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Polynomial Curve Fitting

Abstract—This document contains theory involved in curve fitting.

1 Objective

The objective is to fit best line for the polynomial curve using regularization.

2 Generate Dataset

Create a sinusoidal function of the form

$$y = A \sin 2\pi x + n(t)$$
 (2.0.1)

n(t) is the random noise that is included in the training set. This set consists of N samples of input data i.e. x expressed as shown below

$$x = (x_1, x_2, ..., x_N)^T$$
 (2.0.2)

which give the corresponding values of y denoted as

$$y = (y_1, y_2, ..., y_N)^T$$
 (2.0.3)

The Fig 0 is generated by random values of x_n for

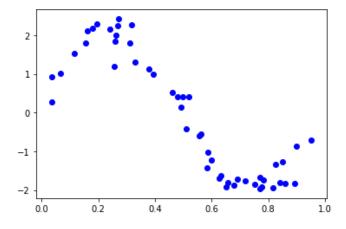


Fig. 0: Sinusoidal Dataset with added noise

n = 1,2,...,N. where N = 50 in the range [0,1].

The corresponding values of y were generated from the Eq (2.0.1). The first term $A \sin 2\pi x$ is computed directly and then random noise samples having a normal (Gaussian) distribution are added inorder to get the corresponding values of y.

import numpy as np
import matplotlib.pyplot as plt

N = 50
np.random.seed(20)
x = np.sort(np.random.rand(N,1),axis=0)
noise = np.random.normal(0,0.3,size=(N,1))
A = 2.5
y = A*np.sin(2*np.pi*x) + noise

plt.scatter(x,y,c='b',marker='o',label='Data with noise')

#Generate the sine curve

plt.xlabel('x');plt.ylabel('y')

The following code generates the input matrix F

The generated matrix would look like

$$\mathbf{F} = \begin{pmatrix} 1 & x_0 & x_0^2 & \dots & x_0^{N-1} \\ 1 & x_1 & x_1^2 & \dots & x_1^{N-1} \\ 1 & x_2 & x_2^2 & \dots & x_2^{N-1} \\ \vdots & \vdots & & \vdots \\ 1 & \dots & \dots & x_N^{N-1} \end{pmatrix}$$
 (2.0.4)

3 POLYNOMIAL CURVE FITTING

The goal is to find the best line that fits into the pattern of the training data shown in the graph. We shall fit the data using a polynomial function of the form,

$$y(w, x) = \sum_{j=0}^{M} w_j x^j$$
 (3.0.1)

(3.0.2)

M is the order of the polynomial The polynomial coefficient are collectively denoted by the vector

w. The proposed vector \mathbf{w} of the model referring to Eq (2.0.4) is given by

$$\hat{\mathbf{w}} = \left(\mathbf{F}^T \mathbf{F}\right)^{-1} \mathbf{F}^T y \tag{3.0.3}$$

Now, adding a regularization term to the error function controls the over-fitting and the total error function takes the form

$$E_D(w) + \lambda E_W(w) \tag{3.0.4}$$

One of the simplest forms of the regularizer is given by the sum of the squares of the weight vector element

$$E_W(w) = \frac{1}{2} w^T w (3.0.5)$$

The values of the coefficients are determined by fitting the polynomial to the training data. This can be done by minimizing an **error function** that measures the misfit between the function y and the training set data points. The sum-of-squares error function is given by

$$\sum_{n=1}^{N} (y_n - w^T f(n))^2$$
 (3.0.6)

where F = f(n) Thus, the total error function becomes

$$\frac{1}{2} \sum_{n=1}^{N} \left(y_n - w^T f(n) \right)^2 + \frac{\lambda}{2} w^T w$$
 (3.0.7)

Eq (3.0.7) can be further expressed as

$$(\mathbf{y} - \mathbf{w}\mathbf{F})^T (\mathbf{y} - \mathbf{w}\mathbf{F}) + \lambda \|\mathbf{w}\|^2$$
 (3.0.8)

where $\|\mathbf{w}\|^2 = \mathbf{w}^T \mathbf{w}$. Expand Eq (3.0.8). Let

$$E = (\mathbf{y} - \mathbf{w}\mathbf{F})^{T} (\mathbf{y} - \mathbf{w}\mathbf{F}) + \lambda \mathbf{w}^{T}\mathbf{w}$$

$$(3.0.9)$$

$$= \mathbf{y}^{T}\mathbf{y} - \mathbf{y}^{T}\mathbf{w}\mathbf{F} - \mathbf{w}^{T}\mathbf{F}^{T}\mathbf{y} + \mathbf{w}^{T}\mathbf{F}^{T}\mathbf{F}\mathbf{w} + \lambda \mathbf{w}^{T}\mathbf{w}$$

$$(3.0.10)$$

$$= \mathbf{y}^{T}\mathbf{y} - \mathbf{w}^{T}\mathbf{F}^{T}\mathbf{y} - \mathbf{w}^{T}\mathbf{F}^{T}\mathbf{y} + \mathbf{w}^{T}\mathbf{F}^{T}\mathbf{F}\mathbf{w} + \mathbf{w}^{T}\lambda\mathbf{I}\mathbf{w}$$

$$= \mathbf{y}^{T} \mathbf{y} - \mathbf{w}^{T} \mathbf{F}^{T} \mathbf{y} - \mathbf{w}^{T} \mathbf{F}^{T} \mathbf{y} + \mathbf{w}^{T} \mathbf{F}^{T} \mathbf{F} \mathbf{w} + \mathbf{w}^{T} \lambda \mathbf{I} \mathbf{w}$$
(3.0.11)

$$= \mathbf{y}^{T}\mathbf{y} - 2\mathbf{w}^{T}\mathbf{F}^{T}\mathbf{y} + \mathbf{w}^{T}(\mathbf{F}^{T}\mathbf{F} + \lambda \mathbf{I})\mathbf{w}$$
(3.0.12)

Evaluate **w** that minimizes E. Here, we make use of matrix differentiation rule given as

$$\frac{\partial x A^T x}{\partial x} = (A + A^T)x = 2Ax \tag{3.0.13}$$

We get 2Ax when A is symmetric. This can be applied here as $(\mathbf{F}^T\mathbf{F} + \lambda \mathbf{I})$. From Eq (3.0.12)

$$\frac{\partial E}{\partial \mathbf{w}} = -2\mathbf{F}^T \mathbf{y} + 2\left(\mathbf{F}^T \mathbf{F} + \lambda \mathbf{I}\right) \mathbf{w} = 0 \qquad (3.0.14)$$

$$\implies (\mathbf{F}^T \mathbf{F} + \lambda \mathbf{I}) \mathbf{w} = \mathbf{F}^T \mathbf{y} \qquad (3.0.15)$$

$$\implies$$
 $\mathbf{w} = (\mathbf{F}^T \mathbf{F} + \lambda \mathbf{I})^{-1} \mathbf{F}^T \mathbf{y}$ (3.0.16)

The coefficient λ governs the relative importance of the regularization term compared with the sum-of-the-squares term.

A more general regularizer is used for which the regularized error takes the form

$$\frac{1}{2} \sum_{n=1}^{N} \left(y_n - w^T f(n) \right)^2 + \frac{\lambda}{2} \sum_{i=1}^{M} \left| w_i \right|^q$$
 (3.0.17)

q = 2 corresponds to quadratic regularizer. The case of q = 1 in known as the lasso. It has the property that if λ is sufficiently large, some of the coefficients w_j are driven to zero, leading to a sparse model in which the corresponding basis functions play no role.

The error function for q = 1 (Lasso) would look like

$$\frac{1}{2} \sum_{n=1}^{N} \left(y_n - w^T f(n) \right)^2 + \frac{\lambda}{2} \sum_{j=1}^{M} \left| w_j \right|$$
 (3.0.18)

Regularization allows complex models to be trained on data sets of limited size without severe overfitting, essentially by limiting the effective model complexity

First, we take a random guess of the sine curve on the input data

plt.plot(np.linspace(0,1,50),np.sin(2*np.linspace (0,1,50)*np.pi),c='g',linewidth=2,label=' function generating input data')

Now, we use the scikit learn and import Lasso

model = Lasso(alpha = 0.000005) model.fit(F,y)

Plot the predicted output

The plot would look like Fig 0 Python code:

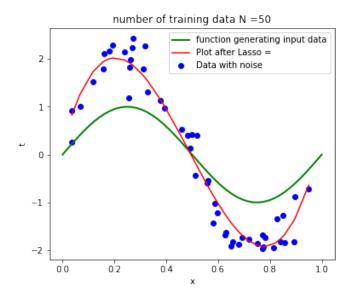


Fig. 0: Curve Fitting after Lasso regression

https://github.com/Hrithikraj2/EE4015_IDP/blob/main/Assignment_4/Assignment_4.ipynb