Multiple Regression:

Linear regression with multiple features

Emily Fox & Carlos Guestrin

Machine Learning Specialization

University of Washington

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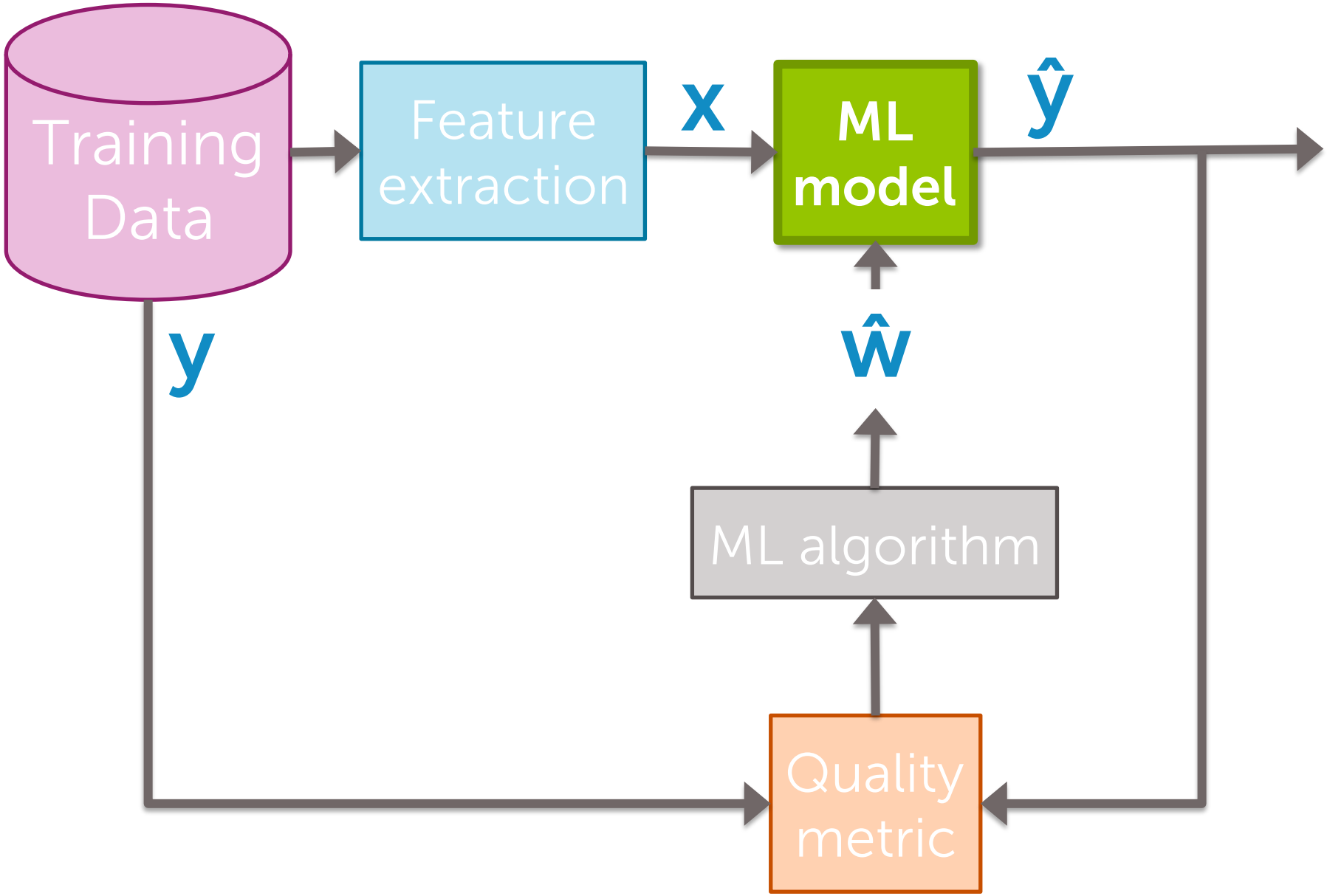

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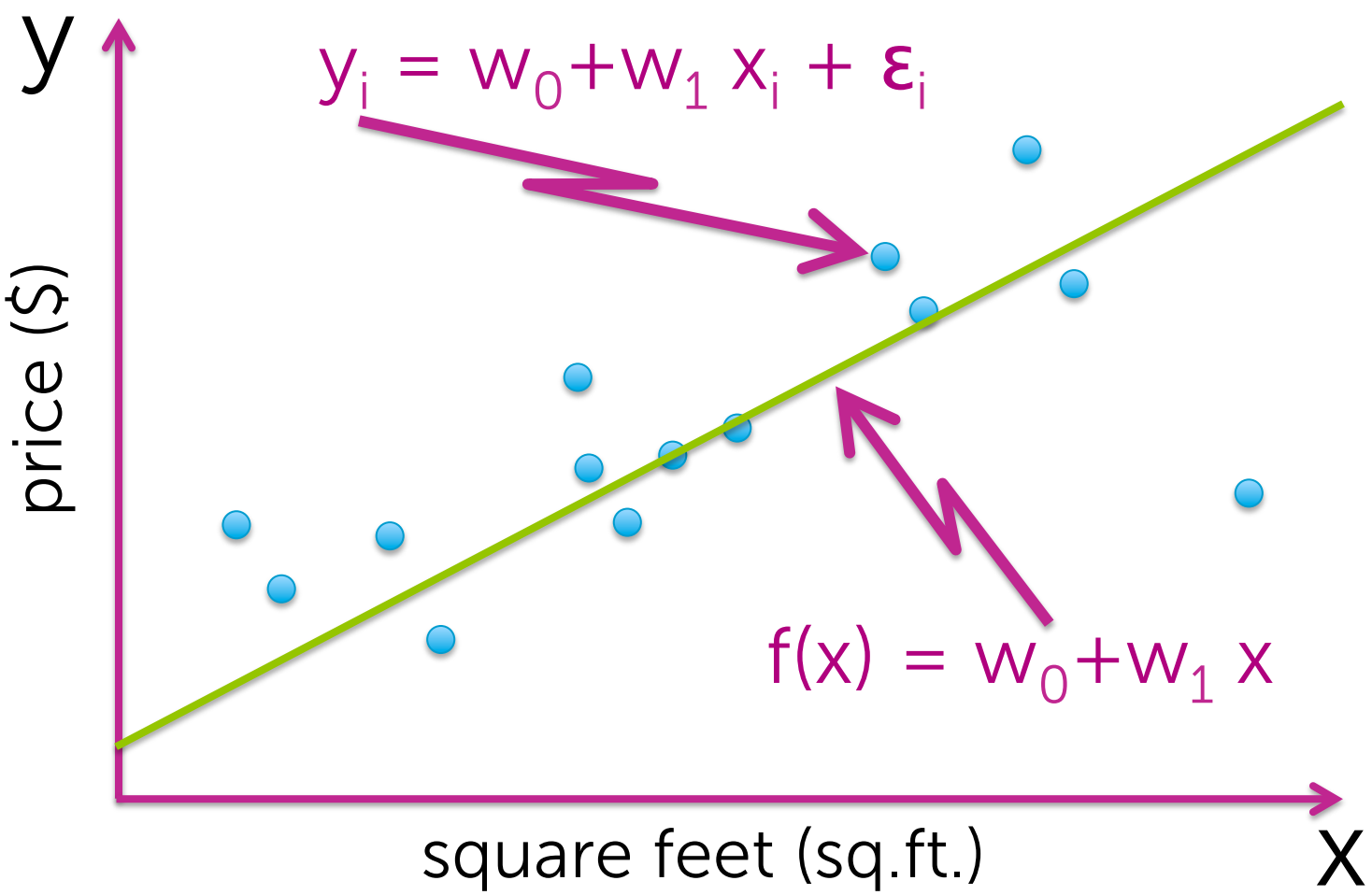
Simple linear regression model



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More complex functions of a single input

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Polynomial regression

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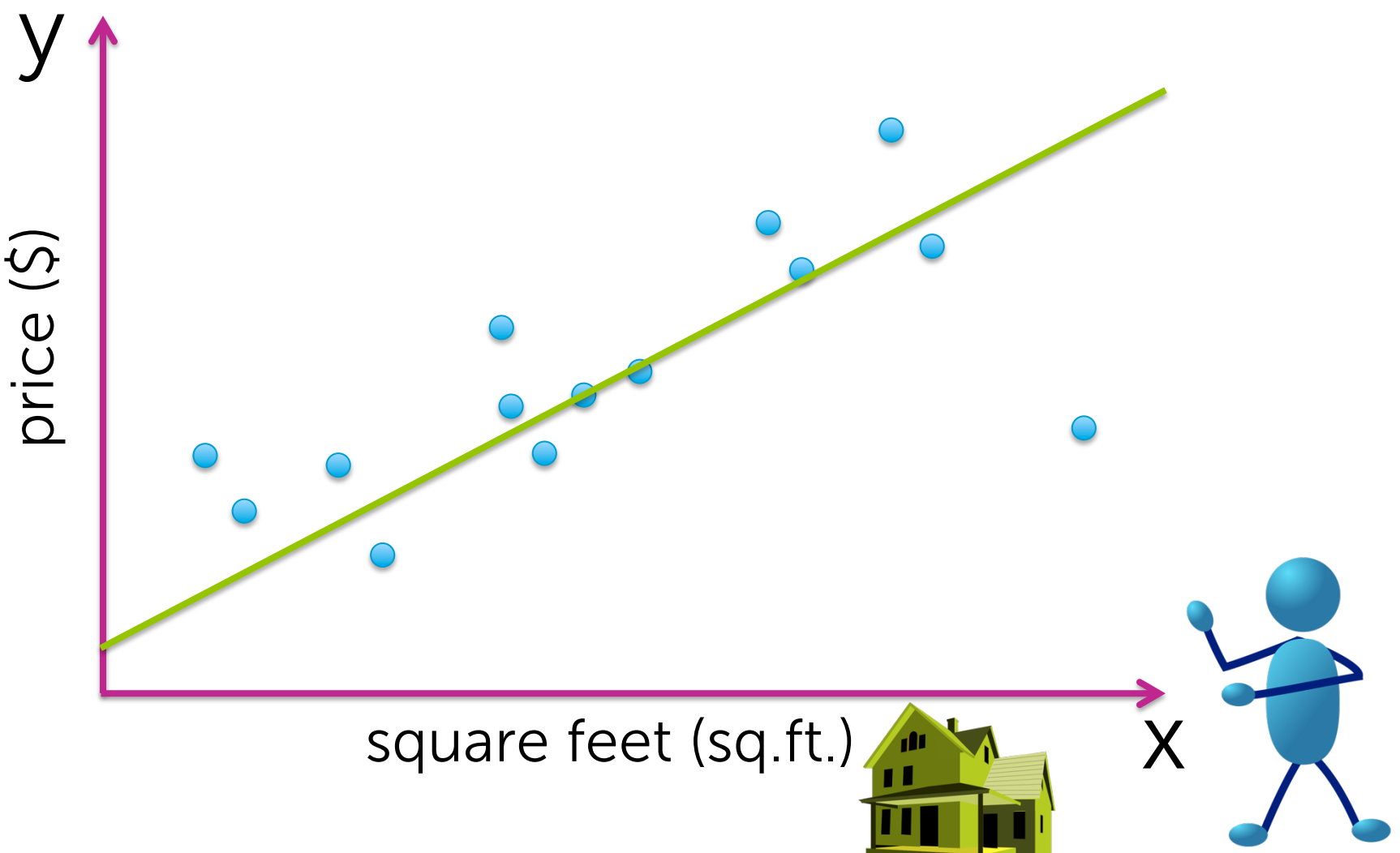
Fit data with a line or … ?



You show your friend your analysis

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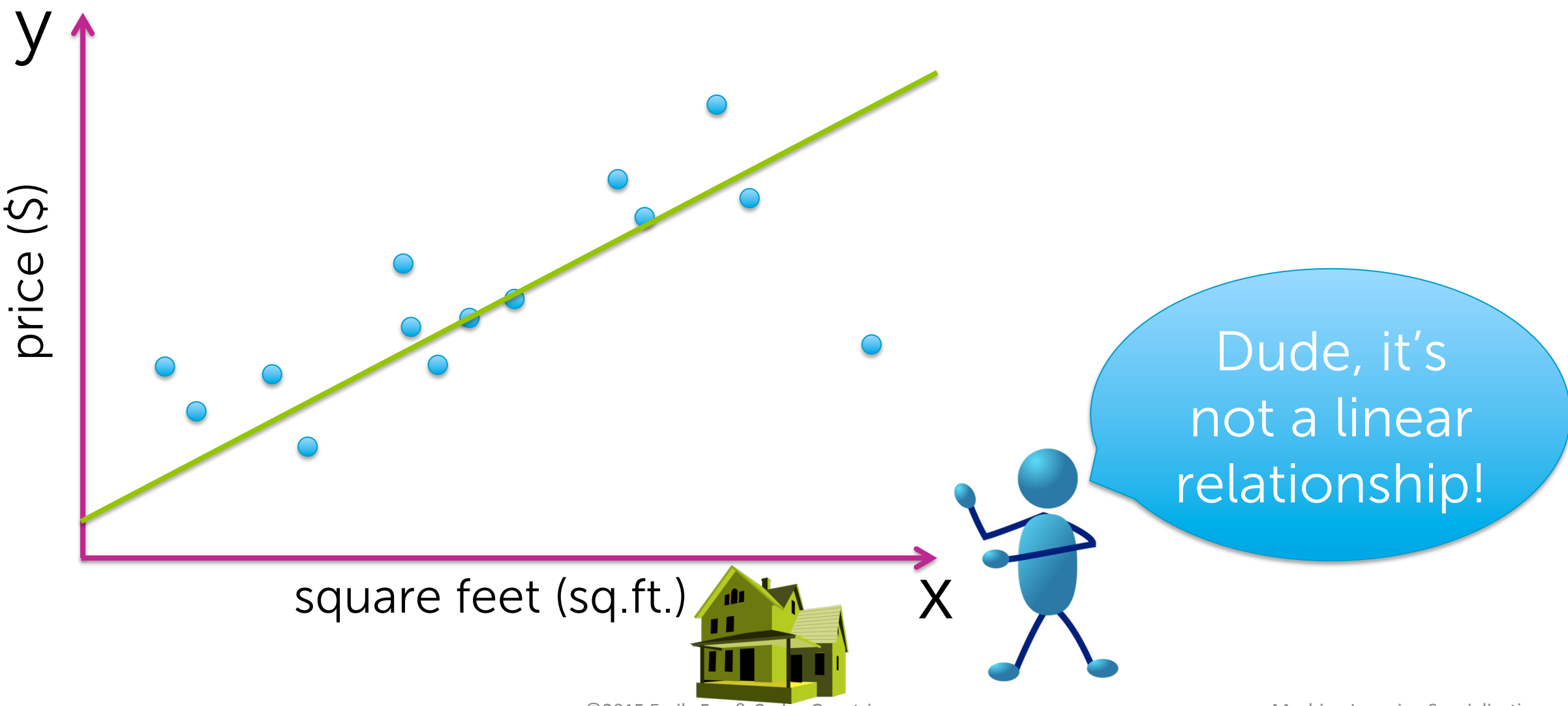
Fit data with a line or … ?



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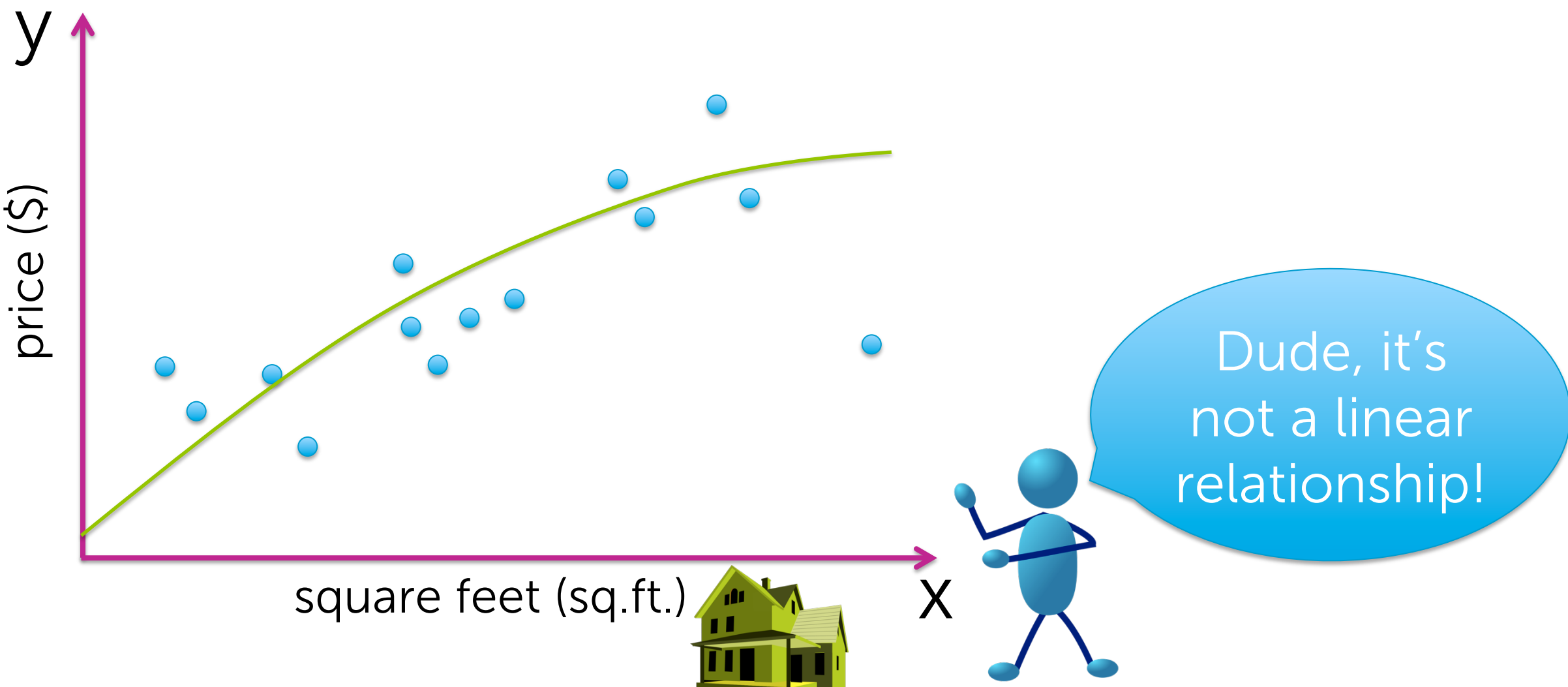
What about a quadratic function?



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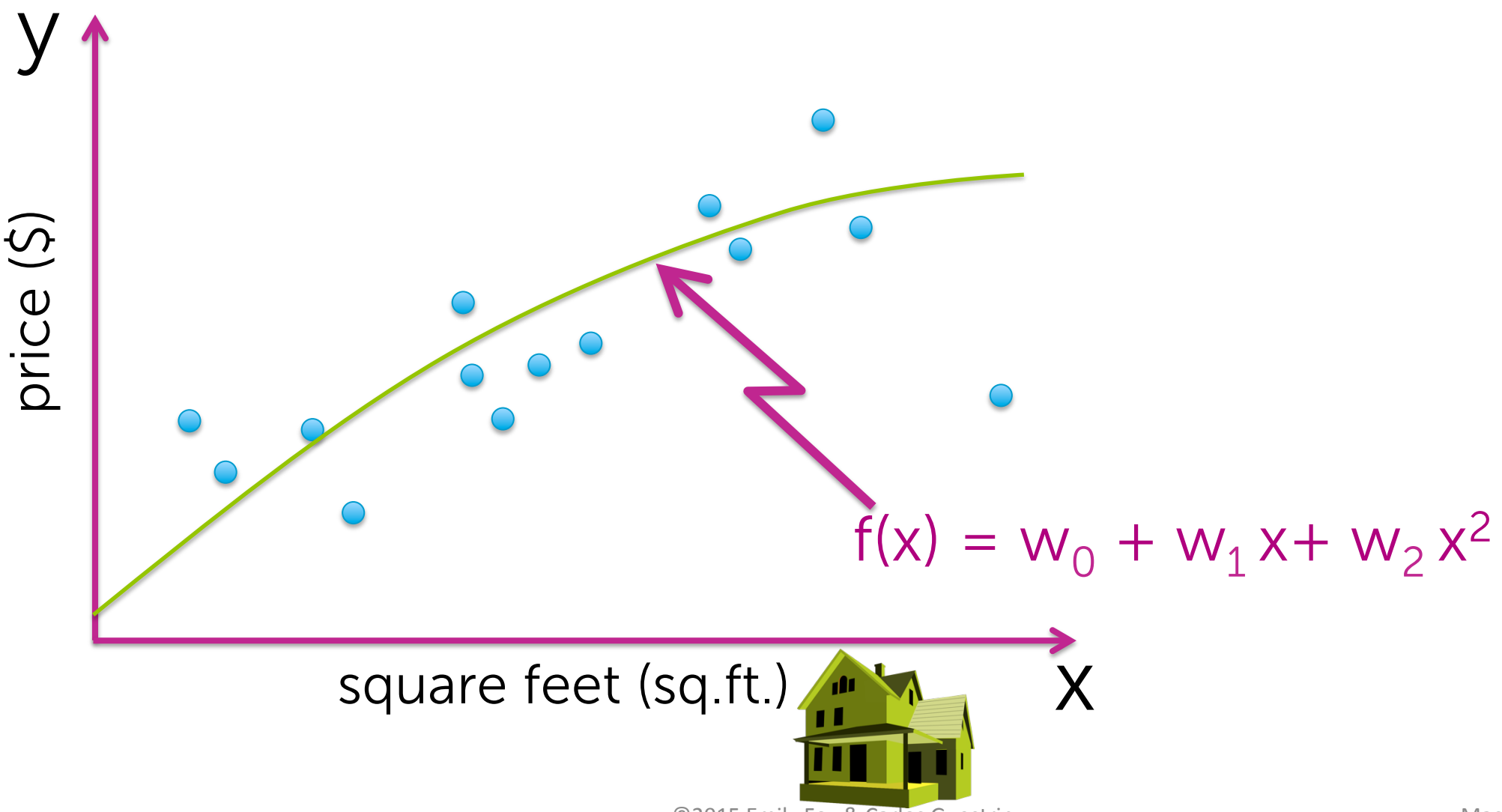
What about a quadratic function?



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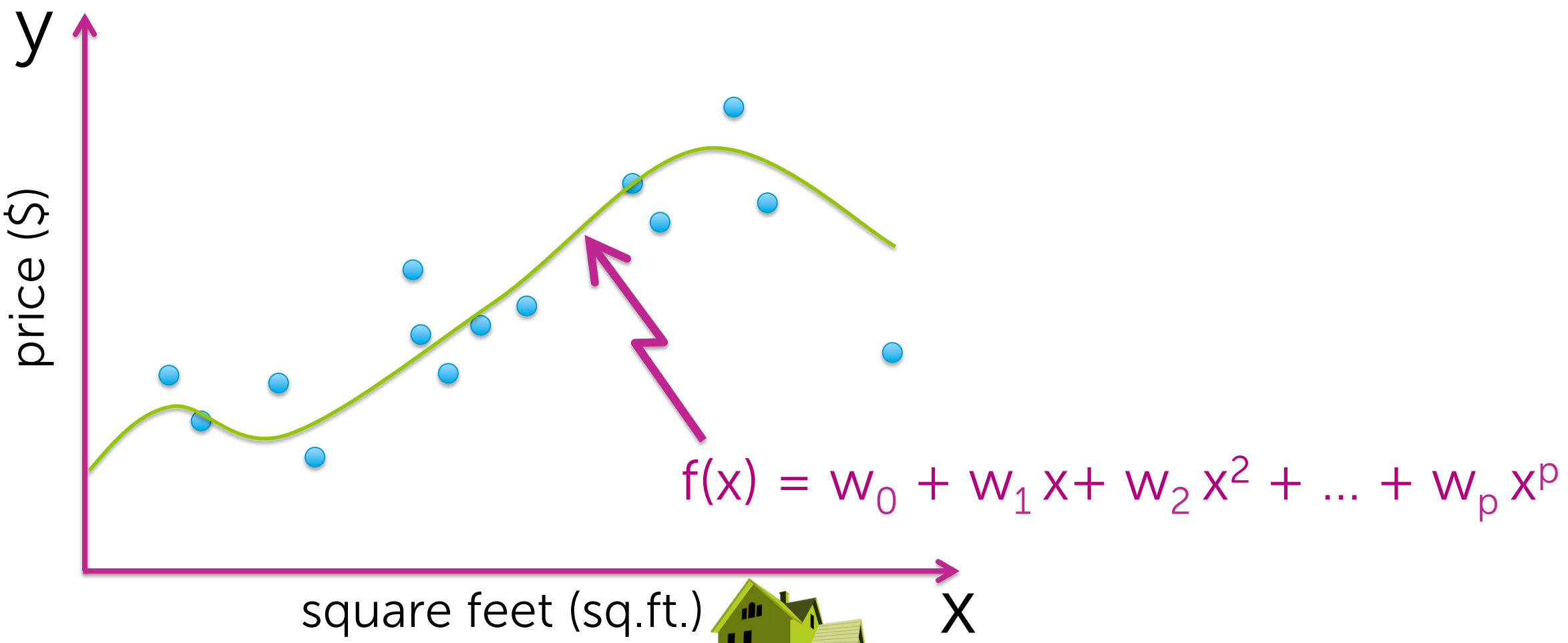
Even higher order polynomial



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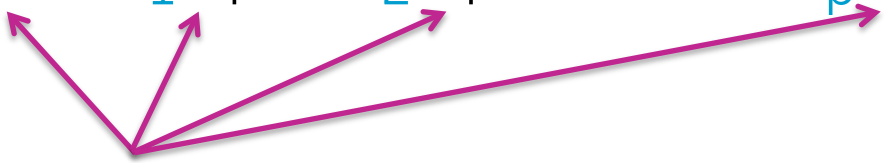
Polynomial regression

Model:

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



treat as different **features**

feature 1 = 1 (constant) *parameter* 1 = w_0

feature 2 = x *parameter* 2 = w_1

feature 3 = x^2 *parameter* 3 = w_2

… …

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

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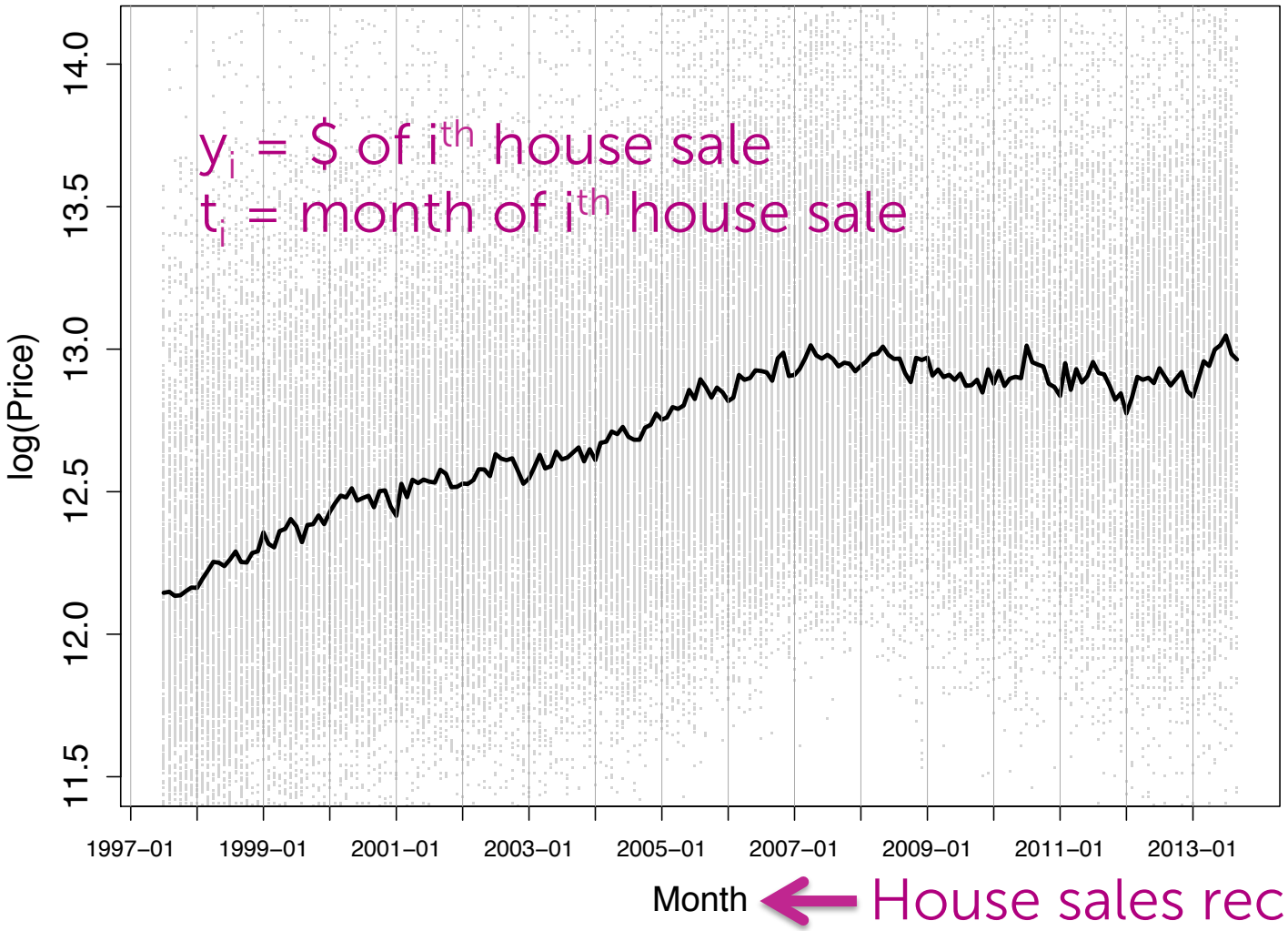
Other functions of one input

Motivating application: Detrending time series



House sales recorded monthly

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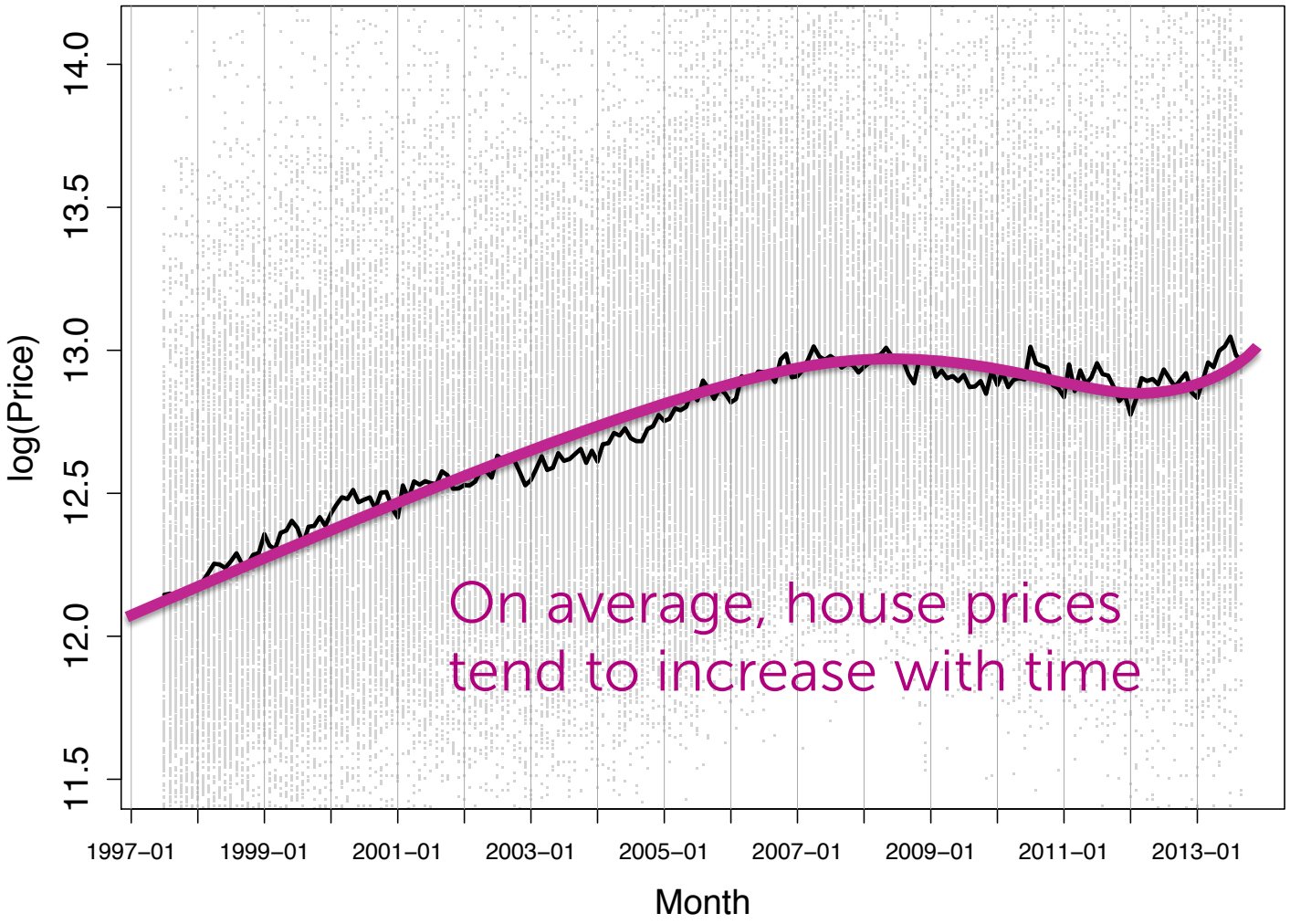
Trends over time



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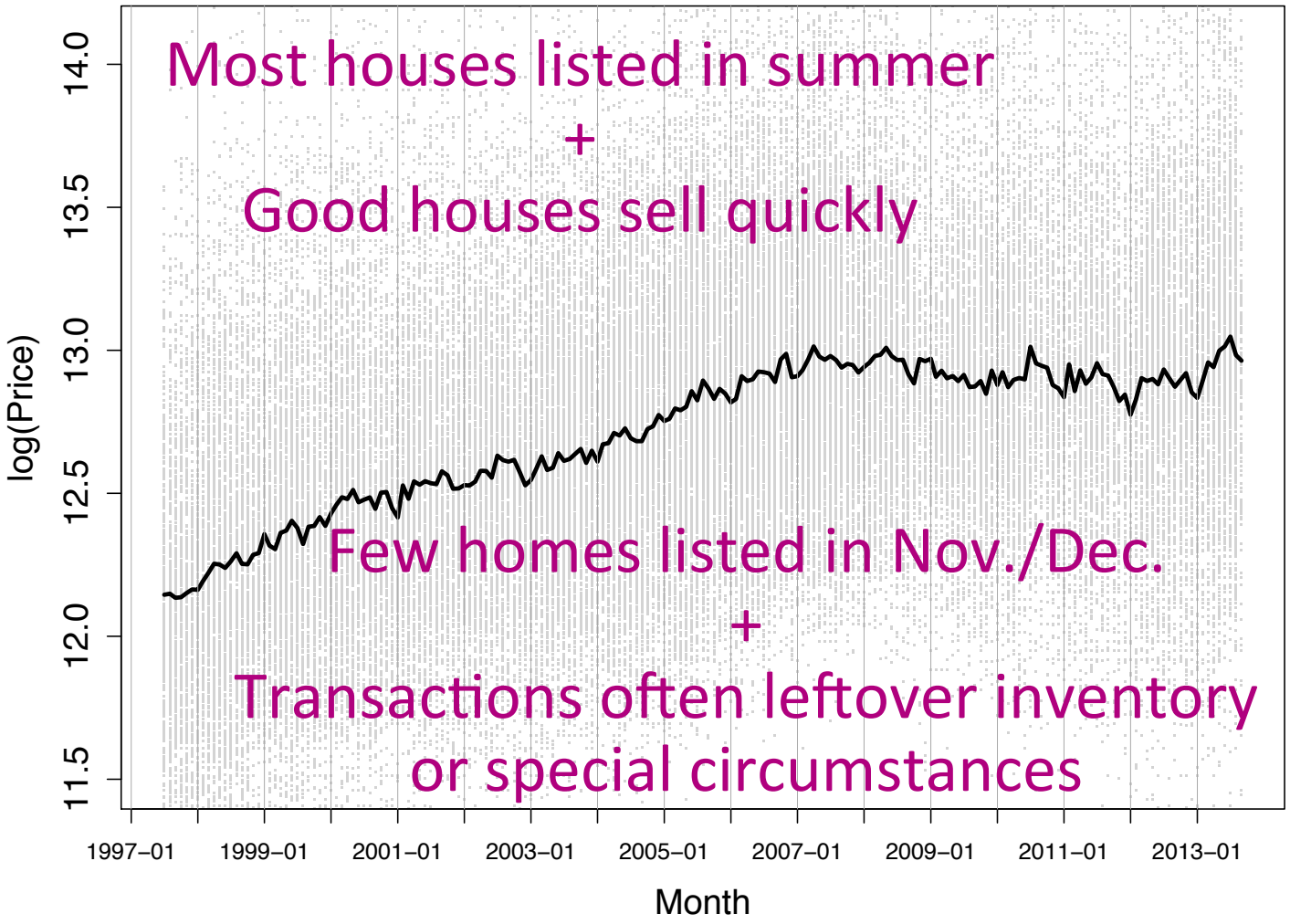
Seasonality



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An example detrending

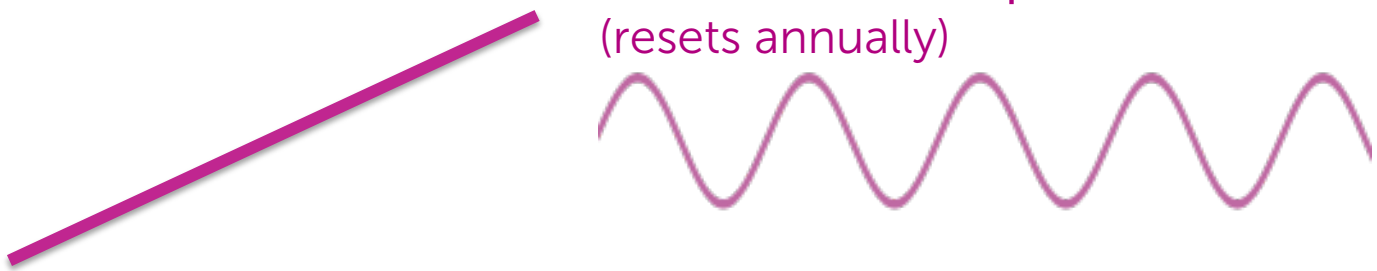
Model:

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

Linear trend

Seasonal component = Sinusoid with period 12 (resets annually)

Unknown phase/shift



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

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

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An example detrending

Equivalently,

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

feature 1 = 1 (constant)

feature 2 = t

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

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

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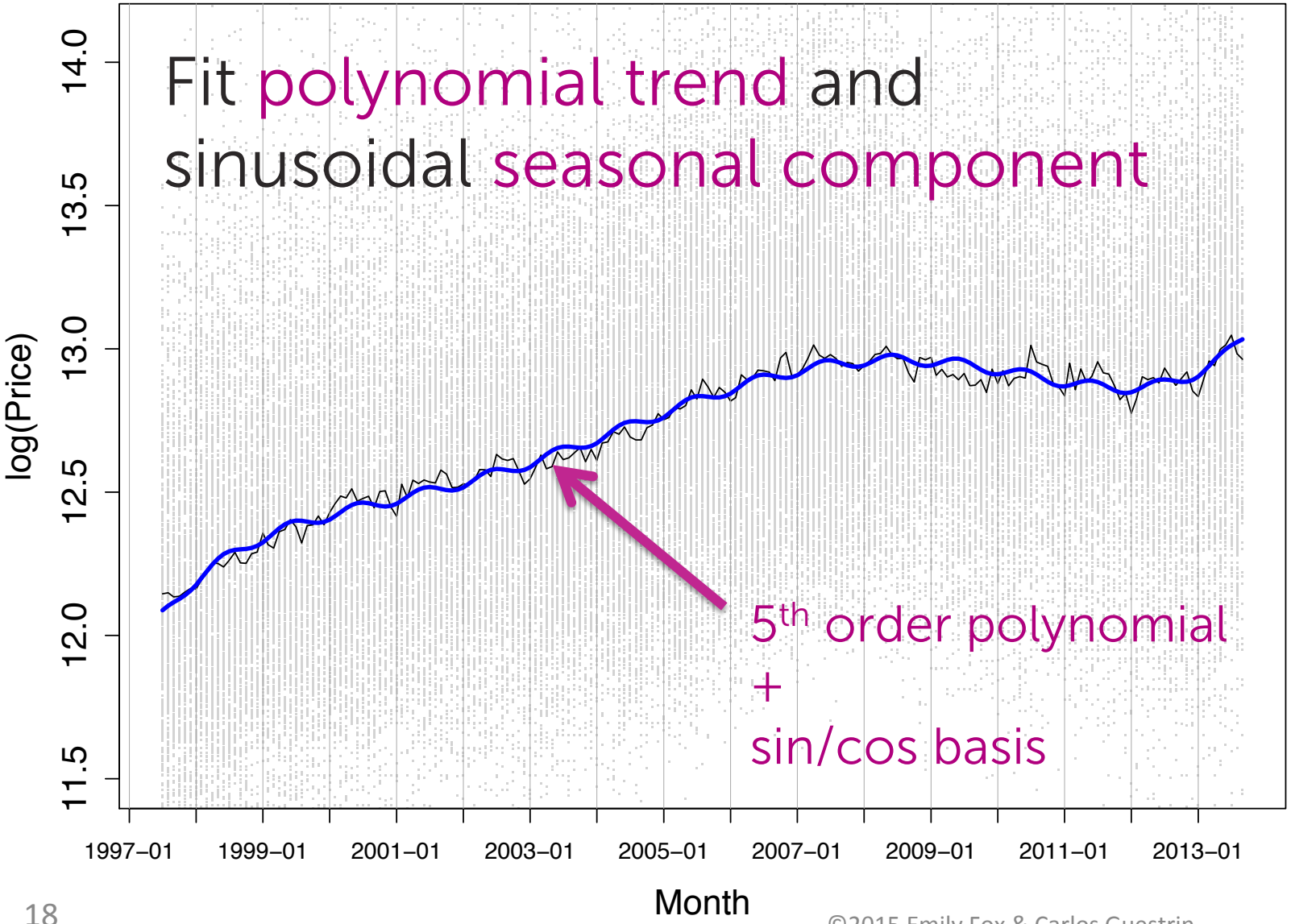
Detrended housing data



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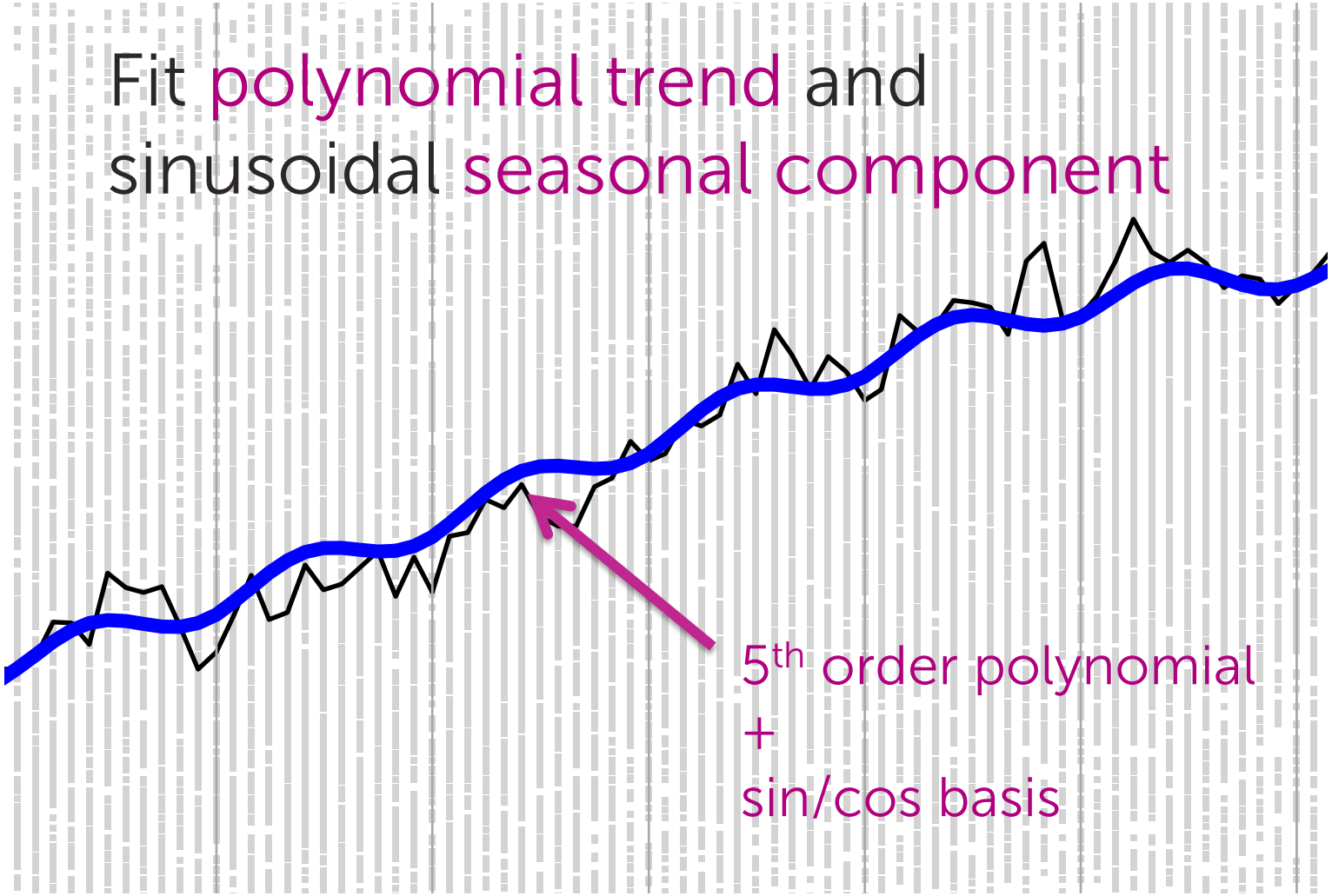
Zoom in…



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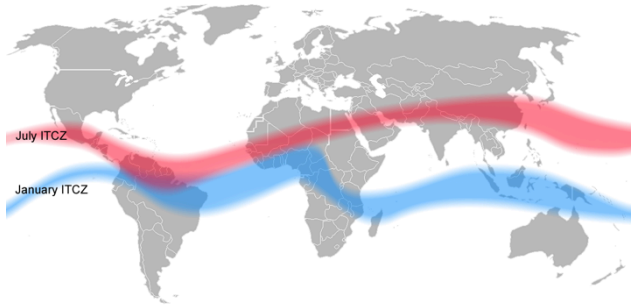
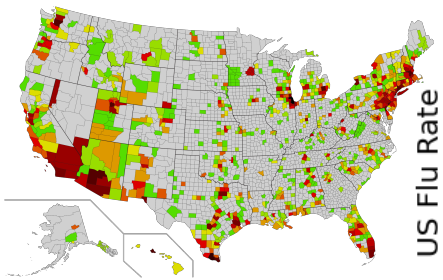
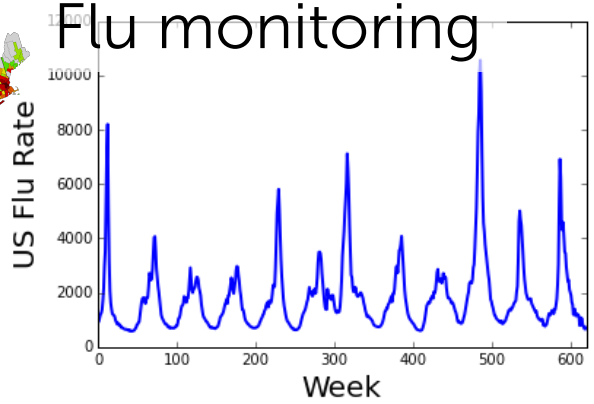
Other examples of seasonality



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

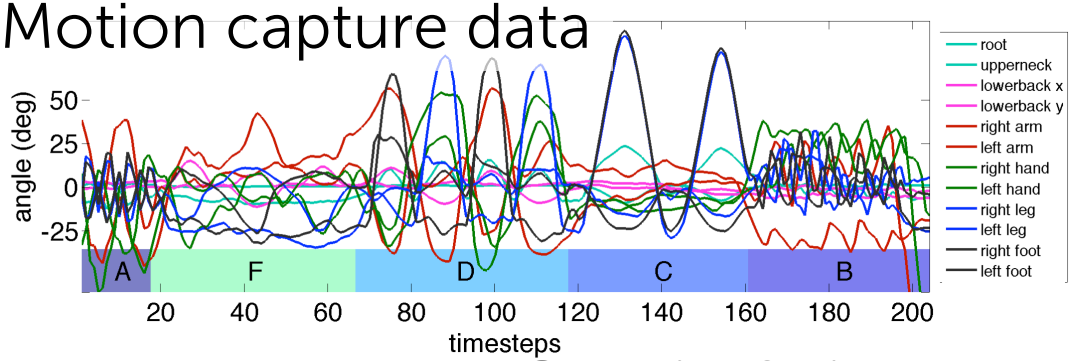


Flu monitoring



Demand forecasting
(e.g., jacket purchases)

Motion capture data



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More generally…

Generic basis expansion

Model:

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

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

j^{th} *feature*

j^{th} *regression coefficient or weight*

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Generic basis expansion

Model:

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

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

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

feature 2 = $h_1(x)$… e.g., x

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

…

feature D+1 = $h_D(x)$… e.g., x^p

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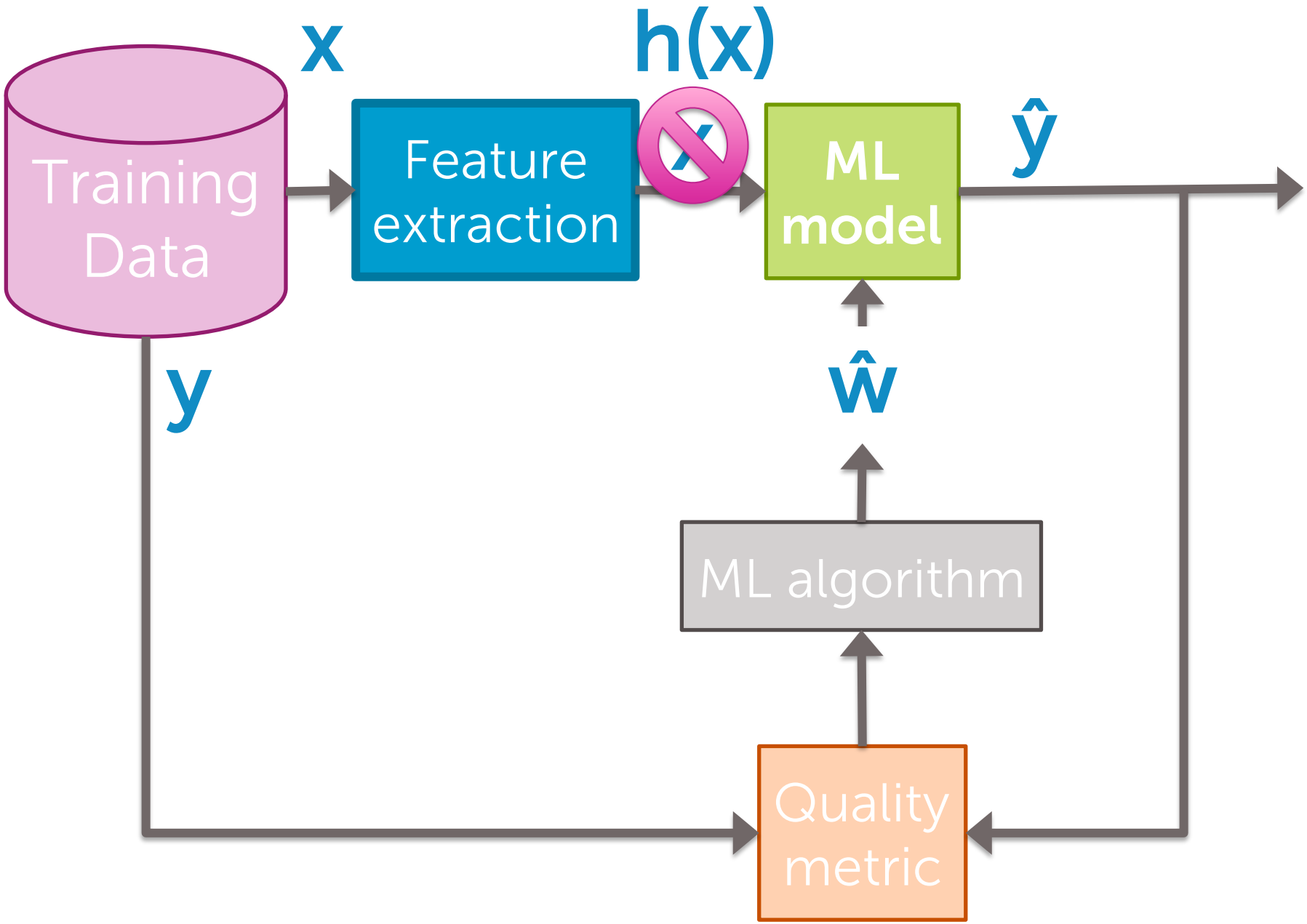

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Incorporating multiple inputs

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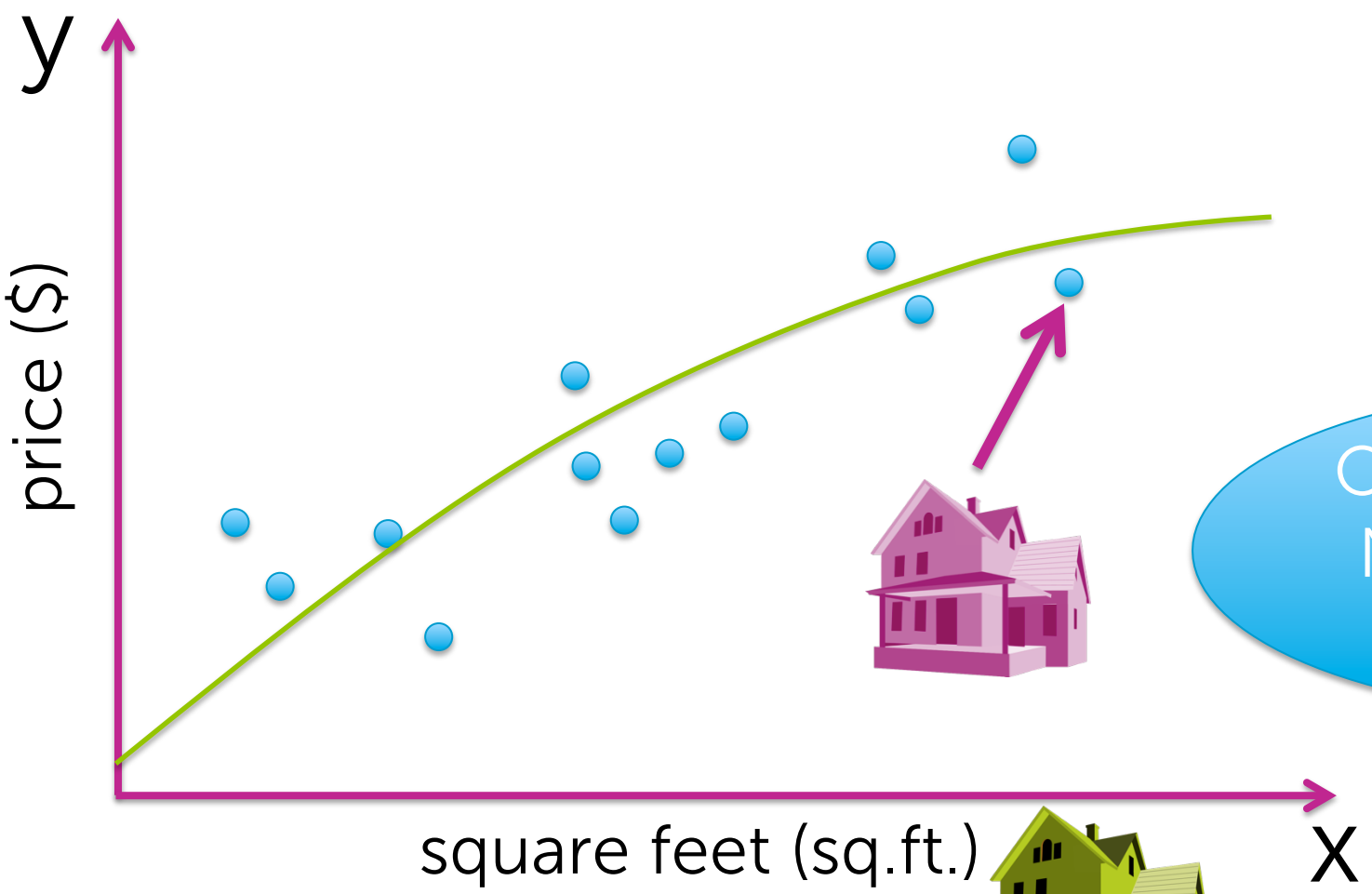
Predictions just based on house size



Only 1 bathroom!
Not same as my
3 bathrooms

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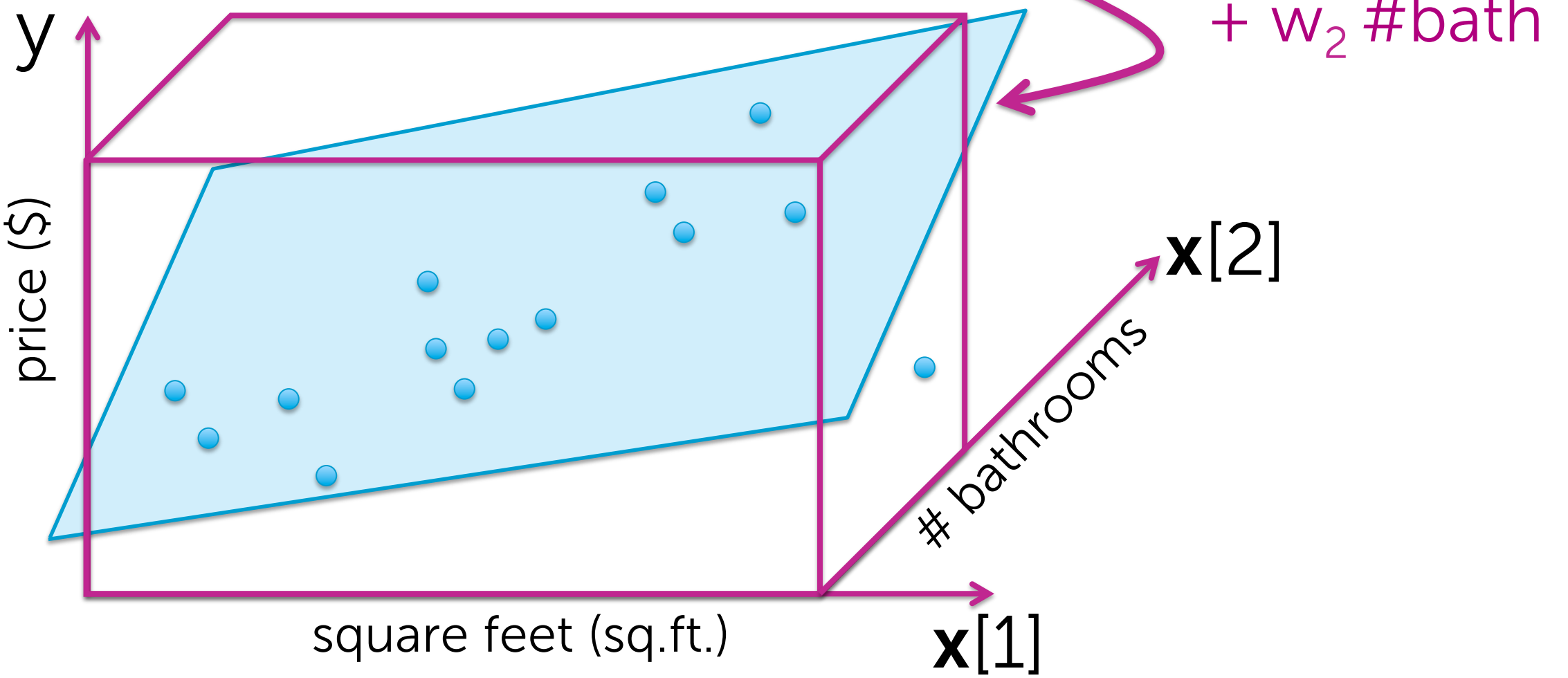
Add more inputs

$f(\mathbf{x}) = w_0 + w_1 \text{ sq.ft.} + w_2 \text{ \#bath}$



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Many possible inputs

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

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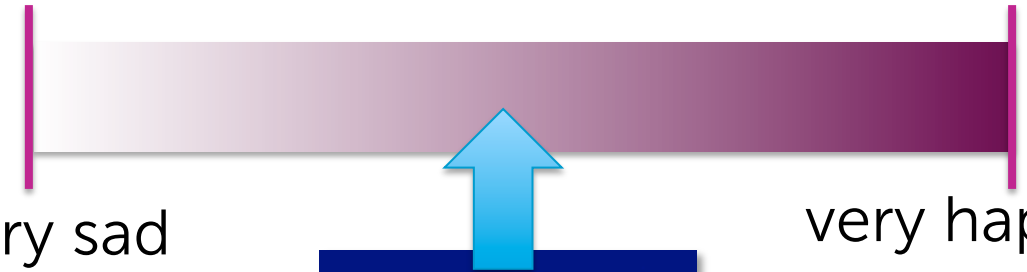
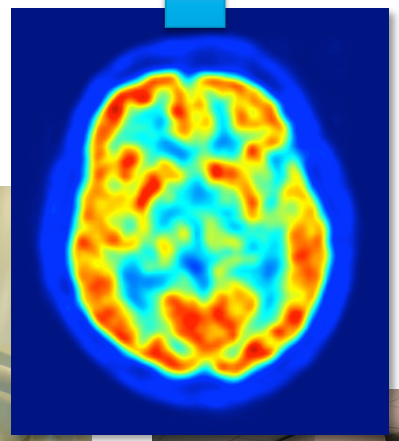
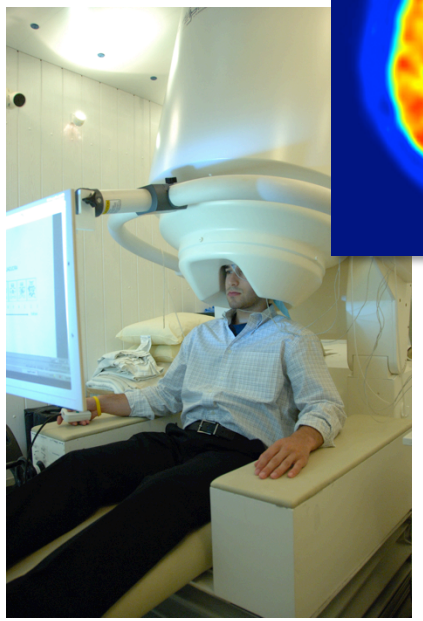
Reading your mind







Features are brain region intensities

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General notation

Output: y ← scalar

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

← d-dim vector

Notational conventions:

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

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Simple hyperplane

Model:

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

feature 1 = 1

feature 2 = **x**[1] … e.g., sq. ft.

feature 3 = **x**[2] … e.g., #bath

…

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

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More generically…
D-dimensional curve

Model:

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

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

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

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

feature 3 = $h_2(\mathbf{x})$ … e.g., $\mathbf{x}$[2] = #bath
or, log($\mathbf{x}$[7]) $\mathbf{x}$[2] = log(#bed) x #bath

…

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

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More on notation

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

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

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

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Interpreting the fitted function

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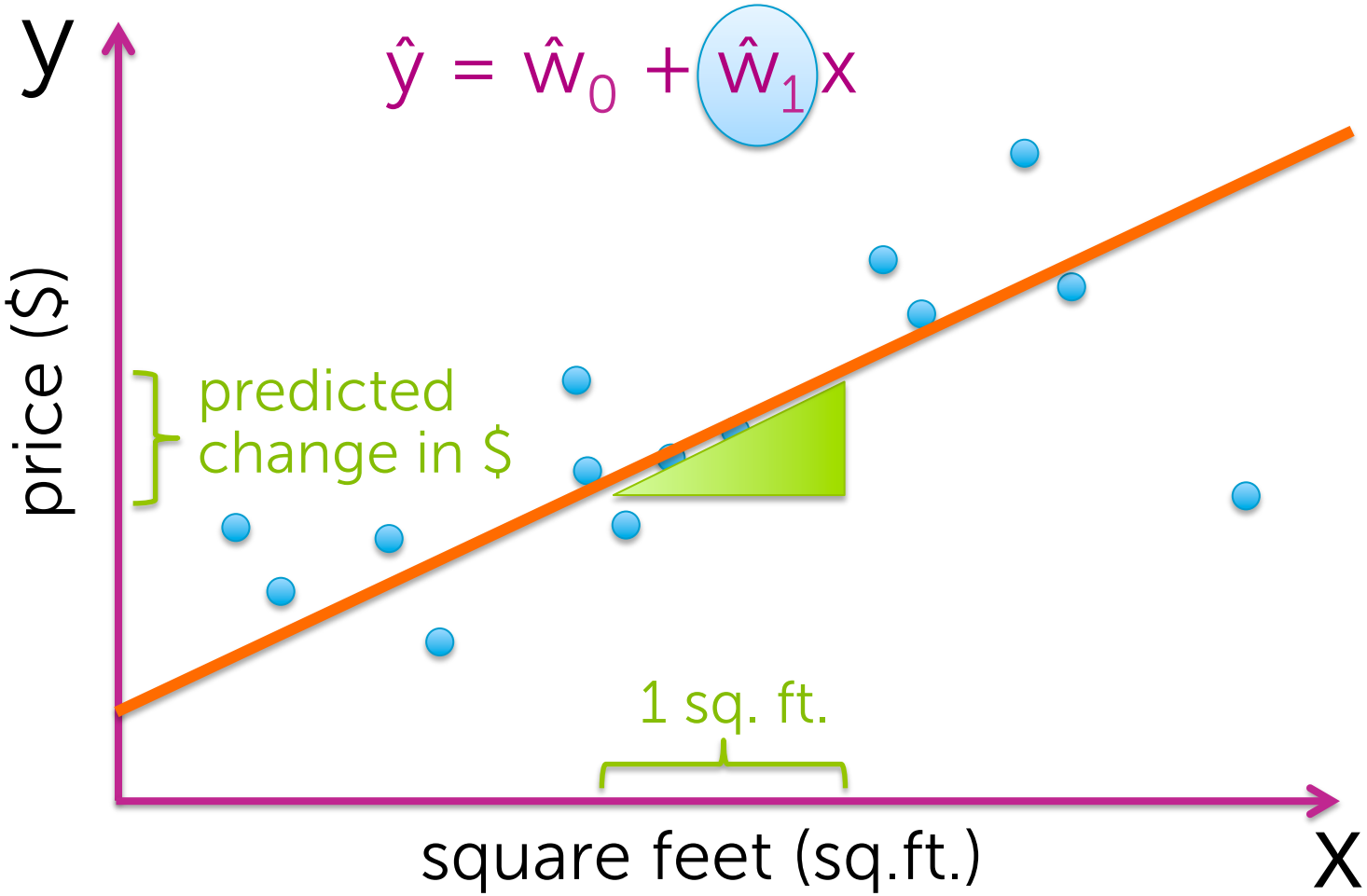
Interpreting the coefficients – Simple linear regression



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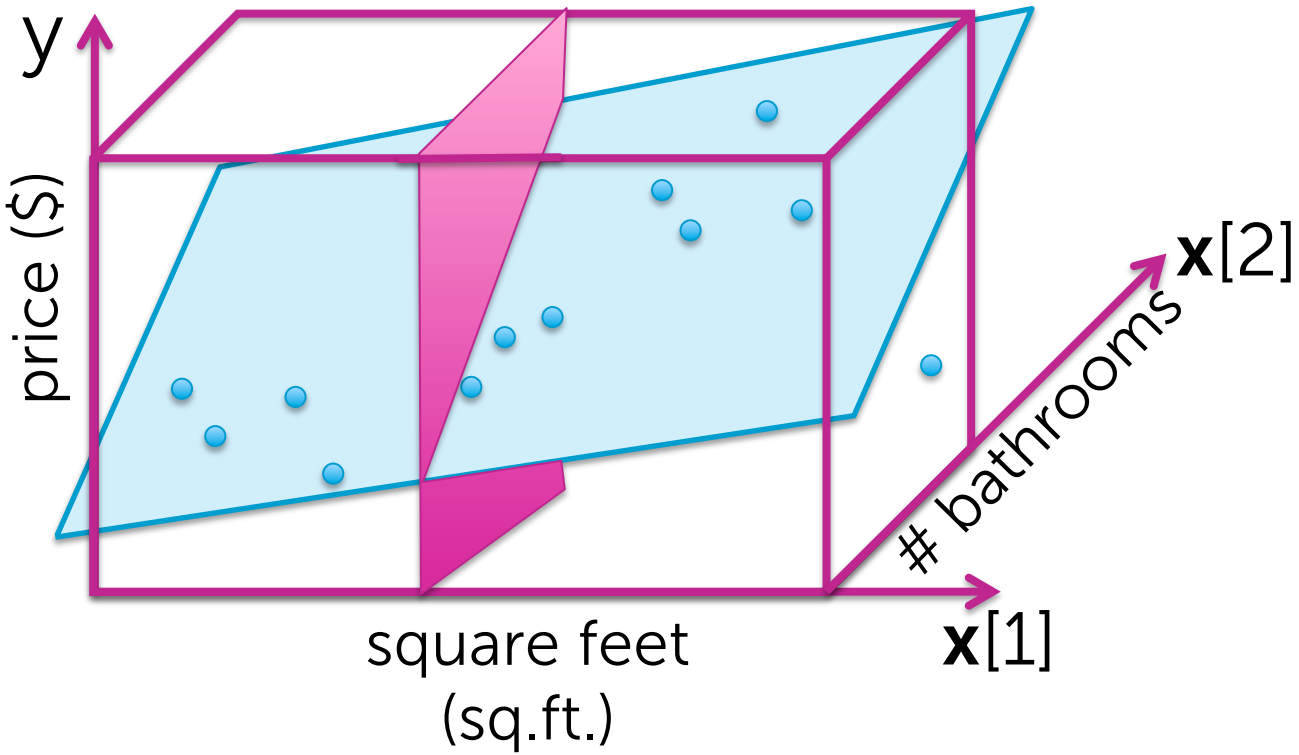
Interpreting the coefficients – Two linear features

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

fix



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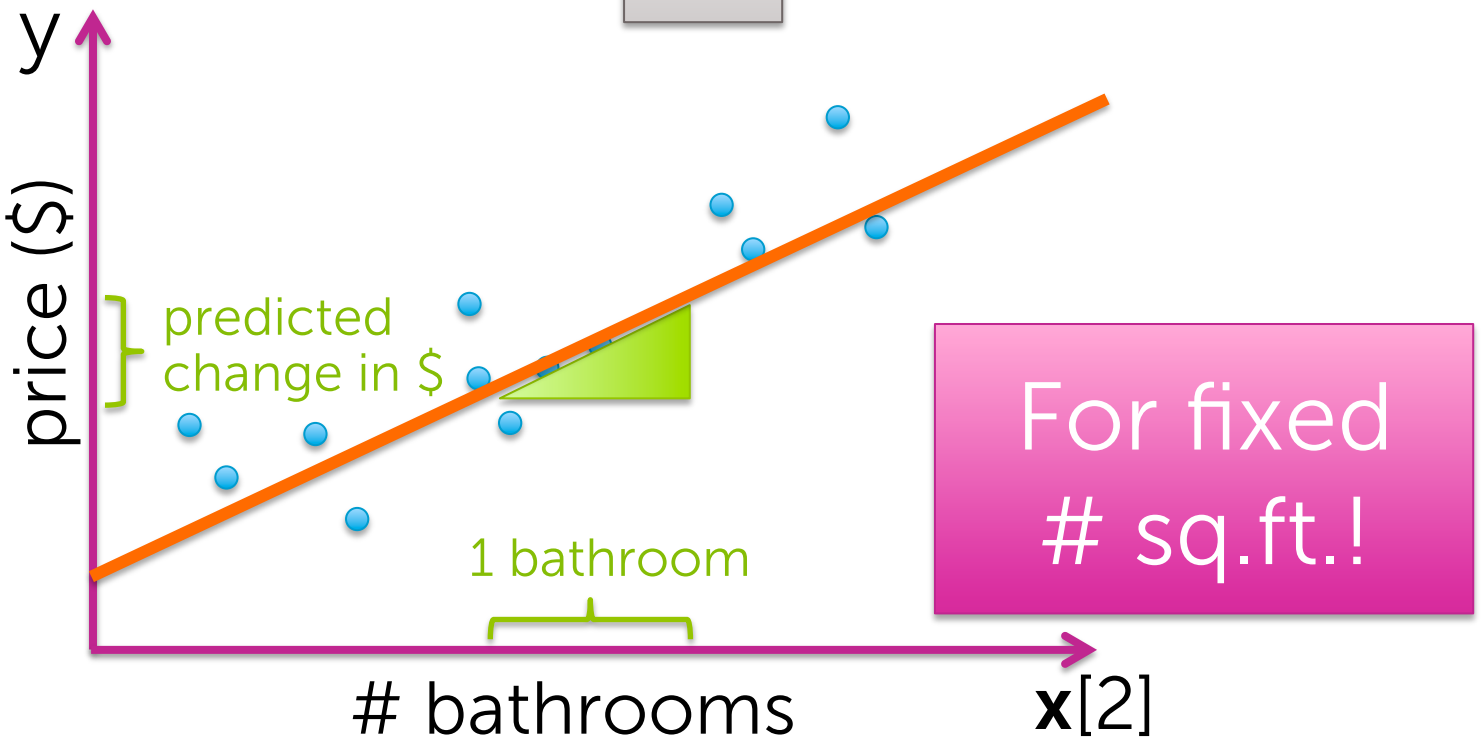
Interpreting the coefficients – Two linear features

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

fix



For fixed # sq.ft.!

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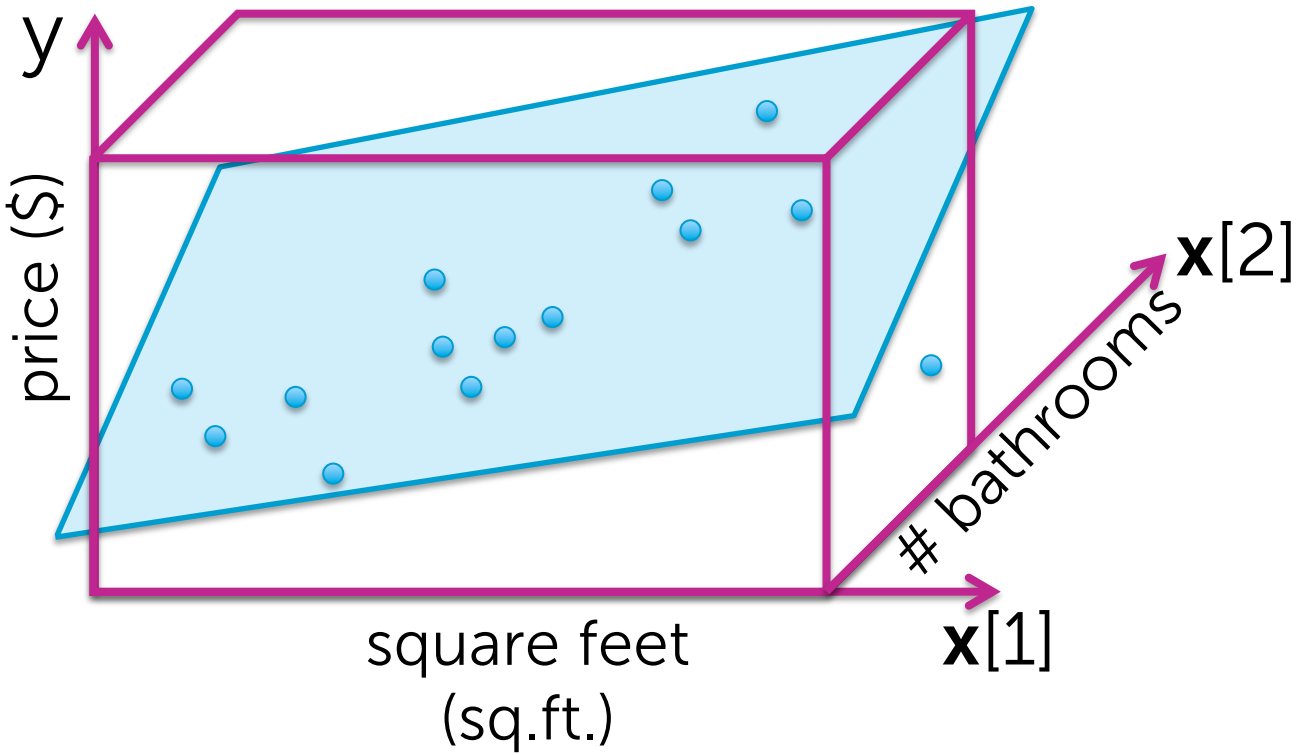
Interpreting the coefficients – Multiple linear features

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

fix fix fix fix



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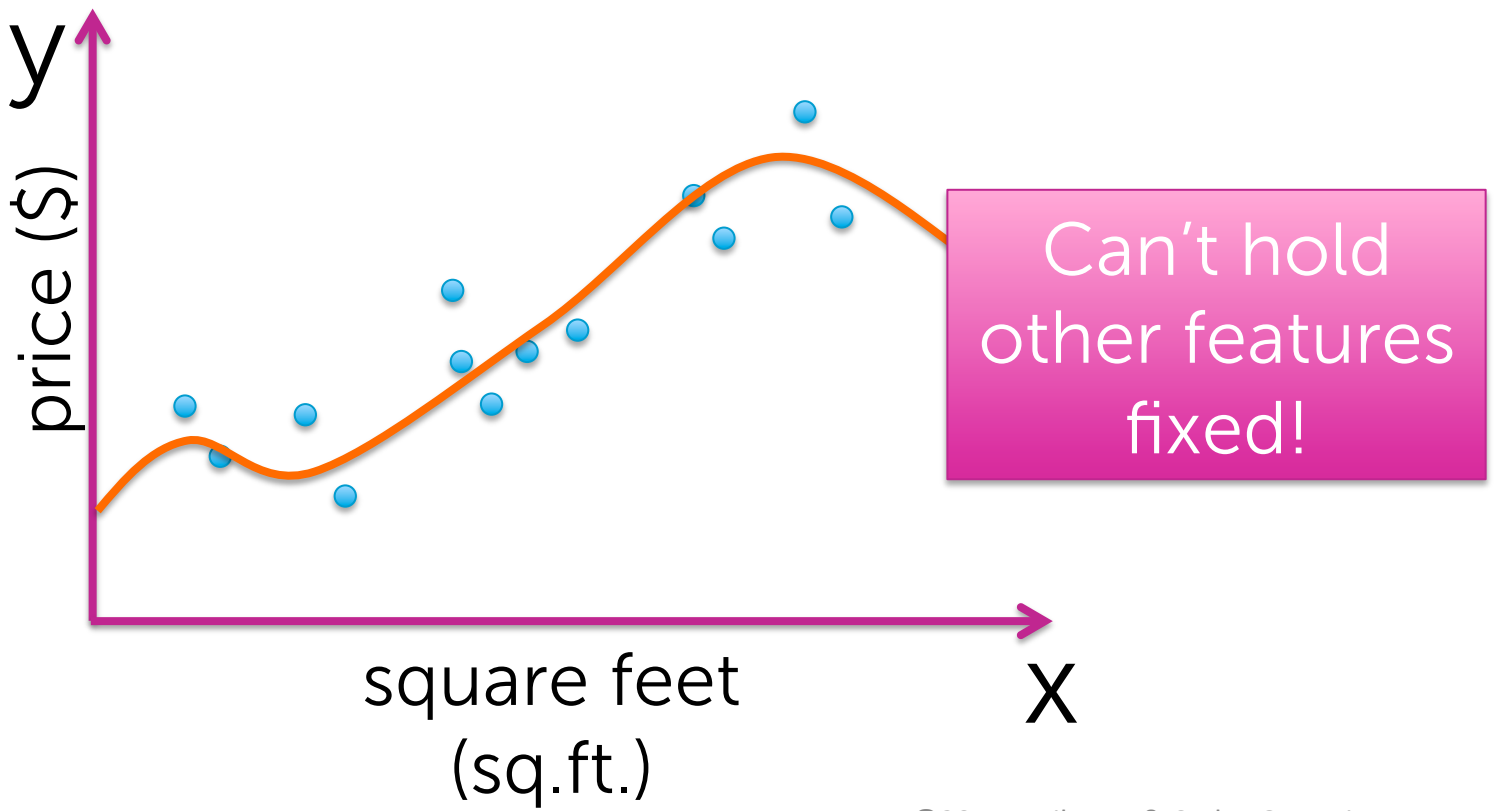
Interpreting the coefficients- Polynomial regression

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



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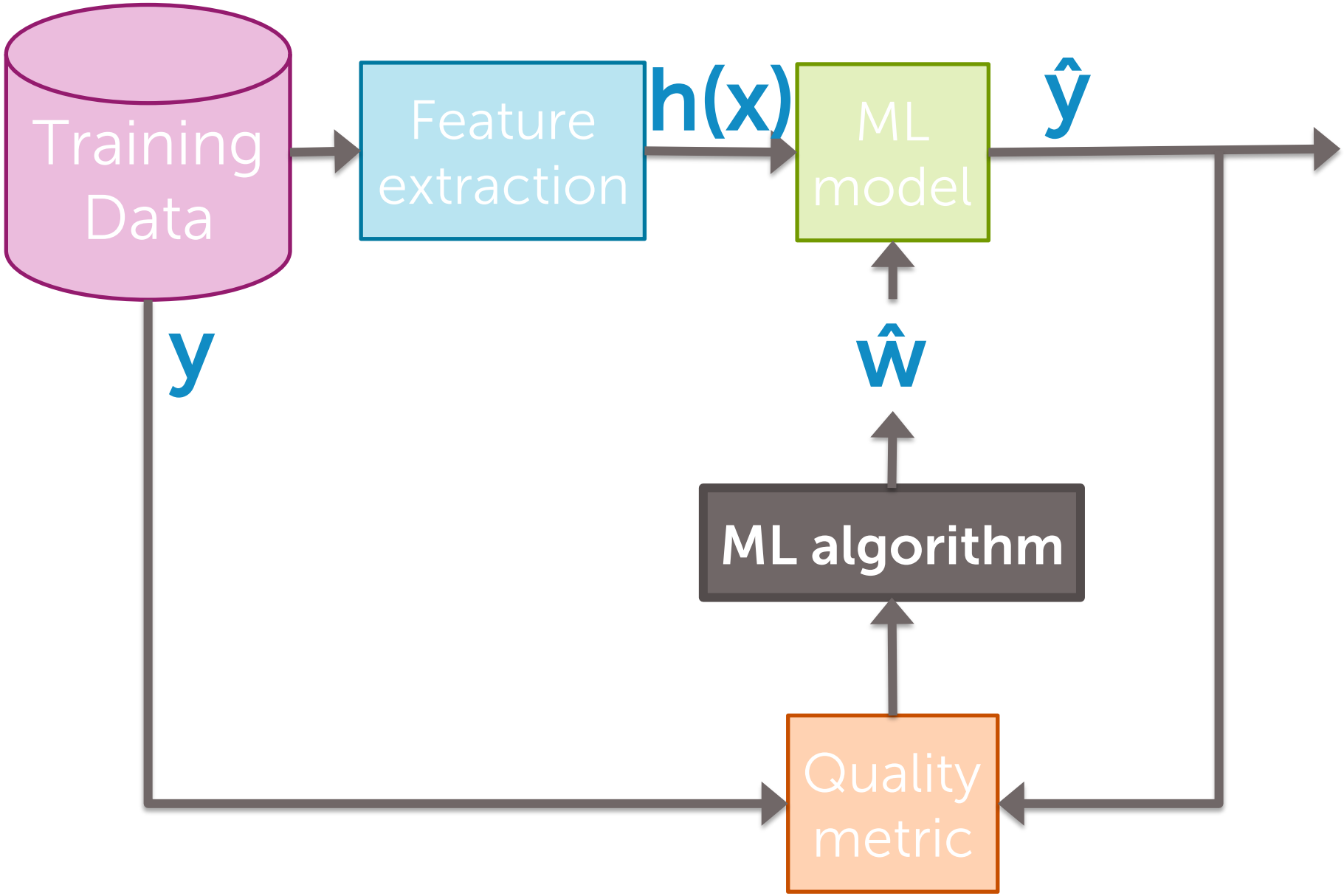
Fitting D-dimensional curves



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Step 1:
Rewrite the regression model

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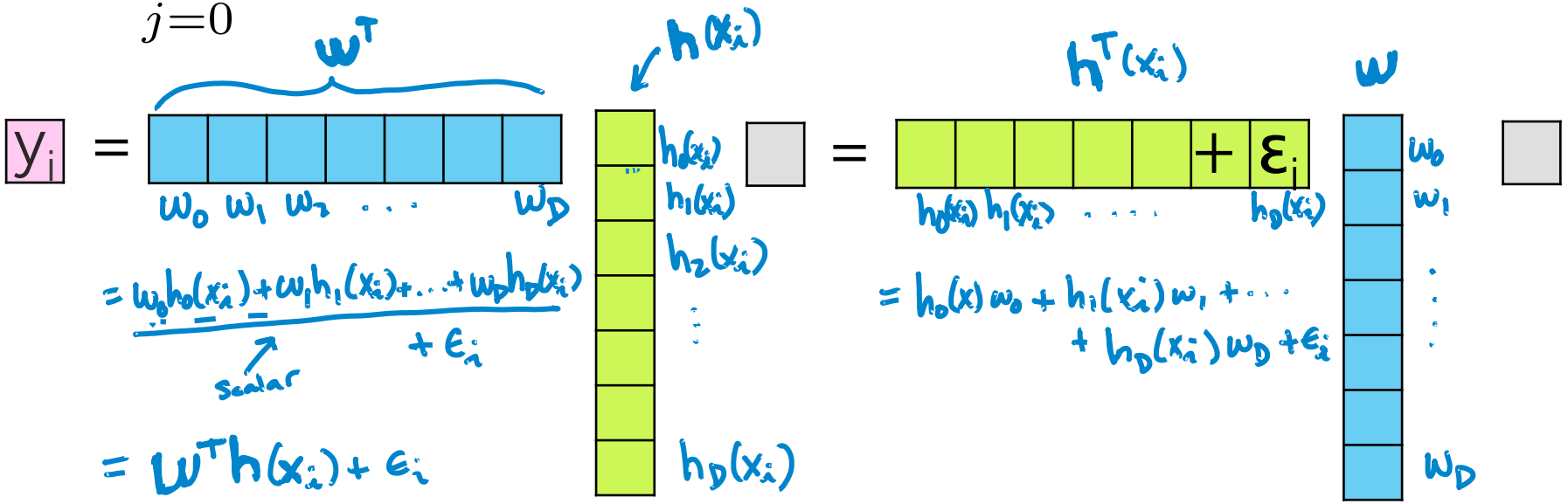
Rewrite in matrix notation

For observation i

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



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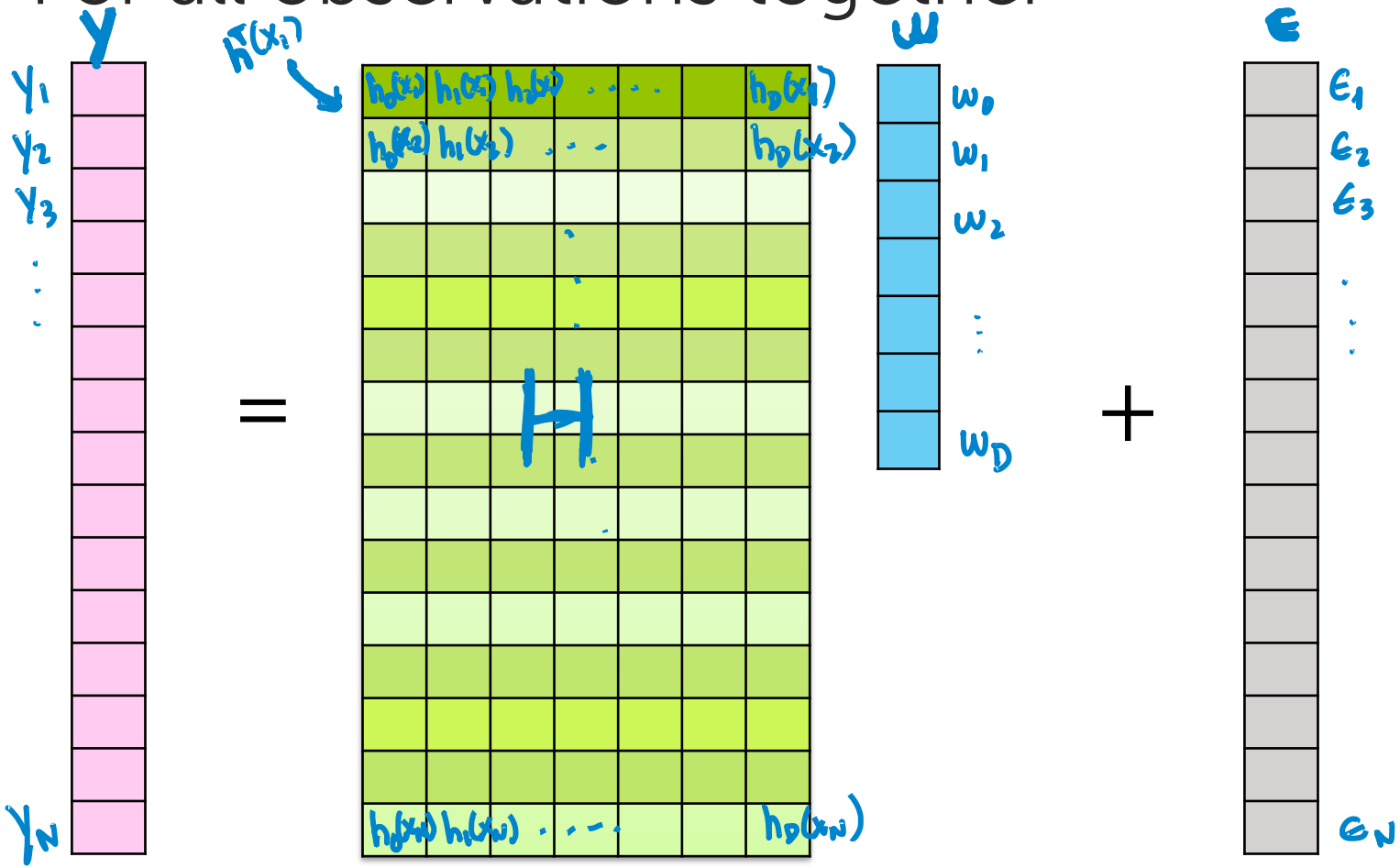
Rewrite in matrix notation

For all observations together



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

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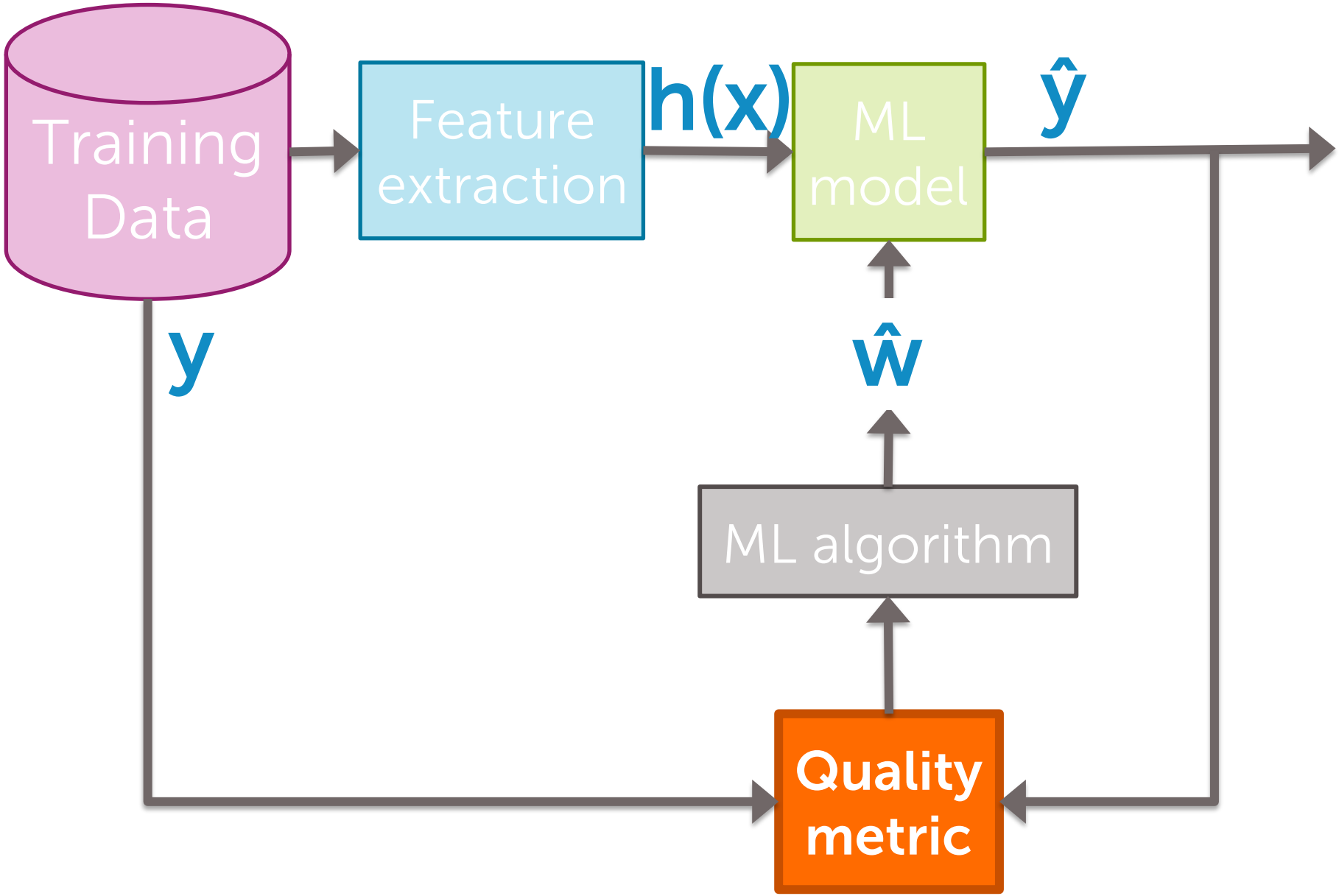
Step 2:
Compute the cost



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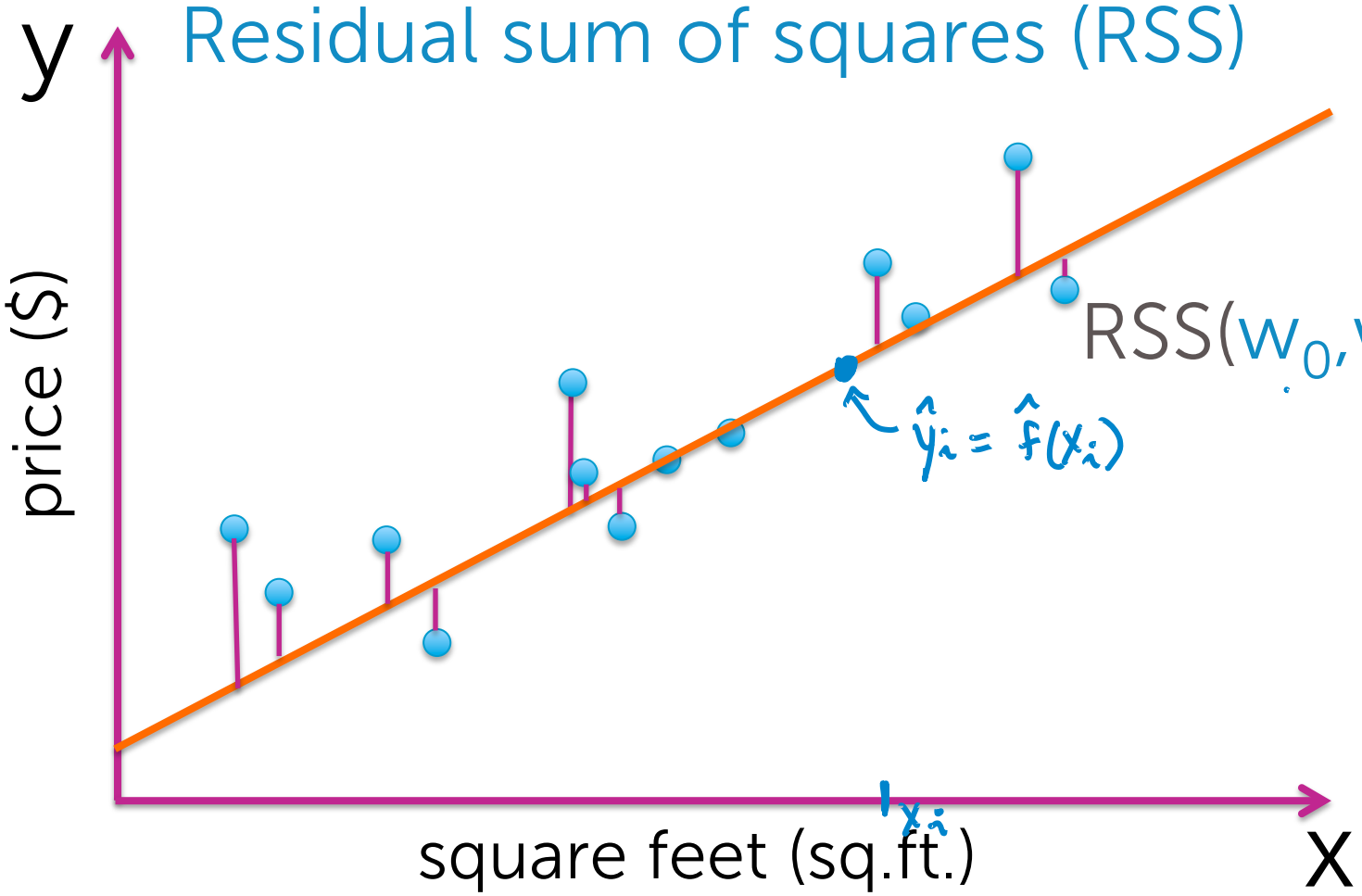
"Cost" of using a given line



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

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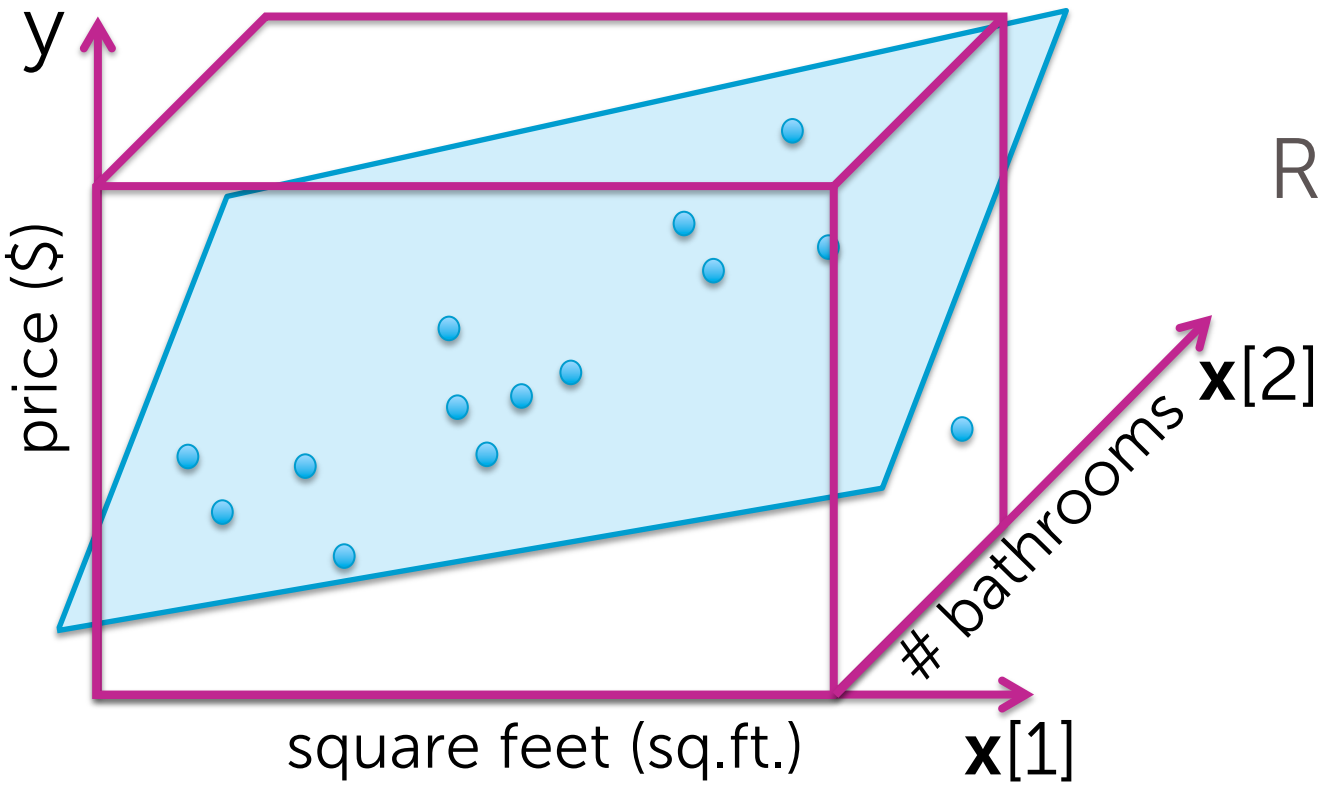
RSS for multiple regression



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

$h^T(x_i)\,\mathbf{w} = \hat{y}_i(\mathbf{w})$

$$\hat{y}_i = h^T(x_i)\,\mathbf{w}$$

$h^T(x_i) = [\,h_0(x_i)\ h_1(x_i)\ \cdots\ h_D(x_i)\,]$

$\mathbf{w} = [\,w_0\ w_1\ w_2\ \cdots\ w_D\,]^T$

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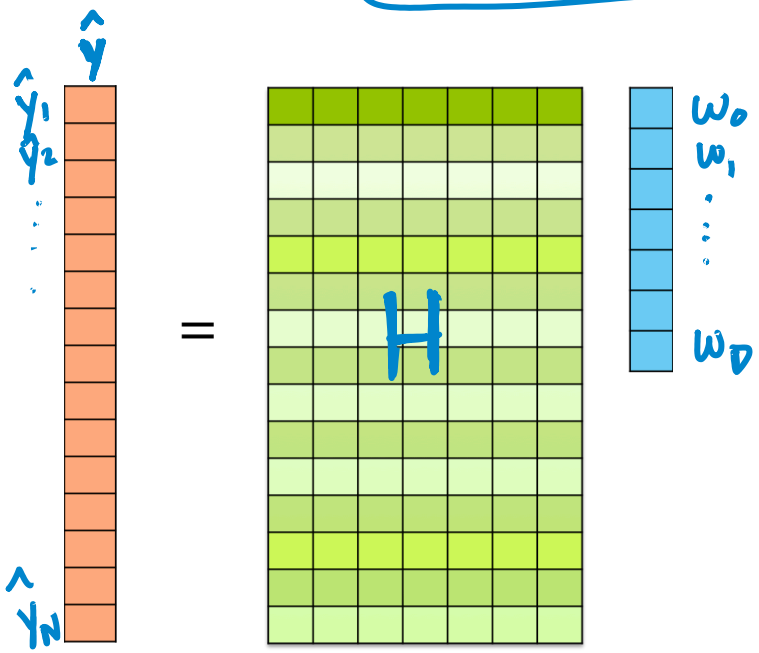
RSS in matrix notation

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

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

Why? (part 1)



$$\hat{y} = Hw$$

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

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

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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 2)

residual_1	residual_2	residual_3	...	residual_N

residual_1
residual_2
residual_3
...
residual_N

$$= (\text{residual}_1^2 + \text{residual}_2^2 + \cdots + \text{residual}_N^2)$$

$$= \sum_{i=1}^{N} \text{residual}_i^2$$

$$\triangleq \text{RSS}(\mathbf{w})$$

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Step 3:
Take the gradient

Gradient of RSS

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

$$= -2\mathbf{H}^T(\mathbf{y}-\mathbf{H}\mathbf{w})$$

Why? By analogy to 1D case:

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

$$= -2h(y-hw)$$

scalars

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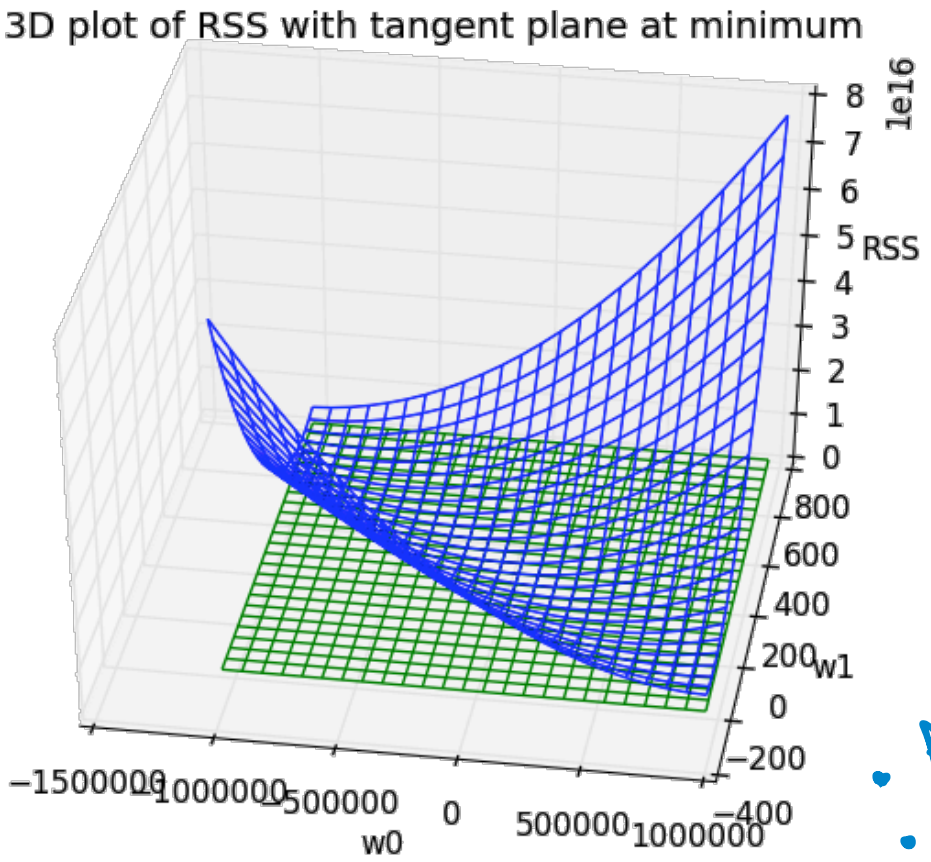
Step 4, Approach 1:
Set the gradient = 0

Closed-form solution



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

Solve for $\mathbf{w}$:

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

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

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

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

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

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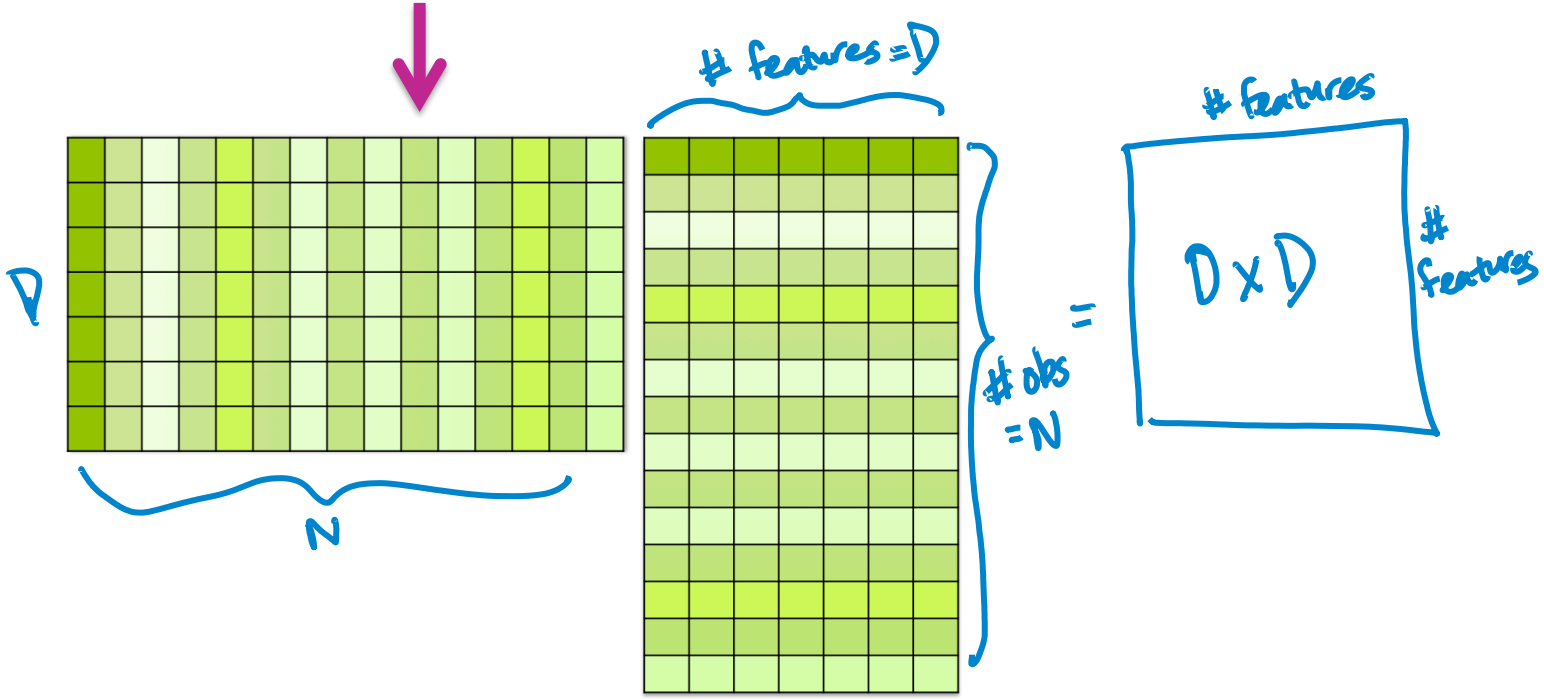
Closed-form solution

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



Invertible if:

really, # of linearly ind. observations

In most cases is $N > D$

Complexity of inverse:

$$O(D^3)$$

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Step 4, Approach 2:
Gradient descent

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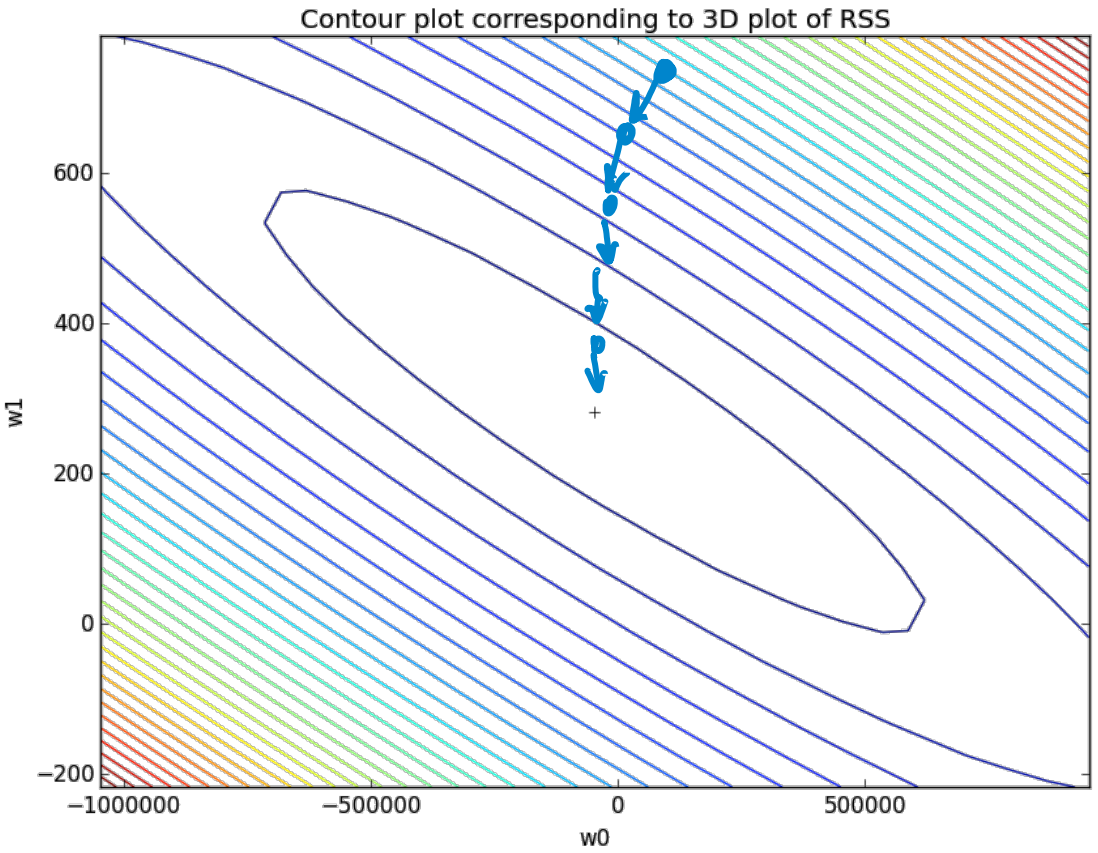
Gradient descent



while not converged

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \eta \nabla \text{RSS}(\mathbf{w}^{(t)})$$

$$-2\mathbf{H}^T(\mathbf{y}-\mathbf{H}\mathbf{w})$$

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

$$\hat{y}(w^{(t)})$$

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Feature-by-feature update

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

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

Partial with respect to w_j

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

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

Update to j^{th} feature weight:

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

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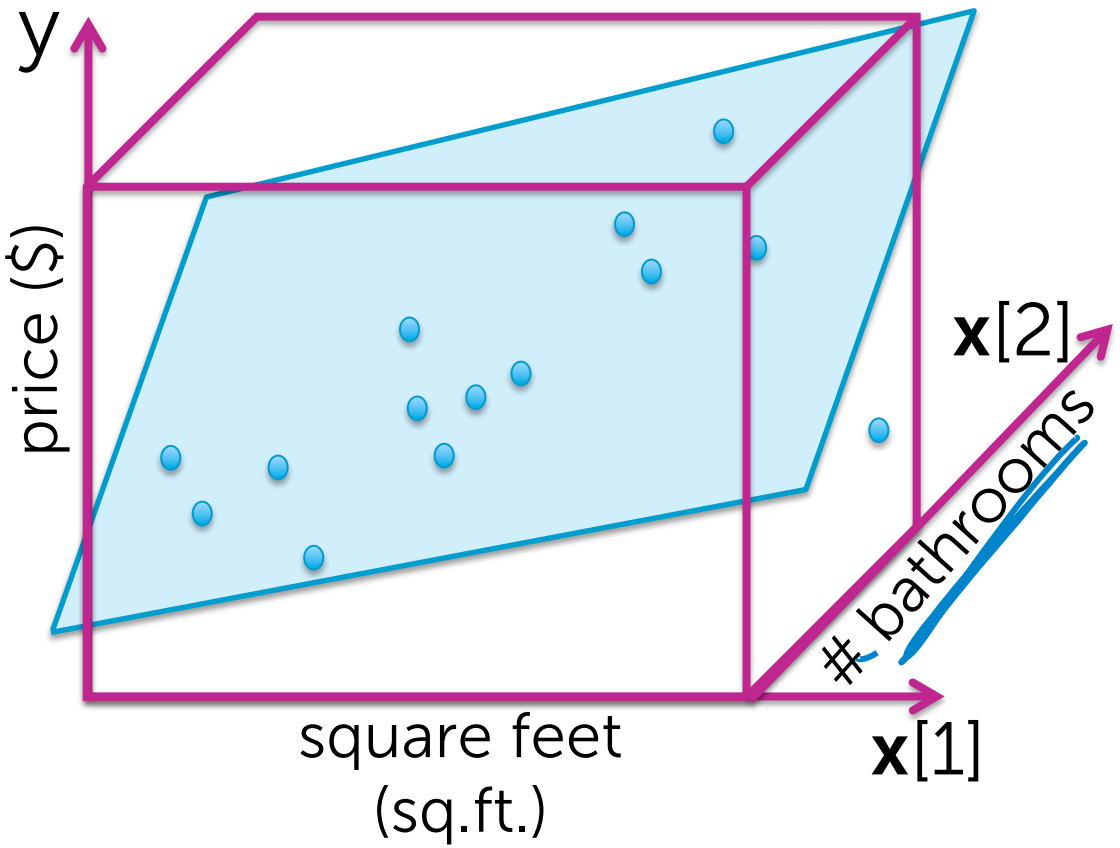
Interpreting elementwise



Update to j^{th} feature weight:

bathrooms

bath for house i

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

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

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

weighted by # bath will be positive

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

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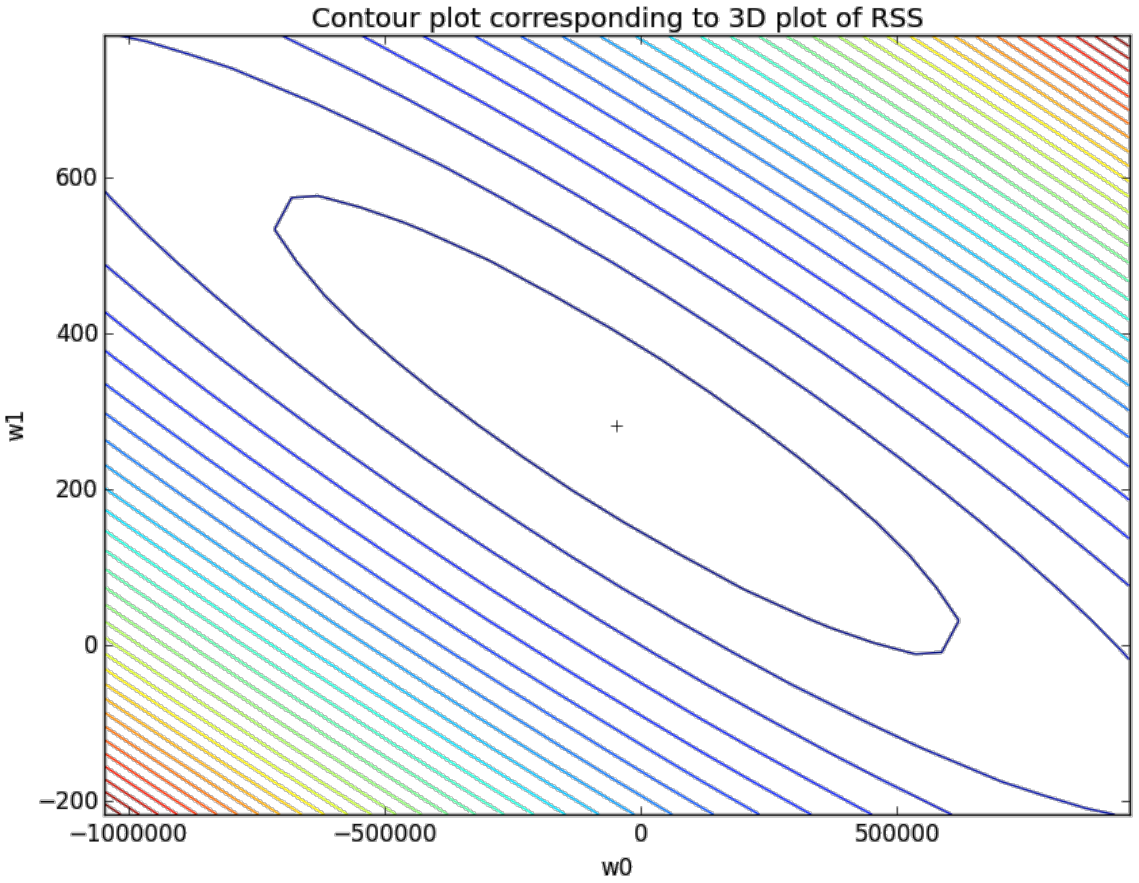
Summary of gradient descent for multiple regression



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

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

  for $j=0,\ldots,D$

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

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

  $t \leftarrow t + 1$

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An extremely useful algorithm

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Summary for multiple linear regression

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What you can do now…

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

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