Linear Regression: Model and Algorithms (part 2)

CSE 446

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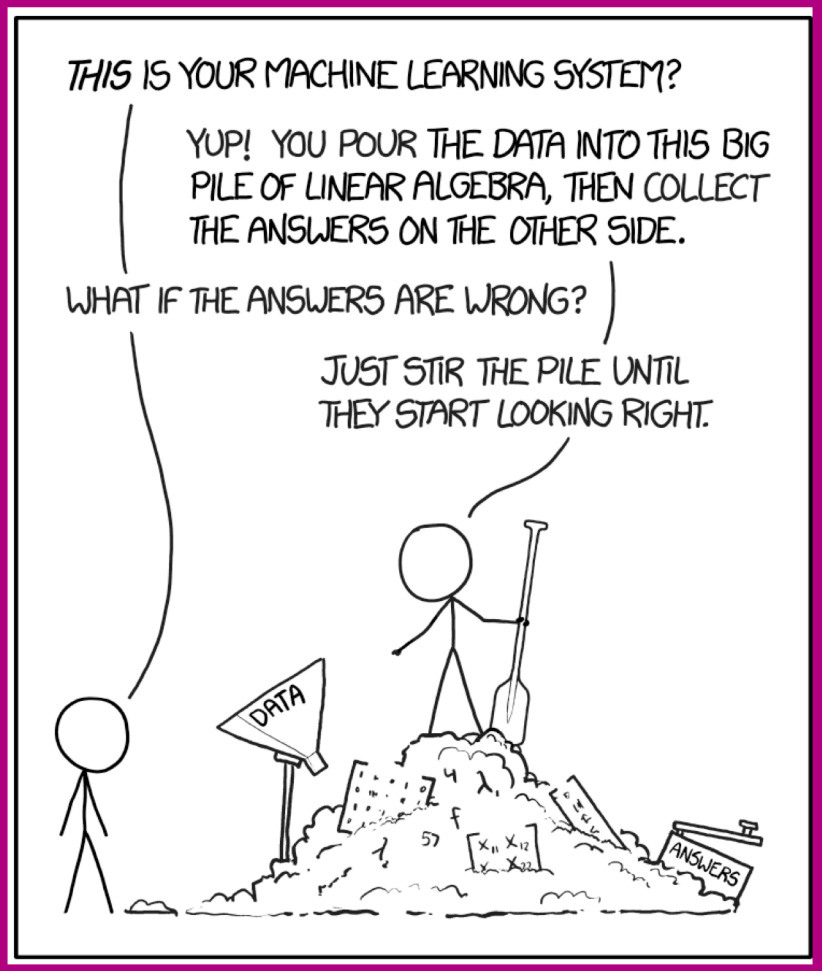
April 8, 2019


THIS IS YOUR MACHINE LEARNING SYSTEM?
YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.
WHAT IF THE ANSWERS ARE WRONG?
JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.
DATA
ANSWERS

XKCD

Linear regression: a supervised learning problem

Goal: to predict some output from some inputs using labelled examples. Example: house sales price from square footage

Supervised learning: Problem of learning a function that maps inputs to outputs based on labelled examples.

Regression: When the labels are real numbers

Linear regression: a supervised learning problem

Goal: to predict some output from some inputs/features. Example: house sales price from square footage

Step 1: Define set up and get data

- a model for how the output y depends on the inputs **x**.
- We assumed that y is a linear function of features + noise.

$$y = \mathbf{w}^T \mathbf{x} + \varepsilon$$

- A training set (labelled examples): $\{(\mathbf{x}_i, y_i)\}_{i=1..n}$

Linear regression: a supervised learning problem

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Step 2: find the parameters **w** that minimize the "loss/cost" on the training set.

- Our **loss function** was residual sum of squares (RSS)
- Find $\hat{w}$ that minimizes RSS = $\sum_{i=1}^{n} (y_i - \sum_{j=1}^{d} w_j x_i[j])^2 = (\mathbf{y}-X\mathbf{w})^T(\mathbf{y}-X\mathbf{w})$
- Found solution by solving for gradient of $(\mathbf{y}-X\mathbf{w})^T(\mathbf{y}-X\mathbf{w}) = \mathbf{0}$

  Solution: $X^TX\hat{w} = X^Ty$ If X^TX is invertible, could write $\hat{w} = (X^TX)^{-1}X^T\mathbf{y}$

Linear regression: a supervised learning problem

Goal: to predict some output from some inputs/features.

Step 1: Define set up ($y = \mathbf{w}^T \mathbf{x} + \varepsilon$) and get data $\{(\mathbf{x}_i, y_i)\}_{i=1..n}$

Step 2: find the parameters $\hat{\mathbf{w}}$ that minimizes RSS = $(\mathbf{y}-X\mathbf{w})^T(\mathbf{y}-X\mathbf{w})$

Step 3: Use $\hat{\mathbf{w}}$ to make predictions.

Given $\mathbf{x}$, predict output: $\hat{\mathbf{w}}^T \mathbf{x}$

Plan for today:

- Gradient descent
- Handling an intercept
- More features/more complex models
- How well does it work?

Linear regression: a supervised learning problem

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Fitting the linear regression model

Gradient descent

Gradient Descent – univariate case

- Repeatedly move in direction that reduces the value of the function.

Use the fact that locally the function behaves like the derivative (and in higher dimensions like the gradient)

$f(x + dx) \sim f(x) + dx * f'(x)$

Want to move in direction of greatest decrease —> opposite of direction of gradient (see directional derivatives for justification)

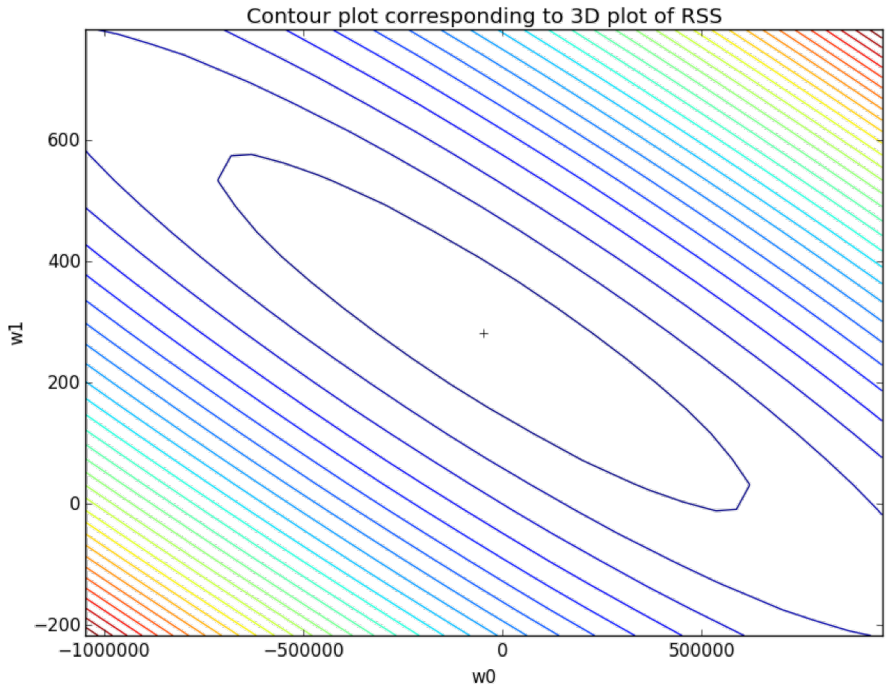
$x_{t+1} = x_t - \eta * f'(x)$

Where eta is the step-size… Only guaranteed to find local minimums; if convex a local min is a unique global min.

Gradient Descent – multivariate case

Gradient descent for linear regression:

repeatedly move in direction of negative gradient

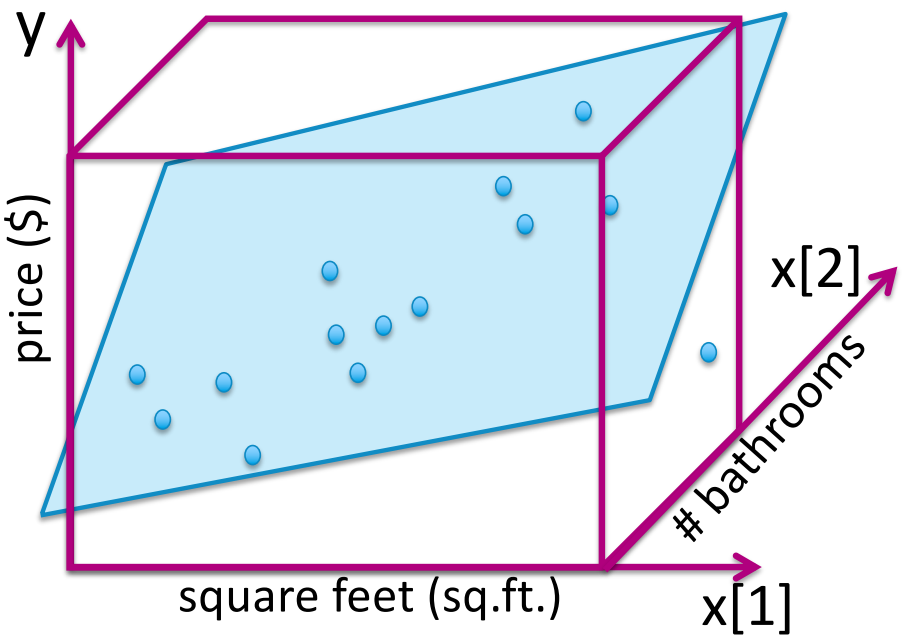


linear regression is a task of finding the minimum error.

while not converged

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

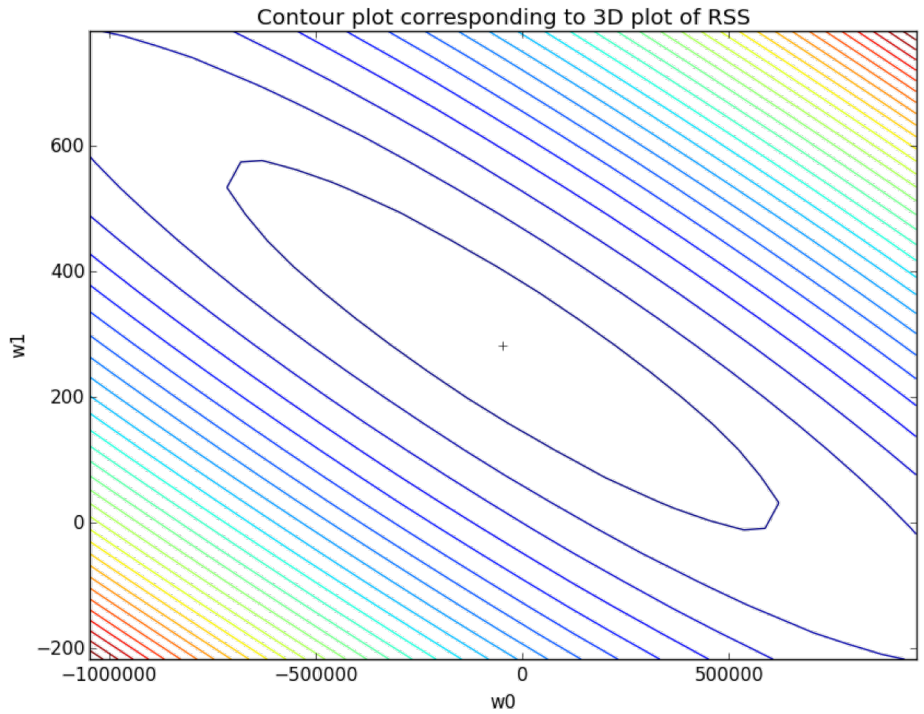
Interpreting elementwise



Update to j^{th} feature weight:

$$w_j^{(t+1)} \leftarrow w_j^{(t)} + 2\eta \sum_{i=1}^{N} x_i[j](y_i - \hat{y}_i(w^{(t)}))$$

Summary of gradient descent for multiple regression



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

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

  for j=1,…,d

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

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

  t ← t + 1

partial = partial derivative of x_j in our RSS model evaluated at the current position w_t

Adding an intercept – “demeaning”

Once we have a fitted function

- We use it to predict the sales price for new houses, by plugging in square footage, number of bathrooms, etc for the new house **x** whose sales price we want to predict.
- Prediction is:

What if we want to allow for an intercept?

Assume that $y = \mathbf{w}^T \mathbf{x} + b + \varepsilon$

Find $\hat{w}, b$ that minimize $RSS = \sum_{i=1}^{n} (y_i - \sum_{j=1}^{d} w_j x_i[j] - b)^2$

$= (\mathbf{y} - X\mathbf{w} - b\mathbf{1})^T(\mathbf{y} - X\mathbf{w} - b\mathbf{1})$

where the 1 above is the vector of all ones.

Handling an intercept (constant term)

Assume that $y = \mathbf{w}^T \mathbf{x} + b + \varepsilon$

Find $\hat{w}, b$ that minimize RSS = $\sum_{i=1}^{n} (y_i - \sum_{j=1}^{d} w_j x_i[j] - b)^2$

$$= (\mathbf{y} - X\mathbf{w} - b\mathbf{1})^T(\mathbf{y} - X\mathbf{w} - b\mathbf{1})$$

Two step approach:

VECTOR: observation x_i = [x_i1, x_i2, x_i3, …, x_in]

1. Show that if $\frac{1}{n}\sum_i \boldsymbol{x}_i = \mathbf{0}$ (*) then solution is simple.

2. Show how to transform, aka ``demean" any linear regression problem so that (*) holds.

I have m measurements of all my variables
x1 = [x1_1, x1_2, …, x1_n]
x2 = [x2_1, x2_2, …, x2_n]

…
xm = [xm_1, …., xm_n]

1. Show that if $\frac{1}{n}\sum_i \boldsymbol{x}_i = \mathbf{0}$ (*) then solution is simple.

VECTOR!

Sum of all columns = 0… all variables have a mean of zero across all our measurements.

Same as saying that $X^T\mathbf{1} = \mathbf{0}$.

Find $\hat{w}$, b that minimize

RSS = $\sum_{i=1}^{n} (y_i - \sum_{j=1}^{d} w_j x_i[j] - b)^2$

= $(\mathbf{y}-X\mathbf{w} - b\mathbf{1})^T(\mathbf{y}-X\mathbf{w} - b\mathbf{1})$

dRSS / dw_j =

partial[w_j] = $-2\sum_{i=1}^{n} x_i[j](y_i - \mathbf{x}_i^T\mathbf{w} - b)$ = 0

goes to zero as sum_i^n x_i[j] b —> as b is just a constant we can pull it out leaving b * sum_i^n x_i [j] = 0 by assumption.
So we can just remove this variable. SAME SOLUTION in coefficients as before!
sum_i x_i [j] (y_i - x_i^T w) = 0

x_i[j] missing in the second case.

partial[b] = $-2\sum_{i=1}^{n} (y_i - \mathbf{x}_i^T\mathbf{w} - b)$ = 0

this middle term goes to zero:
sum_i x_i ^T w = sum_j sum_i x_i[j] w_j
= sum_j w_j sum_i x_i [j]
But sum_i x_i [j] = 0 by assumption

= sum y_i - sum x_i ^T w - nb = 0
—> b = 1/n sum(y_i)

2. Show how to transform, aka ``demean" any linear regression problem so that (*) holds.

Let M = 1\n sum_i x_i —> vector with means for each variable —>

Replace x_i with x_i - M —> demeans all the variables

x1 = [x1[1], x1[2], …., x1[n]]
x2 = [x2[1], x2[2], …., x2[n]]

….
xm = [xm[1], xm[2], …, xm[n]]

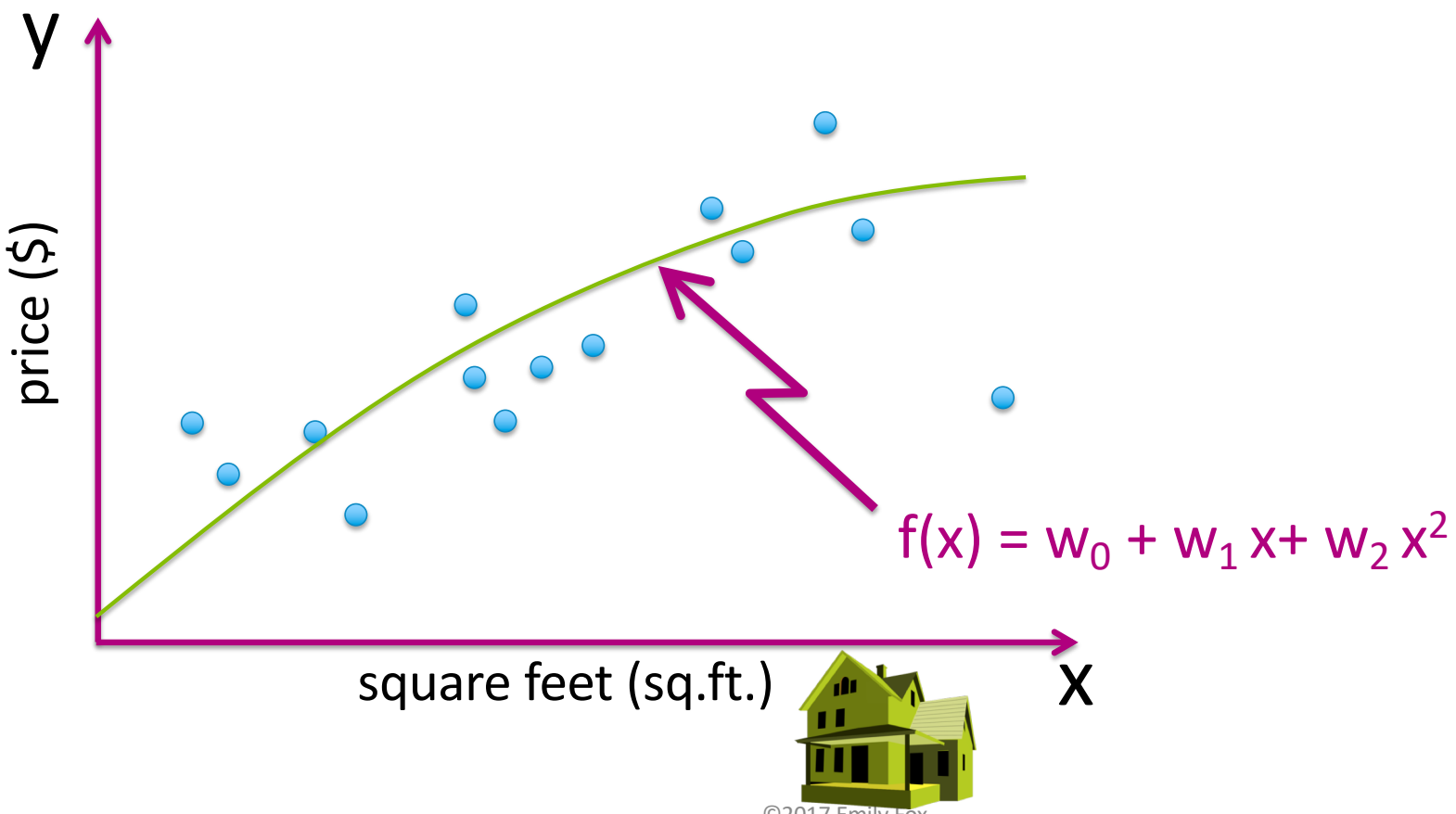
take the mean across each variable

M = [mean(xi[1]), mean(xi[2]), …, mean(xi[n])]

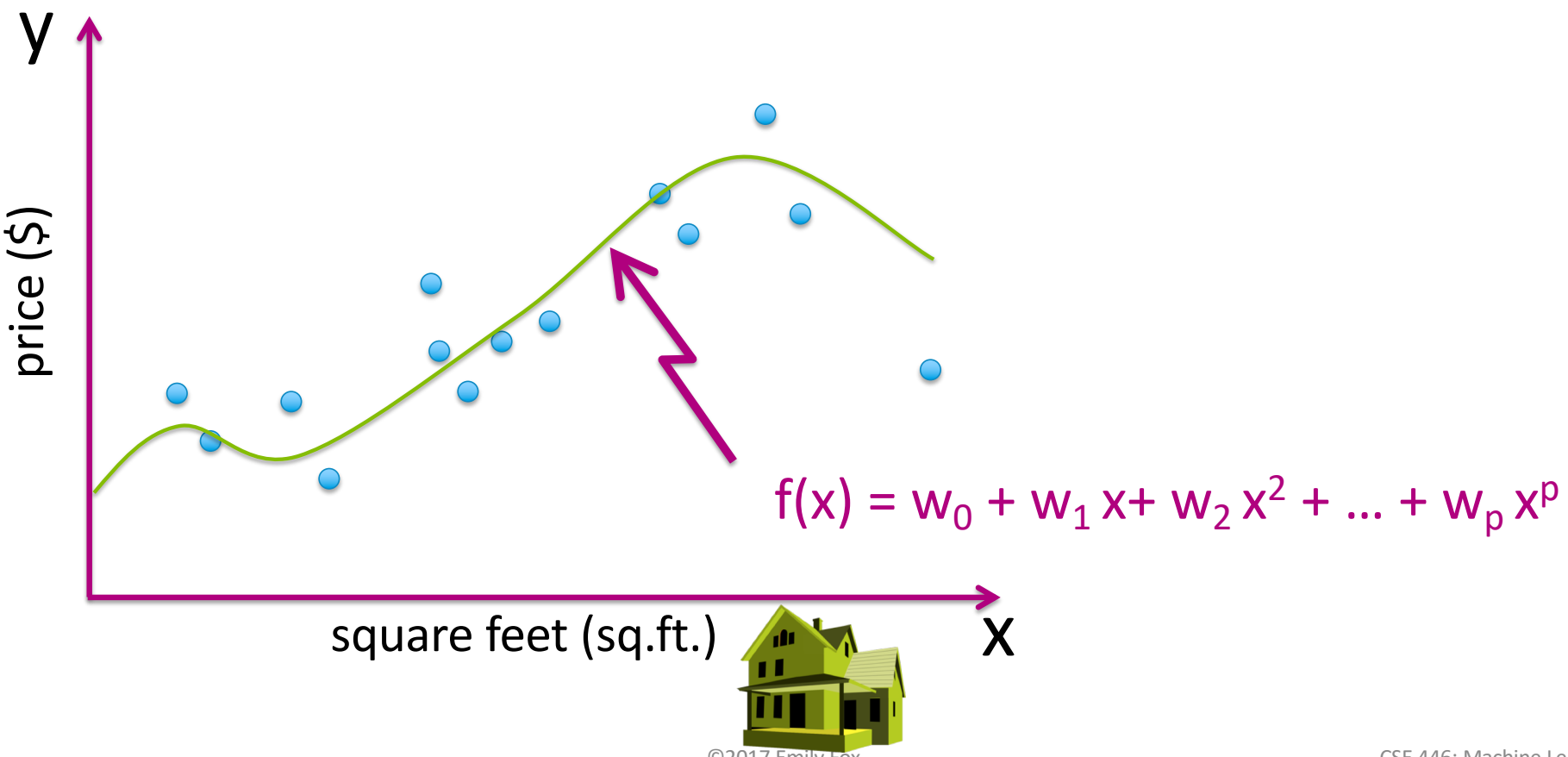
$$\frac{1}{n}\sum_i \boldsymbol{x}_i = \mathbf{0} \quad (*)$$

More features, more complex models

What about a quadratic function?



Even higher order polynomial

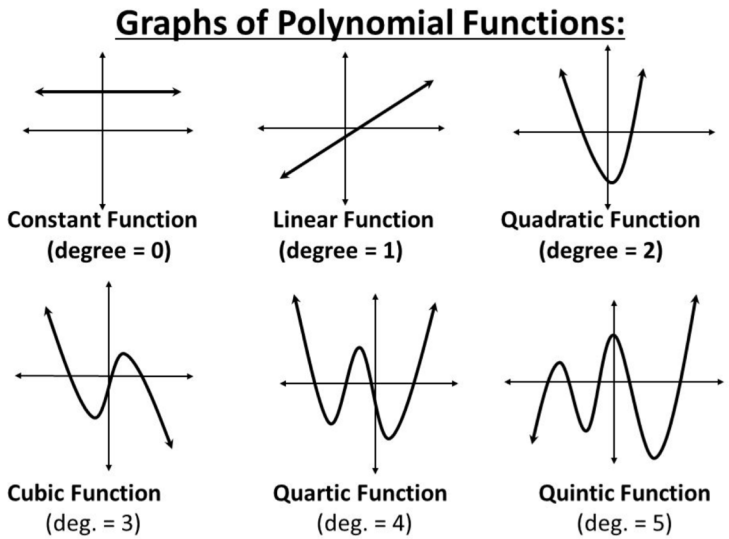


Polynomial regression (single input)

Goal: to predict some output from some inputs/features.

Step 1: Assume that y (sales price) is a polynomial function of feature (square footage)+ noise.

$y_i = \sum_{j=0}^{p} w_j x_i^j + \varepsilon$ A training set (labelled examples):



Polynomial regression

Goal: to predict some output from some inputs/features.

Step 1: $y_i = \sum_{j=0}^{p} w_j x_i^j + \varepsilon$ A training set (labelled examples):

Step 2: find params **w** that minimize the "loss/cost" on training set $\{(x_i, y_i)\}_{i=1..n}$

- **Loss function** is residual sum of squares (RSS)
- Find $\hat{\mathbf{w}}$ that minimizes $\text{RSS} = \sum_{i=1}^{n} (y_i - \sum_{j=0}^{p-1} w_j x_i^j)^2$

Polynomial regression

Goal: to predict some output from some inputs/features.

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- Find $\hat{w}$ that minimizes RSS = $\sum_{i=1}^{n} (y_i - \sum_{j=0}^{p-1} w_j x_i^j)^2$

- **Just as easy to solve!** Just think of x_i^j as one of p features associated with the i^{th} observation.
- Instead of single input x_i, define features **h(x)** = $(1, x, x^2 \ldots, x^p)$

h(x_i**)** = $(h_0(x_i), h_1(x_i), h_2(x_i), h_3(x_i), h_4(x_i), h_5(x_i))$
= $(\ 1\ ,\ x_i\ ,\ x_i^2\ ,\ x_i^3\ ,\ x_i^4\ ,\ x_i^5\ )$

Polynomial regression

Step 1: $y_i = \sum_{j=0}^{p} w_j x_i^j + \varepsilon$

Step 2: find the parameters **w** that minimize the "loss/cost" on the training set.

- Find $\hat{\mathbf{w}}$ that minimizes RSS $= \sum_{i=1}^{n} (y_i - \sum_{j=0}^{p} \mathbf{w}_j x_i^j)^2 = (\mathbf{y}-H\mathbf{w})^T(\mathbf{y}-H\mathbf{w})$
- Find solution by solving for gradient of $(\mathbf{y}-H\mathbf{w})^T(\mathbf{y}-H\mathbf{w}) = \mathbf{0}$

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

Polynomial regression

Step 1: $y_i = \sum_{j=0}^{p} w_j x_i^j + \varepsilon$

Step 2: find the parameters **w** that minimize the "loss/cost" on the training set.

- Find $\hat{\mathbf{w}}$ that minimizes RSS = $\sum_{i=1}^{n} (y_i - \sum_{j=0}^{p} \mathbf{w_j} x_i^j)^2 = (\mathbf{y}-H\mathbf{w})^T(\mathbf{y}-H\mathbf{w})$
- Find solution by solving for gradient of $(\mathbf{y}-H\mathbf{w})^T(\mathbf{y}-H\mathbf{w}) = \mathbf{0}$

  Solution: $H^TH\hat{\mathbf{w}} = H^Ty$

Step 3: Use $\hat{\mathbf{w}} = (\hat{w}_0, \hat{w}_1 \ldots, \hat{w}_p)$ to make predictions. Given x, let

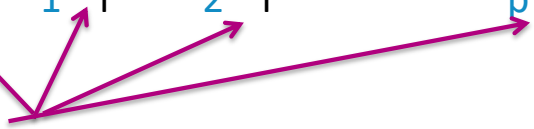
$\mathbf{h}(x) = (1, x, x^2 \ldots, x^p)$ and predict output:

$$\mathbf{h}(x)^T \hat{\mathbf{w}} = \hat{w}_0 + \hat{w}_1 x + \ldots + \hat{w}_p x^p$$

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 transformed inputs 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

Why might we want to use polynomial regression?

- Taylor Series!

More generally

- Start with set of inputs for each observation $\mathbf{x} = (x[1], x[2], \ldots, x[d])$

and training set: $\{(\mathbf{x}_i, y_i)\}_{i=1..n}$

- Define feature map that transforms each input vector $\mathbf{x}_i$ to higher dimensional feature vector $h(\mathbf{x}_i)$.

Example: $x_i[1]$ $x_i[2]$ $x_i[3]$

$h_1(\mathbf{x})$	$h_2(\mathbf{x}_i)$	$h_3(\mathbf{x}_i)$	$h_4(\mathbf{x}_i)$,	$h_5(\mathbf{x}_i)$	$h_6(\mathbf{x}_i)$	$h_7(\mathbf{x}_i)$
1	$x_i[1]$	$x_i[1]^2$	$x_i[1]x_i[2]$	$x_i[2]$	$x_i[2]^2$	$\cos(\pi\, x_i[3]/6)$

General notation

Output: y ← scalar

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

Notational conventions:

- $\mathbf{x}_i$ = input of i^{th} data point (*vector*)
- $x_i[j]$ = j^{th} input of i^{th} data point (*scalar*)
- $\mathbf{h}(\mathbf{x}) = (h_1(\mathbf{x}), h_2(\mathbf{x}), \ldots, h_p(\mathbf{x}))$ feature map applied to input $\mathbf{x}$ (*vector*)
- $h_j(\mathbf{x})$ = j^{th} feature associated with input x (*scalar*) (j^{th} basis function)

H = n by p matrix whose ith row is $\mathbf{h}(\mathbf{x}_i)$

To fit these more general functions

- Start with input features $\mathbf{x}$ = (x[1],x[2],…, x[d])

and training set: $\{(\mathbf{x}_i, y_i)\}_{i=1..n}$

- Define feature map that transforms each $\mathbf{x}_i$ to higher dimensional feature vector $\mathbf{h}(\mathbf{x}_i)$.
- Model: $y_i = \sum_{j=1}^{p} w_j \, h_j(\mathbf{x}_i) + \varepsilon_i$
- Find $\hat{\mathbf{w}}$ that minimizes RSS = $\sum_{i=1}^{n} (y_i - \sum_{j=1}^{p} w_j \, h_j(\mathbf{x}_i))^2$

  $= (\mathbf{y}\text{-}H\mathbf{w})^T(\mathbf{y}\text{-}H\mathbf{w})$
- Solution: $H^T H\hat{\mathbf{w}} = H^T y$

Recap of concepts

What you can do now…

- Describe linear regression (and feature maps)
- Write a regression model using multiple inputs or features thereof.
- 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