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ML-course

2. Regression in Python Scikit-learn

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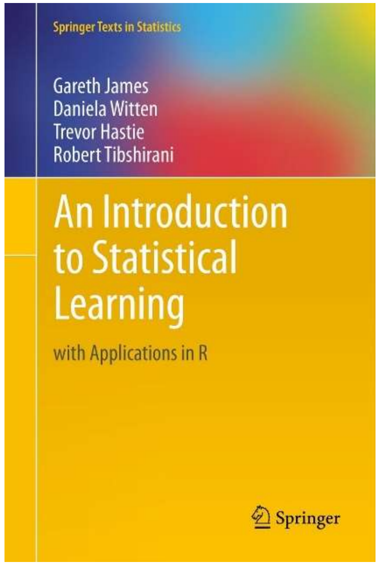
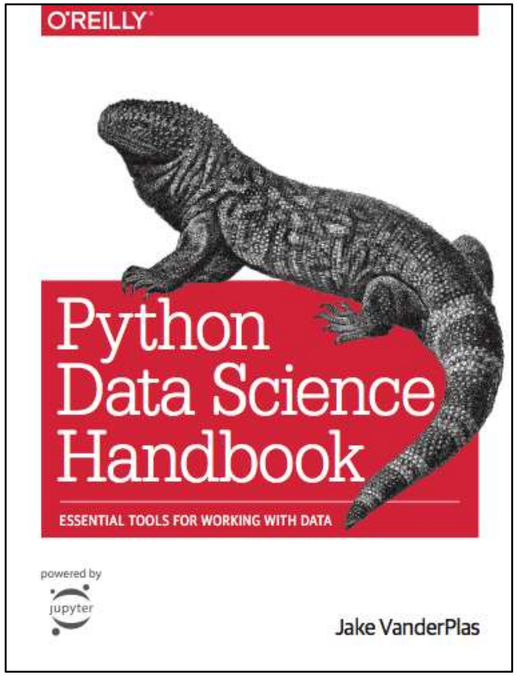
Reference

An Introduction to Statistical Learning by Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani, http://www-bcf.usc.edu/~gareth/ISL/ (available online for free)



Reference



Jake VanderPlas

Python Data Science Handbook
https://jakevdp.github.io/PythonDataScienceHandbook/

Video
https://www.youtube.com/watch?v=L7R4HUQ-eQ0&t=6033s

Reference

http://scikit-learn.org

Supervised vs. Unsupervised Learning

Supervised	Unsupervised
Data: 1) n observations; 2) p variables X1, X2, . . .,Xp, measured on each observation; 3) response Y measured on same n observations Y Continuous: Regression Discrete: Classification	Data: 1) n observations; 2) p variables X1, X2, . . .,Xp, measured on each observation Clustering…

Regression / Classification Problem

Steps to solve

- ***Working with data***
- ***Modeling***

Representation of data in Scikit-learn

- **X**

  two-dimensional ***numpy array***
  shape – (n_samples, m_features)

- **Y**

  one-dimensional ***numpy array***
  shape – (n_samples,)

Modeling

- Choose a class of model
- Fit the model to data
- Validate the model and optimize hyperparameters
- Predict for unknown data

Mathematical model

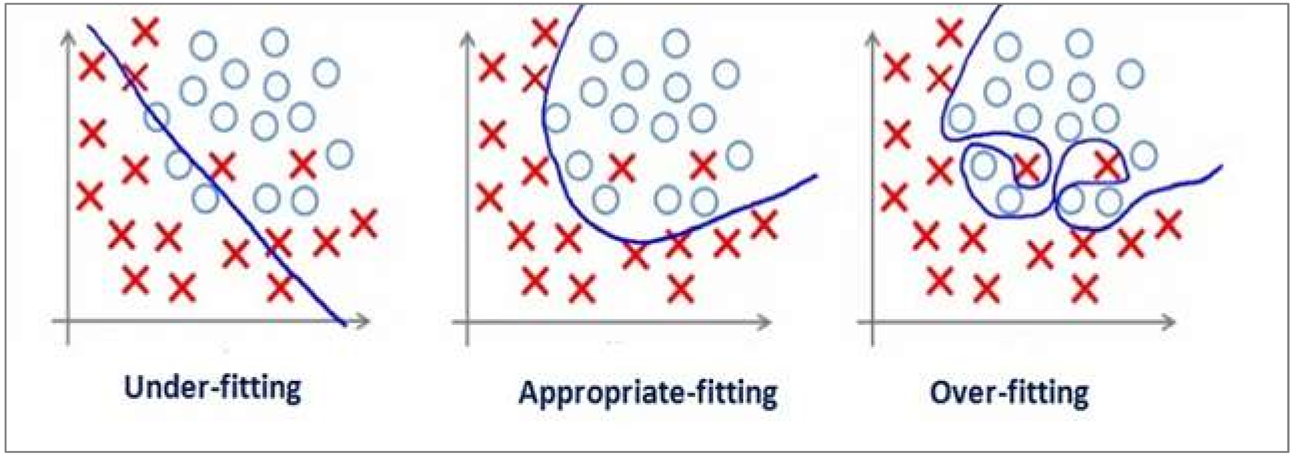
$$Y = f(X) + \epsilon$$

f is some fixed but unknown function of *X*1, . . . , *Xp*, and *e* is a random *error term*, which is independent of *X* and has mean zero. In this formulation, *f* represents the *systematic* information that *X* provides about *Y* .

We can predict *Y* using our estimate for *f*

$$\hat{Y} = \hat{f}(X)$$

Bias-Variance Trade-Off



Underfitting *(high bias)* - algorithm is missing the relevant relations between features and target outputs

Overfitting *(high variance)* - modeling the random noise in the training data, rather than the intended outputs.

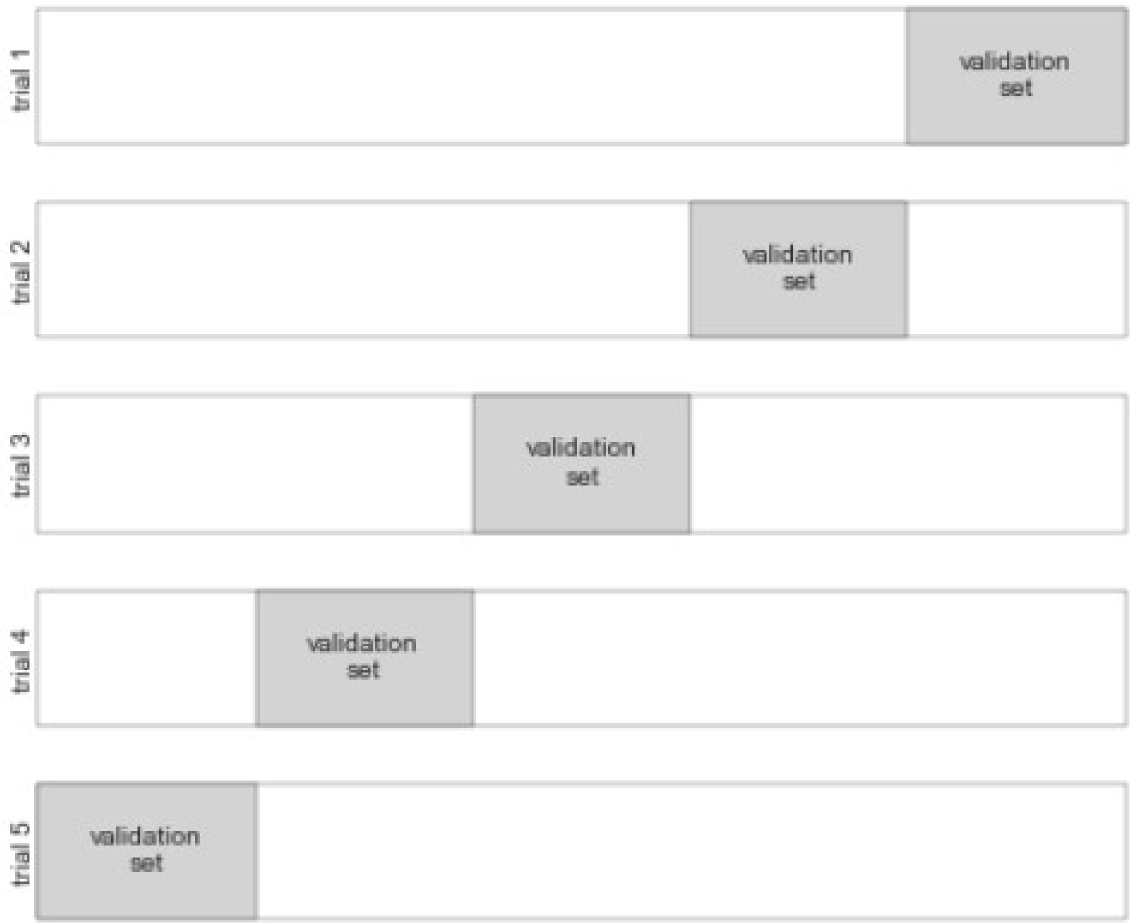
Model validation

- **Data**
  - train + test (e.g. 75% + 25%)
  - train + valid + test (e.g. 60% + 20% + 20%)
  - train with cross-validation + test (e.g. 80% + 20%)

- **Metrics**
  - Regression: **R^2**, MSE, MAE,…

  http://scikit-learn.org/stable/modules/classes.html#sklearn-metrics-metricsmodel.score()

Model validation via cross-validation



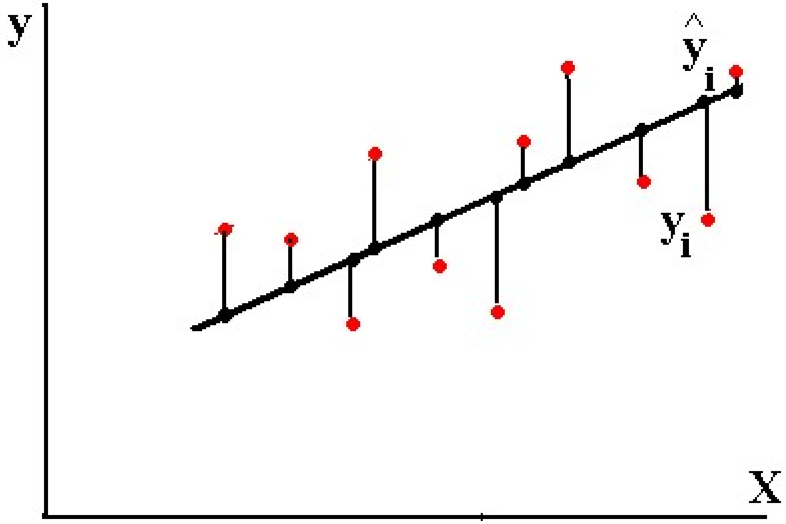
Some models for Regression in Python scikit-learn

- **Generalized Linear Models**
  - Linear Regression
  - Ridge Regression
  - Lasso Regression

example of Linear, Ridge and Lasso Regressions in regression.ipynb

- **Ensemble methods**
  - Random Forests
  - Gradient Tree Boosting

Linear Regression with one variable



(x_i, y_i), $i=1,n$ – number of observations (red points)

$$\hat{y} = ax + b$$

$$\hat{y} = \theta_0 + \theta_1 x_1 = \theta_0 x_0 + \theta_1 x_1, \qquad x_0 = 1$$

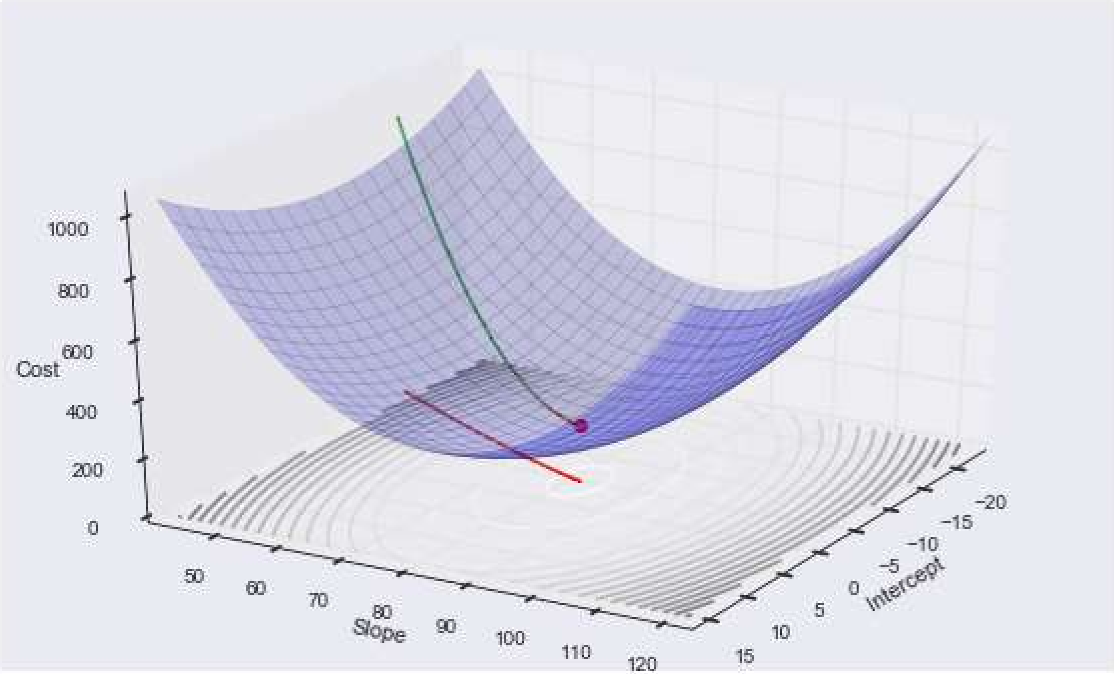
θ_0 - *intercept*, θ_1 - *slope*

The method of least squares

$$Cost = J(\theta_0, \theta_1) = \sum_{i=1}^{n} (\widehat{y^i} - y^i)^2 = \sum_{i=1}^{n} (\theta_0 x_0^i + \theta_1 x_1^i - y^i)^2$$

Our aim - $\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$

Gradient descent to find $\min\limits_{\theta_0,\theta_1} J(\theta_0,\theta_1)$



Need to choose

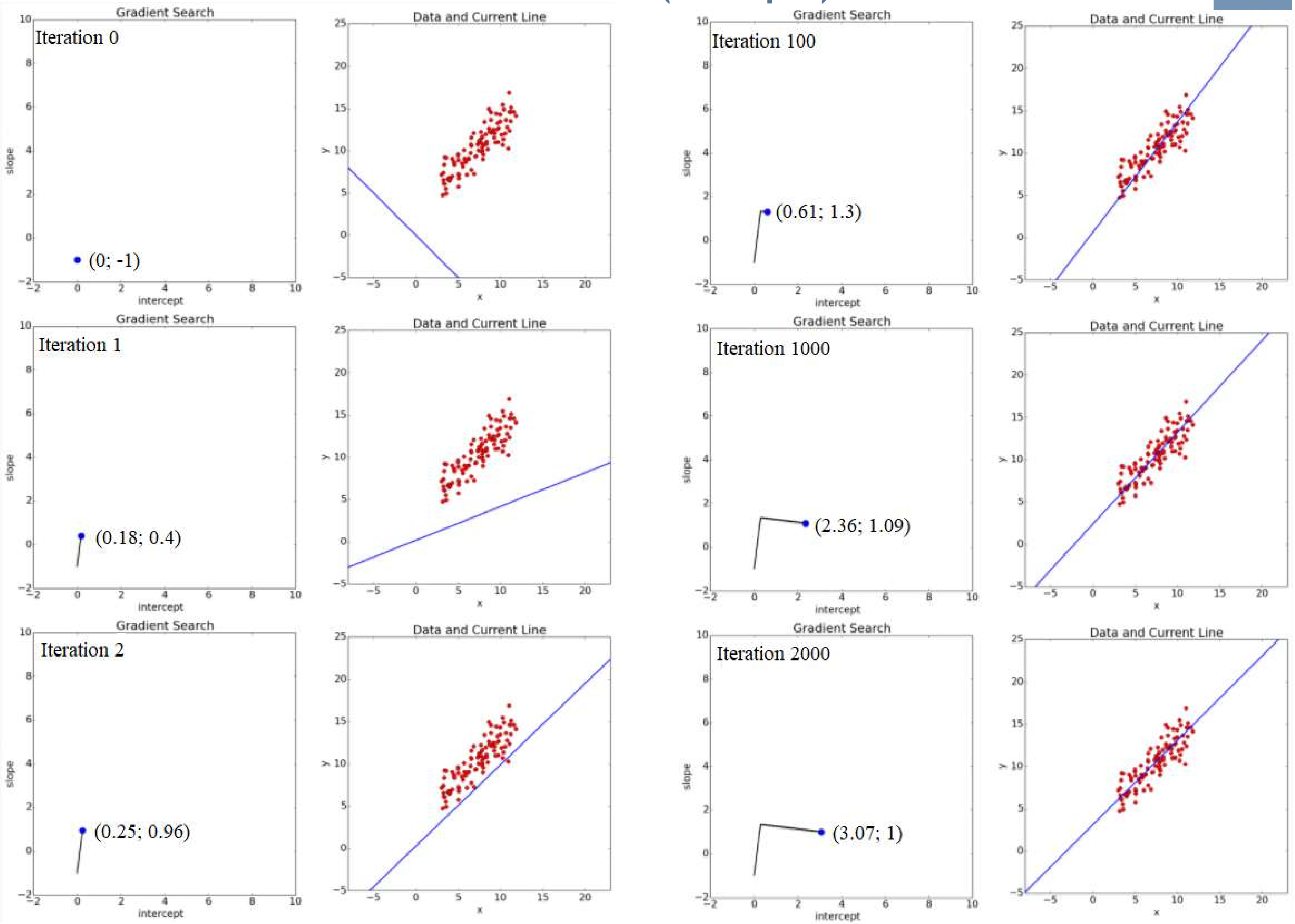
α *– learning rate (step size)*
(θ_0, θ_1) *- start point*

Repeat until convergence

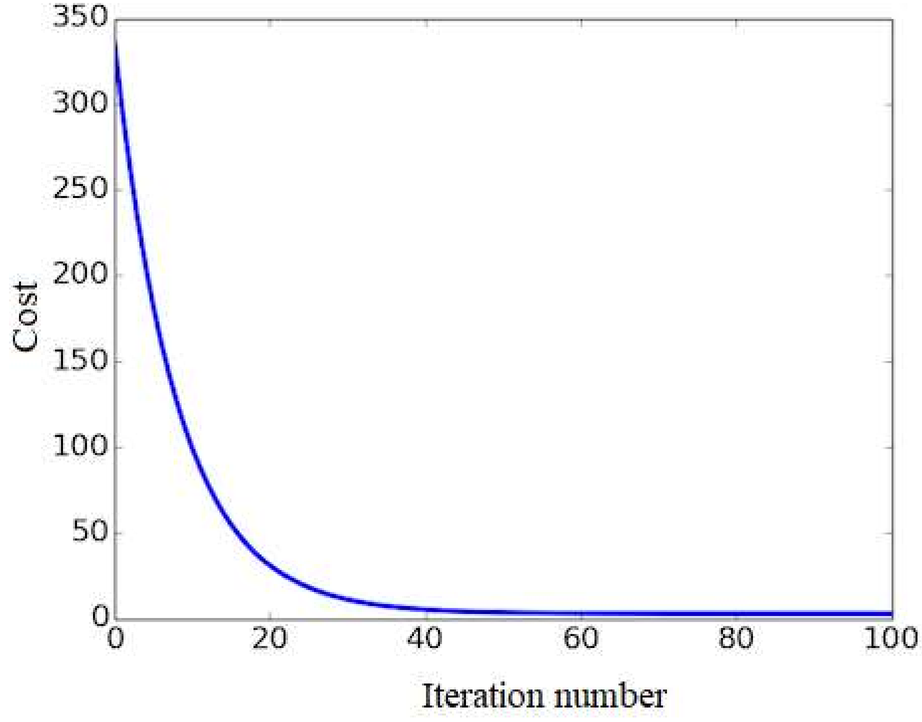
$$\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \theta_0 - 2\alpha \sum_{i=1}^{n} (\theta_0 x_0^i + \theta_1 x_1^i - y^i) x_0^i$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \theta_1 - 2\alpha \sum_{i=1}^{n} (\theta_0 x_0^i + \theta_1 x_1^i - y^i) x_1^i$$

Gradient descent (example)



Gradient descent (example)



Linear Regression with multiple variables

***m** variables, **n** observations*

$$\hat{y} = \theta_0 x_0 + \theta_1 x_1 + \dots + \theta_m x_m, \qquad x_0 = 1$$

$$X = [1, x_1, \dots, x_m] \qquad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \dots \\ \theta_m \end{bmatrix} \qquad \boldsymbol{\hat{y}} = \boldsymbol{h_\theta(X)} = \boldsymbol{X\theta}$$

Dataset for training: $X^{(i)} = \left[1, x_1^{(i)}, \dots, x_m^{(i)}\right], y^{(i)}, i = 1, \dots, n$

$$\boldsymbol{Cost = J(\theta) = \sum_{i=1}^{n}(h_\theta\left(X^{(i)}\right) - y^{(i)})^2} \qquad \textbf{\textit{Our aim}} - \min_\theta J(\theta)$$

Repeat until convergence:

for j=0…m

$$\theta_j = \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) = \theta_j - 2\alpha \sum_{i=1}^{n} (h_\theta\left(X^{(i)}\right) - y^{(i)}) x_j^{(i)}$$

Cost functions for Linear Regression, Ridge and Lasso in scikit-learn

***m** variables, **n** observations*

$$\hat{y} = \theta_0 x_0 + \theta_1 x_1 + \cdots + \theta_m x_m, \qquad x_0 = 1$$

$$X = [1, x_1, \ldots, x_m] \qquad \theta = \begin{bmatrix} \theta_0 \\ \theta_{01} \\ \ldots \\ \theta_m \end{bmatrix} \qquad \boldsymbol{\hat{y} = h_\theta(X) = X\theta}$$

Linear Regression $\quad Cost = J(\theta) = \sum_{i=1}^{n} (X^{(i)}\theta - y^{(i)})^2$

Ridge (*regularization **l2***) $\quad Cost = J(\theta) = \sum_{i=1}^{n} (X^{(i)}\theta - y^{(i)})^2 + \boldsymbol{\alpha \sum_{j=0}^{m} \theta_j{}^2}$

Lasso (*regularization **l1***) $\quad Cost = J(\theta) = \sum_{i=1}^{n} (X^{(i)}\theta - y^{(i)})^2 + \boldsymbol{\alpha \sum_{j=0}^{m} |\theta_j|}$

Regression metrics

R² score, the coefficient of determination

$$R^2(y,\hat{y}) = 1 - \frac{\sum_{i=1}^{n}\left(y^{(i)} - \hat{y}^{(i)}\right)^2}{\sum_{i=1}^{n}(y^{(i)} - \bar{y})^2}, \qquad where \;\; \bar{y} = \frac{\sum_{i=1}^{n} y^{(i)}}{n}$$

Mean squared error

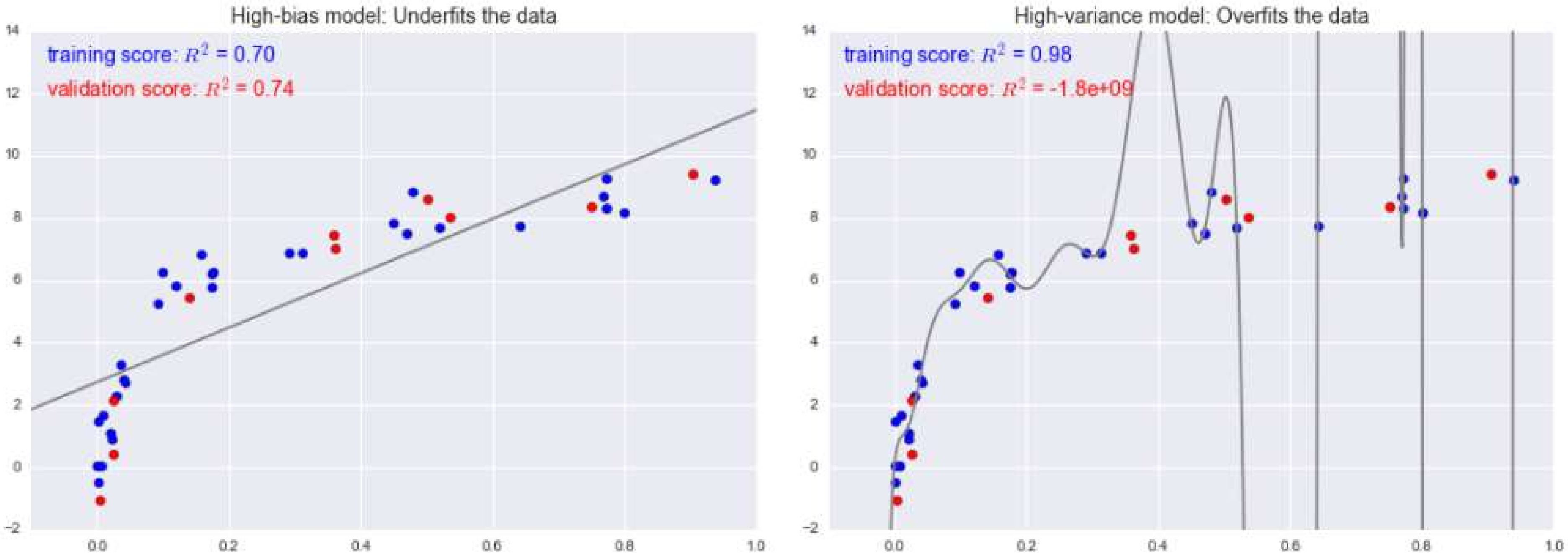
$$MSE(y,\hat{y}) = \frac{1}{n}\sum_{i=1}^{n}\left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

Mean absolute error

$$MAE(y,\hat{y}) = \frac{1}{n}\sum_{i=1}^{n}\left|y^{(i)} - \hat{y}^{(i)}\right|$$

http://scikit-learn.org/stable/modules/model_evaluation.html#regression-metrics

Bias-Variance Trade-Off



- For **high-bias** models, the **performance** of the model on the **validation** set is **similar** to the performance on the **training set** *(but the performance is worse than for appropriate fitting)*.

- For **high-variance** models, the **performance** of the model on the **validation** set is **far worse** than the performance on the **training** set.

Bias-Variance Trade-Off

What to do in case of high-bias or high variance?

Change

- Model complexity (e.g. via regularization)
- Quantity of training samples
- Set of features

Reading

Jake VanderPlas ***Python Data Science Handbook*** *(05.03-Hyperparameters-and-Model-Validation)*

Andrew Ng ***ML: Advice for Applying Machine Learning***

Ways to fix high bias/variance in linear models

High bias (underfitting)	High variance (overfitting)
• Add more features • Add polynomial features	• More training examples • Smaller set of features • Use regularization • Increase regularization strength (coefficient)

Choose the best model

Models	R^2	
	train	test
LinearRegression()		
LinearRegression(normalize = True)		
LinearRegression with PolynomialFeatures		
n=2		
Ridge with Polynomial Features, n=2		
a=0.1		
a=1		
a=10		
a=100		
Lasso with Polynomial Features, n=2		
a=0.1		
a=1		
a=10		
a=100		

Q & A

Thank you!