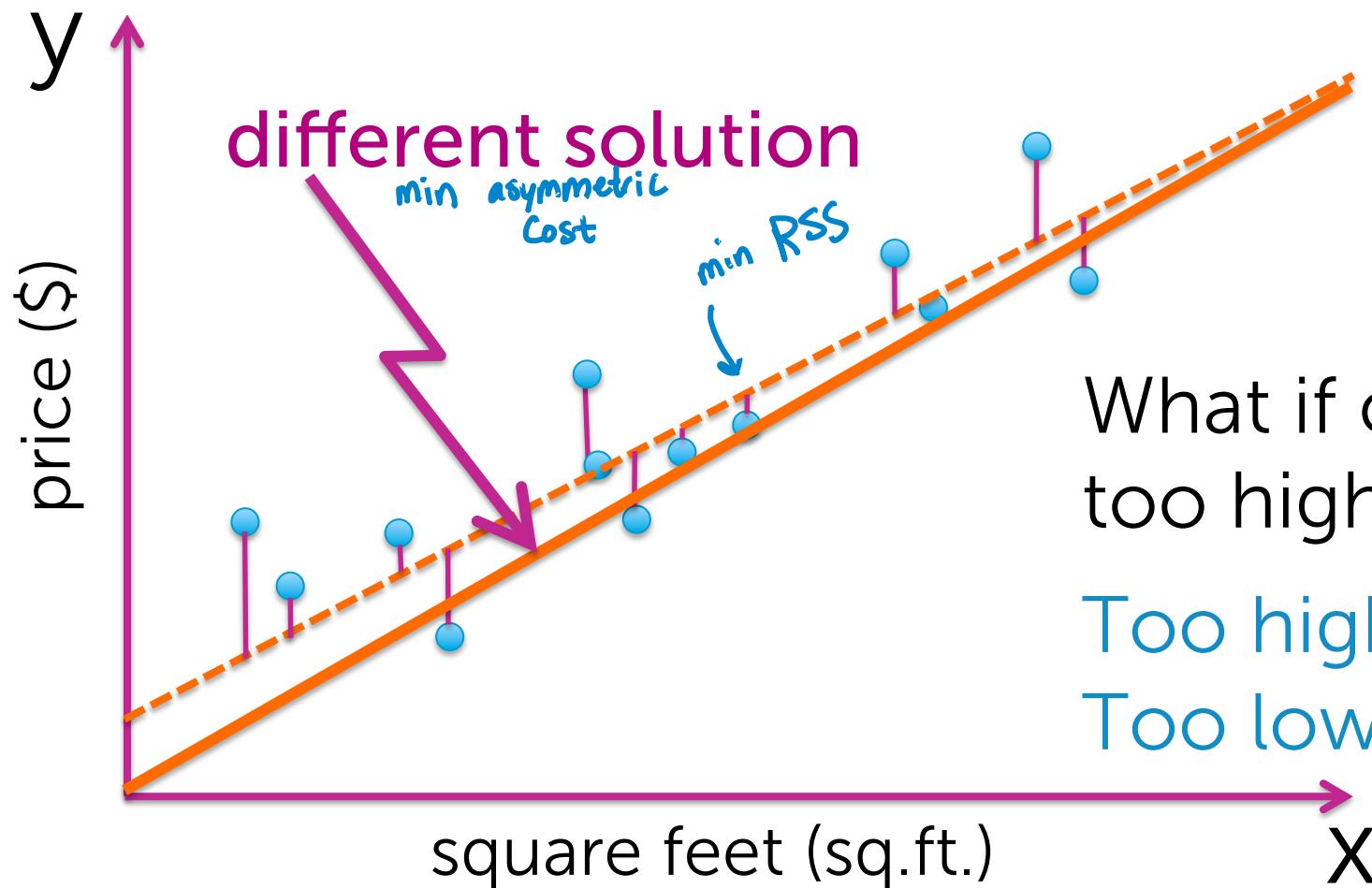
Symmetric cost functions



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

Assumes cost of over-estimating sales price is same as under-estimating

Asymmetric cost functions



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

Too high \rightarrow no offers ($\$=0$)

Too low \rightarrow offers for lower $\$$

Summary for simple linear regression

What you can do now...

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