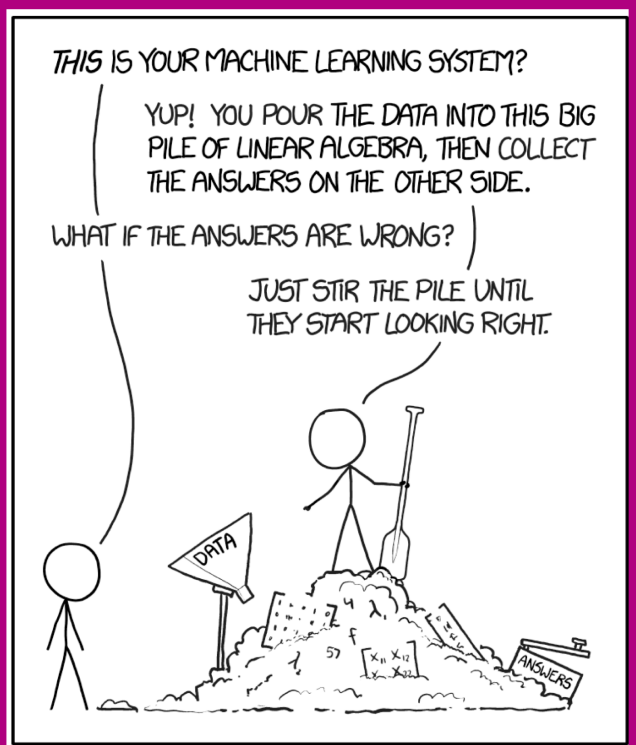
Linear Regression: Model and Algorithms (part 2)

CSE 446

Most slides by Emily Fox
Presented by Anna Karlin
April 8, 2019



- panopto
- latex
- HW1

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.

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

$$w = \begin{pmatrix} w_1 \\ \vdots \\ w_d \end{pmatrix} \qquad x = \begin{pmatrix} x_1 \\ \vdots \\ x_d \end{pmatrix}$$

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

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 **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 $\hat{w} = (X^TX)^{-1}X^T\mathbf{y}$

prediction

$$y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \quad X = \begin{pmatrix} \text{---} & x_i^T & \text{---} \end{pmatrix}$$

Linear regression: a supervised learning problem

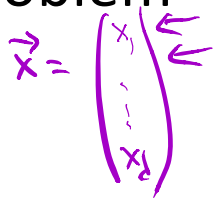
Goal: to predict some output from some inputs/features.

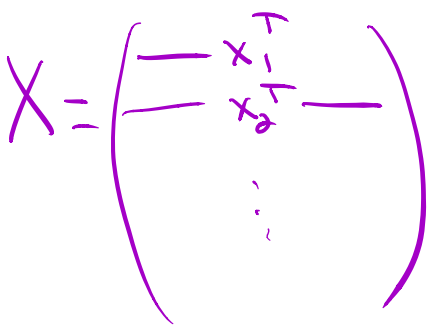
Step 1: Define set up ($y = \mathbf{w}^T \mathbf{x} + \varepsilon$) and get data $\{(\mathbf{x}_i, y_i)\}_{i=1..n}$

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

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

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 $RSS = \sum_{i=1}^{n} (y_i - \sum_{j=1}^{d} \mathbf{x}_i{}^T \mathbf{w}_j)^2 = (\mathbf{y}-X\mathbf{w})^T(\mathbf{y}-X\mathbf{w})$
- 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 $\hat{w} = (X^TX)X^t\mathbf{y}$

Step 3: Use $\hat{w}$ to make predictions, Given **x**, predict output: $\mathbf{w}^T \mathbf{x}$

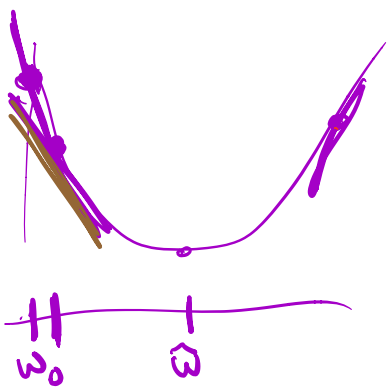
Fitting the linear regression model

Gradient descent

$f(w)$ function convex, cont, nice

Gradient Descent – univariate case

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



$f(w+s) \approx f(w) + s f'(w)$ if s very small

$f'(w) < 0$ s to be positive

> 0 s negative

initialize w_0 $t := 0$

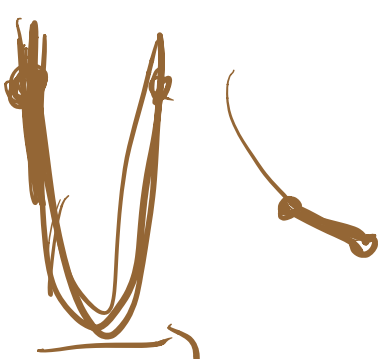
as long as $|f'(w_t)| > \epsilon$

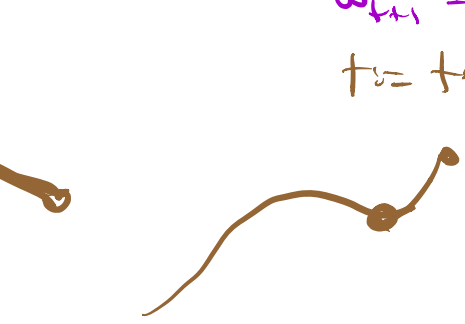
$w_{t+1} = w_t - \eta f'(w_t)$

$t := t+1$

step size

step size





$\frac{\epsilon}{t}$

Gradient Descent – multivariate case

$f(w_1, \ldots, w_d)$

$$f(\vec{w} + \vec{s}) \approx f(w) + \sum_{j=1}^{d} s_j \frac{\partial f}{\partial w_j}(\vec{w}) = f(w) + s^T \nabla f(w)$$

$\|s\| \|\nabla f(w)\| \cos\theta$

angle between $\nabla f(w)$ and $\vec{s}$

to make the fn ↓ as quickly as possible

want to move in direction of negative gradient

initialize $\vec{w}_0$

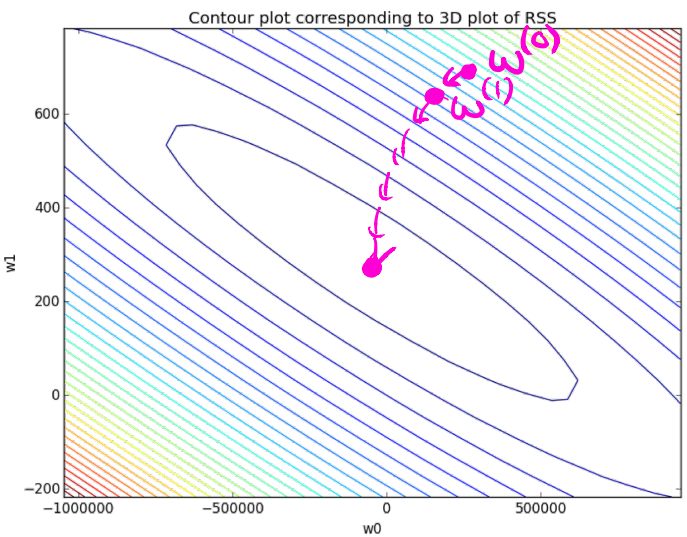
while $\|\nabla f(w_t)\| \geq \varepsilon$

$w_{t+1} = w_t - \eta \nabla f(w_t)$

$\|x\| = \sqrt{\sum x_i^2}$

Gradient descent for linear regression:

repeatedly move in direction of negative gradient

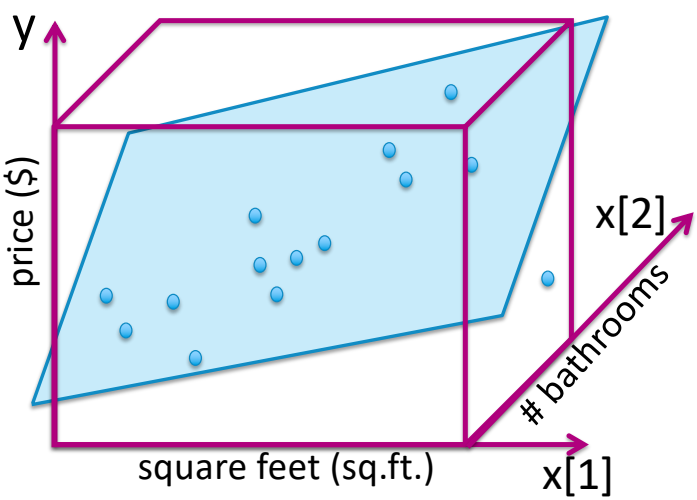


while not converged

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

$$-2X^T(y - Xw^{(t)})$$

Interpreting elementwise



Update to j^{th} feature weight:

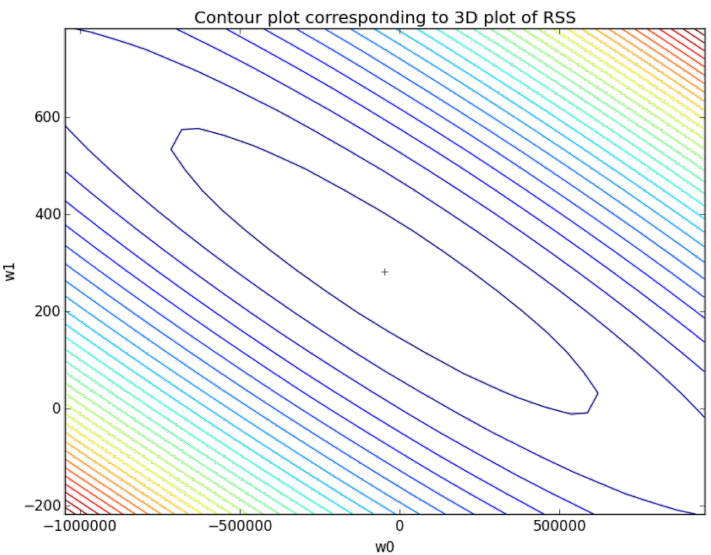
$$w_j^{(t+1)} \leftarrow w_j^{(t)} + 2\eta \sum_{i=1}^{N} x_i[j](y_i - \hat{y}_i(w^{(t)}))$$

predict for x_i using current $w^{(t)}$

$x_i^T w^{(t)}$ =

Summary of gradient descent for multiple regression

$\frac{\partial RSS(w^{(t)})}{\partial w_j}$



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]

  $t \leftarrow t + 1$

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

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

Handling an intercept (constant term)

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

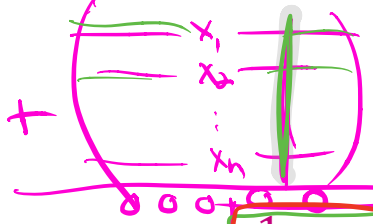
Find $\hat{w}, b$ that minimize $RSS = \sum_{i=1}^{n} (y_i - \sum_{j=1}^{d} w_j x_i[j] - b)^2$

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

Two step approach:

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.



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

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

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

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

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

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

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

$\nabla_w = 0$

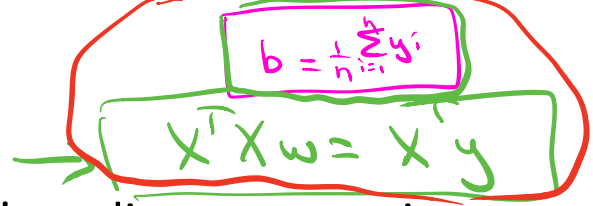
coeff of b is $2\sum_{i=1}^{n} x_i[j]$

$\sum_i x_i[j]y_i - \sum_i x_i[j]x_i^T w - \sum_i x_i[j]b = 0$

$\sum_i y_i - \sum_i x_i^T w - nb = 0 \Rightarrow b = \frac{1}{n}\sum_i y_i$

$(\sum_i x_i^T) w = 0$

$\nabla_w RSS = -2X^T(y - Xw)$



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

$(\vec{x}_i, y_i) \longrightarrow (\vec{x}_i - \vec{\mu}, y_i)_{i=1}^{n}$

$\vec{\mu} = \frac{1}{n}\sum_{i=1}^{n} \vec{x}_i$

$\tilde{X} = \begin{bmatrix} \leftarrow & \vec{x}_1^T - \vec{\mu}^T & \rightarrow \\ \leftarrow & \vec{x}_2^T - \vec{\mu}^T & \rightarrow \end{bmatrix}$

$\sum_{i=1}^{n} \vec{x}_i' = \sum_{i=1}^{n} (\vec{x}_i - \vec{\mu}) = \sum \vec{x}_i - n\vec{\mu} = \vec{0}$

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

$\tilde{X}^T \tilde{X} \hat{w} = \tilde{X}^T y$

$\hat{b} = \frac{1}{n}\sum_{i=1}^{n} y_i$

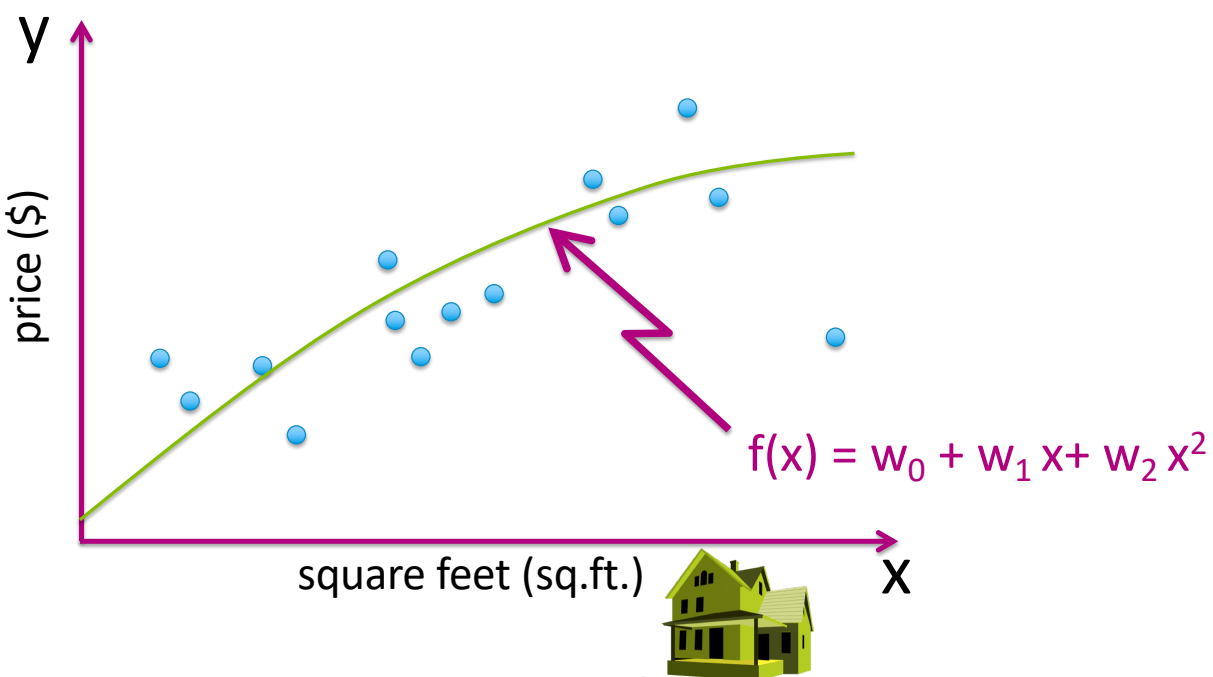
Soln: $\hat{w}, \hat{b}$

$\vec{x}$

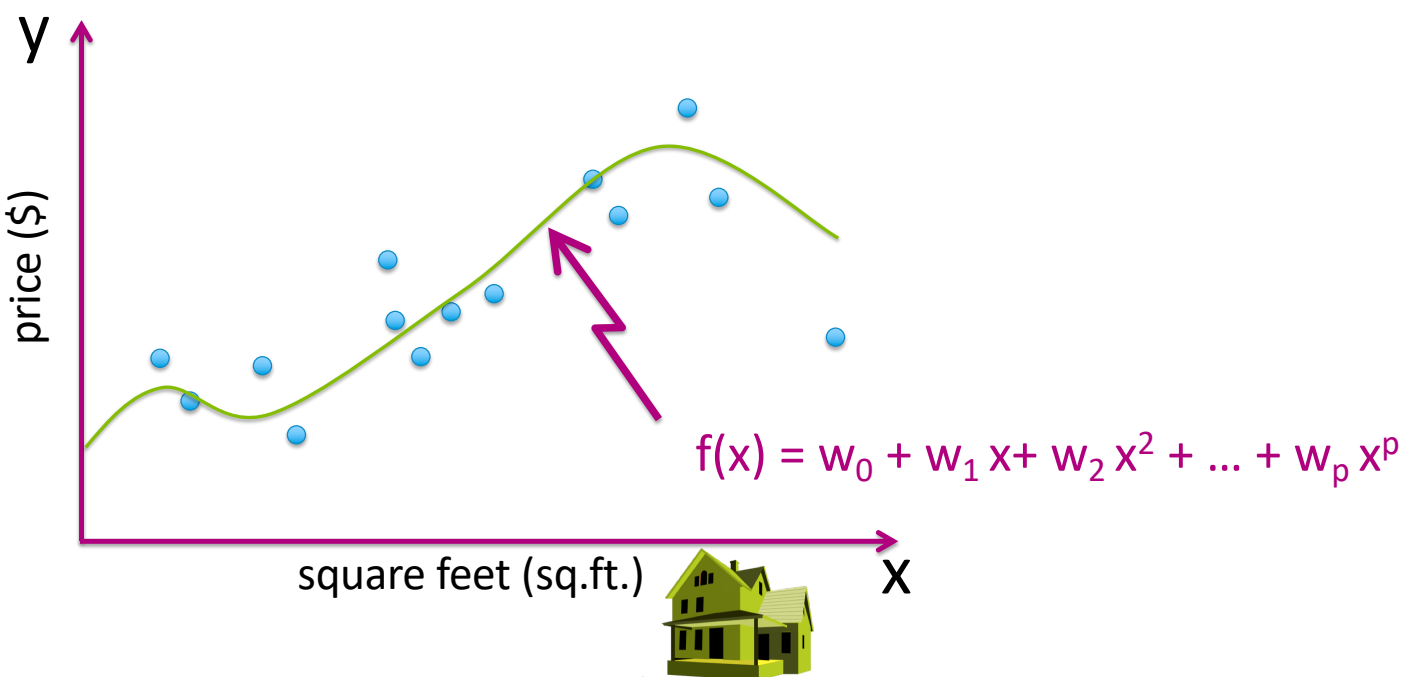
predict $(\vec{x}^T - \vec{\mu}^T)\hat{w} + \hat{b}$

More features, more complex models

What about a quadratic function?



Even higher order polynomial

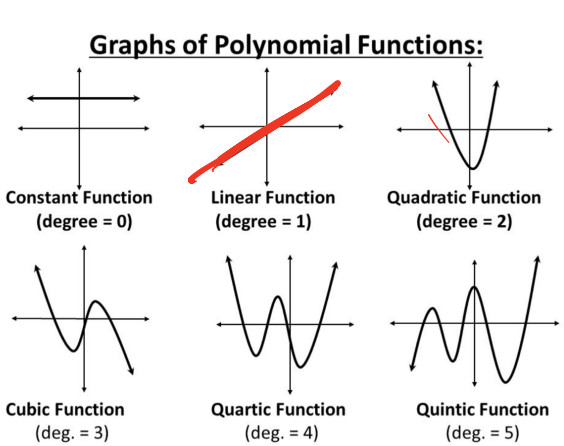


Polynomial regression (single input)

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

Polynomial regression

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

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 $\{(x_i, y_i)\}_{i=1..n}$

- 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 $\mathbf{h(x_i)} = (1, x, x^2 \ldots, x^p)$

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

find w to min

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

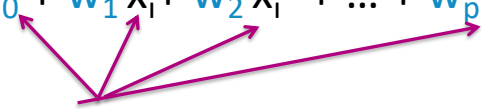
Step 3: Use $\hat{\mathbf{w}} = (\hat{w}_0, \hat{w}_1 \ldots, \hat{w}_p)$ to make predictions. Given x, let $\mathbf{h}(x) = (1, x, x^2 \ldots, x^p)$ and predict output:

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

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!

$$f(x) = f(0) + f'(0)x + \frac{f''(0)}{2!}x^2 + \cdots$$

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

sq footage # baths time of year when the house sold.

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

$\vec{x} = (x_1, x_2, x_3) \rightarrow (h_1(\vec{x}), h_2(\vec{x}), \ldots, h_7(\vec{x}))$

General notation

Output: y ← scalar

Inputs: **x** = (x[1],x[2],…, 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*)

→ **h** (**x**) = $(h_1(\mathbf{x}), h_2(\mathbf{x}), \ldots, h_p(\mathbf{x}))$ feature map applied to input **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 **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 = $\sum_{i=1}^{n} (y_i - \sum_{j=1}^{p} w_j \, h_j(\mathbf{x}_i))^2$

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