Linear Regression

Training set o	f housing	prices
(Portland, OR)		

Size in feet ² (x)	Price (\$) in 1000's (y)
2104	460
1416	232
1534	315
852	178

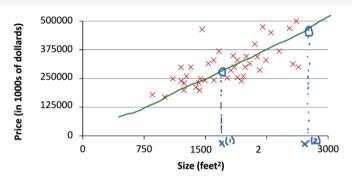
Notation:

m = Number of training examples

x's = "input" variable / features

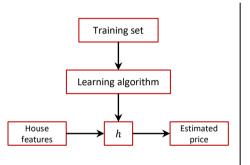
y's = "output" variable / "target" variable

Housing Prices (Portland, OR)



Supervised Learning: Given the "right answer" for each example in the data.

Regression problem: Predict real-valued output



How do we represent h?

- We represent hypothesis about the data using parameters $\theta = (\theta_0, \theta_1)$.
- If the data is correctly predicted according to the hypothesis h_{θ} , then $y \approx h_{\theta}(x) = \theta_0 + \theta_1 x$
- The learning algorithm finds the best hypothesis h_{θ} for the training set.
- We can then estimate the values of y for the test set using that h_{θ}
- If h_{\theta}(x) is a linear function of a real number x of , this procedure is called linear regression.

Training Set

Size in feet ² (x)	Price (\$) in 1000's (y)
2104	460
1416	232
1534	315
852	178

Hypothesis:
$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

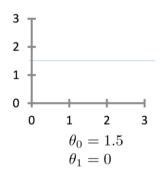
where θ_0 , θ_1 are learnable parameters.

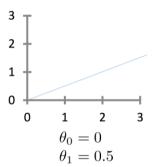
Question: how to choose

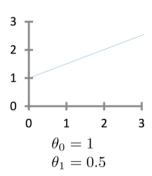
5

Observation

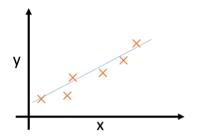
$$h_{\theta}(x) = \theta_0 + \theta_1 x$$







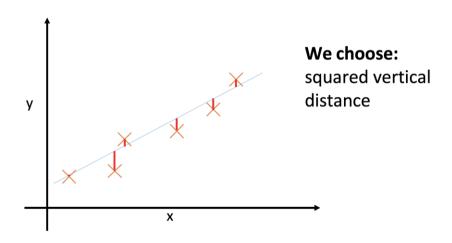
Observation



Idea: Choose θ_0, θ_1 so that $h_{\theta}(x)$ is close to y for our training examples (x, y)

But what does "close" mean?

Observation

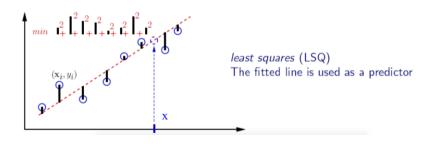


Linear Regression

Hypothesis:

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d = \sum_{j=0} \theta_j x_j$$
 Assume $\mathbf{x_0}$ = 1

Fit model by minimizing sum of squared errors



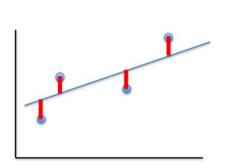
9

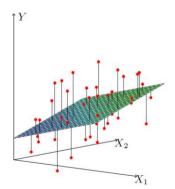
Least Squares Linear Regression

Cost Function

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

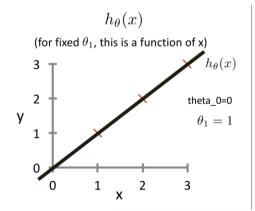
• Fit by solving $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

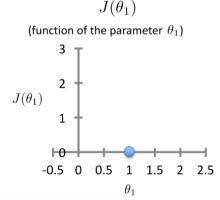




$$J(\boldsymbol{\theta}) = \frac{1}{2n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^{2}$$

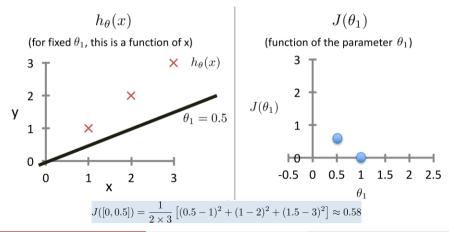
For insight on J(), let's assume $\,x\in\mathbb{R}\,$ so $\,m{ heta}=[heta_0, heta_1]\,$





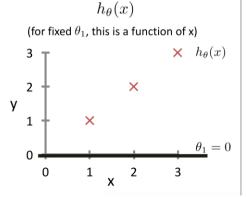
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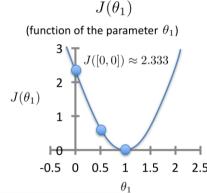
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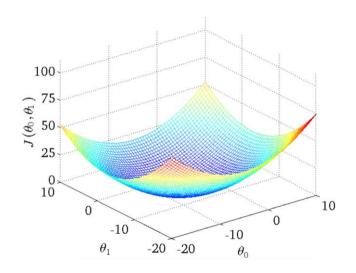


$$J(\boldsymbol{\theta}) = \frac{1}{2n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^{2}$$

For insight on J(), let's assume $\,x\in\mathbb{R}\,$ so $\,oldsymbol{ heta}=[heta_0, heta_1]\,$







Formulation

Hypothesis:
$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

Parameters: θ_0, θ_1

Cost Function:
$$J(\theta_0, \theta_1) = \frac{1}{2n} \sum_{i=1}^{n} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

Goal:
$$\min_{\theta_0, \theta_1} \text{minimize } J(\theta_0, \theta_1)$$

Formulation

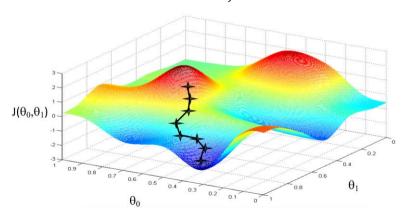
Have some function
$$J(\theta_0,\theta_1)$$
 Want $\min_{\theta_0,\theta_1}J(\theta_0,\theta_1)$

Outline:

- Start with some θ_0, θ_1
- Keep changing $\, heta_0, heta_1\,$ to reduce until we hopefully end up at a minimum $\,J(heta_0, heta_1)\,$

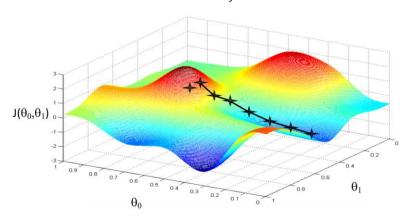
- Choose initial value for θ .
- Until we reach the minimum, update θ to reduce $J(\theta)$:

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



- Choose initial value for θ .
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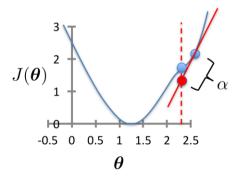


- Initialize θ
- · Repeat until convergence

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

simultaneous update for $j = \emptyset \frac{1}{n}$. d

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

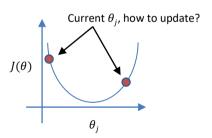


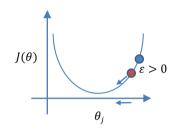
- Initialize θ
- · Repeat until convergence

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

simultaneous update for j = 0.1. d

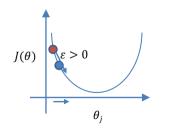
Why minus?





$$\frac{\partial J(\theta)}{\partial \theta_{j}} = \lim_{\varepsilon \to 0} \frac{J(\theta|\theta_{j} + \varepsilon) - J(\theta|\theta_{j})}{\varepsilon} > 0$$

 $ightarrow heta_j$ moves to the **negative direction** ightarrow **counter-direction** w.r.t. the partial derivative.



$$\frac{\partial J(\theta)}{\partial \theta_j} = \lim_{\varepsilon \to 0} \frac{J(\theta | \theta_j + \varepsilon) - J(\theta | \theta_j)}{\varepsilon} < 0$$

 $\rightarrow \theta_j$ moves to the **positive direction** \rightarrow **counter-direction** w.r.t. the partial derivative.

- Initialize θ
- · Repeat until convergence

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

simultaneous update for $j = \emptyset$ 1. d

For Linear Regression:
$$\begin{split} \frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^n \left(h_{\theta} \left(x^{(i)} \right) - y^{(i)} \right)^2 \\ &= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^n \left(\sum_{k=0}^d \theta_k x_k^{(i)} - y^{(i)} \right)^2 \\ &= \frac{1}{n} \sum_{i=1}^n \left(\sum_{k=0}^d \theta_k x_k^{(i)} - y^{(i)} \right) \times \frac{\partial}{\partial \theta_j} \left(\sum_{k=0}^d \theta_k x_k^{(i)} - y^{(i)} \right) \\ &= \frac{1}{n} \sum_{i=1}^n \left(\sum_{k=0}^d \theta_k x_k^{(i)} - y^{(i)} \right) x_j^{(i)} \end{split}$$

What happens with $\frac{\partial}{\partial \theta_0} J(\theta)$???

$$j = 0 : \frac{\partial}{\partial \theta_0} J(\theta) = \frac{1}{n} \sum_{i=1}^n \left(\sum_{k=0}^d \theta_k x_k^{(i)} - y^{(i)} \right)$$

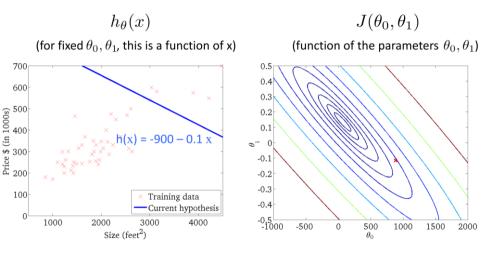
$$j = 1 : \frac{\partial}{\partial \theta_1} J(\theta) = \frac{1}{n} \sum_{i=1}^n \left(\sum_{k=0}^d \theta_k x_k^{(i)} - y^{(i)} \right) x_j^{(i)}$$

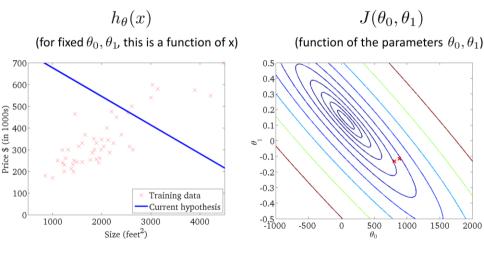
- Initialize θ
- · Repeat until convergence

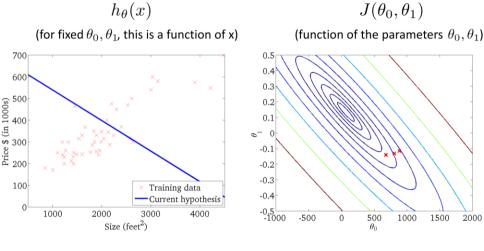
$$\theta_j \leftarrow \theta_j - \alpha \frac{1}{n} \sum_{i=1}^n \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right) x_j^{(i)} \quad \text{simultaneous update for j = 0.1. d}$$

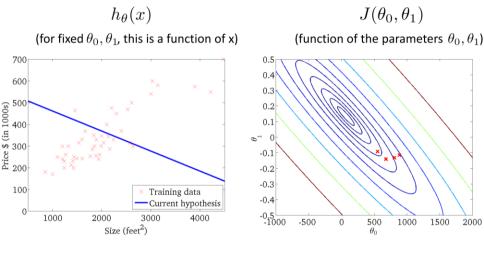
- To achieve simultaneous update
 - At the start of each GD iteration, compute $h_{oldsymbol{ heta}}\left(oldsymbol{x}^{(i)}
 ight)$
 - Use this stored value in the update step loop
- Assume convergence when $\|oldsymbol{ heta}_{new} oldsymbol{ heta}_{old}\|_2 < \epsilon$

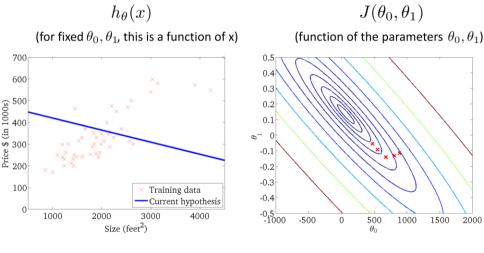
$$\mathsf{L_2} \ \mathsf{norm} \colon \qquad \| m{v} \|_2 = \sqrt{\sum_i v_i^2} = \sqrt{v_1^2 + v_2^2 + \ldots + v_{|v|}^2}$$

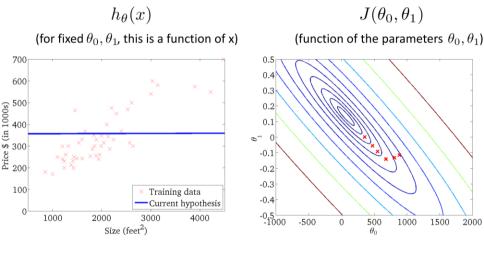


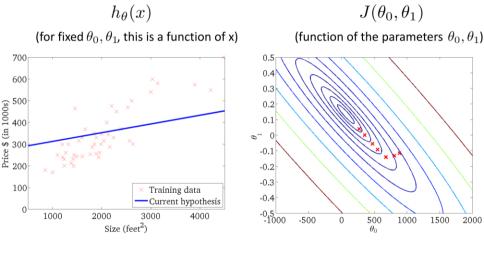


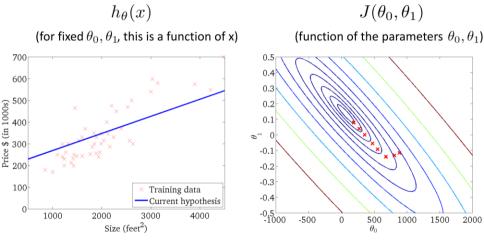


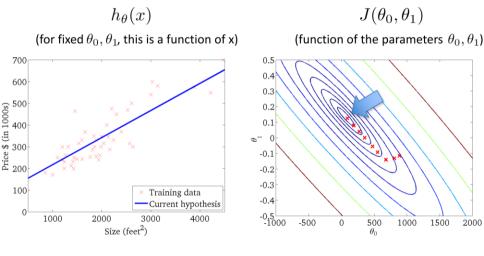












Gradient Descent Variants

There are three variants of gradient descent.

- Batch gradient descent
- · Stochastic gradient descent
- · Mini-batch gradient descent

The difference of these algorithms is the **amount of data**.

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

This term is different with each method

Batch gradient descent

This method computes the gradient of the cost function with the **entire training dataset**.

We need to calculate the gradients for the whole dataset to perform **just one update**.

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

```
for i in range(nb_epochs):
    params_grad = evaluate_gradient(loss_function, data, params)
    params = params - learning_rate * params_grad
```

Batch gradient descent

Advantage

 It is guaranteed to converge to the global minimum for convex error surfaces and to a local minimum for nonconvex surfaces.

Disadvantages

- It can be very slow.
- It is intractable for datasets that do not fit in memory.
- It does not allow us to update our model online.

Stochastic gradient descent

- This method performs a parameter update for **each training** example $x^{(i)}$ and label $y^{(i)}$.
- We need to calculate the gradient for each training example to perform one update.
- · Note: we shuffle the training data at every epoch

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta, x^{(i)}, y^{(i)})$$

```
for i in range(nb_epochs):
    np.random.shuffle(data)
    for example in data:
        params_grad = evaluate_gradient(loss_function, example, params)
        params = params - learning_rate * params_grad
```

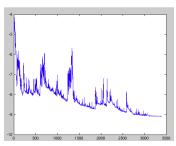
Stochastic gradient descent

Advantage

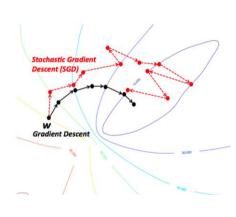
- It is usually much faster than batch gradient descent.
- It can be used to learn online.

Disadvantage

 It performs frequent updates with a high variance that cause the objective function to fluctuate heavily.



The fluctuation: Batch vs SGD



Batch gradient descent converges to the minimum of the basin the parameters are placed in and the fluctuation is small.

SGD's fluctuation is large but it enables to jump to new and potentially better local minima.

However, this ultimately complicates convergence to the exact minimum, as SGD will keep overshooting.

Learning rate of SGD

When we **slowly decrease the learning rate**, SGD shows the same convergence behavior as batch gradient descent

It **almost certainly converging** to a local or the global minimum for non-convex and convex optimization respectively.

Mini-batch gradient descent

This method takes the best of both **batch** and **SGD**, and performs an update for every **mini-batch** of **k** training examples.

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta, x^{(i:i+k)}, y^{(i:i+k)})$$

```
for i in range(nb_epochs):
    np.random.shuffle(data)
    for batch in get_batches(data, batch_size = 50):
        params_grad = evaluate_gradient(loss_function, batch, params)
        params = params - learning_rate * params_grad
```

Mini-batch gradient descent

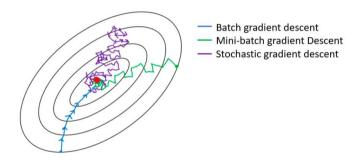
Advantage

- It reduces the variance of the parameter updates.
 - o This can lead to more stable convergence.
- It can make use of highly optimized matrix optimizations common to deep learning libraries that make computing the gradient very efficiently.

Disadvantage

- We have to set mini-batch size.
 - Common mini-batch sizes range between 50 and 256, but can vary for different applications.

Gradient Descent Variants



Gradient descent variants' trajectory towards minimum

Trade-off

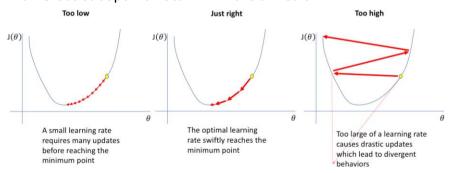
Depending on the amount of data, they make a trade-off:

- The accuracy of the parameter update
- The time it takes to perform an update.
- The memory it takes to perform an update.
- Capability of online learning.

Method	Accuracy	Time	Memory Usage	Online Learning
Batch gradient descent	0	Slow	High	×
Stochastic gradient descent	Δ	High	Low	0
Mini-batch gradient descent	0	Medium	Medium	0

Choosing Learning Rate

- Choosing a proper learning rate is difficult.
- The settings of learning rate schedule is difficult.
- Changing learning rate for each parameter is difficult.
- Avoiding getting trapped in highly non-convex error functions' numerous suboptimal local minima is difficult.

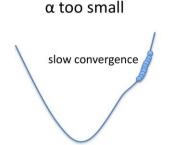


Learning Rate with Exponential Decay

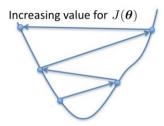
 When training a model, it is often recommended to lower the learning rate as the training progresses. This function applies an exponential decay function to a provided initial learning rate

```
decayed_learning_rate = learning_rate *
                               decay_rate ^ (global_step / decay_steps)
global_step = tf.Variable(0, trainable=False)
starter learning rate = 0.1
learning rate = tf.train.exponential decay(starter learning rate, global step.
                                              100000. 0.96. staircase=True)
  Passing global_step to minimize() will increment it at each step.
learning_step = (
    tf.train.GradientDescentOptimizer(learning_rate)
    .minimize(...my loss..., global_step=global_step)
                                                Learning rate
  .train.exponential_decav(
                                                         - learning rate
    learning_rate,
                                    0.08
    global_step,
                                    0.06
    decay_steps.
                                    0.04
    decay_rate,
    staircase=False.
                                    0.03
    name=None
                                    0.00
```

Choosing a



α too large



- May overshoot the minimum
- May fail to converge
- May even diverge

To see if gradient descent is working, print out $J(\theta)$ each iteration

- · The value should decrease at each iteration
- If it doesn't, adjust α

Extending Linear Regression to More Complex Models

- The inputs **X** for linear regression can be:
 - Original quantitative inputs
 - Transformation of quantitative inputs
 - e.g. log, exp, square root, square, etc.
 - Polynomial transformation a.k.a. Polynomial (linear) regression!
 - example: $y = \beta_0 + \beta_1 \cdot x + \beta_2 \cdot x^2 + \beta_3 \cdot x^3$
 - Basis expansions
 - Dummy coding of categorical inputs
 - Interactions between variables
 - example: $x_3 = x_1 \cdot x_2$

This allows use of linear regression techniques to fit non-linear datasets.

Linear Basis Function Models

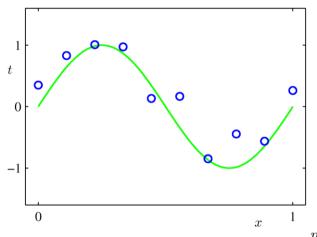
Generally,

$$h_{m{ heta}}(m{x}) = \sum_{j=0}^d heta_j \phi_j(m{x})$$
 basis function

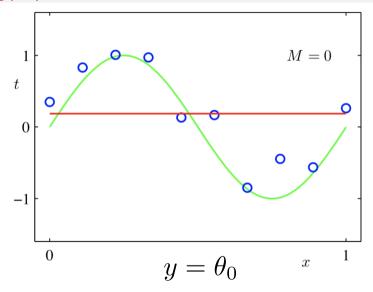
- Typically, $\phi_0(oldsymbol{x})=1$ so that $heta_0$ acts as a bias
- In the simplest case, we use linear basis functions:

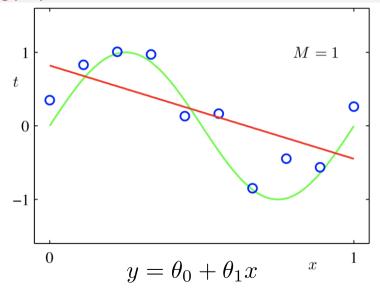
$$\phi_j(\boldsymbol{x}) = x_j$$

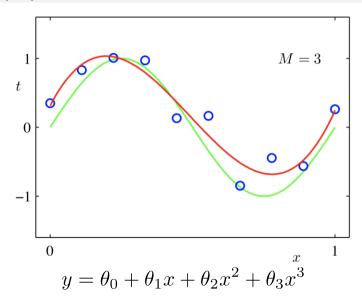
Example of Fitting a Polynomial Curve with a Linear Model

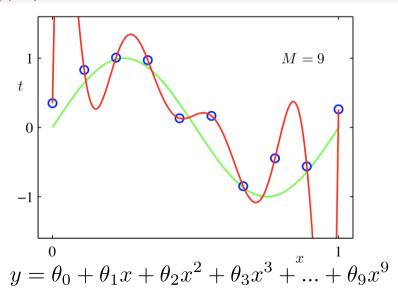


$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \ldots + \theta_p x^p = \sum_{j=0}^{p} \theta_j x^j$$



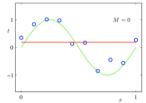




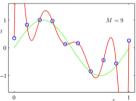


Generalization

Underfitting: The model is too simple - does not fit the data.

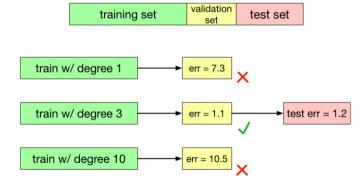


Overfitting: The model is too complex - fits perfectly, does not generalize.



Generalization

- We would like our models to generalize to data they haven't seen before
- The degree of the polynomial is an example of a hyperparameter, something we can't include in the training procedure itself
- We can tune hyperparameters using a validation set:



Foreshadowing

Feature maps aren't a silver bullet:

- It's not always easy to pick good features.
- In high dimensions, polynomial expansions can get very large!

Until the last few years, a large fraction of the effort of building a good machine learning system was feature engineering

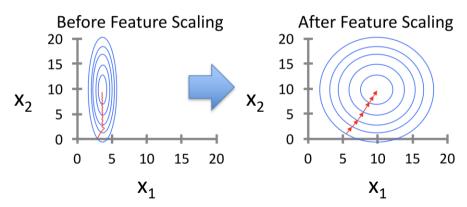
We'll see that neural networks are able to learn nonlinear functions directly, avoiding hand-engineering of features

Linear Basis Function Models

• Basic Linear Model: $h_{m{ heta}}(m{x}) = \sum_{j=0}^u heta_j x_j$

- Generalized Linear Model: $h_{m{ heta}}(m{x}) = \sum_{j=0}^{\infty} heta_j \phi_j(m{x})$
- Once we have replaced the data by the outputs of the basis functions, fitting the generalized model is exactly the same problem as fitting the basic model

Idea: Ensure that feature have similar scales



Makes gradient descent converge much faster

Standardization

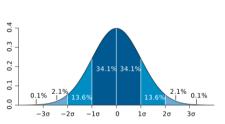
- · Rescales features to have zero mean and unit variance
 - Let μ_j be the mean of feature j: $\mu_j = \frac{1}{n} \sum_{i=1}^n x_j^{(i)}$
 - Replace each value with:

$$x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{s_j} \qquad \qquad \begin{cases} \text{for } j = 1 \dots d \\ (\text{not } x_0!) \end{cases}$$

- s_i is the standard deviation of feature j
- Could also use the range of feature $j \hspace{0.1cm} \text{(max}_i \text{min}_i \text{) for } s_i$
- Must apply the same transformation to instances for both training and prediction
- Outliers can cause problems

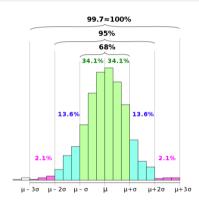
This redistributes the features with their mean $\mu=0$ and standard deviation $\sigma=1$. *sklearn.preprocessing.scale* helps us implementing standardization in python.

Standardization



Standard deviation

$$s_j = \sqrt{\frac{\sum\limits_{i=1}^{n} |x_j^{(i)} - \mu_j|}{n}}$$



68-95-99.7 rule

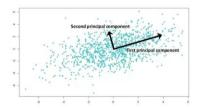
$$egin{aligned} &\Pr(\mu - 1\sigma \leq X \leq \mu + 1\sigma) pprox 0.6827 \ &\Pr(\mu - 2\sigma \leq X \leq \mu + 2\sigma) pprox 0.9545 \ &\Pr(\mu - 3\sigma \leq X \leq \mu + 3\sigma) pprox 0.9973 \end{aligned}$$

Mean Normalization

$$x' = \frac{x - mean(x)}{max(x) - min(x)}$$

This distribution will have values between [-1,1] with μ =0.

Standardization and **Mean Normalization** can be used for algorithms that assumes zero centric data like **Principal Component Analysis (PCA)**.



Min-Max Scaling

$$x' = \frac{x - min(x)}{max(x) - min(x)}$$

This scaling brings the value in [0,1].

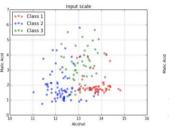
Unit Vector

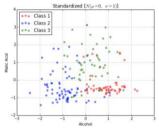
$$x' = \frac{x}{||x||}$$

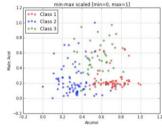
Scaling is done considering the whole feature vector to be of unit length.

Min-Max Scaling and **Unit Vector** techniques produces values of range **[0,1]**. When dealing with features with hard boundaries this is quite useful. For example, when dealing with image data, the colors can range from only 0 to 255.

(255, 0, 0)	(0, 255, 0)	(0, 0, 255)
(0, 255, 255)	(255, 0, 255)	(255, 255, 0)
(0, 0, 0)	(255, 255, 255)	(127, 127, 127)



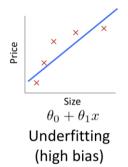


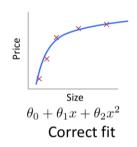


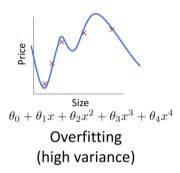
$$x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{s_j}$$

$$x' = \frac{x - min(x)}{max(x) - min(x)}$$

Quality of Fit







Overfitting:

- The learned hypothesis may fit the training set very well ($J({m heta}) pprox 0$)
- ...but fails to generalize to new examples

Regularization

- A method for automatically controlling the complexity of the learned hypothesis.
- Idea: penalize for large values of $heta_j$
- Can incorporate into the cost function
- Works well when we have a lot of features, each that contributes a bit to predicting the label.
- Can also address overfitting by eliminating features (either manually or via model selection).

Regularization

Linear regression objective function

$$J(\boldsymbol{\theta}) = \frac{1}{2n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^2 + \frac{\lambda}{2} \sum_{j=1}^{d} \theta_j^2$$
 model fit to data regularization

- $-\lambda$ is the regularization parameter ($\lambda > 0$)
- No regularization on θ_0 !

Understanding Regularization

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

- Note that $\sum_{i=1}^{a} heta_j^2 = \|oldsymbol{ heta}_{1:d}\|_2^2$
 - This is the magnitude of the feature coefficient vector!
- · We can also think of this as:

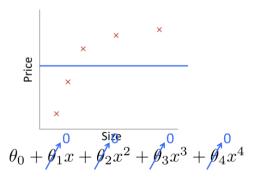
$$\sum_{j=1}^{d} (\theta_j - 0)^2 = \|\boldsymbol{\theta}_{1:d} - \vec{\mathbf{0}}\|_2^2$$

L₂ regularization pulls coefficients toward 0

Understanding Regularization

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

• What happens if we set λ to be huge (e.g., 10¹⁰)?



Regularized Linear Regression

Cost Function

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

- Fit by solving $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
- · Gradient update:

$$\frac{\partial}{\partial \theta_0} J(\theta) \qquad \theta_0 \leftarrow \theta_0 - \alpha \frac{1}{n} \sum_{i=1}^n \left(h_{\theta} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right) \\
\frac{\partial}{\partial \theta_j} J(\theta) \qquad \theta_j \leftarrow \theta_j - \alpha \frac{1}{n} \sum_{i=1}^n \left(h_{\theta} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right) x_j^{(i)} - \lambda \theta_j$$

regularization

Regularized Linear Regression

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

$$\theta_0 \leftarrow \theta_0 - \alpha \frac{1}{n} \sum_{i=1}^n \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)$$
$$\theta_j \leftarrow \theta_j - \alpha \frac{1}{n} \sum_{i=1}^n \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right) x_j^{(i)} - \lambda \theta_j$$

We can rewrite the gradient step as:

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

Summary

Linear regression Cost function

Gradient descent

- · Batch Gradient Descent
- Stochastic Gradient Descent
- Mini-batch Gradient Descent

Learning Rate

· With Exponential Decay

Underfitting & Overfitting

Generalization using Training, Validation and Test set

Feature scaling

- Standardization
- Mean Normalization
- Min-Max scaling
- Unit Vector

Regularization

Q&A

Thank you