Simple Regression:

Linear regression with one input

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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*

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

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

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

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

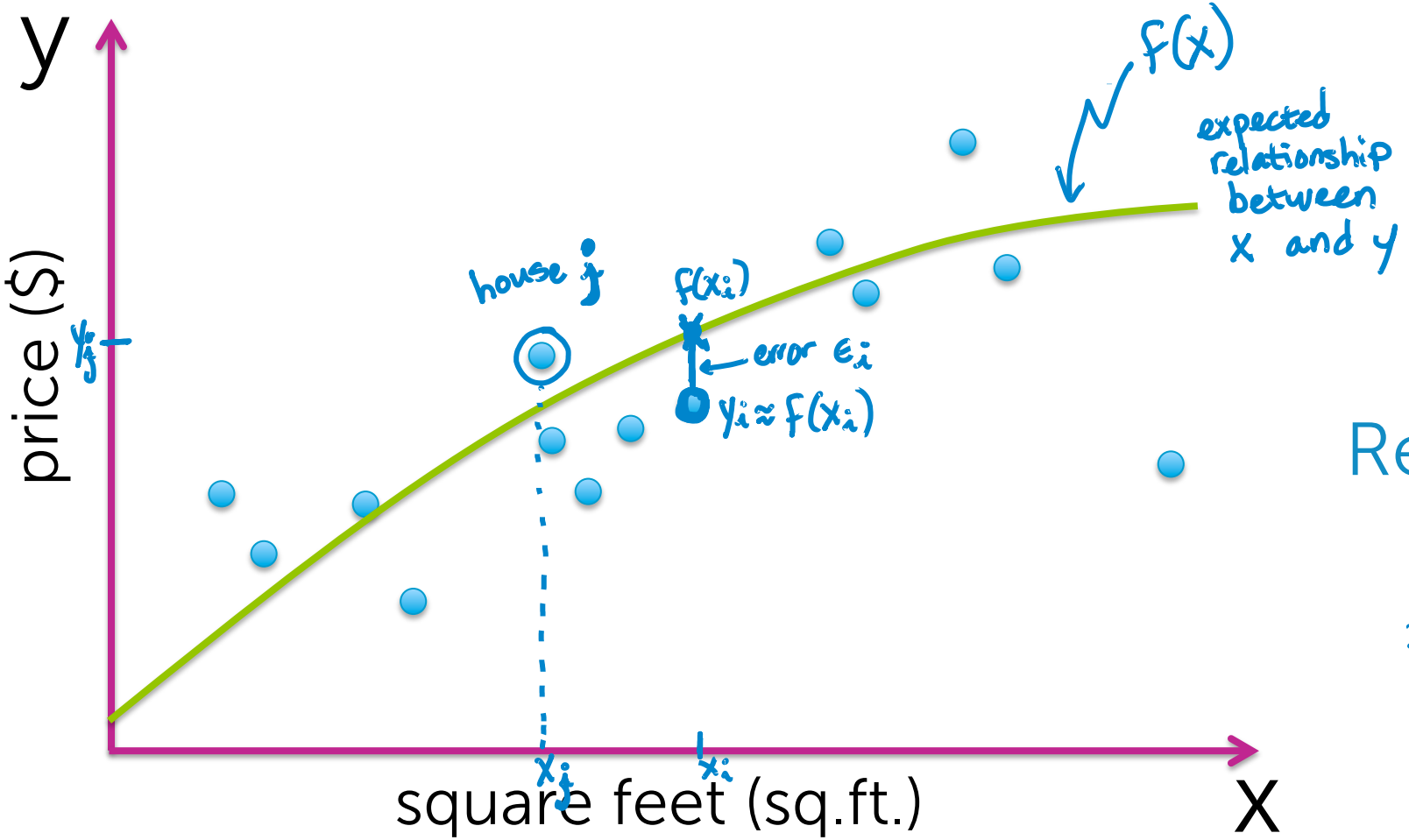
$(x_5 = \text{sq.ft.}, y_5 = \$)$

⋮

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:

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

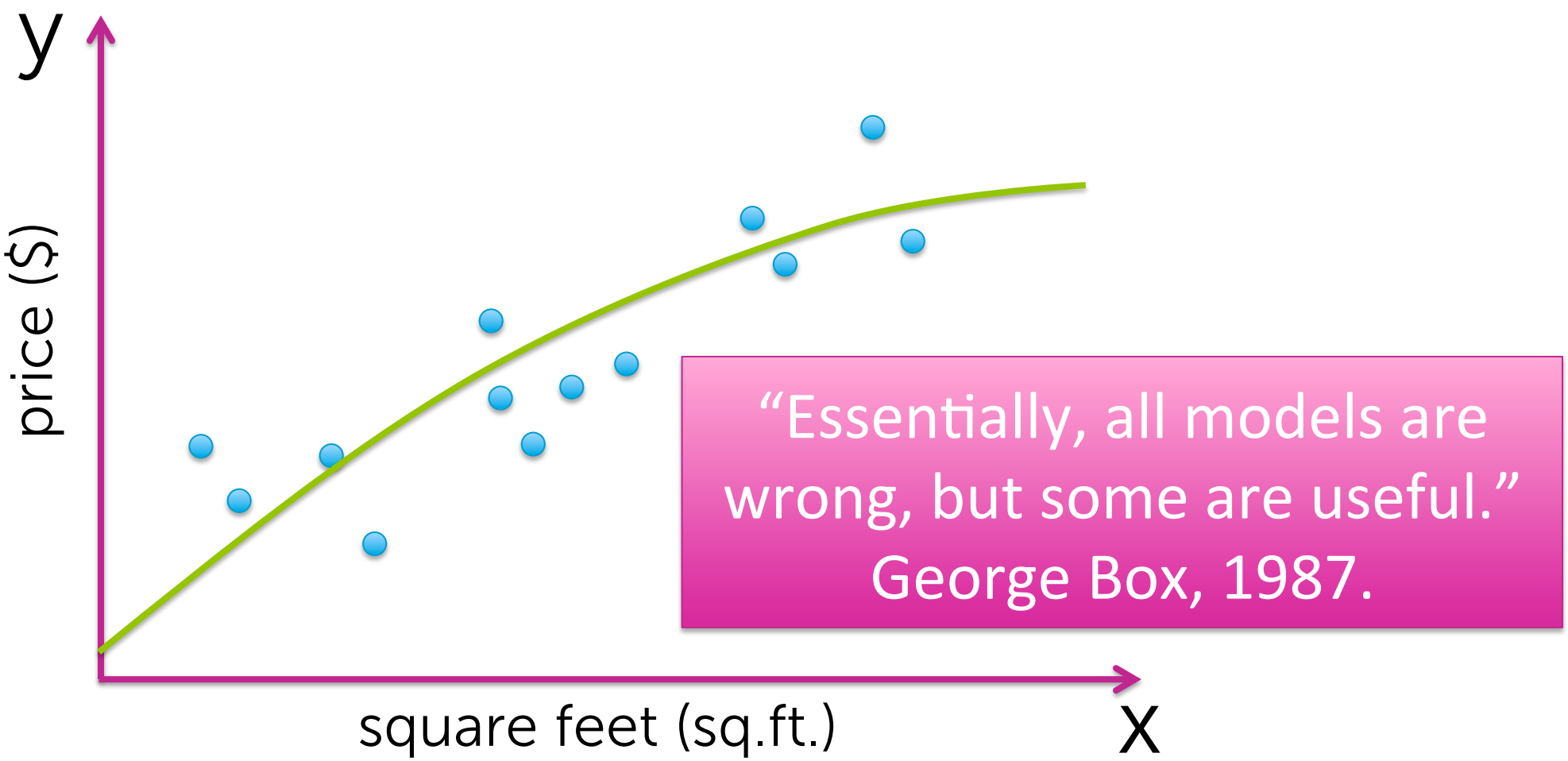
$E[\epsilon_i] = 0$ ← equally likely that error is + or −

↑ expected value

⇓

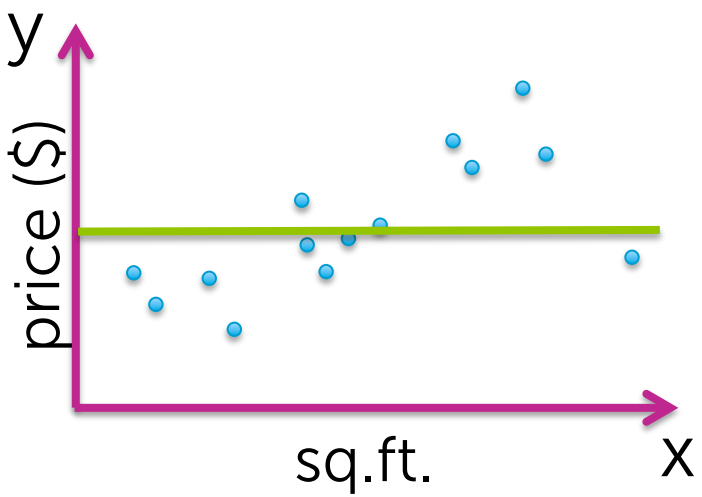
y_i is equally likely to be above or below $f(x_i)$

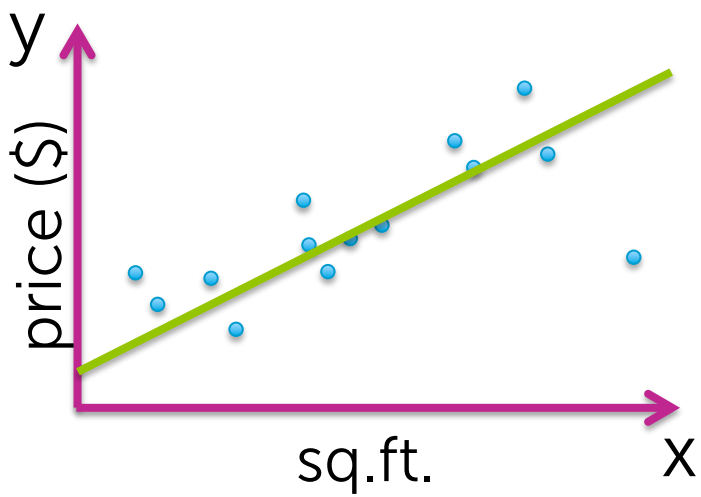
Model –
How we *assume* the world works

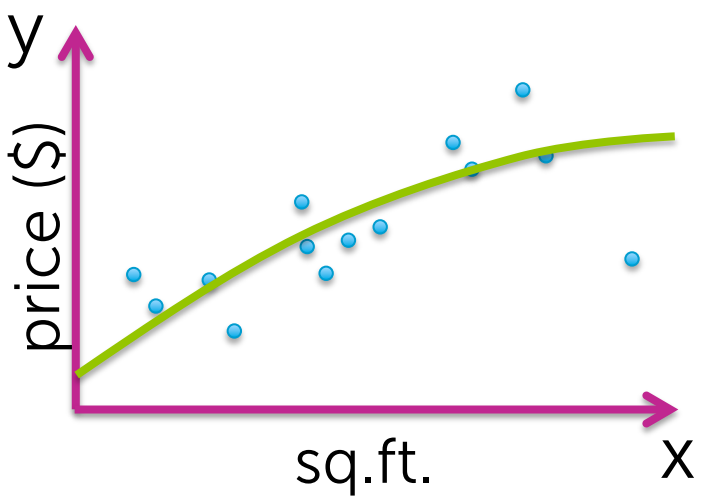


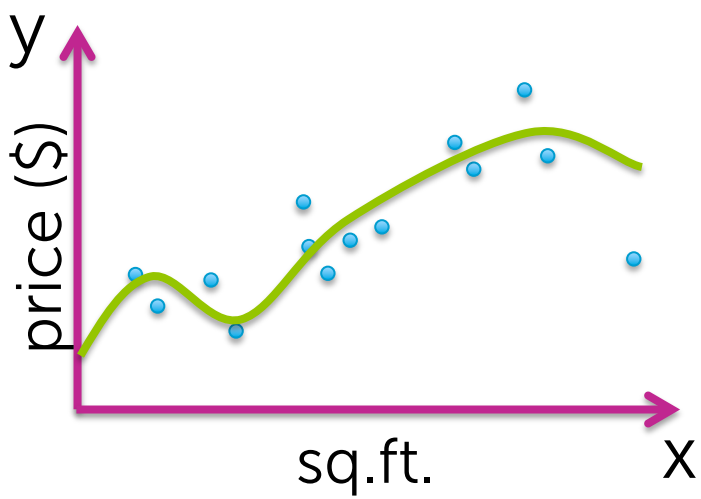
"Essentially, all models are wrong, but some are useful."
George Box, 1987.

Task 1–
Which model f(x)?

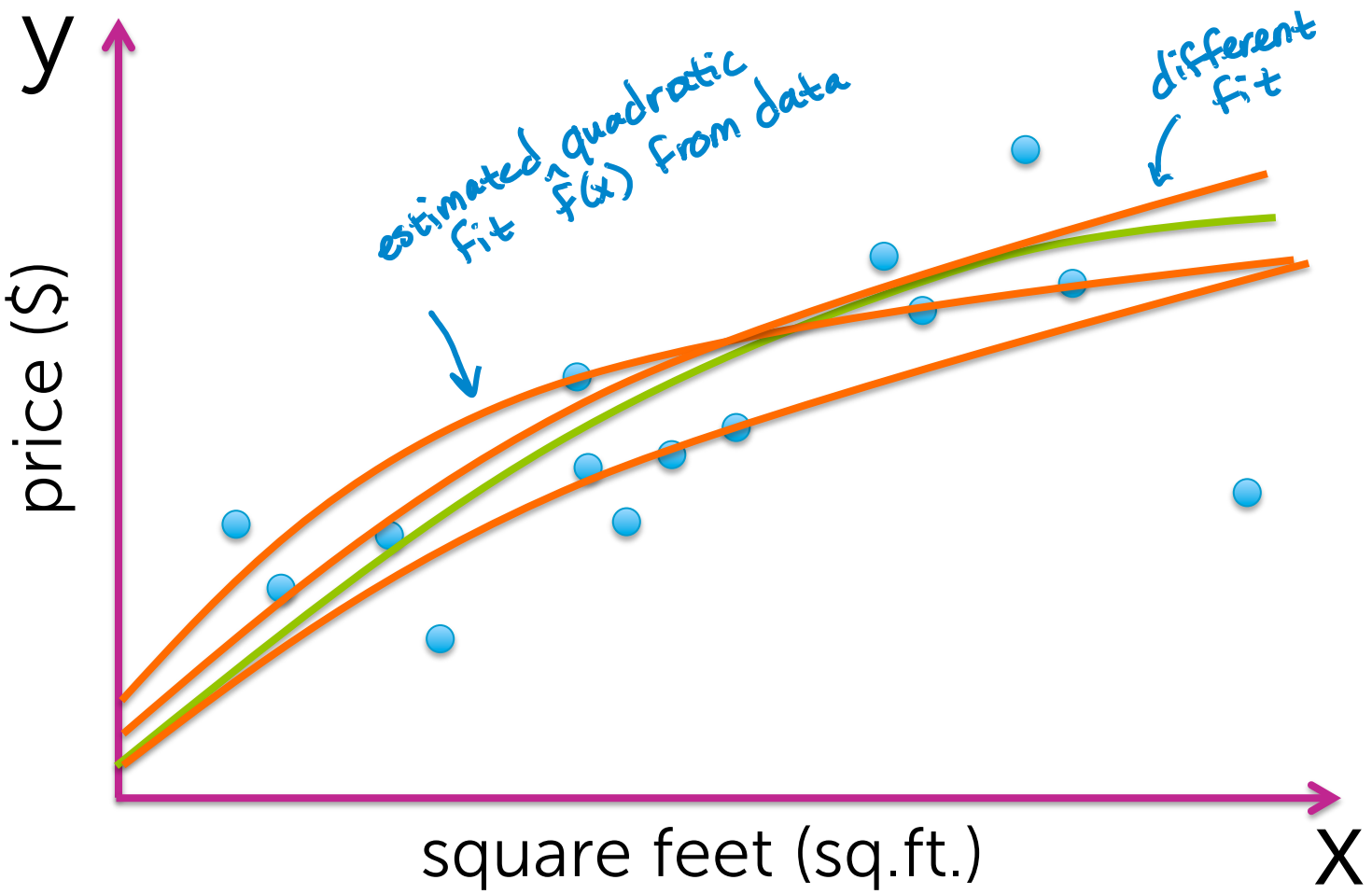




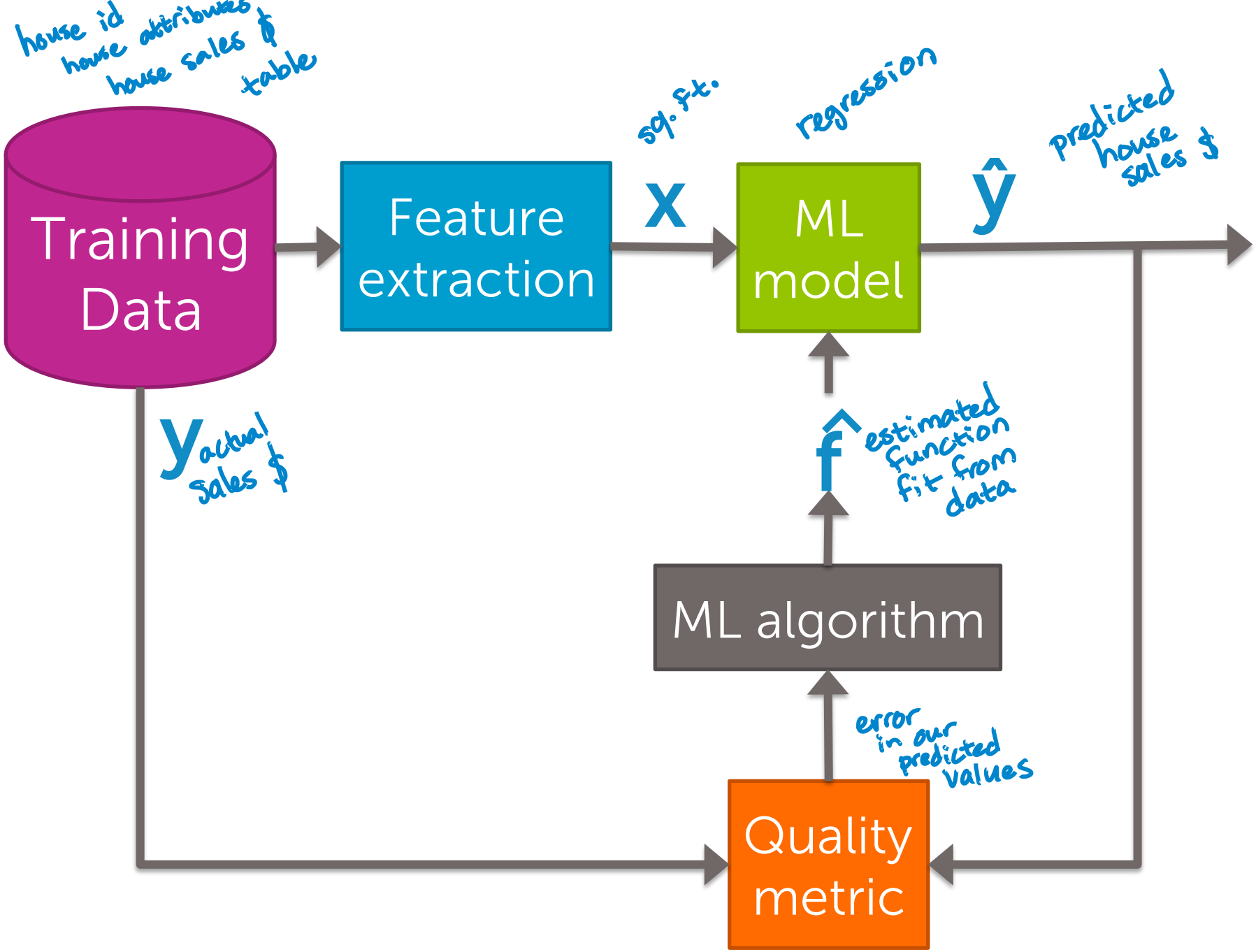




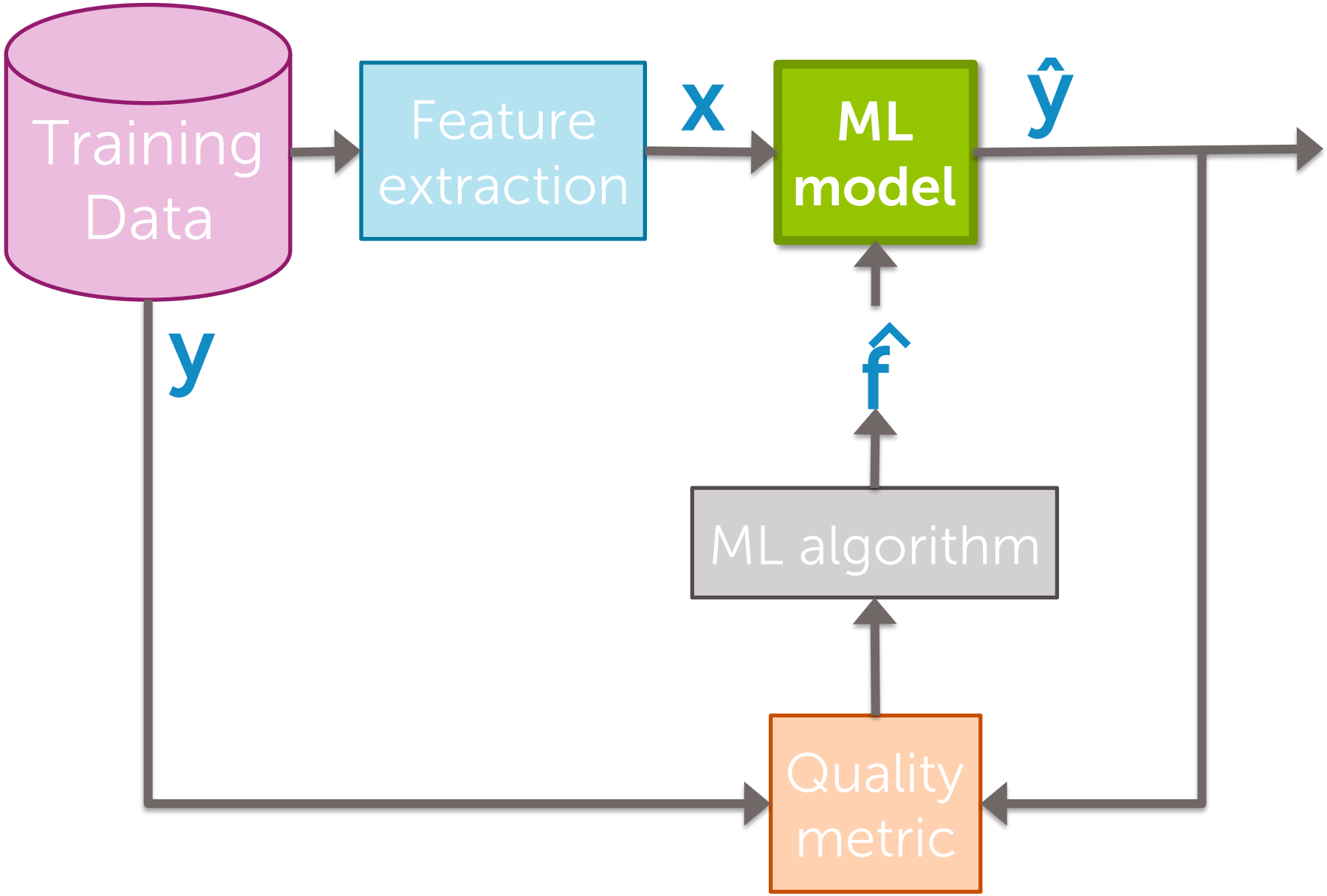
Task 2 – For a given model f(x), estimate function $\hat{f}(x)$ from data



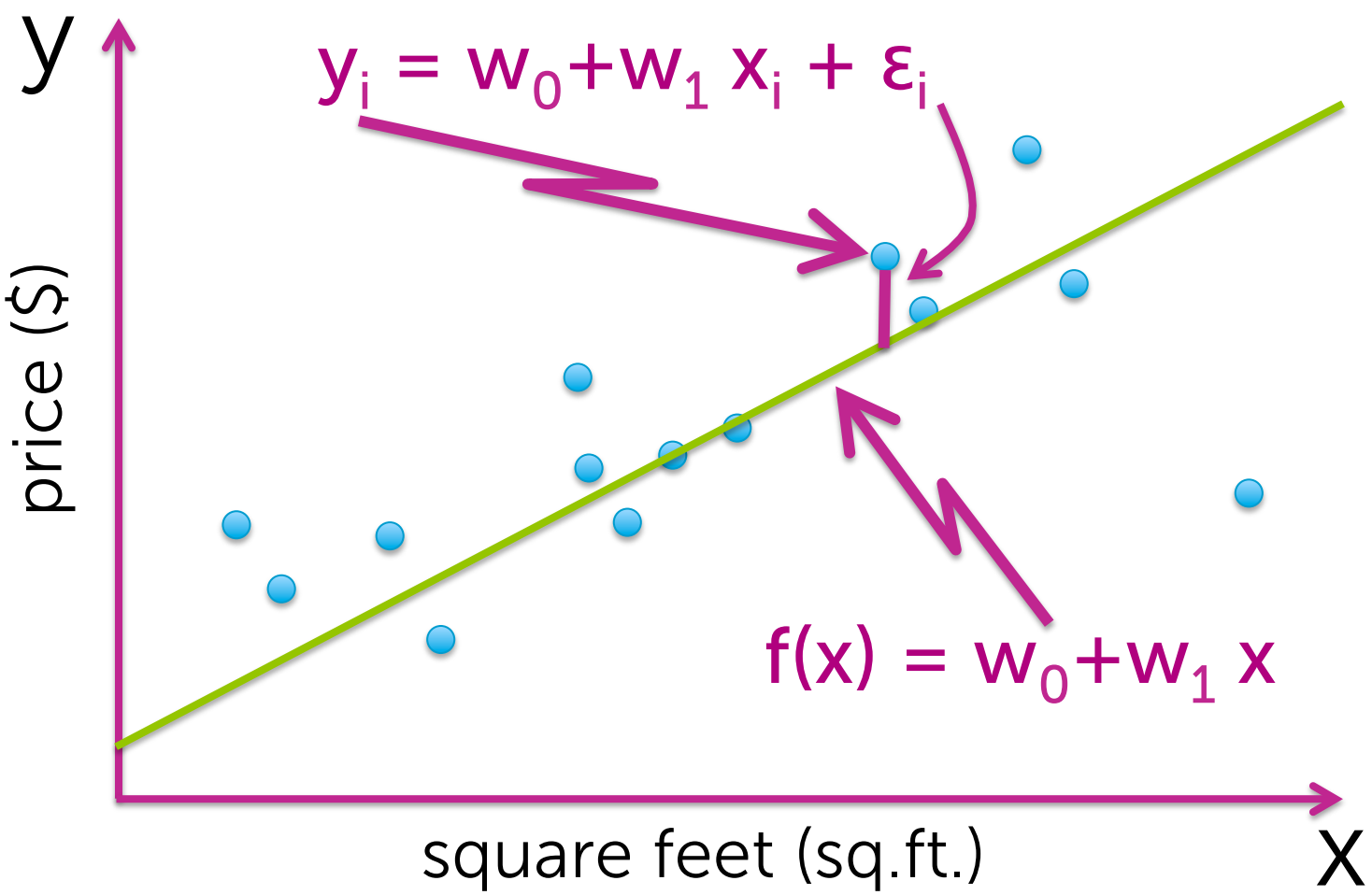
Assume model f(x) is a quadratic function



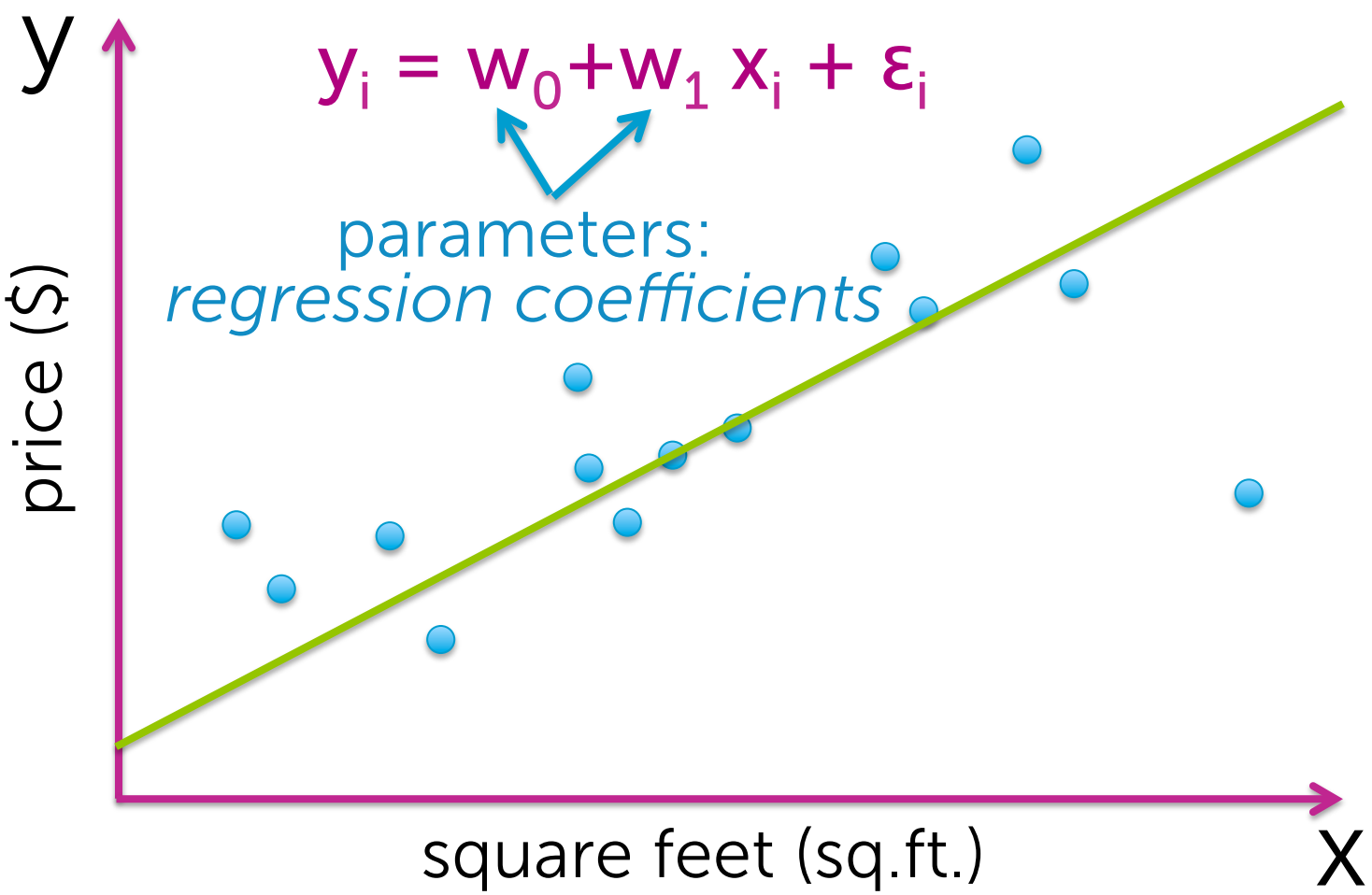
Simple linear regression



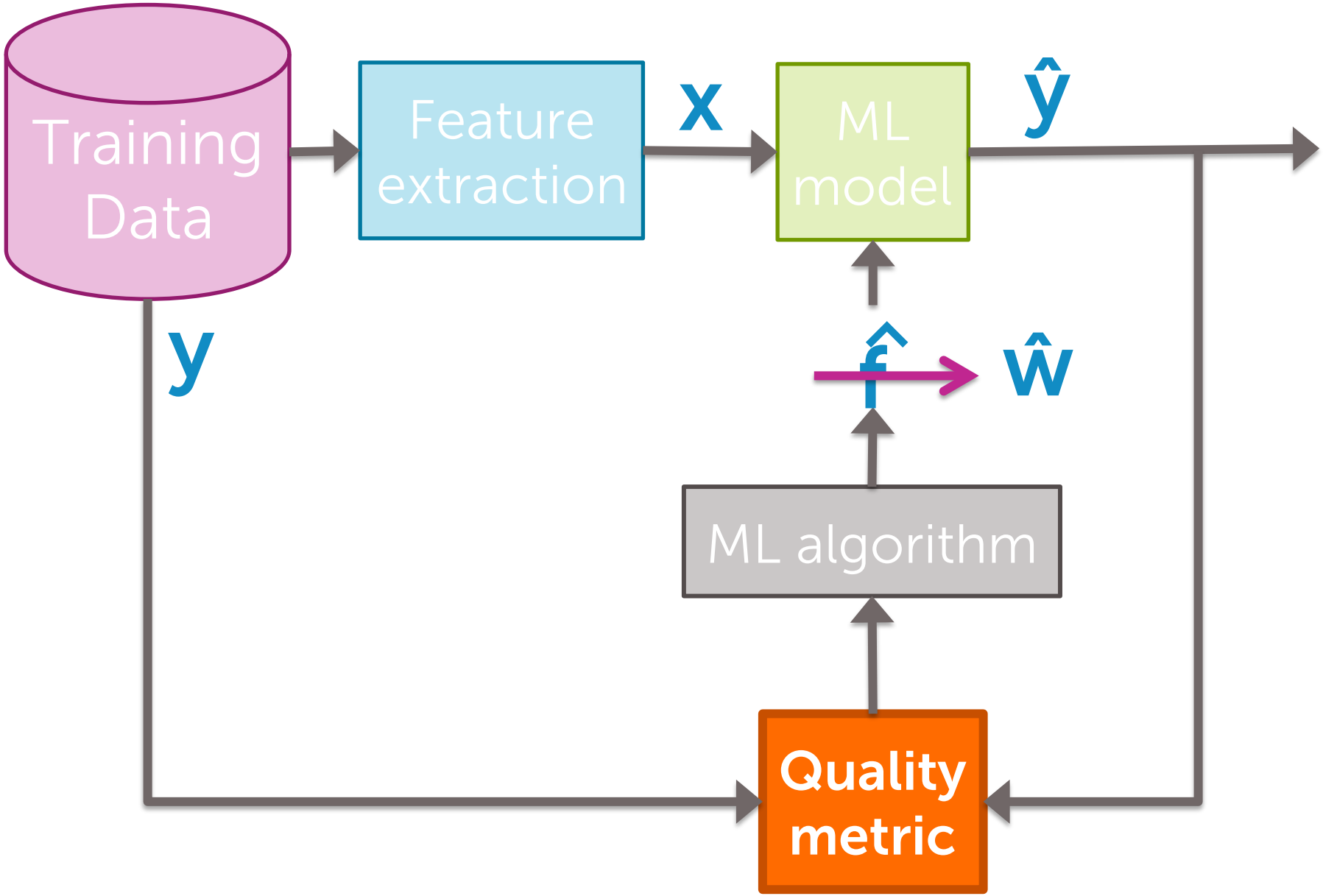
Simple linear regression model



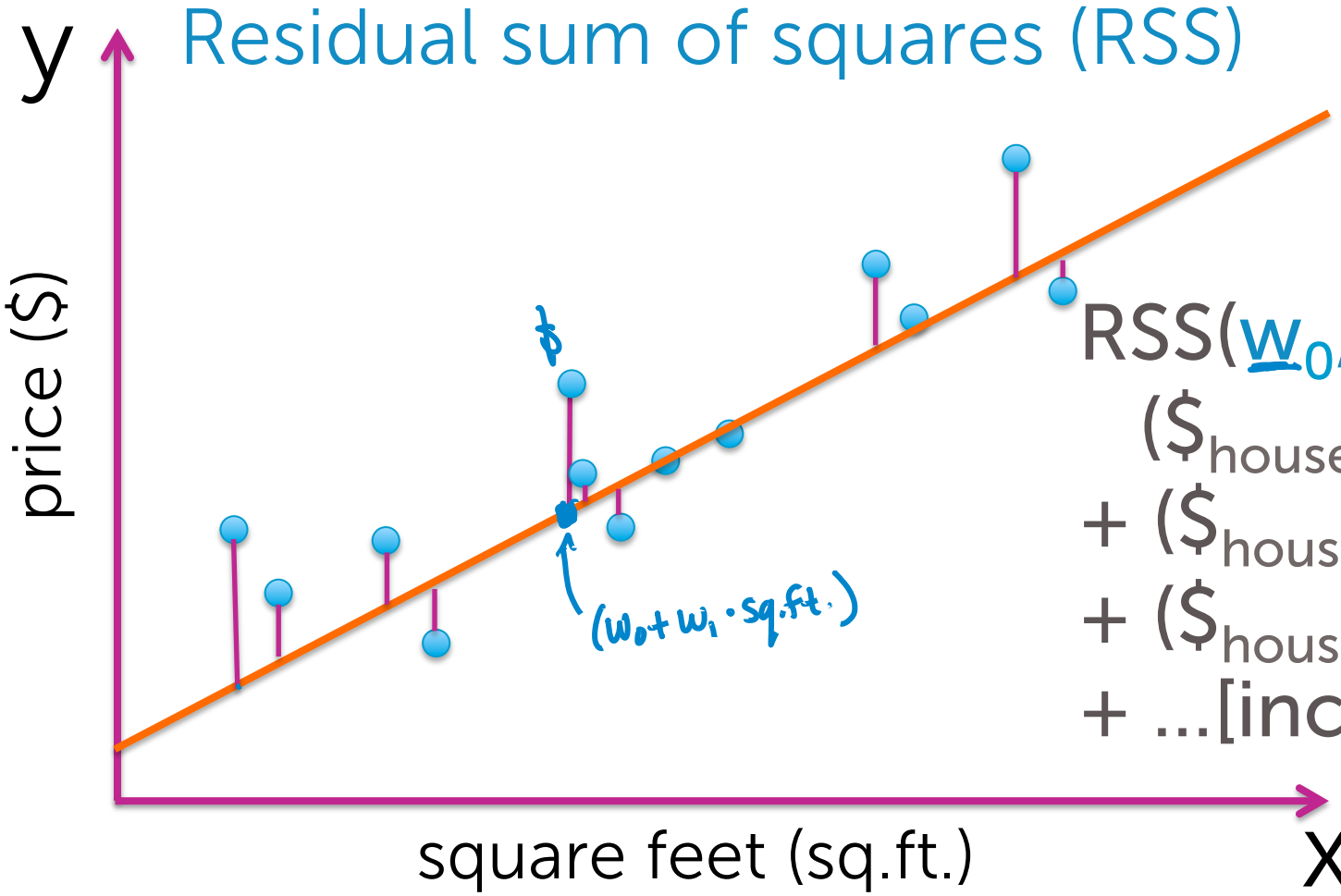
Simple linear regression model



Fitting a line to data



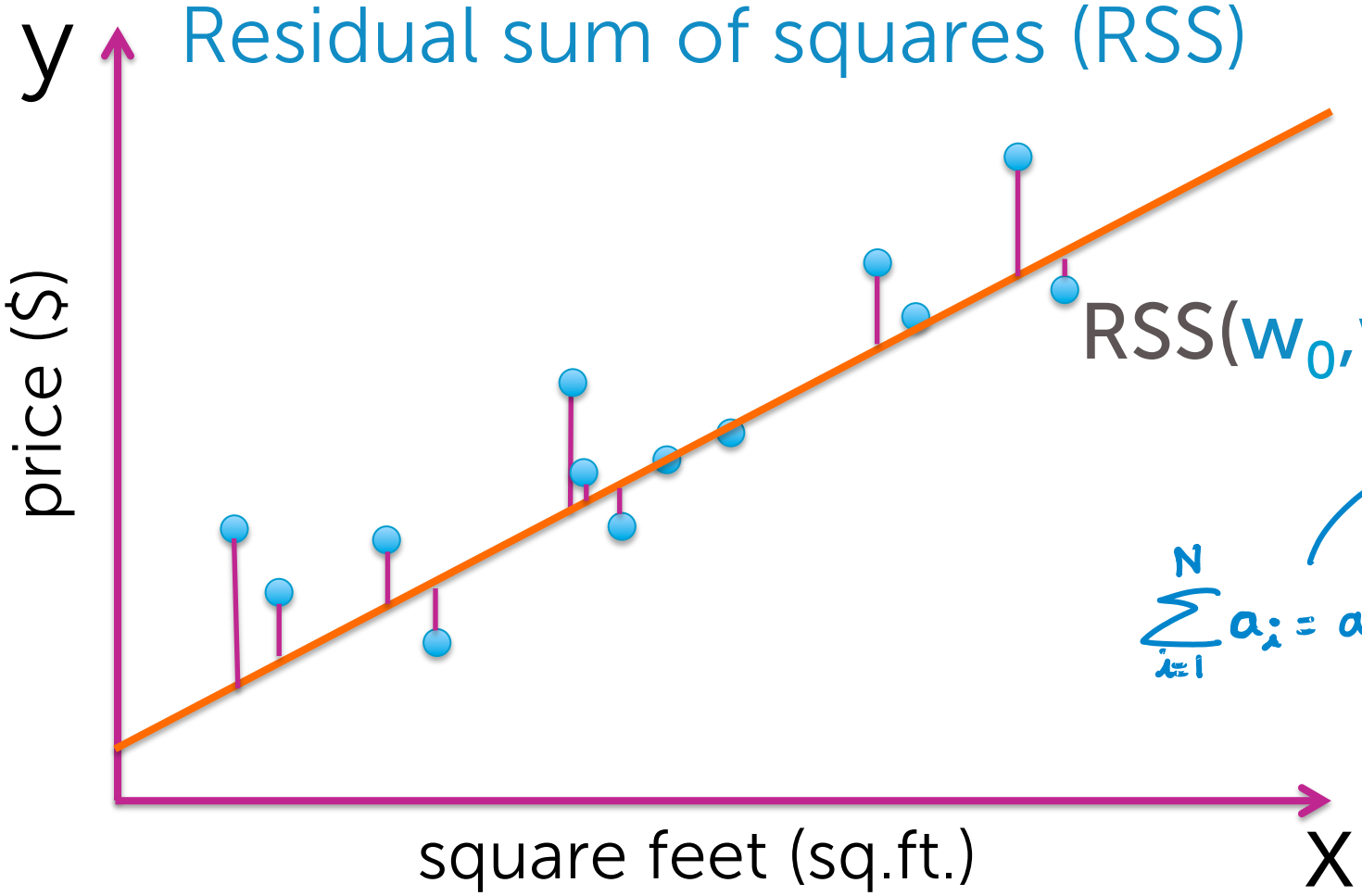
"Cost" of using a given line



Residual sum of squares (RSS)

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

"Cost" of using a given line



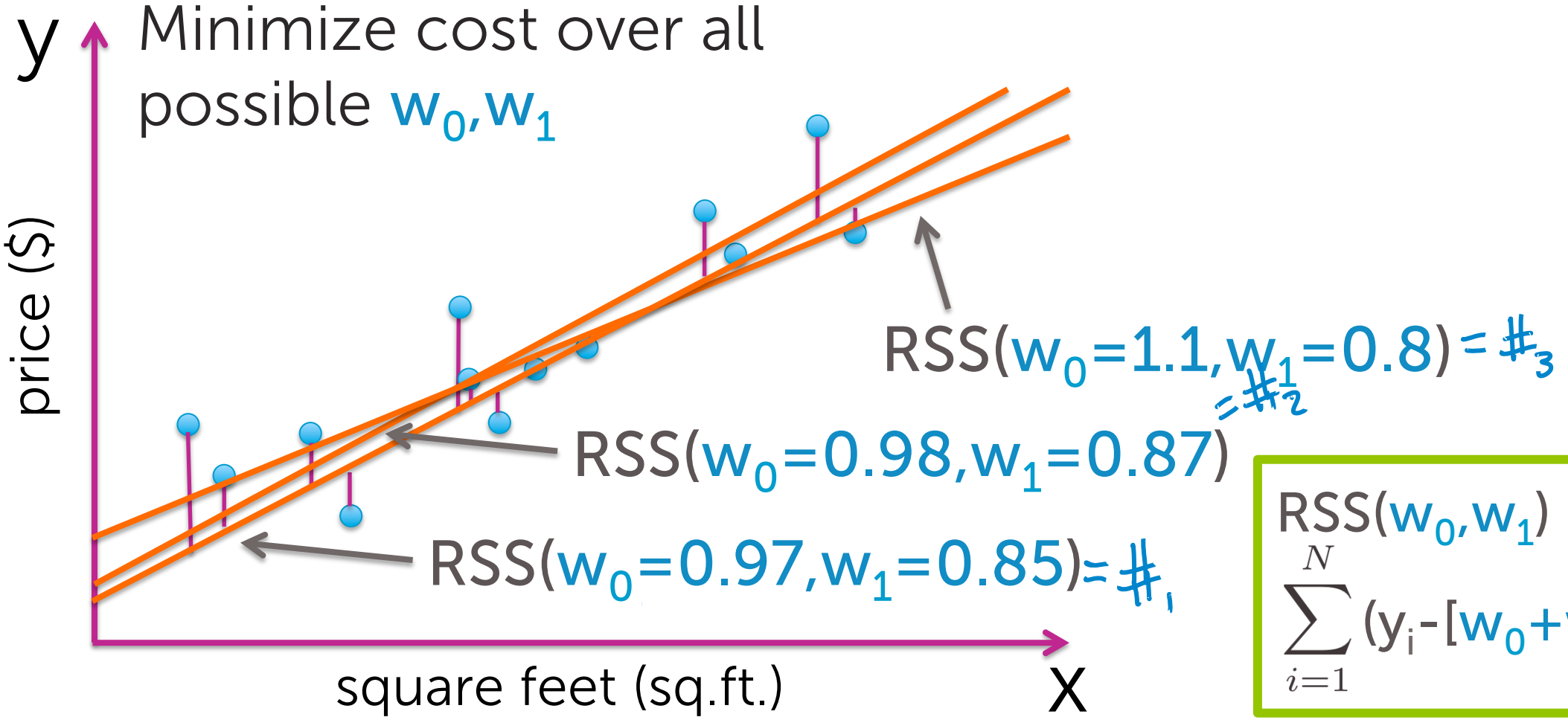
Residual sum of squares (RSS)

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

$$\sum_{i=1}^{N} a_i = a_1 + a_2 + \ldots + a_N$$

Here, $a_i = (y_i - [w_0 + w_1 x_i])^2$

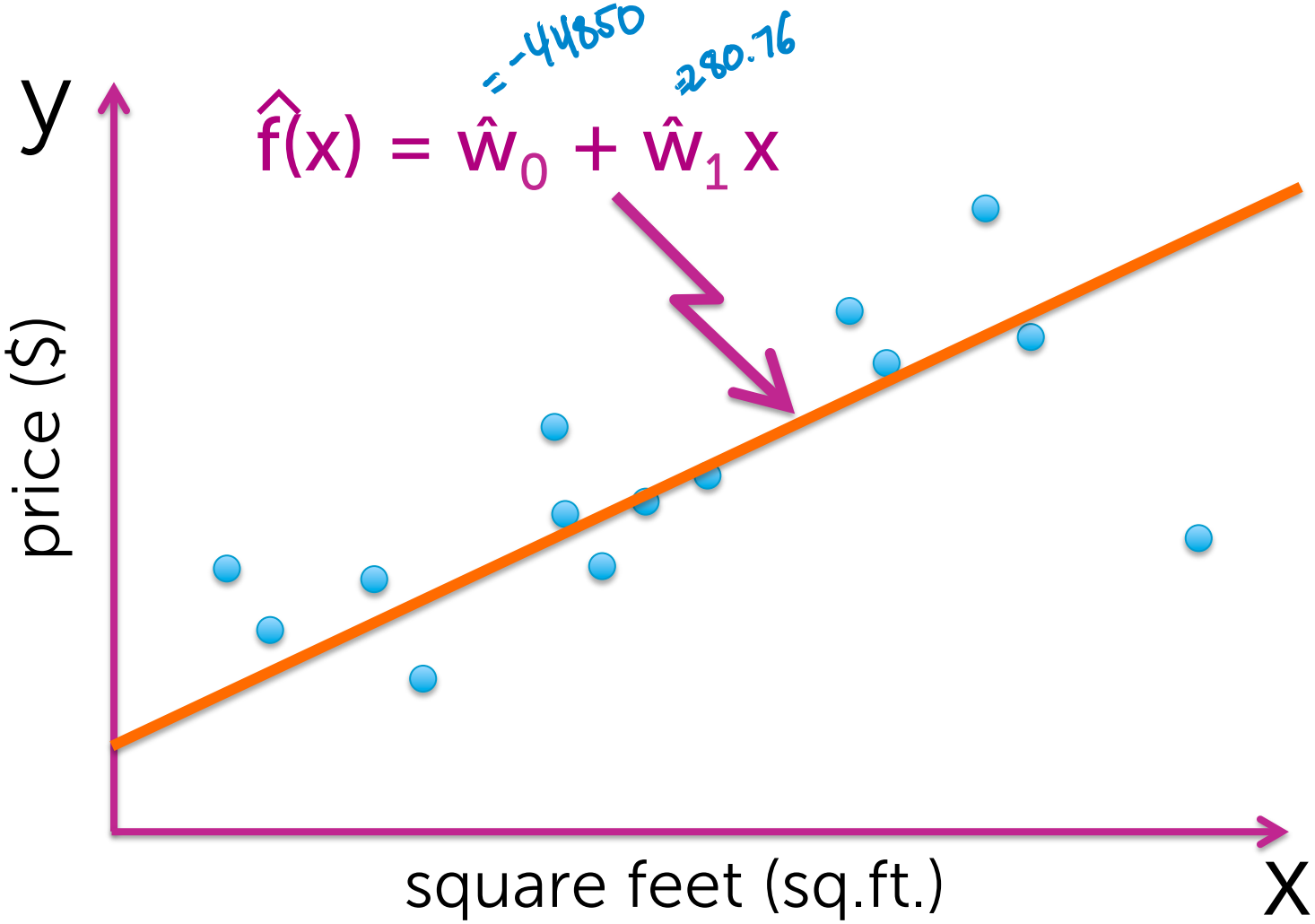
Find "best" line



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

The fitted line: use + interpretation

Model vs. fitted line



Regression model:

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

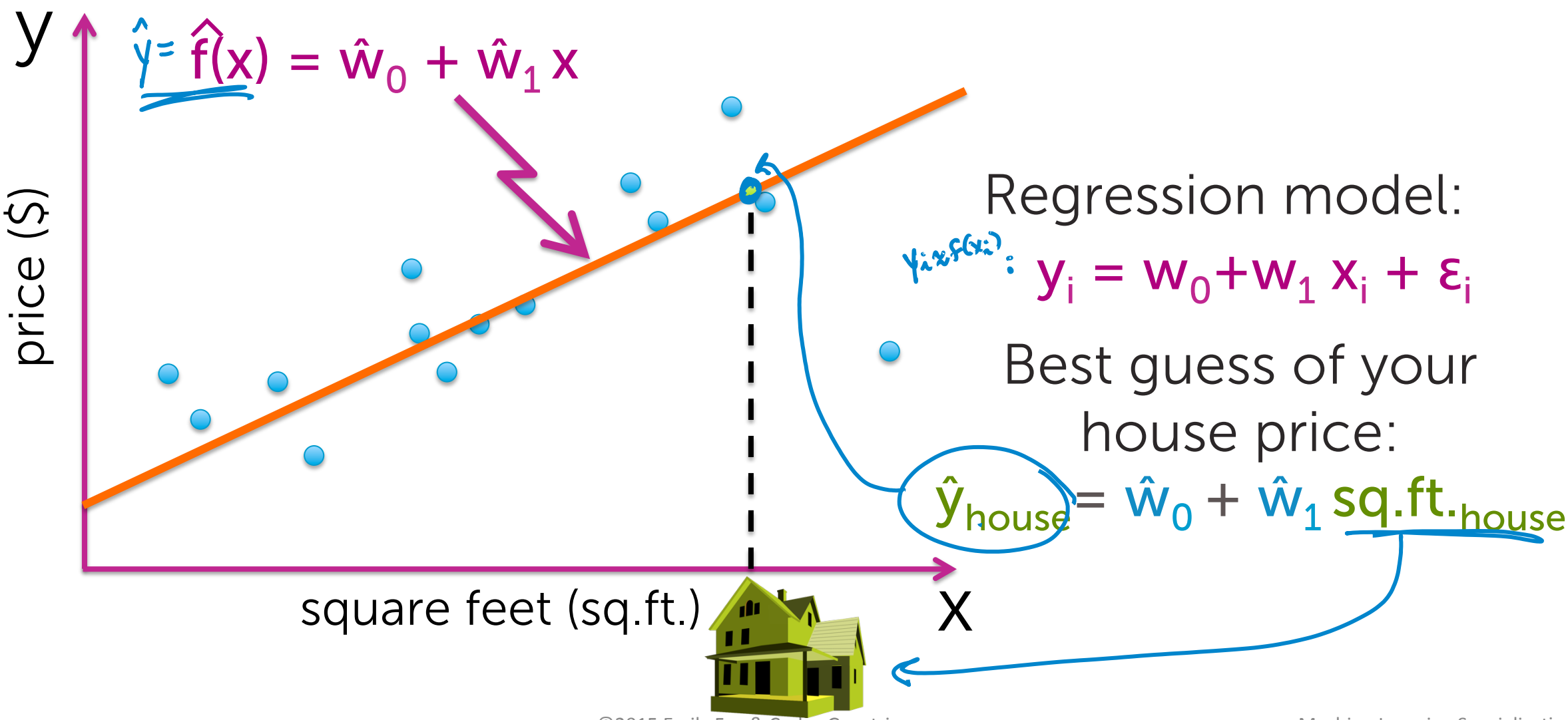
parameters (unknown variables)

Estimated parameters:

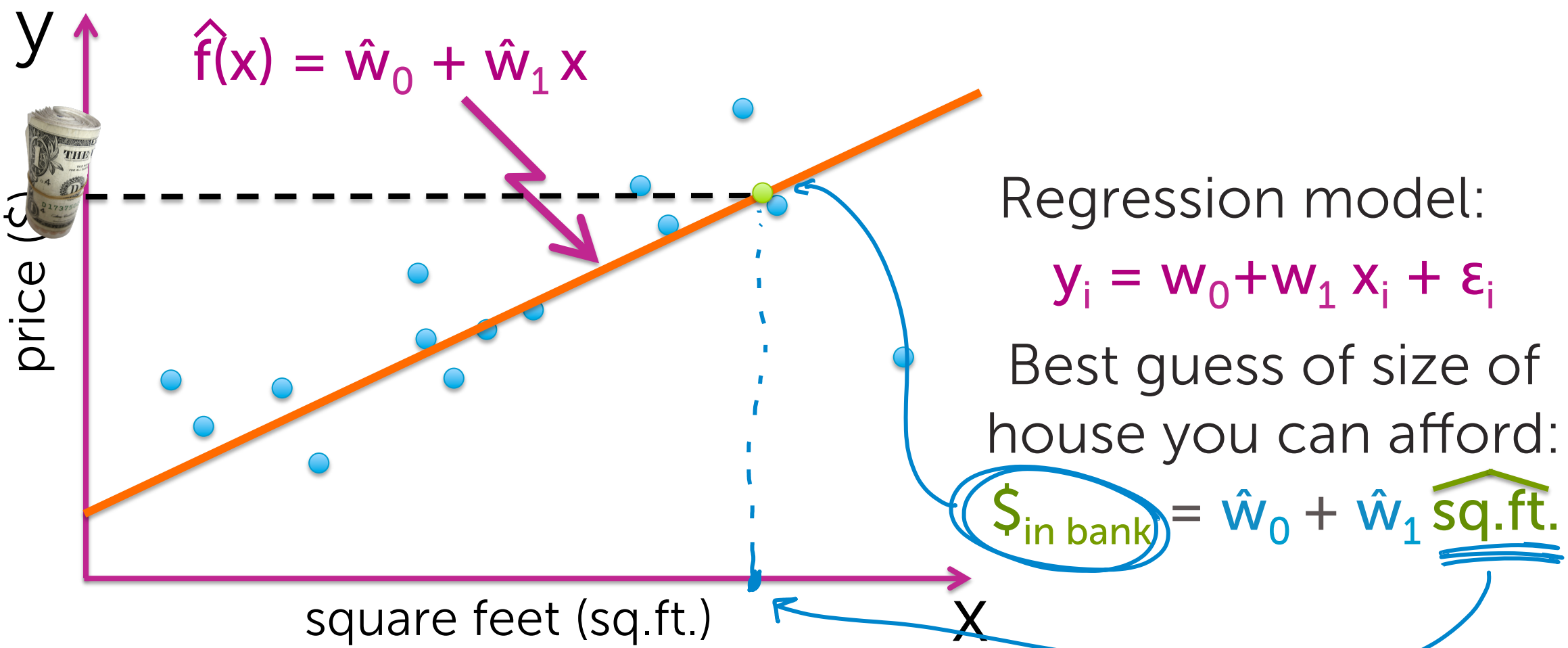
$$\hat{w}_0 \approx -44950, \quad \hat{w}_1 \approx 280.76$$

take actual values

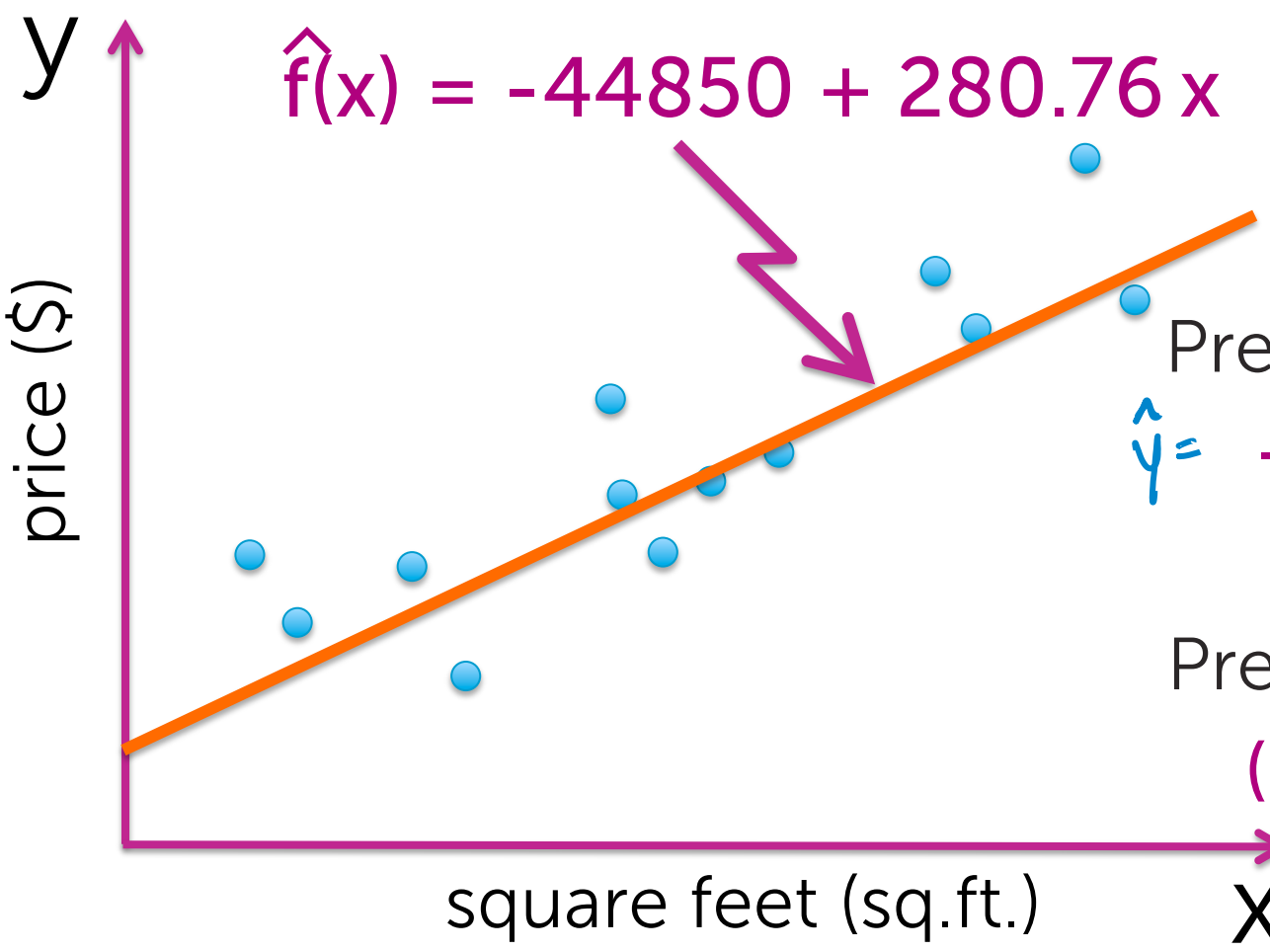
Seller:
Predicting your house price



Buyer:
Predicting size of house



A concrete example



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

$\hat{y} = -44850 + 280.76 * 2{,}640$

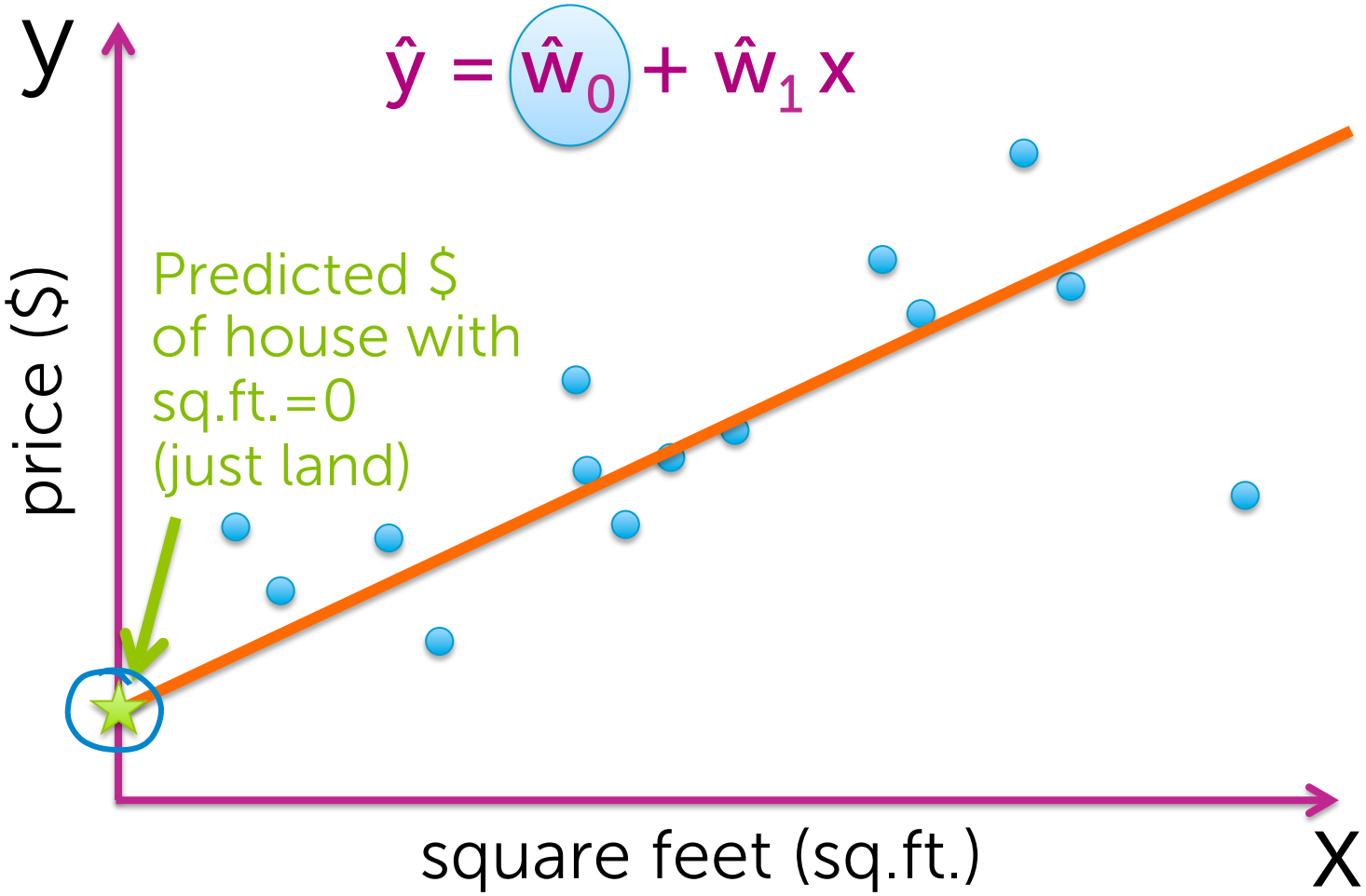
$= \$696{,}356$

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

$(859000+44850)/\ 280.76$

$= 3{,}219$ sq.ft.

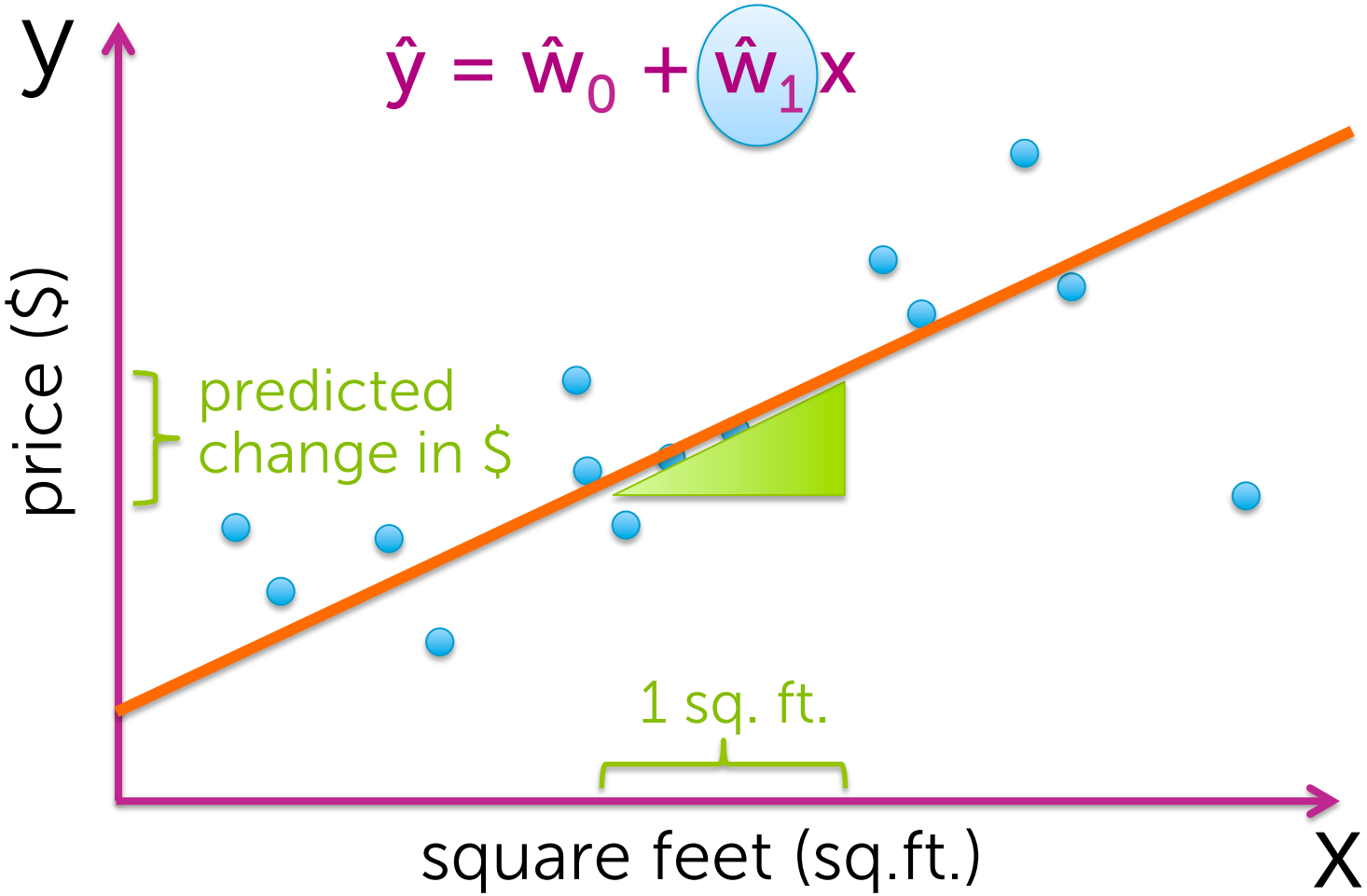
Interpreting the coefficients



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

not very meaningful

Interpreting the coefficients



$$\hat{y} = \hat{w}_0 + \hat{w}_1 x$$

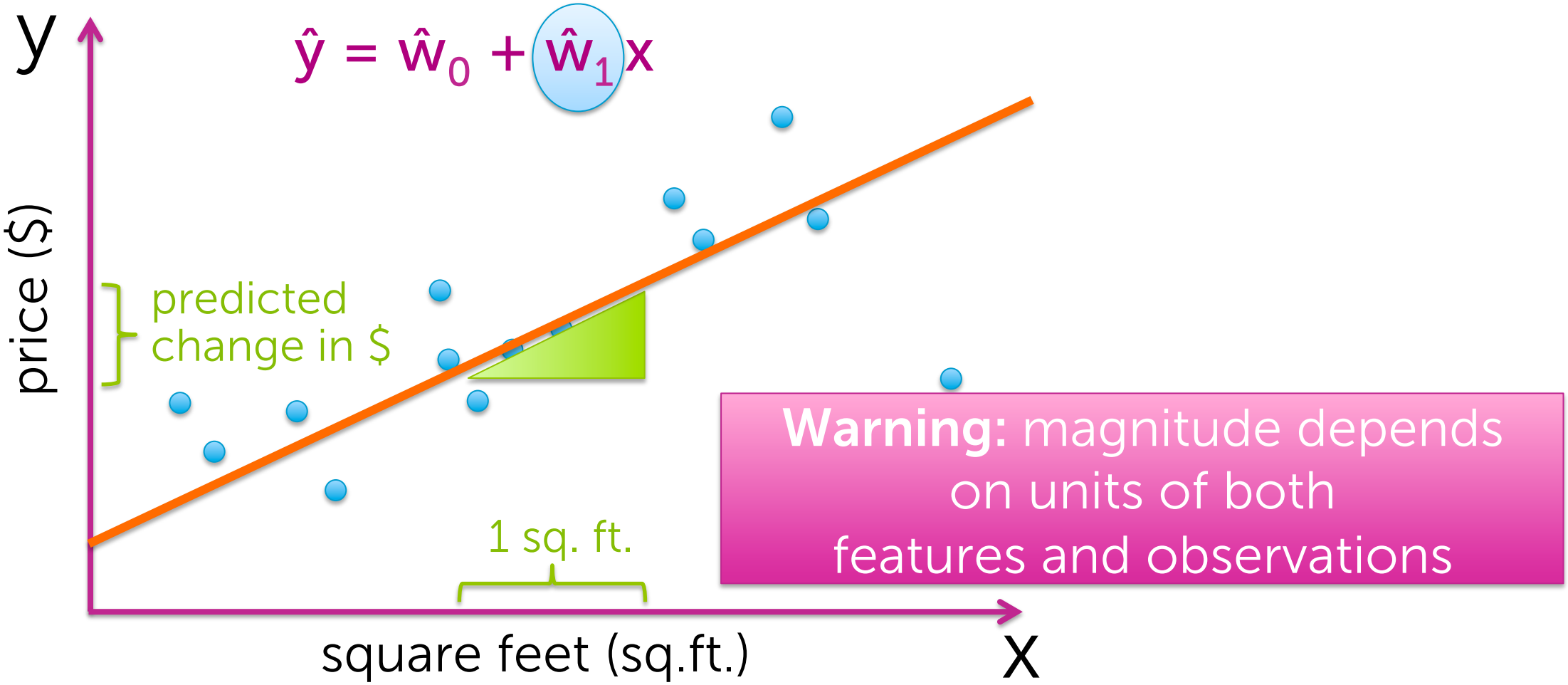
$$\hat{\$}_{1001\ \text{sq.ft.}} - \hat{\$}_{1000\ \text{sq.ft.}}$$

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

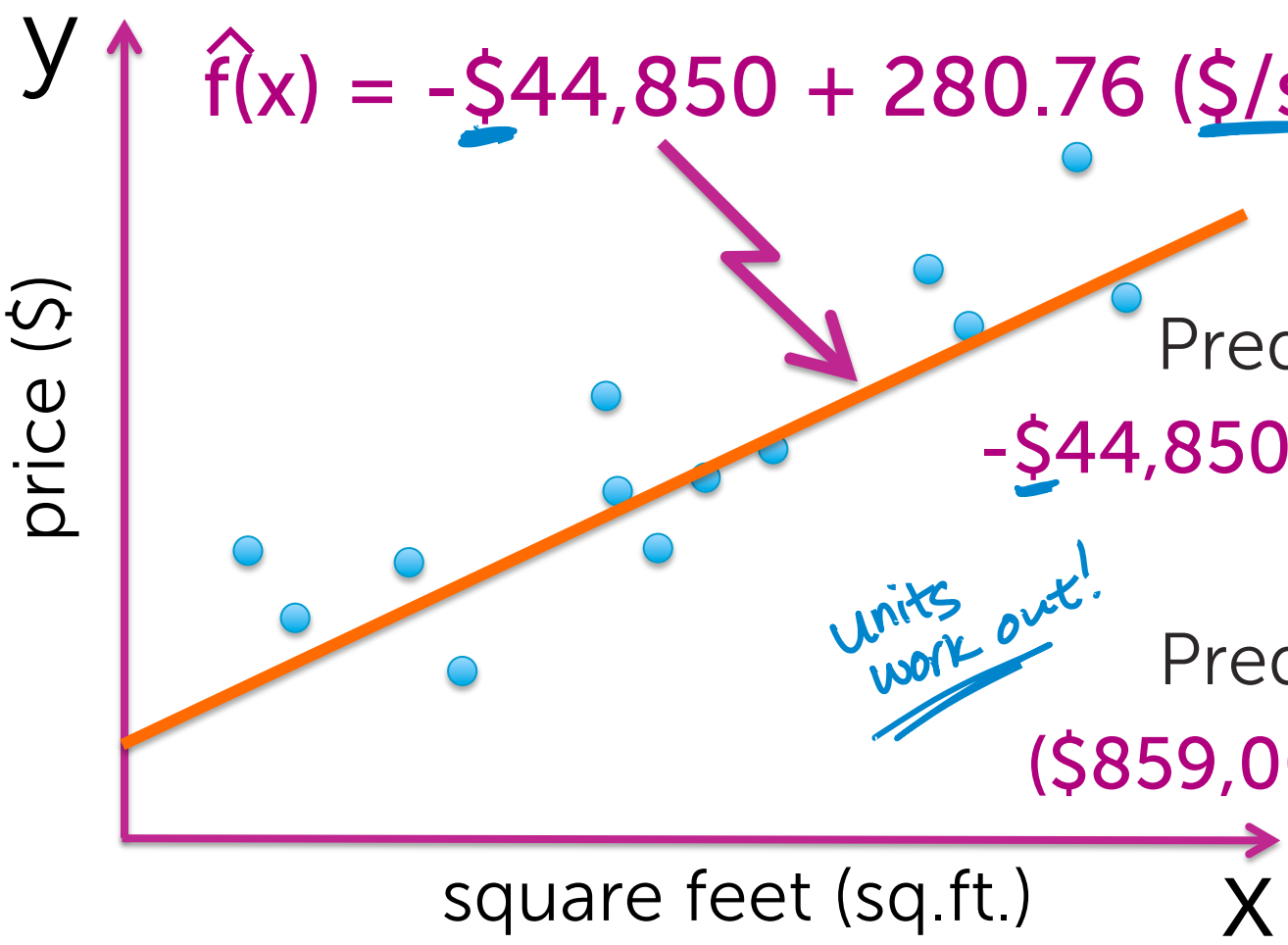
$$= \hat{w}_1$$

predicted change in the output per unit change in input

Interpreting the coefficients



A concrete example



$\hat{f}(x)$ = -$44,850 + 280.76 ($/sq.ft.) x

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

-$44,850 + 280.76 ($/sq.ft.) * 2,640 sq.ft.

= $696,356

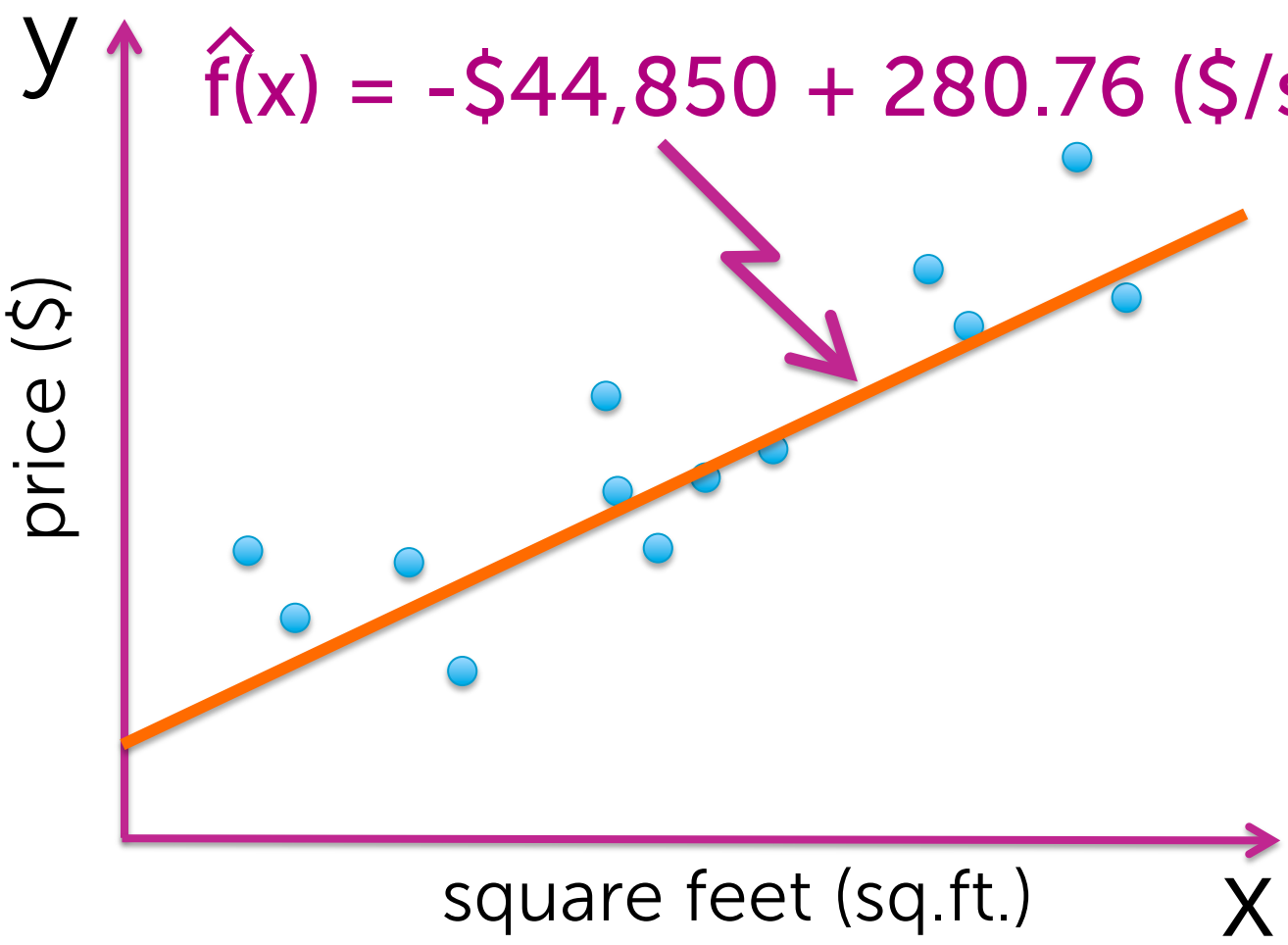
Units work out!

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

($859,000+$44,850)/ 280.76 ($/sq.ft.)

= 3,219 sq.ft.

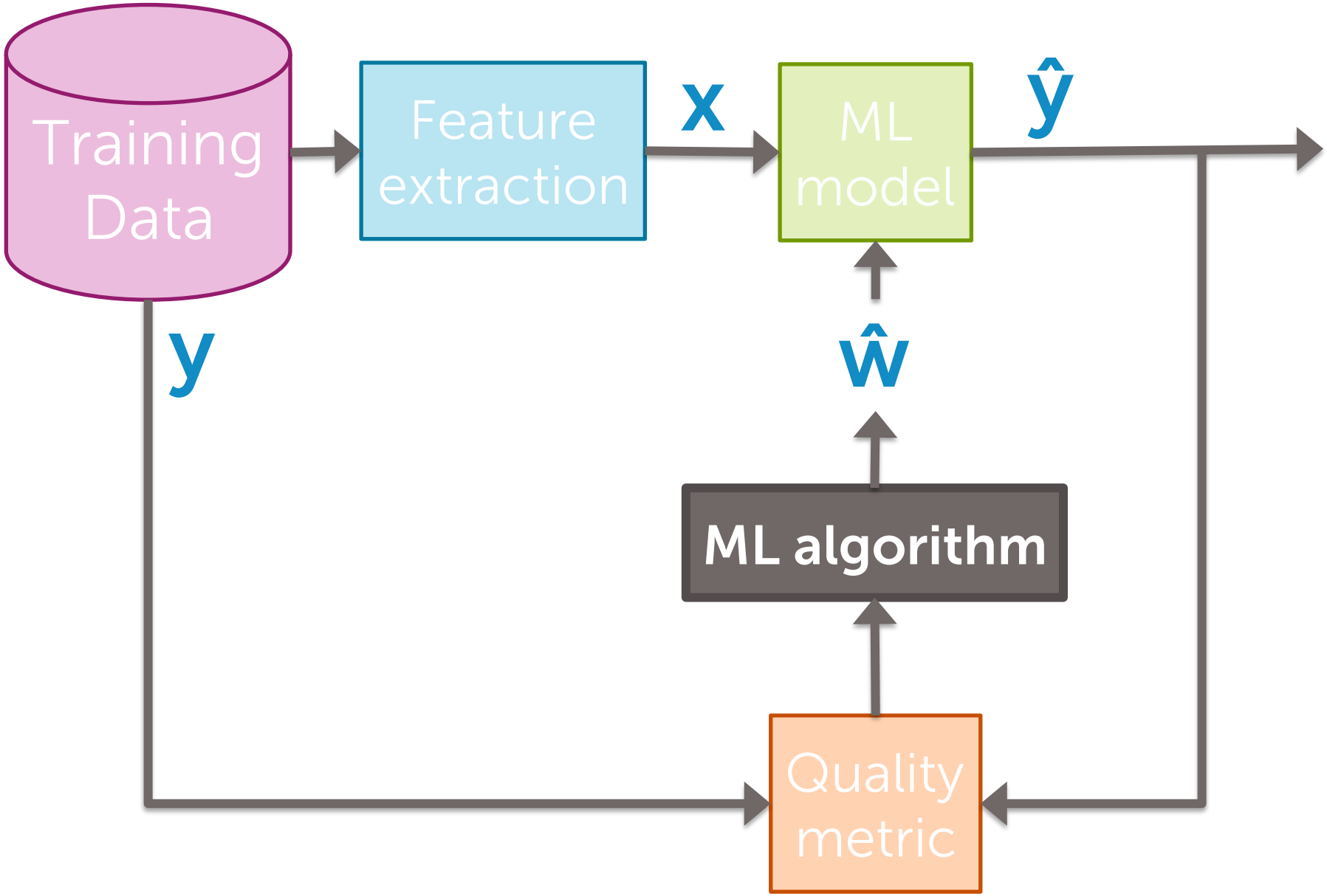
A concrete example



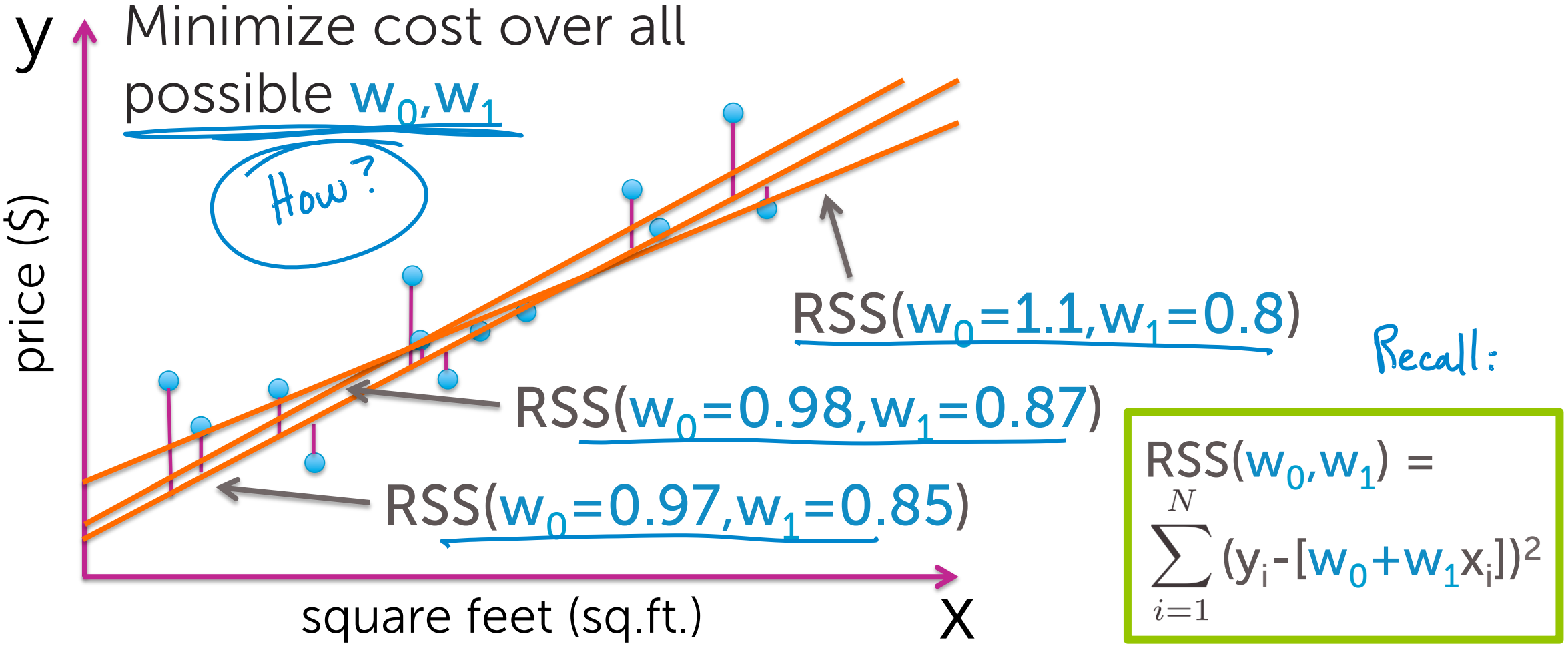
But what if:

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

Algorithms for fitting the model



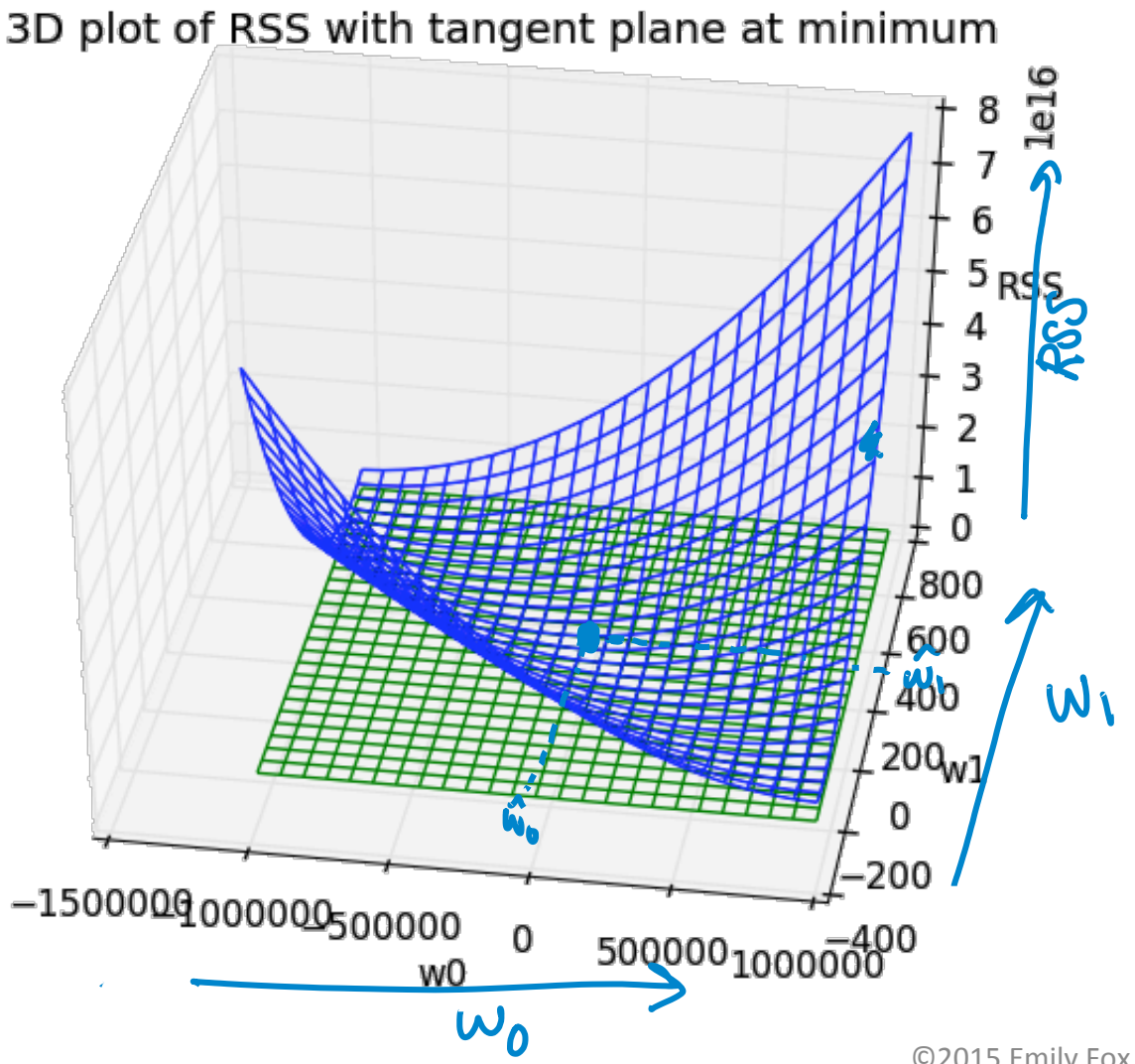
Find "best" line



Recall:

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

Minimizing the cost



Minimize function over all possible w_0, w_1

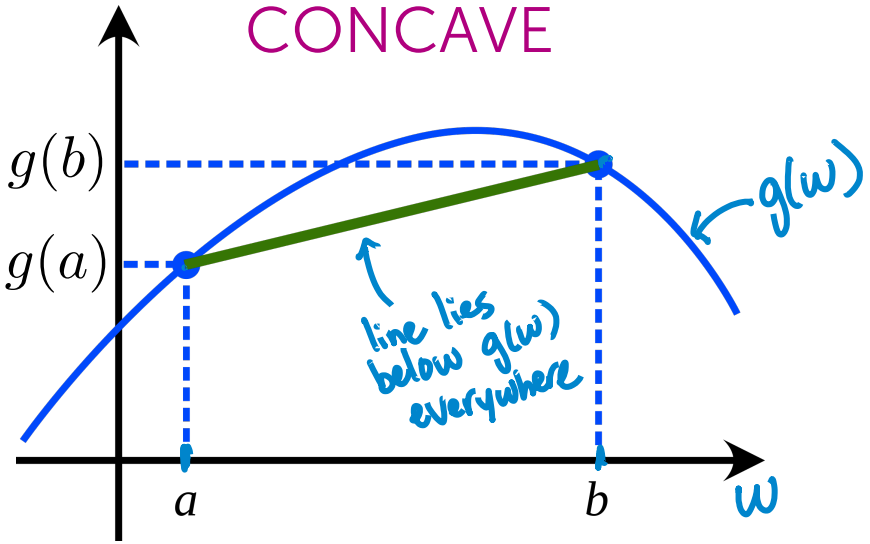
$$\min_{w_0, w_1} \sum_{i=1}^{N} (y_i - [w_0 + w_1 x_i])^2$$

$\text{RSS}(w_0, w_1)$ is a function of 2 variables $= g(w_0, w_1)$

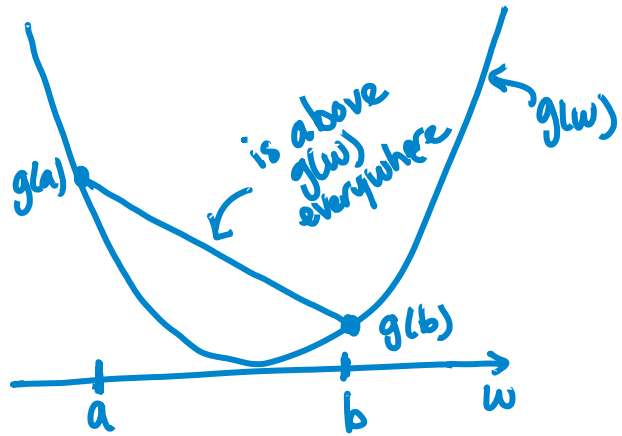
An aside on optimization

Convex/concave functions

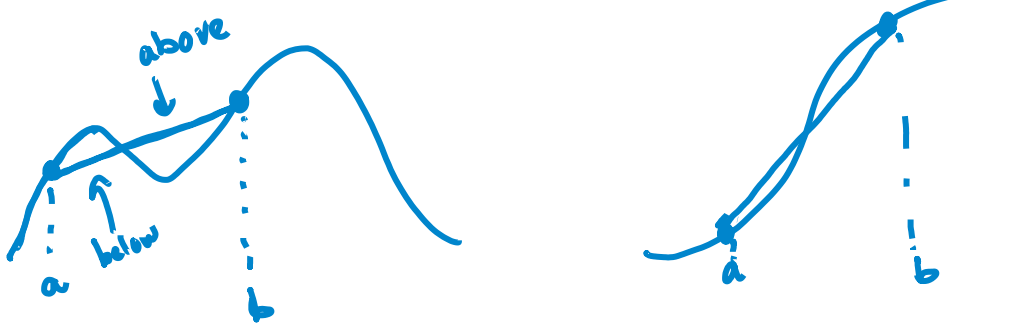
CONCAVE



CONVEX

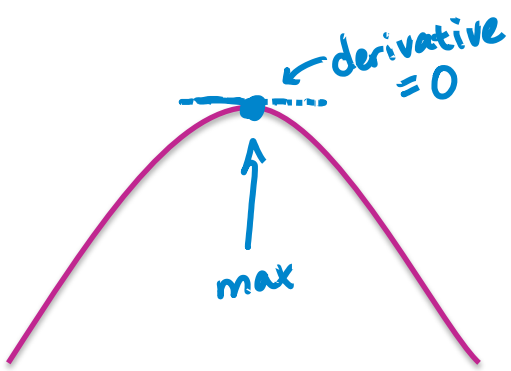


NEITHER

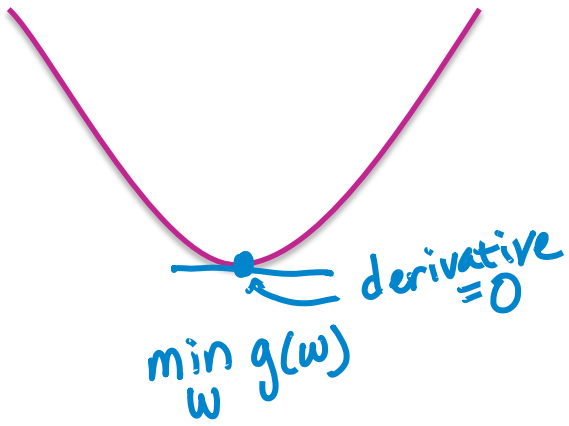


Finding the max or min analytically

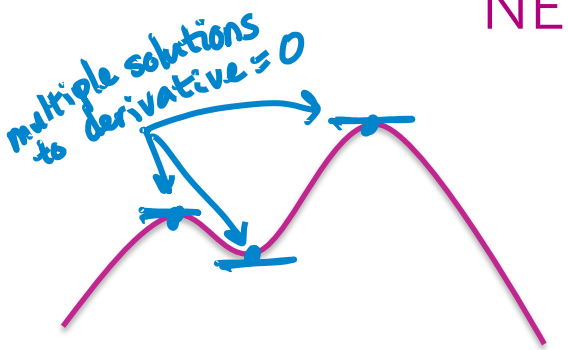
CONCAVE

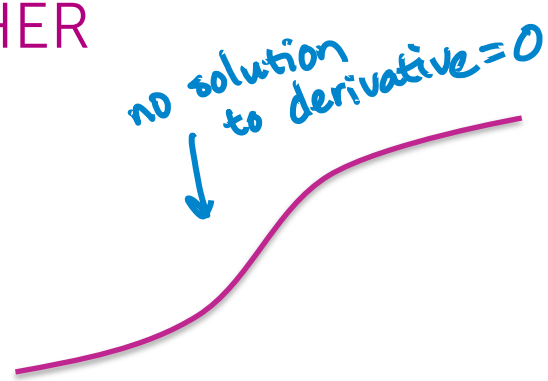


CONVEX



NEITHER





Example:

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

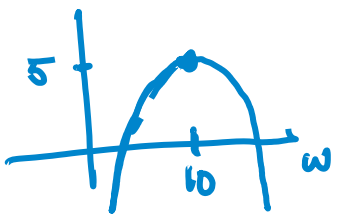
$$\frac{dg(w)}{dw} = 0 - 2(w-10)^1 \cdot 1$$

$$= -2w + 20$$

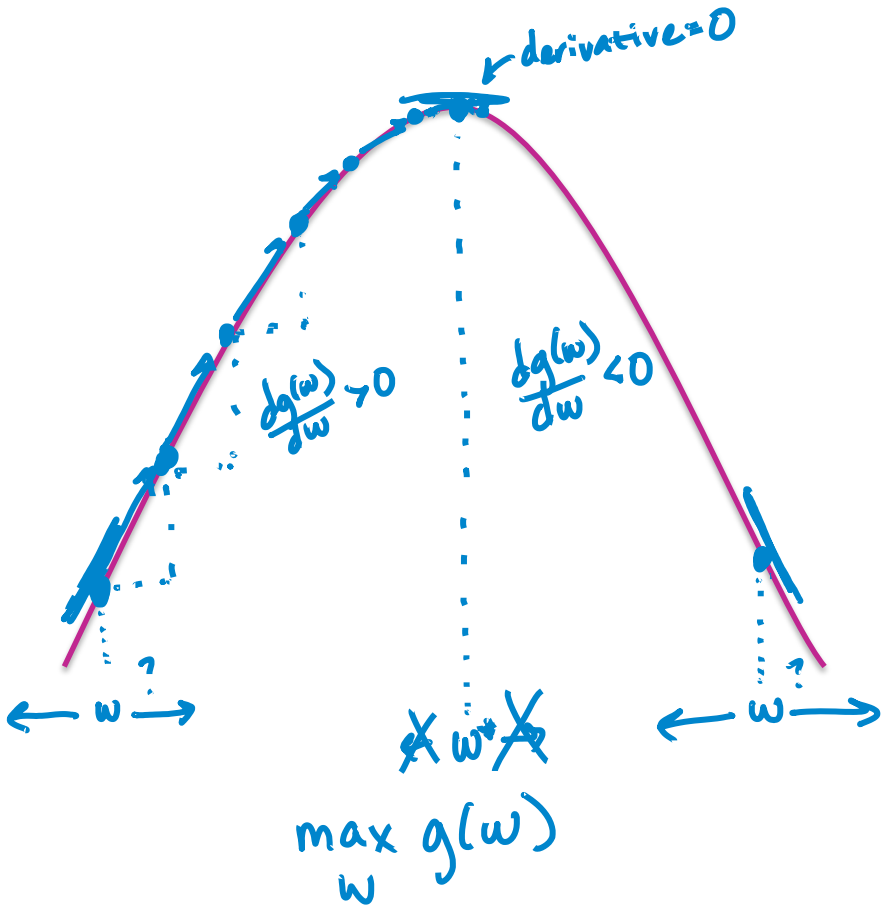
set derivate = 0:

$$-2w + 20 = 0$$

$$w = 10$$



Finding the max via hill climbing



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

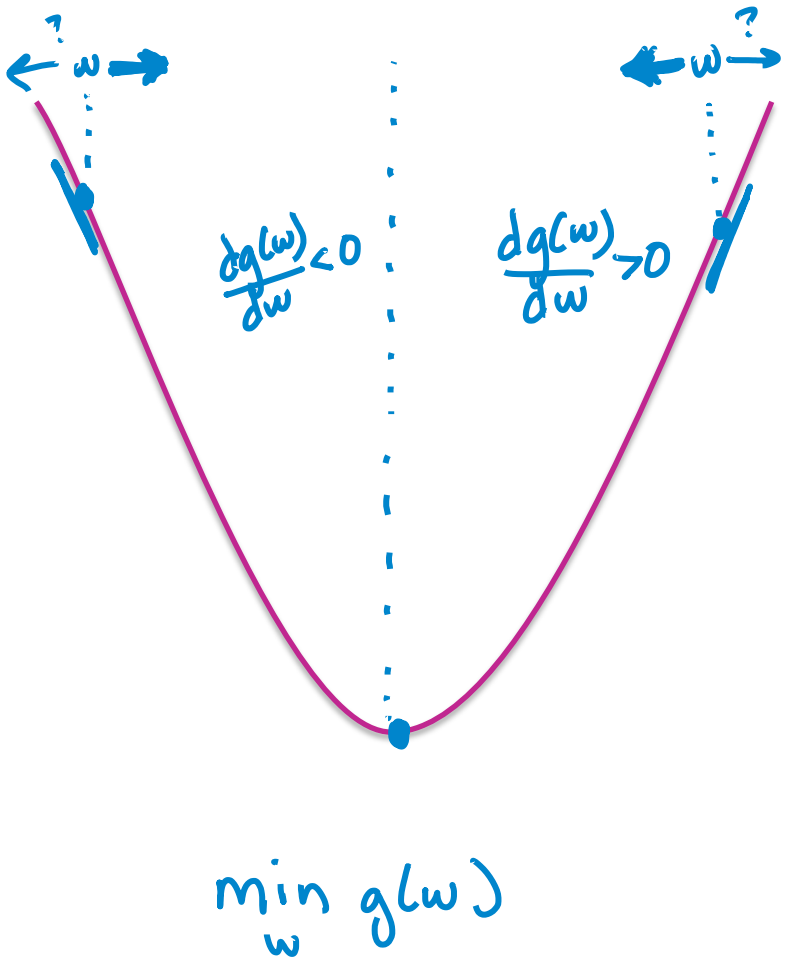
while not converged

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

$w^{(t)}$: iteration t

η: 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:

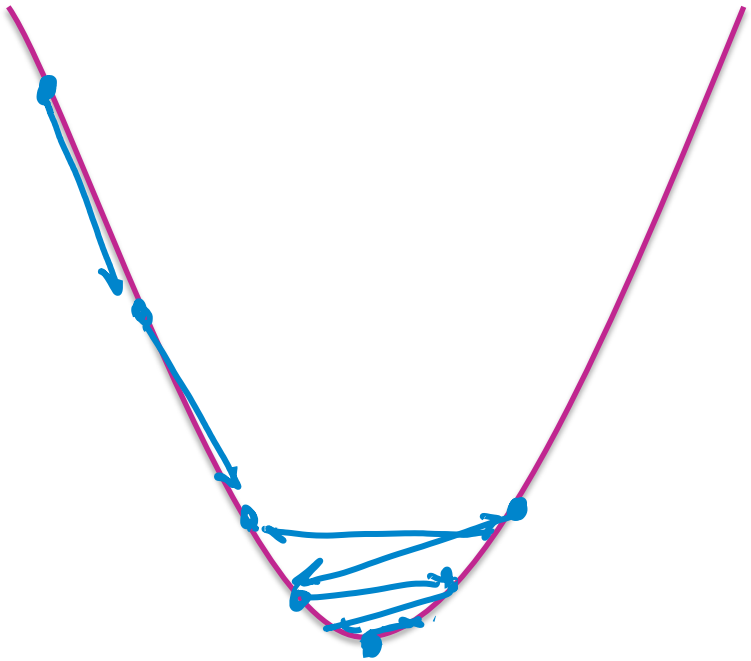
while not converged

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

Choosing the stepsize—

Fixed stepsize

η

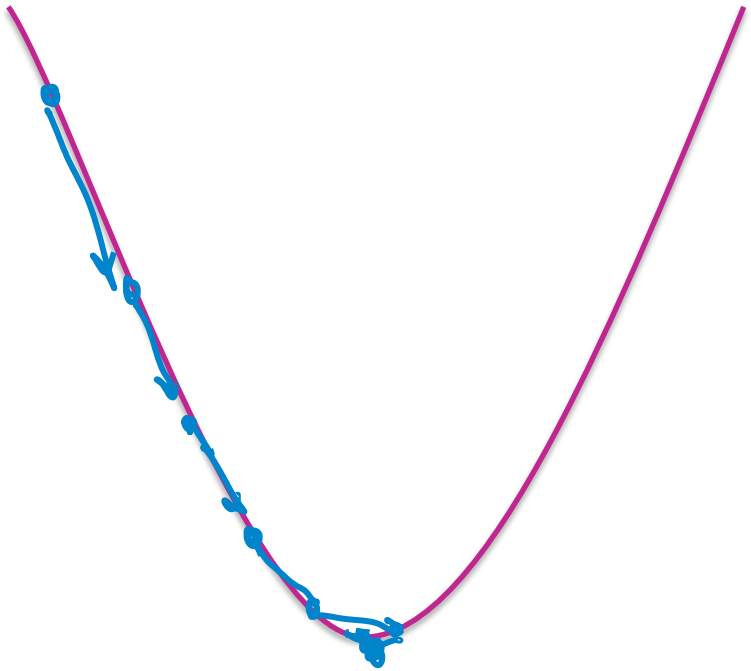


$\eta = 0.1$

Choosing the stepsize—

Decreasing stepsize

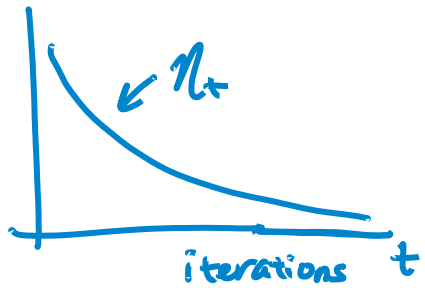
or stepsize schedule



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

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

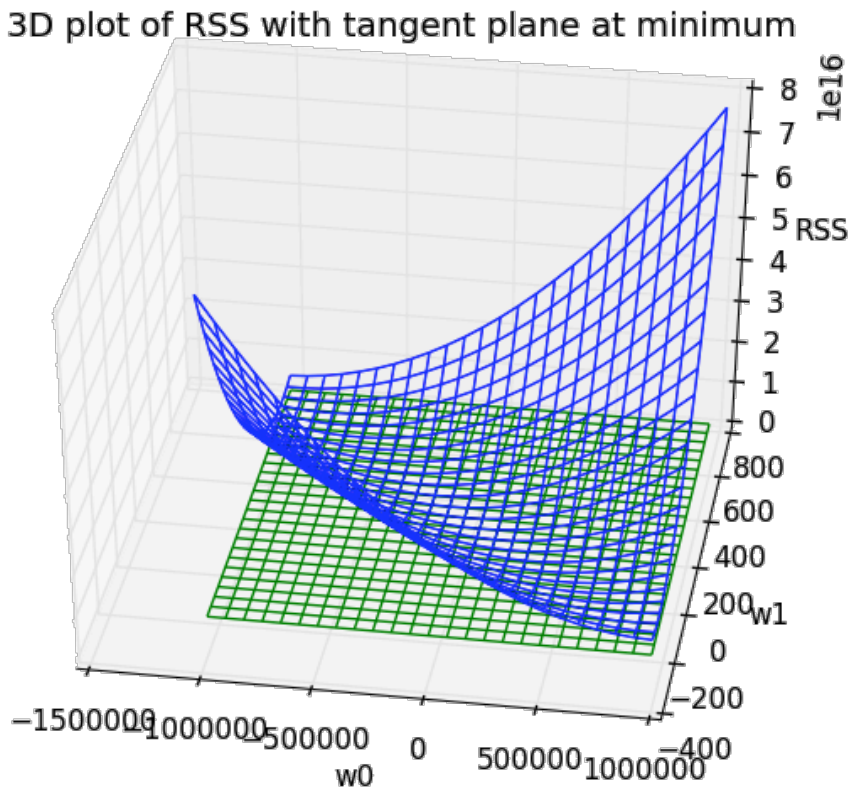
ϵ: threshold to be set

Algorithm:

while not converged

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

Moving to multiple dimensions: Gradients



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

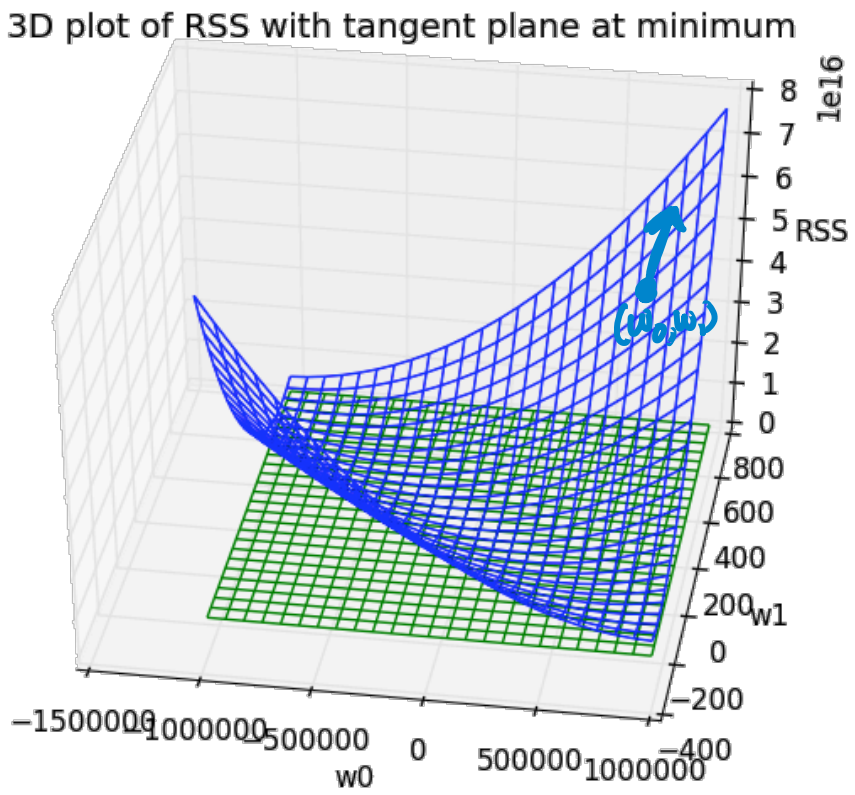
gradient

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

$(p+1)$-dimensional vector

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

Gradient example



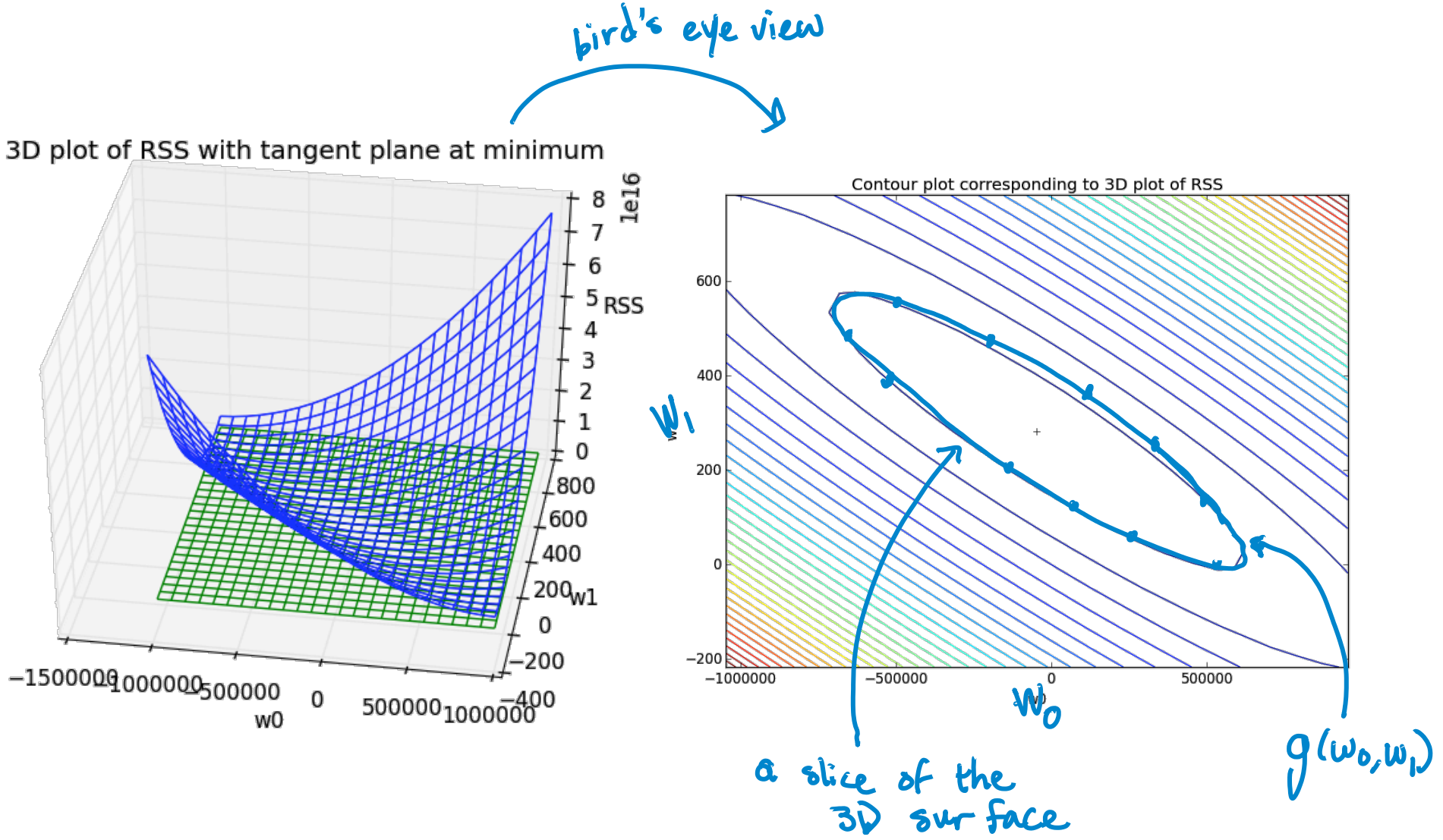
$$g(w) = 5w_0 + 10w_0w_1 + 2w_1^2$$

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

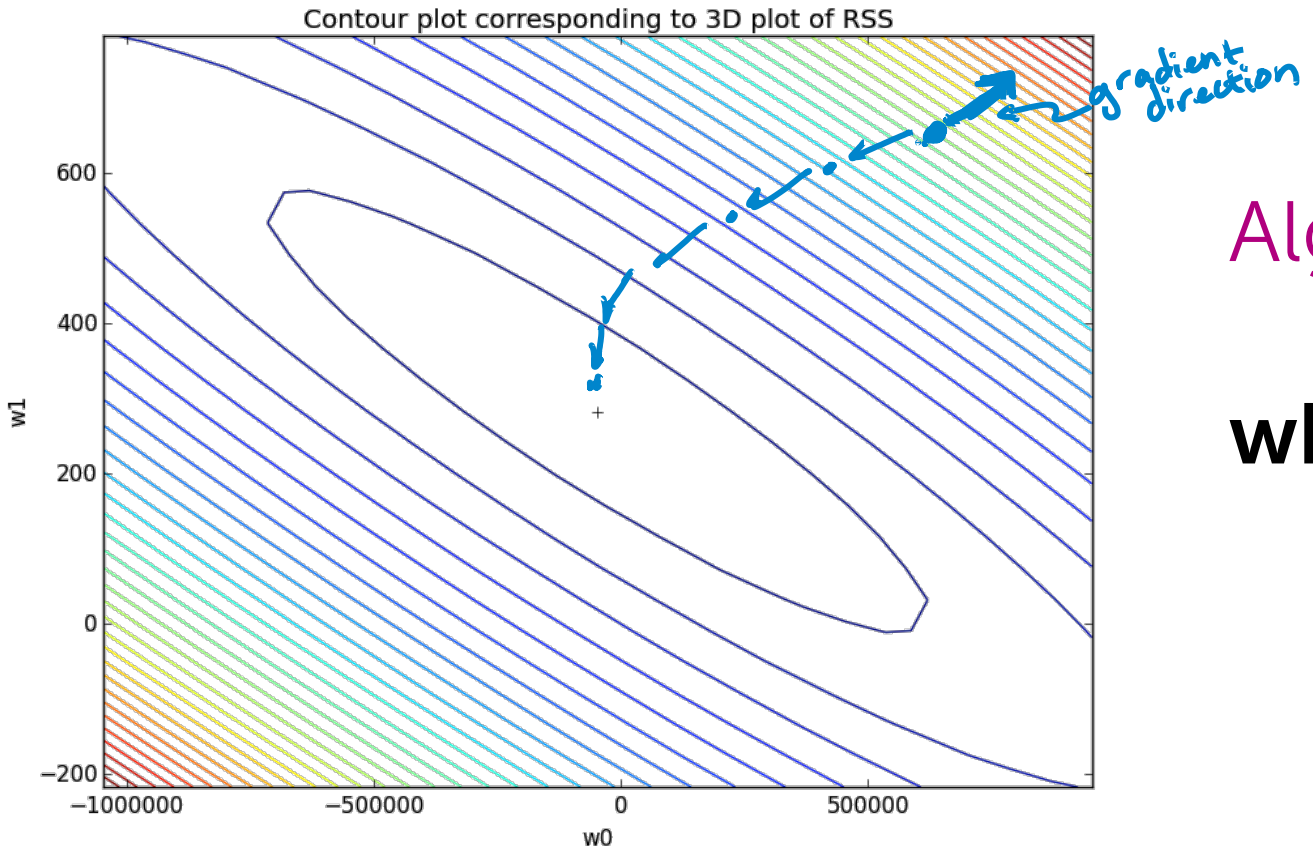
$$\frac{\partial g}{\partial w_1} = 10w_0 + 4w_1$$

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

Contour plots



Gradient descent



Algorithm:

while not converged

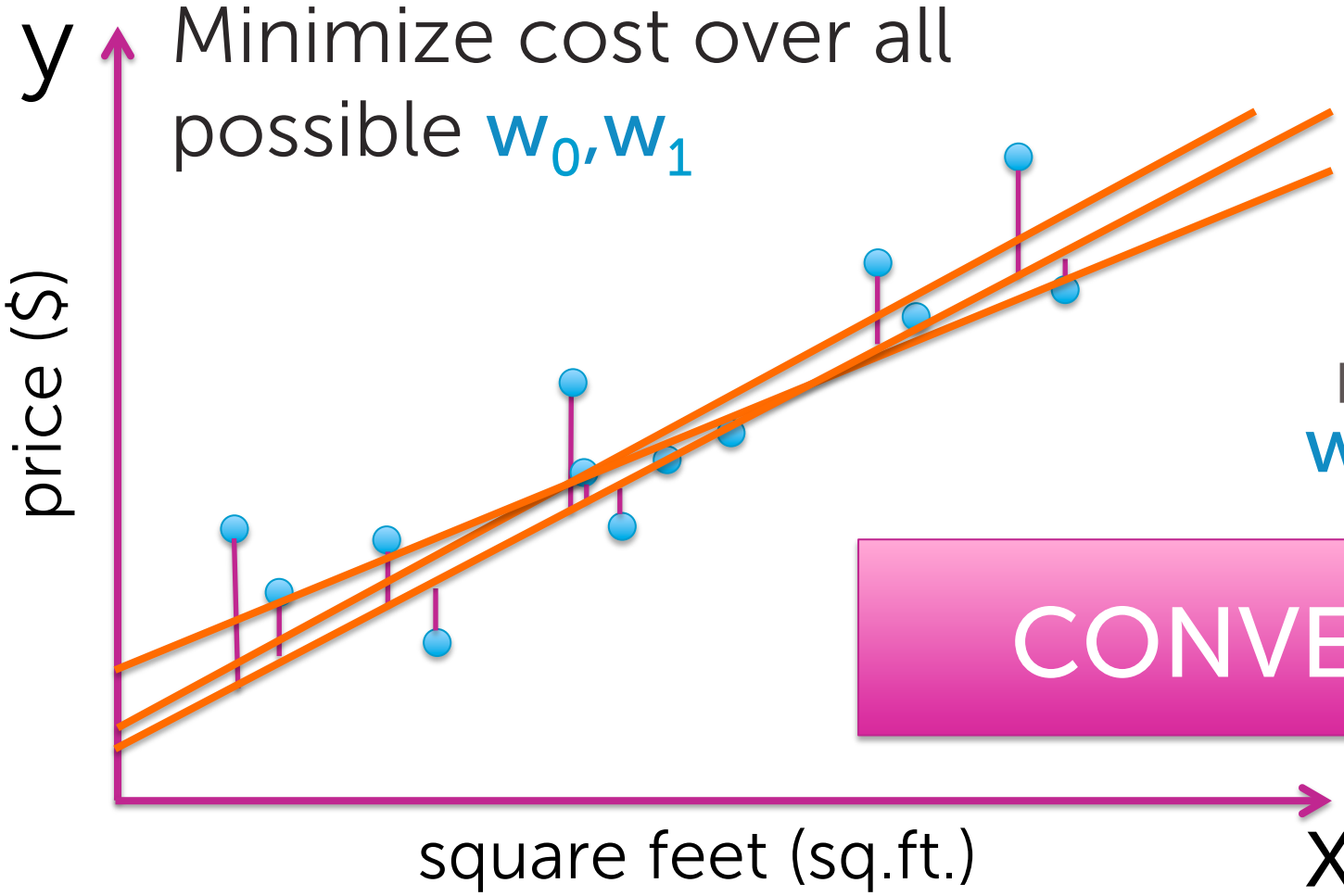
$$w^{(t+1)} \leftarrow w^{(t)} - \eta \nabla g(w^{(t)})$$

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

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

Finding the least squares line

Find "best" line



Minimize cost over all possible w_0, w_1

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

CONVEX

⇒ solution is unique

+ gradient descent alg. will converge to minimum

Compute the gradient

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

Aside:

$$\frac{d}{dw} \sum_{i=1}^{N} g_i(w) = \frac{d}{dw} (g_1(w) + g_2(w) + \dots g_N(w))$$

$$= \frac{d}{dw} g_1(w) + \frac{d}{dw} g_2(w) + \dots \frac{d}{dw} g_N(w)$$

$$= \sum_{i=1}^{N} \frac{d}{dw} g_i(w)$$

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

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

Taking the derivative w.r.t. w_0

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

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

Compute the gradient

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

Taking the derivative w.r.t. w_1

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

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

Compute the gradient

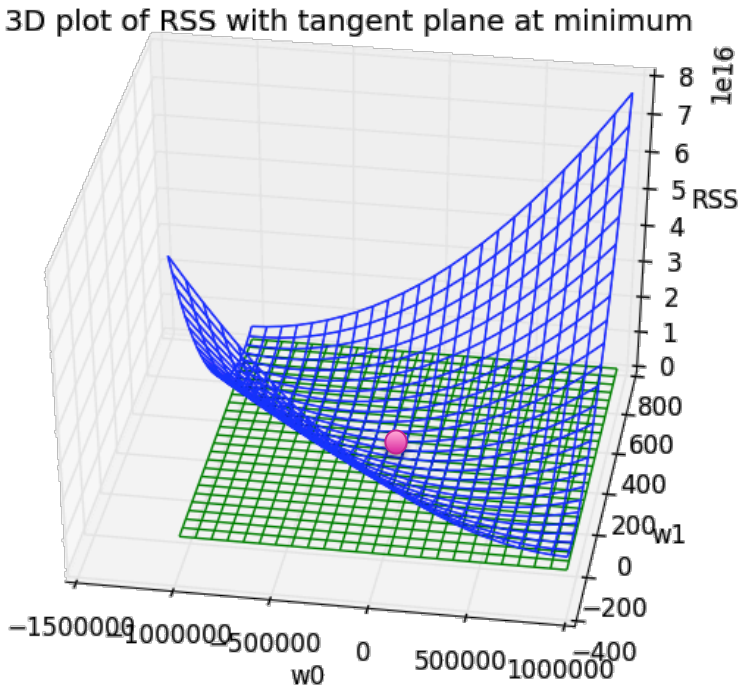
$$\text{RSS}(w_0, w_1) = \sum_{i=1}^{N} (y_i - [w_0 + w_1 x_i])^2$$

Putting it together:

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

Approach 1: Set gradient = 0

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



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:

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

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

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

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

Approach 2: Gradient descent

Interpreting the gradient:

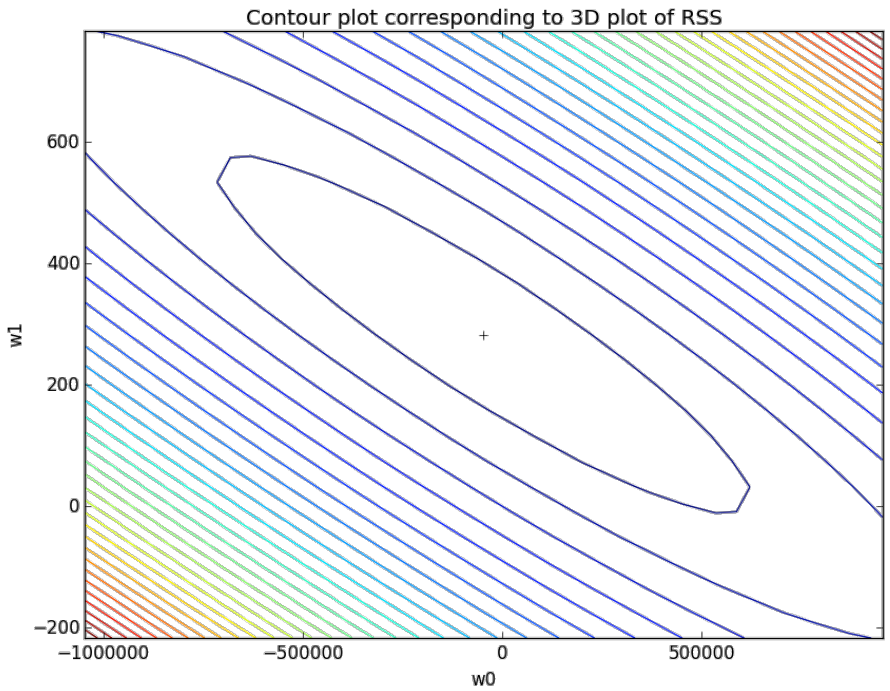
actual house sales observation

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

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

Approach 2: Gradient descent

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



while not converged

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

$(-2)\cdot(-\eta)$

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

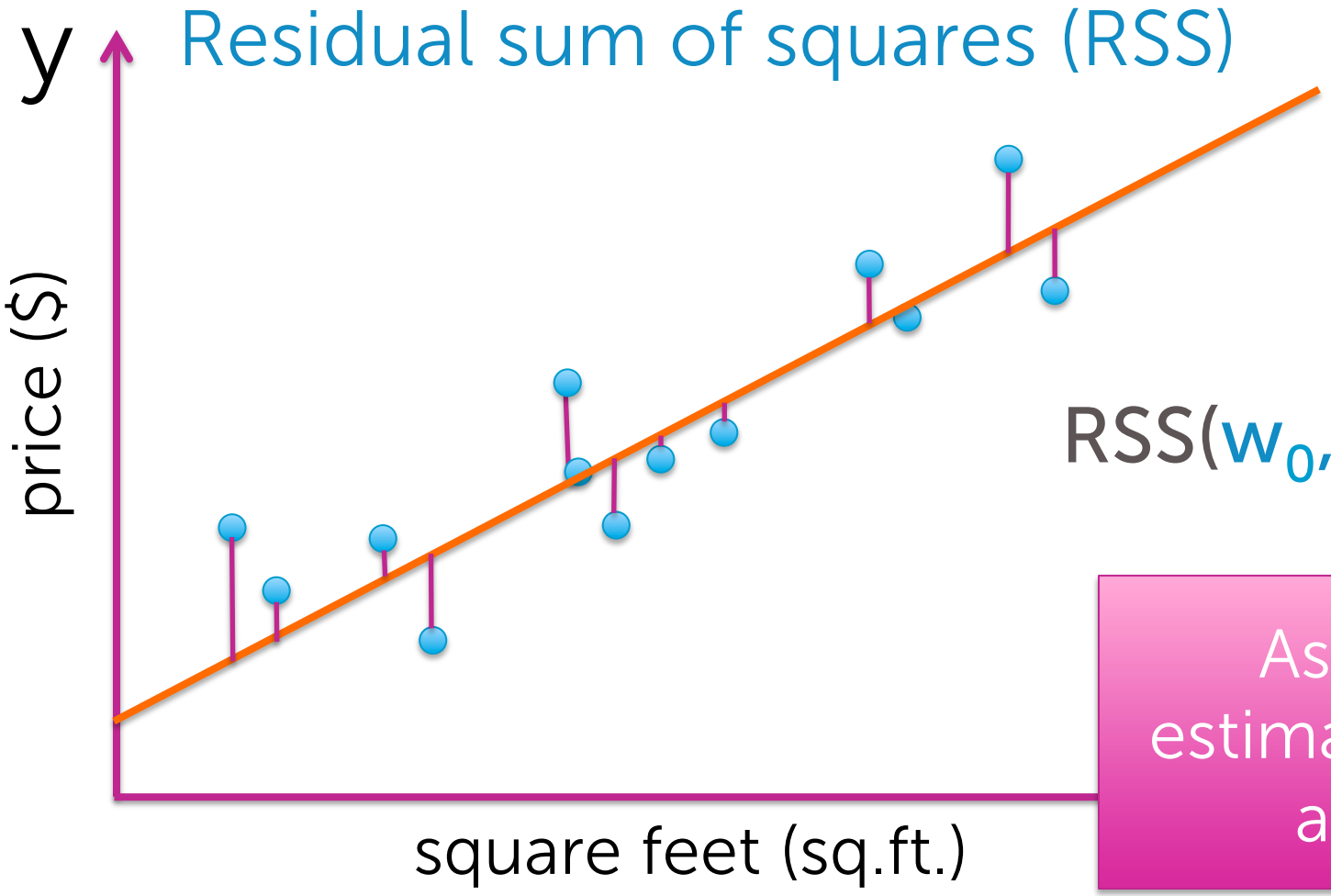
Comparing the approaches

- 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

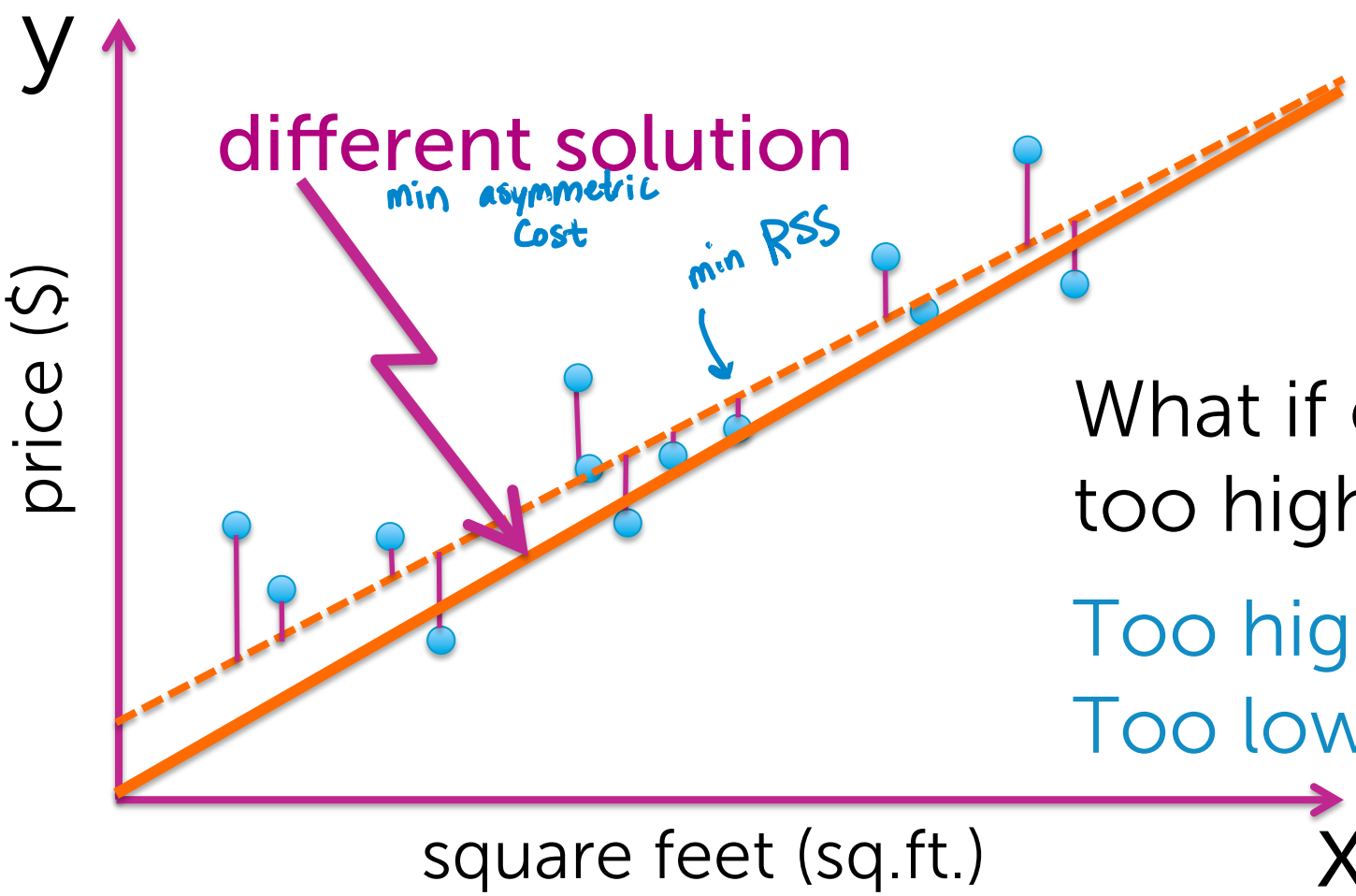


Residual sum of squares (RSS)

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

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 → no offers ($=0)

Too low → 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