Fundamentals of Machine Learning 2020
Linear Regression

ML Instructional Team

April 20, 2020

VEF
ACADEMY

Contents

1. Introduction
2. Linear regression
3. Estimation methods
4. Basis function
5. References

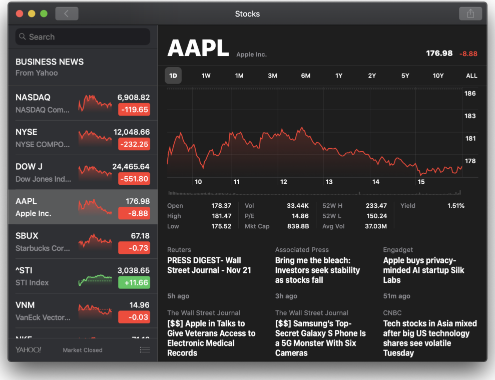
Learning outcomes

- Understanding the mathematical foundations of linear regression
- Define and independently apply a linear regression model on new data
- Differ linear from nonlinear problems and understand the necessary of extending linear to nonlinear models

Possible applications

- Predict tomorrow's stock market **prices** given current market conditions and other possible side information.
- Predict the **age** of a viewer watching a given video on YouTube.
- Predict the **temperature** at any location inside a building using weather data, time, door sensors, etc.
- Predict the **salaries** of graduate students given GPAs, number of social activities, gender, living location, etc.
- Predict the **number of users** sharing your post on Facebook based on your friend list, hashtag popularity, previous posts, etc.

Could you see the trend?



BUSINESS NEWS
From Yahoo

NASDAQ NASDAQ Com...	6,908.82	-119.65
NYSE NYSE COMPO...	12,048.66	-232.25
DOW J Dow Jones Ind...	24,465.64	-551.80
AAPL Apple Inc.	176.98	-8.88
SBUX Starbucks Cor...	67.18	-0.73
^STI STI Index	3,038.65	+11.66
VNM VanEck Vector...	14.96	-0.03

AAPL Apple Inc. 176.98 -8.88

Open	178.37	Vol	33.44K	52W H	233.47	Yield	1.51%
High	181.47	P/E	14.86	52W L	150.24		
Low	175.52	Mkt Cap	839.8B	Avg Vol	37.03M		

Reuters
PRESS DIGEST- Wall Street Journal - Nov 21
5h ago

Associated Press
Bring me the bleach: Investors seek stability as stocks fall
3h ago

Engadget
Apple buys privacy-minded AI startup Silk Labs
51m ago

The Wall Street Journal
[$$] Apple in Talks to Give Veterans Access to Electronic Medical Records

The Wall Street Journal
[$$] Samsung's Top-Secret Galaxy S Phone Is a 5G Monster With Six Cameras

CNBC
Tech stocks in Asia mixed after big US technology shares see volatile Tuesday

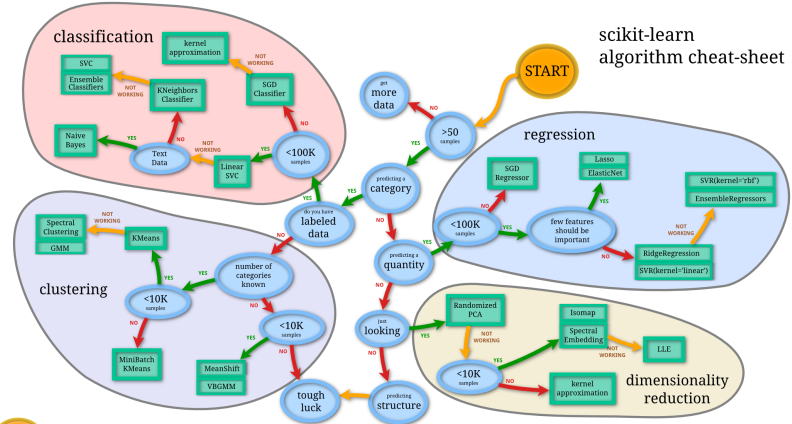
Figure: Apple stock prices (AAPL)

- Normally, we will use stock analysis techniques such as Fibonacci retracement, candlestick, bull/bear signal, etc.
- Can we use Machine Learning methods to help us **automate** the whole process with acceptable results?

How to solve these problems using Machine Learning?

1. Define the problem (e.g. **predicting** some outcome).
2. Collecting the appropriate **data set**.
3. Choose the right machine learning algorithm.
4. Define **evaluation metrics** of the model (e.g. Accuracy, AUC, Precision, Recall, etc.)

Choose the right machine learning algorithm



Back

Figure: Machine learning map (sklearn)

Modeling process

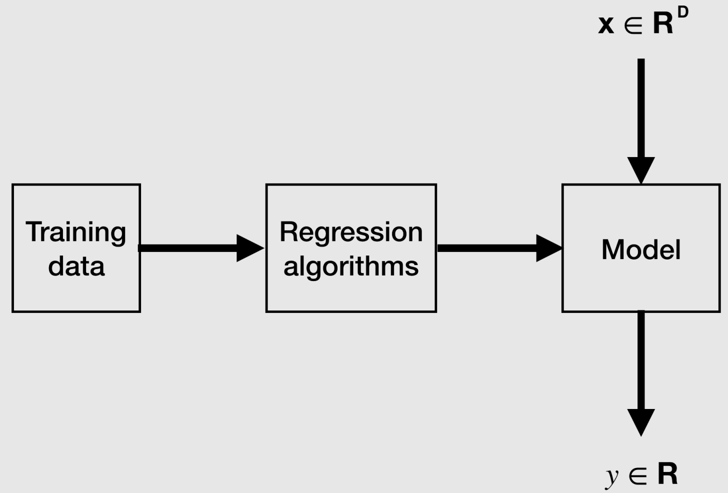
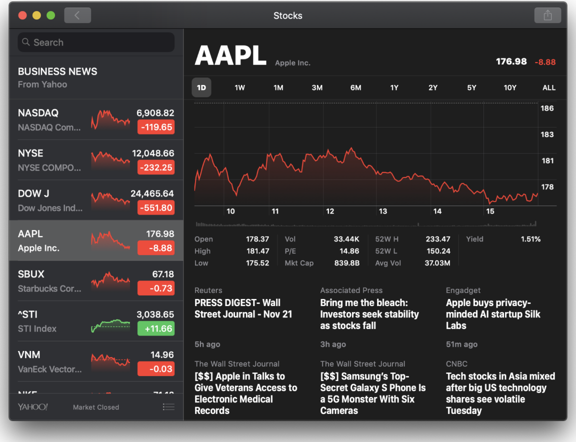


Figure: Regression process

Key points of model

- Need data to build prediction model (training process).
- Could predict *unseen data* in the future (**generalization**).
- **"No Free Lunch"** theorem states that there is no one model that works best for every problem.

Could you see the trend?



BUSINESS NEWS
From Yahoo

NASDAQ NASDAQ Com...	6,908.82	-119.65
NYSE NYSE COMPO...	12,048.66	-232.25
DOW J Dow Jones Ind...	24,465.64	-551.80
AAPL Apple Inc.	176.98	-8.88
SBUX Starbucks Cor...	67.18	-0.73
^STI STI Index	3,038.65	+11.66
VNM VanEck Vector...	14.96	-0.03

AAPL Apple Inc. 176.98 -8.88

Open	178.37	Vol	33.44K	52W H	233.47	Yield	1.51%
High	181.47	P/E	14.86	52W L	150.24		
Low	175.52	Mkt Cap	839.8B	Avg Vol	37.03M		

Reuters
PRESS DIGEST- Wall Street Journal - Nov 21
5h ago

Associated Press
Bring me the bleach: Investors seek stability as stocks fall
3h ago

Engadget
Apple buys privacy-minded AI startup Silk Labs
51m ago

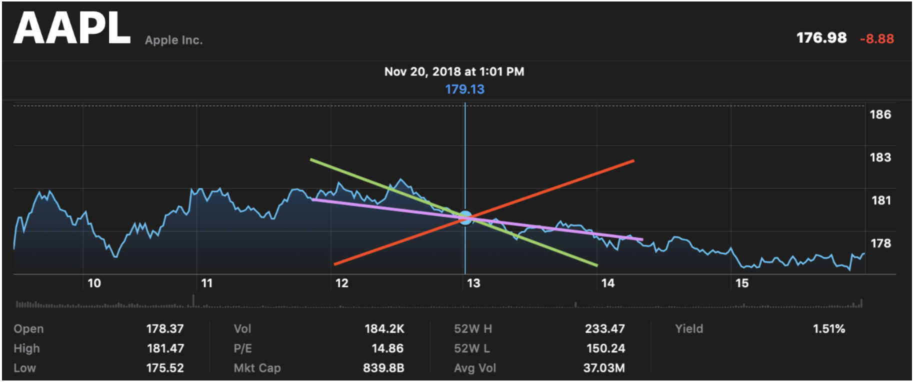
The Wall Street Journal
[$$] Apple in Talks to Give Veterans Access to Electronic Medical Records

The Wall Street Journal
[$$] Samsung's Top-Secret Galaxy S Phone Is a 5G Monster With Six Cameras

CNBC
Tech stocks in Asia mixed after big US technology shares see volatile Tuesday

Figure: Apple stock prices (AAPL)

How to draw a straight line that express the trend of data?



AAPL Apple Inc. 176.98 -8.88

Nov 20, 2018 at 1:01 PM
179.13

Open	178.37	Vol	184.2K	52W H	233.47	Yield	1.51%
High	181.47	P/E	14.86	52W L	150.24		
Low	175.52	Mkt Cap	839.8B	Avg Vol	37.03M		

Figure: There are many possible straight lines for predicting trends

Contents

1 Introduction

2 Linear regression

3 Estimation methods

4 Basis function

5 References

Linear function

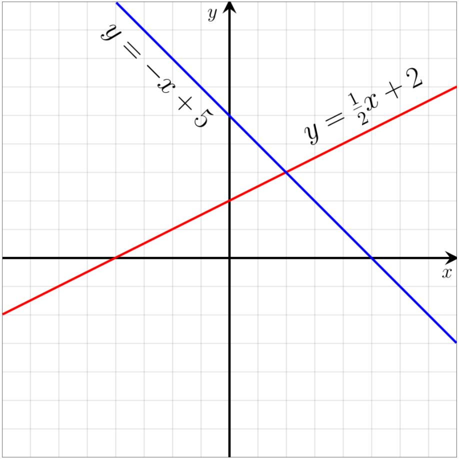


Figure: Linear function (https://en.wikipedia.org/)

Linear model for regression

Linear model for regression is a linear combination of the input variables. It assumes the dependency of the response variable y on the explanatory variables $\mathbf{x}$ is linear.

Formula

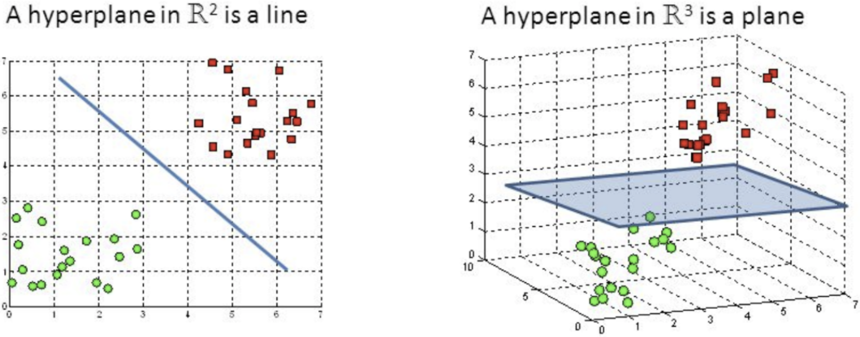
$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + ... + w_D x_D = w_0 + \sum_{j=1}^{D} w_j x_j$$

where

- $y \in \mathbf{R}$: response variable, dependent variable, outcome.
- D: number of dimensions of the input vector $\mathbf{x}$.
- $\mathbf{x} = (x_1, ..., x_D)^T$: input vector (explanatory variable, independent variable, features).
- $\mathbf{w} = (w_0, ..., w_D)$: parameters.
- $D + 1$: total number of parameters.

Hyperplane

Linear is a **straight line** in two-dimensional space, a **plane** in three-dimensional space, and a hyperplane in D-dimensional space.



A hyperplane in $\mathbb{R}^2$ is a line

A hyperplane in $\mathbb{R}^3$ is a plane

Figure: https://towardsdatascience.com/

Assumptions of the (Multiple) Linear Regression Model

Formula

$$y^{(i)}(\mathbf{x}^{(i)}, \mathbf{w}) = w_0 + \sum_{j=1}^{D} w_j x_j^{(i)} + \epsilon^{(i)}$$

- The relationship between the dependent variable (y) and the independent variables $(x_j,\ j = 1, \ldots, D)$ is linear.
- The independent variables $(x_j,\ j = 1, \ldots, D)$ are not random. There is no exact linear relation between two or more of the independent variables (multi-collinearity).
- The expected value of the error term, conditioned on the independent variables, is 0. $E\left[\epsilon^{(i)} | x^{(i)}\right] = 0$
- The variance of the error term is the same for all observations $E\left[\left(\epsilon^{(i)}\right)^2\right] = \sigma_\epsilon^2$ (homoscedasiticity).
- The error term is uncorrelated across observations $E\left[\epsilon^{(i)}\epsilon^{(j)}\right] = 0,\ i \neq j$
- The error term is normally distributed.

Linear regression in one picture

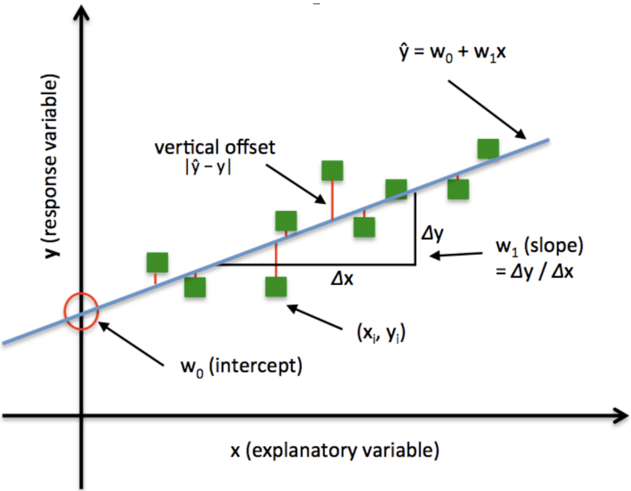


Figure: http://rasbt.github.io/

Loss function

Given the features $\mathbf{x}$, the predicted value of y, $\hat{y}$, is given by
$\hat{y} = f(\mathbf{x}) = w_0 + \sum_{j=1}^{D} w_j x_j$

Loss function

A loss function is a measure of how good a prediction model does in terms of being able to predict the expected outcome.

$$L(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

where N is the number of training examples.

Our goal: find parameters $\mathbf{w}$ that minimize the loss function. How?

Contents

1. Introduction
2. Linear regression
3. Estimation methods
4. Basis function
5. References

Using Ordinary Least Squares

We have

$$L(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}(y^{i} - \mathbf{w}\mathbf{x}^{(i)})^2$$

where we let $x_0^{(i)} = 1$ to simplify the notation.

Our goal is to find $\hat{\mathbf{w}}$:

$$\hat{\mathbf{w}} = argmin_{\mathbf{w}} L(\mathbf{w}) = argmin_{\mathbf{w}} \left(\frac{1}{2}||\mathbf{y} - \mathbf{X}\mathbf{w}||_2^2\right)$$

Using Ordinary Least Squares

$$\begin{aligned} L(\mathbf{w}) &= \frac{1}{2}(y - \mathbf{X}\mathbf{w})^T(y - \mathbf{X}\mathbf{w}) \\ &= \frac{1}{2}\left(y^T y - 2\mathbf{w}^T\mathbf{X}^T y + \mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w}\right). \end{aligned}$$

Setting the gradient to 0:

$$\begin{aligned} \frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} &= -\mathbf{X}^T y + \mathbf{X}^T\mathbf{X}\mathbf{w} = 0 \\ &\iff \mathbf{X}^T\mathbf{X}\mathbf{w} = \mathbf{X}^T y \\ &\iff \mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T y. \end{aligned}$$

Notes:

- The Hessian in this case is $\mathbf{X}^T\mathbf{X}$, which is a positive semidefinite matrix.
- The matrix $\mathbf{X}^T\mathbf{X}$ must be invertible and difficult to scale with high dimension input vector.
- The case in which $\mathbf{X}^T\mathbf{X}$ is non-invertible will be addressed later.

Solve with Gradient descent

Gradient descent algorithm

```
Initialize $\mathbf{w} = [0, ..., 0]$;
for $t = 1, ..., T$ do
    $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla L(\mathbf{w})$
end
```

- η: step size
- $\nabla L(\mathbf{w})$: gradient

- Gradient descent is a *first-order iterative* optimization algorithm for finding a *local minimum of a differentiable function.*
- Pros: Simple idea, no need to compute the second-derivative
- Cons: requires the entire set of data samples to be loaded in memory, since it operates on all of them at the same time

Solve with Stochastic Gradient descent

Stochastic Gradient descent algorithm

```
Initialize $\mathbf{w} = [0, ..., 0]$;
for $t = 1, ..., T$ do
    for $(x, y) \in D_{train}$ do
        $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla L(x, y, \mathbf{w})$
    end
end
```

- Pros: during learning, compute $L(x, y, \mathbf{w})$ before updating **w**, so require less memory.
- Cons: requires a number of hyperparameters such as the regularization parameter and the number of iterations.
- Other gradient descent variants: Batch gradient descent, Mini-batch gradient descent

How about complex data set?

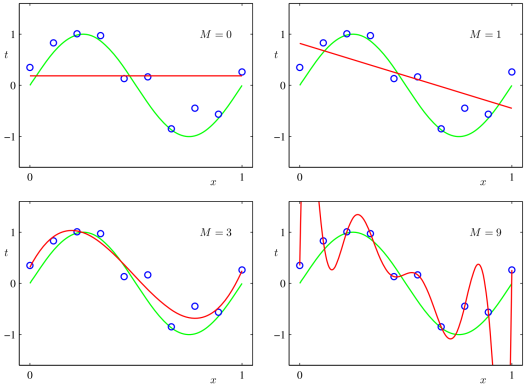


Figure 1.4 Plots of polynomials having various orders M, shown as red curves, fitted to the data set shown in Figure 1.2.

Figure: C. Bishop, Pattern Recognition and Machine Learning

Contents

1. Introduction
2. Linear regression
3. Estimation methods
4. Basis function
5. References

Basis function

Extend the class of models by considering linear combinations of fixed **nonlinear functions** of the form

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x})$$

where $\phi_j(\mathbf{x})$ are known as basis functions. Identity "basis function" is $\phi(\mathbf{x}) = \mathbf{x}$.

Some basis function

Polynomial basis function

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

Gaussian basis function

$$\phi_j(x) = exp\{-\frac{(x-\mu_j)^2}{2s^2}\}$$

Sigmoidal basis function

$$\phi_j(x) = \sigma(\frac{x-\mu_j}{s})$$

where $\sigma(a)$ is the logistic sigmoid function defined by

$$\sigma(a) = \frac{1}{1+exp(-a)}$$

Some basis function

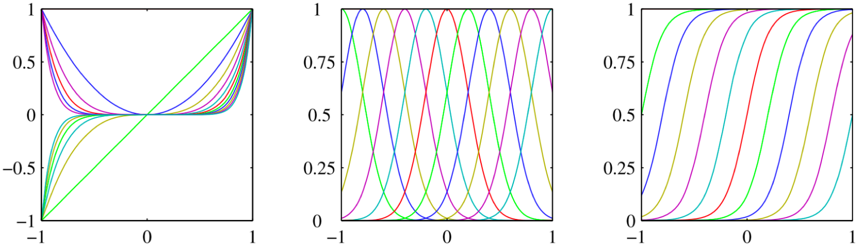


Figure 3.1 Examples of basis functions, showing polynomials on the left, Gaussians of the form (3.4) in the centre, and sigmoidal of the form (3.5) on the right.

Figure: C. Bishop, Pattern Recognition and Machine Learning

Contents

1. Introduction
2. Linear regression
3. Estimation methods
4. Basis function
5. References

References

[1] Bishop, C. M. (2013). Pattern Recognition and Machine Learning. Journal of Chemical Information and Modeling (Vol. 53).

[2] Wikipedia. Gradient descent.

[3] Wikipedia. Ordinary least squares.

[4] Wikipedia. Stochastic gradient descent.