How to Solve Linear Regression Using Linear Algebra

Brownlee on March 5, 2018 in Linear Algebra

Last Updated on December 27, 2020

Linear regression is a method for modeling the relationship between one or more independent variables and a dependent variable.

It is a staple of statistics and is often considered a good introductory machine learning method. It is also a method that can be reformulated using matrix notation and solved using matrix operations.

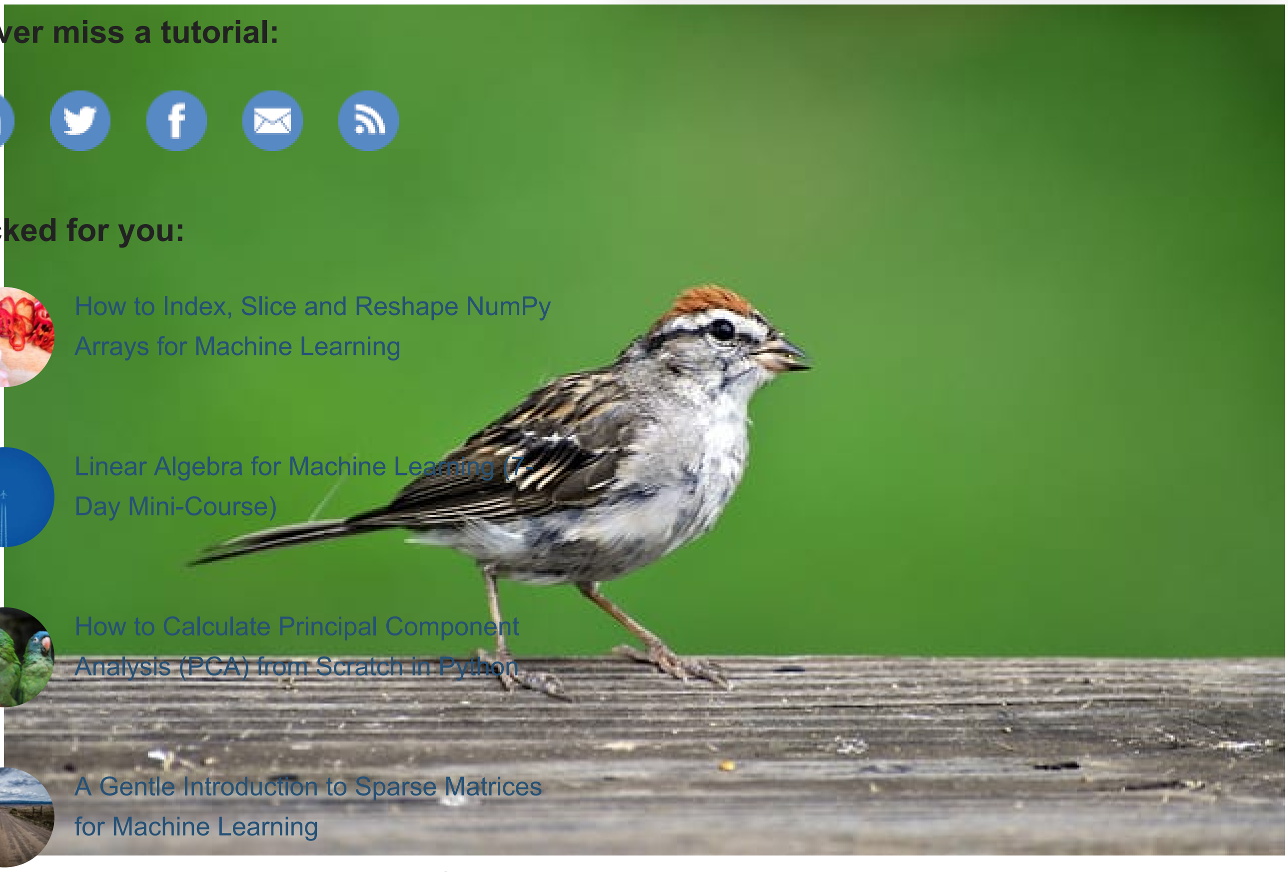
In this tutorial, you will discover the matrix formulation of linear regression and how to solve it using direct and matrix factorization methods.

After completing this tutorial, you will know:

- Linea… ix reformulation with the normal equations.
- How to solve linear regression using a QR matrix decomposition.
- How to solve linear regression using SVD and the pseudoinverse.

Kick-start your project with my new book Linear Algebra for Machine Learning, including *step-by-step tutorials* and the *Python source code* files for all examples.

Let's get started.



How to Solve Linear Regression Using Linear Algebra
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Tutorial Overview

This tutorial is divided into 6 parts; they are:

1. Linear Regression
2. Matrix Formulation of Linear Regression
3. Linear Regression Dataset
4. Solve
5. Solve via QR Decomposition
6. Solve via Singular-Value Decomposition

Linear Regression

Linear regression is a method for modeling the relationship between two scalar values: the input variable x and the output variable y.

The model assumes that y is a linear function or a weighted sum of the input variable.

```
y = f(x)
```

Or, stated with the coefficients.

```
y = b0 + b1 . x1
```

The model can also be used to model an output variable given multiple input variables called multivariate linear regression (below, brackets were added for readability).

```
y = b0 + (b1 . x1) + (b2 . x2) + ...
```

The objective of creating a linear regression model is to find the values for the coefficient values (b) that minimize the error in the prediction of the output variable y.

Matrix Formulation of Linear Regression

Linear regression can be stated using Matrix notation; for example:

```
y = X . b
```

Or, without the dot notation.

```
y = Xb
```

Where X is the input data and each column is a data feature, b is a vector of coefficients and y is a vector of output variables for each row in X.

```
     x11, x12, x13
X = (x21, x22, x23)
     x31, x32, x33
     x41, x42, x43

     b1
b = (b2)
     b3

     y1
y = (y2)
     y3
     y4
```

Reformulated, the problem becomes a system of li... unknown. This type of system is referred to as ove... an there are unknowns, i.e. each coefficient is used o...

It is a challenging problem to solve analytically bec... . multiple possible values for the coefficients. Furthe... is no line that will pass nearly through all points, ther... be able to handle that.

The way this is typically achieved is by finding a solution where the values for b in the model minimize the squared error. This is called linear least squares.

```
||X . b - y||^2 = sum i=1 to m ( sum j=1 to n Xij . bj - yi)^2
```

This formulation has a unique solution as long as the input columns are independent (e.g. uncorrelated).

> *We cannot always get the error e = b – Ax down to zero. When e is zero, x is an exact solution to Ax = b. When the length of e is as small as possible, xhat is a least squares solution.*

— Page 219, Introduction to Linear Algebra, Fifth Edition, 2016.

In matrix notation, this problem is formulated using the so-named normal equation:

```
X^T . X . b = X^T . y
```

This can be re-arranged in order to specify the solution for b as:

```
b = (X^T . X)^-1 . X^T . y
```

This can be solved directly, although given the presence of the matrix inverse can be numerically challenging or unstable.

Linear Regression Dataset

In order to explore the matrix formulation of linear regression, let's first define a dataset as a context.

We will use a simple 2D dataset where the data is easy to visualize as a scatter plot and models are easy to visualize as a line that attempts to fit the data points.

The exam[...]atrix dataset, splits it into X and y components, and plots the dataset as a scatter plot.

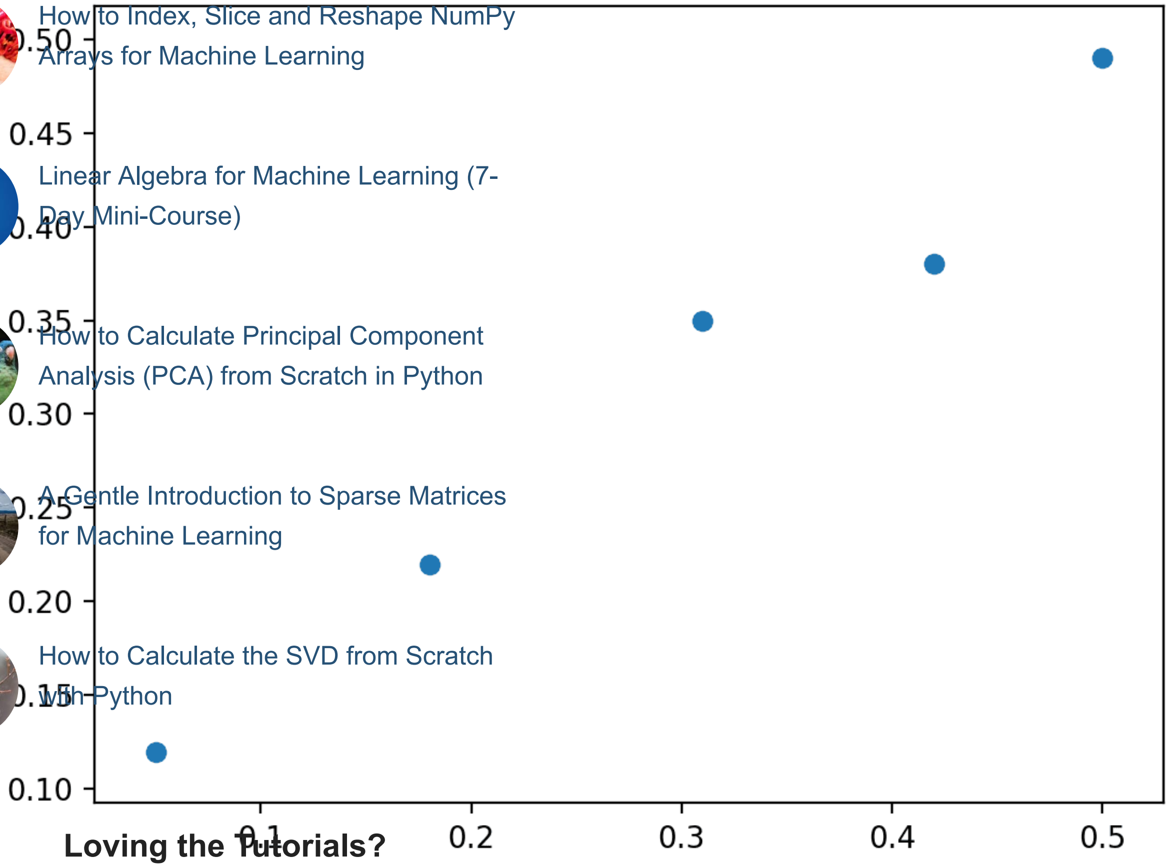
```
from numpy import array
from matplotlib import pyplot
data = array([
    [0.05, 0.12],
    [0.18, 0.22],
    [0.31, 0.35],
    [0.42, 0.38],
    [0.5, 0.49],
    ])
print(data)
X, y = data[:,0], data[:,1]
X = X.reshape((len(X), 1))
# plot dataset
pyplot.scatter(X, y)
pyplot.show()
```

Running the example first prints the defined datase

```
[[ 0.05  0.12]
 [ 0.18  0.22]
 [ 0.31  0.35]
```

```
[ 0.42  0.38]
[ 0.5   0.49]]
```


A scatter plot of the dataset is then created showing that a straight line cannot fit this data exactly.



Scatter Plot of Linear Regression Dataset

Solve

The first approach is to attempt to solve the regression problem directly.

That is, given X, what are the set of coefficients b that when multiplied by X will give y. As we saw in a previous section, the normal equations define how

```
b = (X^T . X)^-1 . X^T . y
```

This can be calculated directly in NumPy using the

```
b = inv(X.T.dot(X)).dot(X.T).dot(y)
```

Once the coefficients are calculated, we can use th

```
yhat = X.dot(b)
```

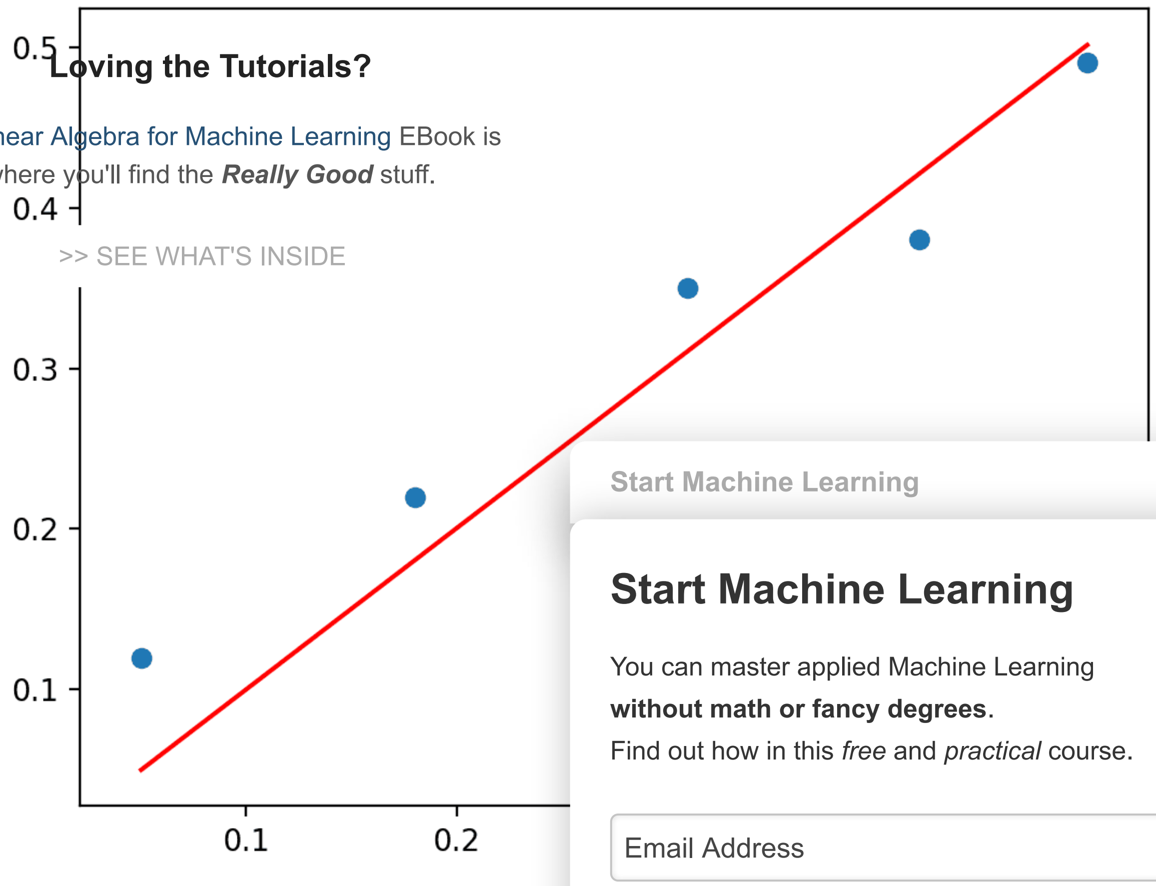
Putting this together with the dataset defined in the below.

```
# solve directly
from numpy import array
from numpy.linalg import inv
from matplotlib import pyplot
data = array([
	[0.05, 0.12],
	[0.18, 0.22],
	[0.31, 0.35],
	[0.42, 0.38],
	[0.5, 0.49],
	])
X, y = data[:,0], data[:,1]
X = X.reshape((len(X), 1))
# linear least squares
b = inv(X.T.dot(X)).dot(X.T).dot(y)
print(b)
# predict using coefficients
yhat = X.dot(b)
# plot data and predictions
pyplot.scatter(X, y)
pyplot.plot(X, yhat, color='red')
pyplot.show()
```


Running the example performs the calculation and prints the coefficient vector b.

```
[ 1.00233226]
```


A scatter plot of the dataset is then created with a line plot for the model, showing a reasonable fit to the data.



Scatter Plot of Direct Solution

A problem with this approach is the matrix inverse that is both computationally expensive and numerically unstable. An alternative approach is to use a matrix decomposition to avoid this operation. We will look at two examples in the following sections.

Solve via QR Decomposition

The QR decomposition is an approach of breaking a matrix down into its constituent elements.

```
A = Q . R
```

Where A is the matrix that we wish to decompose, Q a matrix with the size m x m, and R is an upper triangle matrix with the size m x n.

The QR decomposition is a popular approach for solving the linear least squares equation.

Stepping over all of the derivation, the coefficients can be found using the Q and R elements as follows:

```
b = R^-1 . Q.T . y
```

The approach still involves a matrix inversion, but in this case only on the simpler R matrix.

The QR decomposition can be found using the qr() function in NumPy. The calculation of the coefficients in NumPy looks as follows:

```
# QR decomposition
Q, R = qr(X)
b = inv(R).dot(Q.T).dot(y)
```

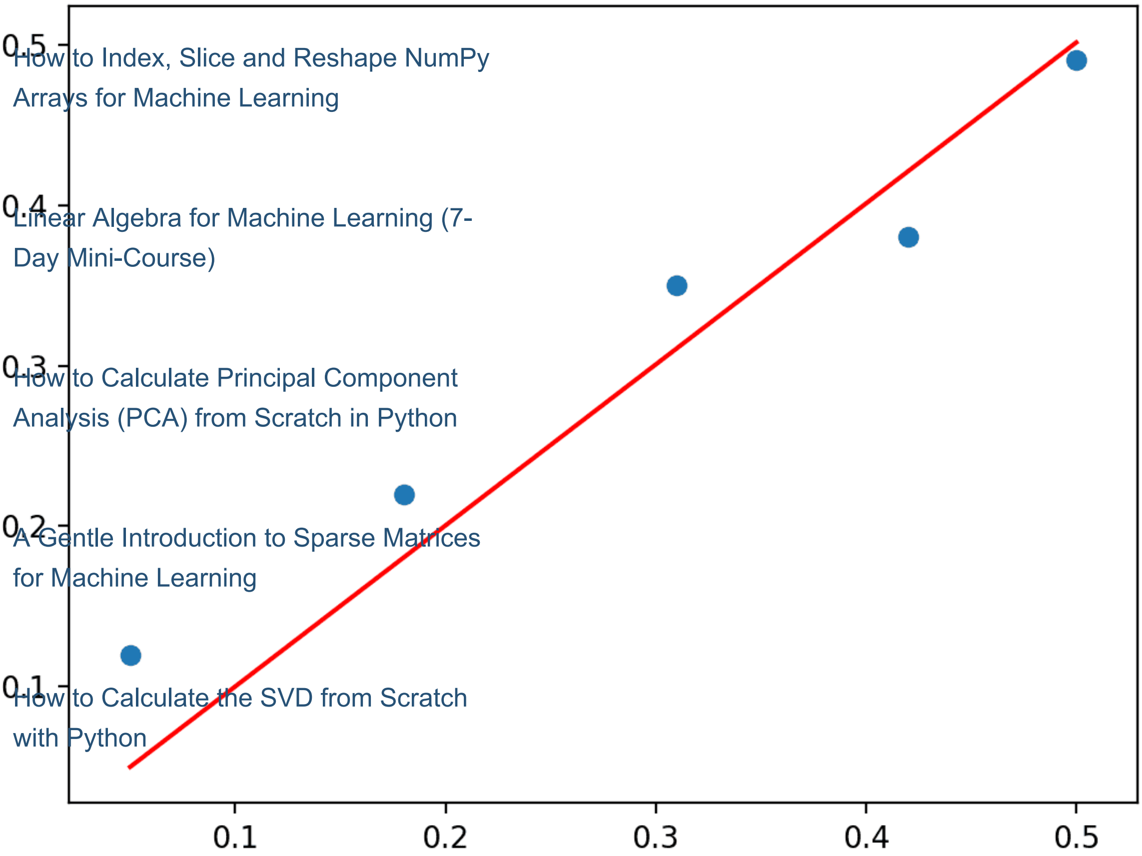
Tying this together with the dataset, the complete example is listed below.


```
# least squares via QR decomposition
from numpy import array
from numpy.linalg import inv
from numpy.linalg import qr
from matplotlib import pyplot
data = array([
[0.05, 0.12],
[0.18, 0.22],
[0.31, 0.35],
[0.42, 0.38],
[0.5, 0.49],
])
X, y = data[:,0], data[:,1]
X = X.reshape((len(X), 1))
# QR decomposition
Q, R = qr(X)
b = inv(R).dot(Q.T).dot(y)
print(b)
# predict using coefficients
yhat = X.dot(b)
# plot data and predictions
pyplot.scatter(X, y)
pyplot.plot(X, yhat, color='red')
pyplot.show()
```

Running the example first prints the coefficient sol

```
[ 1.00233226]
```

The QR decomposition approach is more computationally efficient and more numerically stable than calculating the normal equation directly, but does not work for all data matrices.



Scatter Plot of QR Decomposition Solution to the Linear Regression Problem

Solve via Singular-Value Decomposition

The Singular-Value Decomposition, or SVD for short, is a matrix decomposition method like the QR decomposition.

```
X = U . Sigma . V^*
```

Where A is the real n x m matrix that we wish to de[...] represented by the uppercase Greek letter Sigma) [...]ate transpose of an n x n matrix where * is a superscri[...]

Unlike the QR decomposition, all matrices have ar[...] system of linear equations for linear regression, S[...]

Once decomposed, the coefficients can be found [...] x X and multiplying that by the output vector y.

```
b = X^+ . y
```

Where the pseudoinverse is calculated as followin[...]

```
X^+ = U . D^+ . V^T
```


Where X^+ is the pseudoinverse of X and the + is a superscript, D^+ is the pseudoinverse of the ...ona... ...atri... ...ma... ...d V... the transpose of V^*.

> *Matrix inversion is not defined for matrices that are not square. [...] When A has more columns than rows, then solving a linear equation using the pseudoinverse provides one of the many possible solutions.*

— Page 46, Deep Learning, 2016.

... get U and V from the SVD operation. D^+ can be calculated by creating a diagonal matrix from Sigma and calculating the reciprocal of each non-zero element in Sigma.

```
             s11,   0,   0
Sigma = (      0, s22,   0)
               0,   0, s33

          1/s11,      0,      0
D = (         0,  1/s22,      0)
              0,      0,  1/s33
```

... can calculate the SVD, then the pseudoinverse manually. Instead, NumPy provides the function pinv() that we can use directly.

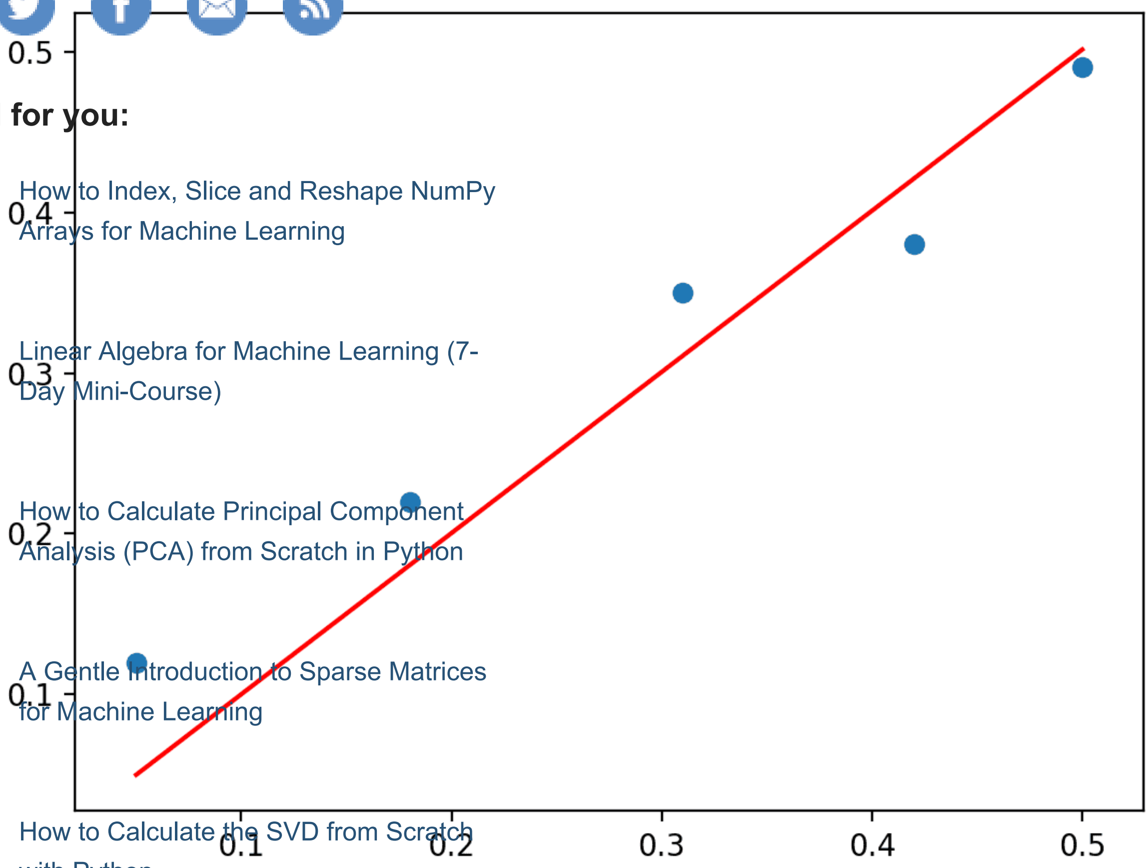
... mplete example is listed below.

```
# least squares via SVD with pseudoinverse
from numpy import array
from numpy.linalg import pinv
from matplotlib import pyplot
data = array([
    [0.05, 0.12],
    [0.18, 0.22],
    [0.31, 0.35],
    [0.42, 0.38],
    [0.5, 0.49],
    ])
X, y = data[:,0], data[:,1]
X = X.reshape((len(X), 1))
# calculate coefficients
b = pinv(X).dot(y)
print(b)
# predict using coefficients
yhat = X.dot(b)
# plot data and predictions
pyplot.scatter(X, y)
pyplot.plot(X, yhat, color='red')
pyplot.show()
```


Running the example prints the coefficient and plo... from the model.

```
[ 1.00233226]
```

In fact, NumPy provides a function to replace these ... directly.



Scatter Plot of SVD Solution to the Linear Regression Problem

Extensions

This section lists some ideas for extending the tutorial that you may wish to explore.

- Imple ing the built-in lstsq() NumPy function
- Test each linear regression on your own small contrived dataset.
- Load a tabular dataset and test each linear regression method and compare the results.

If you explore any of these extensions, I'd love to know.

Further Reading

This section provides more resources on the topic

Books

- Section 7.7 Least squares approximate solutio
- Section 4.3 Least Squares Approximations, In
- Lecture 11, Least Squares Problems, Numeric
- Chapter 5, Orthogonalization and Least Squa
- Chapter 12, Singular-Value and Jordan Decor Statistics, 2014.

- Section 2.9 The Moore-Penrose Pseudoinverse, Deep Learning, 2016.
- Section 15.4 General Linear Least Squares, Numerical Recipes: The Art of Scientific Computing, Third Edition, 2007.

API

- numpy.linalg.inv() API
- numpy.linalg.qr() API
- numpy.linalg.svd() API
- numpy.diag() API
- numpy.linalg.pinv() API
- numpy.linalg.lstsq() API

Articles

- Linear regression on Wikipedia
- Least squares on Wikipedia
- Linear least squares (mathematics) on Wikipedia
- Overdetermined system on Wikipedia
- QR decomposition on Wikipedia
- Singular-value decomposition on Wikipedia
- Moore–Penrose inverse

Tutorials

- The Linear Algebra View of Least-Squares Regression
- Linear Algebra with Python and NumPy

Summary

In this tutorial, you discovered the matrix formulation of linear regression and how to solve it using direct and matri

Specifically, you learned:

- Linear regression and the matrix reformulation with the normal equations.
- How to solve linear regression using a QR ma
- How to solve linear regression using SVD and

Do you have any questions?

Ask your questions in the comments below and I w

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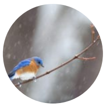
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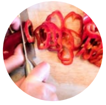
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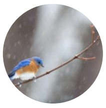
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About Jason Brownlee

Jason Brownlee, PhD is a machine lea … s with modern machine learning methods

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28 Responses to *How to Solve Linear Regression Using Linear Algebra*

John Menzies March 9, 2018 at 10:05 pm #

REPLY

In your introduction you refer to the univariate problem, y=b0+b1*x, or Y=X.b in matrix notation. clear that b is a 2x1 matrix, so X has to be a nx2 matrix.
ever, in your implementation of the various methods of solution you implicitly assume that b0 = 0 and then X is a nx1 matrix and b a 1×1 matrix.
For the example dataset you have chosen, this leads to a plausible solution of b1=1.00233, with a sum uared deviations of 0.00979 and the fitted line looks more or less OK. But it is definitely not a least ares solution for the data set.
If you fit for b0 as well, you get a slope of b1= 0.78715 and b0=0.08215, with the sum of squared deviations of 0.00186. To do this, the X matrix has to be augmented with a column of ones.
data set had been
= array([
[5.05, 0.12],
[5.18, 0.22],
, 0.35],
2, 0.38],
[5.5, 0.49],
])
then fitting for b0 and b1 would give b1=0.78715 as before but using your formalism b1 becomes 0.05963 with sums of squared deviations of 0.00186 as before for the 2-parameter fit, but 0.07130 in your case.
Your presentation is generally quite clear, but I think it is misleading nevertheless in suggesting that it leads t

Jason Brownlee March 10, 2018 at 6:28 am #

REPLY

Thanks John.

Alex November 10, 2018 at 9:00 am #

Hi Jason,

Thank you very much for this great and very helpfu
I wonder how this method can work for quadratic c

Jason Brownlee November 11, 2018 at 5:56 am # REPLY

ca e a r model with inputs raised to exponents, e.g, x^2, x^3, etc. E.g. polynomial regression.

Iyapo kamoru November 1, 2020 at 4:44 pm # REPLY

You are too much. I need more. I would like to tell you that you are excellent in this area. More from you. Thanks

Jason Brownlee November 2, 2020 at 6:39 am # REPLY

Thanks!

Alan April 29, 2019 at 1:15 am # REPLY

Hi Jason,

ve two questions:

Does the coefficient b is always a singular value? I thought it should be a vector containing the coefficients for each Xi.

Also, can this example be applied to fit for example two parallel lines?

il 29, 2019 at 8:23 am # REPLY

It is a vector of coefficients if you have a vector of inputs.

e.g. yhat = X . b

Arthur August 12, 2019 at 5:37 am #

Hi Jason,

Thank you so much for all the encyclopedia of mac

I have one question: when using sklearn's Linear R reg.coef_ outputs "0.78715288" instead of "1.0023

I've passed X and y the same way you did here an you have any ideas why this has happened?

Jason Brownlee August 12, 2019 at 6:41 am #

REPLY

[illegible] the way they perform the calculation may give slightly different coefficients/results.

The sklearn library is developed to be robust to many situations, I would expect they have made useful changes to the base method along these lines.

Javier May 7, 2021 at 5:12 am #

REPLY

Hi Arthur,

This is not a minor difference and has nothing to do with the robustness of scikit-learn.

The difference is that scikit-learn's Linear Regression model includes the intercept, whereas Jason is not here. If you want to omit this term and still get the same result for b as in scikit-learn (0.78715288), you need to subtract the mean from X and y before solving the linear regression model.

Cheers,

Jason Brownlee May 7, 2021 at 6:31 am #

REPLY

Yes, the intercept just centers the data, so to speak. Like a data prep.

Alex September 2, 2019 at 6:31 pm #

REPLY

Hi Jason,

great tutorial. I am solving a problem where my linear regression can be vertical (for example x = 3). For this problem y = X . b does not work. Do you have any ideas how to solve the problem of vertical lines?

Jason Brownlee September 3, 2019 at 6

Do you mean columns of data?

Typically a column represents many observatio

Perhaps rotate your data so that a column bec

Newsha July 21, 2020 at 5:11 pm #

I want to know that is it possible to extract

like Convolutional Neural Networks (CNN) or Autoe

on **wn** July 22, 2020 at 5:27 am # REPLY

You can retrieve and save the model weights directly from a neural net.

Newsha July 22, 2020 at 4:00 pm # REPLY

you're right. but I have another issue.

The goal is to model choice in terms of x1 to x3 and recover the true values of beta1 to beta3 as their coefficients. V and U are unobserved

```
NumberOfObservations = 10000

beta1 = 4 # true values of the parameters of the model (randomly selected)
beta2 = -2
beta3 = 2

# Data generation
data = {'ID': pd.Series(range(1, (NumberOfObservations+1)))}
df = pd.DataFrame(data)

df['x1'] = np.random.normal(loc = 0, scale = 1, size = NumberOfObservations)
df['x2'] = np.random.normal(loc = 0, scale = 1, size = NumberOfObservations)
df['x3'] = np.random.normal(loc = 0, scale = 1, size = NumberOfObservations)

df['V1'] = beta1 * df['x1'] + beta2 * df['x2'] + beta3 * df['x3']

df.loc[df['V1'] >=0, 'choice'] = 1
df.loc[df['V1'] <0, 'choice'] = 0
```

for classification problems, in each layer we have several weights and in the last layer(if we have 2 classes 0 or 1) there are two weights for each Xi, how should I calculate se?

Jason Brownlee July 23, 2020 at 6:02 am # REPLY

I believe you are describing a solution, e.g. a logistic regression – no

rose March 5, 2021 at 7:58 am #

Solve a linear system of equations in the f

vector x, using QR factorization.in QR decompositi

Jason Brownlee March 5, 2021 at 8:16 am # REPLY

this example:
https://machinelearningmastery.com/introduction-to-matrix-decompositions-for-machine-learning/

Rose March 8, 2021 at 7:30 pm # REPLY

No this is not answer my question .my question say that Ax=b find x by qr factorization

Jason Brownlee March 9, 2021 at 5:17 am # REPLY

I believe I have linked to resources that should help.

I do not have the capacity to prepare a code example for you, sorry.

Maybe I'm not the best person to help you with your project.

rose March 9, 2021 at 12:15 am # REPLY

please give me some example about this

Diagonalize a matrix M, such that it can be written in the form D = P −1 MP,

where D is diagonal.

Jason Brownlee March 9, 2021 at 5:21 am # REPLY

This tutorial shows how to calculate a diagonal matrix:
https://machinelearningmastery.com/introduction-to-types-of-matrices-in-linear-algebra/

From there, you will have enough to implemen

rose March 29, 2021 at 3:57 am #

hi dear

in linear algebra
what is a np.linalg.pr
description by linear algebra
plz help

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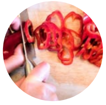
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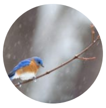
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Jason Brownlee March 29, 2021 at 6:20 am # REPLY

…hap… u ca… eck the API documentation directly: https://numpy.org/doc/stable/reference/routines.linalg.html

Abidex November 9, 2021 at 11:30 pm # REPLY

Using numpy, for a general case of linear regression with one predictor variable and one …ponse variable. Use matplotlib to plot a scatterplot and the fitted line. Also plot the "residuals vs fitted" …h and calculate the $R2$ value. Compare your results with the R function lm() using one of …scombe's quartet as the dataset. You may find numpy.hstack(), np.ones() and numpy.reshape() useful.

… understands questions like this, please? …se I need a feedback. thanks.

adestop0072004@yahoo.ca

Adrian Tam November 14, 2021 at 1:23 pm # REPLY

What is your question?

Leave a Reply

Name (required)

Email (will not be published)

Website

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Welcome!
I'm *Jason Brownlee* PhD
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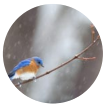

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