Unconstrained Optimization
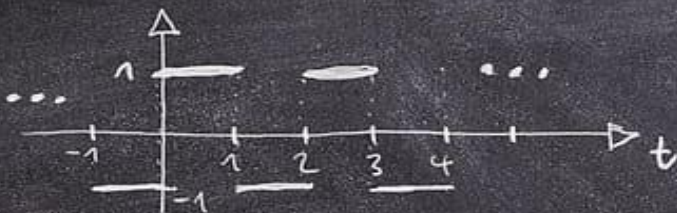
Presentation topics

- Methods used
- Problems analysis
- Final discussion and considerations

Objective: Explore and confirm theoretical assumptions and practical tradeoffs between methods
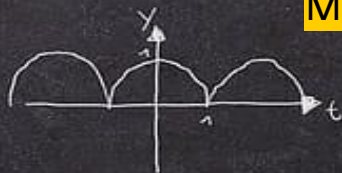
$$f(t) = a_0 + \sum_{n=1}^{\infty} \left[a_n \cdot \cos\left(\frac{n\pi t}{L}\right) + b_n \cdot \sin\left(\frac{n\pi t}{L}\right) \right]$$

$$= a_0 + a_1 \cdot \cos\left(\frac{\pi t}{L}\right) + b_1 \cdot \sin\left(\frac{\pi t}{L}\right) + a_2 \cdot \cos\left(\frac{2\pi t}{L}\right) + b_2 \cdots$$

$$\sqrt{a(\omega)^2 + b(\omega)^2}$$

Methods used

Methods explanation

$$\cdots)dt = \frac{1}{2}\int_{-1}^{1} f(t)\,dt$$

$$= \frac{1}{2}\int_{-1}^{0} f(t)\,dt + \frac{1}{2}\int_{0}^{1} f(t)\,dt$$

$$= \frac{1}{2}\int_{-1}^{0} -1\,dt + \frac{1}{2}\int_{0}^{1} 1\,dt$$

$$= \frac{1}{2}\left[-t\right]_{-1}^{0} + \frac{1}{2}\left[t\right]_{0}^{1}$$

$$= -\frac{1}{2} + \frac{1}{2} = \emptyset$$

$2L=2 \Rightarrow L=1$

$a_n \simeq \frac{1}{n^2}$

$b_n = \emptyset$

$a_n \longrightarrow a(\omega)$

$b_n \longrightarrow b(\omega)$

Methods used

Steepest Descent Method: Informed ($\nabla f(x)$ given)

Conjugate Gradient Method: Informed ($\nabla f(x)$ given)

Inexact Newton Method: Uninformed ($\nabla f(x)$ and $\nabla^2 f(x)$ not given)
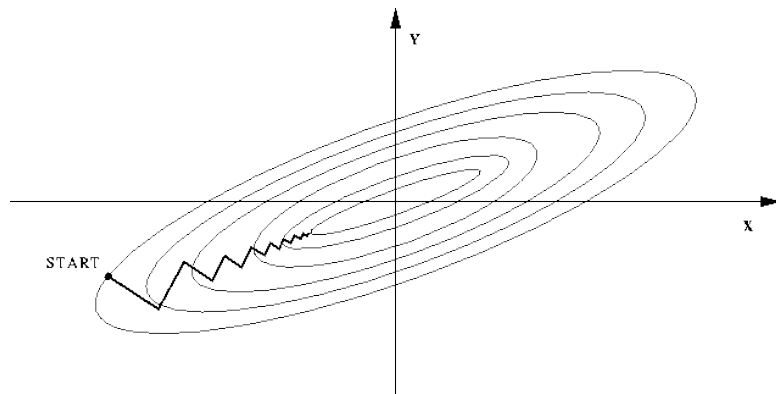**(with finite differences)** and approximated computations

Steepest Descent Method

Takes the **negative gradient as descending direction** everytime.

Best local descent direction, not best descent direction overall.

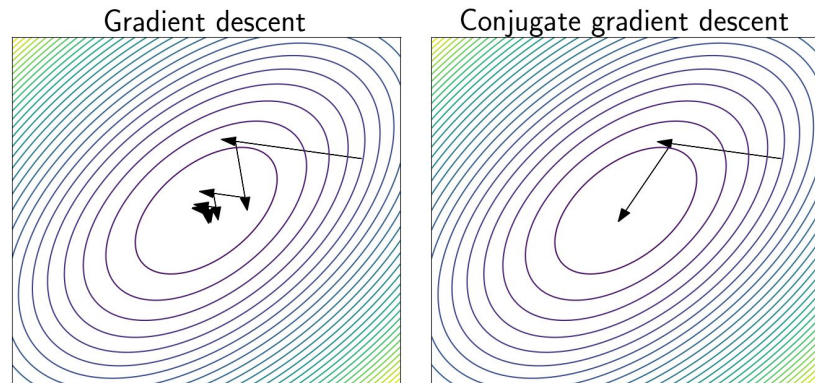Last direction orthogonal to the previous, thus is **conditioning dependent**.

$$p_k = -\nabla f(x_k)$$

Conjugate Gradient Method

Improved SD method.

New descent direction is never orthogonal. It is conjugate to the previous.

Better convergence can be proven.

Gradient descent

Conjugate gradient descent

$$\beta_k = -\frac{(d_k)^T A r^{(k+1)}}{d_k^T A d_k}$$

$$p_{k+1} = -\nabla f_{k+1} + \beta^{k+1} p^k$$

CG method extended to a nonlinear function f:
- Steplength α computed with a line search
- Residual not anymore r = b – Ax, but replaced by ∇f

$$\beta^{k+1} = \frac{\nabla f_{k+1}^T \nabla f_{k+1}}{\nabla f_k^T \nabla f_k} = \frac{||\nabla f_{k+1}||^2}{||\nabla f_k||^2}$$
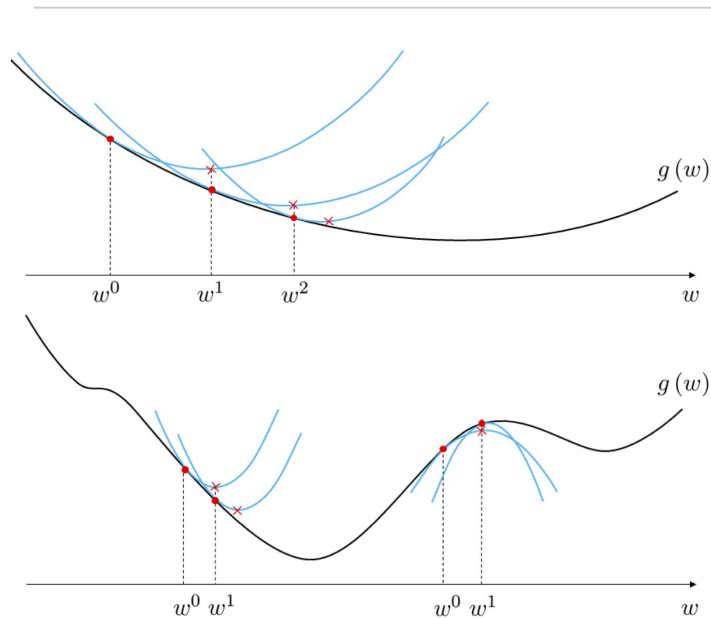
Fletcher & Reeve's version

Newton Method

Exploits the quadratic approximation of the function.

Needs both gradient and hessian of the function.

Hessian has to be SPD, orelse convergence is not guaranteed.

$$p = -(\nabla^2 f(x_k))^{-1} \nabla f(x_k).$$

Inexact Newton Method

Exact descent direction can be hard to compute exactly (exact min of paraboloid):

$$p = -(\nabla^2 f(x_k))^{-1} \nabla f(x_k).$$

We approximate it instead:

$$\|\nabla^2 f(x_k)p + \nabla f(x_k)\| \leq \eta_k \|\nabla f(x_k)\|$$

(!) Updating tolerance: Near the solution → More precise solving

Inexact Newton Method
Forcing Terms

To compute descent direction we use an **iterative solver** (pcg).

More exact → More inner iterations (for Descent Direction)

Less exact → More outer iterations (Newton steps)

Compromise, so use a suitable **forcing term**:

$$||\nabla^2 f(x_k)p + \nabla f(x_k)|| \leq \eta_k ||\nabla f(x_k)|| \qquad \eta_k = \min(0.5, \sqrt{||\nabla f(x_k)||})$$

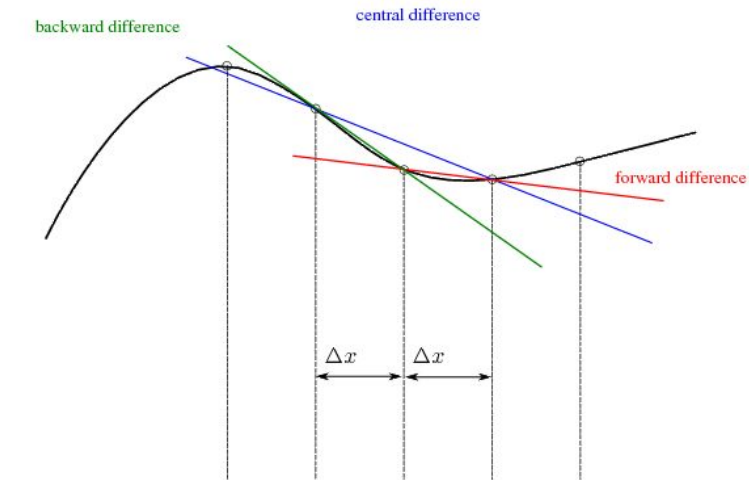(superlinear convergence is not guaranteed, but generally expected)

Newton Method
Finite differences

Gradient and Hessian may be hard to compute.

Approximate them with incremental ratio expressions.

We approximated both:

- ◉ gradient (central difference)
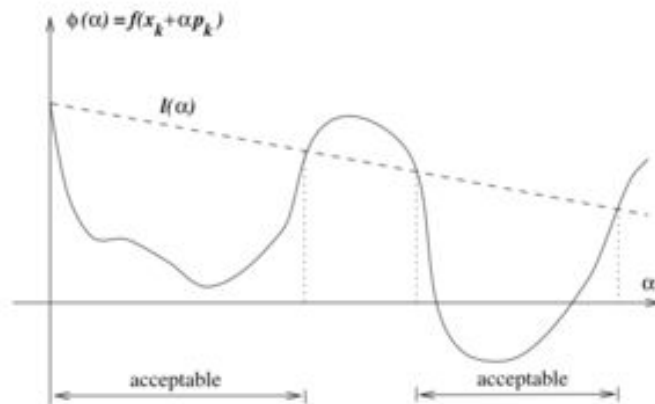- ◉ Hessian (forward difference)

Line search and Armijo condition

In non-linear case we cannot say apriori which is the best step length.

Only 'descent' is not enough.

We must choose one that guarantees 'sufficient descent'.

$$f(\mathbf{x}_k + \alpha_k \mathbf{p}_k) \leq f(\mathbf{x}_k) + c_1 \alpha_k \mathbf{p}_k^{\mathrm{T}} \nabla f(\mathbf{x}_k)$$

Problem analysis
&
Taken approach

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Parameters and approach

- Convergence threshold set as: $\|\nabla f_k(x)\| = 10^{-6}$

- Armijo condition:
  - $\alpha_0 = 5$ ($\alpha_0 = 1$ for NM)
  - $\rho = 0.5$
  - $C_1 = 10^{-4}$

- NM, fully uninformed:
  - Gradient FD: Forward
  - Hessian FD: Central

ROSENBROCK FUNCTION

- All methods converge to the actual minimum x*=(1, 1) with starting point x_0

- Changing the start point to x_1 , SD and CG–FR perform well, while INM does not converge.

$$f(x_1, x_2) = (1 - x_1)^2 + 100\left(x_2 - x_1^2\right)^2$$

$$\overline{x_{(0)}} = (1.2, 1.2), \overline{x_{(1)}} = (-1.2, 1)$$

[P05] GENERALIZED BROYDEN TRIDIAGONAL FUNCTION

- All methods converge but convergence points are distant: problem has multiple minpoints

- Changing the start point to origin they remain distant and NM does not converge ($\nabla^2 f(x)$ non positive definite)

- NM very slow (many computations for Hessian)

$$F(x) = \sum_{i=1}^{n} |(3 - 2x_i)\, x_i - x_{i-1} - x_{i+1} + 1|^p$$

$$p = 7/3, \quad \overline{x_0} = \overline{x_{n+1}} = 0$$

$$\overline{x_i} = -1, \quad i \geq 1.$$

[P13] GENERALIZATION OF THE BROWN FUNCTION 2

- All methods converge to the same point

- The convergence rate respects the theory (relatively to each other):
  - NM: 7 iterations
  - CG–FR: 10 iterations
  - SD: 15 iterations

$$F(x) = \sum_{j=1}^{k} \left[\left(x_{i-1}^2\right)^{\left(x_i^2+1\right)} + \left(x_i^2\right)^{\left(x_{i-1}^2+1\right)} \right],$$

$$i = 2j, \quad k = n/2,$$

$$\overline{x_i} = -1, \text{mod}(i, 2) = 1, \quad \overline{x_i} = 1, \text{mod}(i, 2) = 0.$$

[P14] DISCRETE BOUNDARY VALUE PROBLEM

- No method converges completely
- SD and CG–FR gets to $\|\nabla f_k(x)\| = 10^{-3}$ after 50'000 iterations
- NM stopped after 5 iterations as it wasn't making progress
- Starting from the origin NM converges to the same optimal point (only better convergence criterion)

$$F(x) = \sum_{i=1}^{n} \left[2x_i - x_{i-1} - x_{i+1} + h^2 \left(x_i + ih + 1 \right)^3 / 2 \right]^2,$$

$$h = 1/(n+1), \quad \overline{x_0} = \overline{x_{n+1}} = 0,$$

$$\overline{x}_i = ih(1 - ih), \quad i \geq 1.$$

[P16] BANDED TRIGONOMETRIC PROBLEM

- No method converges completely
- Starting from the origin the situation slightly improves
- Trying with a smaller n (=100) they actually converge: it is only time/computing problem issue

$$F(x) = \sum_{i=1}^{n} i\left[(1 - \cos x_i) + \sin x_{i-1} - \sin x_{i+1}\right]$$

$$x_0 = x_{n+1} = 0 \qquad \bar{x}_i = 1, \quad i \geq 1$$

**Final
Discussion**

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Final Discussion

- Methods, when applicable, do respect theoretical convergence rate (at least in respect to each other)

- Fully uninformed NM has too many computations every iteration, thus takes a lot of time to finish

- NM is unreliable as it's hessian matrix can become non–PD and this can change based on starting point

- *Improvement*: Changing Hessian to become positive definite at each iteration can solve the non–reliability problem

Team Presentation

Florentin-Cristian Udrea
S319029

Sara Rosato
S317547

Thanks for the attention!