Computer Science

Jerzy Świątek

Systems Modelling and Analysis

Choose yourself and new technologies

L.17. Numerical optimization methods

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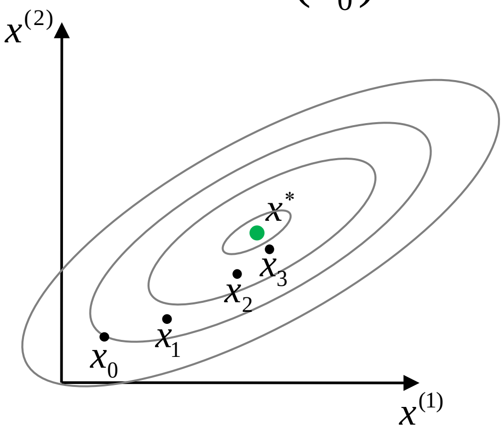
Numerical methods

We only use information about values of objective function $F(x)$ for a given value of x.

$$x_0 \to x_1 \to x_2 \to \cdots \to x_N \approx x^*$$

$$F(x_0) > F(x_1) > F(x_2) > \cdots > F(x_N) \approx F(x^*)$$

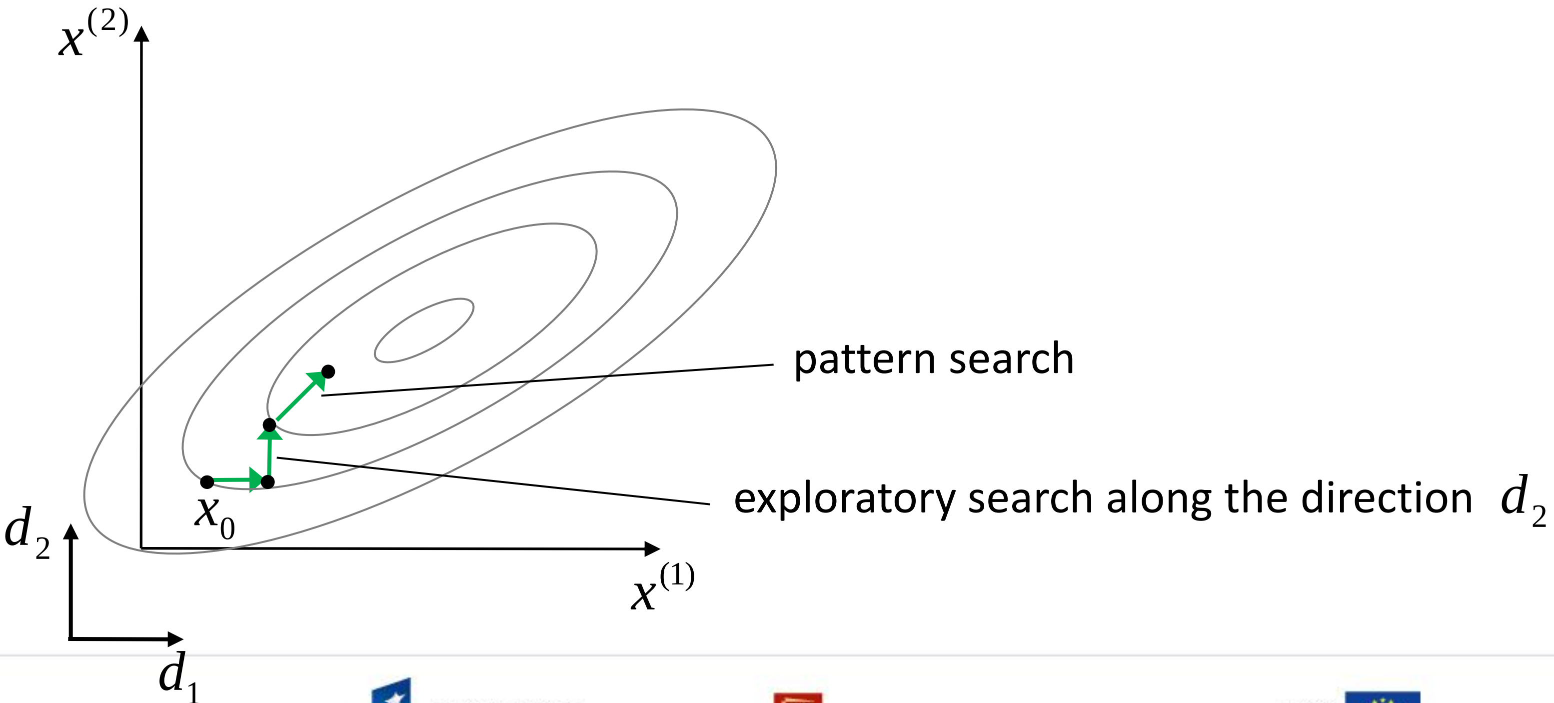


The general idea behind numerical methods.

$$x_{n+1} = G(x_n)$$

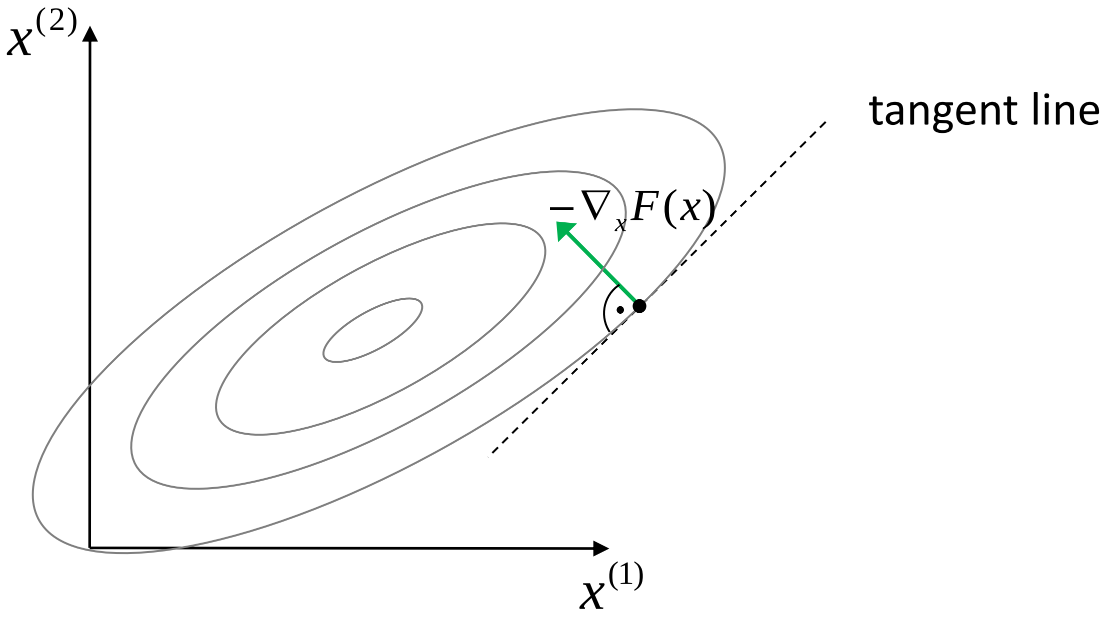
Numerical methods

- Mutlidimensional search without gradient



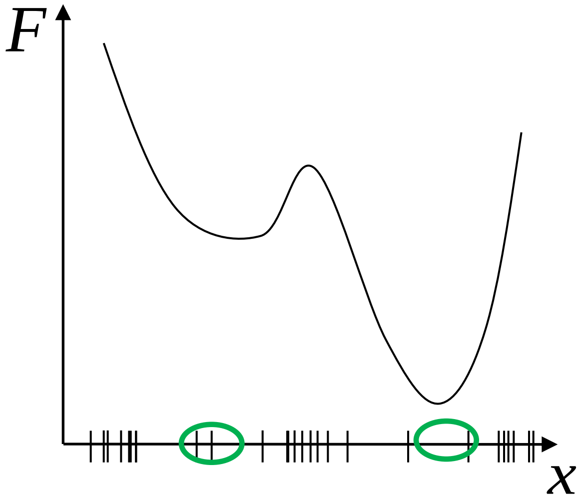
Numerical methods

- Gradient based methods



Numerical methods

- Random search methods



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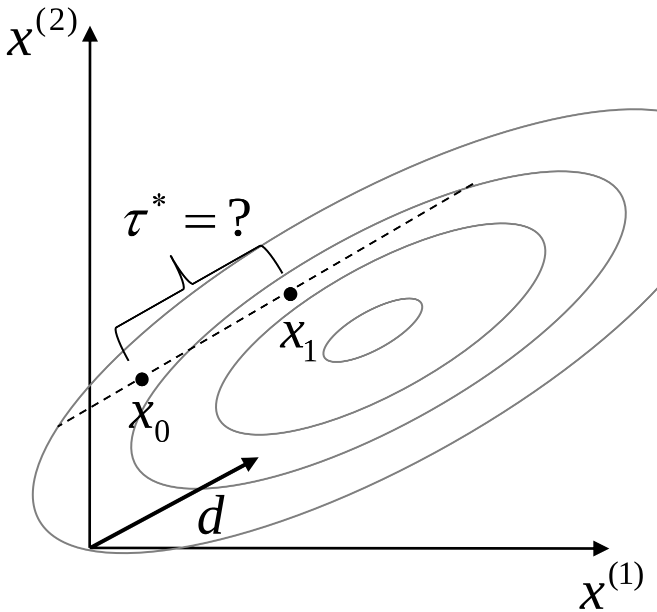
Numerical methods

- Line search methods



$$x_0 \rightarrow x_1 = x_0 + \tau d$$

$$F\left(x_0 + \tau^* d\right) = \min_{\tau} F\left(x_0 + \tau d\right)$$

For given values of x_0, d :

$$F\left(x_0 + \tau d\right) \equiv f(\tau)$$

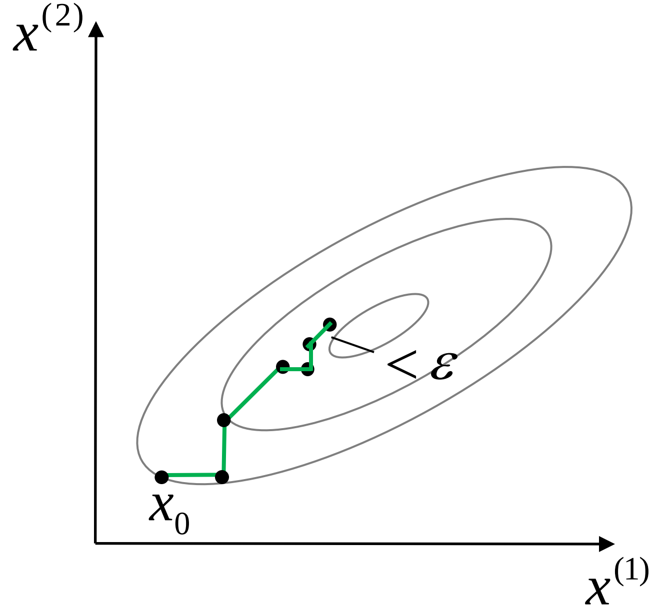
where f is one dimensional function.

Optimization task is: $\tau^* \rightarrow f(\tau^*) = \min_{\tau} f(\tau)$

Numerical methods

- Termination criterion

1) $\left\| x_{n+1} - x_n \right\| < \varepsilon$

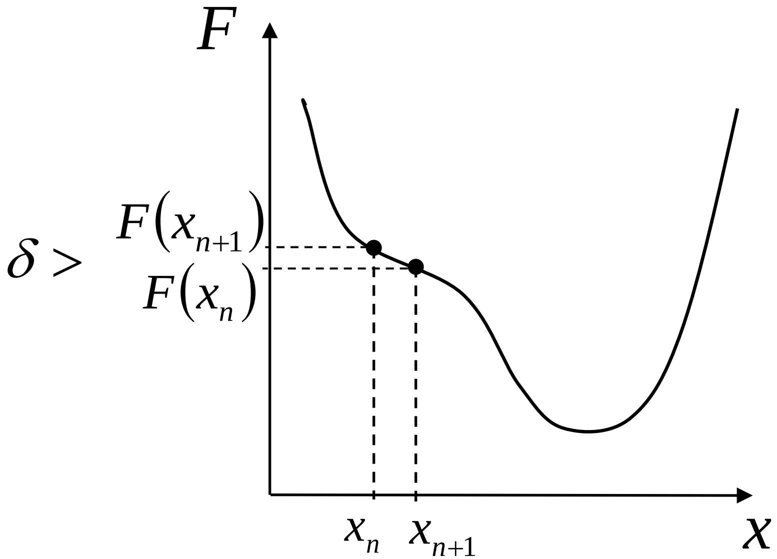


Numerical methods

- Termination criterion

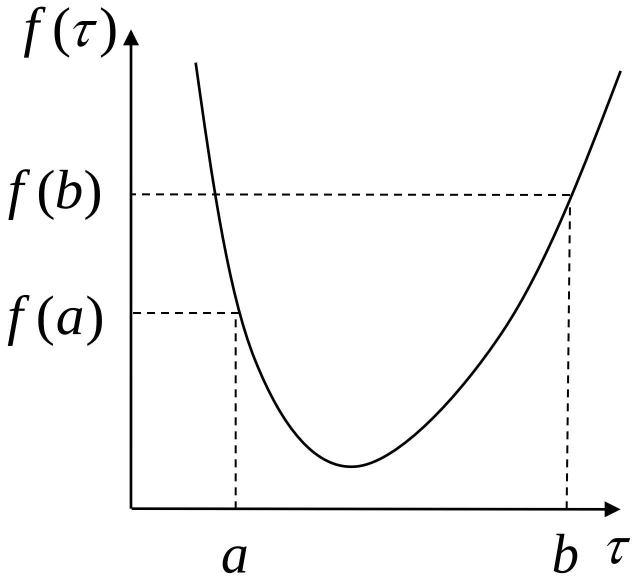
2) $\| F(x_{n+1}) - F(x_n) \| < \delta$

3) $\dfrac{\| F(x_{n+1}) - F(x_n) \|}{\| x_{n+1} - x_n \|} < \delta$



Numerical methods

- Line search



$$x \in \langle a, b \rangle \Rightarrow f(x) < \max\left(f(a), f(b)\right)$$

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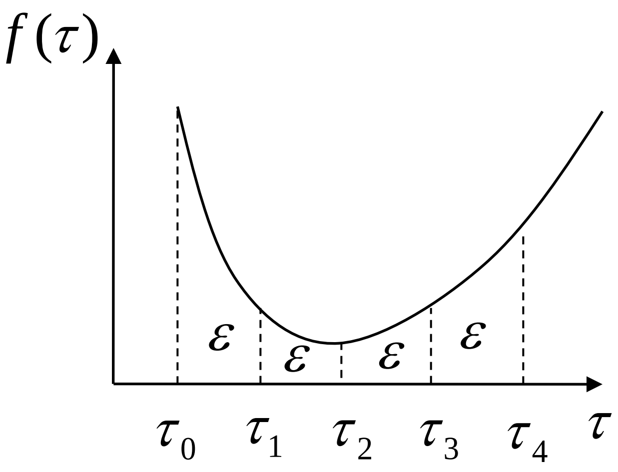
Numerical methods

- Line search – the uniform search method



$$\tau_0 = a$$

$$\tau_n = \tau_0 + n\varepsilon$$

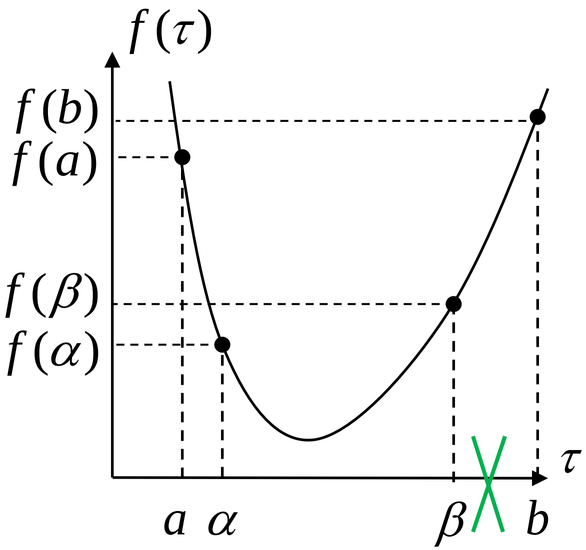
$$N = \left[\frac{b-a}{\varepsilon}\right] + 1$$

N – the number of iterations

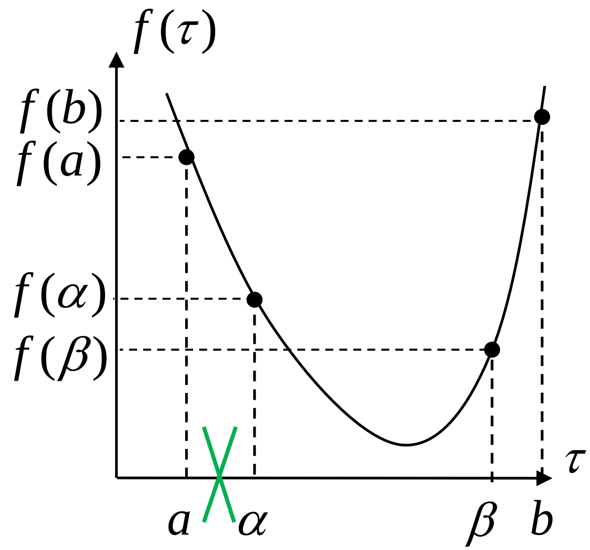
$$\tau^* \approx \tilde{\tau} \rightarrow f(\tilde{\tau}) = \min_{1 \le n \le N} f(\tau_n)$$

Numerical methods

- Line search – the golden section method



$$f(\alpha) < f(\beta) \Rightarrow a := a,\ b := \beta$$



$$f(\alpha) > f(\beta) \Rightarrow a := \alpha,\ b := b$$

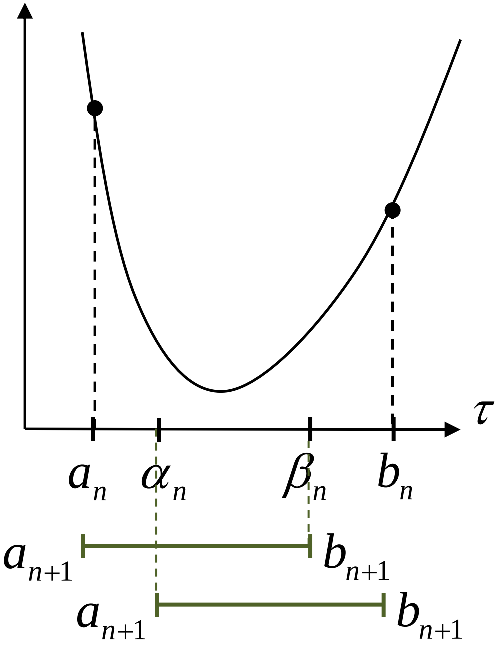
Numerical methods

- Line search – the golden section method

How to determine values of α, β ?

$$\begin{cases} \dfrac{\beta_n - a_n}{b_n - a_n} = \gamma \\ \dfrac{b_n - \alpha_n}{b_n - a_n} = \gamma \end{cases}$$

$$\begin{cases} \beta_n = a_n + \gamma(b_n - a_n) \\ \alpha_n = b_n - \gamma(b_n - a_n) \end{cases}$$

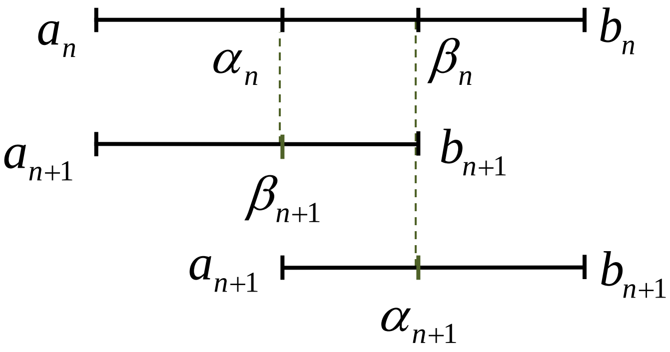


Numerical methods

- Line search – the golden section method

How to determine values of α, β in order to reduce the number of the goal function's calculations?

$$\frac{\beta_{n+1} - a_{n+1}}{b_{n+1} - a_{n+1}} = \gamma$$



We want β_n to become α_{n+1} at the next step.

$$\frac{\alpha_n - a_n}{b_n - a_n} = \gamma$$

Numerical methods

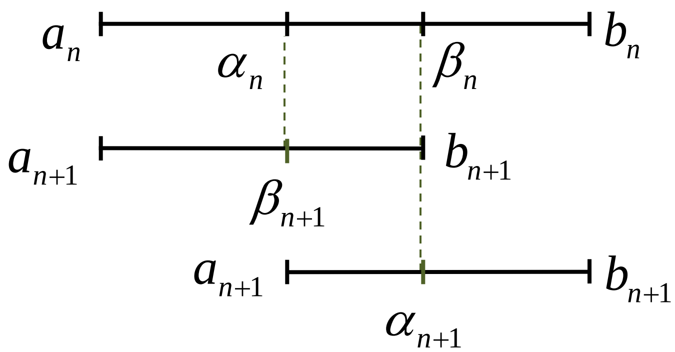
- Line search – the golden section method

$$\frac{b_n - \gamma(b_n - a_n) - a_n}{a_n + \gamma(b_n - a_n) - a_n} = \gamma$$

$$\frac{(b_n - a_n) - \gamma(b_n - a_n)}{\gamma(b_n - a_n)} = \gamma$$

$$\frac{1-\gamma}{\gamma} = \gamma \qquad \gamma^2 + \gamma - 1 = 0$$

$$\gamma = \frac{\sqrt{5}-1}{2}$$



Numerical methods

- Line search – the golden section method

Given: $a_0, b_0, \varepsilon, \gamma = \dfrac{\sqrt{5}-1}{2}$

Step 0: $n = 0,\ \alpha_0 = b_0 - \gamma(b_0 - a_0),\ \beta_0 = a_0 + \gamma(b_0 - a_0)$

Step 1: IF $|b_n - a_n| < \varepsilon$ THEN STOP

Step 2: IF $f(\alpha_n) < f(\beta_n)$ THEN

$$a_{n+1} = a_n,\ b_{n+1} = \beta_n,\ \beta_{n+1} = \alpha_n,\ \alpha_{n+1} = b_{n+1} - \gamma(b_{n+1} - a_{n+1}),\quad n = n+1, \text{GOTO}\,1$$

ELSE

$$a_{n+1} = \alpha_n,\ b_{n+1} = b_n,\ \alpha_{n+1} = \beta_n,\ \beta_{n+1} = a_{n+1} + \gamma(b_{n+1} - a_{n+1}),\quad n = n+1, \text{GOTO}\,1$$

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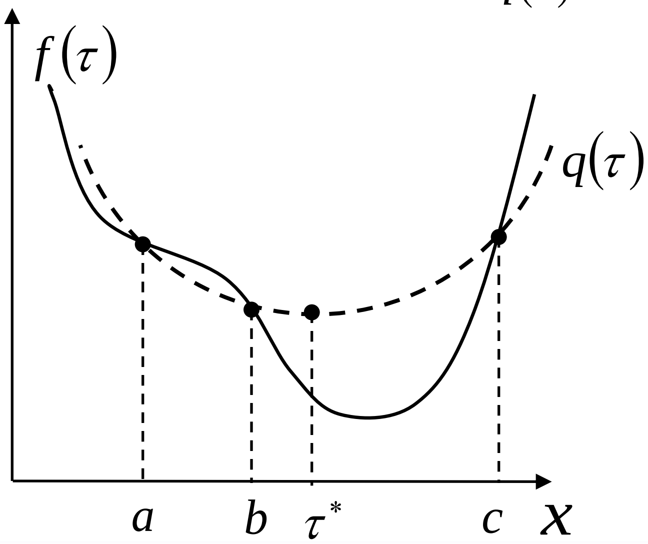
Numerical methods

- Quadratic-fit line search method

$$q(\tau)=\frac{f(a)(\tau-b)(\tau-c)}{(a-b)(a-c)}+\frac{f(b)(\tau-a)(\tau-c)}{(b-a)(b-c)}+\frac{f(c)(\tau-a)(\tau-b)}{(c-a)(c-c)}$$



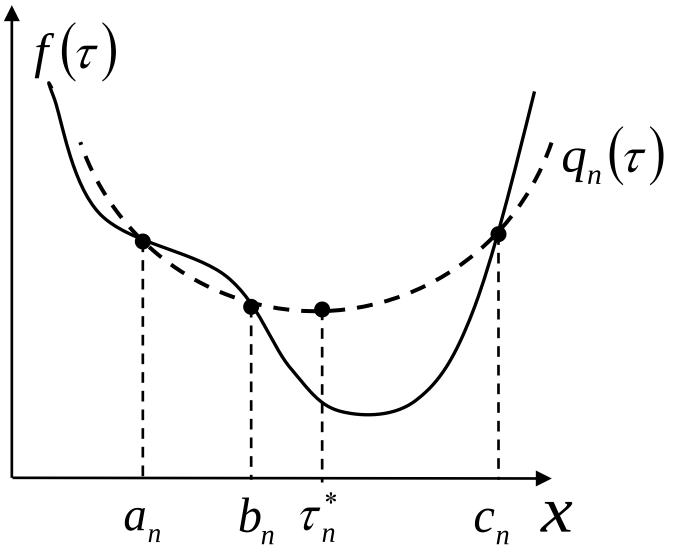
Solution of optimization task: $\tau^* \to q(\tau^*)=\min_{\tau} q(\tau)$

at the current iteration is:

$$\tau^*=\frac{1}{2}\frac{f(a)(b^2-c^2)+f(b)(c^2-a^2)+f(c)(a^2-b^2)}{f(a)(b-c)+f(b)(c-a)+f(c)(a-b)}$$

Numerical methods

- Quadratic-fit line search method



IF $b_n < \tau_n^*$ THEN

IF $f(b_n) > f(\tau_n^*)$ THEN

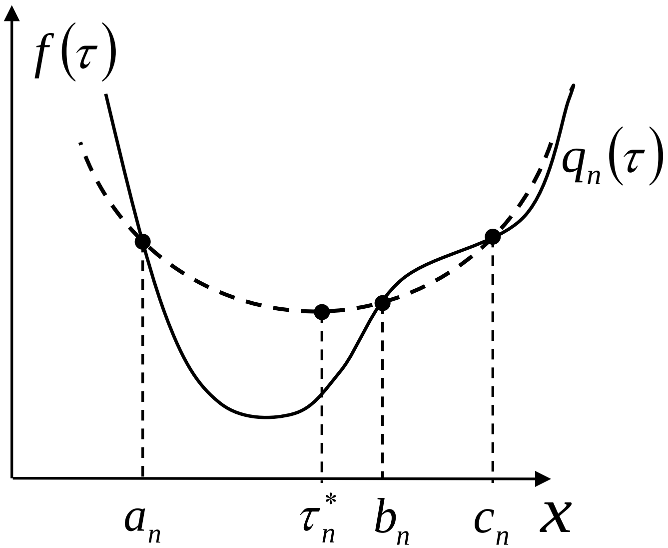
$$a_{n+1} = b_n,\ b_{n+1} = \tau_n^*,\ c_{n+1} = c_n$$

ELSE

$$a_{n+1} = a_n,\ b_{n+1} = b_n,\ c_{n+1} = \tau_n^*$$

Numerical methods

- Quadratic-fit line search method



IF $b_n > \tau_n^*$ THEN

IF $f(b_n) > f(\tau_n^*)$ THEN

$$a_{n+1} = a_n,\ b_{n+1} = \tau_n^*,\ c_{n+1} = b_n$$

ELSE

$$a_{n+1} = \tau_n^*,\ b_{n+1} = b_n,\ c_{n+1} = c_n$$

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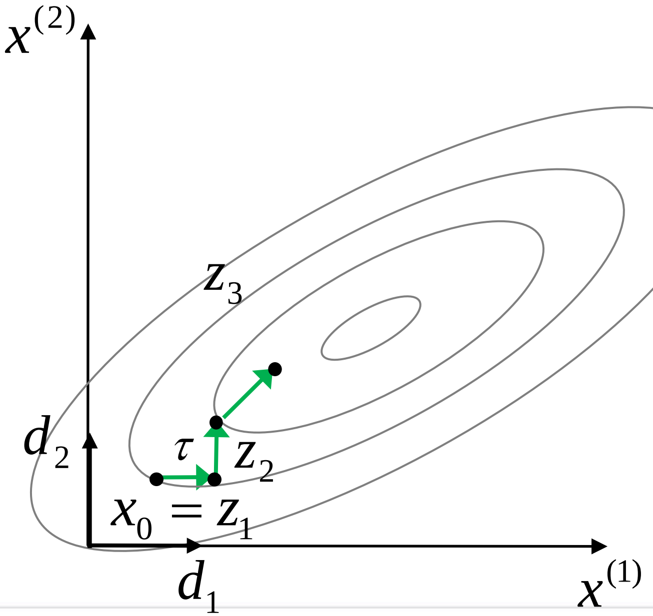
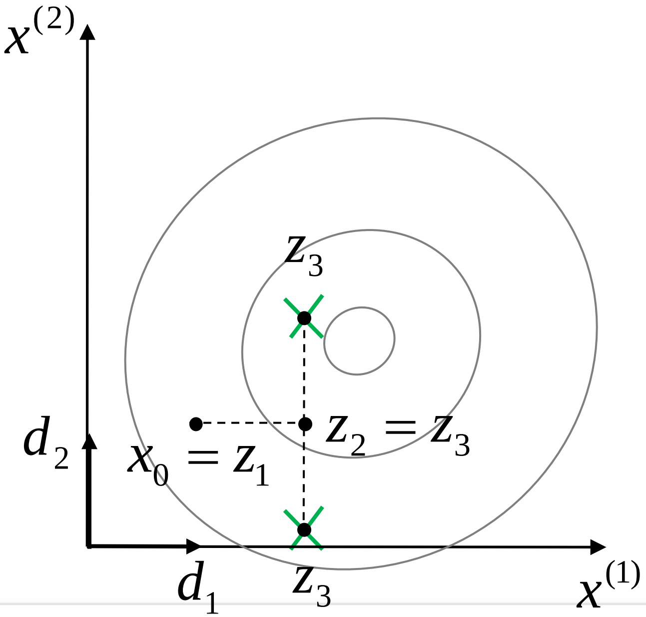
Numerical methods

- Hooke and Jeeves method





Numerical methods

- Hooke and Jeeves method

Given: $d_1, d_2, \ldots, d_S, x_0, \varepsilon, \alpha, \beta, \tau$

Step 0: $z_1 = x_0,\ s = 1,\ n = 0$

Step 1: $z_{s+1} = z_s + \tau d_s$

IF $F(z_{s+1}) < F(z_s)$ THEN GOTO 2

ELSE $z_{s+1} = z_s - \tau d_s$

IF $F(z_{s+1}) < F(z_s)$ THEN GOTO 2

ELSE $z_{s+1} = z_s$, GOTO 2

Numerical methods

- Hooke and Jeeves method

Step 2: IF $s < S$ THEN $s := s+1,$ GOTO 2

IF $F(z_{s+1}) < F(z_1)$ THEN GOTO 3

ELSE $\tau := \beta\tau,$ GOTO 1

Step 3: $x_{n+1} = z_{s+1}$

$z_1 := z_{s+1} + \alpha\left(z_{s+1} - z_1\right)$

IF $\left\| x_{n+1} - x_n \right\| < \varepsilon$ THEN STOP

ELSE $n := n+1, s = 1,$ GOTO 1

Numerical methods

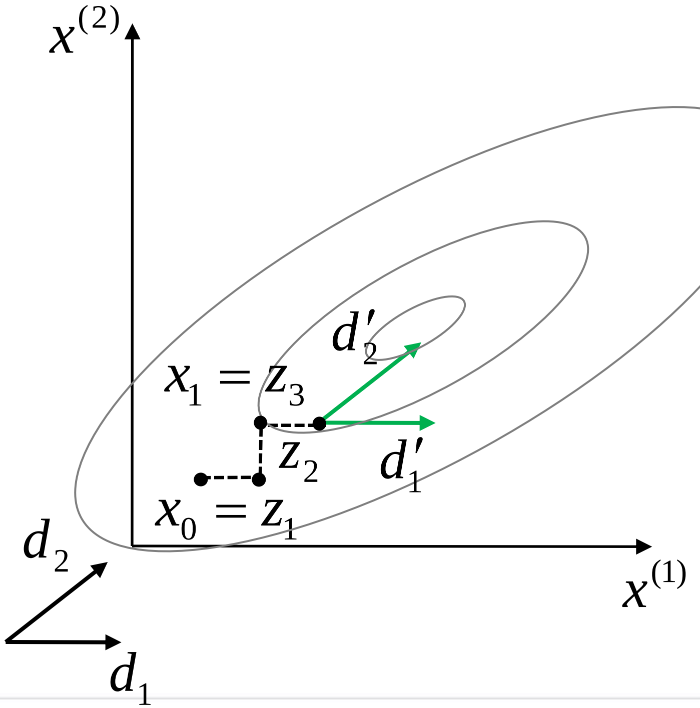
- Rosenbrock method

Conjugate directions $d_1, d_2, \ldots, d_S$:

$$d_i^T A d_j \begin{cases} \neq 0 & \text{for} \quad i = j \\ = 0 & \text{for} \quad i \neq j \end{cases}$$

where A is positively defined, symmetric matrix:

$$F(x) = x^T A x + b^T x + c$$



Numerical methods

- Rosenbrock method

Given: $d_1, d_2, \ldots, d_S, x_0, \varepsilon$

Step 0: $z_1 = x_0 + \tau_s d_s$, where τ_s is minimum along the direction d_s, $s=1,\ n=0$

Step 1: $z_{s+1} = z_s + \tau_s d_s$

IF $s < S$ THEN $s := s+1$ GOTO 1

Step 2: IF $\|x_{n+1} - x_n\| < \varepsilon$ THEN STOP

Numerical methods

- Rosenbrock method

Step 3: $$d = \frac{z_{s+1} - z_1}{\left\| z_{s+1} - z_1 \right\|},$$

$$z_s := z_{s+1} \quad (s = 1,2,\ldots,S-1)$$

$$z_s := d$$

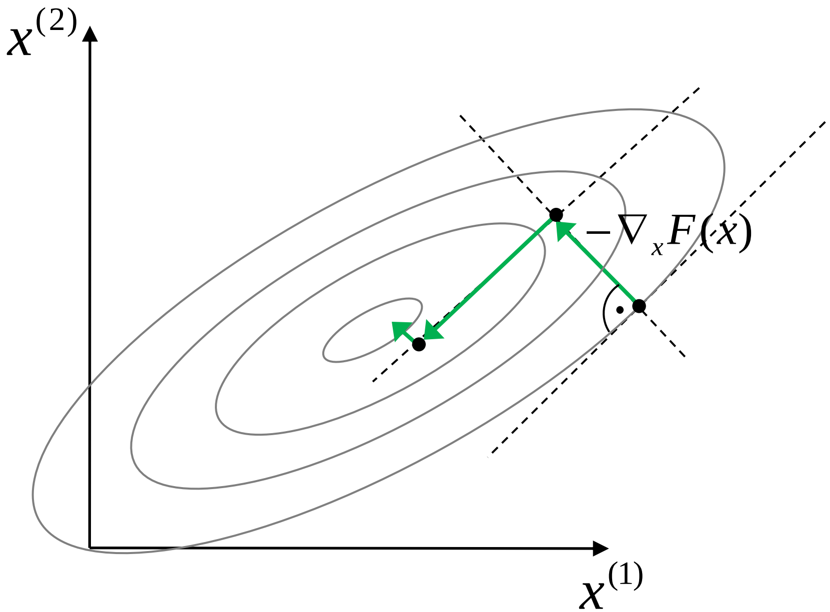
$z_1 := x_{n+1} + \tau d$, where τ is minimum along the direction d,

$$n := n+1, \quad s = 1$$

GOTO 1

Numerical methods

- Steepest descent method



$$x_{n+1} = x_n + \tau_n d_n \qquad d_n = G\left(\nabla_x F(x_n)\right)$$

$$d_n = -\nabla_x F(x_n)$$

$$x_{n+1} = x_n - \tau_n \nabla_x F(x_n), \qquad x_0$$

τ_n is minimum along the direction d_n

Numerical methods

- Newton's method

Taylor's expansion:

$$F(x) = \underbrace{F(x_0) + (x - x_0)^T \nabla_x F(x_0) + \frac{1}{2}(x - x_0)^T H(x_0)(x - x_0)}_{Q(x)} + O_3(\|x - x_0\|)$$

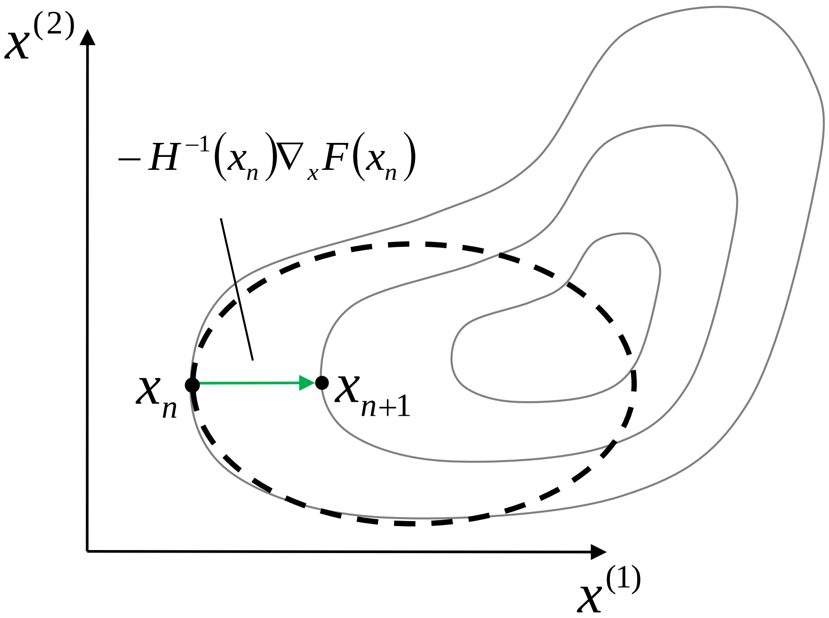
$$\nabla_x Q(x) = \nabla_x F(x_0) + H(x_0)(x^* - x_0) = 0_S$$

$$x^* = x_0 - H^{-1}(x_0)\nabla_x F(x_0)$$

$$\boxed{x_{n+1} = x_n - H^{-1}(x_n)\nabla_x F(x_n)}$$

Numerical methods

- Newton's method



Thank you for attention