AM111 Documentation

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Lecture Location: 375 Geological Museum (3rd floor)

Session Time: Every Monday 17:00-18:00
Session Location: GeoMuseum 103A

TF's Office Hour: Every Tuesday 15:00-16:00, Pierce Hall 108

This website contains supplemental materials made by the TF, Jiawei Zhuang. These materials are **not required** for completing this course, but just provide additional information I find useful. Might also use them for the session. Your grade will **not be affected** if you choose to ignore this website.

CHAPTER 1

Homework Notes

Additional notes (hints, clarifications) for homework.

1.1 Notes on Homework 1

```
In [1]: format compact
```

The last question asks you to use **boolean_print_TT_fn.m** (available on canvas) to print the truth table. Please read this additional note if you have trouble using this function.

1.1.1 Function as an input variable

Typically you pass data (e.g. scalars, arrays...) to a function. But the function `boolean_print_TT_fn()` accepts **another function** as the input variable.

Inline function as an input variable

Let's make two inline functions:

```
In [2]: func1 = @(a) a;
        func2 = @(a,b) a&b;
```

`boolean_print_TT_fn(func,1)` prints the truth table for a function with a single input:

```
In [3]: boolean_print_TT_fn(func1,1)
```

```
_____
a|out
0|0
1|1
```

`boolean_print_TT_fn(func,2)` prints the truth table for a function with two inputs:

```
In [4]: boolean_print_TT_fn(func2,2)
```

```
_______
a|b|out
0|0| 0
0|1| 0
1|0| 0
1|1| 1
```

Standard function as an input variable

However, if you try to pass a standard function (i.e. defined in a separate file) to `boolean_print_TT_fn()`, it will throw you some weird error:

```
In [5]: %%file func2_fn.m
        function s=func2_fn(a,b)
            s = a&b;
        end
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/AM111/docs/func2_fn.m'.
```

```
In [6]: boolean_print_TT_fn(func2_fn,2)
```

```
Not enough input arguments.Error in func2_fn (line 2)     s = a&b;
```

To fix this error, you can put `@` in front of your function, as suggested here.

```
In [7]: boolean_print_TT_fn(@func2_fn,2)
```

```
_______
a|b|out
0|0| 0
0|1| 0
1|0| 0
1|1| 1
```

(That's MATLAB-specific design. Other languages like Python treat inline and standard functions in the same way.)

1.1.2 Print truth table for half adder

Function with multiple return

A Half adder has two return values. One way to return multiple values is

```
In [8]: %%file multi_return.m
        function [carry,s] = multi_return(a,b)
            % This is not a corret adder! You should write your own!
            carry = 0;
            s = 1;
        end
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/AM111/docs/multi_return.m'.
```

However, by default you only get the first output variable `carry` !

```
In [9]: multi_return(0,0)
```

```
ans =
     0
```

To get both `carry` and `s`, you have to use two variables to hold the output results.

```
In [10]: [out1, out2] = multi_return(0,0)
```

```
out1 =
     0
out2 =
     1
```

A perhaps more convenient way is to return a vector containing all outputs you need:

```
In [11]: %%file fake_half_adder.m
         function out = fake_half_adder(a,b)
             % This is not a corret adder! You should write your own!
             carry = 0;
             s = 1;
             out = [carry,s];
         end
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/AM111/docs/fake_half_adder.m'.
```

This time, you don't have to write two variables to hold the output results:

```
In [12]: fake_half_adder(1,1)
```

```
ans =
     0     1
```

Print truth table using boolean_print_TT_fn.m

`boolean_print_TT_fn()` will print the complete result **only if** you use a single vector as the return value for you adder. Use `3` to get the format for half-adder.

```
In [13]: boolean_print_TT_fn(@multi_return,3) % not printing complete result
```

```
_____________
a|b|carry|sum
0|0| 0
0|1| 0
1|0| 0
1|1| 0
```

```
In [14]: boolean_print_TT_fn(@fake_half_adder,3) % can print complete result
```

```
_____________
a|b|carry|sum
0|0| 0  1
0|1| 0  1
1|0| 0  1
1|1| 0  1
```

Print truth table on your own

If you don't want to use boolean_print_TT_fn.m, it is also quite straightforward to print the table on your own:

```
In [15]: disp('a,b|c,s')
         for a=0:1
         for b=0:1
             fprintf('%d,%d|%d,%d \n',a,b,fake_half_adder(a,b))
         end
         end
```

```
a,b|c,s
0,0|0,1
0,1|0,1
```

```
1,0|0,1
1,1|0,1
```

Type `doc fprintf` to see more formatting options.

1.1.3 Print truth table for full adder

Use `4` to get the format for full-adder.

```
In [16]: %%file fake_full_adder.m
         function out = fake_full_adder(a,b,c)
             carry = 0;
             s = 1;
             out = [carry,s];
         end
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/AM111/docs/fake_full_adder.m'.
```

```
In [17]: boolean_print_TT_fn(@fake_full_adder,4)
```

```
_________________
a|b|c|carry|sum
0|0|0|0  1
0|0|1|0  1
0|1|0|0  1
0|1|1|0  1
1|0|0|0  1
1|0|1|0  1
1|1|0|0  1
1|1|1|0  1
```

CHAPTER 2

Lecture & Session Notes

Forget the coding exercises in the class? The following notes might help.

2.1 Lecture 2: Logic Gates & Fibonacci Numbers

Date: 09/05/2017, Tuesday

```
In [1]: format compact
```

2.1.1 Logic gates

nand gate

```
In [2]: nand = @(a,b) ~(a&b)
```

```
nand =
  function_handle with value:
    @(a,b)~(a&b)
```

```
In [3]: nand(1,1) % test if it works
```

```
ans =
  logical
   0
```

print truth table

```
In [4]: help boolean_print_TT_fn % boolean_print_TT_fn.m is available on canvas
```

```
  boolean_print_TT_fn.m
  a function to print the boolean truth table for a given
  supplied function 'func'
```

```
  INPUT
  func: the supplied function (e.g. OR, NAND, XOR)
  input_num: number of inputs
```

```
In [5]: boolean_print_TT_fn(nand,2)
```

```
_______
a|b|out
0|0| 1
0|1| 1
1|0| 1
1|1| 0
```

build "not" gate from "nand" gate

```
In [6]: my_not = @(a) nand(a,a) % "not" is a built-in function so we use my_not to avoid conflicts
```

```
my_not =
  function_handle with value:
    @(a)nand(a,a)
```

```
In [7]: boolean_print_TT_fn(my_not,1)
```

```
_____
a|out
0|1
1|0
```

Why **nand(a,a)** means **not**:

1. **and(a,a) = a**, no matter **a** is 0 or 1
2. **nand(a,a) = not and(a,a) = not a**

2.1.2 Fibonacci Sequence

generate Fibonacci sequences

```
In [8]: %%file fib_fn.m
        function F = fib_fn(n)

            F = zeros(1,n);
            F(1)=1;
            F(2)=1;
            for j=3:n
                F(j)=F(j-1)+F(j-2);
            end

        end
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/AM111/docs/fib_fn.m'.
```

```
In [9]: fib_fn(10)
```

```
ans =
     1     1     2     3     5     8    13    21    34    55
```

Compare with the built-in function fibonacci( )

```
In [10]: fibonacci(1:10)
```

```
ans =
     1     1     2     3     5     8    13    21    34    55
```

golden ratio

```
In [11]: golden_ratio = (sqrt(5)+1)/2 % true value
```

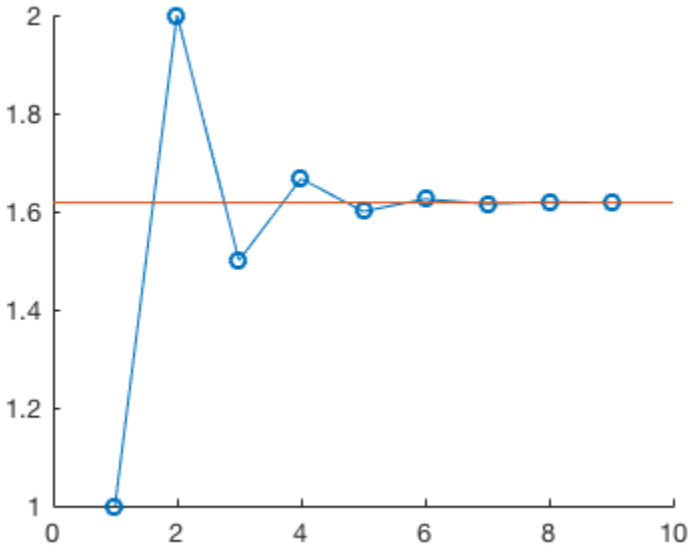
```
golden_ratio =
    1.6180
```

F_n/F_{n-1} Converges to the golden ratio

```
In [12]: F = fib_fn(10);
         F_ratio = F(2:end)./F(1:end-1)
```

```
F_ratio =
  Columns 1 through 7
    1.0000    2.0000    1.5000    1.6667    1.6000    1.6250    1.6154
  Columns 8 through 9
    1.6190    1.6176
```

```
In [13]: %plot --size 400,300
         hold on
         plot(F_ratio,'-o')
         plot([0,10],[golden_ratio,golden_ratio])
```



2.2 Lecture 4: Floats & Random Numbers

Date: 09/12/2017, Tuesday

```
In [1]: format compact
        format long % print more digits
```

2.2.1 Floating point number system

Double precision:

$$x = \pm(1+f)2^e$$
$$0 \le 2^t f < 2^t, t = 52$$
$$-1022 \le e \le 1023$$

(See lecture slides or textbook for more explantion. This website focuses on codes.)

About parameters

How many binary bits are needed to store e:

```
In [2]: log2(2048)
```

```
ans =
    11
```

Maximum value

Calculate the maximum value of x from the formula.

```
In [3]: t=52;
        f=(2^t-1)/2^t;
        (1+f)*2^1023
```

```
ans =
    1.797693134862316e+308
```

Compare with the built-in function

```
In [4]: realmax
```

```
ans =
    1.797693134862316e+308
```

What happens if the value exceeds `realmax`?

```
In [5]: 2e308
```

```
ans =
   Inf
```

Minimum (absolute) value

From the formula

```
In [6]: 2^-1022
```

```
ans =
    2.225073858507201e-308
```

Compare with the built-in function

```
In [7]: realmin
```

```
ans =
    2.225073858507201e-308
```

MATLAB allows you to go lower than `realmin`, but no too much.

```
In [8]: for k=-321:-1:-325
            fprintf('k = %d, 10^k = %e \n',k,10^k)
        end
```

```
k = -321, 10^k = 9.980126e-322
k = -322, 10^k = 9.881313e-323
k = -323, 10^k = 9.881313e-324
k = -324, 10^k = 0.000000e+00
k = -325, 10^k = 0.000000e+00
```

10^{-323} can be scaled up:

```
In [9]: 1e-323 * 1e300
```

```
ans =
     9.881312916824931e-24
```

But 10^{-324} can't, as it becomes exactly 0.

```
In [10]: 1e-324 * 1e300
```

```
ans =
     0
```

Machine precision

Compute machine precision

From the formula $0 \leq 2^t f < 2^t, t = 52$

```
In [11]: 2^(-52)
```

```
ans =
     2.220446049250313e-16
```

Built-in function:

```
In [12]: eps
```

```
ans =
     2.220446049250313e-16
```

Another ways to get `eps`

```
In [13]: 1.0-(0.1+0.1+0.1+0.1+0.1+0.1+0.1+0.1+0.1+0.1) % equals to eps/2
```

```
ans =
     1.110223024625157e-16
```

```
In [14]: 7/3-4/3-1 % equals to eps
```

```
ans =
     2.220446049250313e-16
```

Difference between eps and realmin

`realmin` is about **abosolute** magnitude, while `eps` is about **relative** accuracy. Although a double-precision number can represent a value as small as 10^{-323} (i.e. `realmin`), the relative error of arithmetic operations can be as large as 10^{-16} (i.e. `eps`).

Adding 10^{-16} to 1.0 has no effect at all.

```
In [15]: 1.0+1e-16-1.0
```

```
ans =
     0
```

Adding 10^{-15} to 1.0 has some effect, although the result is quite inaccurate.

```
In [16]: 1.0+1e-15-1.0

ans =
     1.110223024625157e-15
```

Not a number

```
In [17]: 0/0

ans =
   NaN

In [18]: Inf - Inf

ans =
   NaN
```

However, `Inf` can sometimes be meaningful: (MATLAB-only. Not true in low-level languages.)

```
In [19]: 5/Inf

ans =
     0

In [20]: 5/0

ans =
   Inf
```

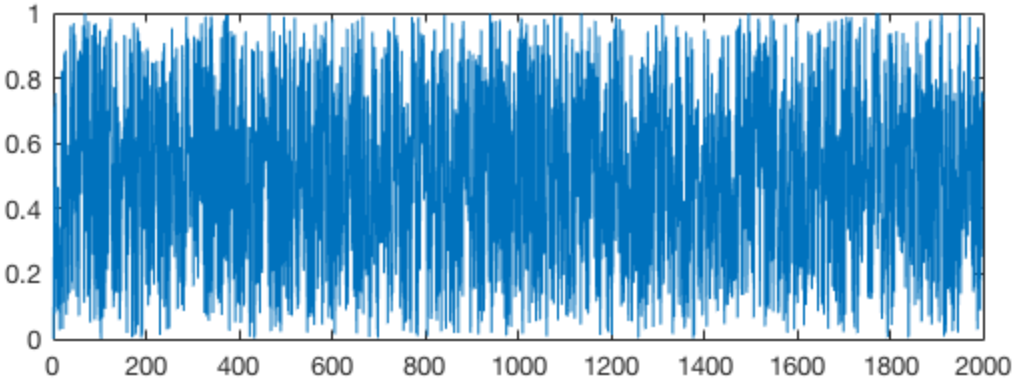
2.2.2 Random numbers

Linear congruential generator

```
In [21]: a = 22695477;
         c = 1;
         m = 2^32;
         N = 2000;

         X = zeros(N,1);
         X(1) = 1000;
         for j=2:N
             X(j)=mod(a*X(j-1)+c,m);
         end

         R = X/m;
```

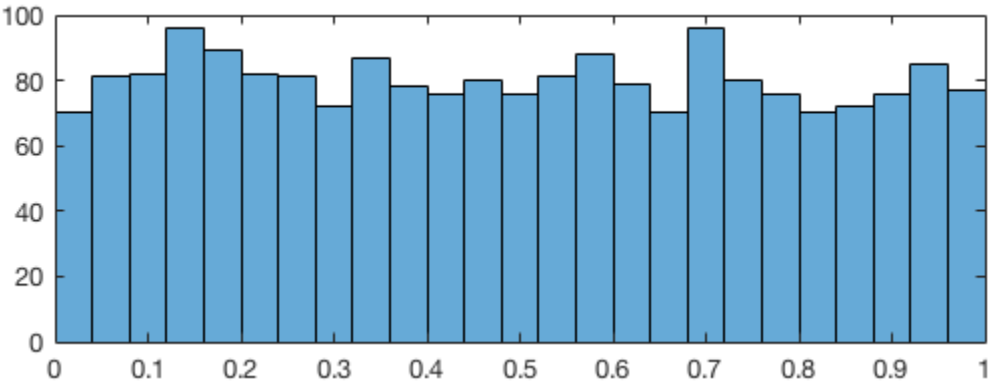
Hmm... looks pretty random

```
In [22]: %plot --size 600,200
         plot(R);
```



The data also looks like evenly-distributed.

```
In [23]: nbins = 25;
         histogram(R, nbins);
```



2.3 Lecture 5: Random Numbers & Complex Numbers

Date: 09/14/2017, Thursday

```
In [1]: format compact
```

2.3.1 Built-in random number generator

`rand` returns a random number between [0,1] (uniform distribution).

```
In [2]: rand
```

```
ans =
    0.8147
```

`rand(N)` returns a $N \times N$ random matrix. You can always type `doc rand` or `help rand` to see the detailed usage.

```
In [3]: rand(5)
```

```
ans =
    0.9058    0.2785    0.9706    0.4218    0.0357
    0.1270    0.5469    0.9572    0.9157    0.8491
    0.9134    0.9575    0.4854    0.7922    0.9340
```

```
    0.6324    0.9649    0.8003    0.9595    0.6787
    0.0975    0.1576    0.1419    0.6557    0.7577
```

`randi(N)` returns an integer between 1 and N.

```
In [4]: randi(100)
```

```
ans =
    75
```

`randn` uses normal distribution, instead of uniform distribution.

```
In [5]: randn(5)
```

```
ans =
   -0.3034   -1.0689   -0.7549    0.3192    0.6277
    0.2939   -0.8095    1.3703    0.3129    1.0933
   -0.7873   -2.9443   -1.7115   -0.8649    1.1093
    0.8884    1.4384   -0.1022   -0.0301   -0.8637
   -1.1471    0.3252   -0.2414   -0.1649    0.0774
```

2.3.2 Complex numbers

Complex number basics

A real number (double-precision) takes 8 Bytes (64 bits). A complex number is a pair of numbers so simply takes 16 Bytes (128 bits)

```
In [6]: x = 3;
        y = 4;
        z = x+i*y;
```

```
In [7]: whos
```

```
  Name      Size            Bytes  Class     Attributes

  ans       5x5               200  double
  x         1x1                 8  double
  y         1x1                 8  double
  z         1x1                16  double    complex
```

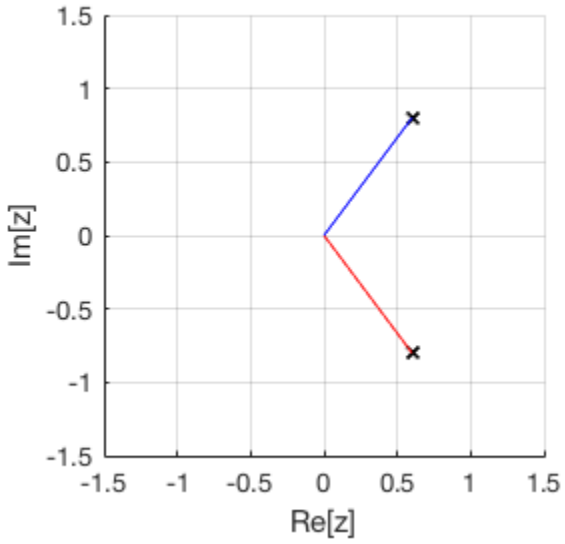
Take conjugate of a complex number:

```
In [8]: conj(z)
```

```
ans =
   3.0000 - 4.0000i
```

Show the number on the complex plane

```
In [9]: %plot --size 300,300
        hold on
        complex_number_plot_fn(conj(z)/5,'r') % complex_number_plot_fn is available on canvas.
        complex_number_plot_fn(z/5,'b')
```



3 equivalent ways to compute $|z|$

```
In [10]: abs(z)
```

```
ans =
     5
```

```
In [11]: sqrt(dot(z,z))
```

```
ans =
     5
```

```
In [12]: norm(z)
```

```
ans =
     5
```

The angle of z in degree:

```
In [13]: angle(z) / pi * 180.0
```

```
ans =
   53.1301
```

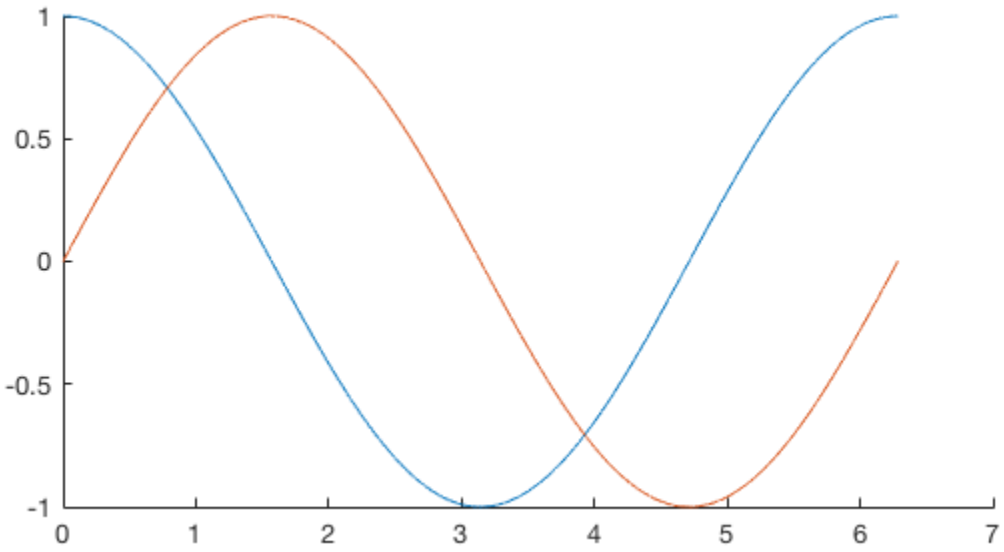
Euler's Formula

$$e^{i\theta} = \cos(\theta) + i\sin(\theta)$$

Verify that MATLAB understands $e^{i\theta}$

```
In [14]: theta = linspace(0, 2*pi, 1e4);
         z = exp(i*theta); % now z is an array, not a scalar as defined in the previou section.
```

```
In [15]: %plot --size 600,300
         hold on
         plot(theta,real(z))
         plot(theta,imag(z))
```

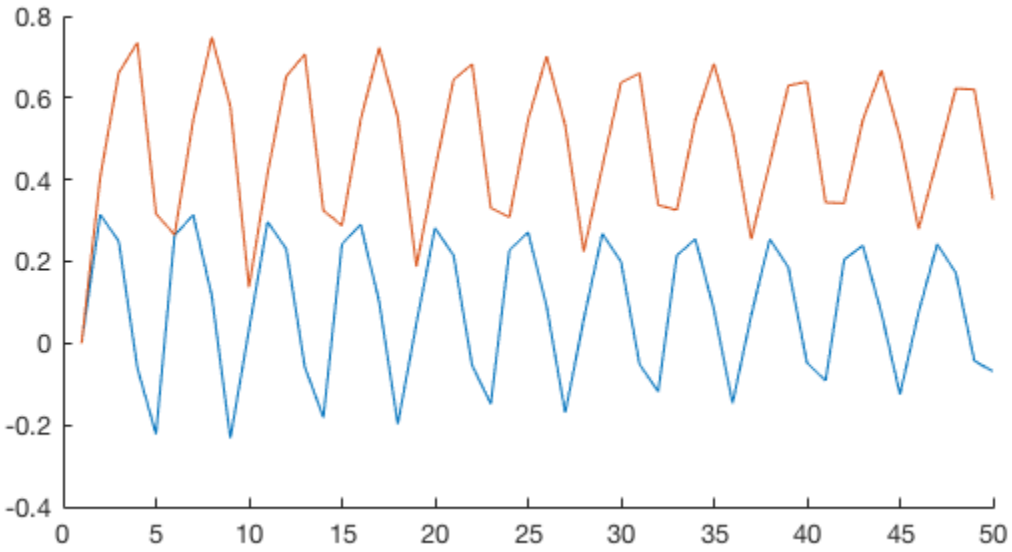


Mandelbrot set

Iteration with a single parameter

```
In [16]: c = rand-0.5 + i*(rand-0.5);

         T = 50;
         z_arr = zeros(T,1); % to hold the entire time series

         z = 0; % initial value
         z_arr(1) = z;

         for t=2:T
             z = z^2+c;
             z_arr(t) = z;
         end
```

```
In [17]: hold on
         plot(real(z_arr))
         plot(imag(z_arr))
```



Run this code repeatedly, you will see sometimes z will blow up, sometime not, according to the initial value of c. Thus we want to figure out what values of c will make z blow up.

Iteration with the entire paremeter space

We want to construct a 2D array containing all possible values of c on the complex plane.

Let's make 1D grids first.

```
In [18]: nx = 100;
         xm = 1.75;
         x = linspace(-xm, xm, nx);
         y = linspace(-xm, xm, nx);
```

```
In [19]: size(x), size(y)
```

```
ans =
     1   100
ans =
     1   100
```

convert 1D grid to 2D grid.

```
In [20]: [Cr, Ci] = meshgrid(x,y);
```

```
In [21]: size(Cr), size(Ci)
```

```
ans =
   100   100
ans =
   100   100
```

```
In [22]: C = Cr + i*Ci; % now C spans over the complex plane
```

```
In [23]: size(C)
```

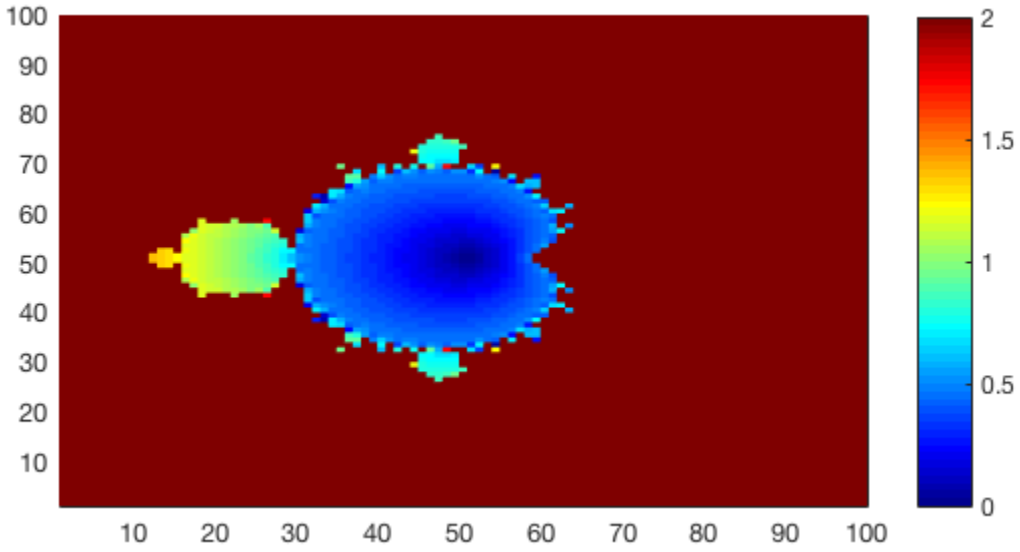
```
ans =
   100   100
```

Run the iteration for every value of C

```
In [24]: T = 50;

         Z_final = zeros(nx,nx); % to hold last value of z, at all possible points.

         for ix = 1:nx
         for iy = 1:nx % we also have nx points in the y-direction

             % get the value of c at current point.
             % note that MATLAB is case-sensitive
             c = C(ix,iy);

             z = 0; % initial value, doesn't matter too much
             for t=2:T
                 z = z^2+c;
             end
             Z_final(ix,iy) = z; % save the last value of z

         end
         end
```

Here's one way to visualize the result.

```
In [25]: pcolor(abs(Z_final)); % plot the magnitude of z

         shading flat; % hide grids
         colormap jet; % change colormap
         colorbar; % show colorbar

         % The default color range is min(z)~max(z),
         % but max(z) is almost Inf so we make the range smaller
         caxis([0,2]);
```



2.4 Lecture 6: Matrix

Date: 09/19/2017, Tuessday

```
In [1]: format compact
```

2.4.1 Matrix operation basics

Making a magic square

```
In [2]: A = magic(3)
```

```
A =
     8     1     6
     3     5     7
     4     9     2
```

Take transpose

```
In [3]: A'
```

```
ans =
     8     3     4
     1     5     9
     6     7     2
```

Rotate by 90 degree. (Not so useful for linear algebra. Could be useful for image processing.)

```
In [4]: rot90(A')
```

```
ans =
     4     9     2
     3     5     7
     8     1     6
```

Sum over each column

```
In [5]: sum(A)
```

```
ans =
    15    15    15
```

Another equivalent way

```
In [6]: sum(A, 1)
```

```
ans =
    15    15    15
```

Sum over each row

```
In [7]: sum(A, 2)
```

```
ans =
    15
    15
    15
```

Extract the diagonal elements.

```
In [8]: diag(A)
```

```
ans =
     8
     5
     2
```

The sum of diagonal elements is also 15, by the definition of a magic square.

```
In [9]: sum(diag(A))
```

```
ans =
    15
```

Determinant

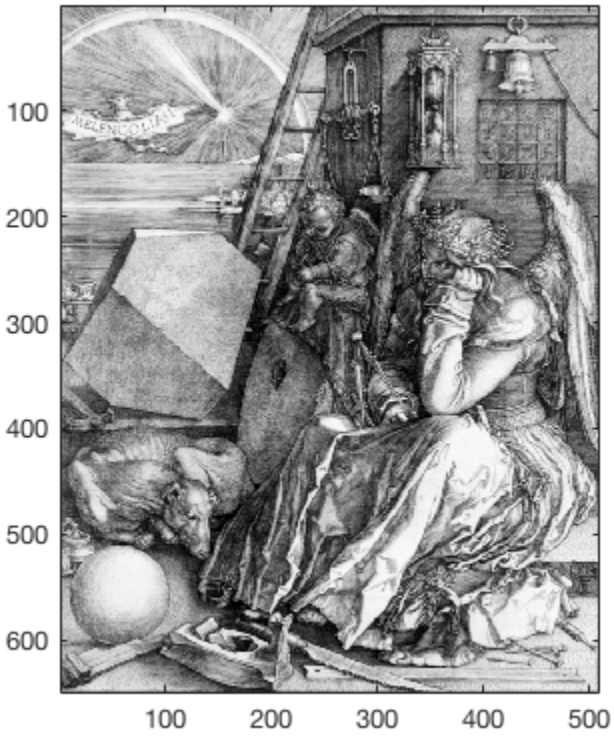
```
In [10]: det(A)

ans =
  -360
```

Matrix inversion A^{-1}

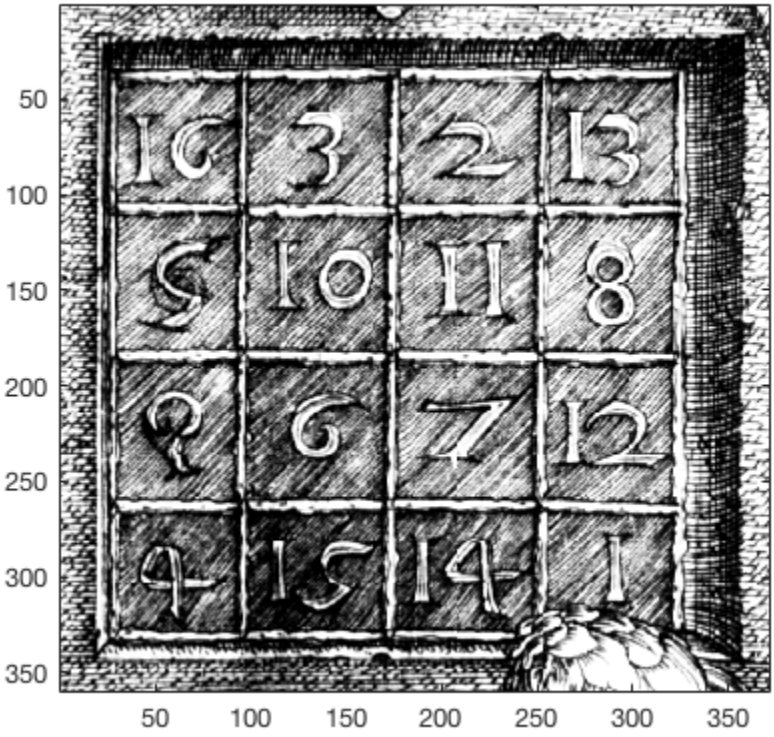
```
In [11]: inv(A)

ans =
    0.1472   -0.1444    0.0639
   -0.0611    0.0222    0.1056
   -0.0194    0.1889   -0.1028
```

2.4.2 Built-in image for magic square

```
In [12]: load durer
         image(X)
         colormap(map)
         axis image
```




```
In [13]: load detail
         image(X)
         colormap(map)
         axis image
```



2.4.3 Vector norms

```
In [14]: x = 1:5 % make a boring vector
```

```
x =
     1     2     3     4     5
```

Calculate p-norm from formula

```
In [15]: my_norm = @(x,p) (sum(abs(x).^p))^(1/p)
```

```
my_norm =
  function_handle with value:
    @(x,p)(sum(abs(x).^p))^(1/p)
```

Check if it works.

```
In [16]: my_norm(x,1)
```

```
ans =
    15
```

As p increases, the norm converges to $\max(|x|)$

```
In [17]: for p=1:10
             my_norm(x,p)
         end
```

```
ans =
    15
ans =
    7.4162
```

```
ans =
    6.0822
ans =
    5.5937
ans =
    5.3602
ans =
    5.2321
ans =
    5.1557
ans =
    5.1073
ans =
    5.0756
ans =
    5.0541
```

It blows up at $p = 442$ because 5^{442} exceeds the `realmin`.

```
In [18]: my_norm(x,441), my_norm(x,442)
```

```
ans =
     5
ans =
   Inf
```

```
In [19]: 5^441
```

```
ans =
  1.7611e+308
```

```
In [20]: 5^442
```

```
ans =
   Inf
```

Built-in function `norm` works for large numbers, though. Think about why.

```
In [21]: norm(x,441), norm(x,442)
```

```
ans =
     5
ans =
     5
```

2.4.4 Conditioning

4x4 magic square

```
In [22]: B = magic(4)
```

```
B =
    16     2     3    13
     5    11    10     8
     9     7     6    12
     4    14    15     1
```

It is singular and ill-conditioned.

```
In [23]: inv(B)
```

```
Warning: Matrix is close to singular or badly scaled. Results may be inaccurate. RCOND =  4.625929e-1
ans =
   1.0e+15 *
```

```
   -0.2649   -0.7948    0.7948    0.2649
   -0.7948   -2.3843    2.3843    0.7948
    0.7948    2.3843   -2.3843   -0.7948
    0.2649    0.7948   -0.7948   -0.2649
```

```
In [24]: det(B)
```

```
ans =
   5.1337e-13
```

```
In [25]: cond(B)
```

```
ans =
   4.7133e+17
```

Use 1-norm instead. All norms should have similar order of magnitude.

```
In [26]: cond(B,1)
```

```
Warning: Matrix is close to singular or badly scaled. Results may be inaccurate. RCOND =  4.625929e-1
> In cond (line 46)
ans =
   2.1617e+17
```

The condition number reaches `1/eps`, leading to large numerical error.

```
In [27]: 1/eps
```

```
ans =
   4.5036e+15
```

2.4.5 Sparse matrix

```
In [28]: A = eye(10)
```

```
A =
     1     0     0     0     0     0     0     0     0     0
     0     1     0     0     0     0     0     0     0     0
     0     0     1     0     0     0     0     0     0     0
     0     0     0     1     0     0     0     0     0     0
     0     0     0     0     1     0     0     0     0     0
     0     0     0     0     0     1     0     0     0     0
     0     0     0     0     0     0     1     0     0     0
     0     0     0     0     0     0     0     1     0     0
     0     0     0     0     0     0     0     0     1     0
     0     0     0     0     0     0     0     0     0     1
```

Store it in the sparse form saves memory.

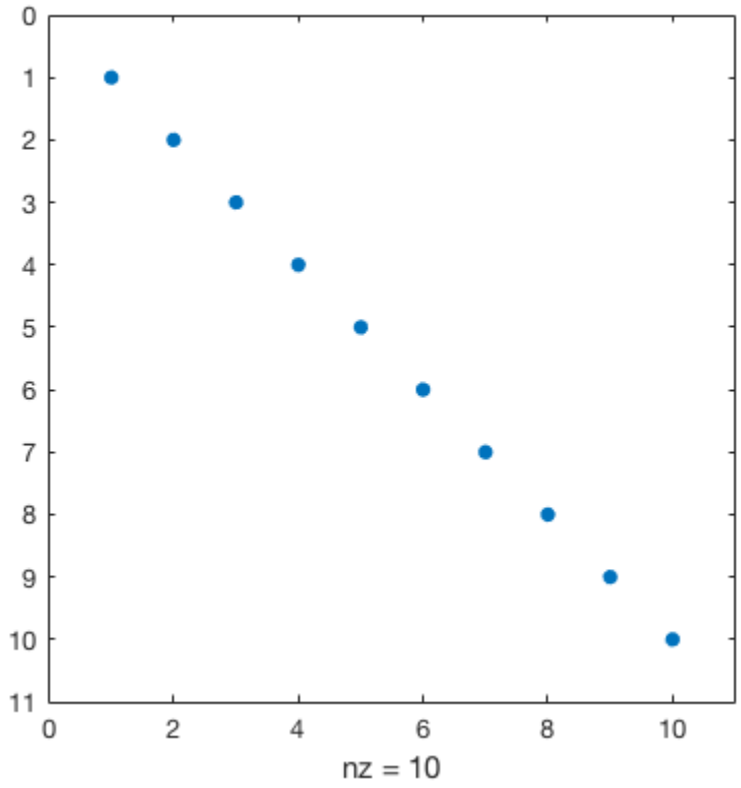
```
In [29]: As = sparse(A)
```

```
As =
   (1,1)        1
   (2,2)        1
   (3,3)        1
   (4,4)        1
   (5,5)        1
   (6,6)        1
   (7,7)        1
   (8,8)        1
   (9,9)        1
  (10,10)       1
```

Use `whos A` and `whos As` to check memory usage.

Visualize sparsity. Also works for `As`

```
In [30]: spy(A)
```



2.5 Lecture 8: Interpolation

Date: 09/26/2017, Tuessday

```
In [1]: format compact
```

2.5.1 A simple example

Make 3 data points

```
In [2]: xp = [-pi/2, 0, pi/2];
        yp = [-1, 0, 1];
```

The two functions below both go through the 3 data points.

```
In [3]: f = @(x) sin(x);
        g = @(x) 2*x/pi;
```

There are ways to plot a function symbolically/analytically (for example), but those methods have a lot of limitations and you don't have detailed controls on them.

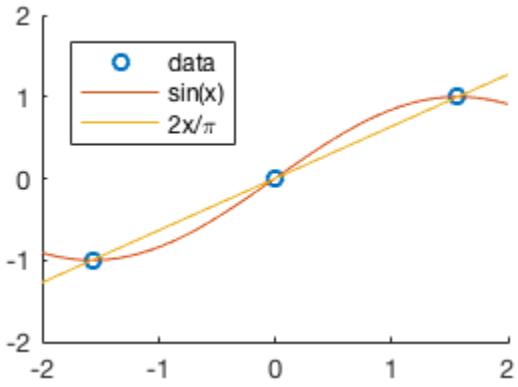
So we stick to the most standard way of plotting: evaluate the function value on a lot of points to make the line look smooth.

```
In [4]: x = linspace(-2,2,1e3); % a 1000 grid points from -2 to 2
```

Always remember to surpress the output (by `;`) when defining this kind of large array. MATLAB WILL print all the elements in an array/matrix no matter how large it is. Sometimes your program will die just because it wants to print 10^{10} numbers.

Now we can plot the functions and data points.

```
In [5]: %plot --size 300,200
        hold on
        plot(xp,yp,'o')
        plot(x,f(x))
        plot(x,g(x))
        legend('data','sin(x)','2x/\pi','Location','northwest')
```



2.5.2 Polynomial interpolation

```
In [6]: % make some data points
        n = 5;
        px = [0 1 2 3 4];
        py = [1 2 2 6 9];
```

n data point can be precisely fitted by a n-1 degree polynomial $p = c_1 + c_2 x + ... + c_n x^{n-1}$.

The coffeicients $c = [c_1, c_2, ...c_n]^T$ satisfy the equation

$$Vc = y$$

where $y = [y_1, y_2, ..., y_n]^T$ is the data points you want to fit, and V is the vandermode matrix only containing powers of x_k, the data points.

```
In [7]: % calculate the vander matrix by loop
        V = zeros(n);
        for j=1:5
            V(:,j) = px.^(j-1);
        end
        V
```

```
V =
     1     0     0     0     0
     1     1     1     1     1
     1     2     4     8    16
     1     3     9    27    81
     1     4    16    64   256
```

The built-in `vander` is flipped left-right. Both forms are correct as long as your algorithm is consistent with the matrix.

```
In [8]: vander(px)
```

```
ans =
     0     0     0     0     1
     1     1     1     1     1
    16     8     4     2     1
    81    27     9     3     1
   256    64    16     4     1
```

Now we can solve $Vc = y$ by $c = V^{-1}y$. In MATLAB backslash form it is `c=V\y`. Note that the actual code never computes V^{-1}, but use something like LU factorization/Gaussian elimination to solve the system. (it is almost always a bad idea to compute the inverse of a matrix). But thinking about $V^{-1}y$ helps you to remember the order of V and y in the command (e.g. is it `V\y` or `y\V` ?).

The code below throws an error because y is a row vector.

```
In [9]: c = V\py
```

```
Error using \Matrix dimensions must agree.
```

You need a column vector on the right side, just like how you write the equation mathematically.

```
In [10]: c = V\py'
```

```
c =
    1.0000
    5.6667
   -7.5833
    3.3333
   -0.4167
```

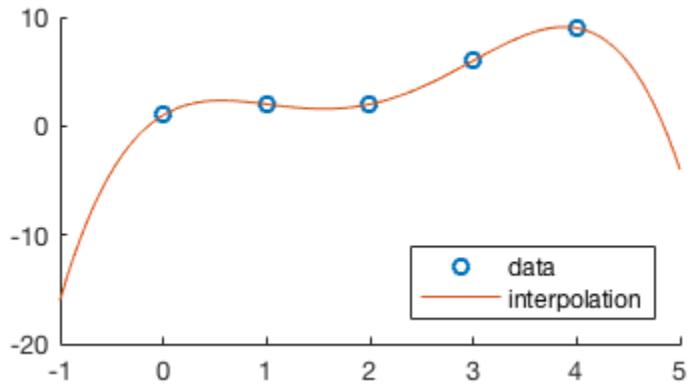
Now we have the coefficients c, we can write the polynomial $p = c_1 + c_2x + ... + c_nx^{n-1}$ as a MATLAB function.

Here's a naive way to evaluate the polynomial. You should write a loop instead. Also consider Horner's method to achieve optimal performance.

```
In [11]: my_ploy = @(c,x) c(1) + c(2)*x + c(3)*x.^2 + c(4)*x.^3 + c(5)*x.^4 ;
```

```
In [12]: % evaluate the function on a lot of data points
         xf = linspace(-1,5,100);
         yf = my_ploy(c,xf);
```

```
In [13]: %plot --size 400,200
         hold on
         plot(px,py,'o')
         plot(xf,yf)
         legend('data','interpolation','Location','southeast')
```



2.6 Lecture 11: Odyssey!!!

Date: 10/05/2017, Thursday

You are expected to finish 8+1 tiny tasks. They will help you get prepared for the final project!

Related resources:

- Ryans's Linux tutorial
- *Intro-to-Odssey-S17_am111.pdf* on Canvas.
- Odyssey quickstart guide
- MATLAB on Odyssey
- Parallel MATLAB on Odyssey

2.6.1 Task 1: Command line on your laptop

Preparation

Read *Session 4 note*, especially Ryans's tutorial if you didn't come to Monday's session.

After reading Chapter 1 to Chapter 5, you should at least know the following Linux commands

- `ls`
- `pwd`
- `mkdir`
- `cd`
- `mv`
- `rm` and `rm -rf`
- `cp` and `cp -r`

If you choose *vi/vim* as your text editor, read Chapter 6. Then you should at least know the following *vim* commands

- `i`
- `esc`
- `:wq`
- `:q!`

Find your own tutorial if you choose other text editors.

Writing code in terminal

Task: Use *vim* or other command line text editer to create a matlab file *hello.m* with the content "disp('hello world!')"

We use *vim* as an example.

First, create a text file by

```
vim hello.m
```

(If *hello.m* already exists, then it will just open that file)

Inside *vim*, type `i` to enter the *Insert Mode*.

Then type the code as usual. For example

```
disp('hello world!')
```

After writting the content, type `esc` to go back to *Command Mode*.

Finally, type `:wq` to save and quit *vim*.

Again, read Chapter 6 for more *vim* usages!

Tips: You can check the content of *hello.m* by a graphic editer. On Mac, you can use `open ./` to open the graphic finder, and then open *hello.m* that you've just created. On Odyssey (See Task 2), there's no graphic editor, so you will also use *vim* to check the file content.

Running MATLAB interactively in terminal

Windows users can jump to Task 2 because I am not sure if the following stuff would work.

Find the MATLAB executable path on your laptop. On Mac it should be something like

```
/Applications/MATLAB_R2017a.app/bin/matlab
```

Running the above command will open the traditional graphic version of MATLAB.

To only use the command line, add 3 options:

```
/Applications/MATLAB_R2017a.app/bin/matlab -nojvm -nosplash -nodesktop
```

Play with this command line version of MATLAB for a while. Type `exit` to quit.

Set shortcut

If you are tired with typing this long command, you can set

```
alias matlab='/Applications/MATLAB_R2017a.app/bin/matlab'
```

Then you can simply type `matlab` to launch the program. However, this shortcut will go away if you close the terminal. To make it a permanent configuration, add the above command to a system file called *~/.bash_profile*. You can edit it by *vim* for example:

```
vim ~/.bash_profile
```

Running MATLAB scripts in terminal

`cd` to the directory where you saved the *hello.m* file. You can execute it by

```
matlab  -nojvm -nosplash -nodesktop
hello
```

Or you can use '-r' to combine two commands together

```
matlab  -nojvm -nosplash -nodesktop -r hello
```

If you didn't set shortcut, the full command would be

```
/Applications/MATLAB_R2017a.app/bin/matlab -nojvm -nosplash -nodesktop -r hello
```

(I actually prefer this command line version to the complicated graphic version!)

2.6.2 Task 2: Command line on Odyssey

Login

Login to Odyssey by

```
ssh am111uXXXX@login.rc.fas.harvard.edu
```

Check Odyssey website if you have any trouble.

Tips: You can open multiple terminals and login to Odyssey, if one is not enough for you.

Basic navigation

Repeat the basic Linux commands, but this time on Odyssey, not on your laptop.

You should see Mac and Linux (Odyssey) commands are almost identical.

File transfer

Use scp

You can transfer files by the built-in `scp` (security-copy) command. **Make sure you are running this command on your laptop, not on odyssey.**

From you laptop to Odyssey (first figure out your Odyssey home directory path by `pwd`)

```
scp local_file_path username@login.rc.fas.harvard.edu:/path_shown_by_pwd_on_Odyssey
```

Try to transfer *hello.m* that you wrote in Task 1 to Odyssey! You will be asked to enter your password again.

From to Odyssey to your laptop is just reversing the arguments

```
scp username@login.rc.fas.harvard.edu:/file_path_on_odyssey local_file_path
```

Use `scp -r` for transfering directory (similar to `cp -r`)

Use other tools

Use Filezilla if you need to transfer a lot of file!

2.6.3 Task 3: MATLAB on Odyssey

Load MATLAB

Load MATLAB by

```
module load matlab
```

(If you get an error, run `source new-modules.sh` and try again.)

It loads the lastest version by default. You can check the version by `which`

```
[username]$ which matlab
alias matlab='matlab -singleCompThread'
/n/sw/matlab-R2017a/bin/matlab
```

Or you can load a specific version

```
module load matlab/R2017a-fasrc01
```

Use this RC portal to find avaiable software and the corresponding loading command. Search for MATLAB. How many different verions do you see?

Run MATLAB

After loading MATLAB, you can run it by: (same as on your laptop)

```
matlab -nojvm -nosplash -nodesktop
```

The 3 options are crucial because there's no graphical user interface on Odyssey.

Play with it, and type `exit` to quit.

Run *hello.m* by `matlab -nojvm -nosplash -nodesktop -r hello`.

2.6.4 Task 4: Interactive Job on Odyssey

After logging into Odyssey, you are on a *home node* with very few computational resources. For any serious computing work you need to switch to a *compute node*. The easiest way is to do this interactively (more about interative mode):

```
srun -t 0-0:30 -c 4 -N 1 --pty -p interact /bin/bash
```

Here we request 30 minutes of computing time (`-t 0-0:30`) on 4 CPUs (`-c 4`), on a single computer (`-N 1`), using interactive mode (`--pty` and `/bin/bash`).

Warning: Don't request too many CPUs! This will make you wait for much longer.

`-p interact` only means you are requesting CPUs on the *interactive partition*, but doesn't mean that you want it to run interactively. The following command starts interactive mode on the *general partition* (more about partition).

```
srun -t 0-0:30 -c 4 -N 1 --pty -p general /bin/bash
```

Then repeat what you've done in Task 3.

2.6.5 Task 5: Batch Job on Odyssey

If your job runs for hours or even days, you can submit it as a *batch job*, so you don't need to keep your terminal open all the time. You are allowed to log out and go away while the job is runnning.

Create a file called *runscript.sh* with the following content. (you can use *vim* to create such a text file)

```
#!/bin/bash
#SBATCH -J Matlabjob1
#SBATCH -p general
#SBATCH -c 1 # single CPU
#SBATCH -t 00:05:00
#SBATCH --mem=400M # memory
#SBATCH -o %j.o # output filename
#SBATCH -e %j.e # error filename

## LOAD SOFTWARE ENV ##
source new-modules.sh
module purge
module load matlab/R2017a-fasrc01

## EXECUTE CODE ##
matlab -nojvm -nodisplay -nosplash -r hello
```

It just puts the options you've used in Task 4 into a text file.

Make sure *runscript.sh* is at the same directory as hello.m, then execute

```
sbatch runscript.sh
```

Use `sacct` to check job status. You should get some output files once it is finished. (more about submitting and monitoring jobs)

Tips: always test your code in interactive mode before submitting a batch job!

2.6.6 Task 6: Use MATLAB-parallel on your laptop

Make sure you've installed the parallel toolbox. To start the command line version, remove the `-nojvm` option when using parallel mode. (The original graphic version works as usual)

```
matlab -nosplash -nodesktop
```

Initialize parallel mode by

```
In [1]: parpool('local', 2)
```

```
Starting parallel pool (parpool) using the 'local' profile ...
connected to 2 workers.

ans =

 Pool with properties:

            Connected: true
           NumWorkers: 2
              Cluster: local
        AttachedFiles: {}
          IdleTimeout: 30 minutes (30 minutes remaining)
          SpmdEnabled: true
```

Then run this script for several times to make sure you get speed-up by using parallel for-loop (`parfor`)

```
In [4]: n = 1e9;

        X = 0;
```

```
        tic
        for i = 1:n
            X = X + 1;
        end
        T = toc;
        fprintf('serial time: %f; result: %d \n',T,X)

        X = 0;
        tic
        parfor i = 1:n
            X = X + 1;
        end
        T = toc;
        fprintf('parallel time: %f; result: %d \n',T,X)
```

```
serial time: 2.724932; result: 1000000000
parallel time: 1.748450; result: 1000000000
```

Tips: For command line version of MATLAB, save the code as *parallel_timing.m*, and then execute `parallel_timing` inside MATLAB.

Finally, quit the parallel mode

```
In [5]: delete(gcp)
```

2.6.7 Task 7: Use MATLAB-parallel on Odyssey interactive mode

Repeat what you've done in Task 6, but on Odyssey. This might **not** be as straightforward as you expected!

You need to request enough memory for the parallel tool box

```
srun -t 0-0:30 -c 4 -N 1 --mem-per-cpu 4000 --pty -p interact /bin/bash
```

Environment variable *SLURM_CPUS_PER_TASK* tells you how many CPUs are available

```
echo $SLURM_CPUS_PER_TASK
4
```

For parallel support, you need to call `matlab-default` instead of `matlab` to launch the program, as described here.

```
module load matlab
matlab-default -nosplash -nodesktop
```

Inside MATLAB, you can again check the number of CPUs by

```
getenv('SLURM_CPUS_PER_TASK')
ans = '4'
```

Initialize parallel mode by (this is a general code for any number of CPUs)

```
parpool('local', str2num(getenv('SLURM_CPUS_PER_TASK')) )
```

The initialization might take severals minutes on Odyssey. Eventually you should see something like

```
ans =

 Pool with properties:

```

```
            Connected: true
           NumWorkers: 4
              Cluster: local
       AttachedFiles: {}
         IdleTimeout: 30 minutes (30 minutes remaining)
         SpmdEnabled: true
```

Then, execute the *parallel_timing.m* script in Task 6. You should see a speed-up like that

```
>> parallel_timing
serial time: 12.228084; result: 1000000000
parallel time: 2.667366; result: 1000000000
```

2.6.8 Task 8: MATLAB-parallel as batch Job

Sightly modify the script *parallel_timing.m* in Task 6. Call it *parallel_timing_batch.m* this time.

```
parpool('local', str2num(getenv('SLURM_CPUS_PER_TASK')))

n = 1e9;

X = 0;
tic
for i = 1:n
    X = X + 1;
end
T = toc;
fprintf('serial time: %f; result: %d \n',T,X)

X = 0;
tic
parfor i = 1:n
    X = X + 1;
end
T = toc;
fprintf('parallel time: %f; result: %d \n',T,X)

X = 0;
tic
parfor i = 1:n
    X = X + 1;
end
T = toc;
fprintf('parallel time: %f; result: %d \n',T,X)

delete(gcp)
```

Then, change the *runscript.sh* in Task 5 correspondingly

```
#!/bin/bash
#SBATCH -J timing
#SBATCH -o timing.out
#SBATCH -e timing.err
#SBATCH -N 1
#SBATCH -c 4
#SBATCH -t 0-00:20
```

```
#SBATCH -p general
#SBATCH --mem-per-cpu 8000

source new-modules.sh
module load matlab
srun -n 1 -c 4 matlab-default -nosplash -nodesktop -r parallel_timing_batch
```

Submit this job. It will take many minutes to finish. Do you get expected speed-up?

In timing.out, you should see something like

```
ans =

 Pool with properties:

            Connected: true
           NumWorkers: 4
              Cluster: local
        AttachedFiles: {}
          IdleTimeout: 30 minutes (30 minutes remaining)
          SpmdEnabled: true

serial time: 7.635188; result: 1000000000
parallel time: 5.901599; result: 1000000000
parallel time: 3.516169; result: 1000000000
Parallel pool using the 'local' profile is shutting down.
```

Explain why the second `parfor` is faster then the first `parfor`

Tips: Using batch job for this kind of small computation is definitely an overkill, as queuing and initializing would take much longer than actual compuation. You will probably use the interactive mode much more often in this class.

2.6.9 Bonus task: make your terminal prettier

Open ~/.bash_profile (for example `vim ~/.bash_profile`), add the following lines

For Mac

```
export CLICOLOR=1
export LSCOLORS=ExFxBxDxCxegedabagacad
```

For Linux (Odyssey)

```
alias ls="ls --color=auto"
```

Type `source ~/.bash_profile` or relaunch the terminal. Notice any difference?

2.7 Session 1: MATLAB Functions and Scripts

Date: 09/11/2017, Monday

```
In [1]: format compact
```

MATLAB's function control can be somewhat confusing... Let me try to explain it.

2.7.1 3 ways to execute MATLAB codes

You can run MATLAB codes in these ways:

- Executing codes directly in the interactive console
- Put codes in a **script** (an m-file), and execute the script in the console
- Put codes in a **function** (also an m-file), and execute the function in the console

Executing codes directly

You know how to run the codes in the interactive console:

```
In [2]: a=1;
        b=2;
        2*a+5*b
```

```
ans =
    12
```

To avoid re-typing the formula `2*a+5*b` over and over again, you can create an inline function in the interative environment.

```
In [3]: f = @(a,b) 2*a+5*b
```

```
f =
  function_handle with value:
    @(a,b)2*a+5*b
```

```
In [4]: f(1,2)
        f(2,3)
```

```
ans =
    12
ans =
    19
```

Writing a script

A script simply allows you to execute many lines of codes at once. It is not a **function**. There's no input and output variables.

To open a new script, type "edit" in the console or click on the "New" Button.

```
In [5]: edit
```

Save the following code into a file with the suffix ".m"

```
In [6]: %%file my_script.m
        a=1;
        b=2;
        2*a+5*b
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/AM111/docs/my_script.m'.
```

Execute the script by typing its file name in the console. Make sure your working directory is the same as the script's directory.

```
In [7]: my_script
```

```
ans =
    12
```

You can definitely change parameters `a, b` in your script and re-run the script over and over again. However, to have a better control on input arguments, you need to write a **function**, a not script.

Writing a function

A function is also a file with the suffix ".m", same as a script. But it contains the `function` head which defines input and output parameters. The function name has to be the same as the file name.

```
In [8]: %%file my_func.m
        function s=my_func(a,b)
            s = 2*a+5*b;
        end
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/AM111/docs/my_func.m'.
```

Now you can provide input arguments to your function.

```
In [9]: my_func(1,2)
```

```
ans =
    12
```

2.7.2 Multi-level functions

An m-file can contain multiple functions. But only the first one can be accessed from the outside. Others are only for internal use.

```
In [10]: %%file mul_by_4.m

         function z=mul_by_4(x)
             y = mul_by_2(x);
             z = mul_by_2(y);
         end

         function y=mul_by_2(x)
             y = 2*x;
         end
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/AM111/docs/mul_by_4.m'.
```

You can call mul_by_4( ), but cannot call mul_by_2( ).

```
In [11]: mul_by_4(2)
```

```
ans =
     8
```

```
In [12]: mul_by_2(2)
```

```
Error using evalUndefined function 'mul_by_2' for input arguments of type 'double'.
```

Note: Since R2016b, you can also add functions in scripts. However, you had better avoid this usage for backward capability. Otherwise, people using an older version of MATLAB will have trouble running your code. Always create a separate file for your function.

2.8 Session 2: Speed-up your code by vectorization

Date: 09/18/2017, Monday

This session is mostly about reviewing Lecture 4 and 5. This page just introduces an additional trick to make your code faster and cleaner.

2.8.1 For loops

You already know how to create a Mandelbrot set by writting tons of "for" loops. If not, see Lecture 5's note.

```
In [1]: %%file mande_by_loops.m
        function Z_final = mande_by_loops(C, T)

            [nx,ny] = size(C);
            Z_final = zeros(nx,ny); % to hold last value of z, at all possible points.

            for ix = 1:nx
            for iy = 1:ny

                % get the value of c at current point.
                % note that MATLAB is case-sensitive
                c = C(ix,iy);
                z = 0; % initial value, doesn't matter too much
                for t=2:T
                    z = z^2+c;
                end
                Z_final(ix,iy) = z; % save the last value of z

            end
            end

        end
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/AM111/docs/mande_by_loops.m'.
```

2.8.2 Vectorization

The above function has 3 "for" loops, but 2 of them are not necessary, because you can operate on the entire array.

```
In [2]: %%file mande_by_vec.m
        function Z = mande_by_vec(C, T)
            % vectorized over C and Z

            [nx,ny] = size(C);
            Z = zeros(nx,ny);
            for t=2:T
                Z = Z.^2+C;
            end

        end
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/AM111/docs/mande_by_vec.m'.
```

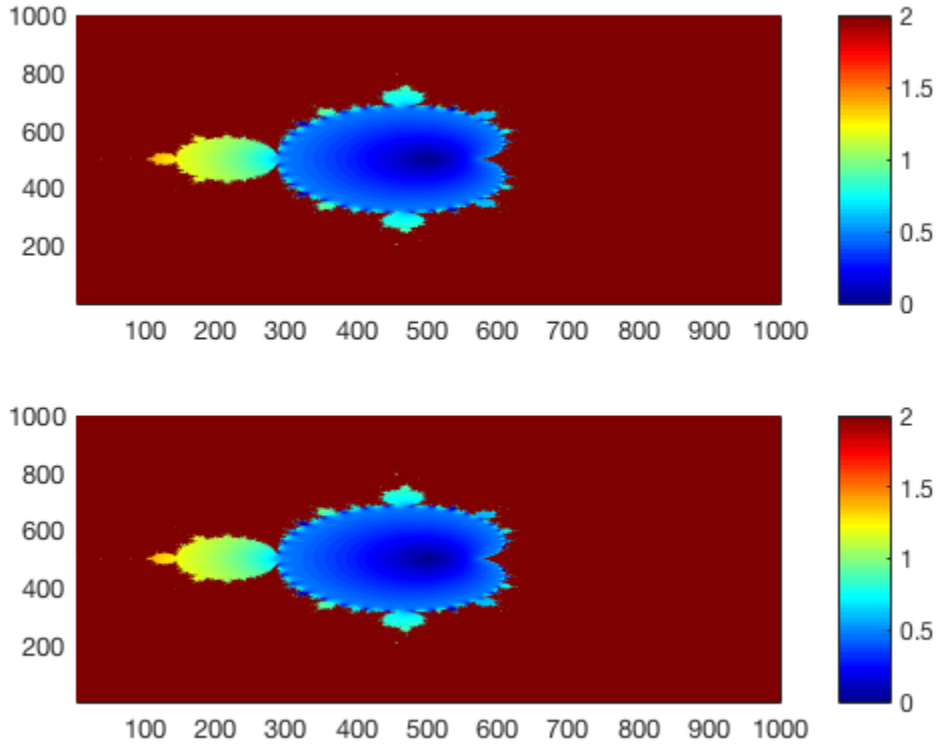
2.8.3 Performance comparision

Compared to the for-loop version, this vectorized version is much shorter, and 20x faster!

```
In [3]: % initialization
        nx = 1000;
        xm = 1.75;
```

```
        x = linspace(-xm, xm, nx);
        y = linspace(-xm, xm, nx);
        [Cr, Ci] = meshgrid(x,y);
        C = Cr + i*Ci;

        T = 50;

        % use loops
        tic
        Z_loop = mande_by_loops(C,T);
        toc

        % use vectorization
        tic
        Z_vec = mande_by_vec(C,T);
        toc

        % check if results are equal
        isequal(Z_vec,Z_loop)

        % plot two results
        subplot(211);pcolor(abs(Z_loop));
        shading flat;colormap jet; colorbar;caxis([0,2]);

        subplot(212);pcolor(abs(Z_vec));
        shading flat;colormap jet; colorbar;caxis([0,2]);
```

```
Elapsed time is 4.883975 seconds.
Elapsed time is 0.255324 seconds.

ans =

  logical

   1
```



MATLAB's loop is notoriously slow because it keeps checking the variable types at every iteration. A rule of thumb is **shorter code is often faster**, in terms of achieving the same functionality. (Only for high-level languages like MATLAB and Python. Loop is fast in low-level languages.)

2.9 Session 3: LU Factorization & Markov Process

Date: 09/25/2017, Monday

```
In [1]: format compact
```

Read Canvas - Files - lectures- linear_algebra.pdf first before looking at this material.

2.9.1 LU=PA Factorization

Gaussian elimination consists of **forward elimination** and **backward substitution**.

The backward substition part is easy – You already have an **upper diagnonal matrix** U, and just need to solve $Ux = b$.

The forward elimination part is more interesting. By doing forward elimination by hand, you transformed the original matrix A to an upper diagnonal matrix U. In fact, during this forward elimination process, you not only produced matrix U, but also constructed two other matrices L and P (even if you didn't even notice it!). They satisfy

$$LU = PA$$

- L is a **lower triangular matrix L** with all diagonal elements being 1. It contains all the multipliers used during the forward elimination.

- P is a **permutation matrix** containing only 0 and 1. It accounts for all row-swapings during the forward elimination.

Row operation as matrix multiplication

Basic idea

To understand how $LU = PA$ works, you should always keep in mind that

```
row operation = left multiply
```

Or more verbosely

```
A row operation on matrix A = left-multiply a matrix L to A (i.e. calculate LA)
```

This is a crucial concept in linear algebra.

Let's see an example:

```
In [2]: A = [10 -7 0; -3 2 6 ;5 -1 5]
```

```
A =
    10    -7     0
    -3     2     6
     5    -1     5
```

Perform the first step of gaussian elimination, i.e. add 0.3*row1 to row2.

```
In [3]: A1 = A; % make a copy
        A1(2,:) = A(2,:)+0.3*A(1,:)
```

```
A1 =
   10.0000   -7.0000         0
         0   -0.1000    6.0000
    5.0000   -1.0000    5.0000
```

There's another way to perform the above row-operation: left-multiply A by an elementary matrix.

```
In [4]: L1 = [1,0,0; 0.3,1,0; 0,0,1] % make our elementary matrix
```

```
L1 =
    1.0000         0         0
    0.3000    1.0000         0
         0         0    1.0000
```

```
In [5]: L1*A
```

```
ans =
   10.0000   -7.0000         0
         0   -0.1000    6.0000
    5.0000   -1.0000    5.0000
```

L1*A gives the same result as the previous row-operation!

Let's repeat this idea again:

```
row operation = left multiply
```

Find elementary matrix

How to find out the matrix L1? Just perform the row-operation to an identity matrix

```
In [6]: L1 = eye(3); % 3x3 identity matrix
        L1(2,:) = L1(2,:)+0.3*L1(1,:) % the row-operation you want to "encode" into this matrix
```

```
L1 =
    1.0000         0         0
    0.3000    1.0000         0
         0         0    1.0000
```

Then you can perform L1*A to apply this row-operation on any matrix A.

Same for the permutation operation, as it is also an elementary row operation.

```
In [7]: Ap = A; % make a copy
        % swap raw 1 and 2
        Ap(2,:) = A(1,:);
        Ap(1,:) = A(2,:);
        Ap
```

```
Ap =
    -3     2     6
    10    -7     0
     5    -1     5
```

You can "encode" this row-swapping operation into an elementary permutation matrix.

```
In [8]: I = eye(3); % 3x3 identity matrix
        P1 = I;

        % swap raw 1 and 2
        P1(2,:) = I(1,:);
        P1(1,:) = I(2,:);
        P1
```

```
P1 =
     0     1     0
     1     0     0
     0     0     1
```

Multiplying A by P1 is equivalent to permuting A directly:

```
In [9]: P1*A % same as Ap
```

```
ans =
    -3     2     6
    10    -7     0
     5    -1     5
```

Get L during forward elimination

For simplicity, assume you don't need permutation steps. Then you just transform an arbrary 3x3 matrix A (non-singular, of course) to an upper-diagnoal matrix U by 3 row operations. Such operations are equivalent to multiplying A by 3 matrices L_1, L_2, L_3

$$A \to L_1 A \to L_2 L_1 A \to L_3 L_2 L_1 A = U$$

We can rewrite it as

$$A = (L_3 L_2 L_1)^{-1} U$$

Or

$$A = LU, \;\; L = (L_3 L_2 L_1)^{-1}$$

It is easy to get L as long as you know L_1, L_2, L_3 from the operations you've performed.

```
In [10]: A % show A's value again
```

```
A =
    10    -7     0
    -3     2     6
     5    -1     5
```

```
In [11]: L1 = [1,0,0; 0.3,1,0; 0,0,1] % repeat L1 again
```

```
L1 =
    1.0000         0         0
    0.3000    1.0000         0
         0         0    1.0000
```

```
In [12]: L1*A % row operation by left-multiply
```

```
ans =
   10.0000   -7.0000         0
         0   -0.1000    6.0000
    5.0000   -1.0000    5.0000
```

```
In [13]: L2 = [1,0,0; 0,1,0; -0.5,0,1] % build the next elimination step
```

```
L2 =
    1.0000         0         0
         0    1.0000         0
   -0.5000         0    1.0000
```

```
In [14]: L2*L1*A % apply the next elimination step
```

```
ans =
   10.0000   -7.0000         0
         0   -0.1000    6.0000
         0    2.5000    5.0000
```

```
In [15]: L3 = [1,0,0; 0,1,0; 0,25,1] % build the last elimination step
```

```
L3 =
     1     0     0
     0     1     0
     0    25     1
```

```
In [16]: U = L3*L2*L1*A % apply the last elimination step
```

```
U =
   10.0000   -7.0000         0
         0   -0.1000    6.0000
         0         0  155.0000
```

Now you've transformed A to an upper-diagonal matrix U. And you also have L:

```
In [16]: L = inv(L3*L2*L1)
```

```
L =
    1.0000         0         0
   -0.3000    1.0000         0
    0.5000  -25.0000    1.0000
```

Or

```
In [17]: L = inv(L1)*inv(L2)*inv(L3)
```

```
L =
    1.0000         0         0
   -0.3000    1.0000         0
    0.5000  -25.0000    1.0000
```

Calculating L is just putting the coefficients in L_1, L_2, L_3 together and negating them (except diagonal elements).

Why? Again, because

```
row operation = left multiply
```

Here we are just encoding multiple row operations $L_1^{-1}, L_2^{-1}, L_3^{-1}$ into a single matrix L. You get this matrix by applying all those operations to an identity matrix.

You can think of L_1^{-1} as "a row operation that cancels the effect of L_1":

```
In [18]: inv(L1)

ans =
    1.0000         0         0
   -0.3000    1.0000         0
         0         0    1.0000
```

Last, let's verify $A = LU$

```
In [19]: L*U

ans =
   10.0000   -7.0000         0
   -3.0000    2.0000    6.0000
    5.0000   -1.0000    5.0000
```

We can say that L represents all forward elimination steps (assume no permutaion). By knowing L, you can easily get U by $U = L^{-1}A$

Get P during forward elimination

Say you have a permutation step P somewhere, for example

$$L_3 P L_2 L_1 A = U$$

It can be shown that P can be "pushed rightward"

$$L_3 L_2 L_1 (PA) = U$$

(The proof is too technical. See P159 of *Trefethen L N, Bau III D. Numerical linear algebra[M]. Siam, 1997* if you are interested).

Thus

$$LU = PA$$

2.9.2 Markov process

There are two towns, both have 100 people (so 200 in total). Everyday, 50% of people in town 1 will move to town 2, while 30% of people in town 2 will move to town 1. Eventually, how many people will each town have?

The initial condition is

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 100 \\ 100 \end{bmatrix}$$

Each day

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \to \begin{bmatrix} x_1 - 0.5x_1 + 0.3x_2 \\ x_2 + 0.5x_1 - 0.3x_2 \end{bmatrix} = \begin{bmatrix} 0.5x_1 + 0.3x_2 \\ 0.5x_1 + 0.7x_2 \end{bmatrix} = \begin{bmatrix} 0.5 & 0.3 \\ 0.5 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

This is a **Markov process**. We can get its **Markov matrix** (or **transition matrix**)

$$A = \begin{bmatrix} 0.5 & 0.3 \\ 0.5 & 0.7 \end{bmatrix}$$

Each column of A has a sum of 1 because it means probability.

```
In [20]: x = [100; 100] % initial condition
         A = [0.5 0.3;0.5 0.7] % Markov matrix
```

```
x =
   100
   100
A =
    0.5000    0.3000
    0.5000    0.7000
```

At the second day, the number of people will be:

```
In [21]: A*x
```

```
ans =
    80
   120
```

Town2 gets more people. This is expected because town1->town2 has a higher probability than town2->town1.

How about after 10 days?

```
In [22]: x10 = A^10*x
```

```
x10 =
   75.0000
  125.0000
```

11 days?

```
In [23]: x11 = A*x10
```

```
x11 =
   75.0000
  125.0000
```

There's no difference between day 10 and day 11, which means the population reaches equilibrium. This is called the **power method** for finding the **state vector** for this **transition matrix**.

This power method is intuitive but not very efficient. For a fancier method for Pset3, see Canvas - Files - scripts_and_code - lin_algebra - pagerank_demo_template.m.

2.10 Session 4: Linux Command Line

Date: 10/02/2017, Monday

This week we are going to use Harvard's Odyssey supercomputer. It is a Linux system, just like most remote servers. Before playing with Odyssey I strongly recommend you to get familiar with Linux basics.

Why command line, not graphical interface?

1. Command line is more like programming so it allows you to do much more, such as renaming 1000 files.

2. When controlling a remote server, the internet bandwidth is typically not enough for showing the graphical user interface. But with command line you only need to transfer texts, not images.

Linux commmand line is **an absolutely essential skill for any programmers** (much more important than MATLAB), so learn it!

2.10.1 Trying Linux command on your Laptop

On Mac

Mac has a built-in app called *Terminial*. You can find it by searching for "Terminial" in *Spotlight Search* (`command+space`, or `control+space` for older OS). Mac command line is almost the same as Linux command line, so you can practice Linux commands on Mac without having to connect to Odyssey. This default terminal is already pretty good for beginners. If you want more advanced terminals, try iTerm2.

For connecting to remote servers, simply execute `ssh username@ip_address` in the terminal.

On Windows

Window's own command line is **very different** from Linux's. On Windows 10, you can follow this official tutorial to install the Linux subsystem, so you can play with Linux on your laptop. If you are using an older windows system, you can try some online Linux "playground" like https://www.tutorialspoint.com/unix_terminal_online.php.

For connecting to remote servers, you can use the old putty or try more advanced ones like MobaXterm.

2.10.2 Linux Command Basics

There are a bunch of Linux tutorials online. I particularly like this one. You should at least read Chapter 1 - Chapter 5.

2.10.3 Text Editors

By default, there are 3 text editors available: *vim*, *emacs* and *nano*. Just pick up one of them. I personally use *vim* but it has the steepest learning curve. There are many discussions on which one to choose (for example, this article).

2.11 Session 5: MATLAB backslash & some pitfalls

Date: 10/16/2017, Monday

```
In [1]: format compact
```

2.11.1 Different behaviors of backslash

You've already used the backslash \ a lot to solve linear systems. But if you look at MATLAB backslash documentation you will find it can do much more than solving linear systems. This powerful feature can sometimes be very confusing if you are not careful.

Standard linear system

First see a standard problem: a 4x4, full rank square matrix A and a 4-element column vector b. We want to solve

$$Ax = b$$

```
In [2]: b = rand(4,1)
```

```
b =
    0.8147
    0.9058
    0.1270
    0.9134
```

```
In [3]: A = rand(4,4)
```

```
A =
    0.6324    0.9575    0.9572    0.4218
    0.0975    0.9649    0.4854    0.9157
    0.2785    0.1576    0.8003    0.7922
    0.5469    0.9706    0.1419    0.9595
```

Well, not big deal...

```
In [4]: x = A\b
```

```
x =
   -0.0486
    0.9204
   -0.0630
    0.0579
```

We can verify the result:

```
In [5]: A*x - b % almost zero
```

```
ans =
   1.0e-15 *
         0
         0
   -0.0555
   -0.1110
```

Incorrect shape

You should already notice that b must be a column vector.

```
In [6]: x = A\b' % row vector doesn't work
```

```
Error using \Matrix dimensions must agree.
```

Also, A and b must have the same number of rows, because A and b come from the following linear system with n rows (equations) and m columns (variables):

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + ... + a_{1m}x_m = b_1 \\ a_{21}x_1 + a_{22}x_2 + ... + a_{1m}x_m = b_2 \\ ... \\ a_{n1}x_1 + a_{n2}x_2 + ... + a_{1m}x_m = b_n \end{cases}$$

```
In [7]: A = rand(3,4) % A has 3 rows but b has 4 rows
```

```
A =
    0.6557    0.9340    0.7431    0.1712
    0.0357    0.6787    0.3922    0.7060
    0.8491    0.7577    0.6555    0.0318
```

```
In [8]: A\b % doesn't work
```

```
Error using \Matrix dimensions must agree.
```

Looks like A has to be a square matrix, but see below...

Over-detemined linear system

In fact, A doesn't have to be a square matrix, just like a linear system doesn't need to have the same number of rows (equations) and columns (variables).

Here we create an over-determined system

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3 \\ a_{41}x_1 + a_{42}x_2 + a_{43}x_3 = b_4 \end{cases}$$

An **over-determined** system means A is **tall** and **narrow** (more rows than columns)

```
In [9]: A = rand(4,3) % more equations (rows) than variables (columns)
```

```
A =
    0.2769    0.6948    0.4387
    0.0462    0.3171    0.3816
    0.0971    0.9502    0.7655
    0.8235    0.0344    0.7952
```

```
In [10]: x = A\b % backslash works
```

```
x =
    0.9798
    0.2901
    0.2142
```

MATLAB does return a set of (x_1, x_2, x_3). But you know this can't be the solution because you can't fulfill 4 equations by just 3 degrees of freedom.

```
In [11]: A*x - b % not zero, so x is not a solution
```

```
ans =
   -0.2479
   -0.6868
    0.4078
    0.0738
```

So what's `x`? It is actually a least-square fit, same as the result from the normal equation

$$A^T Ax = A^T b$$

```
In [12]: (A'*A)\(A'*b) % solve normal equation
```

```
ans =
    0.9798
    0.2901
    0.2142
```

In MATLAB, simply using `A\b` is actually more accurate than `(A'*A)\(A'*b)` for solving least squares, especially for large matrices. That's because the condition number of $A^T A$ could be very large.

```
In [13]: cond(A)
         cond(A'*A)
```

```
ans =
    8.7242
ans =
   76.1114
```

We find $cond(A^T A) = cond(A)^2$. It is not quite large in this tiny case but could explode for large matrices

So how to avoid the normal equation?

Recall that, for a standard, full rank system $Ax = b$, the code `A\b` doesn't compute $A^{-1}b$ at all, because A^{-1} is often ill-conditioned. It uses LU factorization which is better-conditioned.

Similarly, for an over-determined $Ax = b$, the code `A\b` doesn't compute $A^T A$ at all. It uses QR factorization or similar techniques to make the problem better-conditioned.

Under-determined linear system

Now let's look at an under-determined system

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4 + a_{15}x_5 = b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + a_{24}x_4 + a_{25}x_5 = b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + a_{34}x_4 + a_{35}x_5 = b_3 \\ a_{41}x_1 + a_{42}x_2 + a_{43}x_3 + a_{44}x_4 + a_{45}x_5 = b_4 \end{cases}$$

An **under-determined** system means A is **short** and **wide** (more columns than rows)

```
In [14]: A = rand(4,5) % less equations (rows) than variables (columns)
```

```
A =
    0.1869    0.7094    0.6551    0.9597    0.7513
    0.4898    0.7547    0.1626    0.3404    0.2551
    0.4456    0.2760    0.1190    0.5853    0.5060
    0.6463    0.6797    0.4984    0.2238    0.6991
```

```
In [15]: x = A\b % backslash still works
```

```
x =
   -0.1886
    1.4263
    0.2995
   -0.3730
         0
```

We can see x is the solution to $Ax = b$:

```
In [16]: A*x - b % almost zero
```

```
ans =
   1.0e-15 *
    0.4441
    0.3331
    0.0278
    0.1110
```

However, we know that an under-determined system has infinite number of solutions. But MATLAB just returns one value. What's special about this value?

It turns out that the `x` we get here has the smallest norm $||x||_2$ among all possible solutions.

```
In [17]: norm(x) % smaller than any other possible solutions
```

```
ans =
    1.5162
```

2.11.2 Another multiple-behavior example

Because the backslash operator \ has different behaviors under different circumstances, you have to be **very careful**. Sometimes your matrix shape might be wrong, but MATLAB will still return a result. But in that case you might be solving a least square problem instead of a full-rank linear system!

MATLAB has quite a lot of multi-behavior ("poly-algorithm") functions. Another example is the built-in lu() function for LU factorization.

```
In [18]: A = rand(4,4) % to be LU-factorized
```

```
A =
    0.8909    0.1493    0.8143    0.1966
    0.9593    0.2575    0.2435    0.2511
    0.5472    0.8407    0.9293    0.6160
    0.1386    0.2543    0.3500    0.4733
```

Just calling `lu()` with no return, you get a single matrix with L and U stacked together.

```
In [19]: lu(A)
```

```
ans =
    0.9593    0.2575    0.2435    0.2511
    0.5704    0.6938    0.7903    0.4728
    0.9287   -0.1295    0.6905    0.0246
    0.1445    0.3129    0.0978    0.2867
```

Using `[L,U]` to hold the return, you get two separate matrices. Notice that `L` is not a strict lower-triangular matrix, because it also incorporates the pivoting matrix P

```
In [20]: [L,U] = lu(A)
```

```
L =
    0.9287   -0.1295    1.0000         0
    1.0000         0         0         0
    0.5704    1.0000         0         0
    0.1445    0.3129    0.0978    1.0000
U =
    0.9593    0.2575    0.2435    0.2511
         0    0.6938    0.7903    0.4728
         0         0    0.6905    0.0246
         0         0         0    0.2867
```

Using `[L,U,P]` to hold the return, you get all three matrices. Now `L` is strictly lower-triangular.

```
In [21]: [L,U,P] = lu(A)
```

```
L =
    1.0000         0         0         0
    0.5704    1.0000         0         0
    0.9287   -0.1295    1.0000         0
    0.1445    0.3129    0.0978    1.0000
U =
    0.9593    0.2575    0.2435    0.2511
         0    0.6938    0.7903    0.4728
         0         0    0.6905    0.0246
         0         0         0    0.2867
P =
     0     1     0     0
```

```
     0     0     1     0
     1     0     0     0
     0     0     0     1
```

You can ignore the returning `P` by `~`, but keep in mind that the returning `L` is different from that in cell [20], although the code looks very similar.

```
In [22]: [L,U,~] = lu(A)

L =
    1.0000         0         0         0
    0.5704    1.0000         0         0
    0.9287   -0.1295    1.0000         0
    0.1445    0.3129    0.0978    1.0000
U =
    0.9593    0.2575    0.2435    0.2511
         0    0.6938    0.7903    0.4728
         0         0    0.6905    0.0246
         0         0         0    0.2867
```

2.12 Session 6: Three ways of differentiation

Date: 10/23/2017, Monday

```
In [1]: format compact
```

There are 3 major ways to compute the derivative $f'(x)$

- Symbolic differentiation
- Numerical differentiation
- Automatic differentiation

You are already familiar with the first two. The last one is **not required** by this class, but it is just too good to miss. It is the core of modern deep learning engines like Google's TensorFlow, which is used for training AlphaGo Zero. Here we only give a very basic introduction. Enthusiasts can read *Baydin A G, Pearlmutter B A, Radul A A, et al. Automatic differentiation in machine learning: a survey*

Let's compare the pros and cons of each method.

2.12.1 Symbolic differentiation

MATLAB toolbox

MATLAB provides symbolic tool box for symbolic differentiation. It can assist your mathetical analysis and can be used to verify the numerical differentiation results.

```
In [2]: syms x
```

Consider this function

$$f(x) = \frac{1 - e^{-x}}{1 + e^{-x}}$$

```
In [3]: f0 = (1-exp(-x))/(1+exp(-x))

f0 =
-(exp(-x) - 1)/(exp(-x) + 1)
```

The first-order derivative is

```
In [4]: f1 = diff(f0,x)
```

```
f1 =
exp(-x)/(exp(-x) + 1) - (exp(-x)*(exp(-x) - 1))/(exp(-x) + 1)^2
```

We can keep calculating higher-order derivatives

```
In [5]: f2 = diff(f1,x)
```

```
f2 =
(2*exp(-2*x))/(exp(-x) + 1)^2 - exp(-x)/(exp(-x) + 1) + (exp(-x)*(exp(-x) - 1))/(exp(-x) + 1)^2 - (2*
```

```
In [6]: f3 = diff(f2,x)
```

```
f3 =
exp(-x)/(exp(-x) + 1) - (6*exp(-2*x))/(exp(-x) + 1)^2 + (6*exp(-3*x))/(exp(-x) + 1)^3 - (exp(-x)*(exp
```

```
In [7]: f4 = diff(f3,x)
```

```
f4 =
(14*exp(-2*x))/(exp(-x) + 1)^2 - exp(-x)/(exp(-x) + 1) - (36*exp(-3*x))/(exp(-x) + 1)^3 + (24*exp(-4*
```

```
In [8]: f5 = diff(f4,x)
```

```
f5 =
exp(-x)/(exp(-x) + 1) - (30*exp(-2*x))/(exp(-x) + 1)^2 + (150*exp(-3*x))/(exp(-x) + 1)^3 - (240*exp(-
```

We see the expression becomes more and more complicated for higher-order derivatives, even though the original $f(x)$ is fairly simple.

You can imagine that symbolic diff can be quite inefficient for complicated functions and higher-order derivatives.

Convert symbol to function

We can convert MATLAB symbols to functions, and use them to compute numerical values.

```
In [9]: f0_func = matlabFunction(f0)
```

```
f0_func =
  function_handle with value:
    @(x)-(exp(-x)-1.0)./(exp(-x)+1.0)
```

`f0` is converted to a normal MATLAB function. It is different from just copying the symbolic expression to MATLAB codes, as it is vectorized over input `x` (notice the `./`).

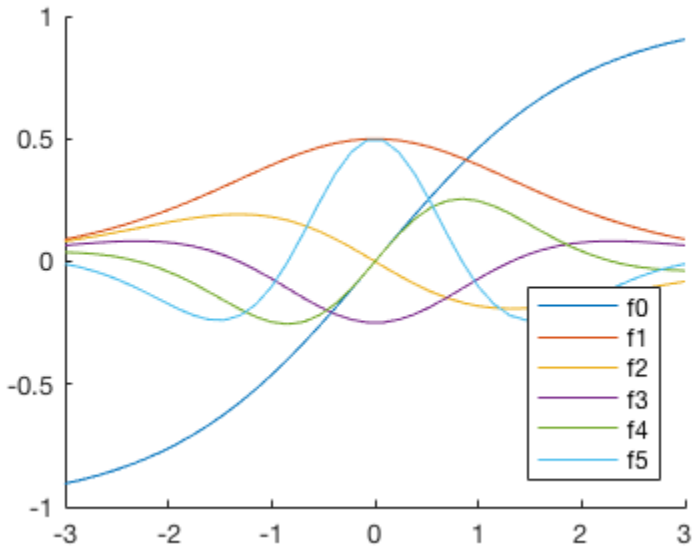
Same for `f0`'s derivatives:

```
In [10]: f1_func = matlabFunction(f1);
         f2_func = matlabFunction(f2);
         f3_func = matlabFunction(f3);
         f4_func = matlabFunction(f4);
         f5_func = matlabFunction(f5);
```

Let's plot all the derivatives.

```
In [11]: xx = linspace(-3,3,40); % for plot
```

```
In [12]: %plot -s 400,300
         hold on
         plot(xx,f0_func(xx))
         plot(xx,f1_func(xx))
         plot(xx,f2_func(xx))
         plot(xx,f3_func(xx))
         plot(xx,f4_func(xx))
         plot(xx,f5_func(xx))
         legend('f0','f1','f2','f3','f4','f5','Location','SouthEast')
```



2.12.2 Numerical differentiation

Is it possible to use the numerical differentiation we learned in class to approximate the 5-th order derivative? Let's try.

```
In [13]: y0 = f0_func(xx); % get numerical data
```

```
In [14]: dx = xx(2)-xx(1) % get step size
```

```
dx =
    0.1538
```

We use the **center difference**, which is much more accurate than **forward** or **backward** difference.

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

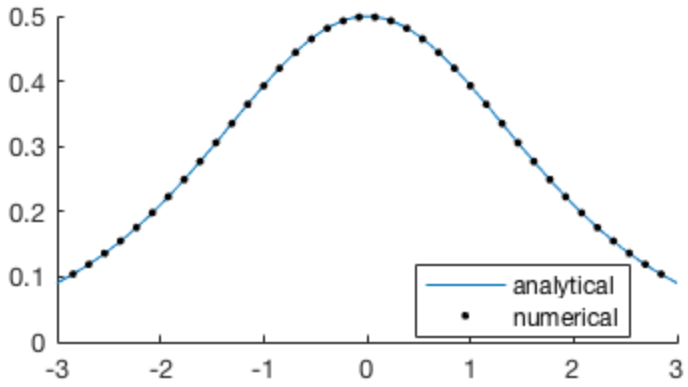
For simplicity, we just throw away the end points `x(1)` and `x(end)`. So the resulted gradient array `y1` is shorter than `y0` by 2 elements. You can also use forward or backward diff to approximate the derivates at the end points. But here we only focus on internal points.

```
In [15]: y1 = (y0(3:end) - y0(1:end-2)) / (2*dx);
         length(y1)
```

```
ans =
    38
```

The numerical diff highly agrees with the symbolic one!

```
In [16]: %plot -s 400,200
         hold on
         plot(xx,f1_func(xx))
         plot(xx(2:end-1),y1,'k.')
         legend('analytical','numerical','Location','Best')
```

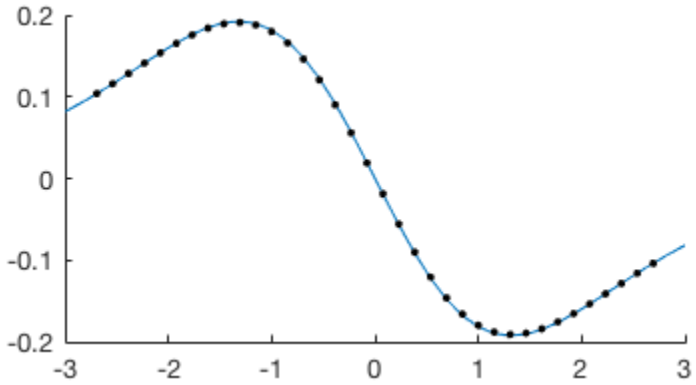


Then we go to 2-nd order:

```
In [17]: y2 = (y1(3:end) - y1(1:end-2)) / (2*dx);
         length(y2)
```

```
ans =
    36
```

```
In [18]: %plot -s 400,200
         hold on
         plot(xx,f2_func(xx))
         plot(xx(3:end-2),y2,'.k')
```

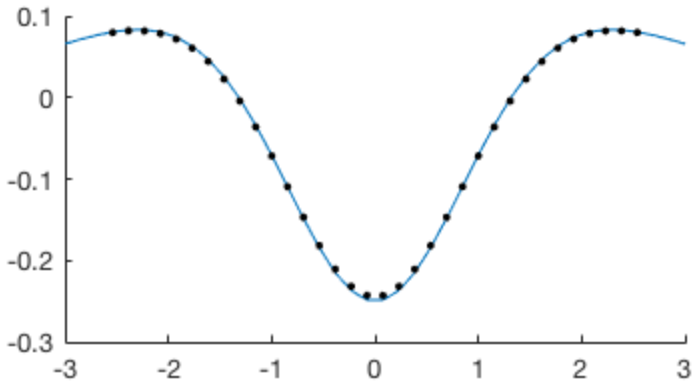


Also doing well. 3-rd order?

```
In [19]: y3 = (y2(3:end) - y2(1:end-2)) / (2*dx);
         length(y3)
```

```
ans =
    34
```

```
In [20]: %plot -s 400,200
         hold on
         plot(xx,f3_func(xx))
         plot(xx(4:end-3),y3,'.k')
```



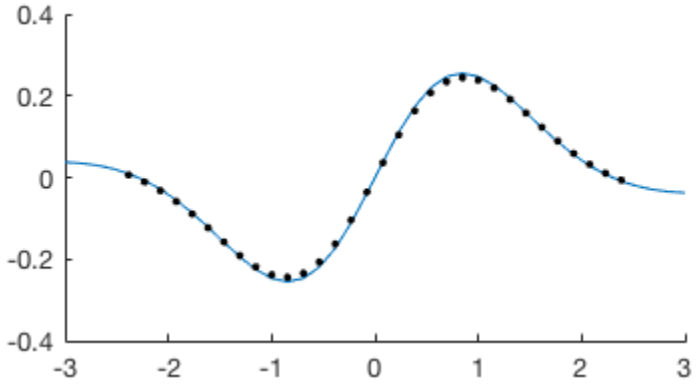
Looks like center diff is doing a really good job.

4-th order?

```
In [21]: y4 = (y3(3:end) - y3(1:end-2)) / (2*dx);
         length(y4)
```

```
ans =
     32
```

```
In [22]: %plot -s 400,200
         hold on
         plot(xx,f4_func(xx))
         plot(xx(5:end-4),y4,'.k')
```



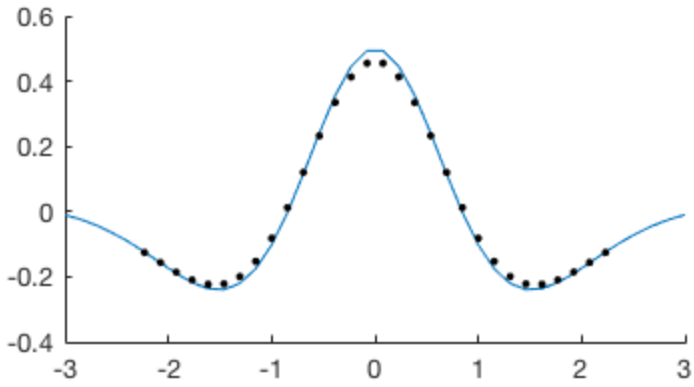
Some points start to deviate, but not too much.

5-th order?

```
In [23]: y5 = (y4(3:end) - y4(1:end-2)) / (2*dx);
         length(y5)
```

```
ans =
     30
```

```
In [24]: %plot -s 400,200
         hold on
         plot(xx,f5_func(xx))
         plot(xx(6:end-5),y5,'.k')
```



Now we get some noticeable error! The relative error at the peak is ~10%.

```
In [25]: format long
         max(y5) % numerical
         max(f5_func(xx))  % analytical
```

```
ans =
   0.455250196326829
ans =
   0.493735580546680
```

Even though the center diff is doing a really good job for low-order derivatives, the error accumulates as the order gets higher. The situation will be even worse for forward or backward diff. Also, the $f(x)$ we choose here is pretty smooth. For a steep $f(x)$, numerical differentiation tends to perform badly.

You might want to use symbolic differentiation instead, but it could be very slow for complicated functions. Is there a better method?

2.12.3 Automatic differentiation

Theoretical explanation

Automatic differentiation ("autodiff" for short) kind of gets the best of both worlds.

- It is not numerical differentiation. Autodiff has no truncation error. The result is as accurate as symbolic method.
- It is not symbolic differentiation. Autodiff doens't compute the complicated symbolic/analytical expression, so it is much faster than the symbolic way.

How can this magic happen? The easiest explanation is using dual numbers.

Consider $f(x) = x^2$. Instead of using a real number like 1.0 or 1.5 as the function input, we use a dual number

$$x + \epsilon$$

where x is still a normal number but ϵ is a special number with property

$$\epsilon^2 = 0$$

It is analogous to the imaginary unit i. You can add or multiply i as usual, but whenever you encounter i^2, replace it by -1. Similarly, you can add or multiply ϵ as usual, but when ever you encounter ϵ^2, replace it by 0.

$$f(x + \epsilon) = x^2 + 2x\epsilon + \epsilon^2 = x^2 + 2x\epsilon$$

The coefficient of ϵ is?

$2x$!! which is just $f'(x)$

We didn't perform any "differentiating" at all. Just by carrying an additional "number" ϵ through a function, we got the derivative of that function as well.

Let's see another example $f(x) = x^3$

$$(x+\epsilon)^3 = x^3 + 3x^2\epsilon + 3x\epsilon^2 + \epsilon^3 = x^3 + 3x^2\epsilon$$

The coeffcient is $3x^2$, which is just the derivative of x^3.

If the function is not a polynomial? Say $f(x) = e^x$

$$e^{x+\epsilon} = e^x e^\epsilon = e^x(1 + \epsilon + \frac{1}{2}\epsilon^2 + ...) = e^x(1+\epsilon)$$

The coeffcient of ϵ is e^x, which is the derivative of e^x. (If you wonder how can a computer know the Taylor expansion of e^ϵ, think about how can a computer calculate e^x)

Code example

MATLAB doesn't have a good autodiff tool, so we use a Python package autograd developed by *Harvard Intelligent Probabilistic Systems Group*.

You don't need to try this package right now (since this is not a Python class), but just keep in mind that if you need a fast and accurate way to compute derivative, there are such tools exist.

Don't worry if you don't know Python. We will explain as it goes.

```
In [1]: %matplotlib inline
        import matplotlib.pyplot as plt # contains all plotting functions
        import autograd.numpy as np # contains all basic numerical functions
        from autograd import grad # autodiff tool
```

We still differentiate $f(x) = \frac{1-e^{-x}}{1+e^{-x}}$ as in the MATLAB section.

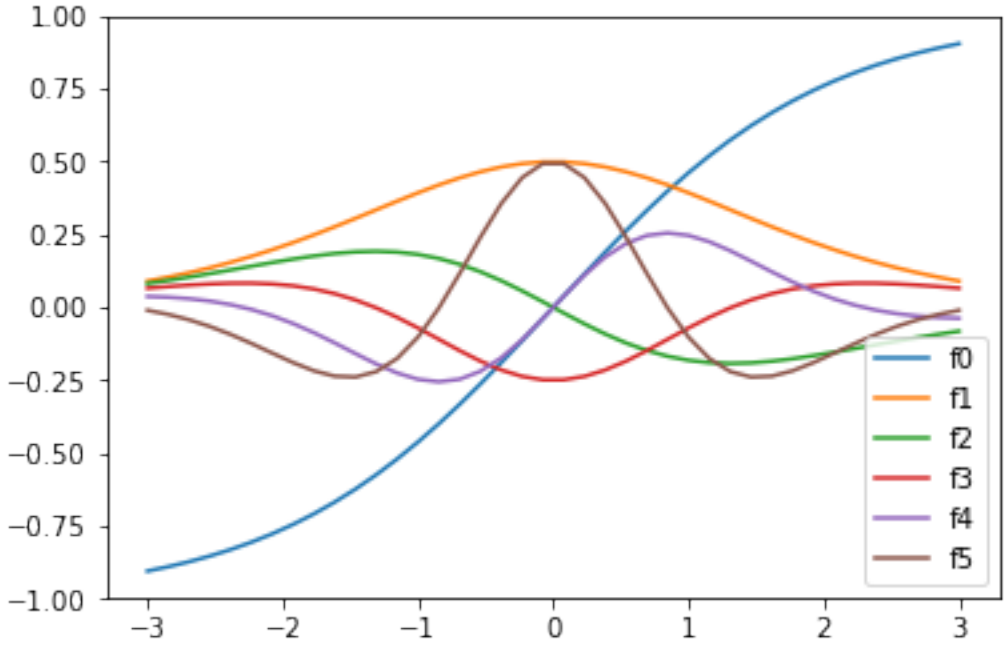
```
In [2]: # Define a Python function
        # Python has no "end" statement
        # It uses code indentation to determine the end of each block
        def f0(x):
            y = np.exp(-x)
            return (1.0 - y) / (1.0 + y)
```

```
In [3]: # grad(f0) returns the gradient of f0
        # f1 is not a symbolic expression!
        # It is just a normal numerical function,
        # but it returns the exact gradient thanks to the autodiff magic
        f1 = grad(f0)
        f2 = grad(f1)
        f3 = grad(f2)
        f4 = grad(f3)
        f5 = grad(f4)
```

```
In [4]: xx = np.linspace(-3, 3, 40) # for plot
```

```
In [5]: # plot all derivatives
        # as in cell[12] of the MATLAB section
        plt.plot(xx, f0(xx), label='f0')
        plt.plot(xx, f1(xx), label='f1')
        plt.plot(xx, f2(xx), label='f2')
        plt.plot(xx, f3(xx), label='f3')
        plt.plot(xx, f4(xx), label='f4')
```

```
plt.plot(xx, f5(xx), label='f5')
plt.legend();
```



The peak of the 5-th order derivative is the same as the result given by MATLAB symbolic tool box. There's no truncation error here.

```
In [6]: f5(xx).max() # the result is exact.
```

```
Out[6]: 0.49373558054667849
```

While being able to give the exact result, autodiff is much faster than the symbolic way!

Another code example: differentiating custom programs

Another advantage of autodiff is that it can differentiate arbitrary **programs**, not just **mathematical expressions**. Many complicated functions cannot be expressed by a combination of basic functions (e.g. the Bessel function in HW5), and in this case symbolic diff will have trouble.

However, the theory of autodiff is simply "carrying an additional number through your program", so as long as you can **code** the program, you can differentiate it. The dual number will just go through all `while` and `if` statements as usual.

Let's make a weird funcition.

```
In [7]: def custom_func(x):
            assert x > 0 # raise an error for negative x

            y = 0 # initial value

            # Again, Python has no "end" statement
            # It uses code indentation to determine the end of this while block
            while y+x < 10:
                y += x

            return y
```

This function initializes `y` as `0` and keeps accumulating the input `x` to `y`, until `y` reaches 10. In other words

- `y` is a multiple of `x`, i.e. `y=N*x`.
- `y` is smaller than but very close to `10`

For $x = 1$, $f(x) = 9x = 9$, because $10x$ will exceed 10.

```
In [8]: custom_func(1.0)
```

```
Out[8]: 9.0
```

For $x = 1.2$, $f(x) = 8x = 9.6$, because $9x = 10.8$ will exceed 10.

```
In [9]: custom_func(1.2)
```

```
Out[9]: 9.6
```

We can still take derivative of this weird function.

```
In [10]: custom_grad = grad(custom_func) # autodiff magic
```

For $x = 1$, $f(x) = 9x$, so $f'(x) = 9$

```
In [11]: print(custom_grad(1.0))
```

```
9.0
```

For $x = 1.2$, $f(x) = 8x$, so $f'(x) = 8$

```
In [12]: print(custom_grad(1.2))
```

```
8.0
```

Symbolic diff will have a big trouble with this kind of function.

2.12.4 So why use numerical differentiation?

If autodiff is so powerful, why do we need other methods? Well, you need symbolic diff for pure mathematical analysis. But how about numerical diff?

Well, the major application of numerical diff (forward difference, etc.) is not getting the derivative of a known function $f(x)$. It is for solving differential equations

$$f'(x) = \Phi(f, x)$$

In this case, $f(x)$ is not known (your goal is to find it), so symbol diff or autodiff can't help you. Numerical diff gives you a way to solve this ODE

$$\frac{f(x+h) - f(x)}{h} \approx f'(x) = \Phi(f, x)$$

2.13 Session 7: Error convergence of numerical methods

Date: 10/30/2017, Monday

```
In [1]: format compact
```

2.13.1 Error convergence of general numerical methods

Many numerical methods has a "step size" or "interval size" h, no mattter numerical differentiation, numerical intergration or ODE solving. We denote $f(h)$ as the numerical approximation to the exact answer f_{true}. Note that f can be a derivate, an integral or an ODE solution.

In general, the numerical error gets smaller when h is reduced. We say a method has $O(h^k)$ convergence if

$$f(h) - f_{true} = C \cdot h^k + C_1 \cdot h^{k+1} + ...$$

As $h \to 0$, we will have $f(h) \to f_{true}$. Higher-order methods (i.e. larger k) leads to faster convergence.

2.13.2 Error convergence of numerical differentiation

Consider $f(x) = e^x$, we use finite difference to approximate $g(x) = f'(x) = e^x$. We only consider $x = 1$ here.

```
In [2]: f = @(x) exp(x); % the function we want to differentiate
```

```
In [3]: x0 = 1; % only consider this point
        g_true = exp(x0) % analytical solution
```

```
g_true =
    2.7183
```

We try both forward and center schemes, with different step sizes h.

```
In [4]: h_list = 0.01:0.01:0.1; % test different step size h
        n = length(h_list);
        g_forward = zeros(1,n); % to hold forward difference results
        g_center = zeros(1,n); % to hold center difference results

        for i = 1:n % loop over different step sizes
            h = h_list(i); % get step size

            % forward difference
            g_forward(i) = (f(x0+h) - f(x0))/h;

            % center difference
            g_center(i) = (f(x0+h) - f(x0-h))/(2*h);
        end
```

The first element in `g_forward` is quite accurate, but the error grows as the step size h gets larger.

```
In [5]: g_forward
```

```
g_forward =
  Columns 1 through 7
    2.7319    2.7456    2.7595    2.7734    2.7874    2.8015    2.8157
  Columns 8 through 10
    2.8300    2.8444    2.8588
```

Center difference scheme is much more accurate.

```
In [6]: g_center
```

```
g_center =
  Columns 1 through 7
    2.7183    2.7185    2.7187    2.7190    2.7194    2.7199    2.7205
  Columns 8 through 10
    2.7212    2.7220    2.7228
```

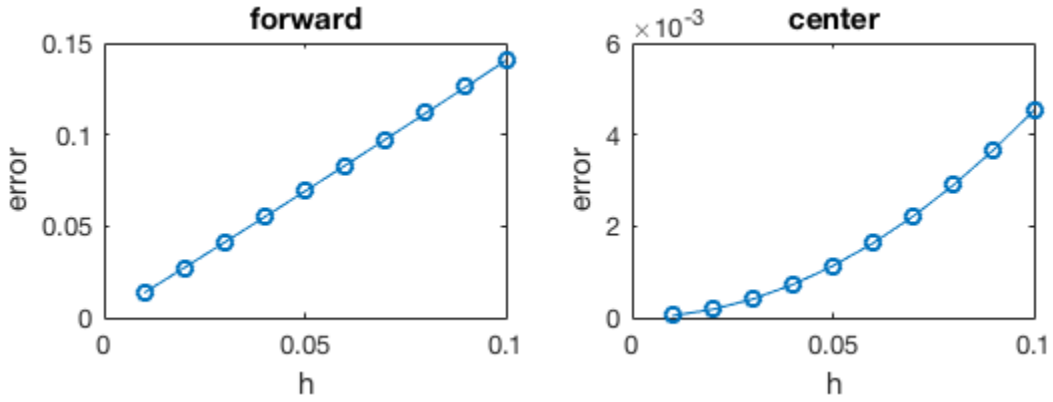
Compute the absolute error of each scheme

```
In [7]: error_forward = abs(g_forward - g_true)
        error_center = abs(g_center - g_true)
```

```
error_forward =
  Columns 1 through 7
    0.0136    0.0274    0.0412    0.0551    0.0691    0.0832    0.0974
  Columns 8 through 10
    0.1117    0.1261    0.1406
error_center =
  Columns 1 through 7
    0.0000    0.0002    0.0004    0.0007    0.0011    0.0016    0.0022
  Columns 8 through 10
    0.0029    0.0037    0.0045
```

Make a $h \leftrightarrow error$ plot.

```
In [8]: %plot -s 600,200
        subplot(121); plot(h_list, error_forward,'-o')
        title('forward');xlabel('h');ylabel('error')
        subplot(122); plot(h_list, error_center,'-o')
        title('center');xlabel('h');ylabel('error')
```



- Forward scheme gives a straight line because it is a first-order method and $error(h) \approx C \cdot h$
- Center scheme gives a parabola because it is a second-order method and $error(h) \approx C \cdot h^2$

2.13.3 Diagnosing the order of convergence

But by only looking at the $error(h)$ plot, how can you know the curve is a parabola? Can't it be a cubic $C \cdot h^3$?

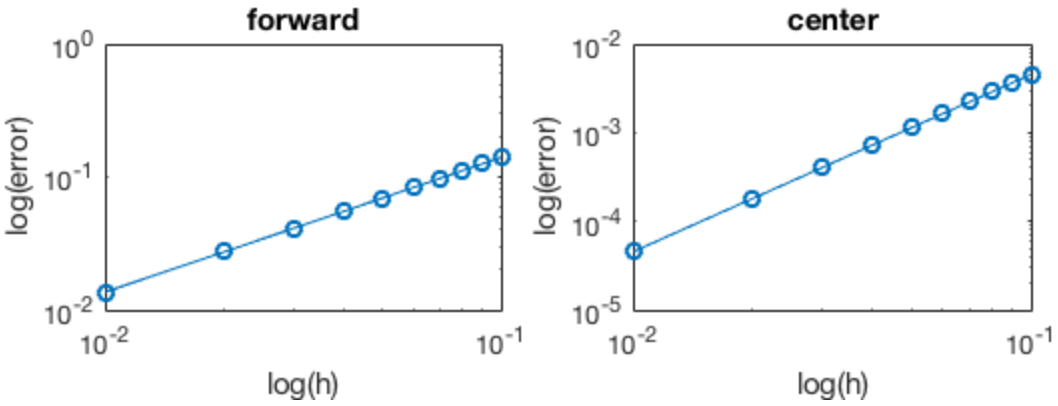
Recall that in HW4 you were fitting a function $R = bW^a$. To figure out the coefficients a and b, you need to take the log. The same thing here.

If $error = C \cdot h^k$, then

$$\log(error) = \log C + k \log h$$

The slope of the $log(error) \leftrightarrow log(h)$ plot is k, i.e. the order of the numerical method.

```
In [9]: %plot -s 600,200
        subplot(121); loglog(h_list, error_forward,'-o')
        title('forward');xlabel('log(h)');ylabel('log(error)')
        subplot(122); loglog(h_list, error_center,'-o')
        title('center');xlabel('log(h)');ylabel('log(error)')
```



To figure out the slope we can do linear regression. You can solve a least square problem as in HW4&5, but here we use a shortcut as described in this example. `polyfit(x, y, 1)` returns the slope and intercept.

```
In [10]: polyfit(log(h_list), log(error_forward), 1)


ans =
    1.0132    0.3662
In [11]: polyfit(log(h_list), log(error_center), 1)
ans =
    2.0002   -0.7909
```

The slopes are 1 and 2, respectively. So we've verified that forward-diff is 1st-order accurate while center-diff is 2nd-order accurate.

If the analytical solution is not known, you can use the most accurate solution (with the smallest h) as the true solution to figure out the slope. If your numerical scheme is converging to the true solution, then the estimate of order will still be OK. The risk is your numerical scheme might be converging to a wrong solution, and in this case it makes no sense to talk about error convergence.

2.13.4 h needs to be small

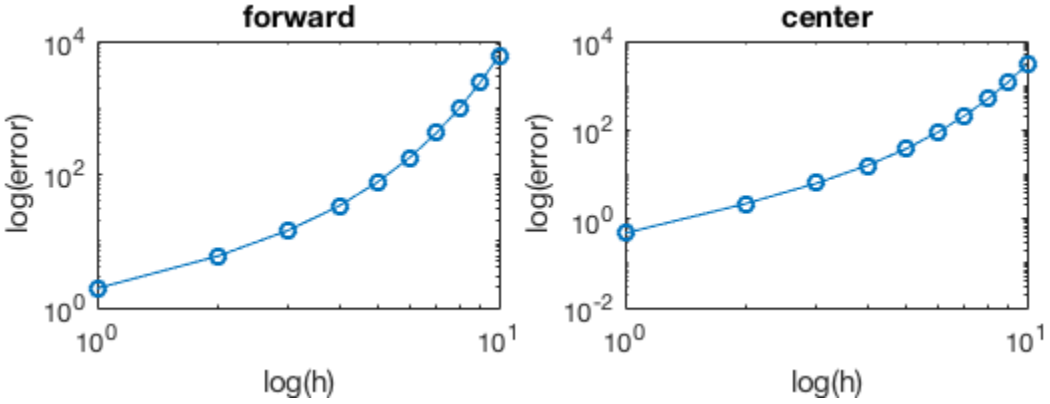
$error(h) \approx C \cdot h^k$ only holds for small h. When h is sufficiently small, we say that it is in the asymptotic regime. All the error analysis only holds in the asymptotic regime, and makes little sense when h is very large.

Let's make the step size 100 times larger and see what happens.

```
In [12]: h_list = 1:1:10; % h is 100x larger than before

         % -- the codes below are exactly the same as before --

         n = length(h_list);
         g_forward = zeros(1,n); % to hold forward difference results
         g_center = zeros(1,n); % to hold center difference results

         for i = 1:n % loop over different step sizes
             h = h_list(i); % get step size

             % forward difference
             g_forward(i) = (f(x0+h) - f(x0))/h;

             % center difference
             g_center(i) = (f(x0+h) - f(x0-h))/(2*h);
         end
```

```
error_forward = abs(g_forward - g_true);
error_center = abs(g_center - g_true);
```

```
In [13]: %plot -s 600,200
         subplot(121); loglog(h_list, error_forward,'-o')
         title('forward');xlabel('log(h)');ylabel('log(error)')
         subplot(122); loglog(h_list, error_center,'-o')
         title('center');xlabel('log(h)');ylabel('log(error)')
```



Now the error is super large and the log-log plot is not a straight line. So keep in mind that for most numerical schemes we always assume small h.

So how small is "small"? It depends on the scale of your problem and how rapidly $f(x)$ changes. If the problem is defined in $x \in [0, 0.001]$, then $h = 0.001$ is not small at all!

2.13.5 Error convergence of numerical intergration

Now consider

$$I = \int_0^1 f(x)$$

We still use $f(x) = e^x$ for convenience, as the integral of e^x is still e^x.

```
In [14]: f = @(x) exp(x); % the function we want to integrate
```

```
In [15]: I_true = exp(1)-exp(0)
```

```
I_true =
    1.7183
```

We use composite midpoint scheme to approximate I. We test different interval size h. Note that we need to first define the number of intervals m, and then get the corresponding h, because m has to be an integer.

```
In [16]: m_list = 10:10:100; % number of points
         h_list = 1./m_list; % interval size

         n = length(m_list);
         I_list = zeros(1,n); % to hold intergration results

         for i=1:n % loop over different interval sizes (or number of intevals)
             m = m_list(i);
             h = h_list(i);

             % get edge points
```

```
        x_edge = linspace(0, 1, m+1);

        % edge to middle
        x_mid = (x_edge(1:end-1) + x_edge(2:end))/2;

        % composite midpoint intergration scheme
        I_list(i) = h*sum(f(x_mid));
    end
```

The result is quite accurate.

```
In [17]: I_list
```

```
I_list =
  Columns 1 through 7
    1.7176    1.7181    1.7182    1.7182    1.7183    1.7183    1.7183
  Columns 8 through 10
    1.7183    1.7183    1.7183
```

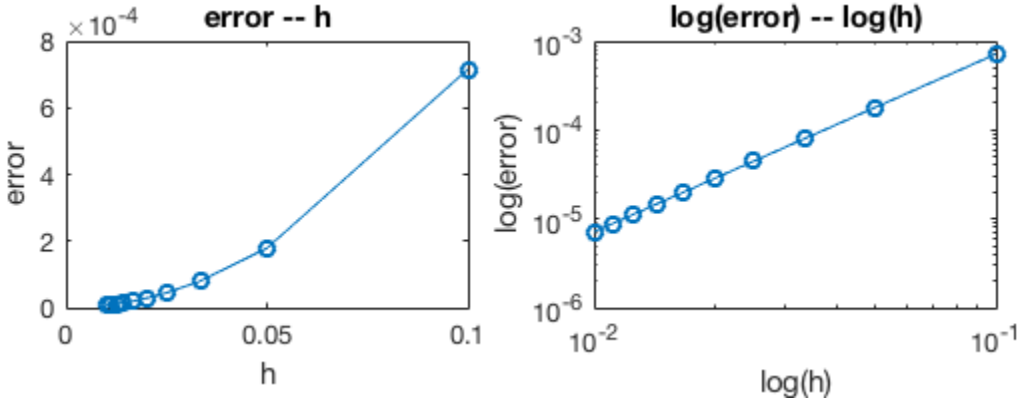
The error is at the order of 10^{-3}.

```
In [18]: error_I = abs(I_list-I_true)
```

```
error_I =
   1.0e-03 *
  Columns 1 through 7
    0.7157    0.1790    0.0795    0.0447    0.0286    0.0199    0.0146
  Columns 8 through 10
    0.0112    0.0088    0.0072
```

Again, a log-log plot will provide more insights about the order of convergence.

```
In [19]: %plot -s 600,200
         subplot(121);plot(h_list, error_I, '-o')
         title('error -- h');xlabel('h');ylabel('error')
         subplot(122);loglog(h_list, error_I, '-o')
         title('log(error) -- log(h)');xlabel('log(h)');ylabel('log(error)')
```



The slope is 2, so the method is second order accurate.

```
In [20]: polyfit(log(h_list), log(error_I), 1)
```

```
ans =
    1.9999   -2.6372
```

We've just applied the same error analysis method on both differentiation and integration. The same method also applies to ODE solving.

2.13.6 Error convergence of ODE solving

Consider a simple ODE

$$\frac{dy(t)}{dt} = y(t), \;\; y(0) = 1$$

The exact solution is $y(t) = e^t$. We use the forward Euler scheme to solve it.

$$\frac{y(t+h) - y(t)}{h} \approx y(t)$$

The iteration is given by

$$y(t+h) = y(t) + h \cdot y(t) = (1+h)y(t)$$

Let's only consider $t \in [0, 1]$. More specifically, we'll only look at the final state $y(1)$, so we don't need to record every step.

```
In [21]: y1_true = exp(1) % true y(1)
```

```
y1_true =
    2.7183
```

Same as in the integration section, we need to first define the number of total iterations m, and then get the corresponding step size h. This ensures we will land exactly at $t = 1$, not its neighbours.

```
In [22]: y0 = 1; % initial condition

         m_list = 10:10:100; % number of iterations to get to t=1
         h_list = 1./m_list; % step size

         n = length(m_list);
         y1_list = zeros(1,n); % to hold the final point

         for i=1:n % loop over different step sizes
             m = m_list(i); % get the number of iterations
             h = h_list(i); % get step size

             y1 = y0; % start with y(0)

             % Euler scheme begins here
             for t=1:m
                 y1 = (1+h)*y1; % no need to record intermediate results here
             end

             y1_list(i) = y1; % only record the final point

         end
```

As h shrinks, our simulated $y(1)$ gets closer to the true result.

```
In [23]: y1_list
```

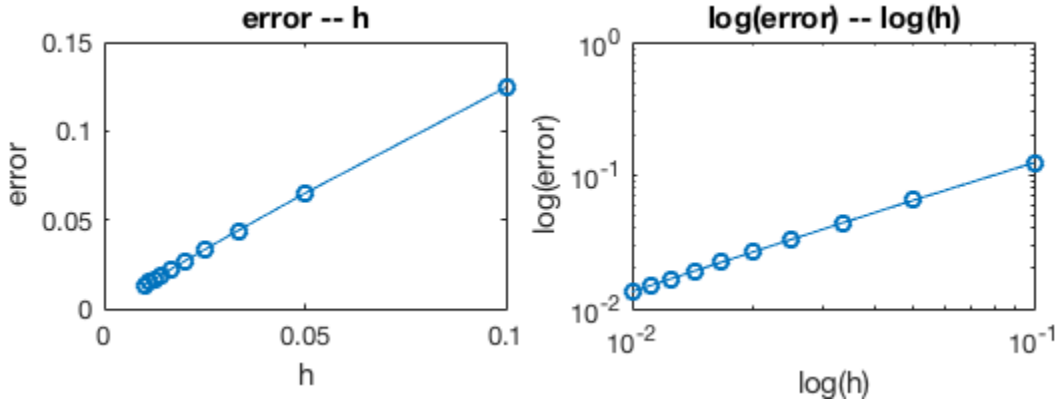
```
y1_list =
  Columns 1 through 7
    2.5937    2.6533    2.6743    2.6851    2.6916    2.6960    2.6991
  Columns 8 through 10
    2.7015    2.7033    2.7048
```

```
In [24]: error_y1 = abs(y1_list-y1_true)
```

```
error_y1 =
  Columns 1 through 7
    0.1245    0.0650    0.0440    0.0332    0.0267    0.0223    0.0192
  Columns 8 through 10
    0.0168    0.0149    0.0135
```

$error \leftrightarrow h$ plot is a straight line, so we know the method is fist order accurate. The log-log plot is not quite necessary here.

```
In [25]: %plot -s 600,200
         subplot(121);plot(h_list, error_y1, '-o')
         title('error -- h');xlabel('h');ylabel('error')
         subplot(122);loglog(h_list, error_y1, '-o')
         title('log(error) -- log(h)');xlabel('log(h)');ylabel('log(error)')
```



Of course we can still calculate the slope of the log-log plot, to double check the forward Euler scheme is a first-order method.

```
In [26]: polyfit(log(h_list), log(error_y1), 1)

ans =
    0.9687    0.1613
```

The take-away is, you can think about the order of a method in a more general sense. We've covered numerical differentiation, intergration and ODE here, and similar analysis also applies to root-finding, PDE, optimization, etc...

2.14 Session 8: ODE stability; stiff system

Date: 11/06/2017, Monday

```
In [1]: format compact
```

2.14.1 ODE Stability

Problem statement

Consider a simple ODE

$$\frac{dy}{dt} = -ay, \;\; y(0) = y_0$$

where a is a **positive** real number.

It can be solved analytically:

$$y(t) = y_0 e^{-at}$$

So the analytical solution decays exponentially. A numerical solution is allowed to have some error, but it should also be decaying. If the solution is instead growing, we say it is **unstable**.

Explicit scheme

Forward Eulerian scheme for this problem is

$$\frac{y_{k+1} - y_k}{h} = -ay_k$$

The iteration is given by

$$y_{k+1} = (1 - ha)y_k$$

The solution at the k-th time step can be written out explicitly

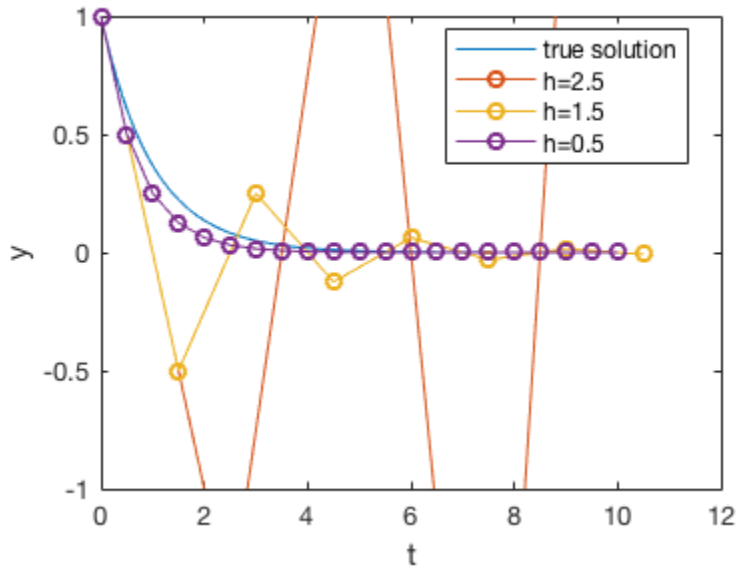
$$y_k = (1 - ha)^k y_0$$

We all know that when h gets smaller the numerical solution will converge to the true result. But here we are interested in relatively large h, i.e. we wonder **what's the largest possible h we can use while still getting an OK result**.

Here are the solutions with different h.

```
In [2]: %plot -s 400,300

        % set parameters, can use different value
        a = 1;
        y0 = 1;
        tspan = 10;

        % build function
        f_true = @(t) y0*exp(-a*t); % true answer
        f_forward = @(k,h) (1-h*a).^k * y0; % forward Euler solution

        % plot true result
        t_ar = linspace(0, tspan); % for plotting
        y_true = f_true(t_ar);
        plot(t_ar, y_true)
        hold on

        % plot Forward Euler solution
        for h=[2.5, 1.5, 0.5] % try different step size
            kmax = round(tspan/h);
            k_ar = 0:kmax;
            t_ar = k_ar*h;

            % we are not doing Forward Euler iteration here
            % since the expression is known, we can directly
            % get the entire time series
            y_forward = f_forward(k_ar, h);

            plot(t_ar, y_forward, '-o')
        end
```

```
% tweak details
ylim([-1,1]);
xlabel('t');ylabel('y');
legend('true solution', 'h=2.5', 'h=1.5', 'h=0.5' , 'Location', 'Best')
```



There all 3 typical regimes, determined by the magnitude of $[1 - ha]$ inside the expression $y_k = (1 - ha)^k y_0$.

1. **Small** h: $0 \leq [1 - ha] < 1$

In this case, $(1 - ha)^k$ will decay with k and always be positve.

We can solve for the range of h:

$$h \leq 1/a$$

This corresponds to h=0.5 in the above figure.

2. **Medium** h: $-1 \leq [1 - ha] < 0$

In this case, the absolute value of $(1 - ha)^k$ will decay with k, but it oscillates between negative and postive. This is not desirable, but not that bad, as our solution doesn't blow up.

We can solve for the range of h:

$$1/a < h \leq 2/a$$

This corresponds to h=1.5 in the above figure.

3. **Large** h: $[1 - ha] < -1$

In this case, the absolute value of $(1 - ha)^k$ will **increase** with k. That's the worst case because the true solution will be **decaying**, but our numerical solution insteads gives **exponential growth**. Here our numerical scheme is totally wrong, not just inaccurate.

We can solve for the range of h:

$$h > 2/a$$

This corresponds to h=2.5 in the above figure.

The take-away is, **to obtain a stable solution, the time step size** h **needs to be small enough. The time step requirement depends on** a, **i.e. how fast the system is changing.** If a is large, i.e. the system is changing rapidly, then h has to be small enough ($h < 1/a$ or $h < 2/a$, depends on what your want) to capture this fast change.

Implicit scheme

But sometimes we really want to use a large step size. For example, we might only care about the steady state where t is very large, so we would like to quickly jump to the steady state with very few number of iterations. Implicit method allows us to use a large time step while still keep the solution stable.

Backward Eulerian scheme for this problem is

$$\frac{y_{k+1} - y_k}{h} = -ay_{k+1}$$

In general, the right hand-side would be some function $f(y_{k+1})$, and we need to solve a nonlinear equation to obtain y_{k+1}. This is why this method is called **implicit**. But in this problem here we happen to have a linear function, so we can still write out the iteration explicitly.

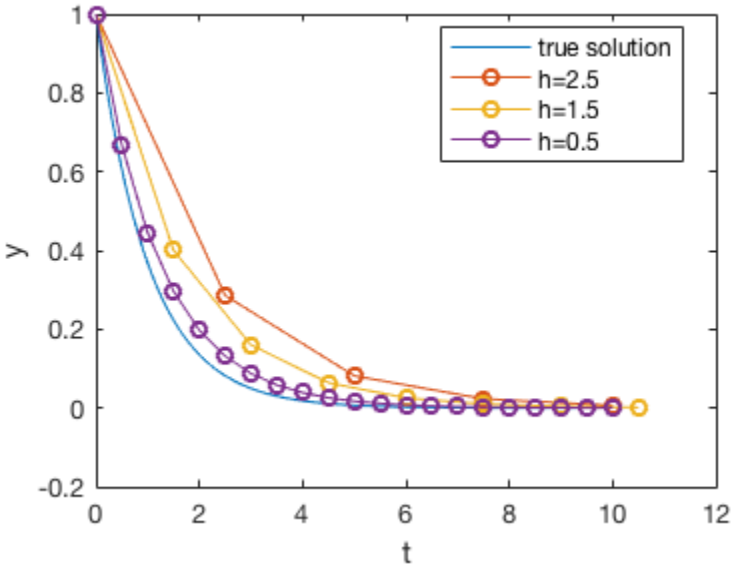
$$y_{k+1} = \frac{y_k}{1 + ha}$$

The solution at the k-th time step can be written as

$$y_k = \frac{y_0}{(1 + ha)^k}$$

Here are the solutions with different h.

In [3]:
```
%plot -s 400,300

% set parameters, can use different value
a = 1;
y0 = 1;
tspan = 10;

% build function
f_true = @(t) y0*exp(-a*t); % true answer
f_backward = @(k,h) (1+h*a).^(-k) * y0; % backward Euler solution

% plot true result
t_ar = linspace(0, tspan); % for plotting
y_true = f_true(t_ar);
plot(t_ar, y_true)
hold on

% plot Forward Euler solution
for h=[2.5, 1.5, 0.5] % try different step size
    kmax = round(tspan/h);
    k_ar = 0:kmax;
    t_ar = k_ar*h;

    % we are not doing Forward Euler iteration here
    % since the expression is known, we can directly
    % get the entire time series
    y_backward = f_backward(k_ar, h);

    plot(t_ar, y_backward, '-o')
end

% tweak details
ylim([-0.2,1]);
xlabel('t');ylabel('y');
legend('true solution', 'h=2.5', 'h=1.5', 'h=0.5' , 'Location', 'Best')
```



Since $\frac{1}{1+ha}$ is always smaller than 1 for any positive h and postive a, $y_k = \frac{y_k}{(1+ha)^k}$ will always decay. So we don't have the instability problem as in the explicit method. A large h simply gives **inaccurate** results, but not **terribly wrong** results.

According to no free lunch theorm, implicit methods must have some additional costs (half joking. that's another theorm). The cost for an implicit method is solving a nonlinear system. In general we will have $f(y,t)$ on the right-hand side of the ODE, not simply $-ay$.

General form

Using $-ay$ on the right-hand side allows a simple analysis, but the idea of ODE stability/instability applies to general ODEs. For example considering a system like

$$\frac{dy}{dt} = -f(t)y \tag{2.1}$$

You can use the typical magnitude of $f(t)$ as the "a" in the previous analysis.

Even for

$$\frac{dy}{dt} = -f(t)y^2 \tag{2.2}$$

You can consider the typical magnitude of $yf(t)$

2.14.2 Stiff system

Consider an ODE system

$$\frac{dy_1}{dt} = -a_1 y_1 \tag{2.3}$$

$$\frac{dy_2}{dt} = -a_2 y_2 \tag{2.4}$$

Using an explicit method, the time step requirement for the first equation is $h < 1/a_1$, while the requirement for the second one is $h < 1/a_2$. If $a_1 >> a_2$, we have to use a quite small h to accomodate the first requirement, but that's an overkill for the second equation. You will be using too many unnecessary time steps to solve y_2

We can define the **stiff ratio** $r = \frac{a_1}{a_2}$. A system is very stiff if r is very large. With explicit methods you often need an unnecessarily large amount of time steps to ensure stability. Implicit methods are particularly useful for a stiff system because it has no instability problem.

You might want to solve two equations separately so we can use a larger time step for the second equation to save computing power. But it's not that easy because in real examples the two equations are often intertwined:

$$\frac{dy_1}{dt} = -a_1 y_1 - a_3 y_2 \tag{2.5}$$

$$\frac{dy_2}{dt} = -a_2 y_2 - a_4 y_1 \tag{2.6}$$

2.15 Session 9: Partial differential equation

Date: 11/13/2017, Monday

```
In [1]: format compact
```

I assume you've learnt very little about PDEs in basic math class, so I would first talk about PDEs from a programmer's perpesctive and come to the math when necessary.

PDE from a programmer's view: You already know that ODE is the evolution of a single value. From the current alue y_t you can solve for the next value y_{t+1}. PDE is the evolution of an array. From the current array $(x_1, x_2, ..., x_m)_t$ you can solve for the array at the next time step $(x_1, x_2, ..., x_m)_{t+1}$. Typically, the array represents some physical field in the space, like 1D temperature distribution.

2.15.1 Naive advection "solver"

Consider a spatial domain $x \in [0, 1]$. We discretize it by 11 points including the boundary.

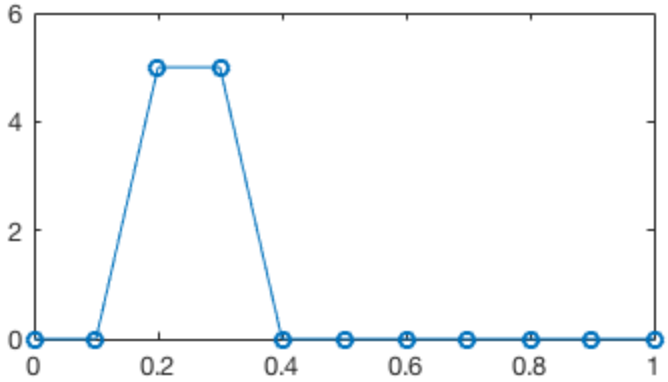
```
In [2]: x = linspace(0,1,11)
        nx = length(x)
```

```
x =
  Columns 1 through 7
         0    0.1000    0.2000    0.3000    0.4000    0.5000    0.6000
  Columns 8 through 11
    0.7000    0.8000    0.9000    1.0000
nx =
    11
```

The initial physical field (e.g. the concentration of some chemicals) is 5.0 for $x \in [0.2, 0.3]$ and zero elsewhere. Let's create the initial condition array.

```
In [3]: u0 = zeros(1,nx); % zero by default
        u0(3:4) = 5.0; % non-zero between 0.2~0.3
```

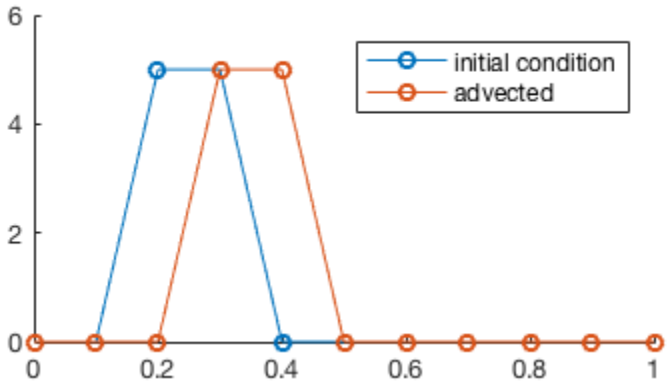
```
In [4]: %plot -s 400,200
        plot(x, u0, '-o')
        ylim([0,6]);
```



Say the chemical is blew by the wind towards the right. At the next time step the field is **shifted rightward by 1 grid point**.

To represent the solution at the next time step, we could create a new array `u_next` and set `u_next(4:5) = 5.0`, based on our knowledge that `u0(3:4) = 5.0`. However, we want to write code that works for any initiatial condition, so the code would look like:

```
In [5]: % initialization
        u = u0;
        u_next = zeros(1,nx); % initialize to 0

        % shift rightward
        u_next(2:end) = u(1:end-1);

        % just plotting
        hold on
        plot(x, u, '-o')
        plot(x, u_next, '-o')
        ylim([0,6]);
        legend('initial condition', 'advected')
```

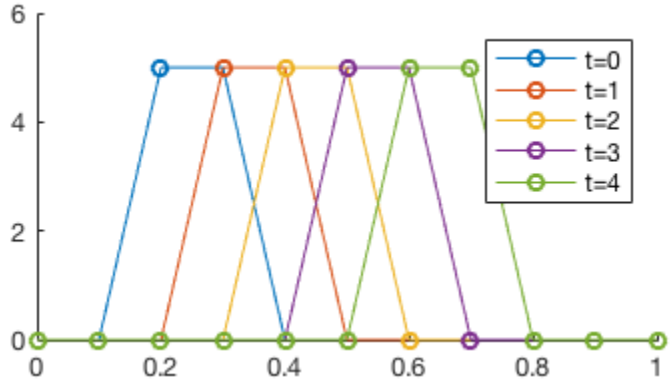


Space-time diagram

We can keep shifting the field and record the solution at 5 time steps.

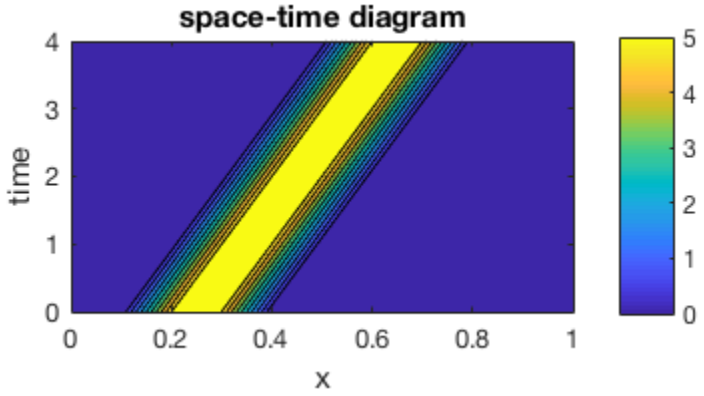
```
In [6]: u = u0; % reset solution
        u_next = zeros(1,nx); % reset solution
        u_ts = zeros(5,nx); % to record the entire time series

        u_ts(1,:) = u; % record initial condition
```

```
for t=2:5
    u_next(2:end) = u(1:end-1); % shift rightward
    u = u_next; % swap arrays for the next iteration
    u_ts(t,:) = u; % record current step
end

% just plotting
hold on
for t=1:5
    plot(x, u_ts(t, :), '-o')
end
ylim([0,6]);
legend('t=0', 't=1', 't=2', 't=3', 't=4')
```



The plot looks quite convoluted with multiple time steps... A better way to visualize it is to plot the time series in a **2D x-t plain**.

```
In [7]: contourf(x,0:4,u_ts)
        colorbar()
        xlabel('x');ylabel('time')
        title("space-time diagram")
```



Here we can clearly see the "chemical field" is moving rightward through time.

2.15.2 Advection equation

We call this rightward shift an **advection** process. Just like the **diffusion** process introduced in the class, advection happens everywhere in the physical world. In general, the physical field won't be shifted by exact one grid point.

Instead, we can have arbitrary wind speed, changing with space and time. To represent this general advection process, we can write a partial differential equation:

Advection equation with initial condition $u_0(x)$

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0, \;\; u(x,0) = u_0(x)$$

This means a phyical field $u(x,t)$ is advected by wind speed c. In general, the wind speed $c(x,t)$ can change with space and time. But if c is a constant, then the analytical solution is

$$u(x,t) = u_0(x - ct)$$

You can verify this solution by bringing it back to the PDE.

We ask, "**what's the chemical concentration at a spatial point** $x = x_j$, when $t = t_n$"? According to the solution, the answer is, "**it is the same as the concentration at** $x = x_j - ct_n$ when $t = 0$". This is physically intuitive. The chemical originally at $x = x_j - ct_n$ was traveling rightward at speed c, so after time period t_n it would reach $x = x_j$. Thus in order to find the concentration at $x = x_j$ right now, what we can do is going backward in time to find where does the current chemical come from.

This solution-finding process means going downward&leftward along the contour line in space-time diagram shown before.

Numerical approximation to advection equation

In practice, c is often not a constant, so we can't easily find an anlytical solution and must rely on numerical methods.

Use first-order finite difference approximation for both $\frac{\partial u}{\partial t}$ and $\frac{\partial u}{\partial x}$:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + c\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0$$

Let $\alpha = \frac{c\Delta t}{\Delta x}$, the iteration can be written as

$$u_j^{n+1} = u_j^n - \alpha(u_j^n - u_{j-1}^n) \tag{2.7}$$

$$= (1-\alpha)u_j^n + \alpha u_{j-1}^n \tag{2.8}$$

Note that, to approximate $\frac{\partial u}{\partial x}$, we use $\frac{u_j - u_{j-1}}{\Delta x}$ instead of $\frac{u_{j+1} - u_j}{\Delta x}$. There's an important physical reason for that. Here we assume c is positive (rightward wind), so the chemical should come from the leftside (u_{j-1}), not the rightside (u_{j+1}).

Finally, notice that when $\alpha = 1$ we effectively get the previous naive "shifting" scheme.

One step integration

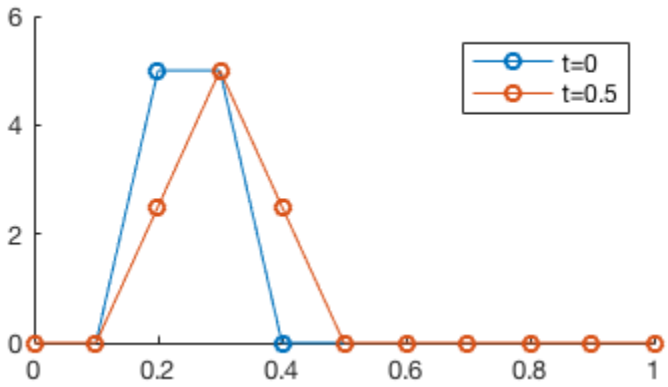
We set $c = 0.1$ and $\Delta t = 0.5$, so after one time step the chemical would be advected by half grid point (recall that our grid interval is 0.1).

Coding up the scheme is straightforward. The major difference from ODE solving is your are updating an array, not a single scalar.

```
In [8]: % set parameters
        c = 0.1; % wind velocity
        dx = x(2)-x(1)
        dt = 0.5;
        alpha = c*dt/dx
```

```
        % initialization
        u = u0;
        u_next = zeros(1,nx);

        % one-step PDE integration
        for j=2:nx
            u_next(j) = (1-alpha)*u(j) + alpha*u(j-1);
            % think about what to do for j=1?
            % we will talk about boundaries later
        end

        % plotting
        hold on
        plot(x, u, '-o')
        plot(x, u_next, '-o')
        ylim([0,6]);
        legend('t=0', 't=0.5')
```

```
dx =
    0.1000
alpha =
    0.5000
```

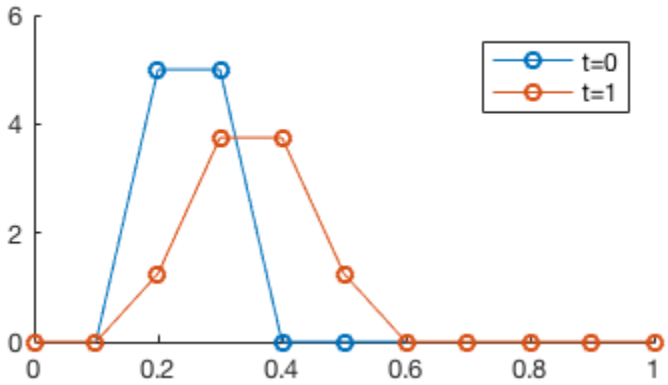


Multiple steps

To integrate for multiple steps, we just add another loop for time.

```
In [9]: % re-initialize
        u = u0;
        u_next = zeros(1,nx);

        % PDE integration for 2 time steps
        for t = 1:2 % loop for time
            for j=2:nx % loop for space
                u_next(j) = (1-alpha)*u(j) + alpha*u(j-1);
            end
            u = u_next;
        end

        % plotting
        hold on
        plot(x, u0, '-o')
        plot(x, u, '-o')
        ylim([0,6]);
```

```
legend('t=0', 't=1')
```



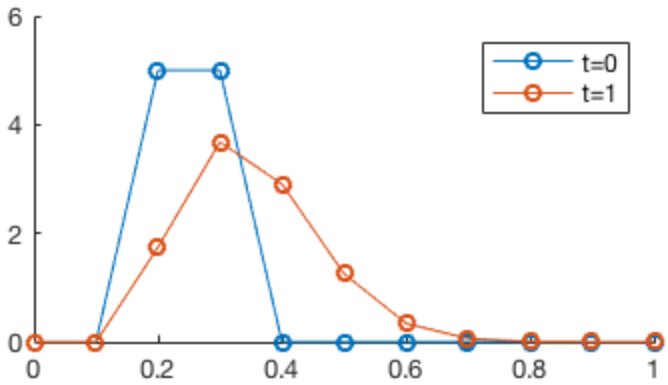
We got a pretty huge error here. After $t = 0.5 \times 2 = 1$, the solution should just be shifted by one grid point, like in the previous naive PDE "solver". Here the center of the chemical field seems alright (changed from 0.25 to 0.35), but the chemical gets diffused pretty badly. That's due to the numerical error of the first-order scheme.

Does decreasing time step size help?

In ODE solving, we can always reduce time step size to improve accuracy. Does the same trick help here?

```
In [10]: c = 0.1;
         dx = x(2)-x(1);
         dt = 0.1; % use a much smaller time step
         nt = round(1/dt) % calculate the number of time steps needed
         alpha = c*dt/dx


         % === exactly the same as before ===
         u = u0;
         u_next = zeros(1,nx);

         for t = 1:nt
             for j=2:nx
                 u_next(j) = (1-alpha)*u(j) + alpha*u(j-1);
             end
             u = u_next;
         end

         hold on
         plot(x, u0, '-o')
         plot(x, u, '-o')
         ylim([0,6]);
         legend('t=0', 't=1')
```

```
nt =
    10
alpha =
    0.1000
```



Oops, there is no improvement.

That's because we have both **time discretization error** $O(\Delta t)$ **spatial discretization error** $O(\Delta x)$ in PDE solving. The total error for our scheme is $O(\Delta t) + O(\Delta x)$. Simply decreasing the time step size is not enough. To improve accuracy you also need to increase the number of spatial grid points (`nx`).

Another way to improve accuracy is to use high-order scheme. But designing high-order advection scheme is quite challenging. You can find tons of papers by searching something like "high-order advection scheme".

2.15.3 Boundary condition

So far we've ignored the boundary condition. Because the field is shifting rightward, the leftmost grid point is able to receive information from the "outside". Think about a pipe where new chemicals keep coming in from the left.

Our previous specification of the advection equation is not complete. The complete version is:

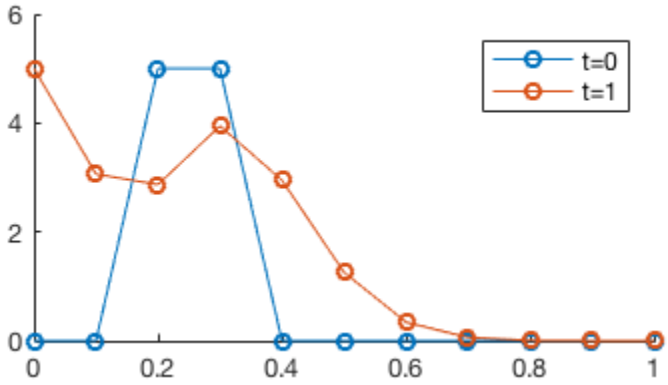
Advection equation with initial condition $u_0(x)$ **and left boundary condition** $u_{left}(t)$

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$$
$$u(x,0) = u_0(x)$$
$$u(0,t) = u_{left}(t)$$

Here we assume $u_{left}(t) = 5$. In the code, you just need to add one line.

```
In [11]: c = 0.1;
         dx = x(2)-x(1);
         dt = 0.1;
         nt = round(1/dt);
         alpha = c*dt/dx;

         u = u0;
         u_next = zeros(1,nx);

         for t = 1:nt

             u_next(1) = 5.0; % the only change!!
             for j=2:nx
                 u_next(j) = (1-alpha)*u(j) + alpha*u(j-1);
             end
             u = u_next;
         end

         hold on
```

```
plot(x, u0, '-o')
plot(x, u, '-o')
ylim([0,6]);
legend('t=0', 't=1')
```



We can now see new chemicals are "injected" from the left side.

2.15.4 Stability

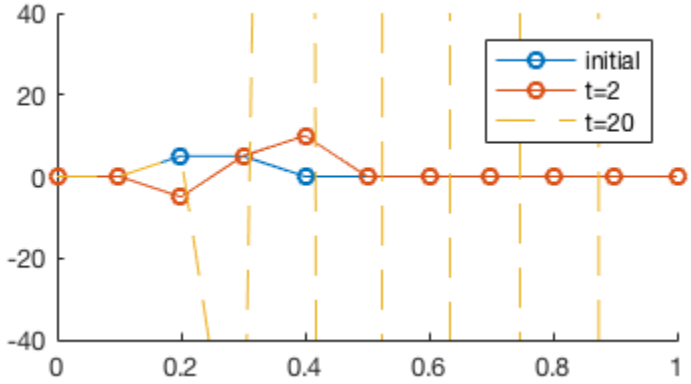
Numerical experiment

PDE solvers also have stability requirements, just like ODE solvers. The general idea is the **time step needs to be small enough, compared to the spatial step**. This holds for advection, diffusion, wave and various forms of PDEs, although the exact formula for time step requirement can be different depending on the problem.

Here we use a much larger time step to see what happens.

```
In [12]: c = 0.1;
         dx = x(2)-x(1);
         dt = 2; % a much larger time step
         alpha = c*dt/dx

         u = u0;
         u_next = zeros(1,nx);

         for t = 1:10
             for j=2:nx
                 u_next(j) = (1-alpha)*u(j) + alpha*u(j-1);
             end
             u = u_next;

             if t == 1 % record the first time step
                 u1 = u;
             end
         end

         hold on
         plot(x, u0, '-o')
         plot(x, u1, '-o')
         plot(x, u, '--')
         ylim([-40,40]);
         legend('initial', 't=2', 't=20')
```

```
alpha =
     2
```



The simulation blows very quickly.

Intuitive explanation

In the previous experiment we have $\alpha = 2$, so one of the coeffcients in the formula becomes negative:

$$u_j^{n+1} = (1-\alpha)u_j^n + \alpha u_{j-1}^n = (-1) \times u_j^n + 2 \times u_{j-1}^n$$

Negative coefficients are meaningless here, because a grid point x_j shouldn't get "negative contribution" from a nearby grid point x_{j-1}. It makes no sense to advect "negative density" or "negative concentration".

To keep both coefficients (α and $1-\alpha$) postive, we require $0 \leq \alpha \leq 1$. Recall $\alpha = \frac{c\Delta t}{\Delta x}$, so we essentially require the time step to be small.

This is just an intuitive explanation. To rigorously derive the stability requirement, you would need some heavy math as shown below.

Stability analysis (theoretical)

The time step requirement can be derived by von Neumann Stability Analysis (also see *PDE_solving.pdf* on canvas).

The idea is we want to know how does the magnitude of u_j^n change with time, under the iteration (first-order advection scheme for example):

$$u_j^{n+1} = (1-\alpha)u_j^n + \alpha u_{j-1}^n$$

It is troublesome to track the entire array $[u_1^n, u_2^n, ..., u_m^n]$. Instead we want a single value to represent the magnitude of the array. The general idea is to perform Fourier expansion on the spatial field $u(x)$. From Fourier analysis we know any 1D field can viewed as the sum of waves of different wavelength:

$$u(x) = \sum_{k=-\infty}^{\infty} T_k e^{ikx}$$

Thus we can track how a single component, $T_k e^{ikx}$, evolves with time. We omit the subscript k and add the time index n, so the component at the n-th time step can be written as $T(n)e^{ikx}$. The iteration for this component is

$$T(n+1)e^{ikx} = (1-\alpha)T(n)e^{ikx} + \alpha T(n)e^{ik(x-\Delta x)}$$

Divide both sides by e^{ikx}

$$T(n+1) = (1-\alpha)T(n) + \alpha T(n)e^{-ik\Delta x}$$

$$\frac{T(n+1)}{T(n)} = 1 - \alpha + \alpha e^{-ik\Delta x}$$

Define **amplification factor** $A = \frac{T(n+1)}{T(n)}$. We want $|A| \leq 1$ so the solution won't blow up, just like what we did in the ODE stability analysis.

We thus require

$$|1 - \alpha + \alpha e^{-ik\Delta x}| \leq 1$$

So we've transformed the requirement on an array to the requirement on a scalar.

We want this inequality to be true for any k. It will finally lead to a requirement for α, which is the same as the previous intuitive analysis that $0 \leq \alpha \leq 1$. Fully working this out needs some math, see this post for example.

2.15.5 High-order PDE

The wave equation is a typical 2nd-order PDE

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0$$

Compared to the advection equation, the major differences are

- The wave can go both rightward and leftward, at speed c or $-c$.
- It needs both left and right boundary condition. Periodic boundary conditions are often used.
- It needs both 0th-order and 1st-order initial conditions, i.e. $u(x,t)|_{t=0}$ and $\frac{\partial u}{\partial t}|_{t=0}$. Otherwise you can't start your intergration, because a 2nd-order time derivative means u^{n+1} would rely on both u^n and u^{n-1}. 0th-order initial condition only gives you one time step, but you need two time steps to get started.

2.16 Session 10: Fast Fourier Transform

Date: 11/27/2017, Monday

```
In [1]: format compact
```

2.16.1 Generate input signal

Fourier transform is widely used in signal processing. Let's looks at the simplest cosine signal first.

Define

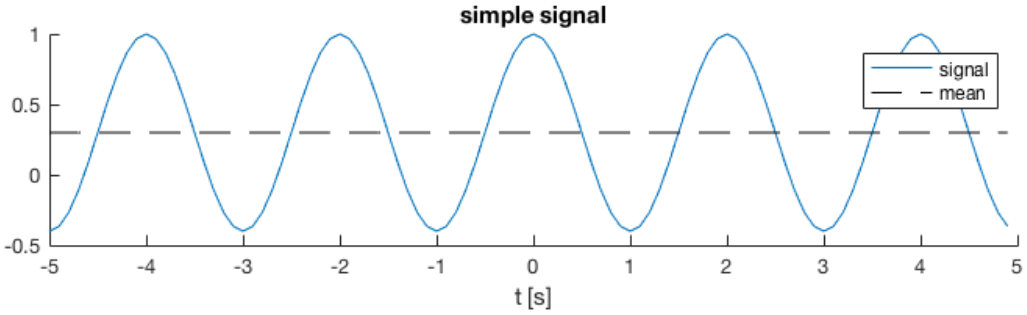
$$y_1(t) = 0.3 + 0.7\cos(2\pi f_1 t)$$

It has a magnitude of 0.7, with a constant bias term 0.3. We choose the frequency $f_1 = 0.5$.

```
In [2]: t = -5:0.1:4.9; % time axis
        N = length(t) % size of the signal

        f1 = 0.5; % signal frequency
        y1 = 0.3 + 0.7*cos(2*pi*f1*t); % the signal
```

```
N =
   100
```

```
In [3]: %plot -s 800,200
        hold on
        plot(t, y1)
        plot(t, 0.3*ones(N,1), '--k')
        title('simple signal')
        xlabel('t [s]')
        legend('signal', 'mean')
```



2.16.2 Perform Fourier transform on the signal

You can hand code the Fourier matrix as in the class, but here we use the built-in function for convenience.

```
In [4]: F1 = fft(y1);
        length(F1) % same as the length of the signal
```

```
ans =
   100
```

There are two different conventions for the normalization factor in the Fourier matrix. One is having the normalization factor $\frac{1}{\sqrt{N}}$ in the both the Fourier matrix A and the inverse transform matrix B

$$A = \frac{1}{\sqrt{N}} \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \cdots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \cdots & \omega^{2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \cdots & \omega^{(N-1)(N-1)} \end{bmatrix}$$

$$B = \frac{1}{\sqrt{N}} \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega^{-1} & \omega^{-2} & \cdots & \omega^{-(N-1)} \\ 1 & \omega^{-2} & \omega^{-4} & \cdots & \omega^{-2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{-(N-1)} & \omega^{-2(N-1)} & \cdots & \omega^{-(N-1)(N-1)} \end{bmatrix}$$

MATLAB uses a different convention that

$$A = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \cdots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \cdots & \omega^{2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \cdots & \omega^{(N-1)(N-1)} \end{bmatrix}$$

$$B = \frac{1}{N}\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega^{-1} & \omega^{-2} & \cdots & \omega^{-(N-1)} \\ 1 & \omega^{-2} & \omega^{-4} & \cdots & \omega^{-2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{-(N-1)} & \omega^{-2(N-1)} & \cdots & \omega^{-(N-1)(N-1)} \end{bmatrix}$$

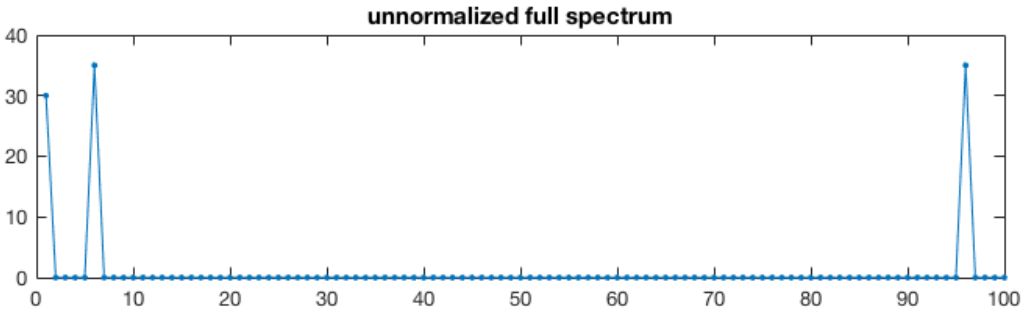
The difference doesn't matter too much as long as you use one of them consistently. In both cases there is

$$F = AY \text{ (Discrete Fourier transfrom)} \tag{2.9}$$
$$Y = BF \text{ (Inverse transfrom)} \tag{2.10}$$

Full spectrum

The spectrum `F1` (the result of the Fourier transfrom) is typically an array of complex numbers. To plot it we need to use absolute magnitude.

```
In [5]: %plot -s 800,200
        plot(abs(F1),'- .')
        title('unnormalized full spectrum')
```



The first term in `F1` indicates the magnitude of the constant term (zero frequency). Diving by `N` gives us the actual value.

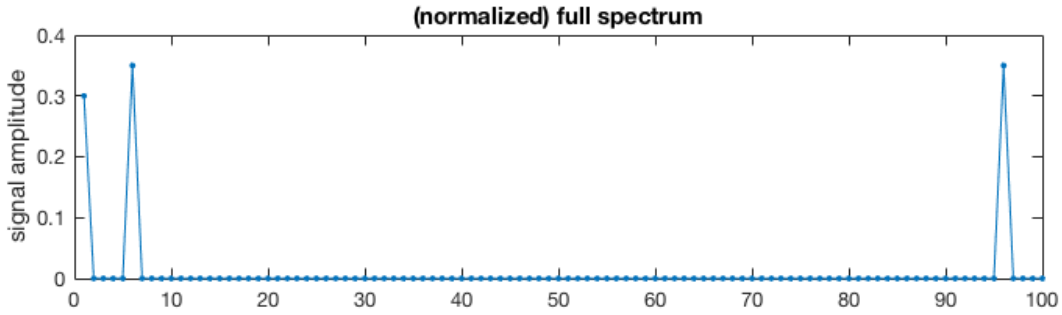
```
In [6]: F1(1)/N % equal to the constant bias term specified at the beginning

ans =
    0.3000
```

Besides the constant bias `F1(1)`, there are two non-zero pointings in `F1`, indicating the cosine signal itself. The magnitude 0.7 is evenly distributed to two points.

```
In [7]: F1(2+4)/N, F1(end-4)/N % adding up to 0.7

ans =
  -0.3500 - 0.0000i
ans =
  -0.3500 + 0.0000i
```

Plotting `F1/N` shows more clearly the magnitude of signals at different frequencies:

```
In [8]: %plot -s 800,200
        plot(abs(F1)/N,'- .')
        title('(normalized) full spectrum')
        ylabel('signal amplitude')
```



Half-sided spectrum

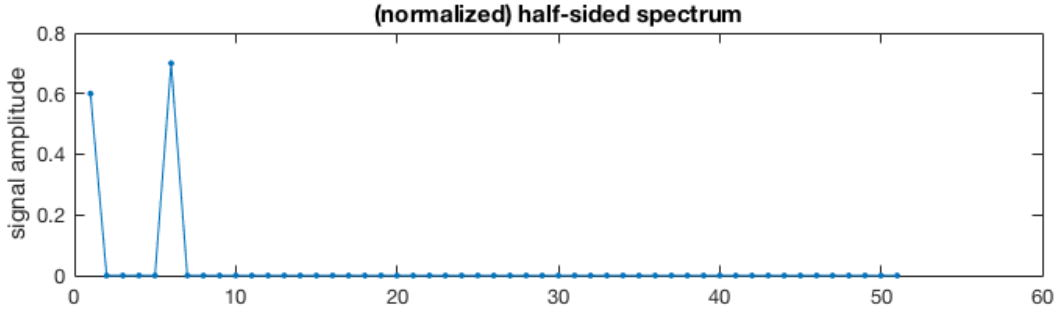
From the matrix A it is easy to show that, the first element `F(1)` in the resulting spectrum is always a real number indicating the constant bias term, while the rest of the array `F(2:end)` is symmetric, i.e. `F(2) == F(end)`, `F(3) == F(end-1)`. (`F(2)` is actually the conjugate of `F(end)`, but we only care about magnitude here.)

Due to such symmetricity, we can simply plot half of the array (scaled by 2) without loss of information.

```
In [9]: M = N/2 % need to cast to integer if N is an odd number
```

```
M =
    50
```

```
In [10]: %plot -s 800,200
         plot(abs(F1(1:M+1))/N*2, '- .')
         title('(normalized) half-sided spectrum')
         ylabel('signal amplitude')
```



2.16.3 Understanding units!

The Discrete Fourier Transform, by defintion, is simply a matrix multiplication which acts on pure numbers. But real physical signals have units. You cannot just treat the resulting array `F1` as some unitless frequency. If the signal is a time series then you need to deal with seconds and hertz; if it is a wave in the space then you need to deal with the wave length in meters.

In order to understand the unit of the resulting spectrum `F1`, let's look at the original time series `y1` first.

The "time step" of the signal is

```
In [11]: dt = t(2)-t(1) % [s]
```

```
dt =
    0.1000
```

This is the finest temporal resolution the signal can have. It corresponds the highest frequency:

```
In [12]: f_max = 1/dt % [Hz]
```

```
f_max =
   10.0000
```

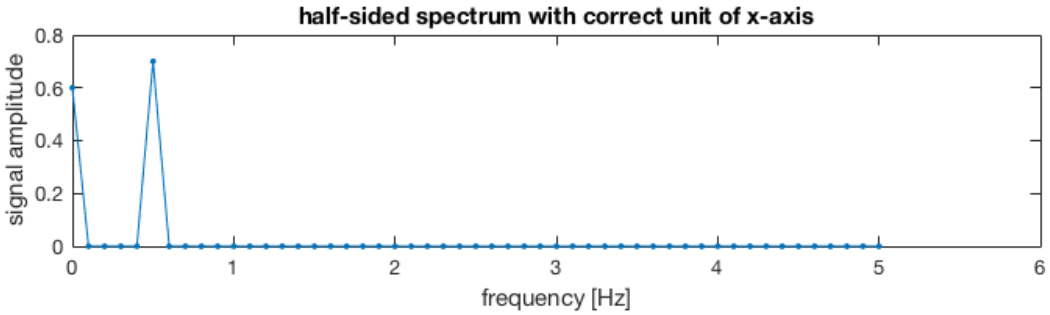
On the contrary, the longest time range (`dt*N`, the time span of the entire signal) corresponds to the lowest frequency:

```
In [13]: df = f_max/N % [Hz]
```

```
df =
    0.1000
```

With the lowest frequency `df` being the "step size" in the frequency axis, the value of the frequency axis is simply the array [0, df, 2*df, ...]. Now we can use correct values and units for the x-axis of the spectrum plot.

```
In [14]: %plot -s 800,200
         plot(df*(0:M), abs(F1(1:M+1))/N*2,'- .')
         title('half-sided spectrum with correct unit of x-axis')
         ylabel('signal amplitude')
         xlabel('frequency [Hz]')
```



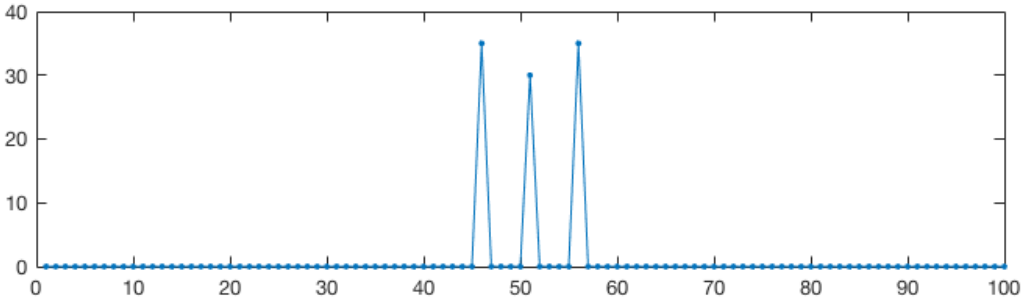
The peak is at 0.5 Hz, consistent with our original signal which has a period of 2 s, since 0.5 Hz = 1/(2s). Thus our unit specification is correct.

2.16.4 Deal with negative frequency

The right half of the spectrum array (`F1(M+2:end)`, not plotted in the above figure) corresponds to negative frequency [-M*df, ..., -2*df, -df]. Thus each element in the entire `F1` array corresponds to each element in the frequency array [0, df, 2*df, ..., M*df, -M*df, ..., -2*df, -df].

You can perform `fftshift` on the resulting spectrum `F1` to swap its left and right parts, so it will align with the motonically increasing axis [-M*df, ..., -2*df, -df, 0, df, 2*df, ..., M*df]. That feels more natural from a mathematical point of view.

```
In [15]: F_shifted = fftshift(F1);
         plot(abs(F_shifted),'- .')
```



2.16.5 Perform inverse transform

Performing inverse transform is simply `ifft(F1)`. Recall that MATLAB performs the $\frac{1}{N}$ scaling during the inverse transform step.

We use `norm` to check if `ifft(F1)` is close enough to `y1`.

```
In [16]: norm(ifft(F1) - y1) % almost zero
```

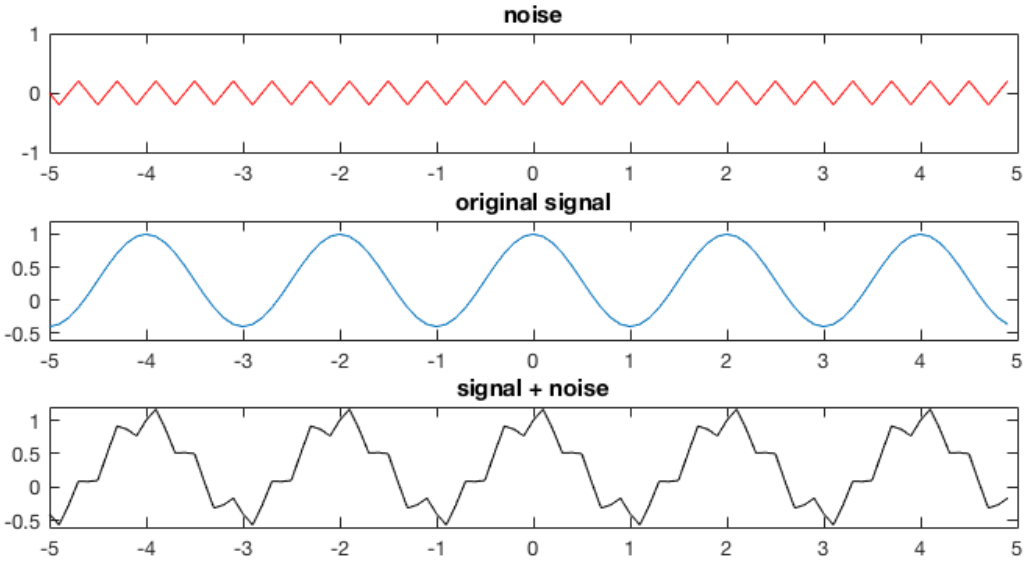
```
ans =
   1.2269e-15
```

2.16.6 Mix two signals

Fourier transform and inverse transform are very useful in signal filering. Let's first add a high-frequency noise to our original signal.

```
In [17]: f2 = 5; % higher frequency
         y2 = 0.2*sin(f2*pi*t); % noise
         y = y1 + y2; % add up original signal and noise
```

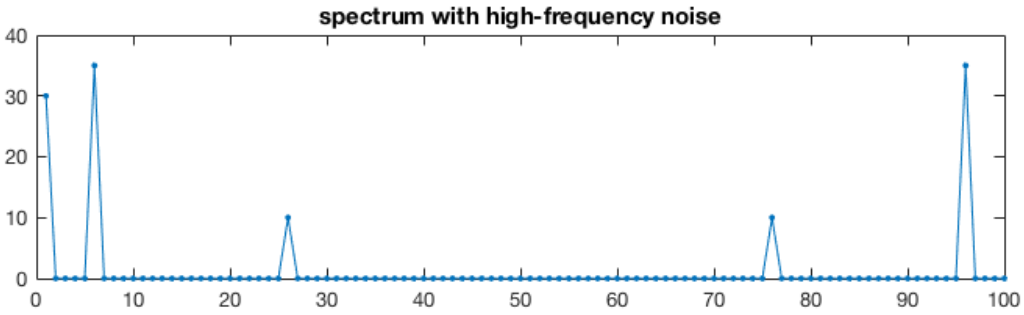
```
In [18]: %plot -s 800,400
         subplot(311);plot(t, y2, 'r');
         ylim([-1,1]);title('noise')

         subplot(312);plot(t, y1);
         ylim([-0.6,1.2]);title('original signal')

         subplot(313);plot(t, y, 'k');
         ylim([-0.6,1.2]);title('signal + noise')
```



After the Fourier transform, we see two new peaks at a relatively higher frequency.

```
In [19]: F = fft(y);
```

```
In [20]: %plot -s 800,200
         plot(abs(F), '- .')
         title('spectrum with high-frequency noise')
```



Again, the noise magnitude 0.2 is evenly distributed to positive and negative frequencies. Here we got complex conjugates:

```
In [21]: F(2+24)/N, F(end-24)/N % magnitude of noises
```

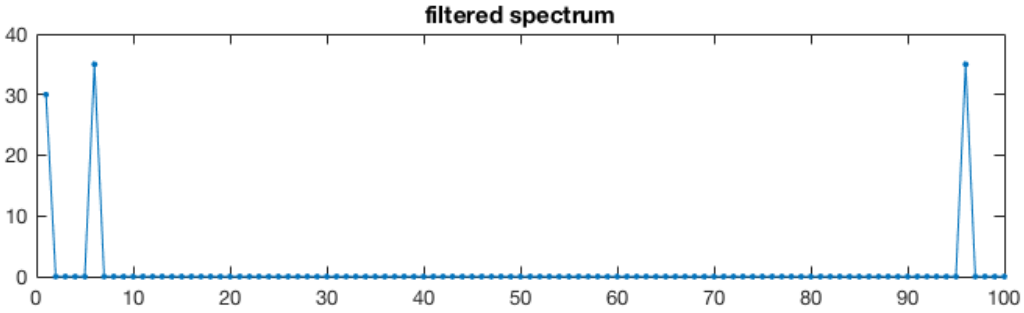
```
ans =
  -0.0000 + 0.1000i
ans =
  -0.0000 - 0.1000i
```

2.16.7 Filter out high-frequency noise

Let's wipe out this annoying noise. It's very difficult to do so in the original signal, but very easy to do in the spectrum.

```
In [22]: F_filtered = F; % make a copy
         F_filtered(26) = 0; % remove the high-frequency noise
         F_filtered(76) = 0; % same for negative frequency
```

```
In [23]: plot(abs(F_filtered), '- .')
         title('filtered spectrum')
```

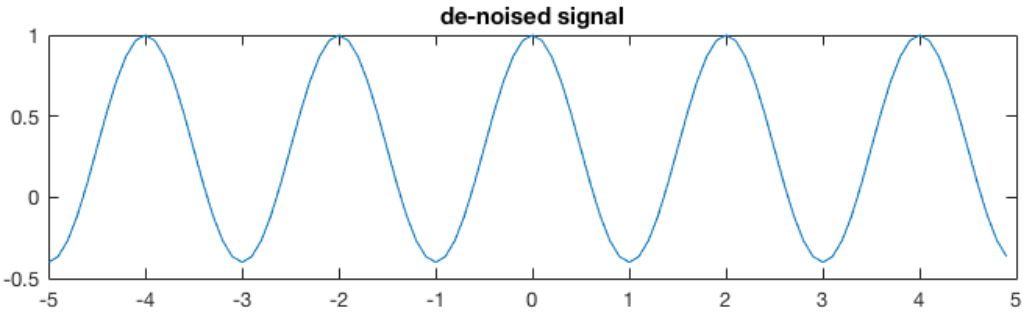


Then we can transform the spectrum back to the signal.

```
In [24]: y_filtered = ifft(F_filtered);
```

If the filtering is done symmetrically (i.e. do the same thing for positive and negative frequencies), the recovered signal will only contain real numbers.

```
In [35]: %plot -s 800,200
         plot(t, y_filtered)
         title('de-noised signal')
```



The de-noised signal is almost the same as the original noise-free signal:

```
In [36]: norm(y_filtered - y1) % almost zero
```

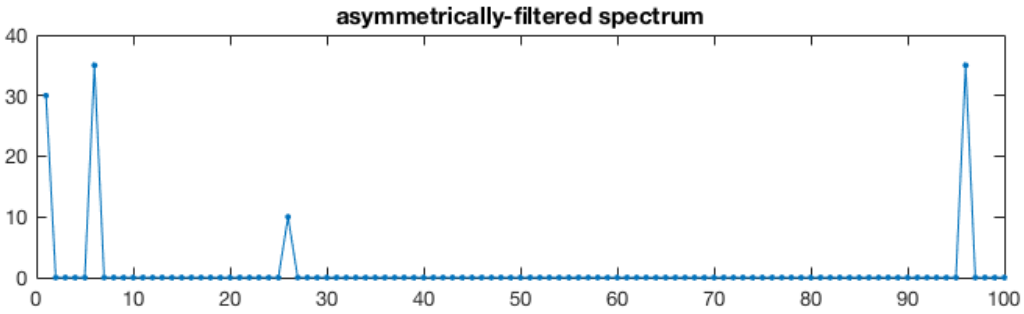
```
ans =
   5.6847e-15
```

2.16.8 Filter has to be symmetric

What happens if the filtering done asymmetrically?

```
In [37]: F_wrong_filtered = F; % make another copy
         F_wrong_filtered(76) = 0; % only do negative frequency
```

```
In [39]: plot(abs(F_wrong_filtered), '- .')
         title('asymmetrically-filtered spectrum')
```



The recovered signal now contains imaginary parts. That's unphysical!

```
In [40]: y_wrong_filtered = ifft(F_wrong_filtered);
```

```
In [42]: y_wrong_filtered(1:5)' % print the first several elements
```

```
ans =
  -0.4000 - 0.1000i
  -0.4657 + 0.0000i
  -0.2663 + 0.1000i
  -0.0114 - 0.0000i
   0.0837 - 0.1000i
```

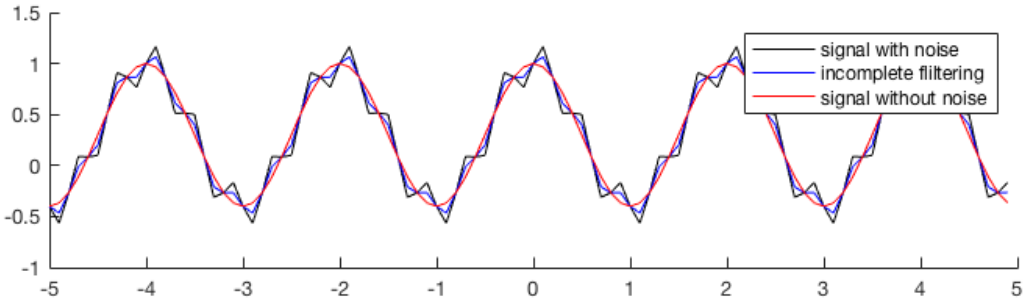
```
In [43]: norm(imag(y_wrong_filtered)) % not zero
```

```
ans =
    0.7071
```

You can plot the real part only. It is something between the unfiltered and filtered signals, i.e. the filtering here is incomplete.

```
In [45]: hold on
         plot(t, y, 'k')
```

```
plot(t, real(y_wrong_filtered), 'b')
plot(t, y1, 'r')
legend('signal with noise', 'incomplete fliltering', 'signal without noise')
```



These notes combine codes and results together. You can just copy the codes to your MATLAB console or script.

If you wonder how I wrote codes in this format and want to try it yourself, see the section below.

CHAPTER 3

MATLAB in Jupyter Notebooks

This course is taught in MATLAB. One thing you could try is to run MATLAB codes in Jupyter Notebooks. Jupyter Notebook is a must-learn tool for data scientists, and it is also becoming popular in the traditional scientific computing community. It is a great tool for interactive computing and allows you to combine codes, simulation results, and descriptions such as latex equations in a single file.

See how to install and use it at:

3.1 Install Jupyter-MATLAB

Prerequisites

- We assume that you are comfortable with Linux command line. If not, checkout out Ryans' tutorial for example.
- We also assume that you already have MATLAB installed and working. This tutorial is tested successfully with MATLAB R2017a on Mac/Linux/Windows.

3.1.1 Install the standard Jupyter-Python notebook

Jupyter relies on Python, so the first thing is to install Anaconda, a popular distribution of scientific Python. Experienced users prefer Miniconda to only install necessary packages, but the standard Anaconda is more convenient for beginners, especially on Windows.

Once you have conda installed, you should test the standard IPython notebook. For example, in the notebook execute

```
In [1]: %%python
        # I am in a MATLAB kernel so need to add the above IPython magic to use the python kernel ins
        # You can skip this magic in a standard python kernel
        print('hello from Python')
```

```
hello from Python
```

3.1.2 On Mac/Linux

(1) Python-side configuration

Open the terminal, execute the following command to check your installation of anaconda and python:

```
which conda pip python
```

All of them should be inside anaconda's directory "…/anaconda3/bin"

MATLAB R2017a only interfaces with Python3.5, so we need to create a new virtual environment:

```
conda create -vv -n jmatlab python=3.5 jupyter
```

Enter this Python environment. **Stay in this environment when executing any terminal commands (pip, python, jupyter) for rest of this tutorial.**

```
source activate jmatlab
```

Then, install the Matlab kernel for Jupyter.

```
pip install matlab_kernal

python -m matlab_kernel install
```

Check if the kernel is installed correctly

```
jupyter kernelspec list
```

You should see both Python and MATLAB.

(2) MATLAB-side configuration

Now we need to expose the MATLAB executable to Jupyter.

Find your MATLAB directory. On Mac it will be like "/Applications/MATLAB_R2017a.app".

Go to the "extern/engines/python" subdirectory and install the Python engine.

```
cd "/Applications/MATLAB_R2017a.app/extern/engines/python"

python setup.py install
```

(3) Start Jupyter notebook

```
cd your_working_directory

jupyter notebook
```

Now you should see both Python and MATLAB options when launching a new notebook. Check if the MATLAB kernel is working by:

```
In [2]: disp('hello from MATLAB')

hello from MATLAB
```

See *Use MATLAB in Jupyter Notebooks* for more usages.

3.1.3 On Windows

Windows is always tricker when it comes to configuring software, but all you need is basically translating Linux commands into Windows commands.

Commonly used Linux/Mac <-> Windows command mappings are:

- `cd folder/subfolder` <-> `cd folder\subfolder` (type `e:` to change the disk E)
- `pwd` <-> `cd`
- `ls` <-> `dir`

You might also need to set environment variables if commands like "python" and "conda" cannot be recognized. Add the following directories to the PATH variable:

- `path_to_Anaconda_dir\`
- `path_to_Anaconda_dir\Scripts\`

All steps are exactly the same as in the Mac/Linux section. Windows is indeed a litte bit annoying, but it doesn't prevent Jupyter+MATLAB from working. Please contact me if you have any troubles.

3.2 Use MATLAB in Jupyter Notebooks

Jupyter Notebook is a great tool for interactive computing. It allows you to combine codes, simulation results, and descriptions such as latex equations in a single file. It works for many langueges including MATLAB, the choice of this class.

For installation, see *Install Jupyter-MATLAB*.

3.2.1 Jupyter basics

The most commonly used Jupyter commands are

- enter – (in command mode) enter edit mode
- shift+enter – (in edit mode) execute current cell
- esc – (in edit mode) enter command mode, so you can use arrow keys to move to other cells
- b – (in command mode) insert empty cell below
- x – (in command mode) cut current cell
- v – (in command mode) paste the cell you've cut
- esc+m/y – change current code cell to markdown cell / reverse

For all commands see "Help" - "Keyboard shortcuts" in the toolbar.

3.2.2 Printing formats

The default output format is "loose", which takes a lot of space.

```
In [1]: format loose
        for i=1:2
            i+1
        end
```

```
ans =

     2


ans =

     3
```

"compact" is a better option for notebook.

```
In [2]: format compact
        for i=1:2
            i+1
        end
```

```
ans =
     2
ans =
     3
```

3.2.3 Use help functions

"help" will print docs inside the notebook, same as Python's help( )

```
In [3]: help sin
```

```
 SIN    Sine of argument in radians.
    SIN(X) is the sine of the elements of X.

    See also ASIN, SIND.

    Reference page in Doc Center
       doc sin

    Other functions named sin

       codistributed/sin    gpuArray/sin    sym/sin
```

"?" will prompt a small text window, same as IPython magic "?". (not shown on the webpage)

```
In [4]: ?sin
```

"doc" will prompt MATLAB's detailed documentations. (not shown on the webpage)

```
In [5]: doc sin
```

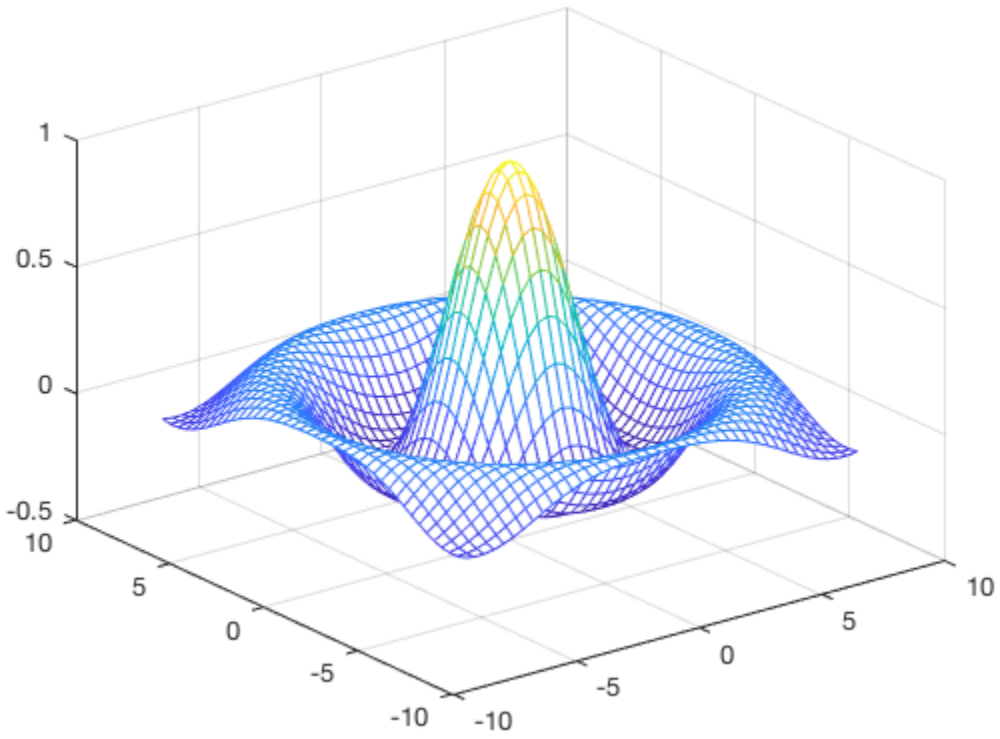
3.2.4 Plotting

Make a cool surface for plotting :)

```
In [6]: tx = linspace (-8, 8, 41);
        ty = tx;
        [xx, yy] = meshgrid (tx, ty);
        r = sqrt (xx .^ 2 + yy .^ 2) + eps;
        tz = sin (r) ./ r;
```

The "%plot inline" magic (default) will plot inside the notebook, same as "%matplotlib inline" in IPython.

```
In [7]: %plot inline
        mesh(tx, ty, tz);
```



The "%plot native" magic will plot in an external window as the original MATLAB's interface, which allows you to rotate, zoom in/out (not shown on the webpage).

```
In [8]: %plot native
        mesh(tx, ty, tz);
```

You can still use "close all" to close the window that was opened by cell above.

```
In [9]: close all
```

"?%plot" will show more plotting options including how to control the figure size (not shown on the webpage)

```
In [10]: ?%plot
```

3.2.5 User-defined functions

For Python programmers it is so common to define a custom function inside a notebook and reuse it over and over again.

A ridiculous design of MATLAB is the function has to be in a separate file, with the function name being the file name. Local functions are allowed since R2016b, but it has many restrictions and doesn't work in either Jupyter Notebook or MATLAB's own Live Script.

Inline functions

By default, matlab only allows **inline functions** within a script.

```
In [11]: f=@(x) x^3+x-1;
```

We can easily find the root of such a function.

```
In [12]: fzero(f,[0 1],optimset('Display','iter'))
```

```
 Func-count     x          f(x)             Procedure
     2              1             1        initial
     3            0.5        -0.375        bisection
     4       0.636364     -0.105935        interpolation
     5        0.68491     0.00620153        interpolation
     6       0.682225  -0.000246683        interpolation
     7       0.682328  -5.43508e-07        interpolation
     8       0.682328   1.50102e-13        interpolation
     9       0.682328             0        interpolation

Zero found in the interval [0, 1]
ans =
    0.6823
```

Standard functions

But inline functions must only contain a single statement, too limited in most cases.

If you try to define a standard function, it will fail:

```
In [13]: function p = multi_line_func(a,b)
             a = a+1;
             b = b+1;
             p = a+b;
         end
```

```
Error: Function definitions are not permitted in this context.
```

Fortunately, Jupyter's "%%file" magic allows us to write a code cell to a file.

```
In [14]: %%file multi_line_func.m

         function p = multi_line_func(a,b)
             % in-file comments can be added like this
             a = a+1;
             b = b+1;
             p = a+b;
         end
```

```
Created file '/Users/zhuangjw/Research/Computing/personal_web/matlab_code/multi_line_func.m'.
```

The output file and this Notebook will be in the same directory, so you can call it directly, as if this function is defined inside the notebook.

```
In [15]: multi_line_func(1,1)
```

```
ans =
     4
```

By doing this, you get Python-like working environment – create a function, test it with several input parameters, go back to edit the function and test it again. This REPL workflow will greatly speed-up your prototyping.

It might take 1~2 seconds for a function cell to take effect, because we are writting files to disk. But you **don't** need to restart the kernel to activate any modifications to your function.

warning: you should avoid adding a MATLAB comment (start with %) at the beginning of a cell, because it might be interpreted as Jupyter magic and thus confuse the kernel.

3.2.6 Markdown cells

Markdown cells are a great way to add descriptions to your codes. Here are examples stolen from the official document. See Jupyter notebook's document for details.

Latex equations

How to write an inline eqution: `$e^{i\pi} + 1 = 0$`

Result: $e^{i\pi} + 1 = 0$

How to write a standalone equation:

```
$$e^x=\sum_{i=0}^\infty \frac{1}{i!}x^i$$
```

Result:

$$e^x = \sum_{i=0}^{\infty} \frac{1}{i!} x^i$$

Tables

How to make a table:

```
| This | is    |
|------|------|
|   a  | table|
```

Result:

This	is
a	table

Not-executing codes

You can put your codes inside a markdown cell, to only show the codes without executing them.

Here's the way to get syntax highlighting for python codes:

````
```python
python codes
```
````

"MATLAB" is not a highlighting option, but you can use "OCTAVE", an open-source clone of MATLAB, to get the same effect.

````
```OCTAVE
disp("Hello World")
for i=1:2
 i+1
end
```
````

Result:

```
disp("Hello World")
for i=1:2
    i+1
end
```

Headings

Headings are an important way to structure your notebook.

```
# Heading 1
## Heading 2
### Heading 3
#### Heading 4
```

Some basic understanding of Linux command line and Python will be useful for installation. **If you are just new to programming, you should simply use MATLAB's original, basic user interface and come back to this tutorial later when you are interested.**

If you feel good about this tool, you can choose to submit notebooks for your homework, Again, **your grade will not be affected by the file format of your homework**.