

**Optimization
Techniques**


UNCONSTRAINED NLP EXAMPLE

Consider the problem:

Minimize $f(x_1, x_2, x_3) = (x_1)^2 + x_1(1 - x_2) + (x_2)^2 - x_2x_3 + (x_3)^2 + x_3$

First, we find the gradient with respect to x_i :

$$\nabla f = \begin{bmatrix} 2x_1 + 1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 + 1 \end{bmatrix}$$



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Next, we set the gradient equal to zero:

$$\nabla f = 0 \quad \Rightarrow \quad \begin{bmatrix} 2x_1 + 1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 + 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

So, we have a system of 3 equations and 3 unknowns. When we solve, we get:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$$


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So we have only one candidate point to check.

Find the Hessian:

$$\nabla^2 f = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$$

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The eigenvalues of this matrix are:

$$\lambda_1 = 3.414 \quad \lambda_2 = 0.586 \quad \lambda_3 = 2$$

All of the eigenvalues are > 0 , so the Hessian is positive definite.


So, the point $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$ is a minimum



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Unlike in Linear Programming, unless we know the shape of the function being minimized or can determine whether it is convex, we cannot tell whether this point is the global minimum or if there are function values smaller than it.




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UNCONSTRAINED NLP EXAMPLE

9.2: Taylor Series

Brook Taylor was an accomplished musician and painter. He did research in a variety of areas, but is most famous for his development of ideas regarding infinite series.



Brook Taylor
1685 - 1731

Greg Kelly, Hanford High School, Richland, Washington

Optimization Techniques

Suppose we wanted to find a fourth degree polynomial of the form:

$$P(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4$$

that approximates the behavior of $f(x) = \ln(x+1)$ at $x = 0$

If we make $P(0) = f(0)$ and the first, second, third and fourth derivatives the same, then we would have a pretty good approximation.

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$P(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4$ $f(x) = \ln(x+1)$

$f(x) = \ln(x+1)$ $f(0) = \ln(1) = 0$	$P(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4$ $P(0) = a_0 \rightarrow a_0 = 0$
$f'(x) = \frac{1}{1+x}$ $f'(0) = \frac{1}{1} = 1$	$P'(x) = a_1 + 2a_2x + 3a_3x^2 + 4a_4x^3$ $P'(0) = a_1 \rightarrow a_1 = 1$
$f''(x) = -\frac{1}{(1+x)^2}$ $f''(0) = -\frac{1}{1} = -1$	$P''(x) = 2a_2 + 6a_3x + 12a_4x^2$ $P''(0) = 2a_2 \rightarrow a_2 = -\frac{1}{2}$

→

Optimization

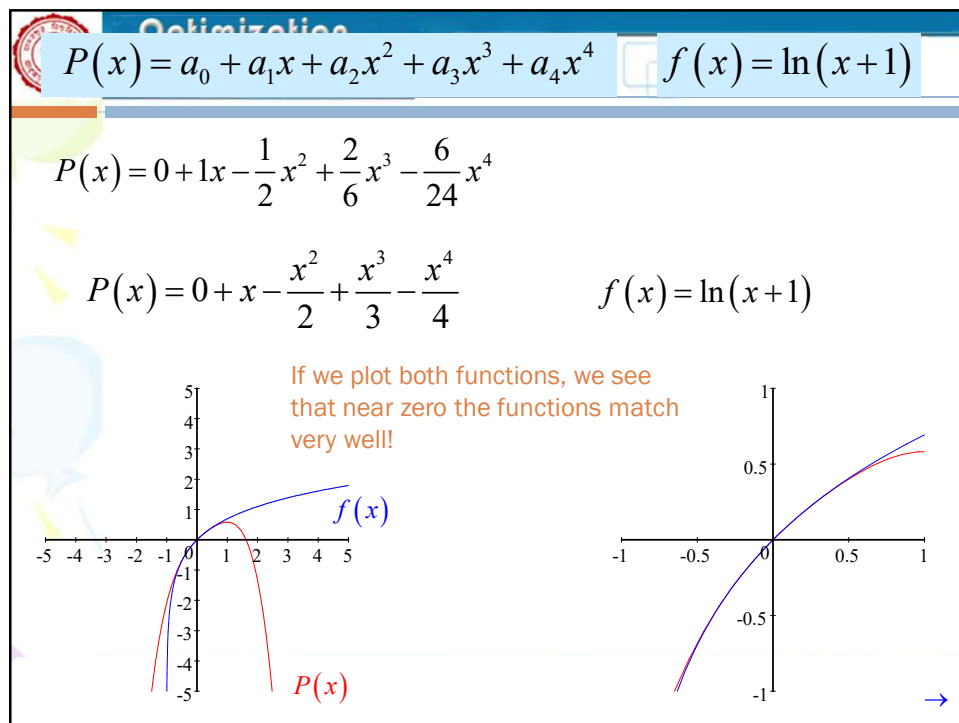
$P(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4$ $f(x) = \ln(x+1)$

$f''(x) = -\frac{1}{(1+x)^2}$ $P''(x) = 2a_2 + 6a_3x + 12a_4x^2$
 $f''(0) = -\frac{1}{1} = -1$ $P''(0) = 2a_2 \rightarrow a_2 = -\frac{1}{2}$

$f'''(x) = 2 \cdot \frac{1}{(1+x)^3}$ $P'''(x) = 6a_3 + 24a_4x$
 $f'''(0) = 2$ $P'''(0) = 6a_3 \rightarrow a_3 = \frac{2}{6}$

$f^{(4)}(x) = -6 \frac{1}{(1+x)^4}$ $P^{(4)}(x) = 24a_4$
 $f^{(4)}(0) = -6$ $P^{(4)}(0) = 24a_4 \rightarrow a_4 = -\frac{6}{24}$

→



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Our polynomial: $0 + 1x - \frac{1}{2}x^2 + \frac{2}{6}x^3 - \frac{6}{24}x^4$

has the form: $f(0) + f'(0)x + \frac{f''(0)}{2}x^2 + \frac{f'''(0)}{6}x^3 + \frac{f^{(4)}(0)}{24}x^4$

or: $\frac{f(0)}{0!} + \frac{f'(0)}{1!}x + \frac{f''(0)}{2!}x^2 + \frac{f'''(0)}{3!}x^3 + \frac{f^{(4)}(0)}{4!}x^4$

This pattern occurs no matter what the original function was!

Optimization

Maclaurin Series:

(generated by f at $x = 0$)

$$P(x) = f(0) + f'(0)x + \frac{f''(0)}{2!}x^2 + \frac{f'''(0)}{3!}x^3 + \dots$$

If we want to center the series (and its graph) at some point other than zero, we get the Taylor Series:

Taylor Series:

(generated by f at $x = a$)

$$P(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \dots$$

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example: $y = \cos x$

$$f(x) = \cos x \quad f(0) = 1 \quad f'''(x) = \sin x \quad f'''(0) = 0$$

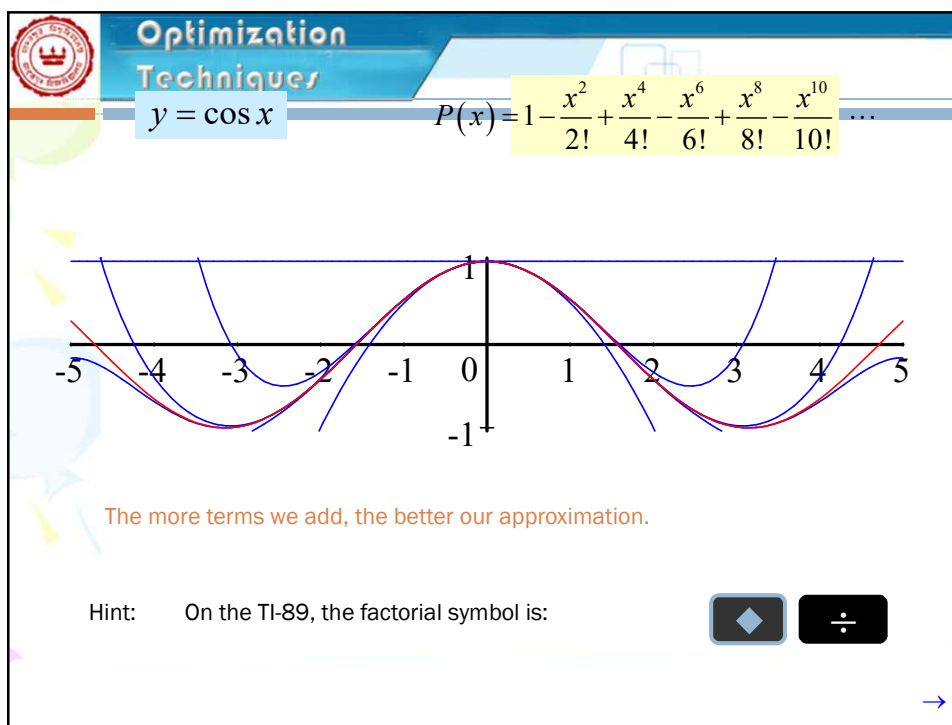
$$f'(x) = -\sin x \quad f'(0) = 0 \quad f^{(4)}(x) = \cos x \quad f^{(4)}(0) = 1$$

$$f''(x) = -\cos x \quad f''(0) = -1$$

$$P(x) = 1 + 0x - \frac{1x^2}{2!} + \frac{0x^3}{3!} + \frac{1x^4}{4!} - \frac{0x^5}{5!} + \frac{1x^6}{6!} - \dots$$

$$P(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \frac{x^8}{8!} - \frac{x^{10}}{10!} + \dots$$

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example: $y = \cos(2x)$

Rather than start from scratch, we can use the function that we already know:

$$P(x) = 1 - \frac{(2x)^2}{2!} + \frac{(2x)^4}{4!} - \frac{(2x)^6}{6!} + \frac{(2x)^8}{8!} - \frac{(2x)^{10}}{10!} \dots$$

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example: $y = \cos(x)$ at $x = \frac{\pi}{2}$


$$f(x) = \cos x \quad f\left(\frac{\pi}{2}\right) = 0 \quad f'''(x) = \sin x \quad f'''\left(\frac{\pi}{2}\right) = 1$$

$$f'(x) = -\sin x \quad f'\left(\frac{\pi}{2}\right) = -1 \quad f^{(4)}(x) = \cos x \quad f^{(4)}\left(\frac{\pi}{2}\right) = 0$$

$$f''(x) = -\cos x \quad f''\left(\frac{\pi}{2}\right) = 0$$

$$P(x) = 0 - 1\left(x - \frac{\pi}{2}\right) + \frac{0}{2!}\left(x - \frac{\pi}{2}\right)^2 + \frac{1}{3!}\left(x - \frac{\pi}{2}\right)^3 + \dots$$


$$P(x) = -\left(x - \frac{\pi}{2}\right) + \frac{\left(x - \frac{\pi}{2}\right)^3}{3!} - \frac{\left(x - \frac{\pi}{2}\right)^5}{5!} + \dots$$



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There are some Maclaurin series that occur often enough that they should be memorized. They are on your formula sheet.

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Optimization

When referring to Taylor polynomials, we can talk about **number of terms**, **order** or **degree**.

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!}$$

This is a polynomial in **3 terms**.

It is a **4th order** Taylor polynomial, because it was found using the 4th derivative.

It is also a **4th degree** polynomial, because x is raised to the 4th power.

The **3rd order** polynomial for $\cos x$ is $1 - \frac{x^2}{2!}$, but it is **degree 2**.




A recent AP exam required the student to know the difference between *order* and *degree*.

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The TI-89 finds Taylor Polynomials:

taylor (expression, variable, order, [point])

taylor (cos(x), x, 6) $\frac{-x^6}{720} + \frac{x^4}{24} - \frac{x^2}{2} + 1$


taylor (cos(2x), x, 6) $\frac{-4x^6}{45} + \frac{2x^4}{3} - 2x^2 + 1$

taylor (cos(x), x, 5, $\pi/2$) $\frac{-(2x-\pi)^5}{3840} + \frac{(2x-\pi)^3}{48} - \frac{2x-\pi}{2}$ π

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Summary

- A first order approximation of $f(x)$ around point \bar{x} is given by
- $f_1(x) = f(x') + f'(x') * (x - x')$
- *Taylor Approximation around a vector x*
- $f_1(x) = f(x^k) + \nabla f(x^k)^T (x - x^k)$
- $f_1(x) = f(x^k) + \sum_{j=1}^n \frac{\partial f(x^k)}{\partial x_j} (x_j - x_j^k)$
- Determine first order Taylor approximation of the function
 - $f(x_1, x_2) = x_1^4 + x_1^2 + 2x_2^2 - 2x_1x_2$ around a point $(x_1, x_2) = (1, 1)$




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Summary

- A second order approximation of $f(x)$ around point \bar{x} for single variable is given by
- $f_2(x) = f(x') + f'(x')(x - x') + \frac{1}{2} f''(x')(x - x')^2$
- *A second order Taylor Approximation around a vector x*
- $f_2(x) = f(x^k) + \nabla f(x^k)^T (x - x^k) + \frac{1}{2} (x - x^k)^T H(x^k) (x - x^k)$
- $f_1(x) = f(x^k) + \sum_{j=1}^n \frac{\partial f(x^k)}{\partial x_j} (x_j - x_j^k) + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2 f(x^k)}{\partial x_i \partial x_j} (x_i - x_i^k) (x_j - x_j^k)$


$f(x_1, x_2) = x_1^4 + x_1^2 + 2x_2^2 - 2x_1x_2$ around a point $(x_1, x_2) = (1, 1)$



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METHOD OF SOLUTION


- In the previous example, when we set the gradient equal to zero, we had a system of 3 linear equations & 3 unknowns.
- For other problems, these equations could be nonlinear.
- Thus, the problem can become trying to solve a system of nonlinear equations, which can be very difficult.



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METHOD OF SOLUTION

- To avoid this difficulty, NLP problems are usually solved numerically.
- We will now look at examples of numerical methods used to find the optimum point for single-variable NLP problems. These and other methods may be found in any numerical methods reference.



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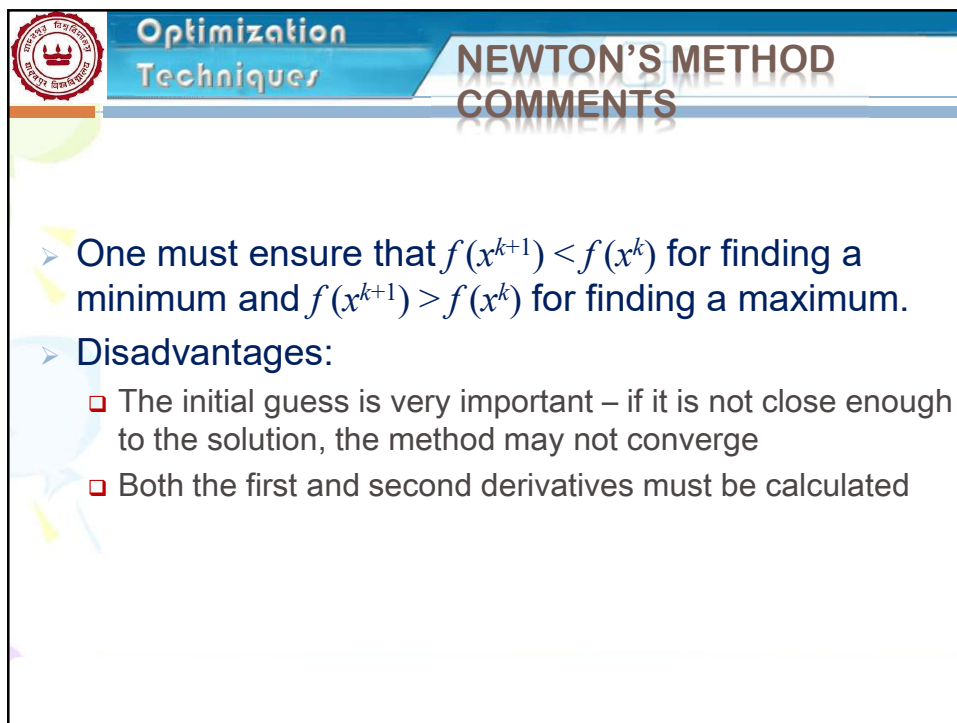
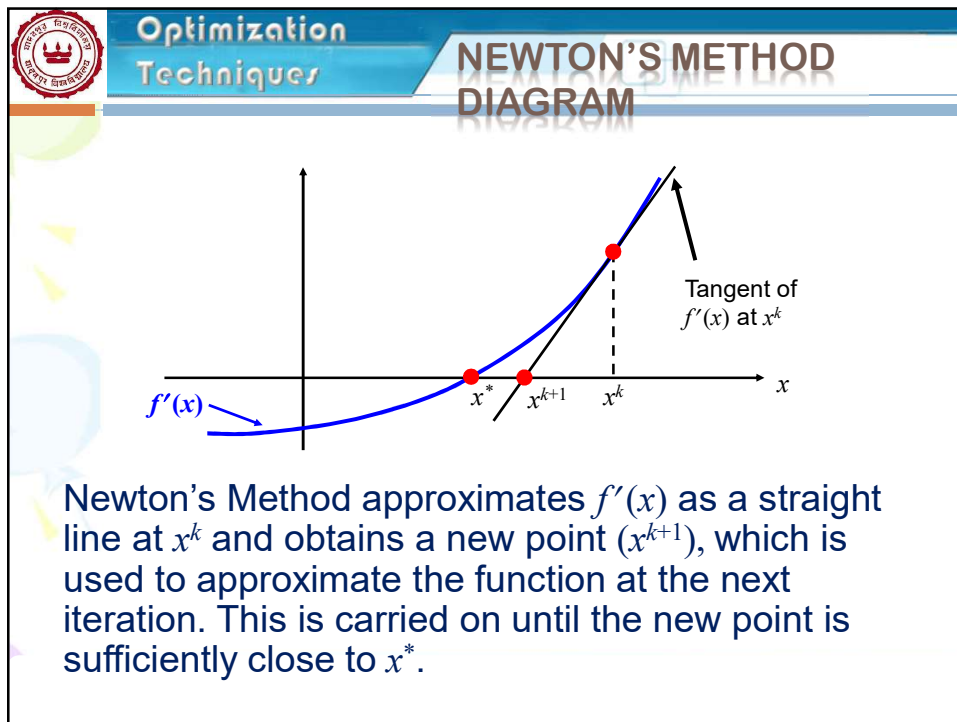
NEWTON'S METHOD


When solving the equation $f'(x) = 0$ to find a minimum or maximum, one can use the iteration step:

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

where k is the current iteration.

Iteration is continued until $|x^{k+1} - x^k| < \varepsilon$ where ε is some specified tolerance.






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REGULA-FALSI METHOD

This method requires two points, x^a & x^b that bracket the solution to the equation $f'(x) = 0$.

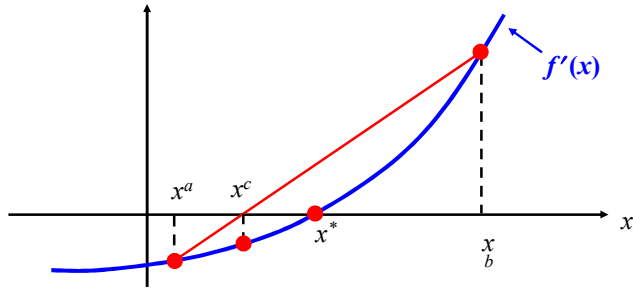
$$x^c = x^b - \frac{f'(x^b) \cdot (x^b - x^a)}{f'(x^b) - f'(x^a)}$$

where x^c will be between x^a & x^b . The next interval will be x^c and either x^a or x^b , whichever has the sign opposite of x^c .




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REGULA-FALSI DIAGRAM




The Regula-Falsi method approximates the function $f'(x)$ as a straight line and interpolates to find the root.



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REGULA-FALSI COMMENTS

- This method requires initial knowledge of two points bounding the solution
- However, it does not require the calculation of the second derivative
- The Regula-Falsi Method requires slightly more iterations to converge than the Newton's Method




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MULTIVARIABLE OPTIMIZATION

- Now we will consider unconstrained multivariable optimization
- Nearly all multivariable optimization methods do the following:
 1. Choose a search direction \mathbf{d}^k
 2. Minimize along that direction to find a new point:

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha^k \mathbf{d}^k$$


where k is the current iteration number and α^k is a positive scalar called the step size.



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THE STEP SIZE

- The step size, α^k , is calculated in the following way:
- We want to minimize the function $f(\mathbf{x}^{k+1}) = f(\mathbf{x}^k + \alpha^k \mathbf{d}^k)$ where the only variable is α^k because \mathbf{x}^k & \mathbf{d}^k are known.
- We set $\frac{df(\mathbf{x}^k + \alpha^k \mathbf{d}^k)}{d\alpha^k} = 0$ and solve for α^k using a single-variable solution method such as the ones shown previously.



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STEEPEST DESCENT METHOD

- This method is very simple – it uses the gradient (for maximization) or the negative gradient (for minimization) as the search direction:

$$\mathbf{d}^k = \begin{cases} + \\ - \end{cases} \nabla f(\mathbf{x}^k) \text{ for } \begin{cases} \max \\ \min \end{cases}$$

So, $\mathbf{x}^{k+1} = \mathbf{x}^k + \begin{cases} + \\ - \end{cases} \alpha^k \nabla f(\mathbf{x}^k)$

