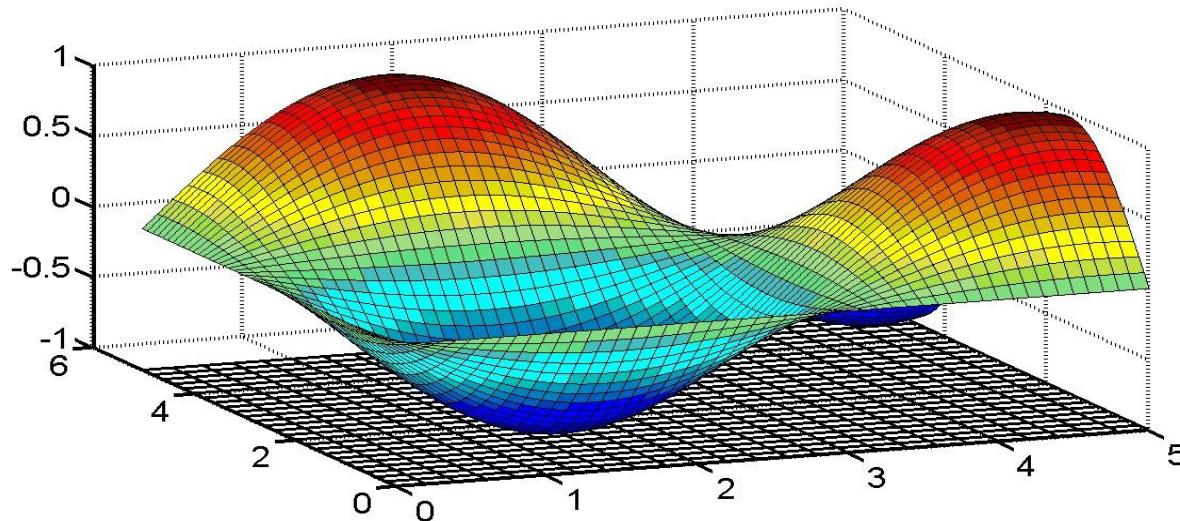


Chapter 8. Method of coordinate descent for finding a minimum of a multivariable function



Let we have a function of n variables

$$F(x_1, x_2, \dots, x_n) \quad a_i < x_i < b_i$$

and we seek coordinates of a point at which the function attains a minimum.

(If you need to find a maximum, then consider the function $-F$ and seek a minimum.)

The most primitive way is to introduce a lot of nodes in the domain of definition, then calculate F at the nodes and use computer command “if . . . less . . . then” for identifying the node at which minimum is attained.

This may be very time-consuming. For example, if $n=7$ and each segment $[a_i, b_i]$ contains 101 node, then total number of nodes is $101^7 > 10^{14}$

If calculation of F at a single node requires, for example, 50 arithmetic operations, then total number of necessary operations is more than 5×10^{15} .

Intel Core i7-7700K Processor performs roughly 38 billion = $38 \cdot 10^9$ floating point operations per second. It will take $5 \times 10^{15} / 38 \cdot 10^9 = 131600$ seconds ≈ 36.5 hours to do this job.

Therefore, there is need in more efficient methods of finding minimum.

Method of coordinate descent:

an idea is to vary coordinates by turns for the search of a minimum.

Let us choose some initial point

$$\mathbf{x}^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)})$$

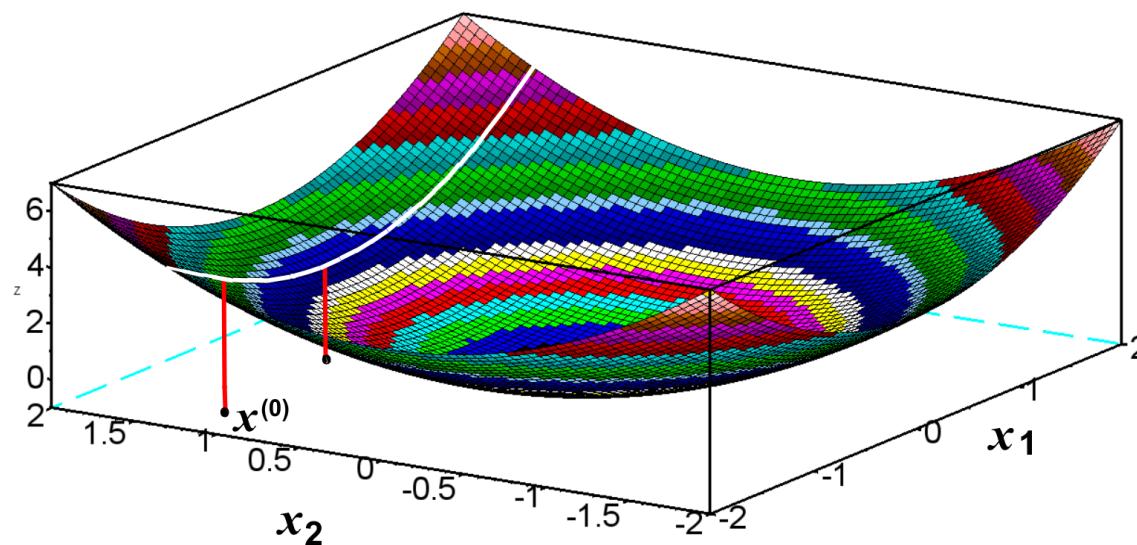
and vary the first coordinate, keeping others:

$$(x_1, x_2^{(0)}, \dots, x_n^{(0)})$$

$$a_1 \leq x_1 \leq b_1$$

By calculation of F at nodes on this segment, one can find a point of minimum

$$(x_1^{(1)}, x_2^{(0)}, \dots, x_n^{(0)}).$$



After that, we fix all coordinates except for x_2 and search a minimum under variation of x_2 :

$$(x_1^{(1)}, x_2, \dots, x_n^{(0)})$$

$$(x_1^{(1)}, x_2^{(1)}, \dots, x_n^{(0)})$$

• • • • • • • • • •

$$(x_1^{(1)}, x_2^{(1)}, \dots, x_n^{(1)}) = x^{(1)}$$

$$x^{(2)}$$

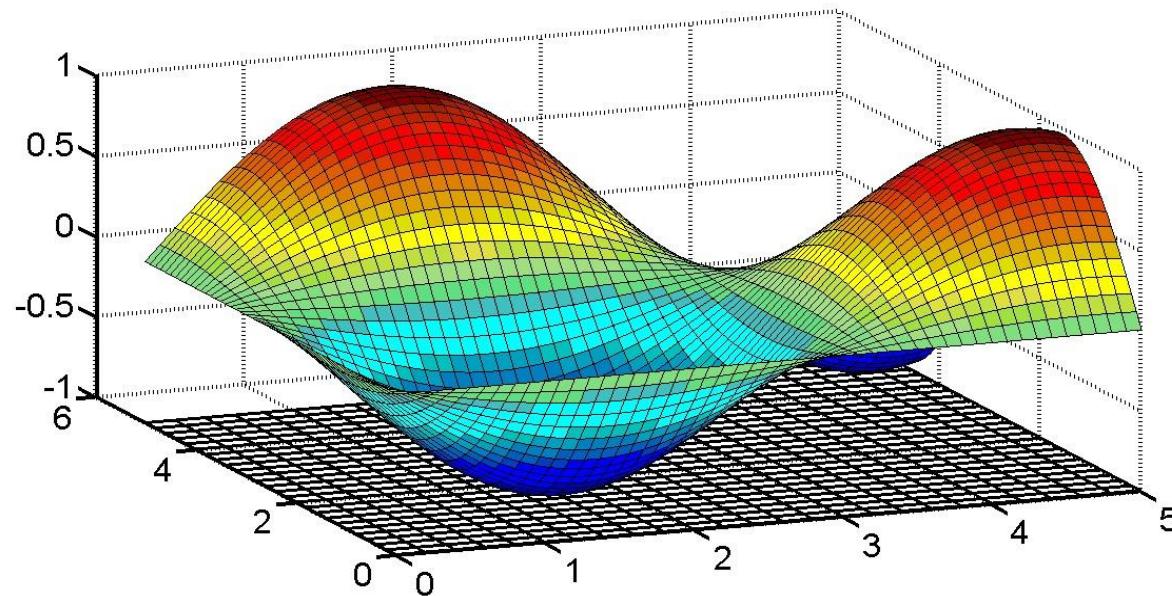
$$x^{(3)}$$

$$x^{(k)}$$

At each step, $F(x^{(k)}) \leq F(x^{(k-1)})$

Method of gradient descent for finding a minimum of a multivariable function

https://en.wikipedia.org/wiki/Gradient_descent



Again, we have a function of n variables

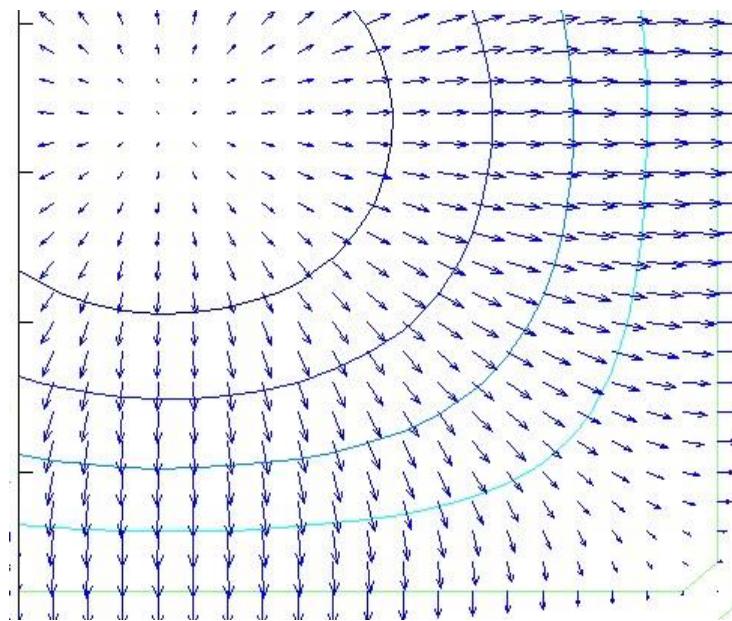
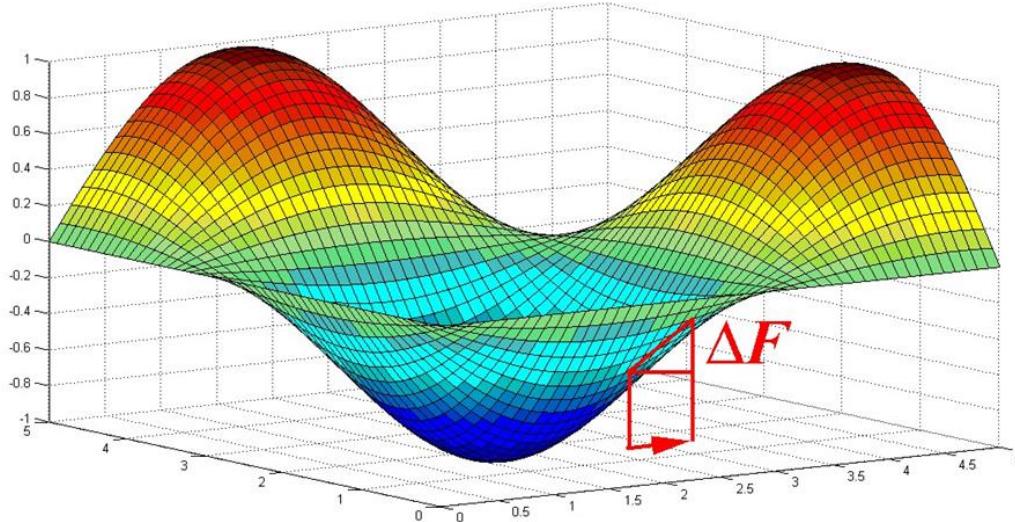
$$F(x_1, x_2, \dots, x_n)$$

and we seek coordinates of a point at which the function attains a local minimum.

Let us choose an initial point: $x^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)})$,
calculate partial derivatives, and compose the gradient

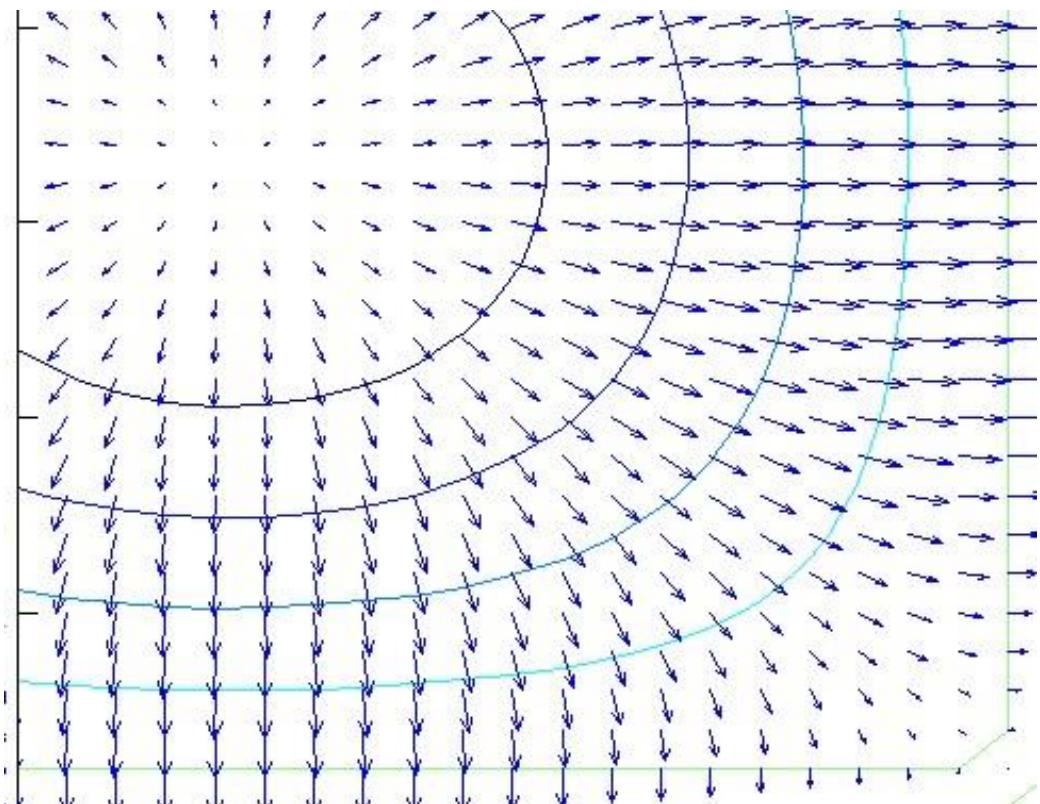
$$\text{grad } F(x^{(0)}) = \sum_{i=1}^n \bar{e}_i \partial F(x^{(0)}) / \partial x_i$$

As known, vector $\text{grad } F(x^{(0)})$ indicates the direction of most rapid rise of the function $F(x)$ at point $x^{(0)}$ in the plane (x,y) .

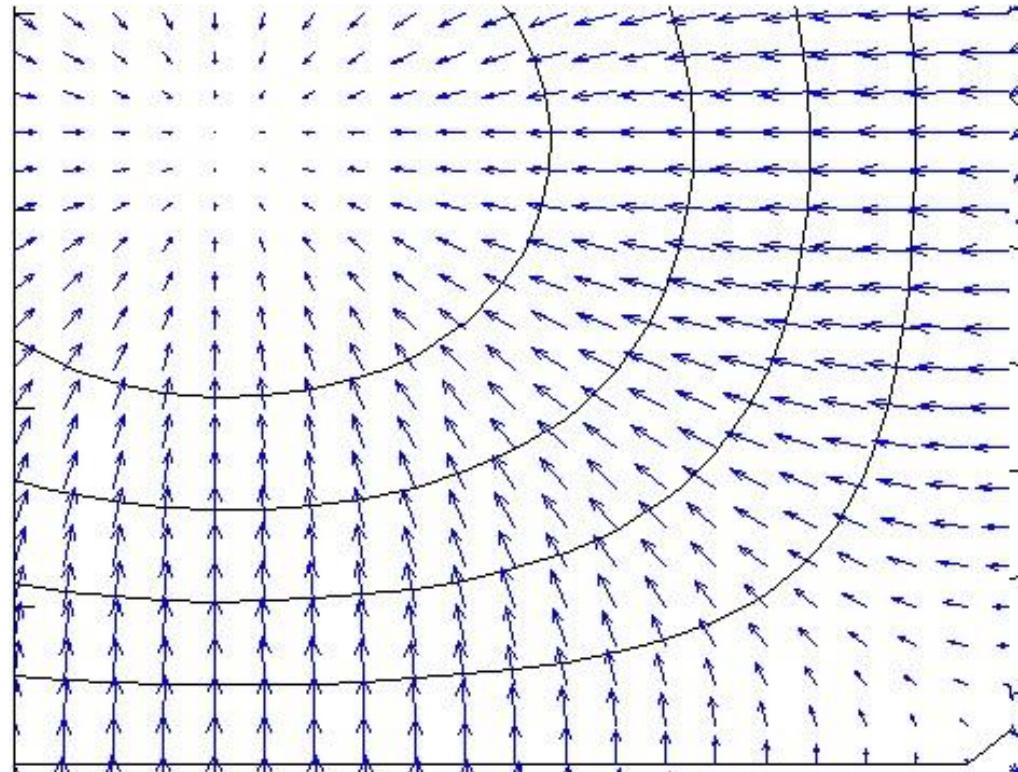


The gradient $\text{grad } F$ is normal to level lines

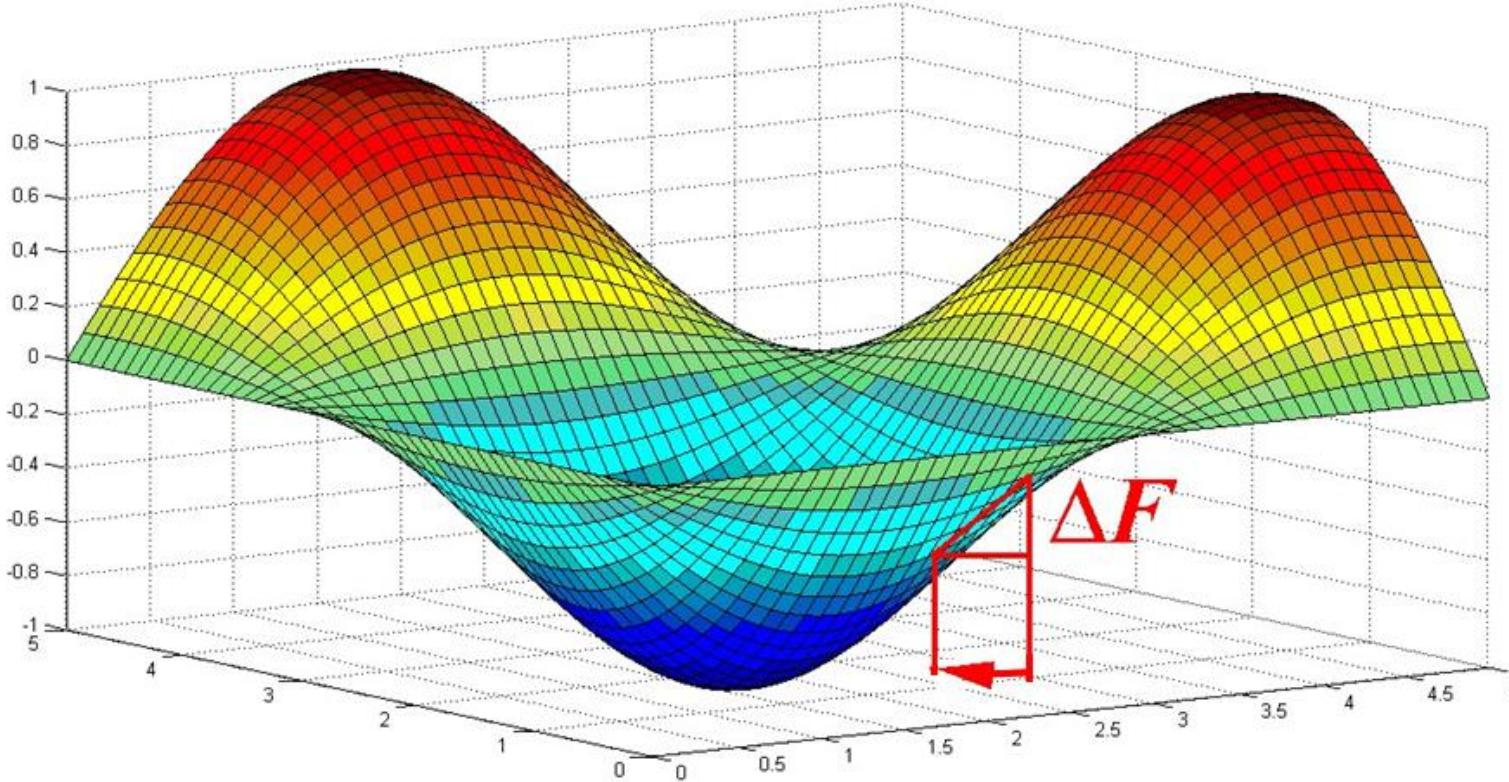
grad F



-grad F

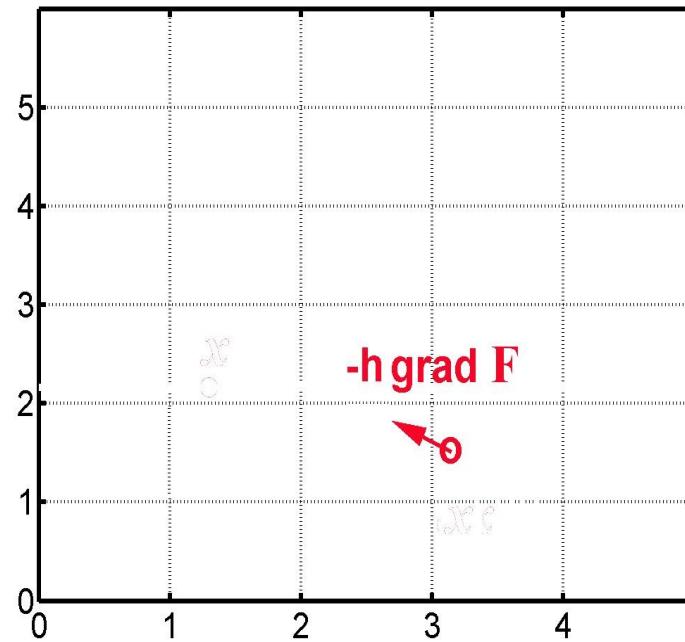
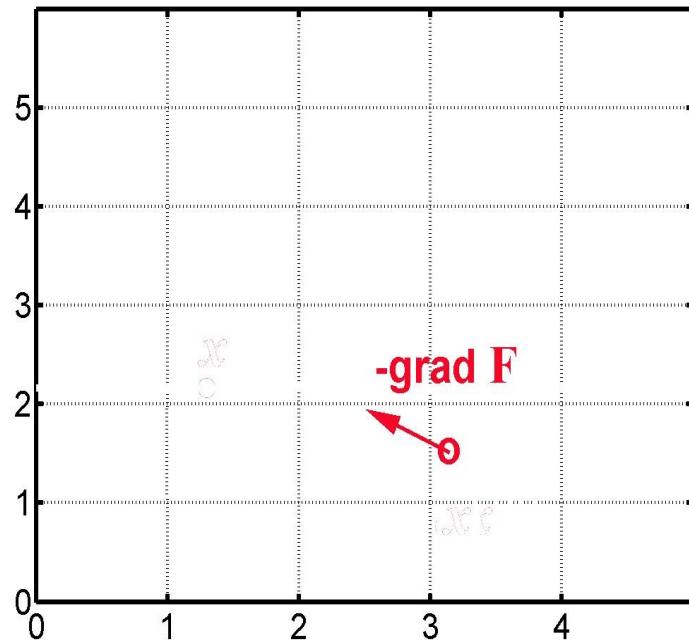


**Antigradient $-\text{grad } F(x^{(0)})$ indicates the direction of fastest
decrease (descent) of the function $F(x)$ at this point**



If we make a step of length $|\text{grad } F(x^{(0)})|$ in the direction of antigradient, then we arrive at a point where gradient changes, therefore, the direction of fastest decrease changes.

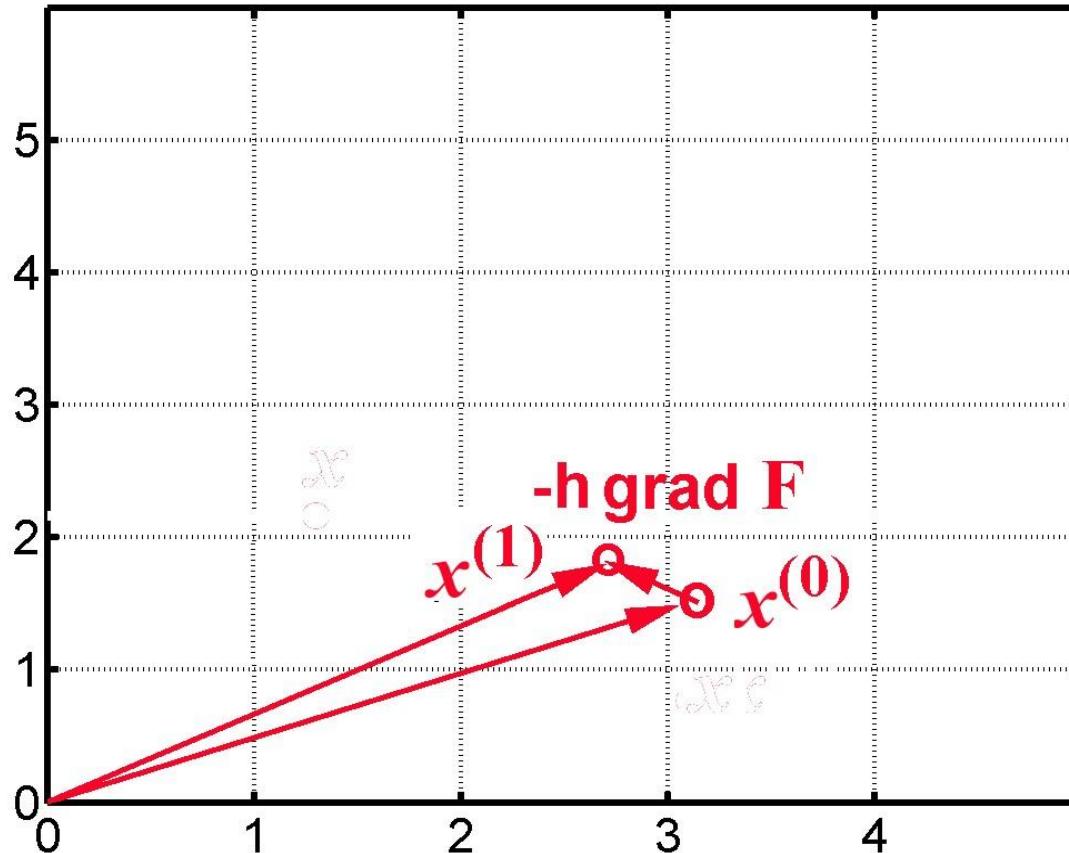
It is reasonable to consider a shorter vector $-h \cdot \text{grad } F(x^{(0)})$, where h is a small parameter, in order to correct the direction of descent:



$x^{(1)} = x^{(0)} - h \cdot \text{grad } F(x^{(0)})$ - in vector form.

Cartesian components:

$$x_i^{(1)} = x_i^{(0)} - h \cdot \frac{\partial F(x^{(0)})}{\partial x_i}$$



Similarly, we perform further steps, which lead to a minimum of $F(x)$:

$$x_i^{(k+1)} = x_i^{(k)} - h \cdot \partial F(x^{(k)}) / \partial x_i$$

$$x_i^{(k+1)} = x_i^{(k)} - h \cdot \partial F(x^{(k)}) / \partial x_i$$

Notice:

As soon as we approach a minimum, the derivatives $\partial F(x^{(k)}) / \partial x_i$ decrease; therefore, the difference $x^{(k+1)} - x^{(k)}$ decreases as well.

Example 1. Find a minimum

$$z=F(x,y)=x^4 + y^4 - 5y + x \quad -2 < x < 3, \quad -2 < y < 4$$

Scilab :

```
for i=1:41
```

```
for j=1:31
```

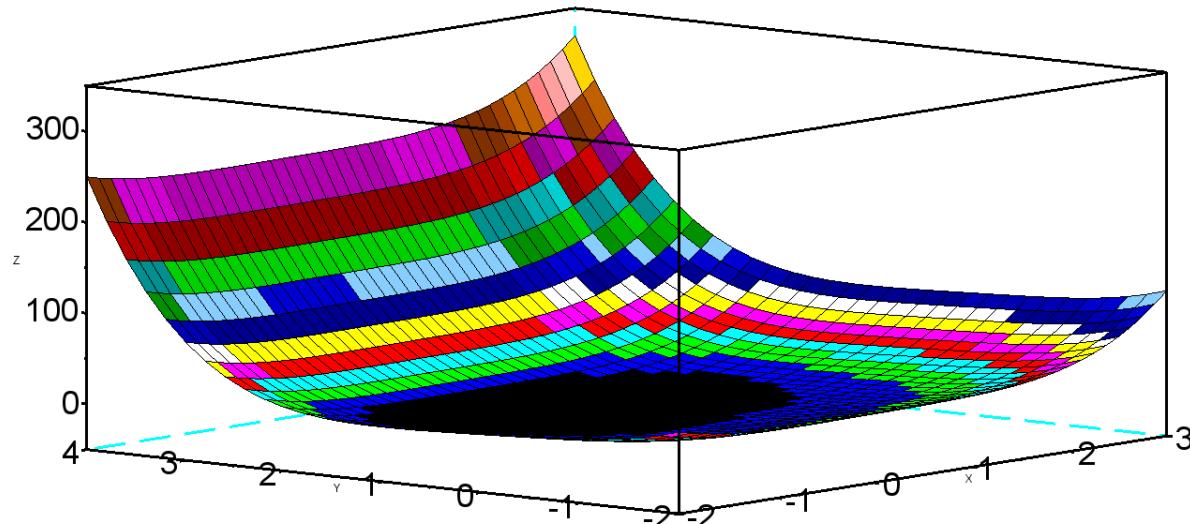
```
  x(i,j)=0.125*(i-1)-2
```

```
  y(i,j)=0.2*(j-1)-2 end
```

```
end
```

```
F=x.^4+y.^4 -5*y+x
```

```
surf(x,y,F)
```



```
h=0.01
xx=2.5
yy=3.5
plot(4,5)
for k=1:300
dFdx=4*xx^3 +1
dFdy= 4*yy^3-5
xx=xx-h*dFdx
yy=yy-h*dFdy
plot(xx, yy,'or','LineWidth',2)
end
disp('xx=',xx,'yy=',yy,'k=',k)
```

answer: xx= -0.6299189
yy= 1.0772173

In Scilab code, it makes sense to set another condition to stop computations:

$$|x_i^{(k+1)} - x_i^{(k)}| < \epsilon \quad \text{for all } i$$

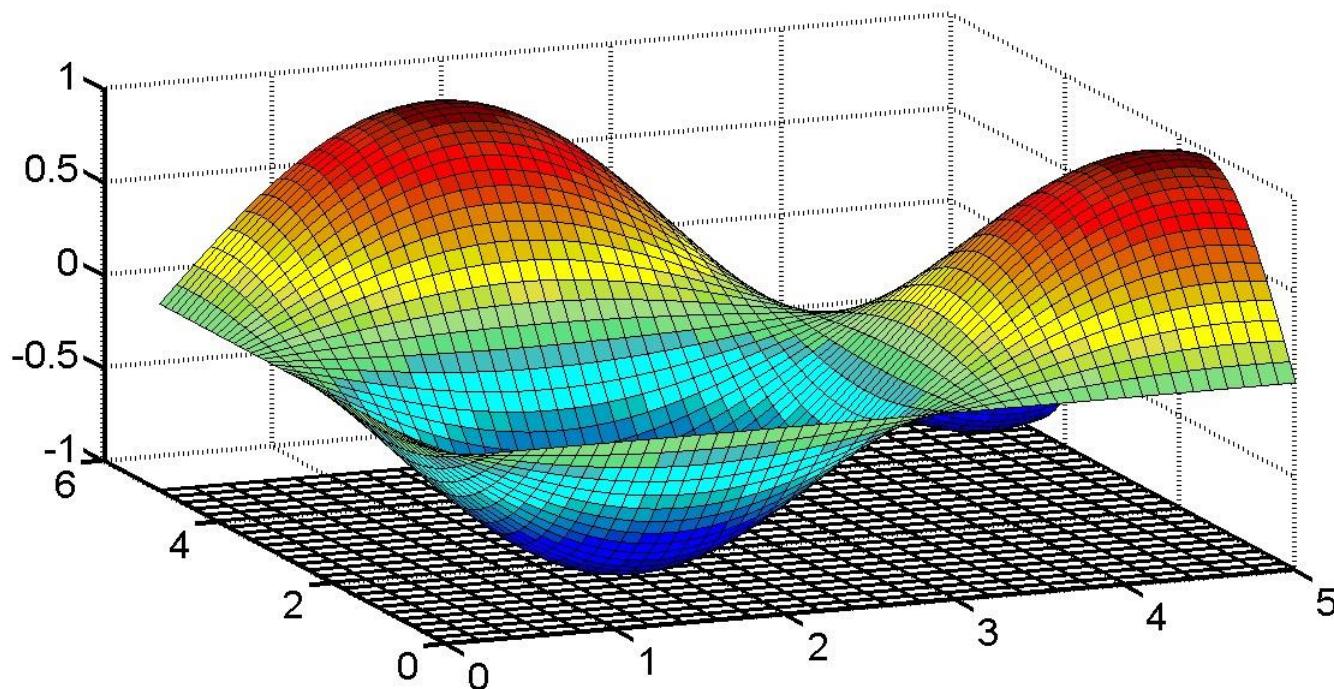
Or

$$|F(x^{(k+1)}) - F(x^{(k)})| < \epsilon$$

(instead of setting total number of steps $k=1:300$)

Remark 1.

Possible non-uniqueness of local minima:



Remark 2.

Often, in the method of gradient descent, one cannot find an analytical expression for partial derivatives of F .

Then some numerical methods for finding the derivatives can be used, see Chapter 11.

Method of most rapid gradient descent for finding a minimum of a function

$$z = F(x_1, x_2, \dots, x_n)$$

Recall Method of gradient descent:

Choose some $x^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)})$

Calculate

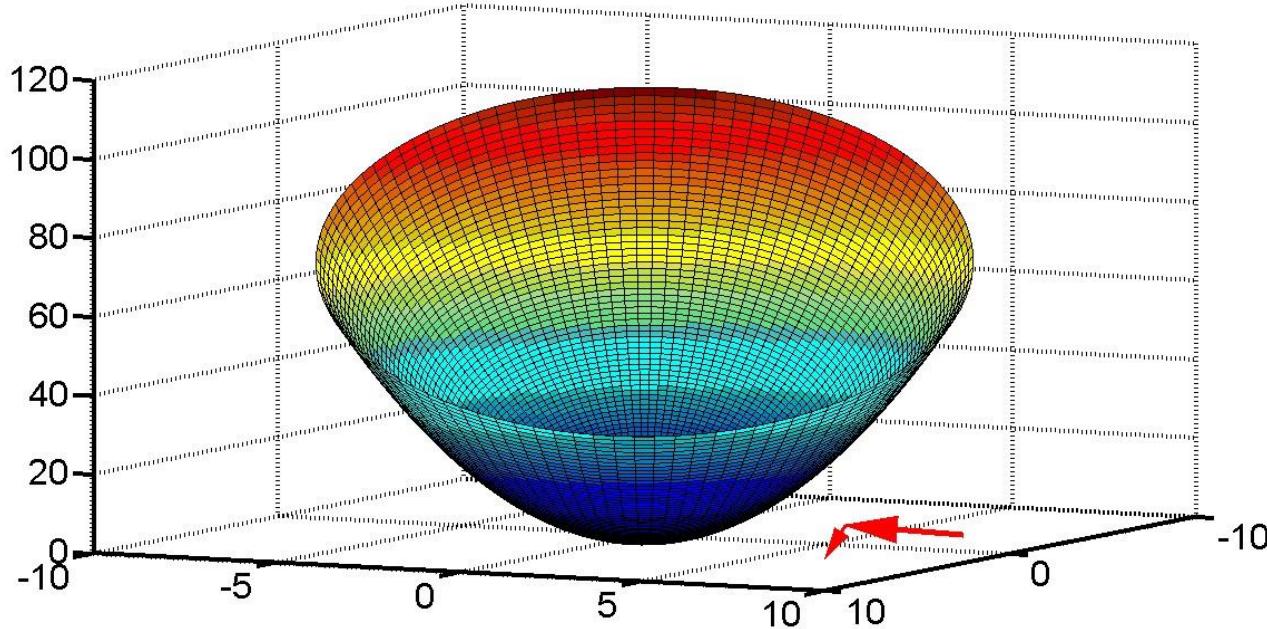
$$\text{grad } F(x^{(0)}) = \sum_i \bar{e}_i \frac{\partial F(x^{(0)})}{\partial x_i}$$

Sequential approximations:

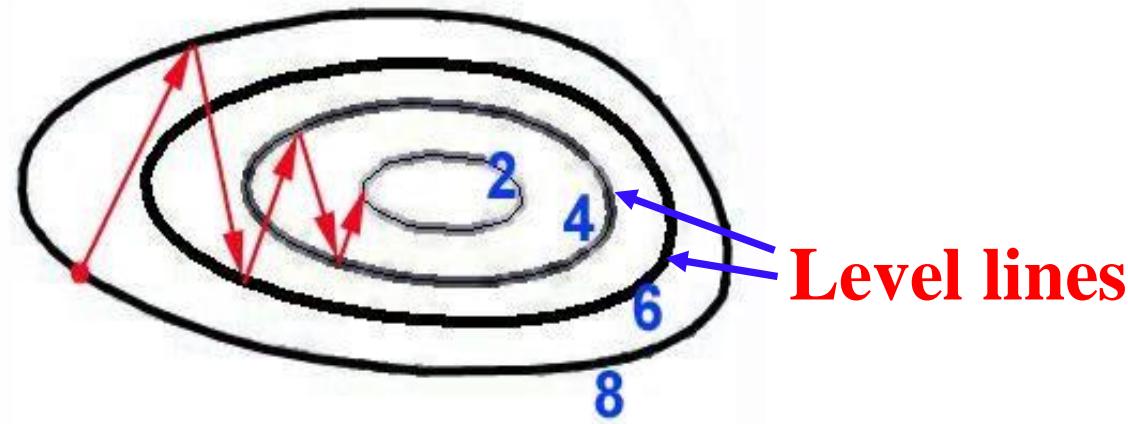
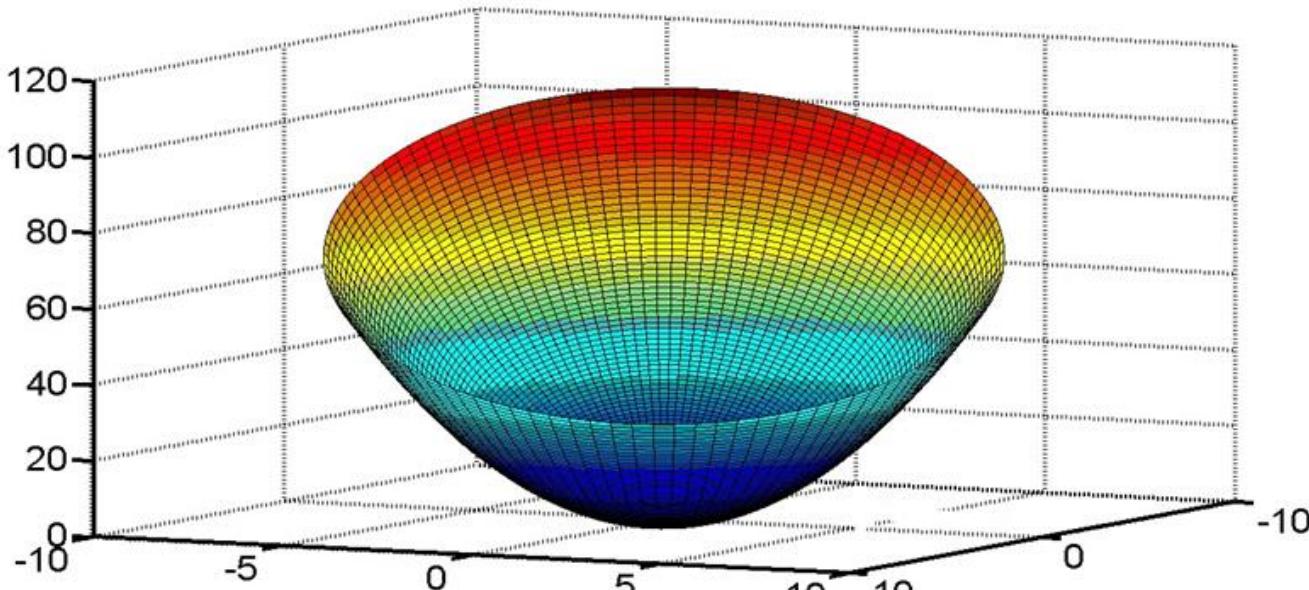
$$x_i^{(k+1)} = x_i^{(k)} - h \cdot \frac{\partial F(x^{(k)})}{\partial x_i}$$

The parameter h governs the length of vector.

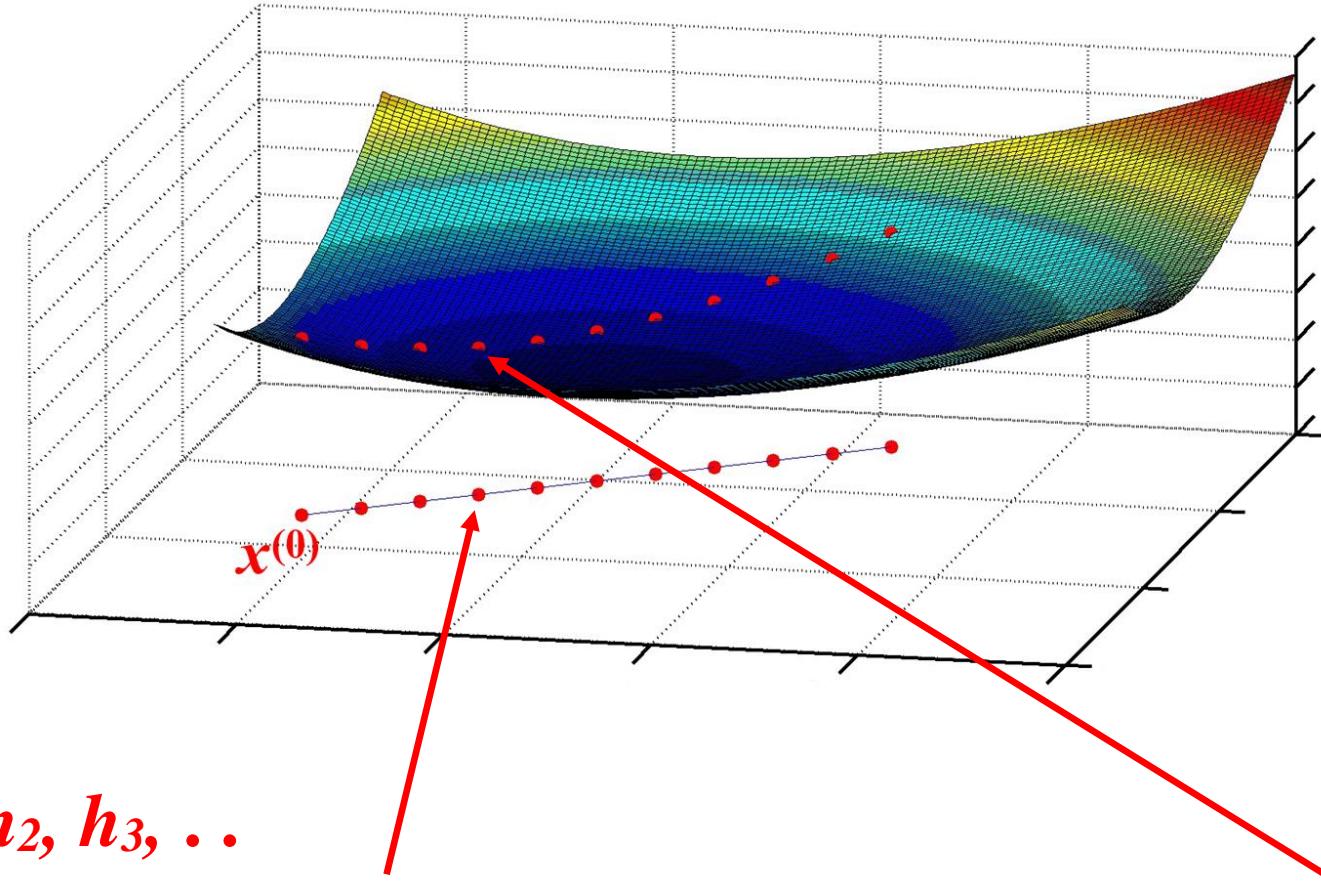
If h is too small, then sequence $X^{(k)}$ approaches a solution slow, as it takes too many steps and a lot of computing time.



If h is too large, then sequence $x^{(k)}$ may converge slow as well, as it may pass by a minimum:



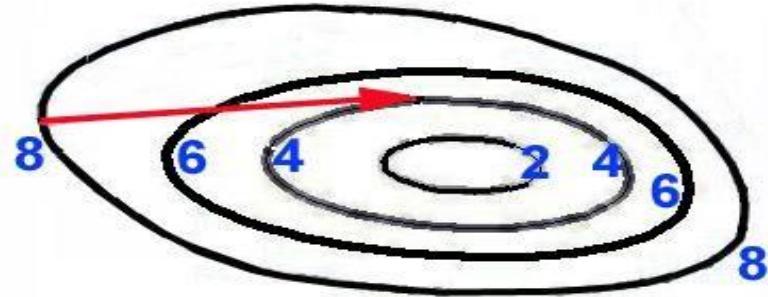
(or the sequence may happen to diverge if h is very large).
What is the optimal value of h ?



Consider various h_1, h_2, h_3, \dots

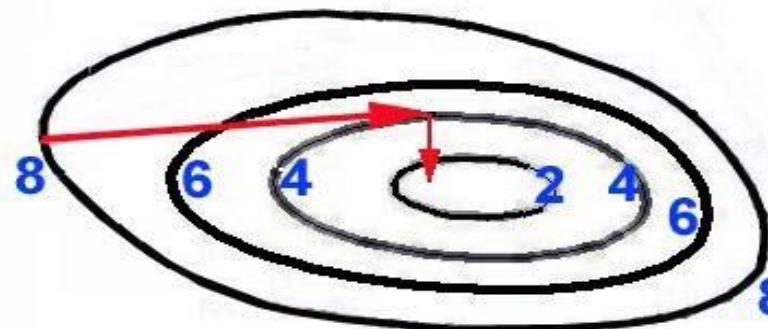
Suppose we have found such h_{opt} , that F attains a minimum F_{\min} in the direction of antigradient. This can be achieved with a method of 1D optimization, for example method of golden section, see the end of this chapter.

As soon as we found such optimum \mathbf{h}_{opt} , that ensures a minimum of F , we move from $x_i^{(0)}$ to $\mathbf{x}^{(1)} = x_i^{(0)} - \mathbf{h}_{\text{opt}} \cdot \partial F(\mathbf{x}^{(0)}) / \partial x_i$

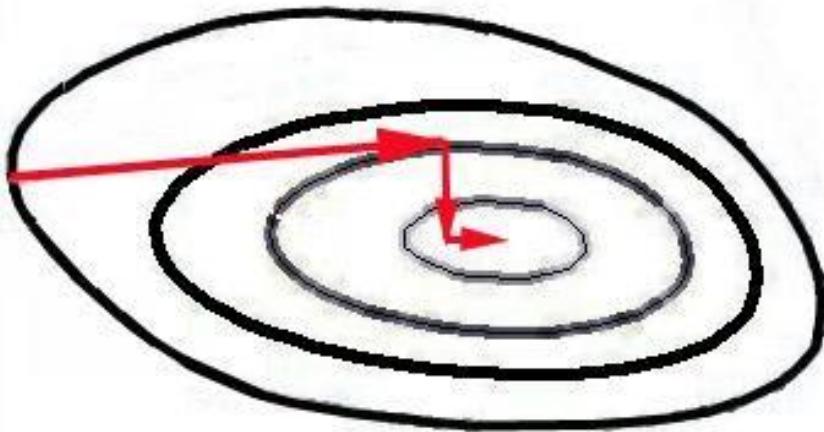


At the point of minimum $\mathbf{x}^{(1)}$, the direction, in which the step was made, is tangent to a level line.

Antigradient calculated at this point will be normal to the level line:



Therefore next step from $\mathbf{x}^{(1)}$ to $\mathbf{x}^{(2)}$ will be made in the normal (orthogonal) direction, as antigradient is normal to the level line that passes through point $\mathbf{x}^{(1)}$.

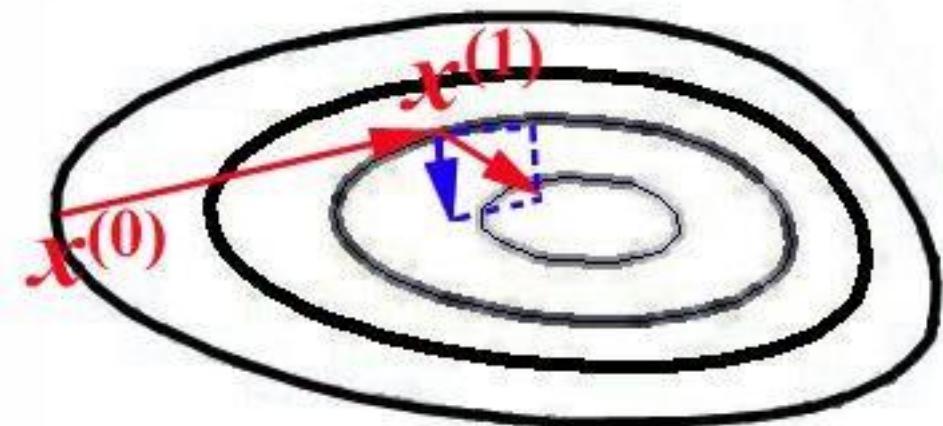


In the same way, at next steps, we seek $\mathbf{h}^{(k)}_{\text{opt}}$ and move on:

$$\mathbf{x}_i^{(k+1)} = \mathbf{x}_i^{(k)} - \mathbf{h}^{(k)}_{\text{opt}} \cdot \partial \mathbf{F}(\mathbf{x}^{(k)}) / \partial \mathbf{x}_i$$

Practice showed that method of fastest gradient descent is more efficient (from the viewpoint of necessary computing time) than method of gradient descent with a constant \mathbf{h} .

Conjugate Gradient Method



Most rapid gradient descent:

$$x^{(1)} = x^{(0)} - h_{\text{opt}} \cdot \text{grad}F(x^{(0)}) , \quad x^{(2)} = x^{(1)} - h_{\text{opt}} \cdot \text{grad}F(x^{(1)})$$

Conjugate gradient method:

$$x^{(2)} = x^{(1)} - h_{\text{opt}} [\text{grad}F(x^{(1)}) + \beta^{(1)} \cdot \text{grad}F(x^{(0)})]$$

correction of the direction of step

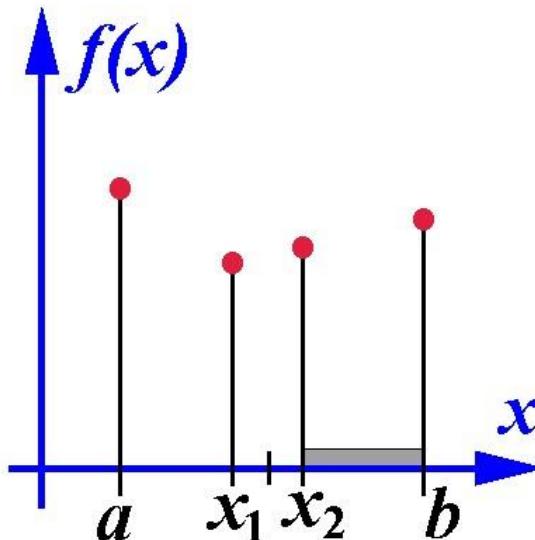
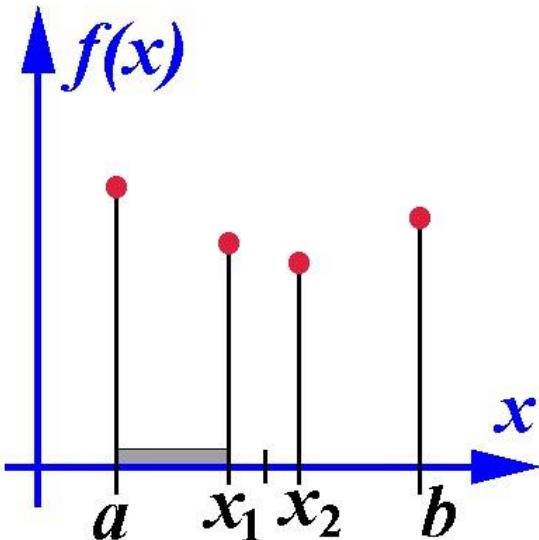
Scilab built-in command: **fminsearch**

```
function y=HIT(x)
  y = x(2)^2 + (1-x(1))^2;
endfunction
[x, fval] = fminsearch ( HIT, [1 -1] )
```

Computes the unconstrained minimum of given function HIT with the Nelder-Mead algorithm.

Same command “fminsearch” in **Matlab**. In addition, “gradient”
[FX,FY] = gradient(F)
returns the x and y components of the two-dimensional numerical gradient of matrix F.

Search of a minimum in case of a function of single independent variable. A bisection method.



Let $f(x)$ be given on $[a,b]$. We divide the segment into two equal parts and consider two points x_1 and x_2 located symmetrically about the midpoint

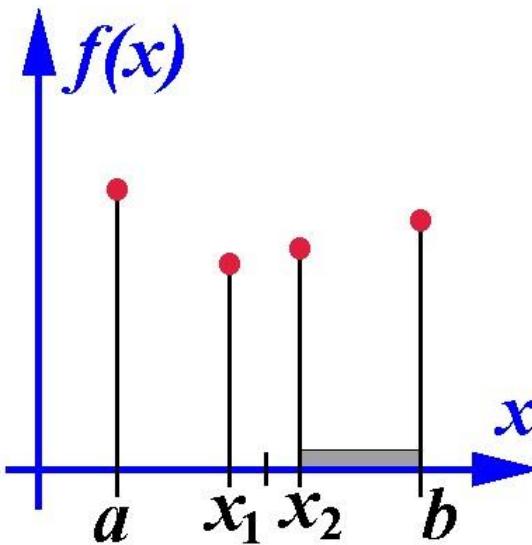
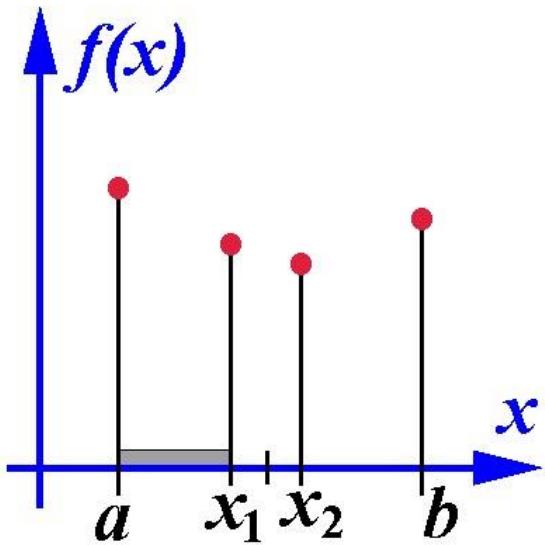
$$x_1 = 0.5 (a+b) - \delta , \quad x_2 = 0.5 (a+b) + \delta ,$$

where δ is small.

Let us calculate $f(x_1)$ and $f(x_2)$.

If $f(x_1) > f(x_2)$, then we drop $[a, x_1]$ and retain $[x_1, b]$

If $f(x_1) < f(x_2)$, then we drop $[x_2, b]$ and retain $[a, x_2]$

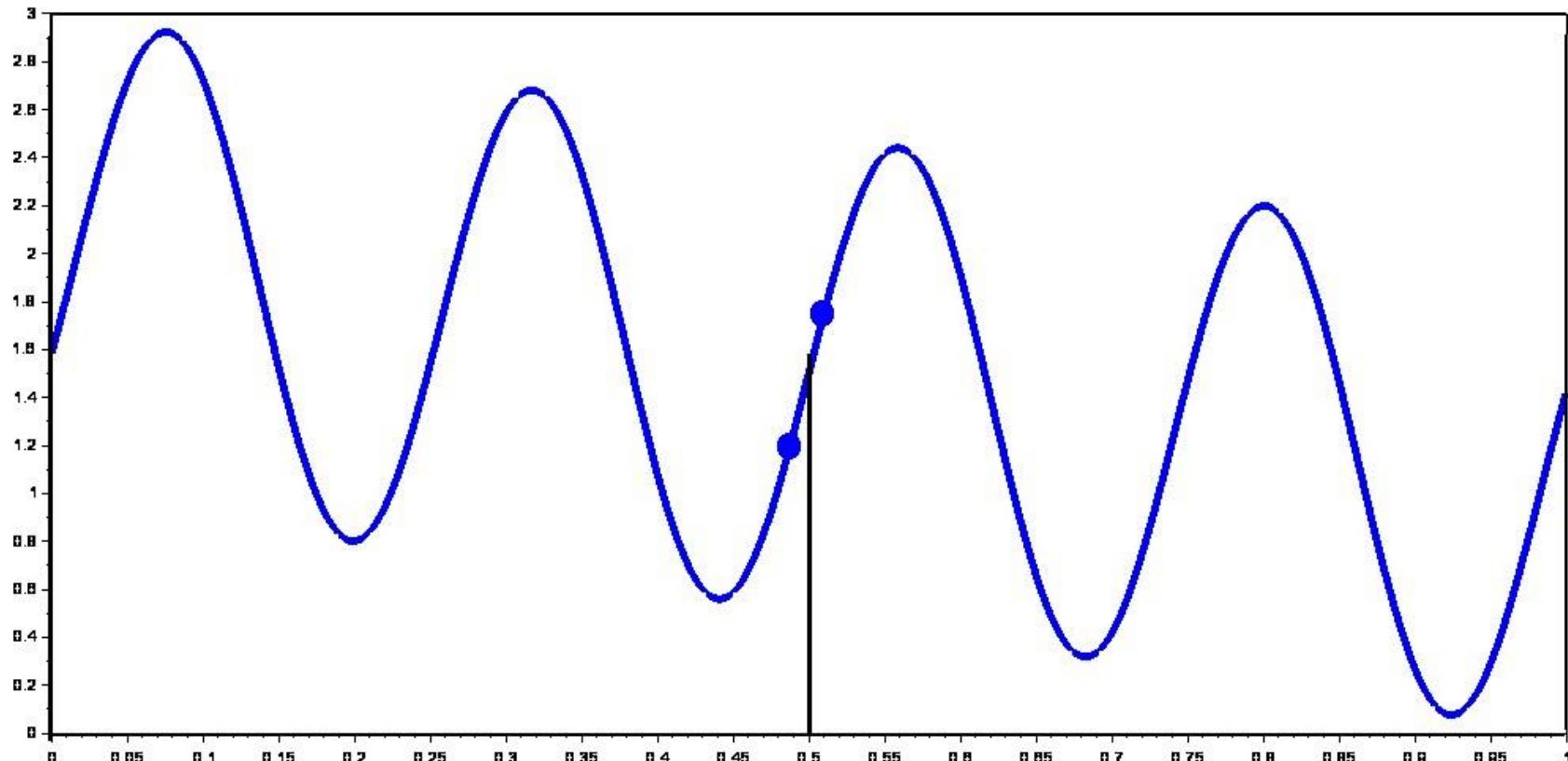


For the obtained segment $[a, x_2]$ or $[x_1, b]$ the procedure of halving the segment keeps on until the length of segment becomes small enough.

```
x=0:0.0002:1
y=x.*exp(x)+50*x.*sin(2*x).^2 -30*x
plot(x,y)
xgrid
x1=0
x2=1
delta=0.0000005
i=1
while x2-x1>.000002
    x3=0.5*(x1+x2)-delta ;
    x4=0.5*(x1+x2)+delta ;
    i=i+1 ;
    y3= x3*(exp(x3)+50*sin(2*x3)^2 -30) ;
    y4= x4*(exp(x4)+50*sin(2*x4)^2 -30) ;
    if y3<y4 then      x2=x4 ;
    else x1=x3 ;
```

```
end  
disp( y3,i)  
end  
xmin=0.5*(x3+x4)  
ymin= xmin*(exp(xmin)+50*sin(2*xmin)^2 -30)  
disp("ymin=",ymin,"xmin=", xmin)
```

It is recommended to plot a graph of the function $f(x)$ in order to avoid a loss of a minimum.



A golden section method.

In the bysection method, at each step, one needs to calculate $f(x)$ at two new points x_1, x_2 .

In a golden section method, at each step, one calculates $f(x)$ only at one new point. This can be performed by choosing

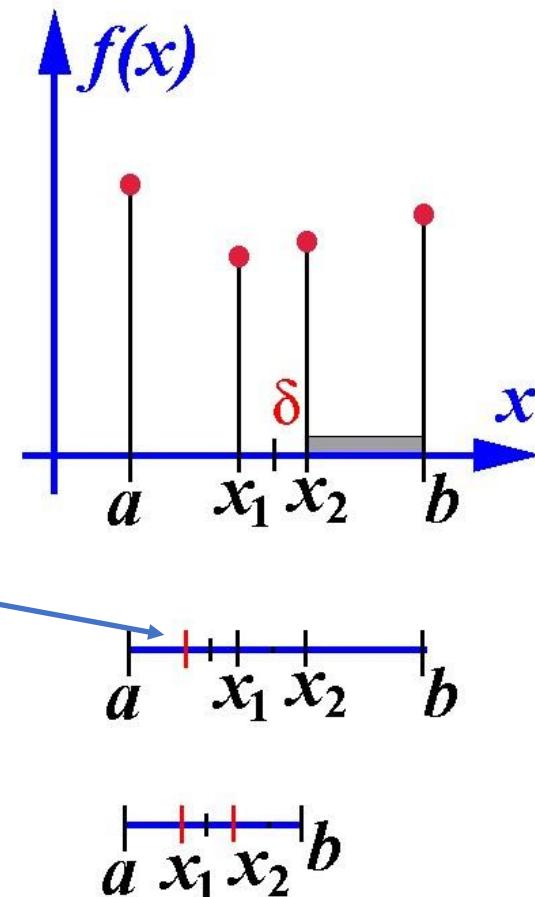
$$\delta = (\sqrt{5}/2 - 1) * (b-a)$$

In such a case, after dropping $[x_2, b]$, on the retained segment $[a, x_2]$ we already know $f(x_1)$, and x_1 is well located with respect to the middle of the retained segment $[a, x_2]$. Therefore, we only need to calculate f at the symmetric point indicated by a bar |

On the new segment $[a, x_2]$, all proportions between locations of points are the same as ones on $[a, b]$:

$$(b-a)/(x_2-a) = (x_2-a)/(x_1-a).$$

As a consequence, further reduction of the segment can be performed in the same way.



In the method of golden section, we need two times smaller amount of computations of $f(x)$; meanwhile the length of segment is reduced at each step by the smaller factor

1.618033988... .

(not by factor 2). Therefore, the eventual gain of computational time is:

2 / 1.618033988