Introduction to Scientific and Engineering Computing, BIL108E

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INTRODUCTION TO SCIENTIFIC & ENGINEERING COMPUTING BIL 108E, CRN24023

Dr. S. Gökhan Karaman

Technical University of Istanbul

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TENTATIVE SCHEDULE

Introduction to Scientific and Engineering Computing, BIL108E

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Week	Date	Topics
1	Feb. 10	Introduction to Scientific and Engineering Computing
2	Feb. 17	Introduction to Program Computing Environment
3	Feb. 24	Variables, Operations and Simple Plot
4	Mar. 03	Algorithms and Logic Operators
5	Mar. 10	Flow Control, Errors and Source of Errors
6	Mar. 17	Functions
6	Mar. 20	Exam 1
7	Mar. 24	Arrays
8	Mar. 31	Solving of Simple Equations
9	Apr. 07	Polynomials Examples
10	Apr. 14	Applications of Curve Fitting
11	Apr. 21	Applications of Interpolation
11	Apr. 24	Exam 2
12	Apr. 28	Applications of Numerical Integration
13	May 05	Symbolic Mathematics
14	May 12	Ordinary Differential Equation (ODE) Solutions with Built-in Functions

LECTURE # 8

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LECTURE # 8

1. POLYNOMIALS
2. APPROXIMATION OF DATA

POLYNOMIALS

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POLYNOMIALS

- Definition: n^{th} degree polynomial
  $p(x) = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_2 x^2 + a_1 x + a_0$
- Coefficients of the polynomial
  $a_n, a_{n-1}, \ldots, a_2, a_1, a_0$
- n: degree of the polynomial

POLYNOMIALS

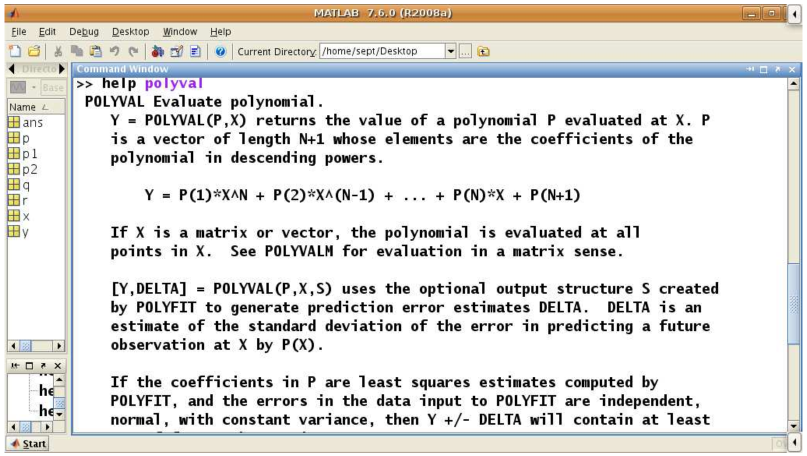
MATLAB toolbox: **polyfun**

- `polyval`: returs the value of the polynomial at a point x.
  Input arguments are vector p and vector x
  p $\longrightarrow a_n, a_{n-1}, \ldots, a_1, a_0$
  x is the abscissae, where the polynomials is evaluated.
- `y = polyval(p, x)`

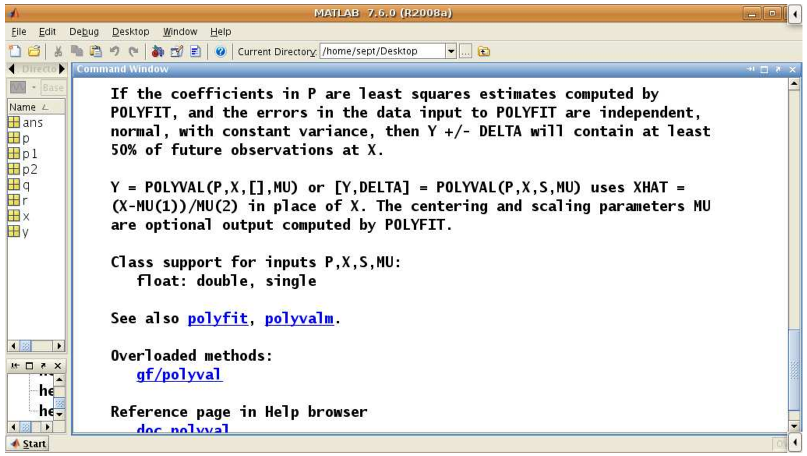
EXAMPLE:

- Given: $p(x) = x^7 + 3x^2 - 1$,
  $x_k = -1 + k/4$ for $k = 0, \ldots, 8$
- Find: Plot the given function.

EXAMPLE cont'd.:



EXAMPLE cont'd.:



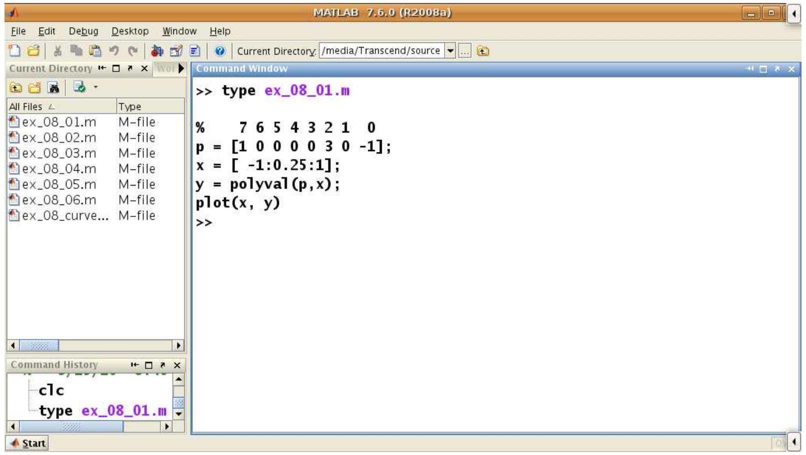
POLYNOMIALS

EXAMPLE cont'd.:

```
%    7 6 5 4 3 2 1  0
p = [1 0 0 0 0 3 0 -1];
x = [ -1:0.25:1];
y = polyval(p,x);
plot(x, y)
```

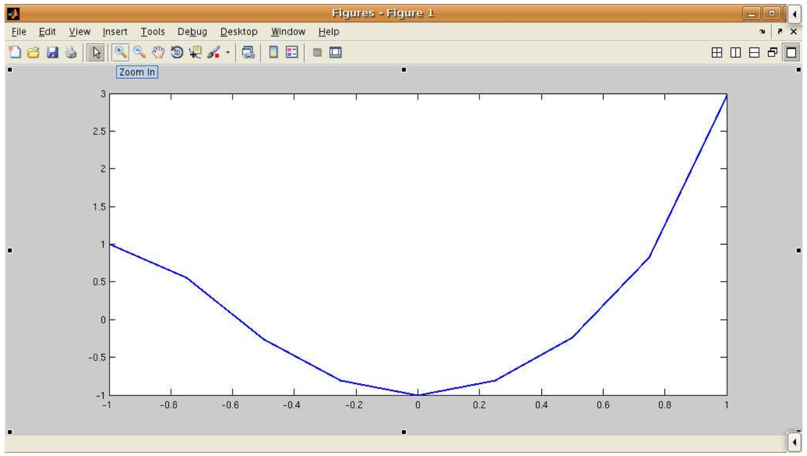
POLYNOMIALS

EXAMPLE cont'd.:



POLYNOMIALS

EXAMPLE cont'd.:



POLYNOMIALS

POLYNOMIALS

- `roots`: provides an approximation of the zeros of a polynomial.
- Usage: `r = roots(p)`
- `poly`: returns the coefficients of the polynomial, whose zeros are given.
- Usage: `p = poly(r)`

POLYNOMIALS

EXAMPLE:

- Given: $p(x) = x^3 - 6x^2 + 11x - 6$
- Find: Compute the zeros of the polynomial.

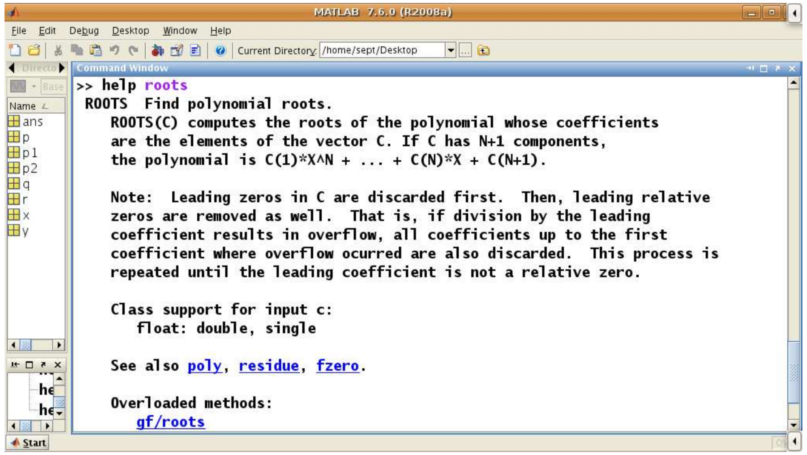
POLYNOMIALS

EXAMPLE cont'd.:

```
p = [1 -6 11 -6]; format long;
roots(p)
```

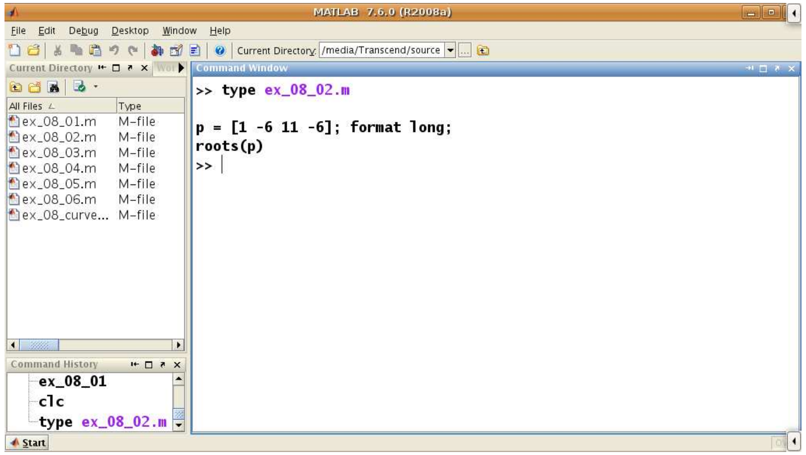

POLYNOMIALS

EXAMPLE cont'd.:



POLYNOMIALS

EXAMPLE cont'd.:



EXAMPLE cont'd.:

```
>> type ex_08_02.m

p = [1 -6 11 -6]; format long;
roots(p)
>> ex_08_02

ans =

   3.000000000000002
   1.999999999999998
   1.000000000000000

>>
```

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EXAMPLE: poly

```
>> help poly
 POLY Convert roots to polynomial.
    POLY(A), when A is an N by N matrix, is a row vector with
    N+1 elements which are the coefficients of the
    characteristic polynomial, DET(lambda*EYE(SIZE(A)) - A) .

    POLY(V), when V is a vector, is a vector whose elements are
    the coefficients of the polynomial whose roots are the
    elements of V . For vectors, ROOTS and POLY are inverse
    functions of each other, up to ordering, scaling, and
    roundoff error.

    ROOTS(POLY(1:20)) generates Wilkinson's famous example.

    Class support for inputs A,V:
       float: double, single

    See also roots, conv, residue, polyval.
```

POLYNOMIALS

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EXAMPLE cont'd.:

```
>> poly(1:20)

ans =

  Columns 1 through 6

   1.0000e+00  -2.1000e+02   2.0615e+04  -1.2568e+06   5.3328e+07  -1.6723e+09

  Columns 7 through 12

   4.0172e+10  -7.5611e+11   1.1310e+13  -1.3559e+14   1.3075e+15  -1.0142e+16

  Columns 13 through 18

   6.3031e+16  -3.1133e+17   1.2066e+18  -3.6000e+18   8.0378e+18  -1.2871e+19

  Columns 19 through 21

   1.3804e+19  -8.7529e+18   2.4329e+18
```

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EXAMPLE cont'd.:

```
>> roots(poly(1:20))

ans =

   2.0000e+01
   1.8998e+01
   1.8006e+01
   1.6989e+01
   1.6011e+01
   1.4996e+01
   1.3996e+01
   1.3008e+01
   1.1994e+01
   1.1002e+01
   9.9998e+00
   8.9998e+00
   8.0001e+00
   7.0000e+00
   6.0000e+00
```

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EXAMPLE:

The result is not always accurate.

Given: $p(x) = (x+1)^7$

Find: Compute the zeros of the polynomial.

Answer: $\alpha = -1$

In fact, numerical methods for the computation of the polynomial roots with multiplicity larger than one are particularly subject to roundoff errors.

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EXAMPLE cont'd.:

```
p = [1 7 21 35 35 21 7 1];
roots(p)
```

POLYNOMIALS

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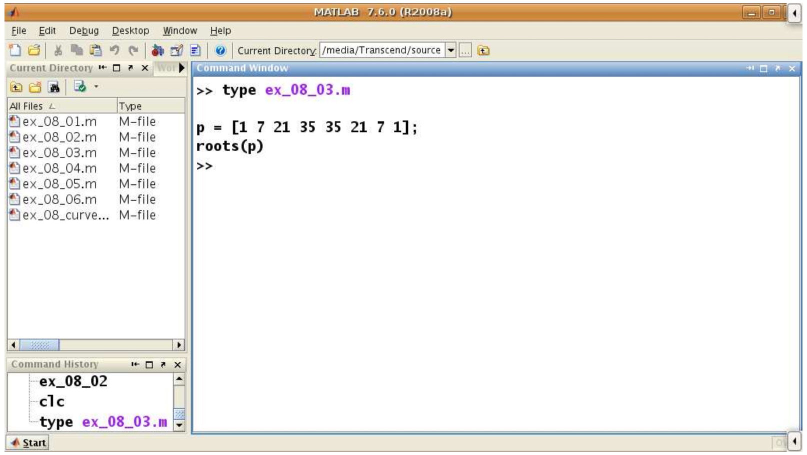
EXAMPLE cont'd.:



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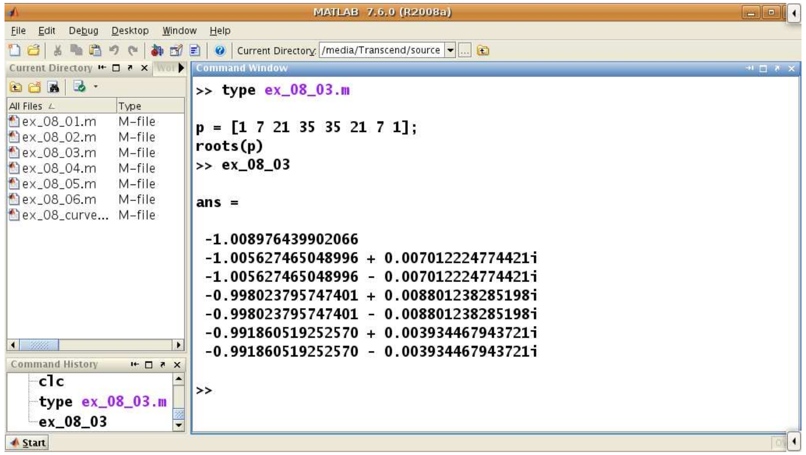
EXAMPLE cont'd.:



ADDITION AND SUBTRUCTION OF POLYNOMIALS

- Polynomial addition and subtraction is the same as vector addition/subtraction operators.
- If the order of two polynomials (size of two vectors) does not match, zero should be added in order to match size of vectors.

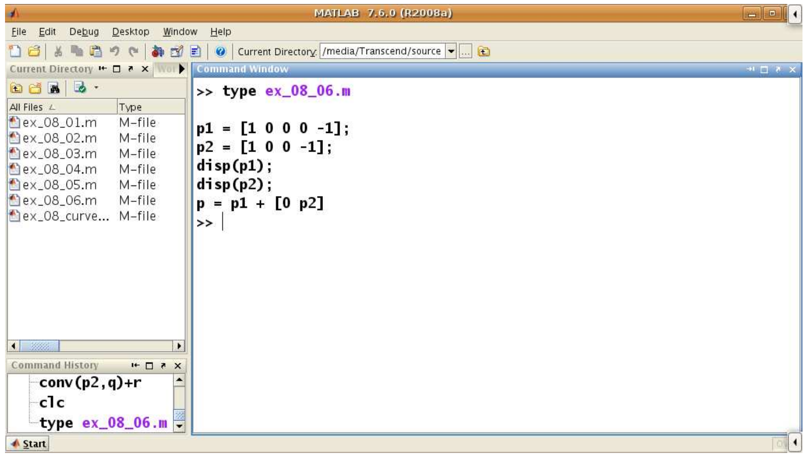
EXAMPLE:

- Given: $p_1(x) = x^4 - 1$, $p_2(x) = x^3 - 1$
- Find: Compute the sum of two polynomials.
- Answer: $p = x^4 + x^3 - 2$

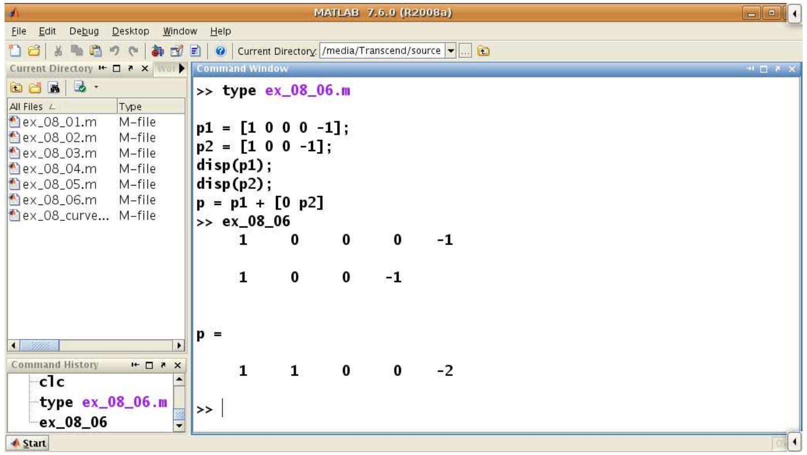
EXAMPLE cont'd.:

```
p1 = [1 0 0 0 -1];
p2 = [1 0 0 -1];
disp(p1);
disp(p2);
p = p1 + [0 p2]
```


EXAMPLE cont'd.:



EXAMPLE cont'd.:



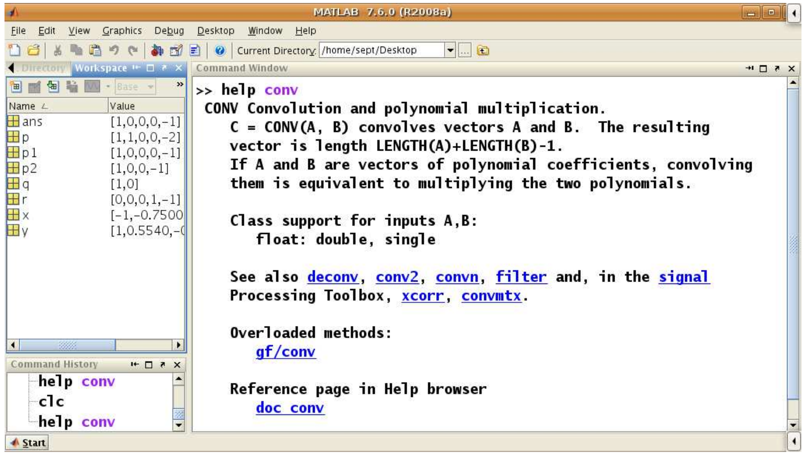
MULTIPLICATION AND DIVISION OF POLYNOMIALS

- `conv`: returns the coefficients of the polynomial given by the product of two polynomials.
- Usage: `conv(p1, p2)`
- `deconv`: provides the coefficients of the polynomials obtained on dividing p1 by p2.
- Usage: `[q, r]=deconv(p1, p2)`
  q: quotient of the division,
  r: remainder of the division
  $p_1(x) = q(x)\,p_2(x) + r(x)$

EXAMPLE:

- Given: $p_1(x) = x^4 - 1$,
  $p_2(x) = x^3 - 1$
- Find: Compute the product of two polynomials.
- Answer: $p = x^7 - x^4 - x^3 + 1$

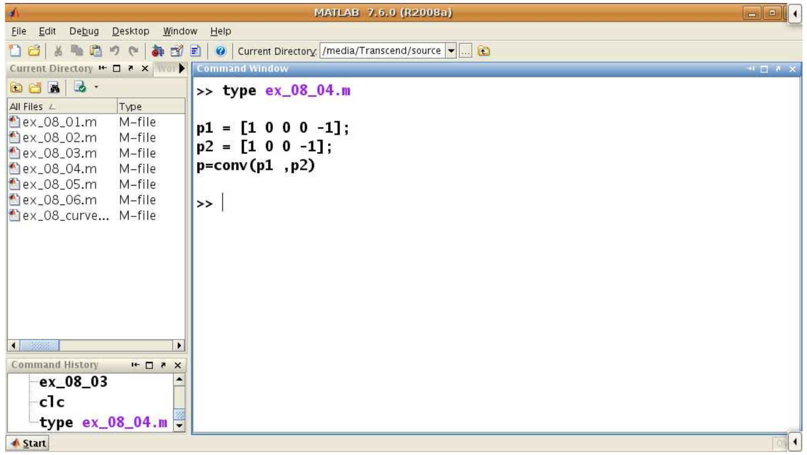
EXAMPLE cont'd.:



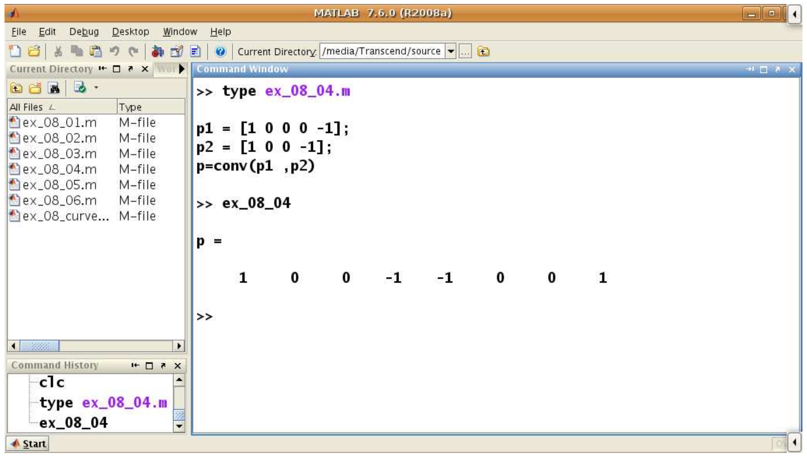
EXAMPLE cont'd.:

```
p1 = [1 0 0 0 -1];
p2 = [1 0 0 -1];
p=conv(p1 ,p2)
```


EXAMPLE cont'd.:



EXAMPLE cont'd.:

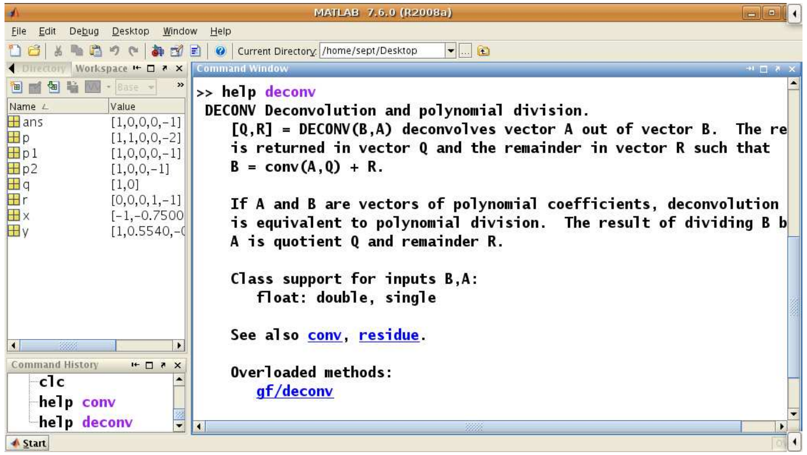


EXAMPLE:

- Given: $p_1(x) = x^4 - 1$, $p_2(x) = x^3 - 1$
- Find: Compute the division of two polynomials.
- Answer: $q(x) = x$, $r(x) = x - 1$

POLYNOMIALS

EXAMPLE cont'd.:



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EXAMPLE cont'd.:

```
p1 = [1 0 0 0 -1];
p2 = [1 0 0 -1];
[q,r]= deconv(p1 ,p2)
```

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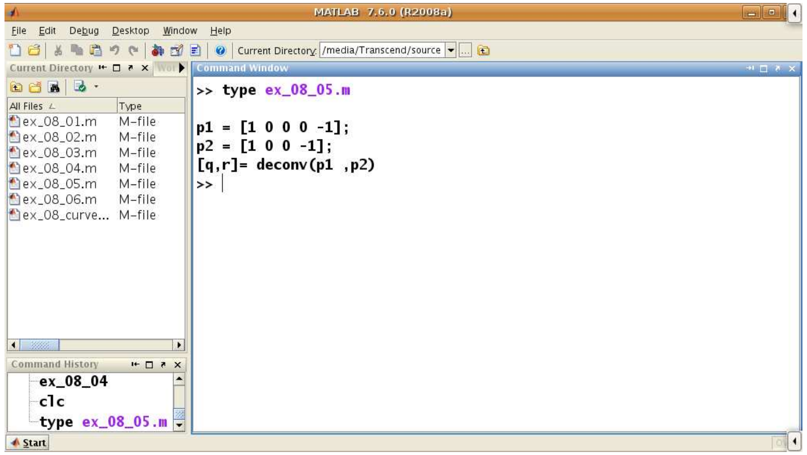
EXAMPLE cont'd.:



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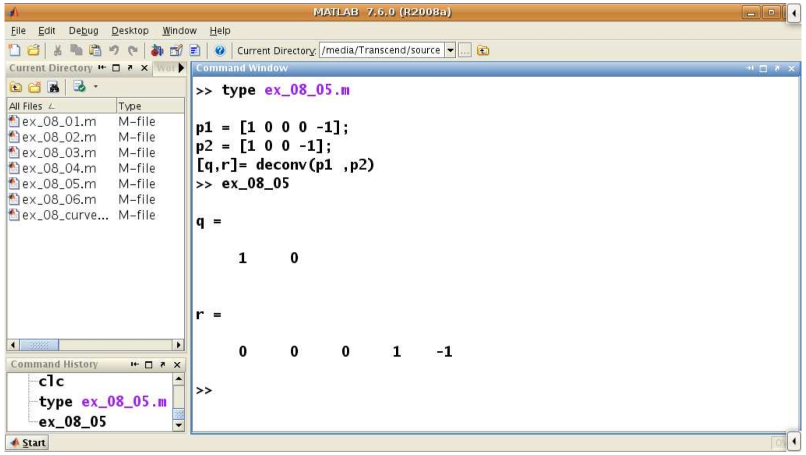
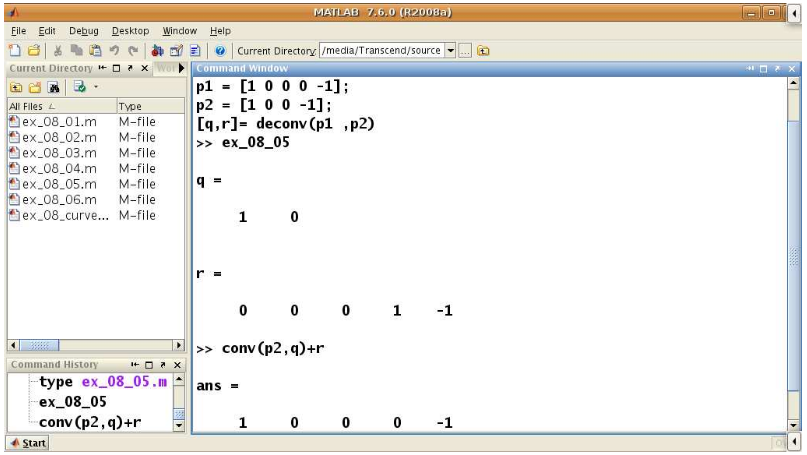
EXAMPLE cont'd.:



POLYNOMIALS

EXAMPLE cont'd.:



POLYNOMIALS

POLYNOMIALS

- `polyint` returns the coefficients of the primitive of the polynomial.
  Usage: `y = polyint(p)`,
  y: coefficients of $\int_0^x p(t)\,dt$
- `polyder`: returns the derivative of the polynomial, whose coefficients are given by the components of the vector p.
  Usage: `y = polyder(p)`,
  y: coefficients of $p'(x)$

CURVE FITTING

CURVE FITTING

- Approximating a function f consists of replacing it by another function $\tilde{f}$.
- A function f can be replaced in a given interval by its Taylor polynomial.
- It requires the knowledge of f and its derivatives up to the order n at a given point x_0.

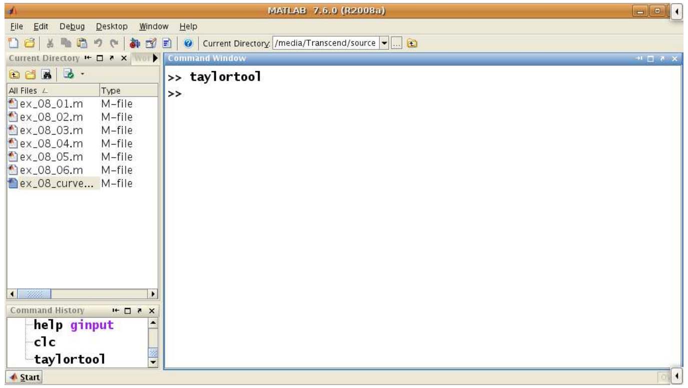
CURVE FITTING

CURVE FITTING

- Taylor polynomial may fail to accurately represent f far enough from the point x_0.
- Use `taylortool` for the computation of Taylor's polynomial of arbitrary degree for any given function f.
- The agreement between the function and its Taylor polynomial is very good in a small neighborhood of x_0.

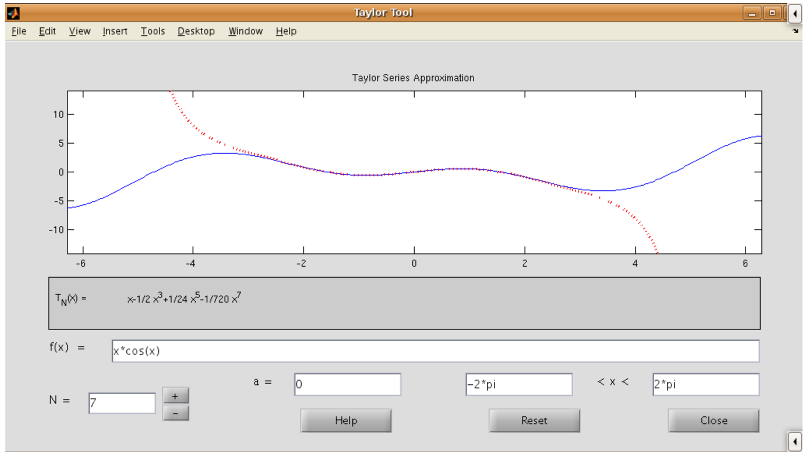
`taylortool`

EXAMPLE

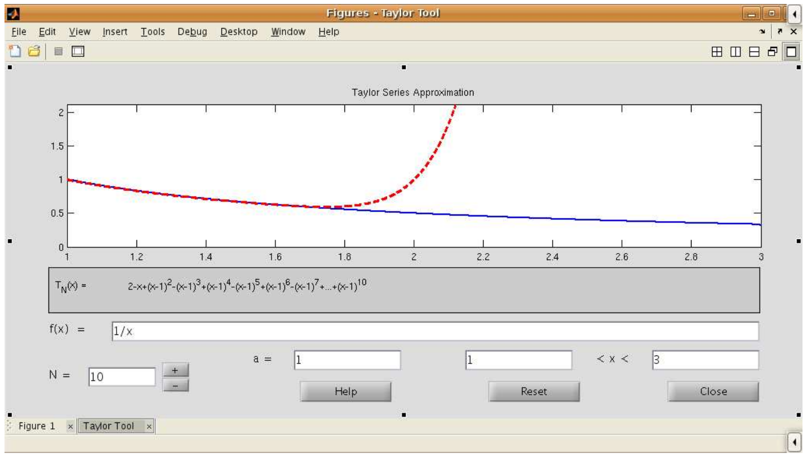


Comparison between the function $f(x) = 1/x$ and its Taylor polynomial of degree 10 for the point $x_0 = 1$.

EXAMPLE cont'd.:



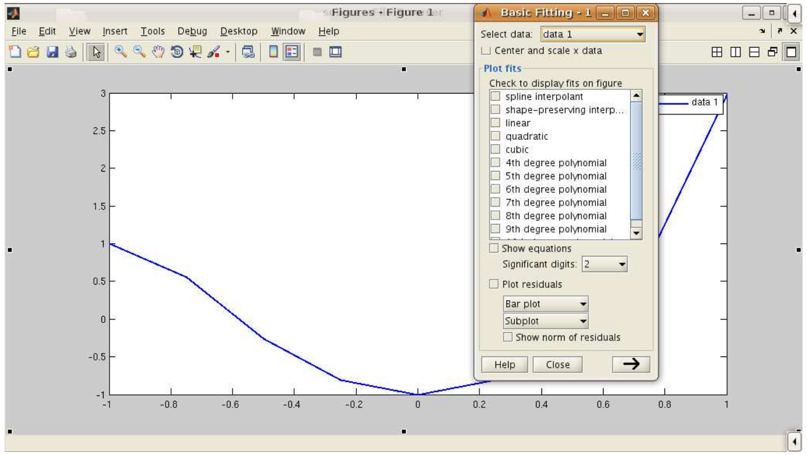
EXAMPLE cont'd.:



CURVE FITTING

- A function is known only through its values at some given points.
- $n+1$ couples (x_i, y_i) are given, $i = 0, 1, 2, \ldots, n+1$.
- Approximate function $\tilde{f}$:
  $\tilde{f}(x_i) = y_i$, where $i = 0, 1, 2, \ldots, n$
- $\tilde{f}$ is called **interpolant** of the set of data
- There exist different types of interpolant:
  - Polynomial interpolant
  - Trigonometric interpolant
  - Rational interpolant

BASIC FITTING:



CURVE FITTING

- The most common method of finding the best fit to data point is the least squares method.
- `polyfit` function uses least squares method.
- `polyfit` function returns the coefficients of a polynomial for a given data set (x_i, y_i).
- Usage: `p = polyfit(x, y, n)`
  n: degree of the polynomial.
  x and y: data set (x_i, y_i).

EXAMPLE

In the table below we report the values of the sea water density ρ(in kg/m^3) corresponding to different values of the temperature T (in degrees Celsius):

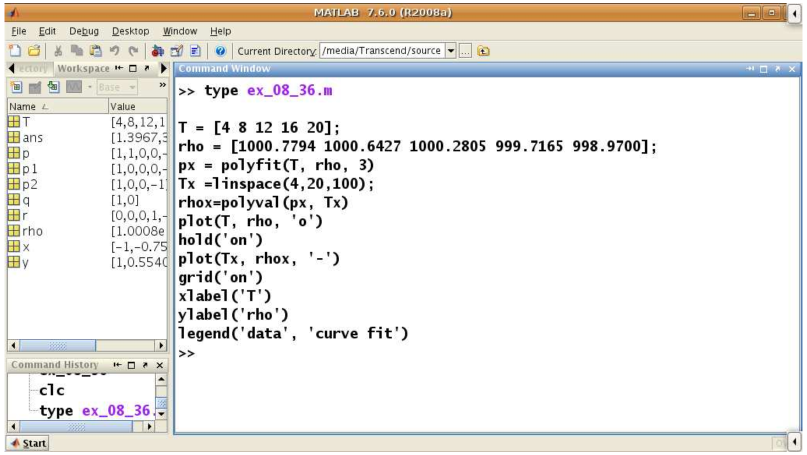
T	4°	8°	12°	16°	20°
ρ	1000.7794	1000.6427	1000.2805	999.7165	998.9700

EXAMPLE cont'd.:

```
T = [4 8 12 16 20];
rho = [1000.7794 1000.6427 1000.2805 999.7165 998.9700];
px = polyfit(T, rho, 3)
Tx =linspace(4,20,100);
rhox=polyval(px, Tx)
plot(T, rho, 'o')
hold('on')
plot(Tx, rhox, '-')
grid('on')
xlabel('T')
ylabel('rho')
legend('data', 'curve fit')
```

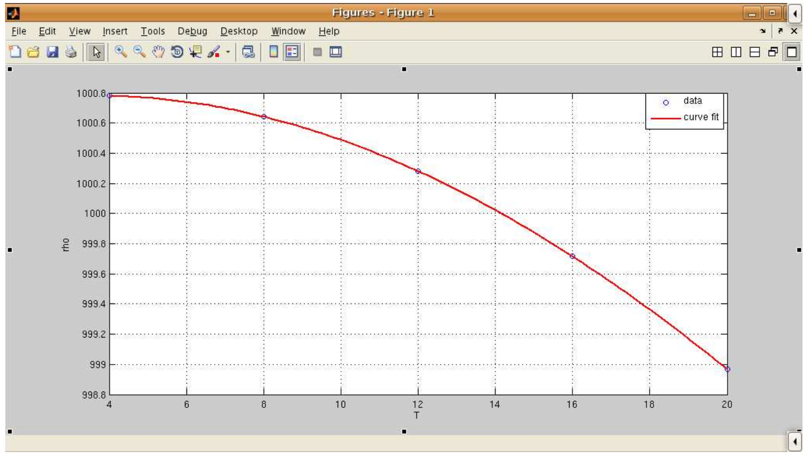
CURVE FITTING

EXAMPLE cont'd.:



CURVE FITTING

EXAMPLE cont'd.:



CURVE FITTING

LEAST SQUARES METHOD

- If the degree of the polynomial increases, interpolation does not guarantee a better approximation of a given function.
- In least – squares approximation we look for an approximant $\tilde{f}$ which is a polynomial of degree m (typically, $m << n$) that minimizes the mean-square error $\frac{1}{n}\sum_{i=0}^{n}[y_i - \tilde{f}(x_i)]^2$. The same minimization criterion can be applied for a class of functions that are not polynomials.

CURVE FITTING

CURVE FITTING WITH FUNCTIONS OTHER THAN POLYNOMIALS

Rewrite the function in a first degree polynomial form.

- Power function:
  $y = b\,x^m \longrightarrow \ln y = m \ln x + \ln b$
- Exponential function:
  $y = b\,e^{mx} \longrightarrow \ln y = m\,x + \ln b$
- Logarithmic function:
  $y = m \ln x + b \longrightarrow y = m \ln x + b$
- Reciprocal function:
  $y = 1/(m\,x + b) \longrightarrow 1/y = m\,x + b$

CURVE FITTING

FUNCTION SELECTION

- For a given data it is possible to foresee which of the functions have the potential for providing a good fit.
- This is done by plotting the data using different combinations of linear and logarithmic axes.

x–axis	y–axis	function
linear	linear	$y = mx + b$
logarithmic	logarithmic	$y = bx^m$
linear	logarithmic	$y = be^{mx}$
logarithmic	linear	$y = m\ln x + b$
linear	linear	$y = 1/(mx + b)$

CURVE FITTING

FUNCTION SELECTION

- Exponential functions can not pass through the origin.
- Exponential functions can only fit data with all positive y's or all negative y's.
- Logarithmic functions cannot model $x = 0$, or negative values of x.
- For the power function $y = 0$ when $x = 0$.
- The reciprocal equation cannot model $y = 0$.

CURVE FITTING

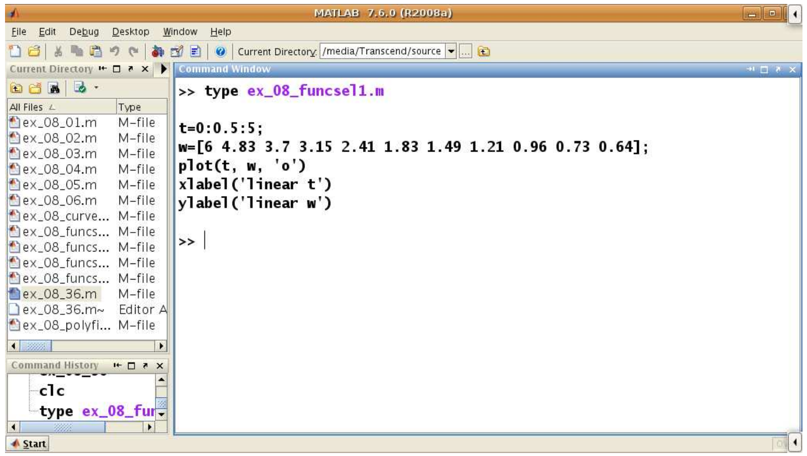
EXAMPLE:

w	0.64	0.73	0.96	1.21	1.49	1.83	2.41	3.15	3.70	4.83	6.00
t	5.0	4.5	4.0	3.5	3.0	2.5	2.0	1.5	1.0	0.5	0.0

- Choose the function for the given data.

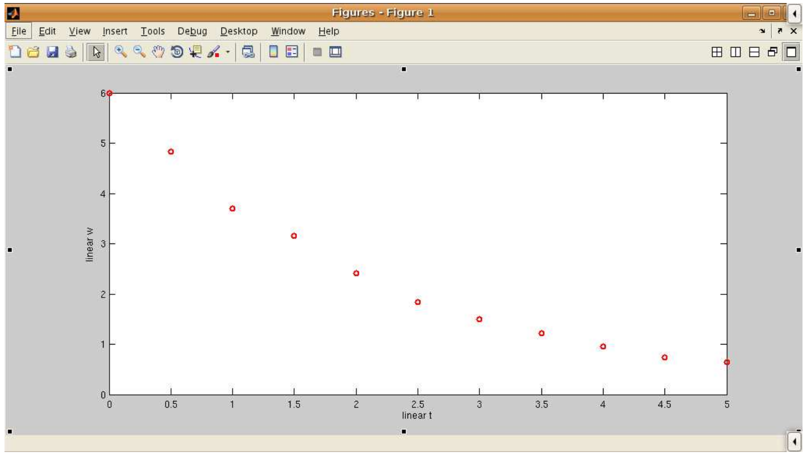
CURVE FITTING

EXAMPLE cont'd.:



CURVE FITTING

EXAMPLE cont'd.:



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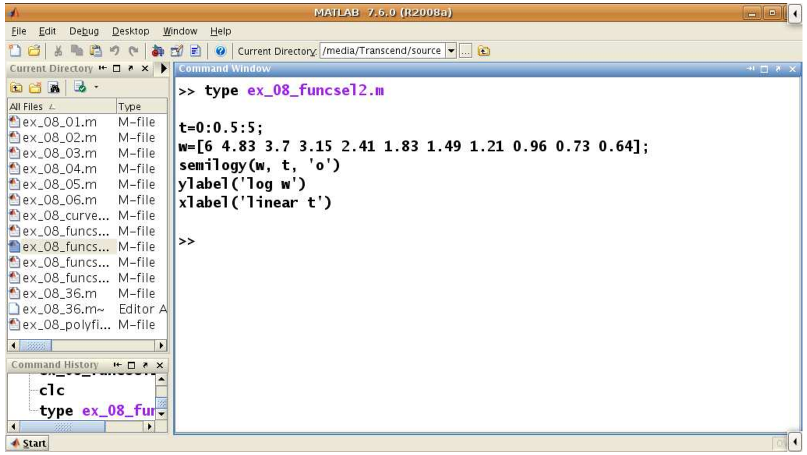
EXAMPLE cont'd.:



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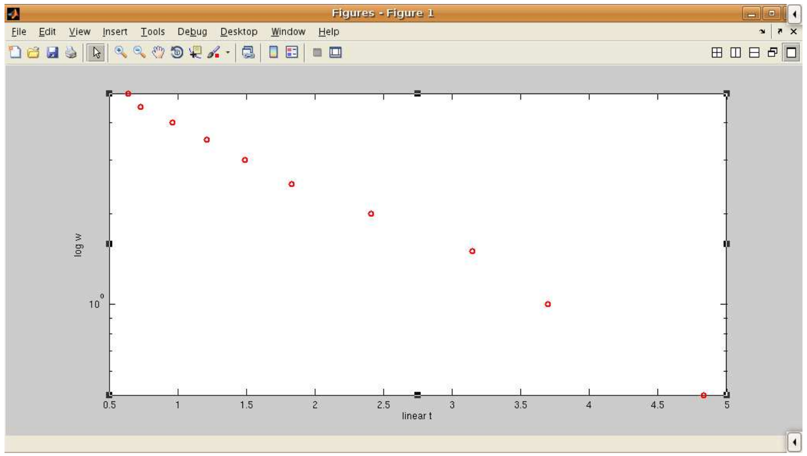
EXAMPLE cont'd.:



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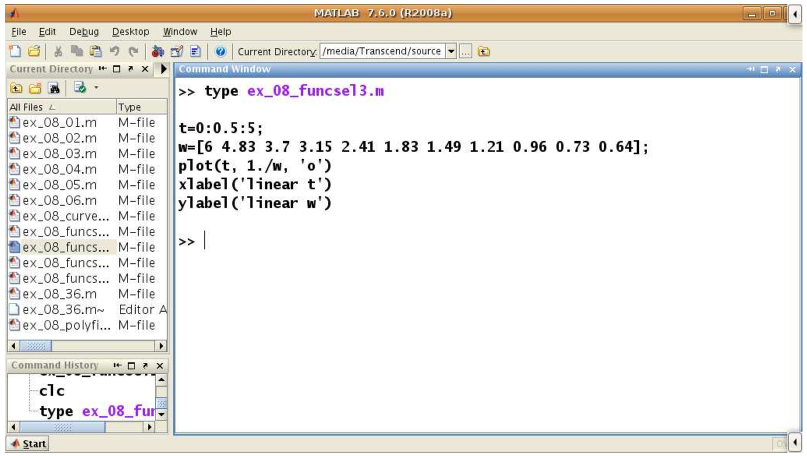
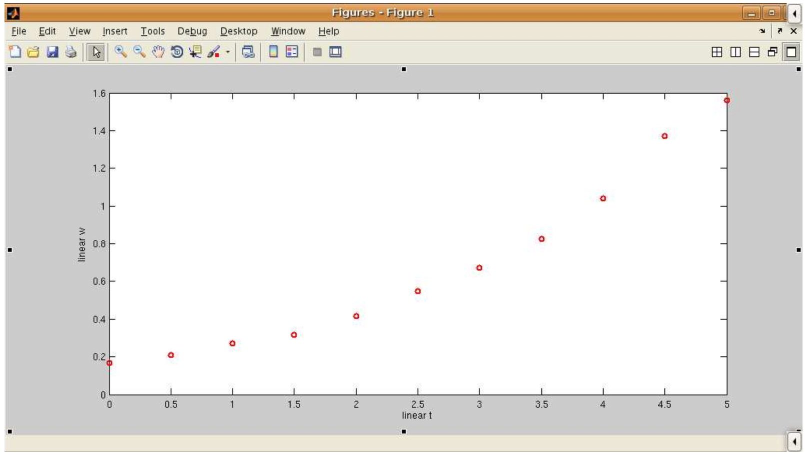
EXAMPLE cont'd.:



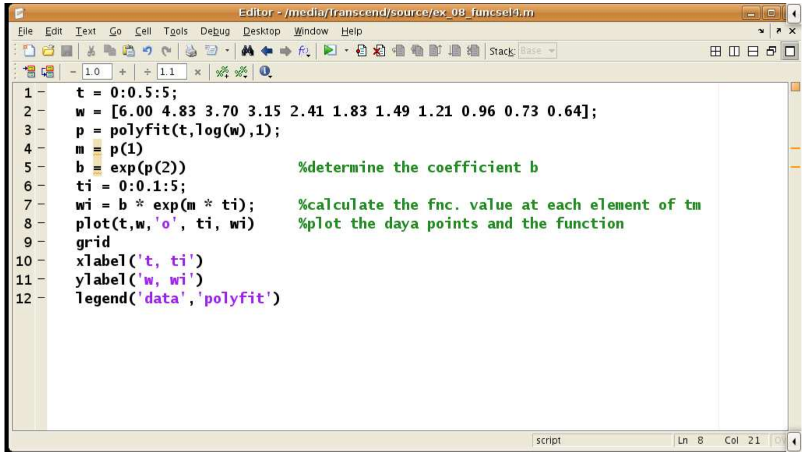
CURVE FITTING

EXAMPLE cont'd.:



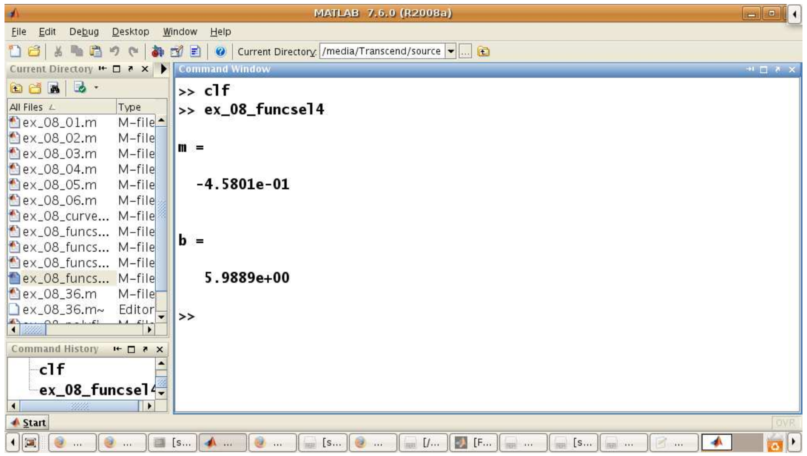
CURVE FITTING

EXAMPLE cont'd.:



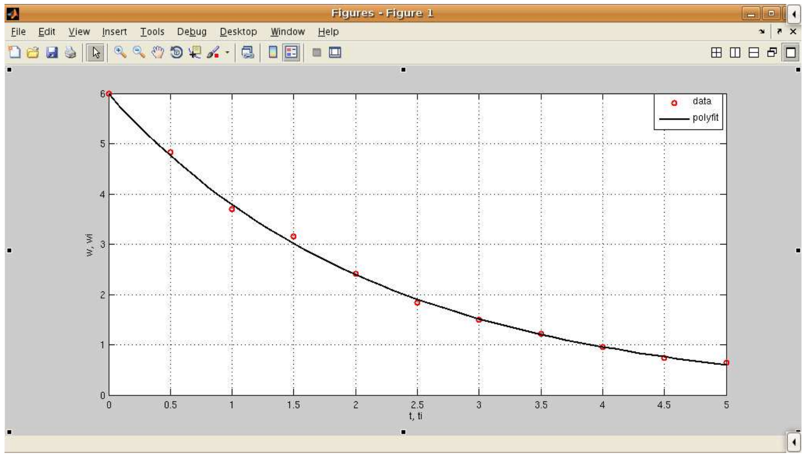
CURVE FITTING

EXAMPLE cont'd.:



CURVE FITTING

EXAMPLE cont'd.:



CURVE FITTING

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EXAMPLE:

	δ_K			
Latitude	$K = 0.67$	$K = 1.5$	$K = 2.0$	$K = 3.0$
65	-3.1	3.52	6.05	9.3
55	-3.22	3.62	6.02	9.3
45	-3.3	3.65	5.92	9.17
35	-3.32	3.52	5.7	8.82
25	-3.17	3.47	5.3	8.1
15	-3.07	3.25	5.02	7.52
5	-3.02	3.15	4.95	7.3
-5	-3.02	3.15	4.97	7.35
-15	-3.12	3.2	5.07	7.62
-25	-3.2	3.27	5.35	8.22
-35	-3.35	3.52	5.62	8.8
-45	-3.37	3.7	5.95	9.25
-55	-3.25	3.7	6.1	9.5

Variation of the average yearly temperature on the Earth for four different values of the concentration K of carbon acid at different latitudes.

- Compute the least-squares polynomial of degree 4 that approximates the values of K reported in the Table given above.

CURVE FITTING

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EXAMPLE:

- The price (in euros) of a magazine has changed as follows:

Nov.87	Dec.88	Nov.90	Jan.93	Jan.95	Jan.96	Nov.96	Nov.00
4.5	5.0	6.0	6.5	7.0	7.5	8.0	8.0

Estimate the price in November 2002 by extrapolating these data.

References

Introduction to Scientific and Engineering Computing, BIL108E

Karaman

References for Week 8

1. Alfio Quarteroni, Fausto Saleri, Scientific Computing with Matlab and Octave, Springer, 2006.
2. Brian Hahn, Daniel T.Valentine, Essential Matlab for Engineers and Scientists, Elsevier, 2010.