10. NON-LINEAR LEAST SQUARE FITTING, OPTIMIZATION

10.1.1 Remember: what we saw during the last lesson

Iterative solution for sparse systems (Jacobi, Gauss Seidel, Matlab `help sparse`)

Non-linear systems Fixed point, Piccard and Newton iterations

Non-linear interpolation

10.1.2 Overview: what you will learn today

Non-linear fitting

Optimization searching for an extremum with-/ out using derivatives

Ordinary differential equations using Euler and Runge-Kutta methods

10.2 Non-linear least square fitting (NAM 6.10, H 6.6)

Example Fit the model function $F(t) = a + b\sin\omega(t - t_0)$ to experimental data.

t	0.5	0.8	1.0	1.2	1.5	1.8	2.0	2.4
y	0.3	0.3	0.5	0.9	1.4	1.1	0.5	0.3

This yields an **overdetermined non-linear system** (4 unknowns, 8 equations)

$$\begin{cases} a + b\sin\omega(0.5 - t_0) \approx 0.3 \\ a + b\sin\omega(0.8 - t_0) \approx 0.3 \\ a + b\sin\omega(1.0 - t_0) \approx 0.5 \\ a + b\sin\omega(1.2 - t_0) \approx 0.9 \\ a + b\sin\omega(1.5 - t_0) \approx 1.4 \\ a + b\sin\omega(1.8 - t_0) \approx 1.1 \\ a + b\sin\omega(2.0 - t_0) \approx 0.5 \\ a + b\sin\omega(2.4 - t_0) \approx 0.3 \end{cases} \quad \text{or} \quad \begin{cases} a + b\sin\omega(0.5 - t_0) - 0.3 \approx 0 \\ a + b\sin\omega(0.8 - t_0) - 0.3 \approx 0 \\ a + b\sin\omega(1.0 - t_0) - 0.5 \approx 0 \\ a + b\sin\omega(1.2 - t_0) - 0.9 \approx 0 \\ a + b\sin\omega(1.5 - t_0) - 1.4 \approx 0 \\ a + b\sin\omega(1.8 - t_0) - 1.1 \approx 0 \\ a + b\sin\omega(2.0 - t_0) - 0.5 \approx 0 \\ a + b\sin\omega(2.4 - t_0) - 0.3 \approx 0 \end{cases}$$

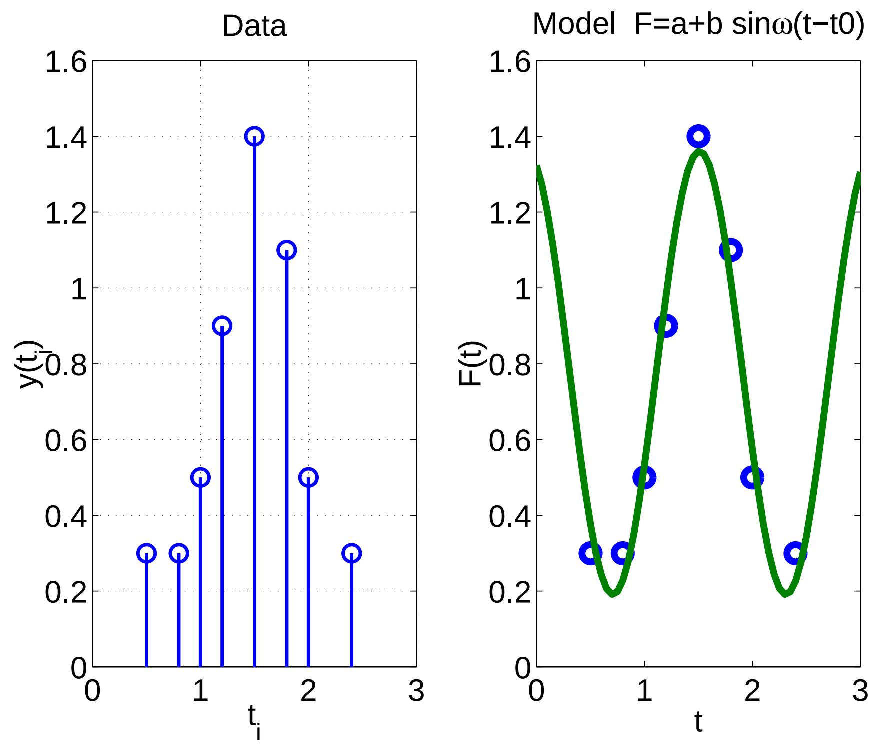
which can be solved by demanding that residuals between the measurements y_i and the model $F(t_i)$ be small $\|\mathbf{y} - \mathbf{F}\|_2 \approx 0$, i.e. $\|\mathbf{y} - \mathbf{F}\|_2 = \mathbf{f}(\mathbf{c}) \approx \mathbf{0}$.

Gauss-Newton solution obtained from $\boxed{\mathbf{c}^{\text{new}} = \mathbf{c}^{\text{old}} + \delta\mathbf{c}, \quad \mathbf{J}^T\mathbf{J}\delta\mathbf{c} = -\mathbf{J}^T\mathbf{f}(\mathbf{c}^{\text{old}})}$

The coefficients $\mathbf{c}$ are obtained from the Newton method for non-linear systems, with an increment $\delta\mathbf{c}$ solving the *overdetermined linear system* $\mathbf{J}\delta\mathbf{c} \approx -\mathbf{f}$. In Matlab, the solution of the normal equations can again be computed with `dc=-f\J`.

Example solution of the non-linear fit with Matlab

```
>> t=[0.5  0.8  1  1.2  1.5 1.8  2  2.4]';
>> y=[0.3  0.3 0.5 0.9  1.4 1.1 0.5 0.3]';
>> subplot(1,2,1), h=stem(t,y), title('Data')
>> a=0.7; b=0.7; w=pi; t0=1.2;
>> c=[a b w t0]';                    %initial guess
>> n=size(t,1); iter=0;dcnorm=1.;
>> while dcnorm>1E-6 & iter<10
>>   u=w*(t-t0); f=a+b*sin(u)-y;
>>   Ji1=ones(n,1);          Ji2=sin(u);
>>   Ji3=b*(t-t0).*cos(u); Ji4=-w*b*cos(u);
>>   J=[Ji1 Ji2 Ji3 Ji4];       % Jacobian
>>   dc=-J\f; c=c+dc;           % Gauss-Newton
>>   dcnorm=norm(dc); iter=iter+1;
>>   a=c(1);  b=c(2);  w=c(3);  t0=c(4);
>>   D=[iter ca b w t0 norm(f) norm(dc) ]
>> end
>> tt=(0:0.05:3)'; Ft=a+b*sin(w*(tt-t0));
>> subplot(1,2,2), plot(t,y,'o',tt,Ft)
```



A solution with an accuracy better than 10^{-6} is obtained with 6 steps:

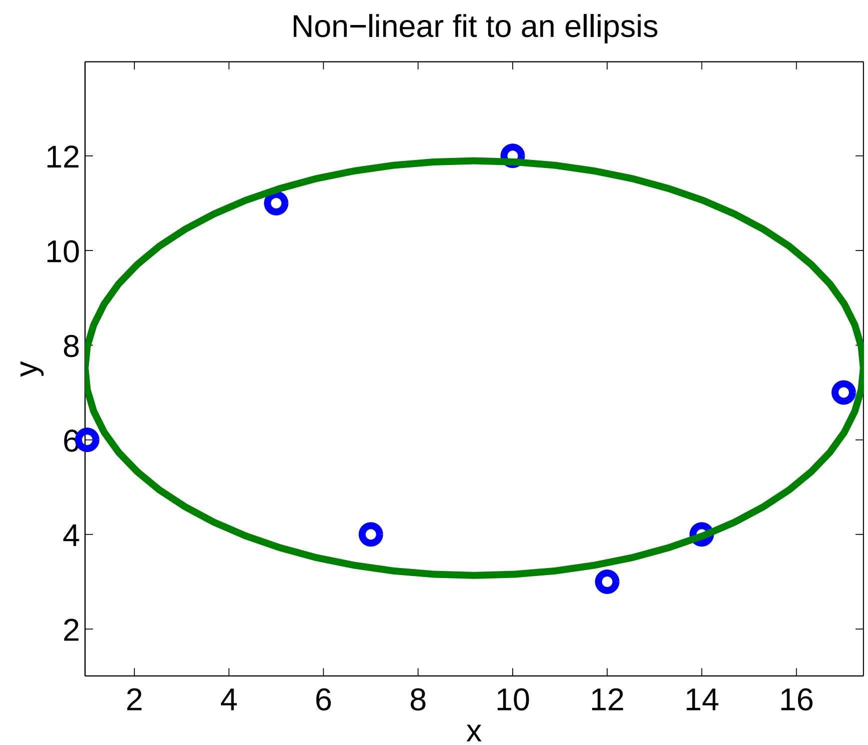
step	a	b	w	t0	||f||	||dc||
1	0.7246	0.4614	3.3935	1.1074	0.8034	0.3600
2	0.7772	0.5428	3.9476	1.1123	0.3688	0.5626
3	0.7762	0.5850	3.9219	1.1089	0.2117	0.0496
4	0.7761	0.5850	3.9225	1.1092	0.1928	0.0007
5	0.7761	0.5850	3.9225	1.1092	0.1928	0.0000
6	0.7761	0.5850	3.9225	1.1092	0.1928	0.0000

Example: fit an ellipsis $F(x,y) = \frac{(x-x_c)^2}{a^2} + \frac{(y-y_c)^2}{b^2} - 1 = 0$ to seven data points.

Set-up the overdetermined non-linear system with 7 equations for 4 unknowns (x_c, y_c, a, b); caluclate the Jacobian $\partial F_i / \partial x_j$

$$\frac{\partial F}{\partial x_c} = -2\frac{x - x_c}{a^2} \qquad \frac{\partial F}{\partial a} = -2\frac{(x-x_c)^2}{a^3}$$
$$\frac{\partial F}{\partial y_c} = -2\frac{y - y_c}{b^2} \qquad \frac{\partial F}{\partial b} = -2\frac{(y-y_c)^2}{b^3}$$

```
>> x=[1 7 10 17  5 12 14]';     %data
>> y=[6 4 12  7 11  3  4]';
>> xc=10; yc=8; a=8; b=3;       %initial guess
>> p=[xc yc a b]'; iter=0; dp=1;
>> while norm(dp)> 1e-6 & iter<10
>>  iter=iter+1; xd=x-xc; yd=y-yc;
>>  f=xd.^2/a^2+yd.^2/b^2-1;
>>  J=-2*[xd/a^2 yd/b^2 xd.^2/a^3 yd.^2/b^3];
>>  dp=-J\f; p=p+dp;            %Gauss-Newton
>> end
>> xc=p(1), yc=p(2), a=p(3), b=p(4)
>> v=0:2*pi/60:2*pi;
>> plot(x,y,'o',xc+a*cos(v),yc+b*sin(v)),
>> axis equal,
xc = 9.1879      yc = 7.5159
a =  8.2298      b =  4.3817
```



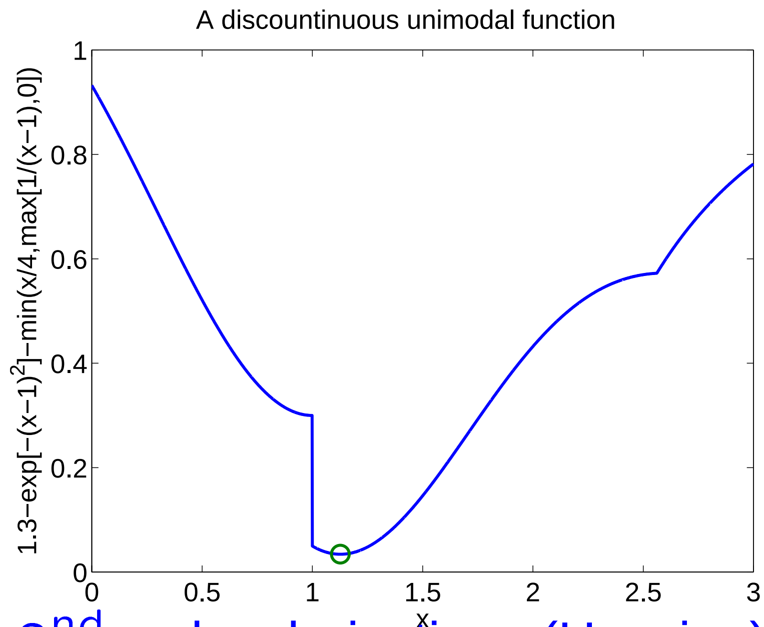
Note that a fit to a circle can be written as a **linear** least square problem (lab 1.3).

10.3 Optimization in one dimension (NAM 7.1, H 6.4)

In Matlab use `fminbnd` for real arguments and `max` for integer arguments argument.

```
>> f=inline('1.3-exp(-(x-1).^2)-min(x/4,max(1./(x-1),0))');
>> [xx,fxx,flag]=fminbnd(f,0,3)
>> x=0:0.001:3; plot(x,feval(f,x),xx,fxx,'o')

xx  = 1.1270    fxx = 0.0342    flag = 1
```



A variety of methods are combined to provide rapid convergence and robust answers; they require *unimodal functions* that are strictly increasing in all the direction from the minimum:

$$f(x) = 1.3 - e^{(x-1)^2} - \min\left[\frac{x}{4}, \max\left[0, \frac{1}{x-1}\right]\right]$$

Methods that use 1st order (Jacobian) and even 2nd order derivatives (Hessian) converge faster... if defined! Check `help optimset` to set the properties.

Here is an example of an optimization where the argument is an integer and the function is cheap to evaluate:

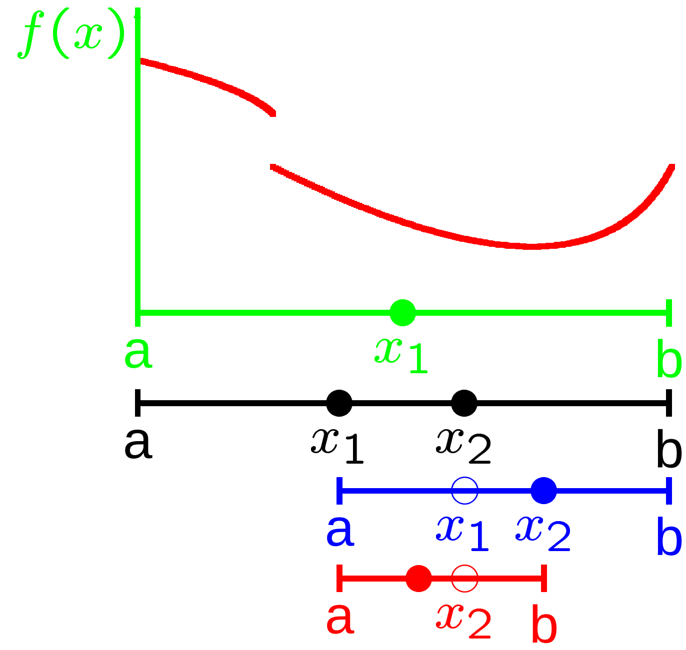
```
>> n=1000000; f=randn(1,n); [fmin,indx]=min(f)

fmin = -4.6365   indx = 198438
```

Golden section search of a minimum $x_* \in [a; b]$ without computing derivatives

Two evaluations are required to decide if the minimum is located in the left or right interval:

if $f(x_1) > f(x_2)$ **then**
  $x_* \in [x_1; b]$
else
  $x_* \in [a; x_2]$
end



For efficiency, choose the proportions so that

$$\tau = \frac{b - x_1}{b - a} = \frac{b - x_2}{b - x_1}$$

in order to reuse the previoius evaluations. By symmetry $(x_2 - a)/(b - a) = \tau$

$$\frac{b - x_2}{b - a} = 1 - \tau \quad \Rightarrow \quad \frac{b - x_2}{b - x_1} = \frac{1 - \tau}{\tau}$$

$$\tau = \frac{1 - \tau}{\tau} \quad \Rightarrow \quad \tau^2 + \tau - 1 = 0 \quad \Rightarrow \quad \tau = \frac{\sqrt{5} - 1}{2} \approx 0.6180$$

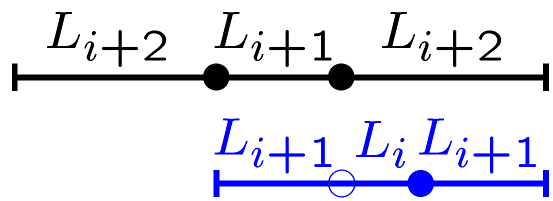
which reminds the *golden ratio* $1 + \sqrt{5}/2 \approx 1.6180$ from the antiquity. Finally

$$\begin{aligned} x_1 &= a + (b - a)(1 - \tau) \\ x_2 &= a + (b - a)\tau \end{aligned}$$

Fibonacci search can be used when the argument is an integer

Write a relation between steps in a golden search

$$L_{i+2} = L_i + L_{i+1}$$



This yields a recursion formula for the Fibonacci numbers

$$F \in \{1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, \ldots\}$$

where consecutive integers approximate the golden section $34/55 = 0.6182 \approx \tau$. This suggests a more efficient algorithm than Matlab's `max` to find the maximum of `Ff(n)` in the interval $i = 0 \ldots 120$ starting from a larger Fibonacci number:

```
function f=Ff(n);
  f=exp(sqrt(n)/10) -cos(n/30+19); return

>> a=0; b=144; n2=89; n1=a+b-n2; F1=Ff(n1); F2=Ff(n2);
>> disp([a n1 n2 b])
>> while b-a>1
>>   if F1>F2, b=n2; n2=n1; F2=F1; n1=a+b-n2; F1=Ff(n1);
>>   else      a=n1; n1=n2; F1=F2; n2=a+b-n1; F2=Ff(n2);
>>   end
>>   disp([a n1 n2 b])
>> end; Fmax=[F1 F2]

 Fmax =     3.6630    3.6629
```

a	n1	n2	n
0	55	89	144
55	89	110	144
89	110	123	144
89	102	110	123
89	97	102	110
97	102	105	110
97	100	102	105
100	102	103	105
100	101	102	103
101	102	102	103
102	102	103	103

10.4 Optimization in higher dimensions n (NAM 7.2, H 6.5)

Efficient methods such as *steepest descent, conjugate-gradients*) do not require evaluating the Jacobian: they are the subject of advanced courses.

Newton's method is however sufficient if the function can differentiated analytically to calculate an extremum by solving

$$\nabla\Phi(x_1, x_2, \ldots, x_n) = 0$$

using iterations

$$\mathbf{x}^{\mathbf{new}} = \mathbf{x}^{\mathbf{old}} + d\mathbf{x}, \qquad \mathbf{J}d\mathbf{x} = -\mathbf{f}(\mathbf{x}^{\mathbf{old}})$$

Example: maximum of $\Phi(x,y) = (x + \sin y)e^{-(x^2+y^2)}$ around $(x,y) = (\frac{1}{4}, \frac{1}{4})$.

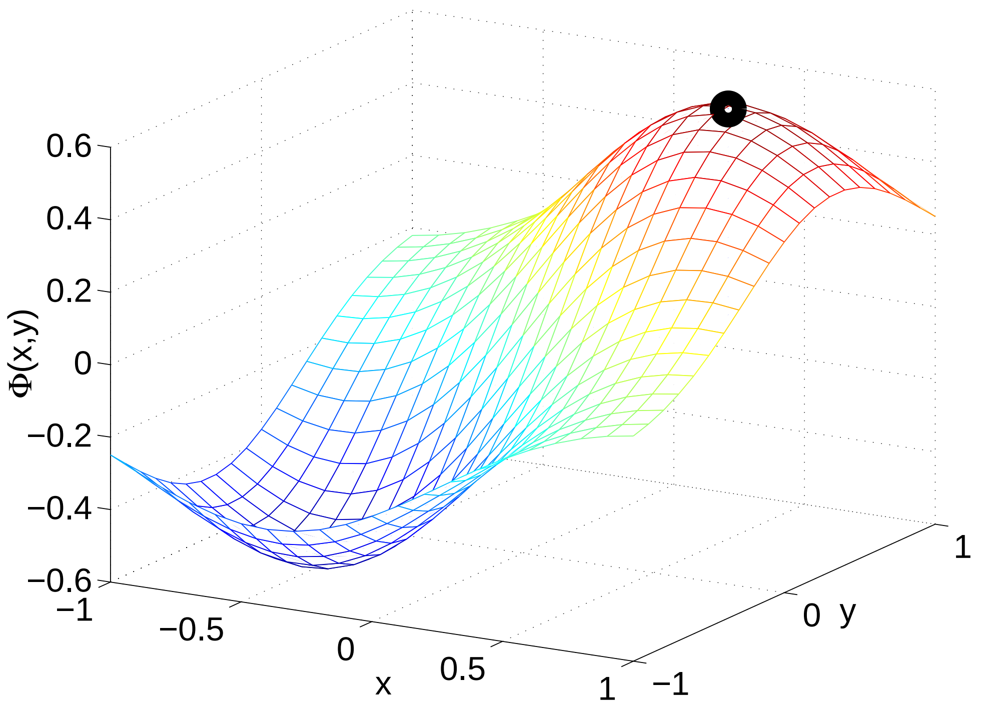
$$\nabla\Phi = \begin{pmatrix} \frac{\partial\Phi}{\partial x} \\ \frac{\partial\Phi}{\partial y} \end{pmatrix} = \begin{pmatrix} (1 - 2x(x + \sin y))e^{-(x^2+y^2)} \\ (\cos y - 2x(x + \sin y))e^{-(x^2+y^2)} \end{pmatrix} = \begin{pmatrix} f_1(x,y) \\ f_2(x,y) \end{pmatrix} = 0$$

To solve this system of the form $\mathbf{f}(\mathbf{x}) = \mathbf{0}$, calculate the Jacobian $J_{ij} = \partial f_i / \partial x_j$

$$\mathbf{J} = \begin{pmatrix} 4x + 2\sin y & 2x\cos y \\ 2y & 2x + 3\sin y + 2y\cos y \end{pmatrix}$$

In matlab the solution is then obtained with

```
>> x=1/4; y=1/4;
>> F=(x+sin(y))*exp(-(x^2+y^2));
>> z=[x y]'; dznorm=1; iter=0;
>> disp([iter dznorm x y F])
>> while dznorm>1e-6 & iter < 30
>>  s=x+sin(y);
>>  f=[1-2*x*s; cos(y)-2*y*s];
>>  J=[-4*x-2*sin(y)  -2*x*cos(y);
>>     -2*y -2*x-3*sin(y)-2*y*cos(y)];
>>  dz=-J\f; z=z+dz;
>>  dznorm=norm(dz,inf); iter=iter+1;
>>  x=z(1); y=z(2);
>>  F=(x+sin(y))*exp(-(x^2+y^2));
>>  disp([iter dznorm x y F])
>> end
```



iter	||dz||	x	y	
0	1.0000	0.2500	0.2500	0.4390
1.0000	0.4055	0.6555	0.5497	0.5666
2.0000	0.1240	0.5315	0.4695	0.5950
3.0000	0.0133	0.5182	0.4635	0.5953
4.0000	0.0002	0.5181	0.4634	0.5953
5.0000	0.0000	0.5181	0.4634	0.5953

11. ORDINARY DIFFERENTIAL EQUATIONS (ODEs)

11.2 Euler and Runge-Kutta methods (NAM 8.2, H 9.3)

Problem: numerically solve the ordinary differential equation for $\mathbf{y}(\mathbf{t})$ for $t > t_0$

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(t, \mathbf{y}), \quad \text{with} \quad \mathbf{y}(t_0) = \mathbf{y_0}$$

using approximations with small steps in time $t_0, t_1, \ldots$ such that $t_{i+1} = t_i + h$.

Euler's method directly follows from the forward difference

$$\frac{\mathbf{y}(t_i + h) - \mathbf{y}(t_i)}{h} \approx \mathbf{f}(t, \mathbf{y}), \quad \Rightarrow \quad \boxed{\mathbf{y}(t_{i+1}) \approx \mathbf{y_i} + h\mathbf{f}(t_i, \mathbf{y_i})}$$

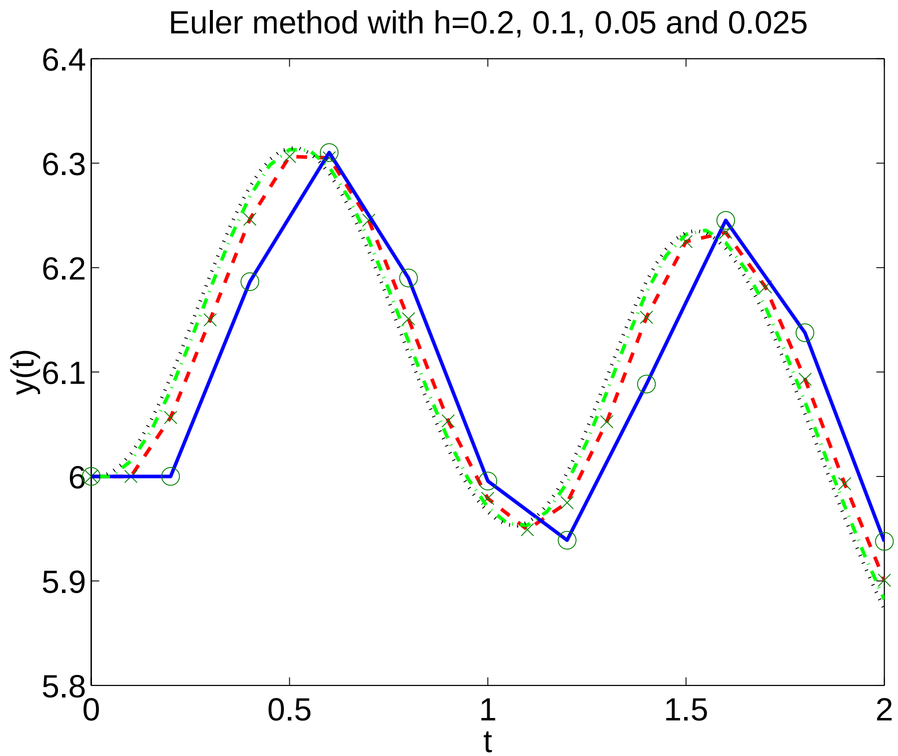
Starting from the *initial condition* $(t_0, \mathbf{y_0})$, one step with Euler's method produces an approximation $(t_1, \mathbf{y}_1)$ with a *local error* $\mathcal{O}(h^2)$; after n steps to reach the final time $t_n = t_0 + nh$, the solution (t_n, y_n) has a *global error* $n\mathcal{O}(h^2) \sim \mathcal{O}(h)$.

Example solve $y'(t) = \sin(ty)$ with $y(0) = 6$ using Euler's method

```
function fend=feuler(h)
 y=6; t=0; tend=2; n=tend/h; T=t; Y=y;
 for i=1:n
   f=sin(t*y); y=y+h*f; t=t+h;
   T=[T; t]; Y=[Y; y];
 end
 fend=y; plot(T,Y,T,Y,'o');
return

>> h=0.2; Y2=[];
>> for k=0:3, Y2=[Y2 feuler(h/2^k)], end;

Y2 = 5.9379  5.9007  5.8823  5.8731
```



A Richardson extrapolation can be used to cancel the leading (global) error in $\mathcal{O}(h)$ and calculate the value $y(2) \approx 5.8731 + \frac{5.8731-5.8823}{2^Q-1} = 5.8639$.

Peer Teaching (2×1 minutes to think, explain to your neighbour and vote)

Richardson extrapolation. Which value for Q should you use here above?

$\leftarrow$ 0 $\qquad$ $\uparrow$ 1 $\qquad$ $\rightarrow$ 2

Runge-Kutta (RK2) achieves a better precision with a global error in $\mathcal{O}(h^2)$

$$\mathbf{y_{i+1}} = \mathbf{y_i} + \frac{h}{2}(\mathbf{k_1} + \mathbf{k_2}), \quad \text{with} \quad \begin{cases} \mathbf{k_1} = \mathbf{f}(t_i, \mathbf{y_i}) \\ \mathbf{k_2} = \mathbf{f}(t_i + h, \mathbf{y_i} + h\mathbf{k_1}) \end{cases}$$

Runge-Kutta (RK4) achieves a high precision with a global error in $\mathcal{O}(h^4)$

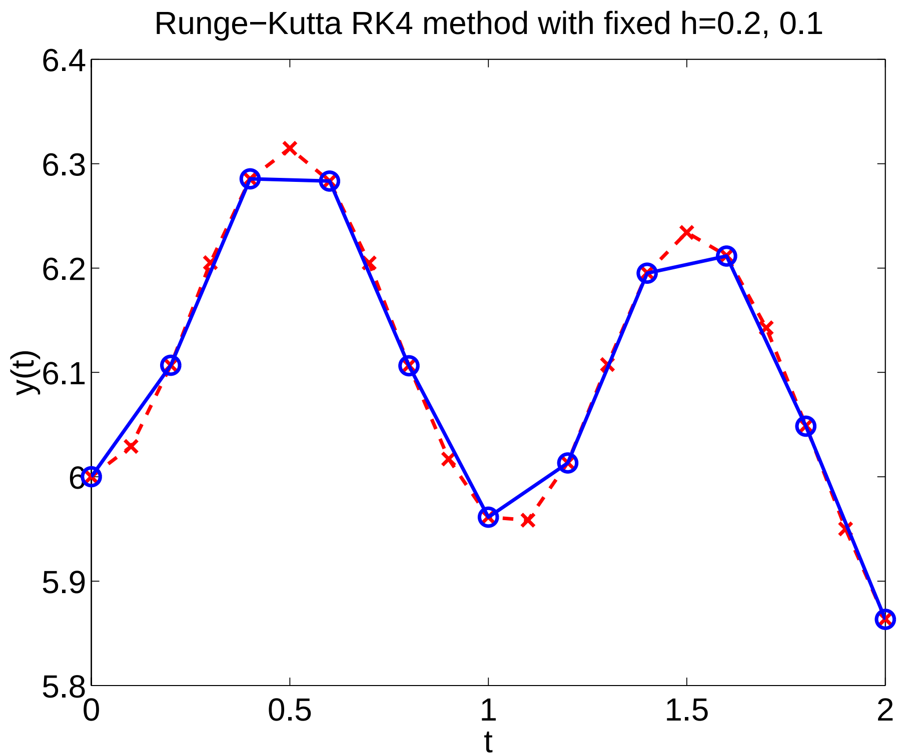
$$\mathbf{y_{i+1}} = \mathbf{y_i} + \frac{h}{6}(\mathbf{k_1} + 2\mathbf{k_2} + 2\mathbf{k_3} + \mathbf{k_4}), \quad \text{with} \quad \begin{cases} \mathbf{k_1} = \mathbf{f}(t_i, & \mathbf{y_i}) \\ \mathbf{k_2} = \mathbf{f}(t_i + \frac{h}{2}, & \mathbf{y_i} + \frac{h}{2}\mathbf{k_1}) \\ \mathbf{k_3} = \mathbf{f}(t_i + \frac{h}{2}, & \mathbf{y_i} + \frac{h}{2}\mathbf{k_2}) \\ \mathbf{k_4} = \mathbf{f}(t_i + h, & \mathbf{y_i} + h\mathbf{k_3}) \end{cases}$$

In Matlab use `help ode23`, `ode45`, `odeset` for RK methods with variable step size, where the step size h is continually adjusted to achieve a specified precision with a minimum number of steps.

Example solve $y'(t) = \sin(ty)$ with $y(0) = 6$ using the RK4 method

```
function f=fsin(t,y),
 f=sin(t*y);
return

function fend=rk4(h)
 y=6; t=0; tend=2; n=tend/h;
 T=t; Y=y; h2=h/2;
 for i=1:n
   k1=fsin(t,   y);
   k2=fsin(t+h2,y+h2*k1);
   k3=fsin(t+h2,y+h2*k2);
   k4=fsin(t+h ,y+h *k3);
   y=y+h/6*(k1+2*k2+2*k3+k4);
   t=t+h;
   T=[T; t]; Y=[Y; y];
 end
 plot(T,Y);  fend=y;
return
```




```
>> h=0.2; YN=[];
>> for k=0:1, YN=[YN rk4(h/2^k)]; Y2=YN(end), end;
Y2 = 5.86346010701075   5.86390480621220

>> % --- Alternative using Matlab's solvers
>> tend=2; y0=6; options=odeset('RelTol',1e-6,'AbsTol',1e-4]);
>> [T,Y]=ode23(@fsin,[0 tend],y0,options);
>> [T,Y]=ode45(@fsin,[0 tend],y0,options);
```

A Richardson extrapolation again cancels the leading (global) error, here in $\mathcal{O}(h^4)$ with $y(2) \approx 5.86390 + \frac{5.86390-5.86346}{2^4-1} = 5.86392.$