

Lecture Module - Numerical Integration and Curve Fitting

ME3001 - Mechanical Engineering Analysis

Mechanical Engineering

Tennessee Technological University

Module 5 - Numerical Integration and Curve Fitting

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- Topic 1 - Overview and Motivation
- Topic 2 - Linear Regression
- Topic 3 - Interpolation and Splines
- Topic 4 - Lagrange Polynomials

Topic 1 - Overview and Motivation

- Problem Definition
- Engineering Applications
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Problem Definition

What is curve fitting?

- various techniques to fit a curve or function to discrete data
- "Data is often given for discrete values along a continuum. However, you may require estimates at points between the discrete values" -
Numerical Methods for Engineers, Chapra and Canale
- additional problem is to find a simpler form of a complicated function by fitting function to data sampled from original function

Problem Definition

Two General Approaches

- 1) Given data with random error, find a single curve that represents the overall trend of the data.
 - "Because any individual data point may be incorrect, we make no effort to intersect every point" - Numerical Methods for Engineers, Chapra and Canale
 - Common method is *regression* (LSR)
- 2) Given data assumed to be precise or specified, find a curve that directly passes through each data point
 - Known as *interpolation, extrapolation*

Engineering Applications

Example Applications in Engineering

- Calibration Curves, Sensors and Instrumentation
- Table Interpolation, Mechanics, Thermo, Statistics
- Velocity Profile Generation, Dynamics of Machinery, Robotics

Two General Problems

- Trend Analysis - predictions from dataset using interpolation polynomial or LSR
- Hypothesis Testing - compare predicted to measured data for model performance or selection

Topic 2 - Linear Regression

- Overview
- Fit Criteria
- Linear Least Squares
- MATLAB Example

Overview

Consider fitting a straight line to a dataset

$$(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$$

with a function

$$y = a_0 + a_1$$

A value y can be defined in terms of the function with an error term e

$$y = a_0 + a_1 + e$$

This can be rearranged to show the **error** as

$$e = y - a_0 - a_1x$$

The goal is to find the coefficients of a function that minimizes the error

Fit Criteria

To find the coefficients of the fit line, the minimization objective must be considered carefully. You might consider fitting a model that minimizes the error directly, but this will not work. The absolute value approach is also problematic.

- $\sum_{i=1}^n e_i = (y_i - a_0 - a_1 x_i)$
- $\sum_{i=1}^n |e_i| = |y_i - a_0 - a_1 x_i|$

To solve these issues, the common technique is to _____ the error.

- $\sum_{i=1}^n e_i^2 = (y_i - a_0 - a_1 x_i)^2$

Linear Least Squares

To fit a straight line to the data, we must find the values a_0 and a_1 that minimize the square of the error. First find the partial derivatives of the squared error and set these equal to zero

$$S_r = \sum_{i=1}^n e_i^2 = (y_i - a_0 - a_1 x_i)^2$$

$$\frac{\delta S_r}{\delta a_0} = -2 \sum (y_i - a_0 - a_1 x_i)$$

$$\frac{\delta S_r}{\delta a_1} = -2 \sum [(y_i - a_0 - a_1 x_i) x_i]$$

$$0 = \sum y_i - \sum a_0 - \sum a_1 x_i$$

$$0 = \sum y_i x_i - \sum a_0 x_i - \sum a_1 x_i^2$$

Linear Least Squares

Use $\Sigma a_0 = na_0$ and the resulting equations can be solved as a linear system in terms of the coefficients a_0 , a_1 , and number of data points n .

$$0 = \Sigma y_i - \Sigma a_0 - \Sigma a_1 x_i$$

$$0 = \Sigma y_i x_i - \Sigma a_0 x_i - \Sigma a_1 x_i^2$$

This leads to the standard equations

$$a_1 = \frac{n \Sigma x_i y_i - \Sigma x_i \Sigma y_i}{n \Sigma x_i^2 - (\Sigma x_i)^2}$$

$$a_0 = \bar{y} - a_1 \bar{x}$$

This alternate form can be found by multiplying by $1 = \frac{-1}{-1}$

$$a_1 = \frac{\Sigma x_i \Sigma y_i - n \Sigma x_i y_i}{(\Sigma x_i)^2 - n \Sigma x_i^2}$$

$$a_0 = \frac{\Sigma x_i \Sigma x_i y_i - \Sigma x_i^2 \Sigma y_i}{(\Sigma x_i)^2 - n \Sigma x_i^2}$$

MATLAB Example

This standard technique is built into the MATLAB function *polyfit*. This function can also be used for higher order regression lines.

```
% ME3001, TNTech, Tristan Hill, October 29, 2024
% Curve fitting with Linear Regression
% this program will
% 1) generate dataset with random noise
% 2) find best fit using 'linear least squares regression' from
    eqs in notes
% 3) find best fit using LSR with MATLAB polyfit()
clear; clc; close all
```

MATLAB Example

```
% step 1) - generate dataset
m=-3; b=1.5;
error_scale=5;

xdata=-5:.5:5;
n=length(xdata);
ydata=m*xdata+b+rand(1,n)*error_scale;

figure(1); hold on
plot(xdata,ydata,'o')
grid on
```

MATLAB Example

`% step 2) - fit line with LSR equations`

```
a1=(n*sum(xdata.*ydata)-sum(xdata)*sum(ydata))/...  
    (n*sum(xdata.^2)-sum(xdata.^2))  
a0=sum(ydata)/n
```

`% compare with equations from ME3023`

```
a1=(sum(xdata)*sum(ydata)-n*sum(xdata.*ydata))/...  
    (sum(xdata)^2-n*sum(xdata.^2))  
a0=(sum(xdata)*sum(xdata.*ydata)-sum(xdata.^2)*sum(ydata))/...  
    (sum(xdata)^2-n*sum(xdata.^2))
```

MATLAB Example

```
% compute and plot values on the best fit line
xfit=-5:.1:5;
yfit=a1*xfit+a0;

plot(xfit,yfit,'-')

% step 3) - fit line with LSR in MATLAB
A=polyfit(xdata,ydata,1) % get second the coefficients

pfit=A(2)+A(1)*xfit; % calculate points on curve
plot(xfit,pfit,':g','LineWidth',5)
```

Download *linear_regression_example1.m* for the complete program.

Topic 3 - Interpolation and Splines

- Polynomial Interpolation Functions
- Polynomial Splines
- Linear Splines
- Cubic Splines

Polynomial Interpolation Functions

Polynomial Interpolation Functions

Polynomial Splines

Polynomial Splines

Linear Splines

Fit a **spline** function consisting of multiple *linear* functions to a set of data.

- the spline must pass through n data points $(x_i, f_i)_{i=1,2,\dots,n}$
- $n - 1$ intervals are defined by spline functions $s_i(x)_{i=1,2,\dots,n-1}$

$$s_i(x) = a_i + b_i(x - x_i)$$

$$a_i = f_i$$

$$b_i = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

- the $(x - x_i)$ term handles the shift to the i^{th} spline function
- substitute b_i into $s_i(x)$ to get the following description of the spline

$$s_i(x) = f_i + \left(\frac{f_{i+1} - f_i}{x_{i+1} - x_i} \right) (x - x_i)$$

Linear Splines

Cubic Splines

"Cubic splines are most commonly used in practice"

Fit a **spline** function consisting of multiple *cubic* functions to the data

- the spline must pass through n data points $(x_i, f_i)_{i=1,2,\dots,n}$
- $n - 1$ intervals are defined by spline functions $s_i(x)_{i=1,2,\dots,n-1}$

$$s_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$$

- coefficients a_i, b_i, c_i, d_i must be found $\implies 4(n - 1)$ unknowns
- the slope at each point must match for a smooth spline
- two additional conditions are required due to no slope match at ends

$$2 * (n - 1) + 2 * (n - 1) - 2 + 2 = 4(n - 1)$$

Cubic Splines

The functions passes through all the data points

$$s_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$$

$$s_i(x_i) = f_i$$

$$f_i = a_i + b_i(x_i - x_i) + c_i(x_i - x_i)^2 + d_i(x_i - x_i)^3 = a_i$$

The a_i coefficients can be replaced with the function values f_i

$$f_i = a_i$$

$$s_i(x) = f_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$$

Define the i^{th} stepsize for convenience

$$h_i = x_{i+1} - x_i$$

Cubic Splines

The function values are equal at each point

$$f_i + b_i (h_i) + c_i (h_i)^2 + d_i (h_i)^3 = f_{i+1}$$

The slope (first derivative) matches at each point between intervals

$$s'_i(x) = b_i + 2c_i(x - x_i) + 3d_i(x - x_i)^2$$

$$\begin{aligned} & b_i + 2c_i(x_{i+1} - x_i) + 3d_i(x_{i+1} - x_i)^2 \\ &= b_{i+1} + 2c_{i+1}(x_{i+1} - x_{i+1}) + d_{i+1}(x_{i+1} - x_{i+1}) \\ &\implies b_i + 2c_i h_i + 3d_i h_i^2 = b_{i+1} \end{aligned}$$

The second derivative is also matches at the nodes for a *natural spline*

$$s''_i(x) = 2c_i + 6d_i(x - x_i)$$

$$2c_i + 6d_i h_i = 2c_{i+1} + 6d_i(x_{i+1} - x_{i+1}) \implies d_i = \frac{c_{i+1} - c_i}{3h_i}$$

Cubic Splines

Topic 3 - Lagrange Polynomials



