

Unconstrained optimization algorithms

Sridharakumar Narasimhan

Professor,

Department of Chemical Engineering

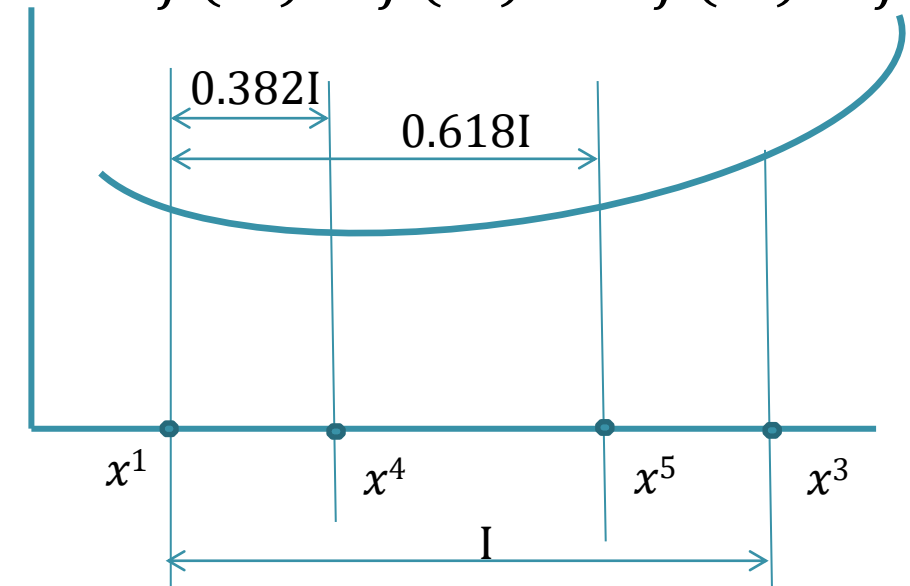
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Univariate unconstrained optimization

- Minimize $f(x)$
- Bracketing:** Find interval containing 3 points such that $f(x^1) > f(x^2)$ and $f(x^2) < f(x^3)$
- Solution lies in interval $x^1 \leq x^* \leq x^3$
- Interval size $I = x^3 - x^1$
- Refinement:**
- Golden section method chooses points

$$x^4 = x^1 + 0.382 I$$

$$x^5 = x^1 + 0.618 I$$
- Evaluate $f(x^4)$ and $f(x^5)$ and identify new interval $[x^1, x^4, x^5]$
- Evaluate at one more point $x^1 + 0.618(x^5 - x^1)$
- Note in either case we need to choose only one more point

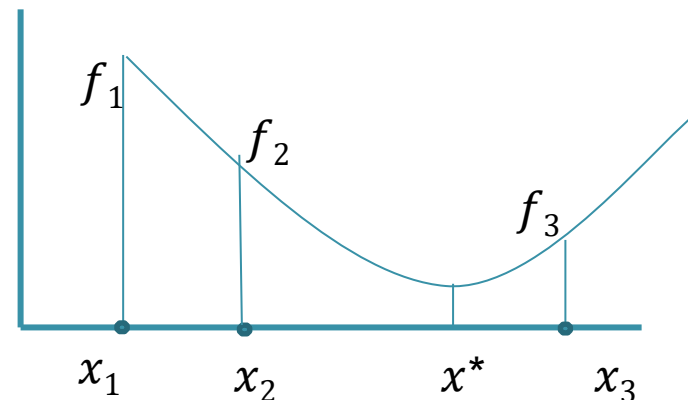


Univariate unconstrained optimization –

- **Refinement based on quadratic or cubic interpolation**
- Fit an approximate quadratic (or cubic) function using three (four) points
 - $f(x) = a + bx + cx^2$
 - Determine constants a, b, c using $[x^1, f(x^1); x^2, f(x^2); x^3, f(x^3)]$ – will get an exact fit
- Determine optimal solution of quadratic approximation

$$x^* = 0.5 \frac{(x_2^2 - x_3^2)f_1 + (x_3^2 - x_1^2)f_2 + (x_1^2 - x_2^2)f_3}{(x_2 - x_3)f_1 + (x_3 - x_1)f_2 + (x_1 - x_2)f_3}$$

- Choose interval consisting of three points such that function decreases and then increase over the interval $[x_2, x^*, x_3]$
- Repeat until convergence




Univariate unconstrained optimization - example

- Minimize $f(x) = x^4 - x + 1$
- Bracketing:**

x	0	-0.5	0.5	1
f(x)	1	1.5625	0.5625	1


- Interval = $[0, 0.5, 1]$
- Refinement:**

- Golden section



x	0	1	0.382	0.618	0.7639	0.5279	
f(x)	1	1	0.6393	0.5279	0.5767	0.5498	

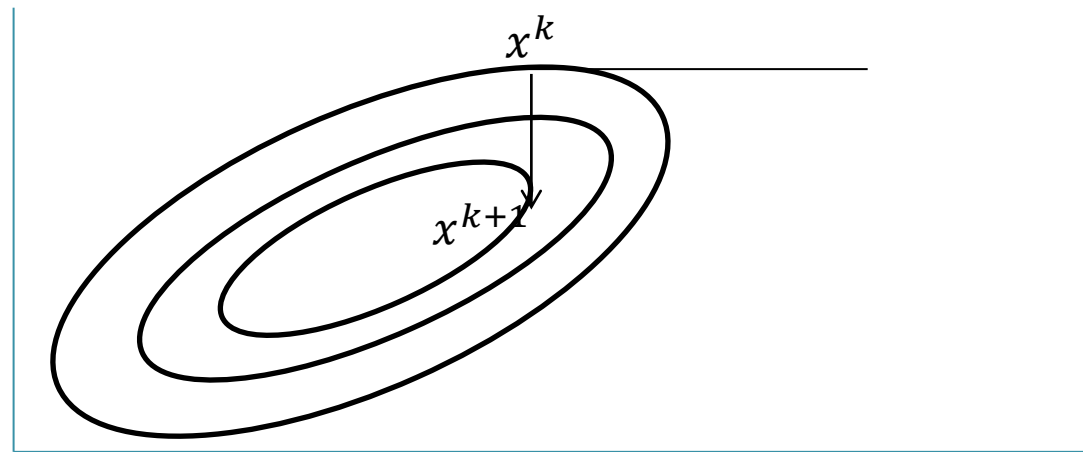
- Quadratic interpolation



x	0	0.382	1	0.5	0.5728	0.5279	
f(x)	1	0.6393	1	0.5625	0.5348	0.5498	

Multivariate unconstrained optimization

- Minimize $f(x_1, x_2, \dots, x_n) = f(x)$
- **Steepest descent**
 - At iteration k starting point is x^k
 - Search direction $s^k =$ Negative of gradient of $f(x) = -\nabla f(x^k)$
 - New point is $x^{k+1} = x^k + \alpha^k s^k$ where α^k is the value of α for which $f(x^{k+1}) = f(\alpha)$ is a minimum (univariate minimization)



Steepest descent method - example

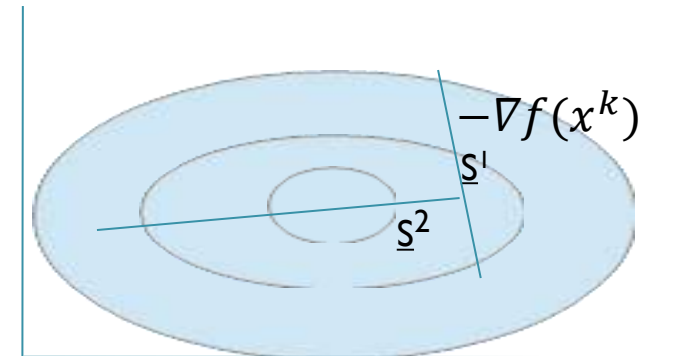
- Minimize $f(x_1, x_2) = x_1^4 - 2x_2x_1^2 + x_2^2 + x_1^2 - 2x_1 + 5$
- Initial point $x^0 = [1 \ 2]$
- $f(x^0) = 5$; $s^0 = -\nabla f(x^0) = [4 \ -2]$
- $x^1 = [1 \ 2] + \alpha[4 \ -2] = [(1 + 4\alpha) \ (2 - 2\alpha)]$
- Bracketing

α	0	0.05	0.1	0.0797
x_1	1	1.2	1.6	1.3188
x_2	2	1.9	1.7	1.8406
$f(\alpha)$	5	4.25	5.1	4.112

Multivariate unconstrained optimization

• Conjugate Gradient Method

- s^{k+1} and s^k are H conjugate if $(s^{k+1})^T H s^k = 0$
- For quadratic function in 2 variables, the optimum is found in 2 steps(iterations) if H is Hessian (matrix of 2nd derivatives) of the objective function



- Without knowing H:
- $$s^{k+1} = -\nabla f(x^{k+1}) + s^k \frac{\nabla^T f(x^{k+1}) \nabla f(x^{k+1})}{\nabla^T f(x^k) \nabla f(x^k)}$$
- For a quadratic function in n variables it can be shown that these successive search directions are H conjugate. After n iterations the quadratic function is minimized

Convergence Criteria

- Terminate when $\|\nabla f(x^k)\|$ is less than some prescribed tolerance
- Terminate if $\|s^k\|$ less than tolerance
- Terminate if maximum absolute or relative change in x_i is less than tolerance
- Terminate if relative change in absolute or relative change in objective function $f(x)$ is less than tolerance
- Terminate if maximum number of iterations reached