Computational Aspects of Econometrics and OR: MATLAB

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1 Overview Matlab part of the course

This document belongs to the course *Computational Aspects of Econometrics and OR*, and specifically the Matlab part of the course. For more information about the course see Blackboard.

1.1 Prerequisites

I expect that you are familiar with the Matlab basics:

- basic array operations (vector/matrix)
  - creating, accessing elements, the `end` index, colon-operator, deleting columns/rows
- mathematical operations
- creating m-files

  - script m-files
  - function m-files

- programming
  - `if`, `for`, `while`, `break`, `continue`, `switch`
  - logical operators: `~`, `<=`, `&`, `|`, etc.

- basic plotting

- important Matlab functions
  - `eye`, `ones`, `zeros`, `diag`, `size`, `length`, `find`, `min`, `max`, `sum`, `sort`, `any`, `all`, `diff`, `repmat`, etc.

If you lack this basic Matlab knowledge, then you should try to learn it as soon as possible. There are many introductory books and tutorial websites you can choose from. Here is a short selection:

- The official "Getting Started with Matlab", which you can also access through the Matlab help function

- Amos Gilat (2011). MATLAB: An Introduction with Applications, SI Version, 4th Edition

- Matlab tutorials on the web

1.2 Learning goals

1.2.1 Know ... (theory: by heart, on paper)

- how to apply the Matlab basics (see prerequisites)

- how to create efficient code by preallocating memory and preventing unnecessary loops by vectorizing computations, logical indexing and using functions such as `find`, `reshape`, `permute`, `min`, `max`, `sort`, `all`, `any`

- basics of anonymous functions

- the (dis)advantages of cell/structure arrays

1.2.2 Be able to use some advanced Matlab tools and techniques in practice (assignment)

1. Matlab tools
   - cell and structure arrays
   - anonymous functions
   - function declarations with variable number of input arguments and default input arguments (`varargin`, `nargin`)

    - import and export data in different formats (e.g. TXT, CSV, MAT files)
    - advanced figure properties (labels, legends, colors, line styles, etc.)
    - 3D-figures (`surf`, `meshgrid`, etc.)

2. Techniques

    - use the help function to *search for* built-in functionality and *use it* (I deliberately give exercises during class and in the assignment for which the solution tool/technique has not been (fully) explained)
    - use the profiler
    - use the debugger
    - appropriate documentation of Matlab code
    - split a problem into smaller pieces and write generic functions for them

1.3 Assignment

The assignment will be announced on Blackboard.

- Work in groups (size to be determined)
- Several small exercises
- Requirements
    - Efficient (preallocation, vectorize, etc.)
    - Well-documented
        * Basic function description
        * Explanation of input/output parameters
        * Comments on long or nontrivial parts of body
    - Generic/flexible: write small generic functions to generalizable or repetitive subproblems instead of one large and inflexible program.

1.4 Exam

See Learning goals (the "*know*" part)

1.5 Course material

Online document—the document you are reading now—containing several topics. For each topic we give

- a short introduction and/or some quick illustrations to get the main idea

- references to the official Matlab documentation, which you can also access by using the Matlab help function, and/or other external online information
- the website YAGTOM is a particularly useful reference for the stuff we are interested in
- exercise(s)

Note that you can easily copy the code snippets in this document and paste them in the Matlab command window, unless it is a function definition for which you'll need to create a m-file.

1.6 Course structure

The classes consist of several blocks consisting of:

- Introduction to topic
- Reading documentation/examples (preferably at home!)
- Hands on: solve exercises
- Recapture: discuss main issues
- *Selected* hints and/or solutions on blackboard after lecture

You probably won't have sufficient time to solve all the exercises during class, especially if you spend a lot of time reading the course materials. Try to **prepare** at home by reading the theory/documentation and give yourself the optimal opportunity to practice, encounter and solve problems during class.

2 Efficient coding

2.1 Introduction

One of the most important things that I want you to take away from this course is that you'll produce efficient Matlab code. By this I mean that I don't want to see code for which there is an obvious better solution. Compared to many other programming languages (such as C++, Java, Delphi, etc.) Matlab often requires a different way of thinking. Many complex tasks can be performed in a few lines of code where other languages need many more. Besides being shorter, usually this concise solution performs much faster than the alternative solution, which can used in Matlab as well.

Let's give an example. Suppose that we have a matrix `A`, say `A = rand(10000,1000)`, and we want to divide all numbers larger than 0.5 by 2. The straightforward approach, used in many other programming languages, would be the following:

```
[m,n] = size(A);
for i=1:m
  for j=1:n
    if A(i,j)>0.5
      A(i,j) = A(i,j)/2;
    end
  end
end
```

This solution gets the job done, and if you are not really interested in the performance of this piece of code (because you don't have to perform it many times and/or for large matrices), then there is not much of a problem. However, you don't always know under what circumstances your code will be used in the future. Therefore, it would be nice if you pick up the habit of automatically coding such as problem as follows:

```
i = A>0.5;
A(i) = A(i)/2;
```

This solution doesn't only perform much faster in Matlab, it has the additional advantage that it also works for numerical arrays with dimensions unequal to two.

The continuous awareness that you should try to develop is "*How can I prevent the use of loops?*"

In this block we will look at tools and techniques that you can use to make your Matlab code more efficient and in particular to prevent loops.

2.2 Preallocation

If you are going to use loops anyway, then make sure that you preallocate memory for output arrays. Adding new elements/rows etc. to an existing array is *very* time consuming.

```
N = 1e6;

tic
x = 0;
for k = 2:N
   x(k) = x(k-1) + 5;           % expand the existing array
end
bad = toc

tic
y = zeros(1, N);                % preallocate the output
for k = 2:N
   y(k) = y(k-1) + 5;
end
good = toc
```

Output

```
bad =

    0.2769


good =

    0.0174
```

Here we used the commands `tic` and `toc` to measure the time elapsed between the two statements.

2.3 Element-wise Arithmetic

Try to operate on multi-dimensional arrays as much as possible. Basic mathematical functions such as `sin`, `exp`, `log` can be applied to multi-dimensional arrays. A bit less familiar, but a great tool to get rid of loops, are the basic arithmetic operators `.*`, `./`, `.^`, that operate on arrays of the same dimension (or scalars). For instance:

```
A = A./B;
B = B.^2;
```

to divide every element in the matrix `A` by the corresponding element in `B` and square the elements in the matrix `B`. Note that the latter is different from `B^2`, which is the matrix product of `B` with itself.

2.4 Useful functions

There is quite a number of built-in functions that prevent the usage of loops. Here is a list with a short description and/or example. Probably, you already know some of these commands. Make sure that you are also familiar with the optional extra input and output arguments, which can often be very useful.

sum `sum(A,2)` sums along the second dimension, i.e., over the columns, of the matrix `A`. For example:

```
A = reshape(1:24, 4, 6)
a1 = sum(A, 1)
a2 = sum(A, 2)
```

With output

```
A =

     1     5     9    13    17    21
     2     6    10    14    18    22
```

```
     3     7    11    15    19    23
     4     8    12    16    20    24


a1 =

    10    26    42    58    74    90


a2 =

    66
    72
    78
    84
```

mean,std,var calculate the mean along a particular dimension of an array. For the `std` and `var` functions, the third input argument refers to the dimenion—and the second denotes wheter you want the population (1) or sample (0/default) standard deviation or variance.

min,max Compute the min/max along a particular dimension (third input argument). Indices of min/max-locations are returned in the second output argument.

```
A = rand(4, 6)
[m1, i1] = min(A, [], 1)
[m2, i2] = min(A, [], 2)
```

Output:

```
A =

    0.0540    0.1299    0.3371    0.5285    0.6541    0.0838
    0.5308    0.5688    0.1622    0.1656    0.6892    0.2290
    0.7792    0.4694    0.7943    0.6020    0.7482    0.9133
    0.9340    0.0119    0.3112    0.2630    0.4505    0.1524


m1 =

    0.0540    0.0119    0.1622    0.1656    0.4505    0.0838


i1 =

     1     4     2     2     4     1
```

```
m2 =

    0.0540
    0.1622
    0.4694
    0.0119


i2 =

     1
     3
     2
     2
```

sort similar to min/max, but dimension is the second input argument

cumsum,cumprod cumulative sum (prod)

find returns the indices of nonzero elements. Useful in combination with logical tests: `i = find(A>1 & A<2)`

all, any test whether all entries (any entry) in a particular dimension of an array are (is) nonzero.

```
A = [1 1 1
     0 1 0
     0 0 0];
rows = [all(A); any(A)]
cols = [all(A,2), any(A,2)]
```

Output

```
rows =

     0     0     0
     1     1     1


cols =

     1     1
     0     1
     0     0
```

diff calculate the difference of the elements of an array. For instance, `diff([1 2 5 8 15])` yields `[1 3 3 7]`. The (optional) second and third input arguments can be used to control the order of the difference and the dimension that should be used. A not so obvious practice of the `diff` function, but very useful, is locating the positions in a vector where the value changes.

```
x = [10 10 10 20 20 20 20 30 30 40 40 40]
d = diff(x)
i = [find(d), length(x)]        % always include the last entry
y = x(i)
```

Output:

```
d =

     0     0    10     0     0     0    10     0    10     0     0


i =

     3     7     9    12


y =

    10    20    30    40
```

2.5 Logical indexing

In the introductory example, we have already seen the use of **logical indexing**. The statement `i = A>0.5` returns a logical (0/1 or false/true) array of the same dimension as `A` indicating whether or not the entry is larger than 0.5. Next, `A(i)` simply returns those entries. If necessary, `find(i)` can be used the get the corresponding indices.

2.6 Linear indexing

Internally, Matlab stores a numerical array, regardless of its dimension and size, as a 1-dimensional vector. Hence, the 3x4 matrix in the following example is actually stored as a vector of size 12. This explains the results of the following Matlab statements.

```
A = [11 12 13 14
     21 22 23 24
     31 32 33 34]

i = find(mod(A,11) == 0)        % find indices of multiples of 11
x = A(i)
```

Output:

```
A =

    11    12    13    14
    21    22    23    24
    31    32    33    34


i =

     1
     5
     9


x =

    11
    22
    33
```

The vector `i` is a linear index into the matrix `A`. Linear indices can be translated in the corresponding regular multi-dimensional indices and vice versa by the functions `ind2sub` and `sub2ind`, respectively. See the Matlab help function for more details of these functions. For example:

```
>> [r,c] = ind2sub([3 4],i')

r =

     1     2     3


c =

     1     2     3
```

2.7 Matrix creation and transformation

You should already be aware of functions like `ones`, `zeros`, `eyes`, `diag`, `tril`, `triu` to create basic arrays of desired size. By adding functions as `repmat`, `reshape` and `permute` a whole new window of opportunities opens.

2.7.1 Example: juggling with matrices

Given a vector $x \in \mathbb{R}^{MN}$. Create a $Mm \times Nn$ matrix with $M \times N$ submatrices of size $m \times n$ with the elements in x.

Let `x=[1 2 3 4 5 6]` and $m = 3, n = 2, M = 2, N = 3$. Hence, we need to produce the matrix

```
x =

     1     1     2     2     3     3
     1     1     2     2     3     3
     1     1     2     2     3     3
     4     4     5     5     6     6
     4     4     5     5     6     6
     4     4     5     5     6     6
```

One way to solve this problem is to use the Kronecker product:

```
kron(reshape(1:6,2,3), ones(3,2))
```

This solution is sufficient for most purposes, but you have to keep in mind that `kron` actually needs to do $MNmn$ multiplications. Hence, if the sizes become larger and the computation has to be repeated several times, then this solution is not so efficient. Even though `kron` does not use loops, it is not necessary to perform the multiplications.

We can solve this exercise in an efficient way without using loops by juggling around with matrices. Perhaps it is not straightforward to get this solution, but it gives a good idea of what these functions can do.

```
>> x = repmat(1:6,6,1)

x =

     1     2     3     4     5     6
     1     2     3     4     5     6
     1     2     3     4     5     6
     1     2     3     4     5     6
     1     2     3     4     5     6
     1     2     3     4     5     6

>> x = reshape(x, [3 2 3 2])

x(:,:,1,1) =

     1     1
     1     1
     1     1


x(:,:,2,1) =

     2     2
```

```
     2     2
     2     2


x(:,:,3,1) =

     3     3
     3     3
     3     3


x(:,:,1,2) =

     4     4
     4     4
     4     4


x(:,:,2,2) =

     5     5
     5     5
     5     5


x(:,:,3,2) =

     6     6
     6     6
     6     6

>> x = permute(x,[1 4 2 3])

x(:,:,1,1) =

     1     4
     1     4
     1     4


x(:,:,2,1) =

     1     4
     1     4
     1     4
```

```
x(:,:,1,2) =

     2     5
     2     5
     2     5


x(:,:,2,2) =

     2     5
     2     5
     2     5


x(:,:,1,3) =

     3     6
     3     6
     3     6


x(:,:,2,3) =

     3     6
     3     6
     3     6

>> x = reshape(x, [6 6])

x =

     1     1     2     2     3     3
     1     1     2     2     3     3
     1     1     2     2     3     3
     4     4     5     5     6     6
     4     4     5     5     6     6
     4     4     5     5     6     6
```

2.8 Memory usage: operating in blocks

As you should now by now, we prefer to operate on arrays (matrices, vectors) as a whole, because this is usually faster than operating on individual entries inside a loop. Unfortunately, sometimes you want to do so many repetitions or your data set is so large, that Matlab experiences memory problems. You may observe that the computation speed slows down, because Matlab has to read and write data to disk instead of using the internal memory of your computer. In some cases, the memory that you require may be simply too much and Matlab returns an error.

One way to deal with this issue is to use a for-loop and load or generate individual entries and operate on them. A more sophisticated method is to use a loop and operate on a large block of your data set. In this way, you still have the advantage of working on large arrays, and you can bypass the memory problem.

You can practice this idea in one of the exercises.

2.9 Profiling

If you are really interested in optimizing your code, then Matlab's profiler is a very useful tool. It presents you an overview of how many times a specific function or line of code was executed and how many time was spent there. This gives you a good indication where you should try to improve your code.

2.10 Debugging

More important than the efficiency of your code is of course that the code should do what it should do. If it doesn't, then you should debug your code. You can do this by looking at your code and try to spot the bug, but sometimes it is more convenient to use Matlab's debugging tools. In that way you can go over the execution of your code step by step. Often that can give you ideas about improving the efficiency of your code as well.

2.11 Final remarks

The tools we have discussed in this block enable a Matlab programmer to write very powerful programs with a few lines of code. The danger exists that this code becomes difficult to read, even to the programmer himself. Therefore, it is the programmer's responsibility to add appropriate comments to the code if necessary.

It's up to you to find the right balance between producing *efficient code* on the one hand, and having an *efficient coding process* on the other hand. It doesn't make sense to spend one hour optimizing your code, if you're applying it only once on a small or medium sized data set. However, it would be nice if you are able to optimize your code if necessary. If you try to change your way of thinking is this respect, it often goes automatically in practice. Hence, *avoid loops* as much as you can *anywhere* during this course (and forever after!). During the exam, some of your abilities in this respect will be tested!

Very useful functions to prevent the use of loops, but outside the scope of our course, are `arrayfun`, `cellfun` and `bsxfun`. If you really need to address speed issues of your Matlab code, then have a look at these functions. See the Matlab help and Yagtom.

2.12 Exercises

2.12.1 Student grades

Define a three-dimensional array using the statements

```
n = [4 2 10]
A = 10*rand(n)
```

Perform the following tasks *without using loops.*

1. Suppose that the entries in the matrix represent grades. Round the grades to halves. The only exception is that the grade 5.5 is not allowed; these grades have to be rounded to 5 or 6.

2. Create a matrix B with three columns for which the rows represent the indices into the matrix A that correspond to sufficient grades (>=6). Hence, if `A(2,1,5)` is greater or equal to 6, then `[2 1 5]` is one of the rows of `B`.

3. The matrix contains the grades for 10 students who each did 2 assignments of 4 questions each. Calculate the students' overall grades, which is determined by the arithmetic mean of the in total 8 questions. Did you use the `mean` function once or twice? Try using it only once.

2.12.2 Square form

Consider the square form $x^T Ax$ with $x \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n\times n}$. Suppose that we want to evaluate this expression for all vectors in the rows of the $m \times n$ matrix X. The standard solution with loops is as follows:

```
[m,n] = size(X);
y = zeros(m,1);
for i=1:m
  y(i) = X(i,:)*A*X(i,:)';
end
```

1. Can you find a method that does not require a loop? *Hint:* look for a combination of a (regular) matrix product and a elementwise-product of matrices.

2. Generate random matrices X and A for $n = 40$, $m = 1000$. Test the performance of the two approaches by replicating the computations, say 1000 times, by putting them in a loop and time the duration using `tic` and `toc`.

3. Also compare the performance of the two methods using the profiler.

2.12.3 Euclidean distance

Let the rows of the $m \times n$ matrix X represent m vectors in n-dimensional space. We want to create a $m \times m$ matrix D such that $D_{ij} = \|x_i - x_j\|_2$, i.e., the distance (2-norm) between the ith and jth row of X. Write a function for this purpose. You could start by implementing the "standard" approach using three loops: two for the combination i and j and one for the dimension. The third loop is easy to get rid of. The second loop can also be deleted. Try to find this solution and compare the solutions using the profiler.

2.12.4 Find the bug

In this exercise you'll have to find an error in a function. It is not a syntax error for which Matlab returns an error, but a logical error, which simply returns an unintended answer. If you can't such an error right away, then a good alternative is to use the Debugger. Walk through the function step by step and examine intermediate output.

Save the file knapsack$_{\text{error}}$.m on your Matlab path. This function is supposed to solve the unbounded knapsack problem where there is an unlimited supply of each item of a certain value and weight. If the problem is solved correctly, then it should give the given output for the example below.

```
value    = [4, 5, 2];
weight   = [4, 6, 3];
capacity = 10;
[X, f] = knapsack_error(value, weight, capacity)
```

Output:

```
X =

     0     0     0
     0     0     0
     0     0     1
     1     0     0
     1     0     0
     0     1     0
     1     0     1
     2     0     0
     2     0     0
     1     1     0


f =

     0
     0
     2
```

```
4
4
5
6
8
8
9
```

Unfortunately, the function does not give the correct output. Find the bug!

2.12.5 Run length decoding

Reconsider the example about the `diff` function. Extend the use of the `diff` function even further by writing a function that also counts the number of subsequent equal values. For a given input vector `x`, the function should return two outputs: a vector `y` (as in the example) and a vector `c` that counts the number of subsequential values in `x`. For the particular example this would be `y = [10 20 30 40]` and `c = [3 4 2 3]`.

2.12.6 Random experiment: operating in blocks

Consider the following experiment. We have a group of n people numbered from 1 to n. They are put in a random sequence and we are interested in the number of occurrences where two people with consecutive numbers are side by side. For instance, if person number 5 is followed by person number 6, then we have a hit. However, if these two persons are in the opposite order, then it does not count. If we have three consecutive numbers in line, then this should count as two.

1. Create a function that takes the size of the group and the number of experiment replications as inputs, and then performs the experiment and returns the fraction of consecutive numbers in the generated sequences. Matlab has a function `randperm`, however, this function can generate random permutations only one by one. We want to generate them all at once. You could do this by using `rand` in combination with (the second output argument) of `sort`. You should not use a loop in your function.

2. Test your function and try different values for the number of replications. Try to find the number where Matlab slows down due to memory problems.

3. Make a new implementation of your function in such a way that it can generate and operate blocks of permutations. For instance, instead of doing 1 billion permutations in one go, you'll do 1000 blocks of 1 million permutations.

4. Try to compare the performance differences with respect to the speed for several block sizes when working with a large number of replications. You might want to use the profiler.

5. Bonus question: add another input argument to your function that indicates the required number of consecutive numbers in the line. In the standard case this was two, but it could be three or any other number.

3 Cell and structure arrays

3.1 Cells

The most used data type in Matlab is without any doubt the "double", which is a data type that represents numerical numbers. Multi-dimensional arrays allow us to represent vectors, matrices and even higher dimensional data. Regardless of the dimension and size of such an array, each and every entry in this array is always a *single* double. Cell arrays are similar in most aspects, but each entry of a cell array can be any other Matlab data type, e.g., a matrix, a string, a double, a structure array or even another cell array. This is especially convenient if you want to store data that somehow belongs together and has different formats and sizes.

Look at this quick introduction about cell arrays. You can stop reading when they start talking about `cellfun`. Although this is a very useful function, especially in combination with function handles, and I encourage the use of it, we don't deal with it in this course.

If you need more information about cell arrays look at the Matlab documentation on the web here, or even better, access the Matlab help function.

3.2 Structures

Structures arrays are an alternative way to store data of different types and size in a single entity. You might know structures from other programming languages, such as Java and c++, and they are very similar in Matlab, however, we don't consider objects as in object oriented programming, just regular Matlab data types.

Read the introduction about structures, and structure arrays, on Yagtom. For more detailed information, again look at the official Matlab documentation.

3.2.1 Example: passing multiple arguments to a function

One of the nice possibilities of structs is to pass multiple input arguments to a function. This is specially useful for large projects.

Suppose that you have a set of functions that share a large set of parameters:

```
function y = main(x,rho,lambda,mu,sigma,A,b)

y = subfun(x,rho,lambda,mu,sigma,A,b);

function y = subfun(x,rho,lambda,mu,sigma,A,b)

y = x + rho/lambda + mu*sigma + A'*A*b;
```

Now suppose that somewhere in the code you call the function by `main(x,mu,sigma,rho,lambd`
This doesn't give you an error message, but the result is probably not as intended and it'll be difficult to spot this bug.

Moreover, suppose that we need to extend the computation in `subfun` and that an additional input argument is needed. Then, we'll need to change the function `main` and all functions that call `main` and `subfun` as well.

We can resolve these inconveniences by using structs:

```
function y = main(x, pars)

y = subfun(x, pars);

function y = subfun(x, pars)

% Extract parameters from struct.  This step is not really necessary,
% because we can use the values directly as well.
rho    = pars.rho;
lambda = pars.lambda;
mu     = pars.mu;
sigma  = pars.sigma;
A      = pars.A;
b      = pars.b;

y = x + rho/lambda + mu*sigma + A'*A*b;
```

3.3 Exercises

3.3.1 Reading from a text file

In this exercise we are also going to practice some data import and export tools. Note that if you are importing/exporting only numerical data, then `dlmread` and `dlmwrite` are convenient functions. Here we have mixed numerical and text data, which is a bit more complicated.

1. Download the file datelist.csv and have a look at it.

2. Import the data in Matlab. You can use any method you like, for instance the import wizard (`uiimport`) or the `textscan` command. Skip the header line. From the data now create the numerical vectors `year`, `day`, and `week`, and cell arrays `month` and `weekday`. If you really get stuck here, then download the Matlab data file datelist.mat and load in your Matlab session.

3. Create a 9x2 cell array `C`. For every year in the data set put the year number (i.e., a scalar value) in the first "column". The second "column" should be filled by two-column matrices containing the day and week numbers of the corresponding year in the data set.

4. Create a 12x1 structure array with the fields: month, day, weekday and year. Of course, the month field only needs to contain a single string (character array). You might need to search for a built-in Matlab function that you can use to compare strings (character arrays) and cells.

5. Check if there are any duplicate dates in the data set. Note that the combination (year,day,week) should be unique for any date, so you don't need to consider any of the text data. Try not to use a loop for locating the duplicates.

6. Write the duplicate dates to a comma-separated-values (CSV) file with a structure exactly similar to the original. Also include the header line. Take a look at the functions `fopen`, `fprintf` and `fclose`.

3.3.2 Combinations totaling to sum

Consider natural numbers n and k. We are interested in creating all possible combinations of k numbers summing to n. For example, if $n = 4$ and $k = 3$, then the combinations are

```
0    0    4
0    1    3
0    2    2
0    3    1
0    4    0
1    0    3
1    1    2
1    2    1
1    3    0
2    0    2
2    1    1
2    2    0
3    0    1
3    1    0
4    0    0
```

For fixed k a straightforward solution comes to mind involving k loops. The problem, however, is that k and hence the number of loops is unknown beforehand. This problem could be solved by recursion, but still that solution uses a lot of loops.

A very elegant solution to this problem, which illustrates the possibilities to do things without loops, is given by the following function. It is instructive to walk through the steps of this function using the debugger.

```
function c = combsum(n,k)
% COMBSUM All combinations of natural numbers totaling to sum
%
% c = combsum(n,k)
```

```
%
% Returns all possible combinations of K numbers totalling to N in the
% rows of the output matrix C.

% All possible placements of internal dividers.
dividers = nchoosek(1:(n+k-1), k-1);
ndividers = size(dividers, 1);

% Add dividers at the beginning and end.
b = [zeros(ndividers, 1), dividers, (n+k)*ones(ndividers, 1)];

% Find distances between dividers.
c = diff(b, 1, 2) - 1;
```

In this exercise, we make another implementation of the function `combsum` by using cell arrays. Initialize a cell array `x` of size $1 \times k$. Use the `ndgrid` function to create k multi-dimensional arrays (tensors) of size $(n+1)^k$ (with values 0 to n) into the cell array that you just created. The left-hand side of this assignment should be `[x{:}]`, which is the same as `[x{1},x{2},...,x{end}]`. This puts the k outputs of `ndgrid` in the cell array `x`. Now reshape the contents of each cell to a vector and put them in a matrix `A` with k columns (you may use a loop for this). This matrix `A` contains all possible combinations of k numbers with values from 0 to n. If you now delete all rows that do not add up to n, then you are done. Test the intermediate steps of the approach with small values for n and k, so that you understand what is going on, and finally write the new implementation of `combsum`.

4 Function handles & anonymous functions

4.1 Introduction

You should already be familiar with the concept of m-file functions, because it's the standard way to define a function in Matlab. M-file functions allow you to divide your computations in independent pieces of code, which can be called whenever you like. However, it is a bit annoying when you have to create a m-file function for a one line function definition. Sometimes this is necessary though, for example when you have to define the objective function of an optimization problem, because the optimization tool requires this as an input. This is where function handles and anonymous functions are extremely convenient as we shall see.

4.2 Function handles

A function handle is nothing more than a *reference* to another function. This is a simple example how to create and use a reference to a built-in Matlab function.

```
f = @sin;                           % reference to the sin function
x = f(pi*(0:0.5:2))                 % evaluate sin through the function handle f

x =

         0    1.0000    0.0000   -1.0000   -0.0000
```

This also works for multiple input and output arguments.

```
g = @min;
A = [1 2
     4 3];
[x,i] = g(A,[],2)                   % find row minimum (traverse along 2nd dimension)

x =

     1
     3


i =

     1
     2
```

4.3 Anonymous functions

An anonymous function is a special type of function handle to a function for which no m-file function exists. You can see it as an alternative to inline functions. Actually, anonymous functions are much more flexible and faster than inline functions, so use anonymous functions from now on.

Here is a simple example of an anonymous function:

```
f = @(x) poisspdf(x, 5)
```

This statement defines a function handle `f` to a function of one variable `x`, which is defined by `poisspdf(x,5)`. Hence, `f(2)` would return the same output as `poisspdf(2,5)`, which is the probability that a Poisson distributed random variable with mean 5 is equal to 2. Note that the variable `x`, which is used in the definition of the anonymous function has no effect on a variable with the same name in the current workspace.

We can also define functions with multiple input arguments and use variables from the workspace in the definition.

```
a = 1;
c = 2;
f = @(x,a) a.*(x-c).^2;
```

Note that we are using element-wise arithmetic operators in the definition. This allows us to call the function with non-scalar inputs (as long as they match in size of course). Another important thing to remember is that changing the value of `c` has no effect on the definition of `f`: only the value of `c` at the time of the definition is relevant! On the other hand, the value of `a` in the workspace has no effect at all on the function `f` where `a` is only used as a (temporary) reference to the second input argument of `f`. These notions explain the results of the following commands.

```
t = [4 4 5 5];
b = [1 2 1 2];
y = f(t,b);
a = 100;
c = 100;
y = [y; f(t,b)]
```

Changing the variables `a` and `c` has no effect on the output as you can see:

```
y =

     4     8     9    18
     4     8     9    18
```

4.4 Illustrative example

Now that we have seen how to define anonymous functions, let's have a look at some examples where anonymous functions are very useful. We can use them

- to pass a function to another function,
- to capture data values for later use by a function,
- to call functions outside of their normal scope.

A useful Matlab function is the `fzero` function, which you can use to find the zero location of a function of a scalar variable. For instance:

```
>> fzero(@log, 2)

ans =

   1
```

`@log` is a function handle of the function for which we want to find the root and the second argument is an initial guess of the location of the root.

Often, you don't want to find the location where a function is equal to zero, but the location where it is equal to a certain value `c`, which is not necessarily equal to zero. What to do if we want to find the location where the gamma function is equal to 10? Without anonymous functions, we would have to define an m-file function that, for a given input `x`, returns `gamma(x)-10`, and use that function as the input for `fzero`. We would have to repeat this procedure for other targets than `10`. Of course, we can easily define a function with a second input argument that represents the target, but `fzero` requires a function with only one input variable.

This problem is easily solved with anonymous functions:

```
f = @(x) gamma(x)-10;
x = fzero(f, 2)
```

We can even do it in one line:

```
x = fzero(@(x) gamma(x)-10, 2)
```

We can take this idea even one step further by defining a function that generalizes the `fzero` function to include an input variable that represents the target. Consider the m-file function

```
function x = ftarget(f, target, x0)

g = @(x)(f(x) - target);
x = fzero(g, x0);
```

Now we can do

```
>> [ftarget(@log, 1, 2), ftarget(@gamma, 120, 3), ftarget(@normcdf, 0.975, 3)]

ans =

    2.7183    6.0000    1.9600
```

Note that we could have obtained the same results from the following anonymous function instead of the m-file function above.

```
ftarget = @(fun, target, x0) fzero(@(x) fun(x)-target, x0)
```

4.5 Exercises

4.5.1 Piecewise linear function

Define the following function as an anonymous function. Make sure that the function allows non-scalar input. Note that you can't use `if` statements or loops in the definition of an anonymous function.

$$f(x) = \begin{cases} x+1 & \text{if } x \leq 1 \\ x+3 & \text{if } 1 < x \leq 2 \\ 7 - x^2/2 & \text{if } x > 2 \end{cases}$$

Plot the function using `fplot`.

4.5.2 Expected value

Let X be a gamma distributed random variable with shape parameter 5 and scale parameter 2. Write an anonymous function `Efx` that returns $E[f(X)]$ for a function $f(.)$. For instance, $E[\log(X)]$ can be calculated by `Efx(@log)`. You'll need to find a (built-in) function you can use to evaluate an integral. Use your version of `Efx` to calculate

1. $E[\log(X)]$
2. $E[1/X]$
3. $E[\cos(X)]$
4. $E[(X-10)^2]$ Note that this should return the variance of X: 20.

4.5.3 Solving nonlinear equations

In this exercise we will try to solve a system of *nonlinear* equations. Note that we will discuss *linear* equations in the section about Linear algebra.

Make an anonymous function for $f : \mathbb{R}^n \to \mathbb{R}^n$ with n an even natural number and

$$f(x) = \begin{bmatrix} g(x) \\ h(x) \end{bmatrix},$$

with

$$g_i(x) = 1 - x_{2i-1}, \qquad i = 1, \ldots, n/2$$

and

$$h_i(x) = 10(x_{2i-1} - x_{2i})^2, \qquad i = 1, \ldots, n/2$$

Note that it is not too difficult to do this without having to define the functions $g(.)$ and $h(.)$ first. For instance, the function $g(.)$ is easily defined by `1-x(1:2:end-1)`. Moreover, you can write a single anonymous function that works for all (even) n.

We are interested in solving the nonlinear system of equations $f(x) = 0$, which has n equations and n unknowns. It can easily be verified that the n-dimensional all-one vector is a solution for this problem.

Now try to find this solution numerically using the `fsolve` function. Read the documentation about how to use this function. Pick a random initial guess—i.e. generate it using a random number generator—and make sure to have the function display some output so that you can check the number of function evaluations.

Now do the same, but also provide `fsolve` with the Jacobian (first derivative) of $f(.)$. This time you can write a m-file function to compute the function f and its Jacobian. However, if you can write an anonymous function for this Jacobian, then I'd be very interested in seeing that solution.

If you run the algorithm again, then you should see that the number of function evaluations is much smaller than in the case without the Jacobian.

5 Generic programming & good documentation

5.1 Introduction

More often than not, Matlab is the number one choice among the tools that I would consider as an alternative to solve a particular problem. One of the things I like about Matlab is that it is so easy to develop advanced algorithms in such a short time. An important reason for this is the possibility to use the many mathematical, statistical and visualization functions that are available right out of the box accompanied with professional documentation and examples. Another advantage is the freedom that the language allows. For instance, contrary to most other programming languages, in Matlab it is not necessary to declare variables and their dimension, size and type before you use them. As a matter of fact, you can change the dimension, size and type of a variable at free will.

It is easy to understand that the last "advantage" can result in ambiguities as well. Combined with the power of this high level programming language this can introduce serious problems. Unfortunately, Matlab makes it very easy to make very powerful code such that even the author cannot understand its meaning after even a week. Needless to say that another person cannot make any sense of it as well.

This block is to give some guidelines how we can prevent this problem.

Generic programming By this I mean that you try to split your problem in smaller subproblems and write separate pieces of code for them. Ideally, the subproblems should be coded in such a way that their applicability goes beyond the use of the particular problem at hand.

Good documentation Add appropriate documentation to your functions and complex pieces of code.

5.2 Generic programming

As explained in the introduction, the idea is to split a problem in smaller subproblems. It is hard to give specific rules here; you will have to find the right balance of the subproblem size. As a guideline you could say that you should consider writing a separate Matlab (sub)function if:

- You are copying pieces of code. For instance, if you want to repeat a certain analysis with minor variations or different data sets, or if you want to produce the same type of plot for different data sets.

- You are writing a rather complex piece of code of more than, say, 10 lines.

If possible, you should try to take the generic programming one step further by trying to anticipate on possible alternative uses of the particular subproblem for which you are writing a Matlab function. You can do this in several different ways as illustrated in the following sections.

5.2.1 Allowing higher dimensional inputs than necessary for your original problem

Suppose that you want to compute the shape and scale parameters of a gamma distribution that correspond to a given mean and standard deviation. Even though it is only two lines of code, this is a typical example of a subproblem that needs to be solved at another time as well. Perhaps, you need to solve it for a multiple combinations of means and standard deviations. Hence, it's convenient if the function allows vector or even higher dimensional input. This can often be accomplished by making the arithmetic element-wise right from the start. Even if you cannot prevent the use of loops in the function, all future caller functions don't have to implement this loop again and again.

5.2.2 Adding additional input arguments that control the behavior of the function

Suppose that you need to compute the 4-period moving average of multiple time series with quarterly data. Because you may need to repeat this computation several times and for different type of time series, it makes sense to write a dedicated Matlab function for it. However, perhaps you need to solve a similar problem in the future for monthly data. You can provide an additional input argument that controls the number of periods for which you want to calculate the moving average.

5.2.3 Providing default values for some input variables

Continuing on the previous example, we can make the additional input argument optional. Hence, the user is not required to use it, and in that case the function should provide a default value. This can be accomplished by the use of the `nargin` statement, possibly in combination with `isempty`. For example:

```
function y = MovingAverage(x, n)

if nargin < 2 || isempty(n)
  % Default: four period moving average
  n = 4;
end

% Start of computations
```

This allows the user to call the function by `MovingAverage(x)`, `MovingAverage(x,4)` as well as `MovingAverage(x,12)`.

By using the `varargin` construct it is even possible to have a variable number of input arguments. The `varargin` construct requires some basic knowledge of cells.

See the Matlab help and Yagtom for some examples.

5.2.4 Providing additional output

Often your computations produce intermediate or side results. These results could be useful in some circumstances. Therefore, it doesn't do any harm to include these results as output variables. Outputs don't necessarily have to be retrieved by the caller function, hence if the user doesn't need the results, then there is no waste of computations or memory. If desired, it is possible to control the flow inside a function depending on the required output arguments by using the `nargout` and possibly even the `varargout` constructs.

5.3 Documenting your code

As noted before, it is important to supply your code with appropriate documentation. I distinguish between two different types of documentation.

5.3.1 Function documentation

If you write a function, then you should always include

- a one-line description of the function
- an overview of the input and output variables
- a description of what the function does

It is important that all three parts of the function documentation are put at the top of your file, directly below the function declaration, in a contiguous block of lines starting with the comment character (`%`) and starting with the one-line description. This entire block will show up in the Matlab command window when the command `help <FunctionName>` is issued. The first line of the documentation is displayed for each m-file when the `help` function is given a directory name as its argument (`help <Directoryname>`).

The idea is explained in the following example.

```
function [y, trimmed] = trim_data(x, fraction, tail)
% TRIM_DATA Trims the tails of input vector
%
% y = trim_data(x, fraction, tail)
%
% For a numerical vector trims away a certain percentage of the lowest
% and/or highest observations.
%
% |----------+------------------------------------------------------|
% | Input    | Description                                          |
% |----------+------------------------------------------------------|
% | x        | vector with numerical data                           |
% | fraction | fraction of observations to trim away (default: 0.2) |
% | tail     | 0: trim away high and low observations (default)     |
% |          | 1: trim away high observations only ...              |
```

```
% |          | -1: trim away low observations only                          |
% |----------+--------------------------------------------------------------|
% |----------+--------------------------------------------------------------|
% | Output   | Description                                                  |
% |----------+--------------------------------------------------------------|
% | y        | sorted vector with observations that are not trimmed away |
% | trimmed  | the trimmed observations                                     |
% |----------+--------------------------------------------------------------|

if nargin < 2 || isempty(fraction)
  % Default trim 20%.
  fraction = 0.2;
end

if nargin < 3 || isempty(tail)
  % Default trim high and low observations.
  tail = 0;
end

if tail == 0
  % Convert to one-sided fraction.
  fraction = fraction / 2;
end

x = sort(x);
n = length(x);

% Compute the number of observations to trim per tail.
k = floor(fraction * n);

switch tail
case 1
  % Trim high observations.
  y = x(1:end-k);
case -1
  % Trim low observations.
  y = x(k+1:end);
otherwise
  % Trim high and low observations.
  y = x(k+1:end-k);
end

% If second output argument required, then return the trimmed values.
if nargout > 1
  switch tail
  case 1
```

```
    trimmed = x(end-k+1:end);
  case -1
    trimmed = x(1:k);
  otherwise
    trimmed = x([1:k, end-k+1:end]);
  end
end
```

5.3.2 Local documentation

You add local documentation, i.e., documentation to the code itself, for several reasons.

- To enhance the understanding of the main flow of the code. This is the type of documentation that is present in the `trim_data` function in section about Function documentation.
- To explain details about nontrivial parts or lines of code
- To explain the idea behind variables

It is certainly not necessary, or even desirable, to comment on each and every line of code. Note that the necessity of local documentation diminishes if you write relatively small functions, because the function already should contain a proper documentation and the number of different variables is usually limited.

5.3.3 Programming style

Code documentation is supported by a good programming style. The programming style gives rules/guidelines about e.g.

- choosing function/file names,
- choosing variables names,
- indentation of `if` statements, `for` and `while` loops, and multi-line statements.

The Matlab editor provides nice support for indentation of code. Choosing variable/function names is specially important for large projects and many different styles and preferences exist. I don't want to add to this discussion.

5.4 Exercise: restructuring code and adding documentation

In this exercise, we consider a script file that is created by copying the commands from the *Command Window* in a Matlab session to an m-file. During this Matlab session I wanted to explore the effect of rounding errors on the approximation of derivatives by taking *finite differences*. For a function f, the central finite difference approximation for $f'(x_0)$ is given by

$$D_h(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h},$$

where h is the step size. For relatively larg step sizes, this approximation is inaccurate because it simply does not capture the curvature at x_0 well enough. On the other hand, very small step sizes could introduce *numerical inaccuracies* due to rounding errors.

Have a look at the script file roundingerror.m. For the sin function and several step sizes I have plotted the errors from the finite difference approximation at $x_0 = 0.5$ and its true derivative, which we know is the cos function. I also marked the step size with the smallest error in the plot. After that, I repeated this procedure for other values of x_0 and added the results to the same figure.

The example illustrates the ease of experimenting in Matlab. However, the resulting script file is not a very generic and flexible piece of code for several reasons.

- If you want to chance the values for x_0, then you'll have to change this at 3 locations in the code. This is what we call *hard coding*.
- If you want to add another point x_0, then you'll have to copy a piece of the code and change the value for x_0 used there. In addition, you'll have to come up with a different color code to distinguish the plot from the other plots in the figure.
- If you want to do the experiment for another function instead of the sine, then you'll have to change the calls to the sine and cosine everywhere in the code (hard coding again).

Restructure the script file such that these drawbacks are resolved.

1. Write a *function* m-file with the following input arguments:
   - reference to a function (a function handle)
   - reference to a derivative function
   - vector with x_0 locations
   - vector with step sizes

   and the following output arguments

   - matrix with absolute errors corresponding to the x_0 locations (in the columns) and the step sizes (in the rows)
   - index locations of step size with minimum error

   Make sure that the function has appropriate documention.

2. Write a *script* m-file that uses this function to repeat the original experiment and plots the results nicely in one figure.

6 Linear algebra

6.1 Basic linear algebra in Matlab

Matlab supports many basic linear algebra operations such as

- Creation of special matrices
  - `eye`, `zeros`, `diag`, `toeplitz`, `hankel`, `hilb`, `vander`
- Fundamental matrix properties
  - `det`, `trace`, `rank`, `norm`, `inv`
- Matrix factorizations
  - `eig`, `qr`, `lu`, `svd`, `chol`

Special attention is given to the problem of solving a system of linear equations, because in practice people often choose the wrong alternative to solve this problem.

Given $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$ such that

$$Ax = b.$$

We can distinguish three cases:

1. **Square** system: $m = n$
2. **Over-determined** system: $m > n$
3. **Under-determined** system: $m < n$

A rule of thumb, regardless of the case, is **always** use the **backslash** operator (\, `mldivide`):

```
x = A\b;
x = mldivide(A,b);                % same as above
```

The computation is **more efficient** (faster) than alternative solutions:

1. Square system (and nonsingular): equivalent to $x = A^{-1}b$ (`x = inv(A)*b`)
2. Over-determined system ($m > n$): equivalent to least-squares solution $x = (A^TA)^{-1}A^Tb$ (`x = inv(A'*A)*A'*b`)
3. Under-determined system ($m < n$): `A\b` gives a solution with as many zeros as possible. Alternative solutions can be obtained by combining this result with the solution(s) to $Ax = 0$, which can be obtained by `null(A)`.

6.2 Exercises

6.2.1 Obtaining different solutions to a under-determined linear system

Create a matrix A and vector b using the following commands.

```
m = 6;
n = 10;
A = randn(m,n);
b = randn(m,1);
```

Verify that the matrix has rank 6, otherwise repeat the procedure. Note that the system $Ax = b$ is under-determined: infinitely many solutions will exist. Recall from your linear algebra course that any solution to the linear system $Ax = b$ can be written as $x = x^0 + y$, where x^0 is an arbitrary solution and y a homogeneous solution, which is in the null space of A, i.e., $Ay = 0$.

1. Obtain an arbitrary particular solution x^0 for the linear system $Ax = b$.

2. Find the particular solution $x \in \mathbb{R}^{10}$ for which the first four elements are equal to zero. Note that if the rank of A is 6, then the null space has dimension 4. Hence, any vector y in the null space can be written as a linear combination of 4 linearly independent vectors $v^1, \ldots, v^4$ in the null space:
$$y = \sum_{i=1}^{4} \alpha_i v^i.$$
You'll need to find the coefficients α_i for which the first four entries of the vector
$$x = x^0 + y = x^0 + \sum_{i=1}^{4} \alpha_i v^i \tag{1}$$
are zero, and you can ignore the other 6 entries of x and y. Hence, you'll need to find the homogeneous solution y for which $y_j = -x^0_j$, for $j = 1, 2, 3, 4$.

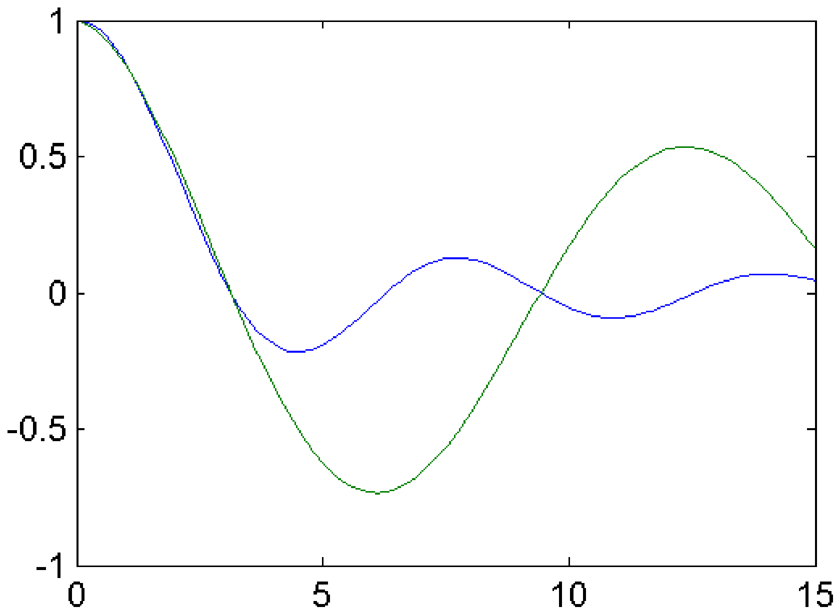
3. Find the particular solution x that, among all solutions, has the smallest 2-norm: $\|x\|_2 = \sqrt{x^T x}$. Ideally, you would like to choose $x = 0$ because its norm is 0, but $x = 0$ is not a solution to our linear system. A solution is always of the form $x = x^0 + y$ with $y = V\alpha$, where V is the matrix with the linear independent vectors from the null space. The ideal solution $x = 0$ corresponds to $y = -x^0$ or $V\alpha = -x^0$. Since the rank of V is 4, this system is underdetermined and no solution will exist. The best solution, therefore, comes from solving the associated least squares problem to this linear system. Check that this solution is equal to `pinv(A)*b`

7 Graphics

7.1 Customizing plots

In this section we'll refresh/introduce some useful graphical commands using examples. First, let's make a data set and plot them.

```
x = (0:0.1:15)';              % column vector
y = [sin(x)./x, exp(-0.05*x).*cos(.5*x)]; % two columns
plot(x,y);
```

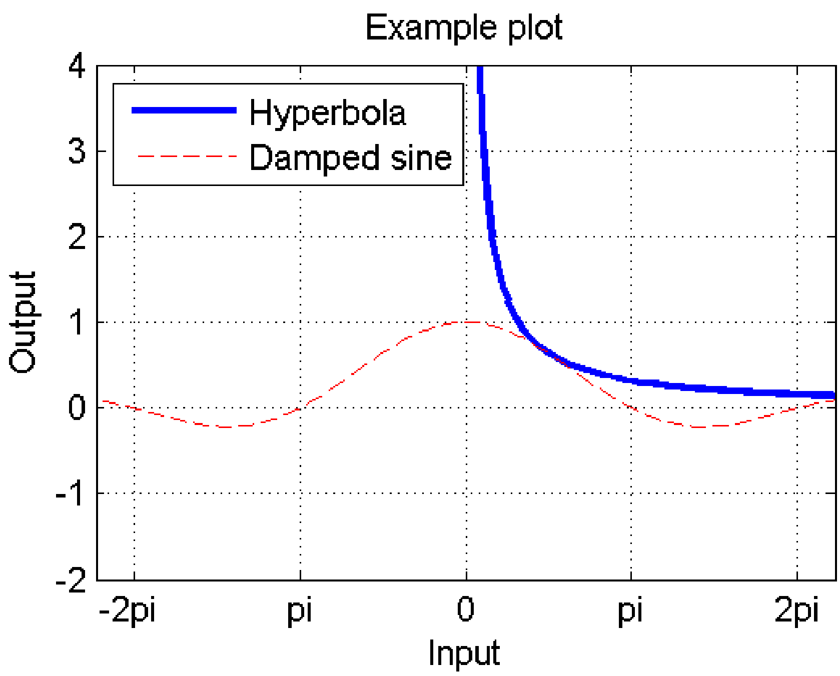


After you have created a plot you can use the figure window to edit the figure. For instance, you can add all kinds of labels, change line types and line colors, etc. If you want to use the same type of plot for different parameter values of data sets, then it is convenient to be able to do this type of figure customization automatically using Matlab code. This prevents repeating the customization manually over and over again.

The next example shows the most common graphic customizations.

```
figure                          % create a new figure
x = 0.1:0.1:7;
plot(x, 1./x, 'r--', 'linewidth', 2); % set line color, line style and
                                      % line width
hold on                         % add the next plot in the same figure (axes)

% With fplot we only have to specify the function and the range instead of
% the x-y vectors.
fplot(@(x) sin(x)./x, [-7 7], 'b');

grid on                         % add x- and y- grid lines
```

```
axis([-7 7 -2 4]);                % change visible axis

% Change the default location and labels of the x-axis.
set(gca, 'xtick', pi*(-2:2));
set(gca, 'xticklabel', {'-2pi', 'pi', '0', 'pi', '2pi'});

% Add some labels
title('Example plot');
xlabel('Input');
ylabel('Output');
legend('Hyperbola', 'Damped sine', ...
       'Location', 'NorthWest'); % force the location of the legend
```



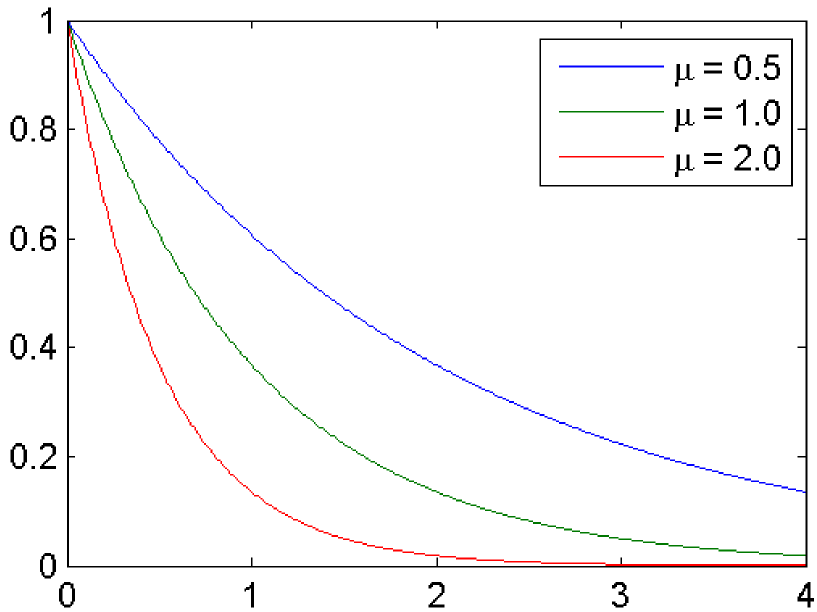
The figure/axis/plot properties that you can access through the figure window can also be changed using Matlab commands. You can use the commands `get` and `set` to retrieve and change these settings. As the first input argument these functions require a so-called handle to a figure/axis/plot. The standard functions `gcf` (get current figure) and `gca` (get current axis) return the handles to the current figure/axis. Try the following commands and check the results and try to change some setting using the command line.

```
get(gcf)
get(gca)
get(gca, 'ygrid');
set(gca, 'ygrid', 'off');
```

If you want to create multiple figures or plots, then it using cell arrays in combination with `sprintf` is useful to set labels/legends.

```
x = (0:0.01:4)'; mu = [0.5, 1, 2];
```

```
y = zeros(length(x), length(mu)); leg = cell(1,length(mu));
for n=1:length(mu)
  y(:,n) = exp(-mu(n)*x);
  leg{n} = sprintf('\\mu = %.1f', mu(n));
end
plot(x, y);
legend(leg{:});                  % passes the cells as arguments to legend
```



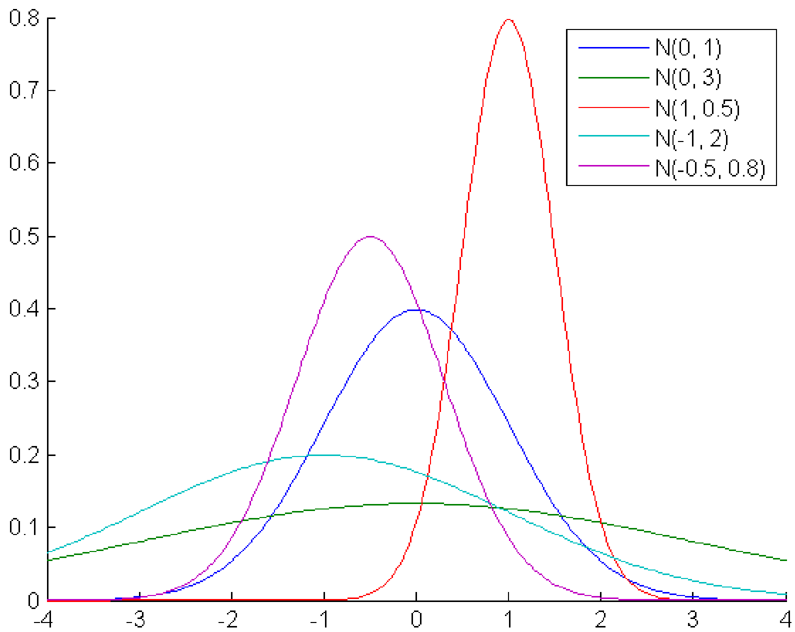
In the example above, we have used a single `plot` statement, which is convenient when you want multiple plots in one figure, because each plots automatically gets its own color. However, sometimes you build up a figure by using several plot-like statements. The default plot color is blue, which means you'll need to specify different colors if you want the plots to have different colors. You can do this manually, for instance:

```
figure;
x = -3:0.5:3;                       % large step size
plot(x, sin(x), 'b');               % plot in blue
hold on                             % add new plots to the same figure
x = -3:0.05:3;                      % small step size
plot(x, sin(x), 'r');               % plot in red
legend('Large step size', 'Small steps');
```

This is okay if you only have two or three plots, but it not so convenient if you have a more and/or arbitrary number of plots in the same figure. In that case, you can specify RGB colors—color values for red, green, and blue—taken from a so-called *colormap*. This is illustrated by the following example.

```
% Define parameter combinations
mu_sigma = [  0,   1
```

```
              0,  3
              1,  0.5
             -1,  2
           -0.5,  0.8];

n   = size(mu_sigma, 1);                % number of plots
x   = linspace(-4, 4, 201);             % define the x-range
leg = cell(n, 1);                       % initialize empty legend cell array

% Get the colors from the 'lines' colormap
colmap = lines(n);

figure;
hold on
for i=1:n
    mu    = mu_sigma(i, 1);
    sigma = mu_sigma(i, 2);
    % Plot using the RGB-colors in the i-th row from the colormap
    plot(x, normpdf(x, mu, sigma), 'color', colmap(i,:));
    leg{i} = sprintf('N(%g, %g)', mu, sigma);
end
legend(leg{:});
```

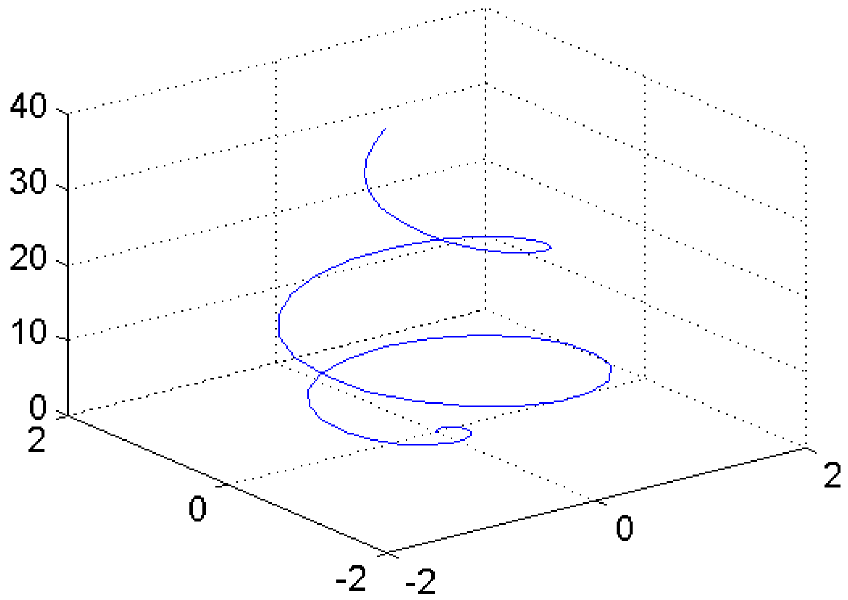


Instead of using the `lines` colormap, you could also use other colormaps such as `gray`, `pink`, `cool`, `bone`, `copper`.

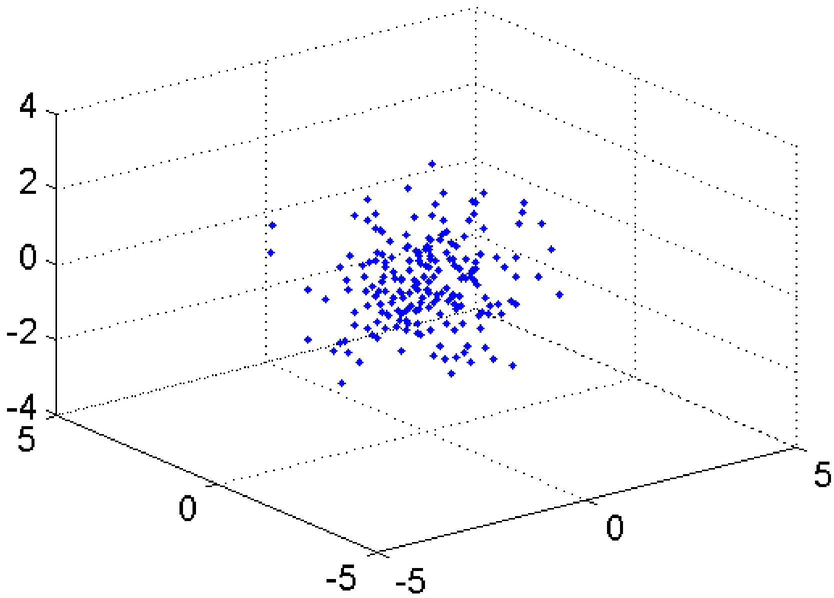
7.2 3D graphics

Making 3D plots is not much different than creating 2D plots. Let's see some examples.

```
t = 0:.1:2*pi;
x = t.^3.*sin(3*t).*exp(-t);
y = t.^3.*cos(3*t).*exp(-t);
z = t.^2;
plot3(x,y,z); grid on
```




```
n = 200;
x = randn(n,1);
y = randn(n,1);
z = randn(n,1);
plot3(x,y,z, '.'); grid on
```



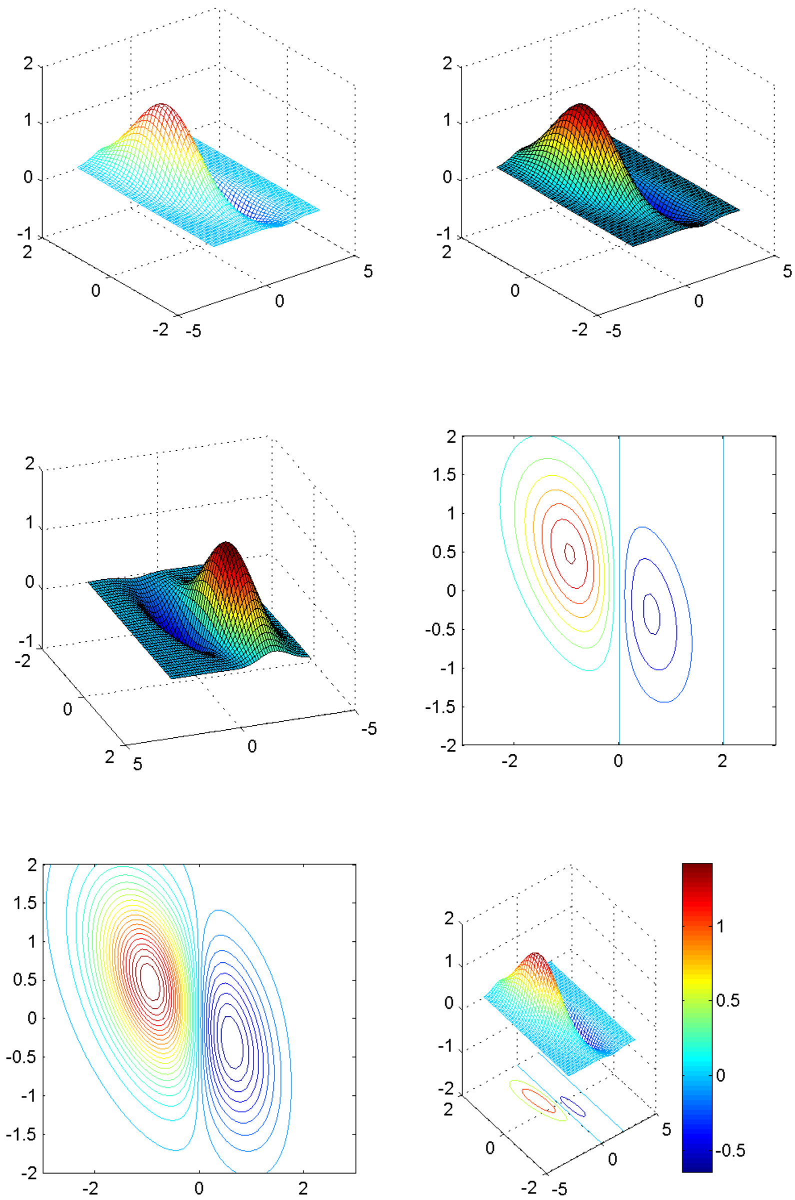
Things become more interesting if we want to plot a function with two input arguments as a surface. We need to create a xy-grid first, which specifies all combinations of x and y values for which we evaluate the function. The following example illustrates the `meshgrid` function.

```
[x,y] = meshgrid(1:5, [10, 20])
z = x + y

x =

     1     2     3     4     5
     1     2     3     4     5


y =

    10    10    10    10    10
    20    20    20    20    20


z =

    11    12    13    14    15
    21    22    23    24    25
```

How we can use the `meshgrid` function to create various 3D plots is illustrated by the next example.

```
[x,y] = meshgrid(-3:0.1:3, -2:0.1:2);
z = (x.^2 - 2*x) .* exp(-x.^2 - y.^2 - x.*y);
```

```
figure;

% Create the first subplot of a figure with 6 (3x2) subplots
subplot(3,2,1);
mesh(x,y,z);

subplot(3,2,2);
surf(x,y,z);

subplot(3,2,3);
surf(x,y,z);
view(-200, 30);

subplot(3,2,4);
contour(x,y,z);

subplot(3,2,5);
contour(x,y,z,30);

subplot(3,2,6);
meshc(x,y,z);
colorbar;
```



Sometimes your two-dimensional function is defined using a single two-dimensional input argument instead of two one-dimensional input arguments. For instance,

```
f = @(x,y) (x.^2 - 2*x) .* exp(-x.^2 - y.^2 - x.*y);
```

defines the same function as

```
g = @(x) (x(:,1).^2 - 2*x(:,1)) .* exp(-x(:,1).^2 - x(:,2).^2 - x(:,1).*x(:,2));
```

Depending on the situation one could be prefered over the other. In the last case, it is a bit more complicated to create a 3D-figure, because the output of meshgrid cannot be directly applied. Fortunately, it is not too difficult to accomplish:

```
[x,y] = meshgrid(-3:0.1:3, -2:0.1:2); % generate the grid as before
X = [x(:) y(:)];                    % put all (x,y) combinations from the grid in
                                    % the rows of a two-column matrix
z = g(X);                           % evaluate the function (this will be a
                                    % column vector)
z = reshape(z, size(x))             % reshape to the same size as x (and y)
mesh(x,y,z)                         % generate the 3D mesh plot
```

7.3 Exercise: probability distributions

For each of the plots that you make in this exercise make sure that you give different plots a different color or line style and include appropriate titles, axis labels and legends.

1. Plot the probability density function (pdf) for the normal distribution with mean $\mu = 1$ and standard deviations $\sigma = 0.1, 0.5, 1, 2$ in one plot.
2. Do the same for the gamma distribution.
3. Plot the pdf of both the normal and gamma distribution (take $\mu = 1$ and $\sigma = 1$) in one plot.
4. Draw 100 random numbers from the $N(1, 1)$ distribution. In one figure plot
   (a) The cdf of the $N(1, 1)$ distribution
   (b) The *empirical cdf* of the first 10, 30 and 100 observations, respectively. You can use `ecdf` for this puropose. You can also use `cdfplot`, but make sure that you give the plots different colors.

8 Regression

8.1 Introduction

Regression using the least squares criterion can be summarized by the following optimization problem

$$\min_{x \in X} \sum_i F_i(x)^2$$

We distinguish the following functional forms for the function F.

$F(x)$	Constraints (X)	Matlab solver
$Ax - b$	None	`\`, `mldivide` or `regress`
$Ax - b$	$x \geq 0$	`lsqnonneg`
$Ax - b$	Bound, linear	`lsqlin`
General $F(x)$	Bound	`lsqnonlin`
$F(x, xdata) - ydata$	Bound	`lsqcurvefit`

The first case simply corresponds the the standard linear regression problem, which we discussed in the section about Linear algebra. The second and third type are extensions to this problem where we put a simple nonnegativity restriction on x or general linear constraints. The last two types correspond to cases where the objective is nonlinear.

8.2 Linear regression

Suppose we have a quadratic function

$$f(x) = \beta_1 x^2 + \beta_2 x + \beta_3$$

for which the coefficient β are unknown. Observations are available from the model

$$y = f(x) + \varepsilon$$

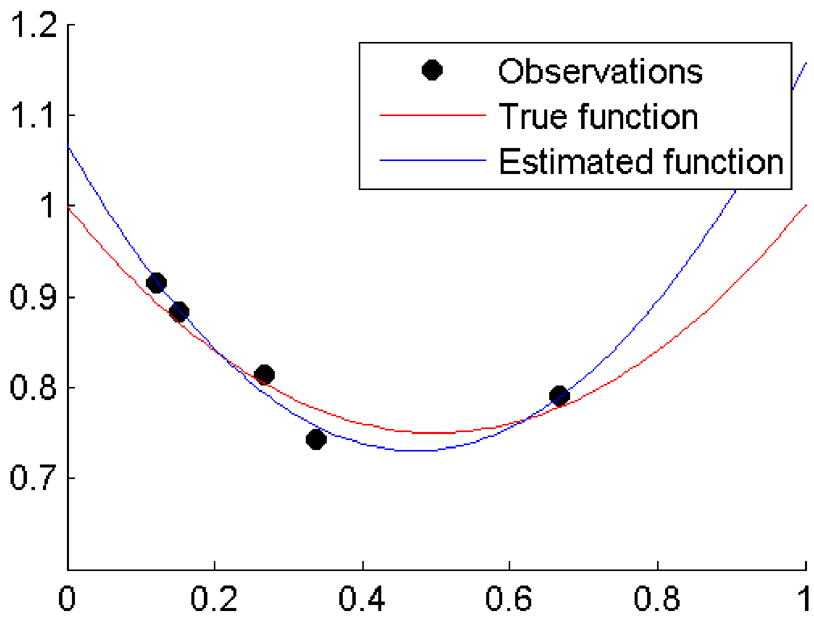
How do we estimate the coefficients from the data? Often students think that they should use one of the nonlinear solvers, because they are dealing with a quadratic model. This is a mistake, because the quadratic function is *linear* in its coefficients and that's what counts.

We would solve this problem as follows.

```
%% First create some data to work with
beta = [1 -1 1]';                % the true coefficients
m = 5;                           % number of observations
sigma = 0.02;                    % st.dev
x = rand(m,1);                   % the locations of the observations
X = [x.^2, x, ones(m,1)]         % data/regression matrix
y = X*beta + normrnd(0, sigma, m, 1); % the perturbed y-values

%% Do the regression and some analysis
b = X\y;                         % estimate
yhat = X*b;                      % predictions
e = y - yhat;                    % errors
sigmahat = sqrt(e'*e/(m-length(b))); % estimate for sigma

% Display results
fprintf(1, 'Coefficients (true and estimated)\n');
fprintf(1, '%8g %8.4f\n', [beta, b]');
fprintf(1, '\nStandard deviation (true and estimated)\n');
fprintf(1, '%8g %8.4f\n', [sigma, sigmahat]');

%% Do some vizualization
fun = @(x,beta) beta(1)*x.^2 + beta(2)*x + beta(3);

figure;
%plot(x, y, 'k.', 'markersize', 12);
scatter(x, y, 'k', 'filled');
```

```
hold on
fplot(@(x) fun(x,beta), [0 1], 'r');
fplot(@(x) fun(x,b), [0 1], 'b');

legend('Observations', 'True function', 'Estimated function');
```

```
Coefficients (true and estimated)
       1    1.5244
      -1   -1.4362
       1    1.0685

Standard deviation (true and estimated)
    0.02    0.0176
```



8.3 Nonlinear regression

Now consider the situation where we have observations from the model

$$y_i = \alpha_1 \exp(\alpha_2 x_i) + \varepsilon$$

We want to estimate α by solving

$$\min_{\alpha} \sum_i (y_i - \alpha_1 e^{\alpha_2 x_i})^2 \quad \Leftrightarrow \quad \min_{\alpha} \|y - f_x(\alpha)\|^2$$

with

$$f_x(\alpha) = \begin{bmatrix} \alpha_1 e^{\alpha_2 x_1} \\ \vdots \\ \alpha_1 e^{\alpha_2 x_m} \end{bmatrix}$$

and Jacobian matrix

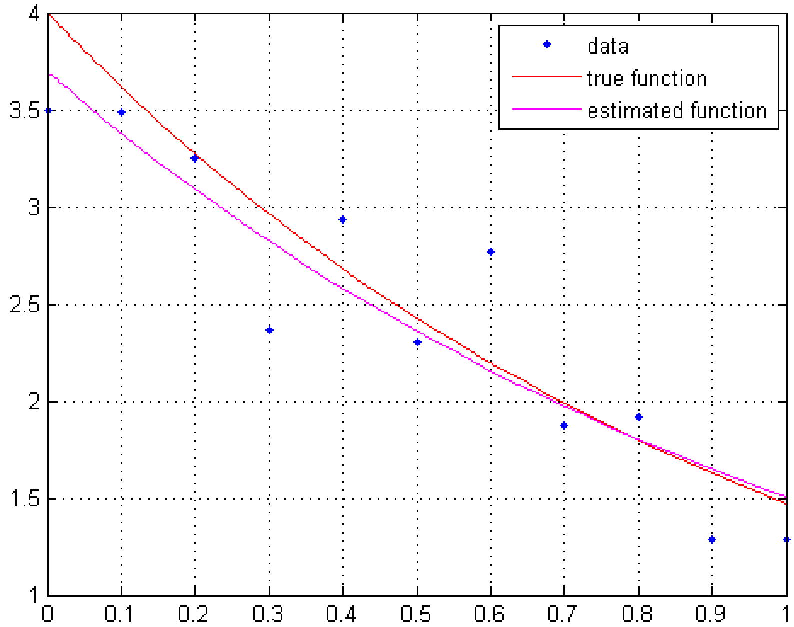
$$Jf_x(\alpha) = \begin{bmatrix} e^{\alpha_2 x_1} & \alpha_1 x_1 e^{\alpha_2 x_1} \\ \vdots & \vdots \\ e^{\alpha_2 x_m} & \alpha_1 x_m e^{\alpha_2 x_m} \end{bmatrix}$$

Note that we consider the function f as a function with two arguments, but for our purposes we choose α as its main (first) argument. The Jacobian information can be passed on the Matlab solver, which makes the optimization more efficient. In Matlab we can create a m-file function:

```
function [f,Jf] = nonlinfun(a,x)

% We split the computation, because we can reuse the results in the Jacobian
% evaluation.
y = exp(a(2)*x);
f = a(1)*y;

% Return the Jacobian only if asked for
if nargout > 1
  Jf = [y, x.*f];
end
```

We solve the problem using `lsqcurvefit`.

```
a = [4; -1];
truefun = @(x)(nonlinfun(a,x)); % the true function

x = (0:0.1:1)';
y = truefun(x) + 0.3*randn(size(x)); % add some noise
a0 = [1; 1]; lb = []; ub = [];  % initial estimate, no lower/upper bounds

% Change some solver options
opt = optimset('lsqcurvefit');
opt = optimset(opt, ...
               'display', 'iter', ...
               'jacobian', 'on', ...
               'derivativecheck', 'on');

ahat = lsqcurvefit(@nonlinfun, a0, x, y, lb, ub, opt);

estimfun = @(x)(nonlinfun(ahat,x)); % the estimated function

% Plot the results
clf; plot(x, y, '.');
hold on; grid on
fplot(truefun, [0 1], 'r');
fplot(estimfun, [0 1], 'm');
legend('data', 'true function', 'estimated function');
```



8.4 Exercises

8.4.1 Nonlinear regression

The data below can be modeled by the equation

$$y = \left(\frac{a + \sqrt{x}}{b\sqrt{x}} \right)^2 + \varepsilon$$

x	y
0.5	11.1
1.0	6.3
2.0	3.7
3.0	2.7
4.0	2.3

Determine the parameters a and b by nonlinear regression

1. using `lsqcurvefit`
2. using `lsqnonlin`
3. using `fminsearch`

Plot the estimated model in a figure and also display the original data set.

Hint. Anonymous functions will be very useful here. Define anonymous functions for the model and each of the objectives to be minimized for `lsqcurvefit`, `lsqnonlin` and `fminsearch`. Carefully look at the required input/output arguments for these objective functions.

8.4.2 Estimating a full quadratic model using linear regression

Consider the full quadratic model

$$y_i = x_i^T A x_i + b^T x_i + c + \varepsilon_i$$

where $x_i \in \mathbb{R}^n$, $A \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$ and $c \in R$. We assume that A is symmetric, thus A, b and c combined form a total of $(n+1)(n+2)/2$ coefficients. Note that the model is linear in these coefficients, hence the coefficients can be estimated by linear regression. This implies that there exist functions

$$r : \mathbb{R}^n \to \mathbb{R}^{(n+1)(n+2)/2} \qquad \text{and} \qquad \alpha : \mathbb{R}^{n\times n} \times \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^{(n+1)(n+2)/2}$$

such that

$$x^T A x + b^T x + c = r(x)^T \alpha(A, b, c)$$

In Matlab, the vector $r(x)$ can be created using the `x2fx` function (look at the documentation for this function). The function α is a straightforward transformation of the coefficients A, b and c.

x(1)	x(2)	x(3)	y
0.7269	-0.1649	-1.4916	7.5925
-0.3034	0.6277	-0.7423	9.8878
0.2939	1.0933	-1.0616	14.9603
-0.7873	1.1093	2.3505	19.1152
0.8884	-0.8637	-0.6156	9.5911
-1.1471	0.0774	0.7481	6.0004
-1.0689	-1.2141	-0.1924	7.1351
-0.8095	-1.1135	0.8886	9.6753
-2.9443	-0.0068	-0.7648	58.0111
1.4384	1.5326	-1.4023	22.5375
0.3252	-0.7697	-1.4224	7.0363
-0.7549	0.3714	0.4882	4.4605
1.3703	-0.2256	-0.1774	11.7823
-1.7115	1.1174	-0.1961	35.6122
-0.1022	-1.0891	1.4193	20.4914
-0.2414	0.0326	0.2916	1.0463
0.3192	0.5525	0.1978	2.4877
0.3129	1.1006	1.5877	12.2703
-0.8649	1.5442	-0.8045	36.4001
-0.0301	0.0859	0.6966	2.5647

1. Import the data in the table above in Matlab.
2. Create the regression matrix R (using `x2fx`) for the full quadratic model and estimate the coefficient vector $\hat{\alpha}$.
3. Derive the estimates $\hat{A}$, $\hat{b}$ and $\hat{c}$ from $\hat{\alpha}$. You'll need to match up the entries of the regression matrix and the parameters A, b and c. See the documentation for `x2fx`. Try to find a link between the variables that works for general dimension n. If that's too difficult, then just get the link for $n = 3$.

4. Verify that $r(x)^T\hat{\alpha} = x^T\hat{A}x + \hat{b}^T x + \hat{c}$ for an arbitrary $x \in \mathbb{R}^3$.

5. Verify that the estimated quadratic function is convex. Note that this can be easily derived from $\hat{A}$, but not from $\hat{\alpha}$.

6. Fix $x_3 = 0$ and generate a 3D visualization of the estimated quadratic function for the range $x_1, x_2 \in [-2, 2]$.

9 Interpolation

Sometimes we want our estimating function to pass through the observations, i.e., the estimate is equal to the observation. In that case, regression is not an option and we need to apply an interpolating method.

9.1 One-dimensional interpolation

The one-dimensional interpolation problem is summarized as follows.

- Given data: $x, y \in \mathbb{R}^n$
- Find an interpolating function $f(x)$ such that

$$f(x_i) = y_i$$

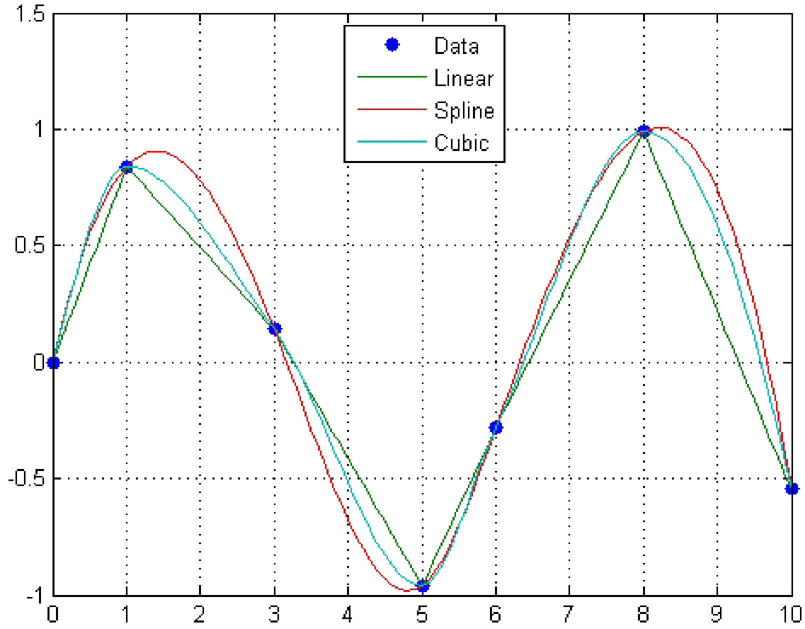
- Evaluate the interpolating function for the points $v_1, \ldots, v_m$

In Matlab this problem is easily solved using `interp1(x,y,v,method)` where `method` is one of

- `nearest`
- `linear`
- `spline`: cubic (3th degree) interpolation → smooth result
- `cubic`: piecewise cubic → preserves shape and monotonicity

This is illustrated by the following example:

```
x = [0 1 3 5 6 8 10]';
y = sin(x);
v = (0:.1:10)';
f = [interp1(x,y,v,'linear'), ...
     interp1(x,y,v,'spline'), ...
     interp1(x,y,v,'cubic')];
h = plot(x, y, '.', v, f);
set(h(1), 'markersize', 18); grid on
legend('Data', 'Linear', 'Spline', 'Cubic', 'Location', 'North');
```



9.2 Higher-dimensional interpolation

Two-dimensional interpolation is solved very similarly using `interp2`. Higher dimension interpolation problems are supported by the functions `interp3`, `interpn` and `ndgrid`.

9.3 Interpolation of scattered data

The interpolation methods we have discussed so far all require that the observations are on a grid. Hence, for the two-dimensional interpolation problem, this implies that the observations (x_i, y_i, z_i) can be represented by three matrices `X`, `Y` and `Z` where the matrices `X` and `Y` are a grid as produced by `meshgrid`.

Sometimes the observation locations (x_i, y_i) are scattered throughout the plane. In that case, we have to use an alternative method. The official Matlab documentation, gives some nice examples for the functions that you can use in that case. In the next section, we shall consider yet another approach.

9.4 Interpolation using Radial Basis Functions

Consider a scattered data set

$$X = \begin{bmatrix} x_1^T \\ \vdots \\ x_m^T \end{bmatrix} \in \mathbb{R}^{m \times n} \qquad \text{and} \qquad y = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} \in \mathbb{R}^m$$

An interpolating Radial Basis Function model is given by

$$f(x) = \sum_{j=1}^{m} \beta_j h_j(x),$$

where $h_j(x)$ is

$$h_j(x) = \phi(\|x - x_j\|).$$

The function $\phi : \mathbb{R} \to \mathbb{R}$ is a radial basis function, such as

- linear : $\phi(t) = t$
- gaussian : $\phi(t) = \exp(-ct^2)$ for some $c > 0$
- multiquadric : $\phi(t) = \sqrt{t^2 + c^2}$ for some $c > 0$
- thin plate spline : $\phi(t) = t^2 \log t$

Note that the model has m coefficients β_j and m basis functions, which are both equal to the number of observations. The coefficients can be estimated from the *linear* system of equations

$$\Phi\beta = y \qquad \text{with} \qquad \Phi_{ij} = h_j(x_i) = \phi(\|x_i - x_j\|), \quad i, j = 1, \ldots, m.$$

If we substitute all results in our model, then we get an interpolating function $f(x)$. Note that for the Gaussian and multiquadric class of basis functions we still have a free parameter c. It's value can be changed—but you'll have to estimate the coefficients again—and it determines the smoothness of the model. It can be selected based upon your preferences, or even better, by minimizing some error criterion.

Remark: If the m observations are all unique, then the matrix Φ is guaranteed to be nonsingular. Unfortunately, when the number of observations m increases, then numerical instabilities can arise because rows become nearly dependent.

9.5 Exercise: interpolation

Load the data in the file `scattered.txt`, which gives some observations (in the third column) of a two-dimensional model.

1. Visualize an interpolating surface using any of the built-in methods in a 3D figure that also shows the observations marked by points.

2. Try to produce some interpolating radial basis approximations using several choices for the radial basis function class and associated constant. Again visualize the results. Your solution to the exercise about the Euclidean distance might be useful in creating the Φ matrix.