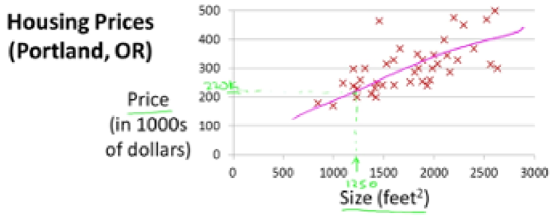
1 Linear regression (for regression)

Model a scalar target with one or more quantitative features.
Although regression computes a linear combination, features can be transformed by nonlinear functions if relationships are known or can be guessed.



1.1 Univariate linear regression

- Description

  Simple linear regression is a statistical method that studies the relationship between two variables:
  - x: the predictor, explanatory, independent variable,
  - y: the response, outcome, dependent variable.

- Model's hypothesis

  $h(x) = \theta_0 + \theta_1 * x = \hat{y}$

- Model's parameters (# 2)

  - θ_0, θ_1

- Cost function (in this case, the squared error function)

  $J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right)^2$

- Goal

  $\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$

- Algorithm

  - notations

    - x: the independent variable
    - y: the dependent variable
    - m: the number of training examples
    - $x^{(i)}$: the input value of the i^{th} training example
    - $y^{(i)}$: the target value of the i^{th} training example
    - $\hat{y}^{(i)}$: the prediction made on the i^{th} training example by the current hypothesis function
    - α: the learning rate; determines how big steps we take when updating the θ parameters

  - gradient descent

    - start with some initial values for θ_0 and θ_1 (usually zero)

    - keep changing θ_0 and θ_1 to reduce $J(\theta_0, \theta_1)$

      - $\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \theta_0 - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right)\right)$

      - $\theta_1 = \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \theta_1 - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right) \cdot x^{(i)}\right)$

  - directly use the following **formulas**

    - $\theta_1 = \frac{\sum_{i=1}^{m} (x^{(i)} - \bar{x})(y^{(i)} - \bar{y})}{\sum_{i=1}^{m} (x^{(i)} - \bar{x})^2}$

    - $\theta_0 = \bar{y} - \theta_1 \bar{x}$

  - hyperparameters

- α: if too small, slow gradient descent; if too large, gradient descent may fail to converge

1.2 Multivariate linear regression

- Description

  Multivariate linear regression is a statistical method that studies the relationship between multiple variables:
  - n variables $x = \{x_1, x_2, \ldots, x_n\}$: the predictor, explanatory, independent variables,
  - one y variable: the response, outcome, dependent variable.

- Model's hypothesis

  $h(x) = \theta_0 + \theta_1 * x_1 + \theta_2 * x_2 + \ldots + \theta_n * x_n = \hat{y}$

- Model's parameters (# $n + 1$)

  $\theta = \{\theta_0, \theta_1, \ldots, \theta_n\}$

- Cost function (in this case, the squared error function)

  $J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left(\hat{y}^{(i)} - y^{(i)}\right)^2$

- Goal

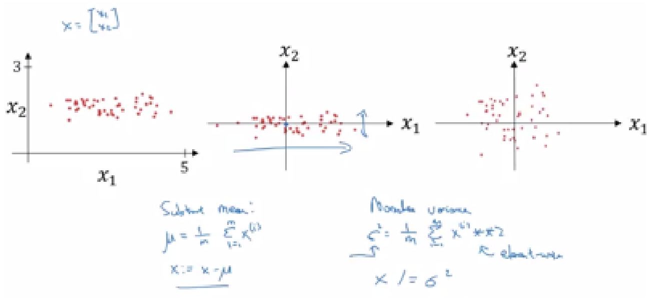
  $\min_{\theta} J(\theta)$

- Algorithm
  - notations
    - x: the independent variables
    - y: the dependent variable
    - m: the number of training examples
    - n: the number of features representing each training example
    - $x^{(i)}$: the input values of the i^{th} training example
    - $x_j^{(i)}$: the value of the j^{th} feature of the i^{th} training example
    - $y^{(i)}$: the target value of the i^{th} training example
    - $\hat{y}^{(i)}$: the prediction made on the i^{th} training example by the current hypothesis function
    - α: the learning rate; determines how big steps we take when updating the θ parameters
  - gradient descent
    - start with some initial values for θ_0, θ_1, ..., θ_n (usually 0)
    - keep changing θs to reduce $J(\theta)$
      - $\theta_0 = \theta_0 - \alpha \frac{\partial J}{\partial \theta_0} = \theta_0 - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right)\right)$
      - $\theta_1 = \theta_1 - \alpha \frac{\partial J}{\partial \theta_1} = \theta_1 - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right) \cdot x_1^{(i)}\right)$
      - ...
      - $\theta_n = \theta_n - \alpha \frac{\partial J}{\partial \theta_n} = \theta_n - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right) \cdot x_n^{(i)}\right)$
  - hyperparameters
    - α

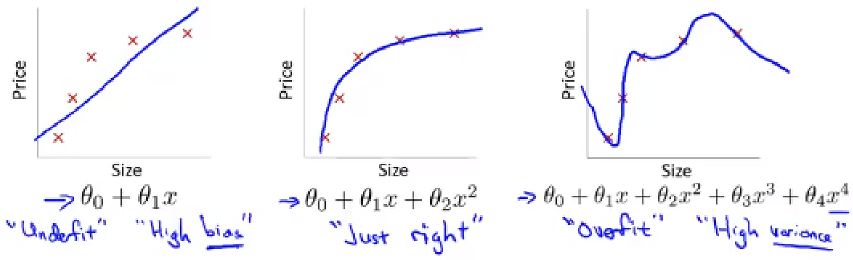
- Performance evaluation
  - R^2 regression score: $R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}$

- Problems
  - make sure features are on similar scales; gradient descent may be slow otherwise
    - feature scaling: $x' = \frac{x - min(x)}{max(x) - min(x)}$
    - feature scaling with mean normalization: $x' = \frac{x - mean(x)}{max(x) - min(x)}$

- feature scaling with standardization: $x' = \frac{x - mean(x)}{std(x)}$



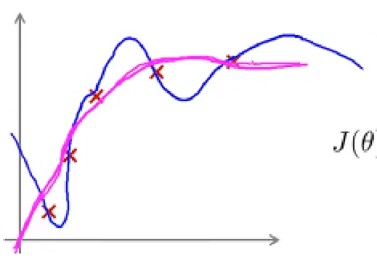
- make sure the gradient descent is working correctly
  - plot the value of the cost function J over the number of iterations (# $epochs$)
  - for a sufficiently small α, $J(\theta)$ should decrease on every iteration
  - if α is too small, the gradient descent can be slow to converge
  - if α is too large, $J(\theta)$ may not decrease on every iteration; may not converge
  - try values $\alpha \in \{\dots, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, \dots\}$
- check model performance



  - in case of **underfitting**
    - try adding new features
      - e.g, use a polynomial regression

$$\theta_0 + \theta_1 * x \quad \Rightarrow \quad \theta_0 + \theta_1 * x + \theta_2 * x^2 + \theta_3 * x^3 + \dots$$

  - in case of **overfitting**
    - get more training examples
    - try reducing the number of features
      - manually select which features to keep
      - use a model-selection algorithm
    - try getting additional features
    - try adding polynomial features
    - use regularization
      - keep all the features, but reduce the magnitude of parameters θ;
        works well when working with a lot of features, each of which contributes a bit to predicting y
      - intuition: *shrink* model parameters in order to *smooth out* the decision boundary (generate a *simpler* hypothesis)



$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} \theta_j^2\right]$$

      - cost function with the *regularization term*

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}\left(\hat{y}^{(i)} - y^{(i)}\right)^2 + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

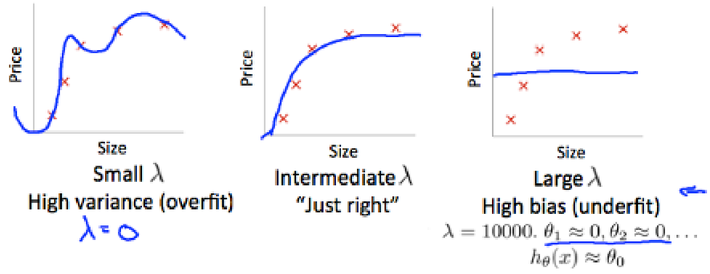
- parameter update in gradient descent (for $j \in \{1, 2, \ldots, n\}$)

$$\theta_j = \theta_j - \alpha\frac{\partial J}{\partial\theta_j} = \theta_j - \alpha\left(\frac{1}{m}\sum_{i=1}^{m}\left(\hat{y}^i - y^{(i)}\right)\cdot x_j^{(i)} + \frac{\lambda}{m}\theta_j\right) = \theta_j\left(1 - \alpha\frac{\lambda}{m}\right) - \alpha\frac{1}{m}\sum_{i=1}^{m}\left(\hat{y}^i - y^{(i)}\right)\cdot x_j^{(i)}$$

- λ is the *regularization parameter* and needs to be tuned;
  it controls the trade-off between the goal of fitting the training data well and the goal of keeping the parameters small;
  try values $\lambda \in \{0, 0.02, 0.04, 0.08, 0.16, \ldots, 10\}$

$$\boxed{h_\theta(x) = \theta_0} + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4 \leftarrow$$

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \boxed{\frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2}$$



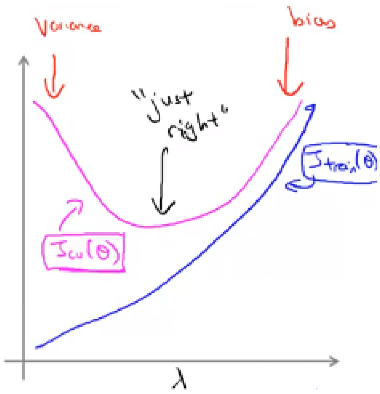
- when using regularization, try increasing or decreasing λ

Bias/variance as a function of the regularization parameter λ

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \boxed{\frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2}$$

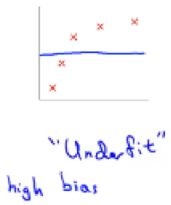
$$J_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

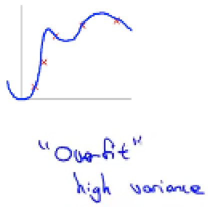
$$\boxed{J_{cv}(\theta)} = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$



- debugging
  - choices to make when dealing with an underfit or an overfit model

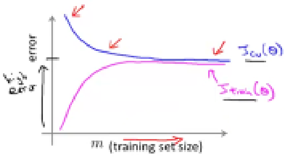
Try getting additional features	Get more training examples
Try adding polynomial features $(x_1^2, x_2^2, x_1x_2, \text{etc})$	Try smaller sets of features
Try decreasing λ	Try increasing λ

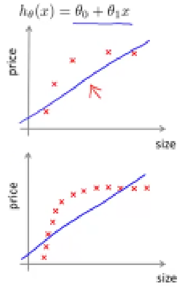




  - machine learning diagnostic
    - gain guidance on how to improve the model's performance
    - draw **learning curves**: check the train and dev set error when training on various sizes of the training data set ($1 \leq i \leq m$)
      - high bias $\Rightarrow$ getting more data won't help
      - high variance $\Rightarrow$ getting more data might help

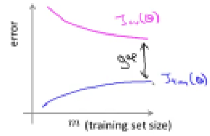
High bias

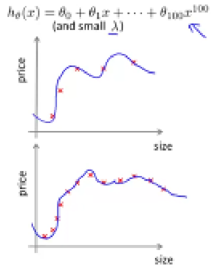




If a learning algorithm is suffering from high bias, getting more training data will not (by itself) help much.

High variance





If a learning algorithm is suffering from high variance, getting more training data is likely to help.