INTRODUCTION TO SCIENTIFIC & ENGINEERING COMPUTING BIL 108E, CRN24023

Dr. S. Gökhan Karaman

Technical University of Istanbul

April 5, 2010

Tentative Course Schedule, CRN 24023

Week	Date	Topics
1	Feb. 08	Introduction to Scientific and Engineering Computing
2	Feb. 15	Introduction to Program Computing Environment
3	Feb. 22	Variables, Operations and Simple Plot
4	Mar. 01	Algorithms and Logic Operators
5	Mar. 08	Flow Control, Errors and Source of Errors
6	Mar. 15	Functions
6	Mar. 20	Exam 1
7	Mar. 22	Arrays
8	Mar. 29	Solving of Simple Equations
9	Apr. 05	Polynomials Examples
10	Apr. 12	Applications of Curve Fitting
11	Apr. 19	Applications of Interpolation
11	Apr. 24	Exam 2
12	Apr. 26	Applications of Numerical Integration
13	May 03	Symbolic Mathematics
14	May 10	Ordinary Differential Equation (ODE) Solutions with Built-in Functions

LECTURE # 9

LECTURE # 9

1. INTERPOLATION
   1. Lagrange Interpolation
   2. Chebyshev Interpolation
   3. Linear Interpolation
   4. Spline Functions
2. APPROXIMATION
   1. Least Squares Approximation
   2. Linear Regression

INTERPOLATION

Data points for a function (x_i, y_i)

$i = 0, 1, 2, \ldots, n$

x_i are all distinct and are called nodes.

Approximate function should satisfy $\tilde{f}(x_i) = y_i,\ i = 0, 1, \ldots, n$

$\tilde{f}$ is called **interpolant** of the set of data y_i

- polynomial interpolant
  $\tilde{f}(x) = a_0 + a_1\, x + a_2\, x^2 + \ldots + a_n\, x^n$
- trigonometric interpolant
  $\tilde{f}(x) = a_{-M}\, e^{-iMx} + \ldots + a_0 + \ldots + a_M\, e^{iMx}$
- rational interpolant

VANDERMONDE MATRIX

$\tilde{f}(x) = \sum_{k=0}^{n} c_k \, \varphi_k(x_j) = y_j$, $j = 0, 1, 2, \ldots, n$

If we choose $\varphi_k(x) = x^k$

$p(x) = \sum_{k=0}^{n} c_k \, x^k$

$$\begin{pmatrix} 1 & x_0 & \ldots & x_0^n \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & \ldots & x_n^n \end{pmatrix} \begin{pmatrix} c_0 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} y_0 \\ \vdots \\ y_n \end{pmatrix}$$

$$X \, c = y$$

$n+1$ equations for $n+1$ unknowns $c_0, c_1, \ldots, c_n$.
The matrix with the given structure is named as **Vandermonde matrix**

INTERPOLATION

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

INERPOLATION WITH POLYNOMIALS

LAGRANGE INTERPOLATION

$$\varphi_k(x) = \prod_{j=0}^{n} \frac{x - x_j}{x_k - x_j}$$

$$\Pi_n(x) = \sum_{k=0}^{n} y_k \varphi_k(x)$$

write the equation for all n+1 points.

$L_j(x) = \prod_{i=0, i \neq j}^{n} \frac{x - x_i}{x_j - x_i}$
$= \frac{(x-x_0)\ldots(x-x_{j-1})(x-x_{j+1})\ldots(x-x_n)}{(x_j-x_0)\ldots(x_j-x_{j-1})(x_j-x_{j+1})\ldots(x_j-x_n)}$

for $j = 0, 1, 2, \ldots, n$ every $L_j(x)$ has the property $L_j(x_j) = 1$ and $L_j(x_i) = 0$ if $i \neq j$.

INTERPOLATION

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

EXAMPLE

Draw the graph of the Lagrange polynom $L_2(x)$ for the $x_j = j$, $j = 0, 1, 2, 3, 4$ supporting points. The supporting points are equispaced.

Lagrange –Polynom $L_2(x) = \frac{(x-x_0)(x-x_1)(x-x_2)(x-x_3)(x-x_4)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)(x_2-x_4)}$

Here $L_2(x_2) = 1$ and $L_2(x_i) = 0$ if $i \neq 0$

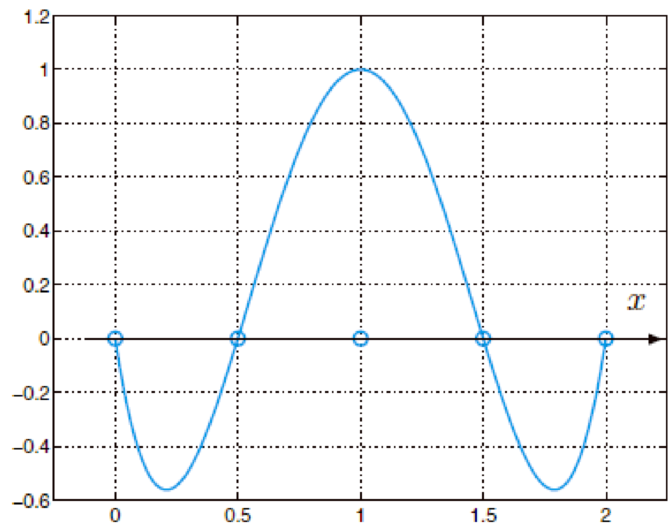
$$p(x) = \sum_{j=0}^{n} y_j \, L_j(x)$$

INTERPOLATION

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

EXAMPLE



INTERPOLATION

EXAMPLE

```
function v = polyinterp(x,y,u)
n = length(x);
v = zeros(size(u));
for k = 1:n
    w = ones(size(u));
    for j = [1:k-1 k+1:n]
        w = (u-x(j))./(x(k)-x(j)).*w;
    end
    v = v + w*y(k);
end
```

To illustrate polyinterp, create a vector of densely spaced evaluation points.

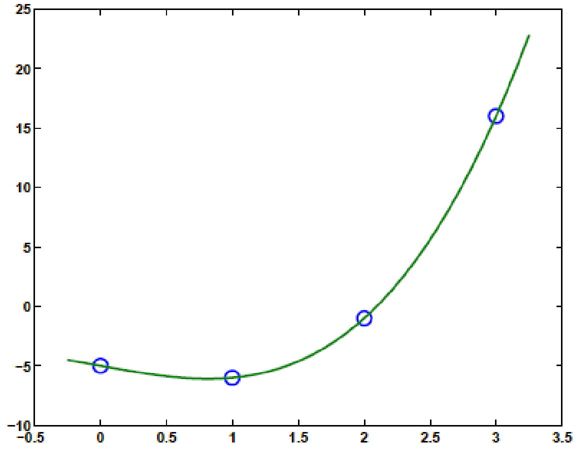
```
u = -.25:.01:3.25;
```

Then

```
v = polyinterp(x,y,u);
plot(x,y,'o',u,v,'-')
```


INTERPOLATION

EXAMPLE



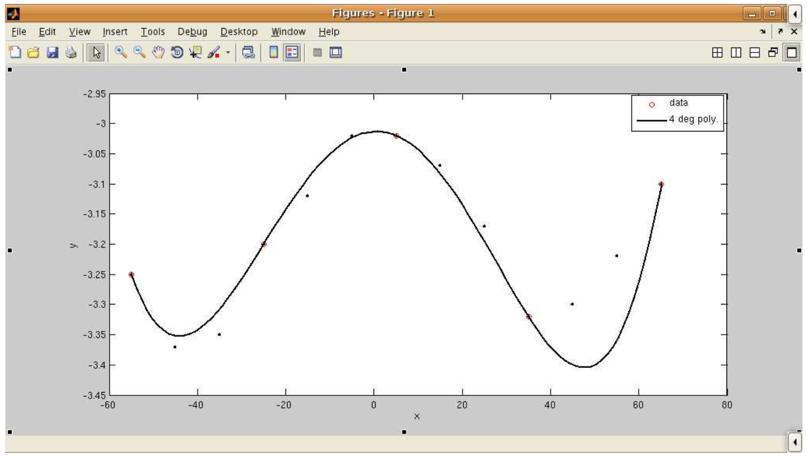
INTERPOLATION

EXAMPLE

```
x = [-55 -25 5 35 65];
y = [-3.25, -3.2, -3.02, -3.32, -3.1];
format short e;
c = polyfit(x, y, 4);
p4x = linspace(x(1), x(end), 100);
p4y = polyval(c,p4x);

plot(x,y,'or')
hold('on')
plot(p4x, p4y, 'k-')
xlabel('x')
ylabel('y')
legend('data', '4 deg poly.')
xdat = [-55:10:65];
ydat = [-3.25, -3.37, -3.35, -3.2, -3.12, -3.02, -3.02 ...
    -3.07, -3.17, -3.32, -3.3, -3.22, -3.1];
plot(xdat,ydat,'.k')
```


INTERPOLATION

EXAMPLE

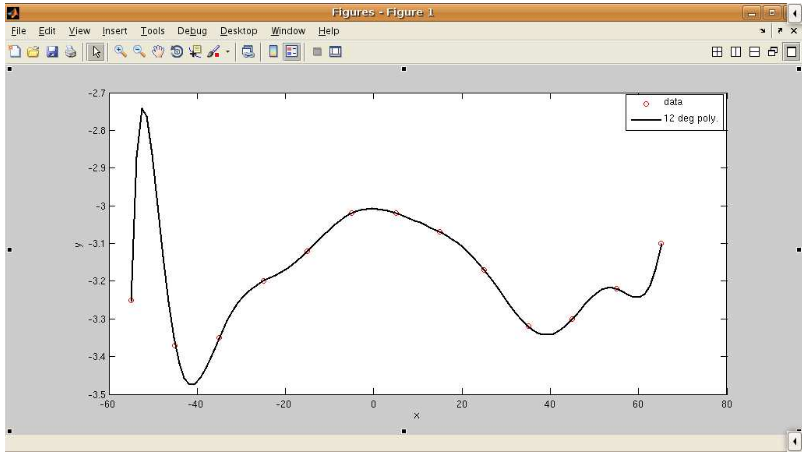


LAGRANGE INTERPOLATION ERROR

EXAMPLE

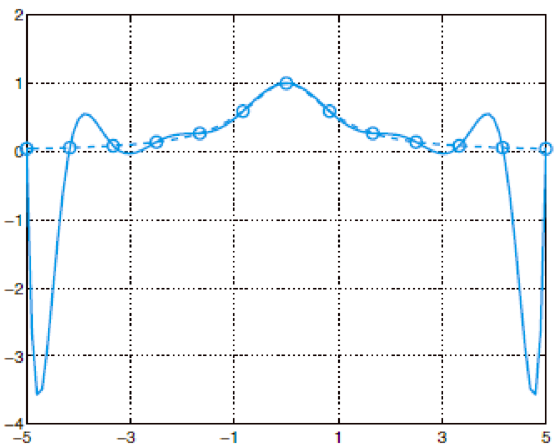
```
clear;
clf;
clc;
x = [-55:10:65];
y = [-3.25, -3.37, -3.35, -3.2, -3.12, -3.02, -3.02 ...
    -3.07, -3.17, -3.32, -3.3, -3.22, -3.1];
format short e;
c = polyfit(x, y, 12);
p12x = linspace(x(1), x(end), 100);
p12y = polyval(c,p12x);

plot(x,y,'or')
hold('on')
plot(p12x, p12y, 'k-')
xlabel('x')
ylabel('y')
legend('data', '12 deg poly.')
```


EXAMPLE



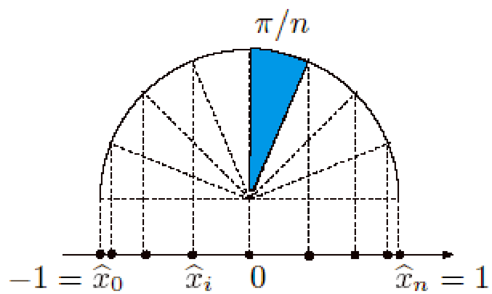
CHEBYSHEV INTERPOLATION

Runge function $f(x) = \frac{1}{1+x^2}$

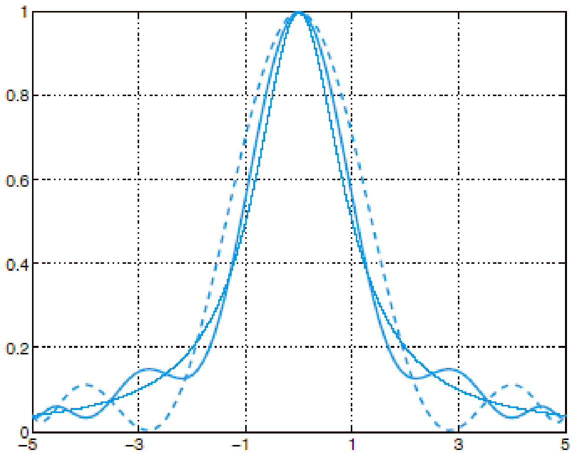


CHEBYSHEV INTERPOLATION

$$x_i = \frac{a+b}{2} + \frac{b-a}{2}\widehat{x}_i, \text{ where } \widehat{x}_i = -\cos(\pi i/n),\ i = 0, \ldots, n$$



CHEBYSHEV INTERPOLATION



PIECEWISE LINEAR INTERPOLATION

Use linear composite interpolation

- When the function f is nonsmooth or
- When f is known by its values at a set of given points

Given: nodes(not necessarily uniform) $x_0 < x_1 < \ldots < x_n$, interval I_i, $|x_i, x_{i+1}|$ Approximate the function f by a continuous function which,on each interval, is given by the segment joining the two points $(x_i, f(x_i))$ and $(x_{i+1}, f(x_{i+1}))$

PIECEWISE LINEAR INTERPOLATION

Piecewise linear interpolation polynomial of f is $\Pi_1^H f$
for $x \in I_i$,

$$\Pi_1^H f(x) = f(x_i) + \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}(x - x_i)$$

The upper – index H denotes the maximum length of the interval I_i.
For all x in the interpolation interval, $\Pi_1^H f(x)$ tends to $f(x)$ when $H \longrightarrow 0$ provided that f is sufficiently smooth.

PIECEWISE LINEAR INTERPOLATION

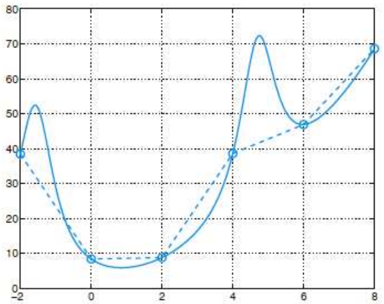
`s1=interp1(x,y,z)` is used to calculate the linear interpolation value in a given interval.
x, y: data points
z: arbitrary points with an arbitrary dimension

INTERPOLATION

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

EXAMPLE



The function $f(x) = x^2 + 10/(\sin(x) + 1.2)$ (*solid line*) and its piecewise linear interpolation polynomial $\Pi_1^H f$ (*dashed line*)

INTERPOLATION

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

EXAMPLE

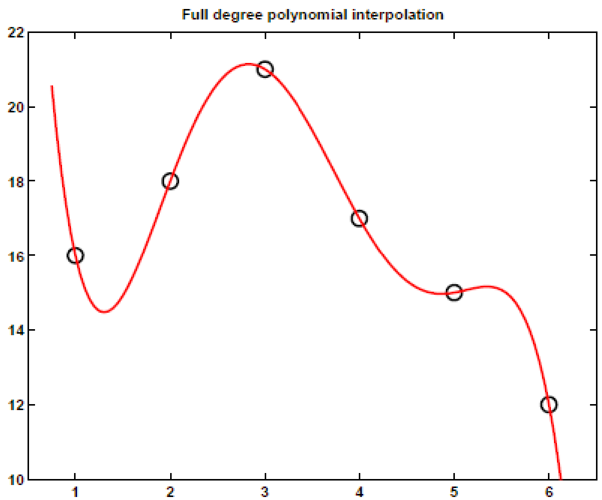
```
x = 1:6;
y = [16 18 21 17 15 12];
plot(x,y,'o',x,y,'-');
```


INTERPOLATION

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

EXAMPLE

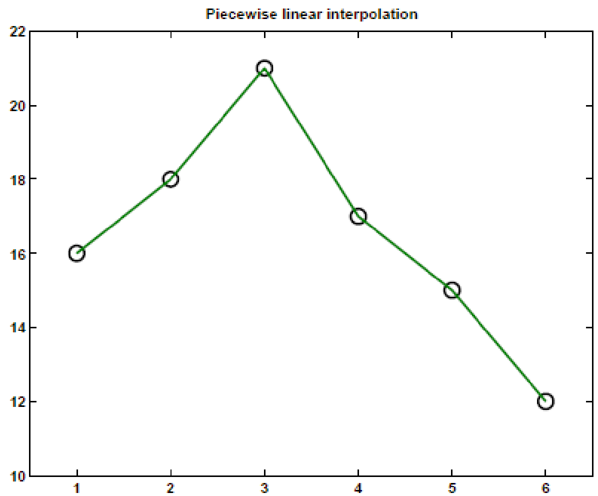


INTERPOLATION

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

EXAMPLE



SPLINE FUNCTIONS

Piecewise polynomial interpolation of degree $n \geq 2$ can be defined. In several applications, it is desirable to get approximation by smooth functions which have at least a continuous derivative. Function properties:

1. on each interval $I_i = [x_i, x_{i+1}]$, for $i = 0, \ldots, n-1$, s_3 is a polynomial of degree 3 which interpolates the pairs of values $(x_j, f(x_j))$ for $j = i, i+1$;
2. s_3 has continuous first and second derivatives in the nodes x_i, $i = 1, \ldots, n-1$

A cubic spline creates a smooth curve, using a third degree polynomial.

SPLINE FUNCTIONS

METHODS

- **Nearest neighbor interpolation** (method = 'nearest'). This method sets the value of an interpolated point to the value of the nearest existing data point.
- **Linear interpolation** (method = 'linear'). This method fits a different linear function between each pair of existing data points, and returns the value of the relevant function at the points specified by x_i. This is the default method for the `interp1` function.

SPLINE FUNCTIONS

METHODS

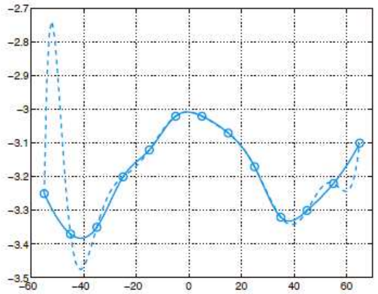
- **Cubic spline interpolation** (method = 'spline'). This method fits a different cubic function between each pair of existing data points, and uses the `spline` function to perform cubic spline interpolation at the data points.
- **Cubic interpolation** (method = 'pchip' or 'cubic'). These methods are identical. They use the `pchip` function to perform piecewise cubic Hermite interpolation within the vectors x and y.

SPLINE FUNCTIONS

- When the **nearest** and **linear** methods are used the values of x_i must be within the domain of x. If the **spline** or the **pchip** methods are used, x_i can have values outside the domain of x and the function **interp1** performs extrapolation.
- The spline method can also return errors if the input data points are nonuniform such that some points are much closer than others.

INTERPOLATION

EXAMPLE



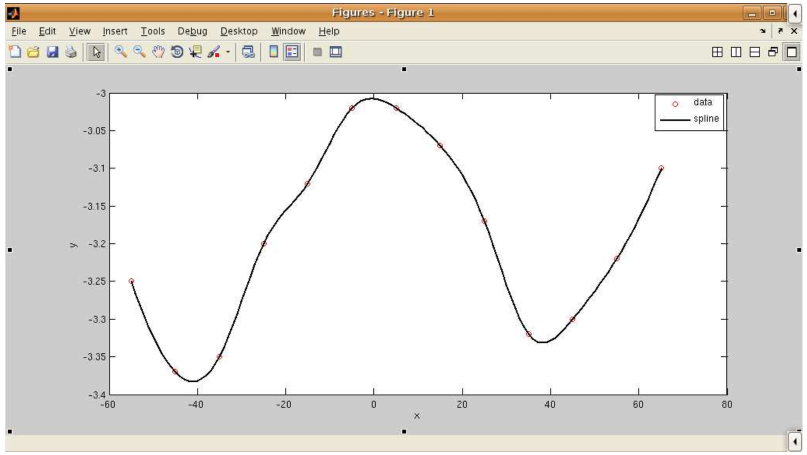
Comparison between the interpolating cubic spline and the Lagrange interpolant for the case considered in Example

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

INTERPOLATION

EXAMPLE

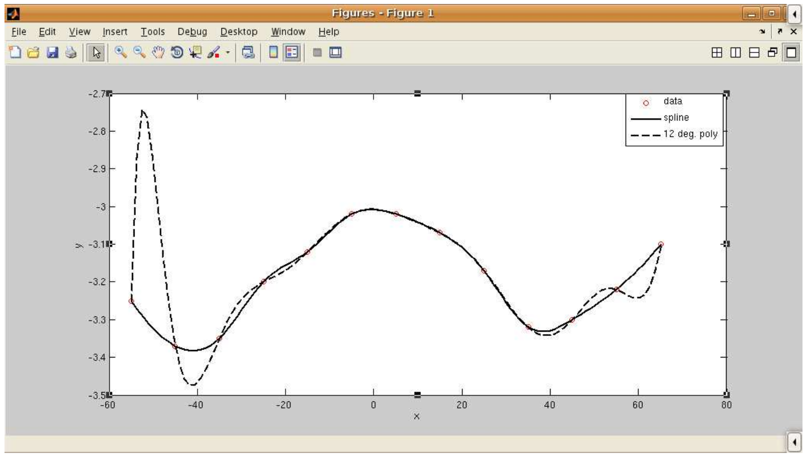


Introduction to Scientific and Engineering Computing, BIL108E

Karaman

INTERPOLATION

EXAMPLE

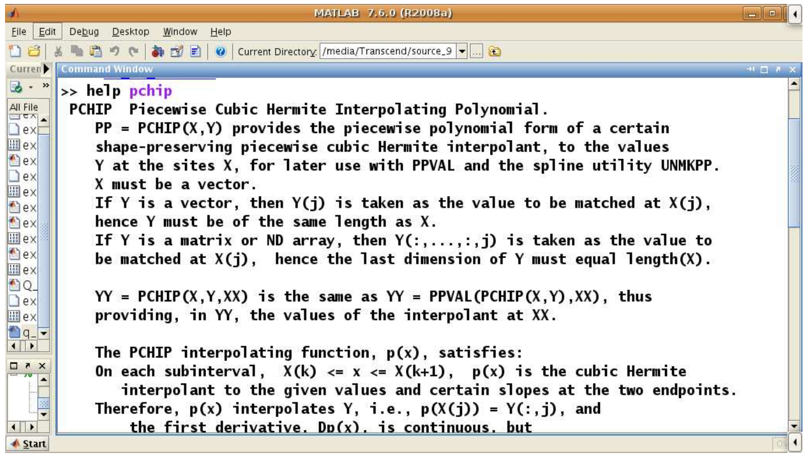


Introduction to Scientific and Engineering Computing, BIL108E

Karaman

APPROXIMATION

EXAMPLE



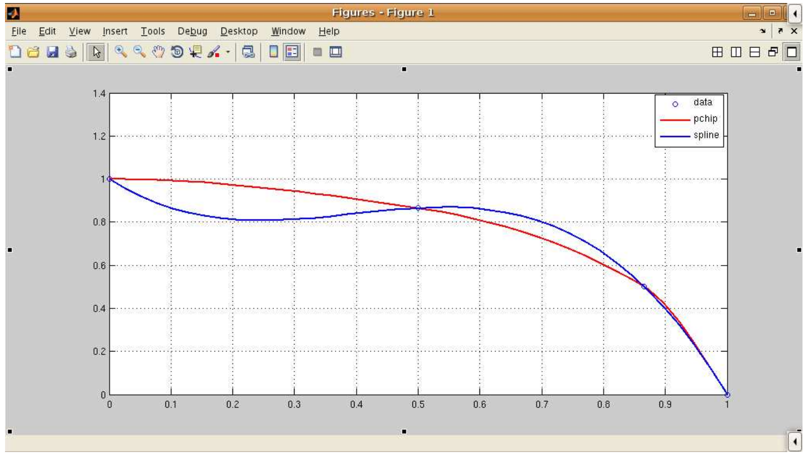
APPROXIMATION

EXAMPLE

```
clear;clf;clc;

t = linspace (0 , pi /2 ,4);
x = cos ( t ); y = sin ( t );
xx = linspace (0 ,1 ,40);
plot (x ,y , 'o');
hold('on');
plot(xx, pchip (x, y, xx))
plot(xx, spline (x, y, xx))
grid('on')
legend('data', 'pchip', 'spline')
```


APPROXIMATION

EXAMPLE



APPROXIMATION

EXAMPLE

The following data points which are points of the function $f(x) = 1.5^x \cos(2x)$ are given.

x	0.0	1.0	2.0	3.0	4.0	5.0
y	1.0	-0.6242	-1.4707	3.2406	-0.7366	6.3717

Use linear, spline and pchip interpolation methods to calculate the value of y between the points. Create a figure for each of the interpolation methods. In the figure show the points, a plot of the function and a curve that corresponds to the interpolation method.

APPROXIMATION

LEAST SQUARES METHOD

For a linear equation:

- If the number of linear equations is less than the unknowns, the equation system is under –determined (or infinite solutions)
- If the number of linear equations is more than the unknowns, the equation system is over –determined.

REGRESSION ANALYSIS

Regression analysis is a process of fitting a function to a set of data points. Curve fitting with polynomials is done with `polyfit` function which uses the least squares method. Experimental data always has a finite amount of error included in it, due to both accumulated instrument inaccuracies and also imperfections in the physical system being measured. Even data describing a linear system won't all fall on a single straight line.

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

LINEAR REGRESSION

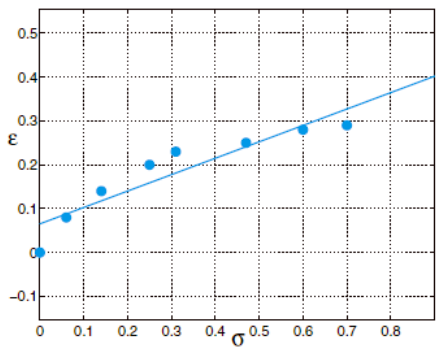
Linear form of the least squares method.

- n+1 functions are given.
- Linear function $y = a + b\,x$ where a and b are constants
- Minimize the euclid norm of the function for the given data points.

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

EXAMPLE



Linear least-squares approximation of the data of Problem

APPROXIMATION

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

LEAST SQUARES METHOD

euclid norm

$||x||_2 = \sqrt{\sum_{j=1}^{n} |x_j|^2}$

$f(x_1, x_2, \ldots, x_n) = ||A\,x - b||_2^2$

$= (A\,x - b)^T\,(A\,x - b) = x^T\,A^T\,A\,x - 2\,x^T\,A^T\,b + b^T\,b$

$= ||(\sum_{j=1}^{n} a_{k,j}\,x_j - b_k)_{k=1}^{m}||_2^2$

$= \sum_{k=1}^{m}(\sum_{j=1}^{n} a_{k,j}\,x_j - b_k)^2$

LEAST SQUARES METHOD

$0 = \frac{df}{dx_i} = 2\sum_{k=1}^{m}(\sum_{j=1}^{n} a_{k,j}\, x_j - b_k) a_{k,i}$

$$\begin{pmatrix} a + b\, x_1 \\ \vdots \\ a + b\, x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

or

$$A \begin{pmatrix} a \\ b \end{pmatrix} = y$$

here

$$\begin{pmatrix} 1 + x_1 \\ \vdots \\ 1 + x_n \end{pmatrix}$$

$$S = \left\| A \begin{pmatrix} a \\ b \end{pmatrix} - y \right\|_2^2 = \sum_{j=1}^{n} (a + b\, x_j - y_j)^2$$

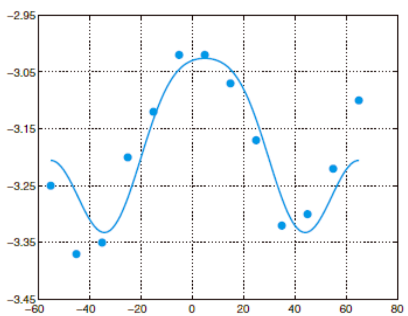
Minimize the euclid norm by finding values of a and b where the derivatives of S with respect to a and b are zero simultaneously.

$$\frac{\partial S}{a} = 2\sum_{j=1}^{n}(a + b\, x_j - y_j) = 0$$

$$\frac{\partial S}{b} = 2\sum_{j=1}^{n} x_j\,(a + b\, x_j - y_j) = 0$$

$$\begin{bmatrix} n & \sum_{j=1}^{n} x_j \\ \sum_{j=1}^{n} x_j & \sum_{j=1}^{n} x_j^2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{n} y_j \\ \sum_{j=1}^{n} x_j\, y_j \end{bmatrix}$$

EXAMPLE



The least-squares approximation of the data of the Problem using a cosine basis. The exact data are represented by the small circles

EXAMPLE:

- Tom and Ben are twin boys born on October 27, 2001. Here is a table of their weights, in pounds and ounces, over their first few months.

```
% Date Tom Ben
W = [10 27 2001 5 10 4 8
     11 19 2001 7 4 5 11
     12 03 2001 8 12 6 4
     12 20 2001 10 14 8 7
     01 09 2002 12 13 10 3
     01 23 2002 14 8 12 0
     03 06 2002 16 10 13 10];
```

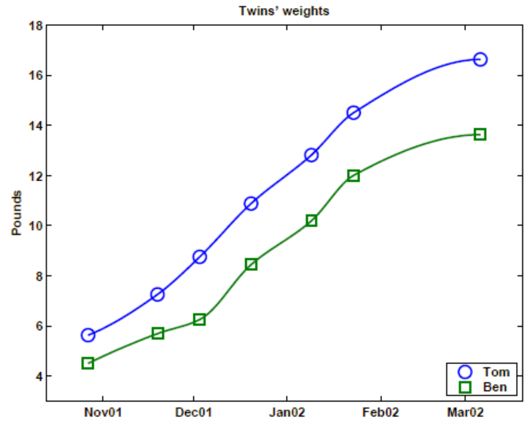
EXAMPLE cont'd.:

Use `datenum` to convert the date in the first three columns to a serial date number measuring time in days.

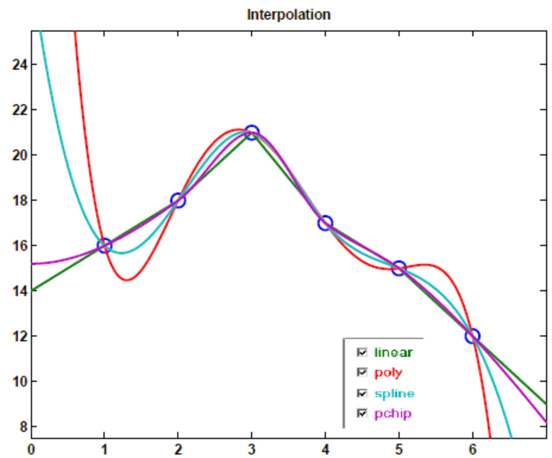
```
t = datenum(W(:,[3 1 2]));
```

Make a plot of their weights versus time, with circles at the data points and the pchip interpolating curve in between. Use datetick to relabel the time axis. Include a title and a legend.

EXAMPLE cont'd.:



EXAMPLE:



References for Week 9

1. Alfio Quarteroni, Fausto Saleri, Scientific Computing with Matlab and Octave, Springer, 2006.
2. Moler C, NumericalComputing with Matlab, Mathworks Inc., 2004 (http://www.mathworks.com/moler).
3. Hans Rudolf Schwarz, Norbert Köckler, Numerische Mathematik, Vieweg + Teubner, 2009.
4. Thomas Huckle, Stefan Schneider, Numerische Methoden, Springer, 2006.