Linear Regression

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The instructor gratefully acknowledges Andrew Ng (Stanford), Eric Eaton (UPenn), David Kauchak (Pomona), and the many others who made their course materials freely available online.

Linear Regression Setup

Learning Goals

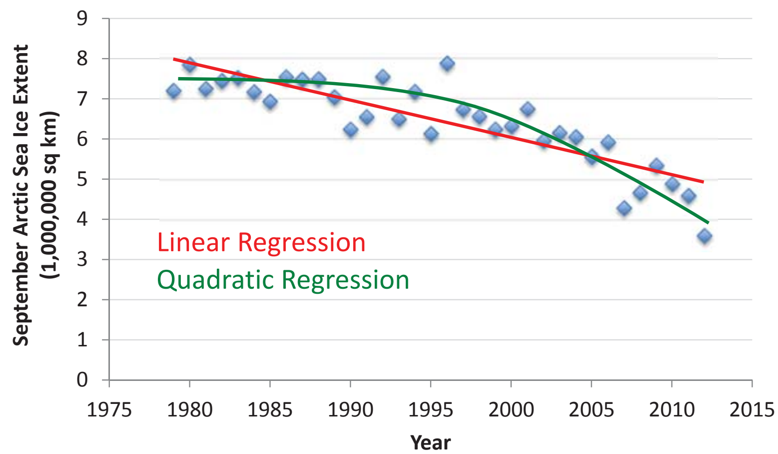
- Describe how regression differs from classification
- Describe the goal of linear regression

Regression

Given:

– Data $\mathbf{X} = \{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n)}\}$ where $\boldsymbol{x}^{(i)} \in \mathbb{R}^d$

– Corresponding labels $\boldsymbol{y} = \{y^{(1)}, \ldots, y^{(n)}\}$ where $y^{(i)} \in \mathbb{R}$



Based on slide by Eric Eaton
[Data from G. Witt. Journal of Statistics Education, Volume 21, Number 1 (2013)]

Linear Regression

Hypothesis

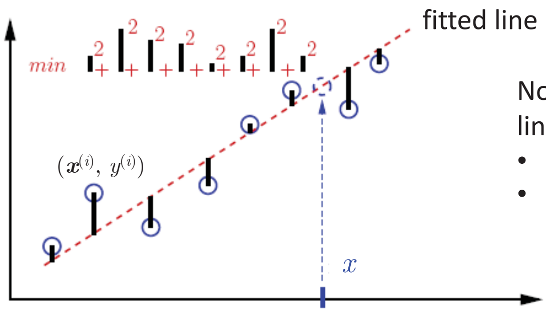
assume $x_0 = 1$

$$y = h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d$$

$$= \sum_{j=0}^{d} \theta_j x_j = \boldsymbol{\theta}^T \boldsymbol{x}$$

θ_j's are parameters (weights)

Fit model (find $\boldsymbol{\theta}$) by minimizing sum of squared errors



fitted line used as predictor

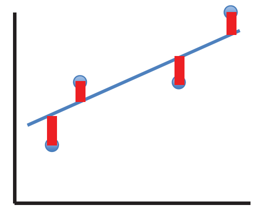
Note:
linear regression is a **parametric** method
- makes inferences about model
- fixed number of parameters (d+1)

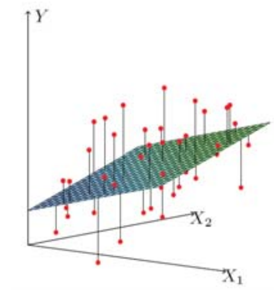
Based on slide by Eric Eaton [Figures courtesy of Greg Shakhnarovich]

Cost Function

$$J(\boldsymbol{\theta}) = \frac{1}{2}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) - y^{(i)}\right)^2$$

Fit by solving $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$





More generally…

$$R_n(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\mathrm{Loss}\left(y^{(i)}, h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})\right)$$

empirical risk / training error

$$z = y^{(i)} - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})$$

Q1: Why use squared error?
Q2: How do we optimize $\boldsymbol{\theta}$?

$$\mathrm{Loss}(z) = \frac{z^2}{2}$$

squared error

different people use $1/(2n)$ vs $1/2$

Based on slide by Eric Eaton

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Probabilistic Interpretation

Learning Goals

- Describe why we minimize squared error

Probabilistic Interpretation

Assume $y^{(i)} = \boldsymbol{\theta}^T \boldsymbol{x}^{(i)} + \epsilon^{(i)}$

What is $\epsilon^{(i)}$?

- error term
- captures un-modeled effects (e.g. missing features)
- captures random noise

How can we model $\epsilon^{(i)}$?

Probabilistic Interpretation

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Maximum Likelihood Estimate (MLE)

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Solving Linear Regression

Learning Goals

- Describe shape of $J(\boldsymbol{\theta})$
- Describe two approaches for optimizing $\boldsymbol{\theta}$
  - Gradient Descent (stochastic and batch version)
  - Normal Equations
- Compare tradeoffs of GD vs Normal Equations

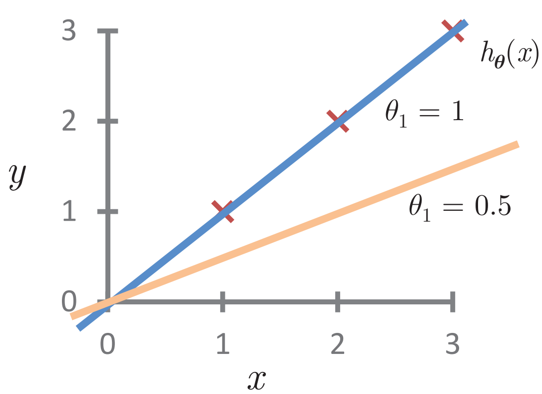
Intuition behind Cost Function

$$J(\boldsymbol{\theta}) = \frac{1}{2}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) - y^{(i)}\right)^2$$

For insight on $J(\boldsymbol{\theta})$, assume $x^{(i)} \in \mathbb{R}$ so $\boldsymbol{\theta} = [\theta_0, \theta_1]^T$. Also fix $\theta_0 = 0$.

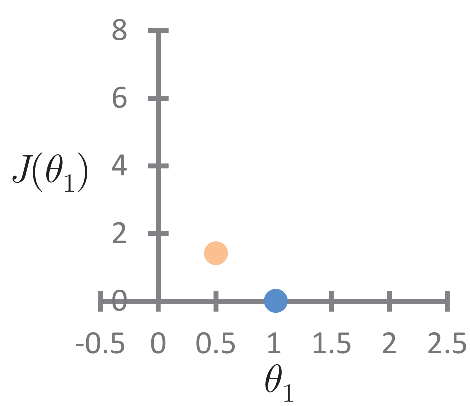
$h_{\boldsymbol{\theta}}(x)$

(for fixed θ_1, this is a function of x)



$J(\theta_1)$

(function of the parameter θ_1)

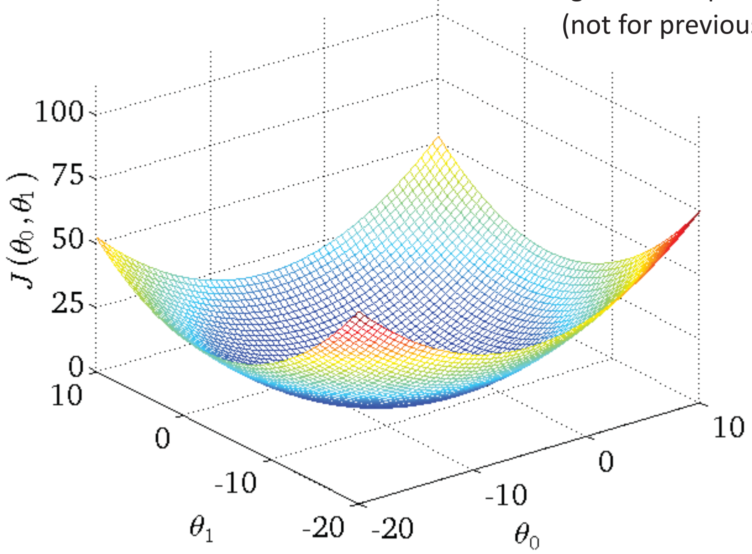


Based on slide by Eric Eaton
[Example by Andrew Ng]

$$J(0.5) = \tfrac{1}{2}\left[(0.5-1)^2 + (1-2)^2 + (1.5-3)^2\right] = 1.75$$

Intuition behind Cost Function

general shape of $J(\theta_0,\theta_1)$
(not for previous example)



Based on slide by Andrew Ng

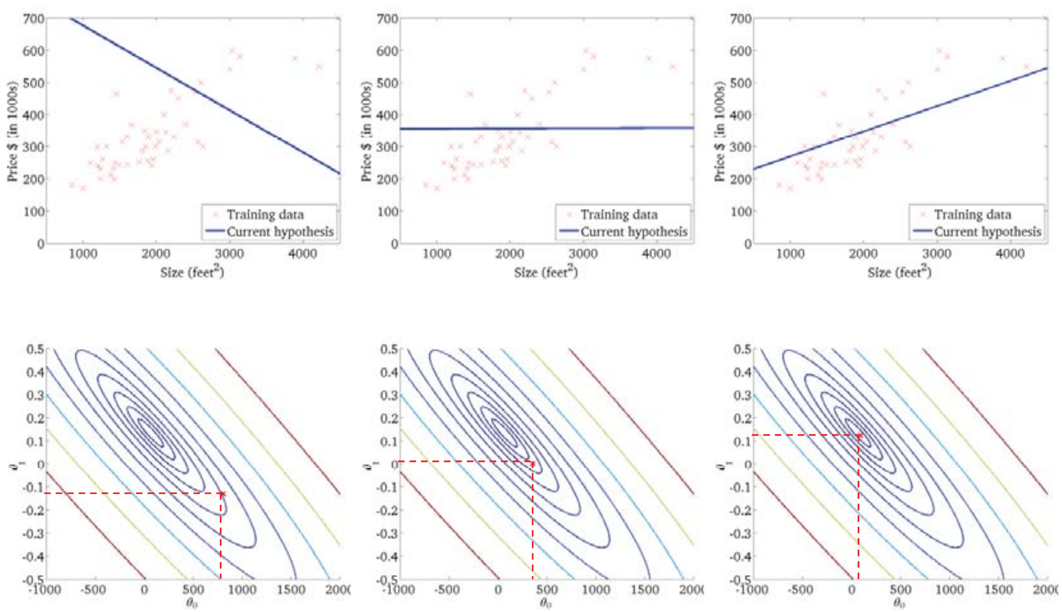
Intuition behind Cost Function

$h_{\boldsymbol{\theta}}(\boldsymbol{x})$

(for fixed (θ_0,θ_1), this is a fcn of x)

$J(\theta_0,\theta_1)$

(fcn of the parameters (θ_0,θ_1))



contour map

Based on slide by Andrew Ng

Solving Linear Regression

Learning Goals

- ✓ Describe shape of $J(\boldsymbol{\theta})$
- Describe two approaches for optimizing $\boldsymbol{\theta}$
  - Gradient Descent (stochastic and batch version)
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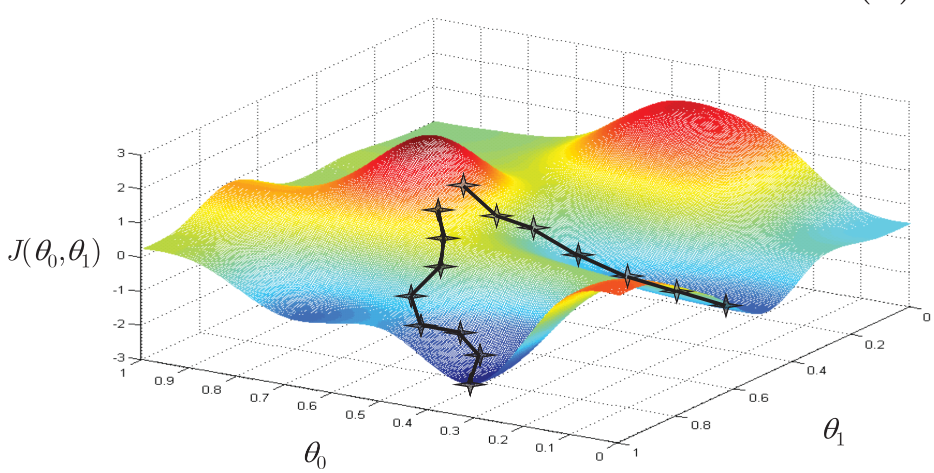
- Compare tradeoffs of GD vs Normal Equations

Basic Search Procedure

Idea

- Choose initial value for $\boldsymbol{\theta}$
- Until we reach minimum
  - Choose new value for $\boldsymbol{\theta}$ to reduce $J(\boldsymbol{\theta})$



since the least squares objective function is convex, we do not need to worry about local minima

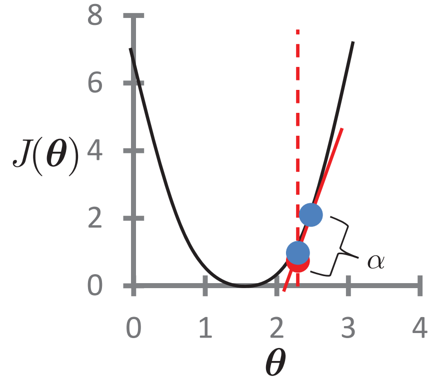
Based on slide by Andrew Ng

Approach 1: Gradient Descent

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

learning rate
(small, e.g., $\alpha = 0.05$)

update simultaneously for all $j = 0, \ldots, d$



For one training example $(\boldsymbol{x}, y)$

Based on slide by Eric Eaton

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Batch versus Stochastic Mode

Batch Gradient Descent (BGD)

repeat until convergence {

$$\theta_j \leftarrow \theta_j - \alpha \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) - y^{(i)} \right) x_j^{(i)}$$

}

converged when $||\boldsymbol{\theta}_{\text{new}} - \boldsymbol{\theta}_{\text{old}}||_2 < \epsilon$

for every *j* **simultaneously**

To achieve simultaneous update:

- At start of each GD iteration, compute $h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})$
- Use this stored value in update step

Stochastic Gradient Descent (SGD)

repeat until convergence {

for $i = 1$ to n {

$$\theta_j \leftarrow \theta_j - \alpha \left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) - y^{(i)} \right) x_j^{(i)}$$

}

}

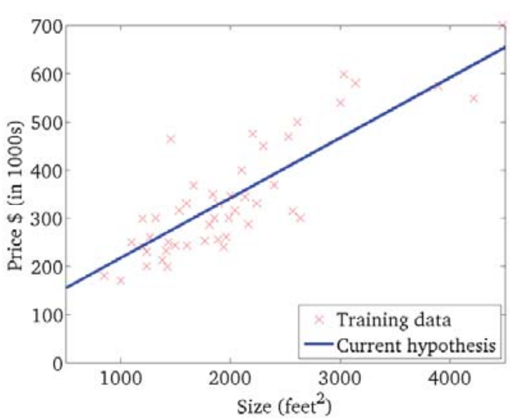
often will randomly shuffle points

for every *j* **simultaneously**

Gradient Descent Example

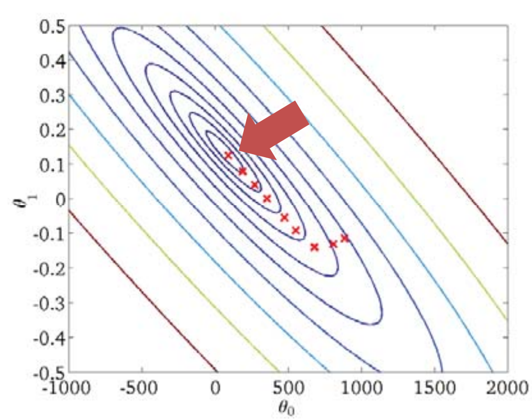
$h_{\boldsymbol{\theta}}(x)$

(for fixed (θ_0,θ_1), this is a function of x)



$J(\theta_0,\theta_1)$

(function of the parameter (θ_0,θ_1))



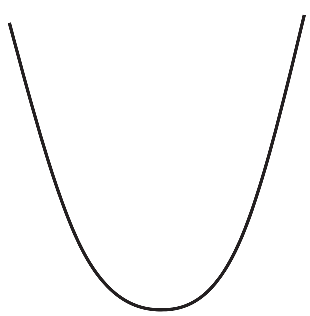
Based on slide by Andrew Ng

Batch versus Stochastic GD

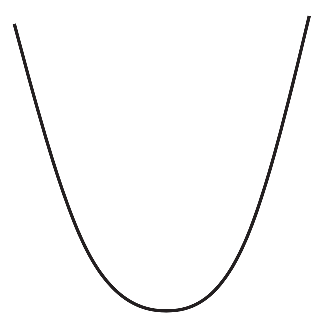
- Batch has to scan through entire training set before taking single step (costly if n is large)
- Stochastic makes progress "right away"
  - often $\boldsymbol{\theta}$ gets "close" to minimum much faster
    - but $\boldsymbol{\theta}$ may never converge if it oscillates around $\arg\min J(\boldsymbol{\theta})$
  - in practice, most values near minimum will be good enough approximation to true minimum
    - alternatively, we can guarantee convergence if we allow step size α to decrease, e.g. $\alpha_k = \frac{1}{1+k}$, where k = outer loop iteration

Choosing step size α

α too small



α too large



To check if GD is working, print out $J(\boldsymbol{\theta})$ each iteration
- value should decrease each iteration
- if it does not, adjust α

Based on slide by Eric Eaton
[Originally by Andrew Ng]

Solving Linear Regression

Learning Goals

✓ Describe shape of $J(\boldsymbol{\theta})$

- Describe two approaches for optimizing $\boldsymbol{\theta}$
  - ✓ Gradient Descent (stochastic and batch version)
  - – Normal Equations
- Compare tradeoffs of GD vs Normal Equations

Approach 2: Normal Equations

(closed form solution)

Vectorization

- more compact equations
- faster code (using optimized matrix libraries)

Let us consider our model

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j x_j$$

Let $\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}$ and $\boldsymbol{x} = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}$. Then $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \boldsymbol{\theta}^T \boldsymbol{x}$.

Matrix-Vector Form

For n instances:

$$h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) = \sum_{j=0}^{d} \theta_j x_j^{(i)}$$

Let

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \qquad \boldsymbol{X} = \begin{bmatrix} - & \left(\boldsymbol{x}^{(1)}\right)^T & - \\ & \vdots & \\ - & \left(\boldsymbol{x}^{(i)}\right)^T & - \\ & \vdots & \\ - & \left(\boldsymbol{x}^{(n)}\right)^T & - \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(i)} & \dots & x_d^{(i)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(n)} & \dots & x_d^{(n)} \end{bmatrix}$$

Then

$$\underset{\mathbb{R}^{n\times 1}}{h_{\boldsymbol{\theta}}(\boldsymbol{X})} = \underset{\mathbb{R}^{n\times(d+1)}}{\boldsymbol{X}}\,\underset{\mathbb{R}^{(d+1)\times 1}}{\boldsymbol{\theta}}$$

predictions for all instances

Matrix-Vector Form of Cost Function

Let

$$\boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

Solve for θ analytically

$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$ attained when $\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = 0$

Expanding $\mathrm{J}(\boldsymbol{\theta})$:

Solve for θ analytically

Take gradient, set equal to 0, then solve for θ:

Closed-Form Solution

Can obtain $\boldsymbol{\theta}$ by plugging in $\boldsymbol{X}$ and $\boldsymbol{y}$ into

$$\boldsymbol{\theta}^* = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

$$\boldsymbol{X} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(i)} & \dots & x_d^{(i)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(n)} & \dots & x_d^{(n)} \end{bmatrix} \quad \boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

- Cost of inverting $\boldsymbol{A} = \boldsymbol{X}^T\boldsymbol{X} \sim O(d^3)$
  – expensive for large d
- If $\boldsymbol{A}$ is not invertible (i.e. $\boldsymbol{A}$ is singular), may need to
  – use pseudo-inverse (`np.linalg.pinv`)
    - Cholesky decomposition better
  – remove redundant (not linearly independent) features
  – remove extra features to ensure $d \leq n$

Based on slide by Eric Eaton

Solving Linear Regression

Learning Goals

✓ Describe shape of $J(\boldsymbol{\theta})$

✓ Describe two approaches for optimizing $\boldsymbol{\theta}$

  ✓ Gradient Descent (stochastic and batch version)

  ✓ Normal Equations

- Compare tradeoffs of GD vs Normal Equations

Gradient Descent vs Normal Equation

Gradient Descent

- requires multiple iterations
- need to choose α
- works well when d is large
- can support online learning

Normal Equations

- non-iterative
- no need for α
- slow if *d* is large
  - matrix inversion is $O(d^3)$

Based on slide by Eric Eaton

What Should You Be Able To Do?

- Name cost function for linear regression and provide rationale
- Given model, find Maximum Likelihood Estimator (MLE)
- Optimize functions by taking derivative / gradient
- State tradeoffs of gradient descent vs normal equations
- Homework
  - Extend linear regression to weighted linear regression
  - Implement (regularized polynomial) regression using SGD and normal equations

(Extra Slides)

Linear Regression Extensions

Learning Goals

- Describe how to extend linear regression to more complex models using basis functions
- Describe why we might scale features

Basis Functions

So far,

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j x_j$$

transform features by ϕ

Generally,

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d'} \theta_j \underbrace{\phi_j(\boldsymbol{x})}_{\text{basis function}}$$

new dimension

Typically, $\phi_0(\boldsymbol{x}) = 1$ so that θ_0 acts as bias.

In the simplest case, we use linear basis functions:

$$\phi_j(\boldsymbol{x}) = x_j$$

More complex basis functions allow use of linear regression techniques to **fit non-linear datasets**.

Based on slide by Eric Eaton
(originally by Chrisopher Bishop [PRML])

Extending Linear Regression to More Complex Models

The inputs $\boldsymbol{X}$ for linear regression can be …

- original quantitative inputs
- transformation of quantitative inputs
  - e.g. $\log$, $\exp$, square root, square, etc
- polynomial transformation
  - e.g. $y = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$
- dummy coding of categorical inputs
- interactions between variables
  - e.g. $x_3 = x_1 x_2$

Based on slide by Eric Eaton

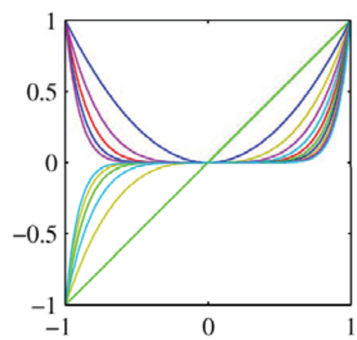
Polynomial Regression

Let $x \in \mathbb{R}$.

Polynomial basis functions:

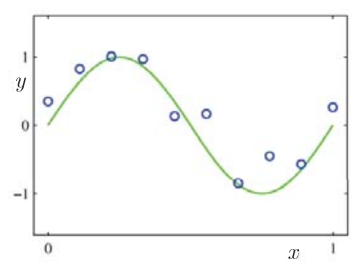
$$\phi_j(x) = x^j$$

These are "global" (a small change in x affects all basis functions).



Fit a polynomial curve with a linear model

$$h_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \ldots + \theta_p x^p = \sum_{j=0}^{p} \theta_j x^p$$



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(originally by Chrisopher Bishop [PRML])

Summary

Basic Linear Model

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j x_j$$

Generalized Linear Model

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d'} \theta_j \phi_j(\boldsymbol{x})$$

Once we have replaced the data by the outputs of the basis functions, fitting the generalized linear model is same problem as fitting the basic model, e.g.

$$\boldsymbol{\Phi} = \begin{bmatrix} - & \left(\boldsymbol{\phi}(\boldsymbol{x}^{(1)})\right)^T & - \\ & \vdots & \\ - & \left(\boldsymbol{\phi}(\boldsymbol{x}^{(i)})\right)^T & - \\ & \vdots & \\ - & \left(\boldsymbol{\phi}(\boldsymbol{x}^{(n)})\right)^T & - \end{bmatrix}$$

$$\boldsymbol{\theta}^* = \left(\boldsymbol{\Phi}^T \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^T \boldsymbol{y}$$

Based on slide by Eric Eaton
(originally by Geoff Hinton)

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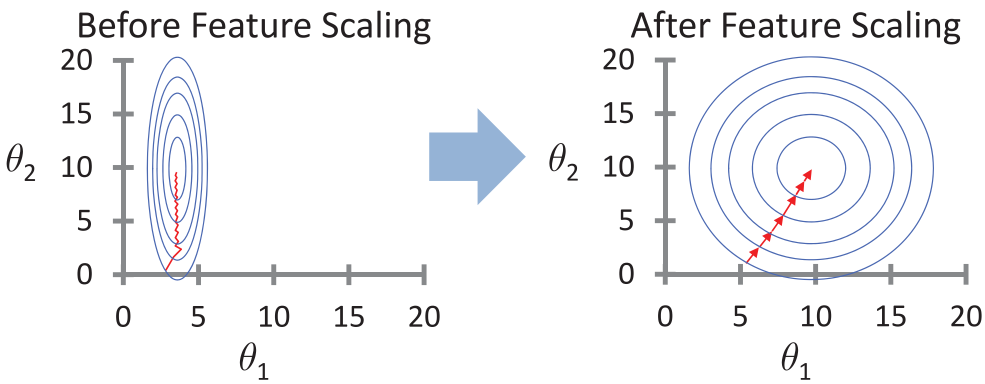
Feature Scaling

Ensure features have similar scales



Why?

- Make GD converge much faster
- Avoid numerical issues in matrix-vector products

Based on slide by Eric Eaton

Feature Standardization

Rescale features to have zero-mean, unit-variance

Let
$$\mu_j = \frac{1}{n}\sum_{i=1}^{n} x_j^{(i)} \qquad \sigma_j = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(x_j^{(i)} - \mu_j\right)^2}$$

Replace each value with
$$x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{\sigma_j}$$
for $j = 1, \ldots, d$
do not rescale x_0

Remember to apply same transformation to both training and prediction

- learn parameters (μ, σ) using only training set
- see `sklearn.preprocessing`
- outliers can cause problems

Based on slide by Eric Eaton