Computer Science

Jerzy Świątek

Systems Modelling and Analysis

Choose yourself and new technologies

L.5b Numerical optimization methods – multidimensional search without derivatives

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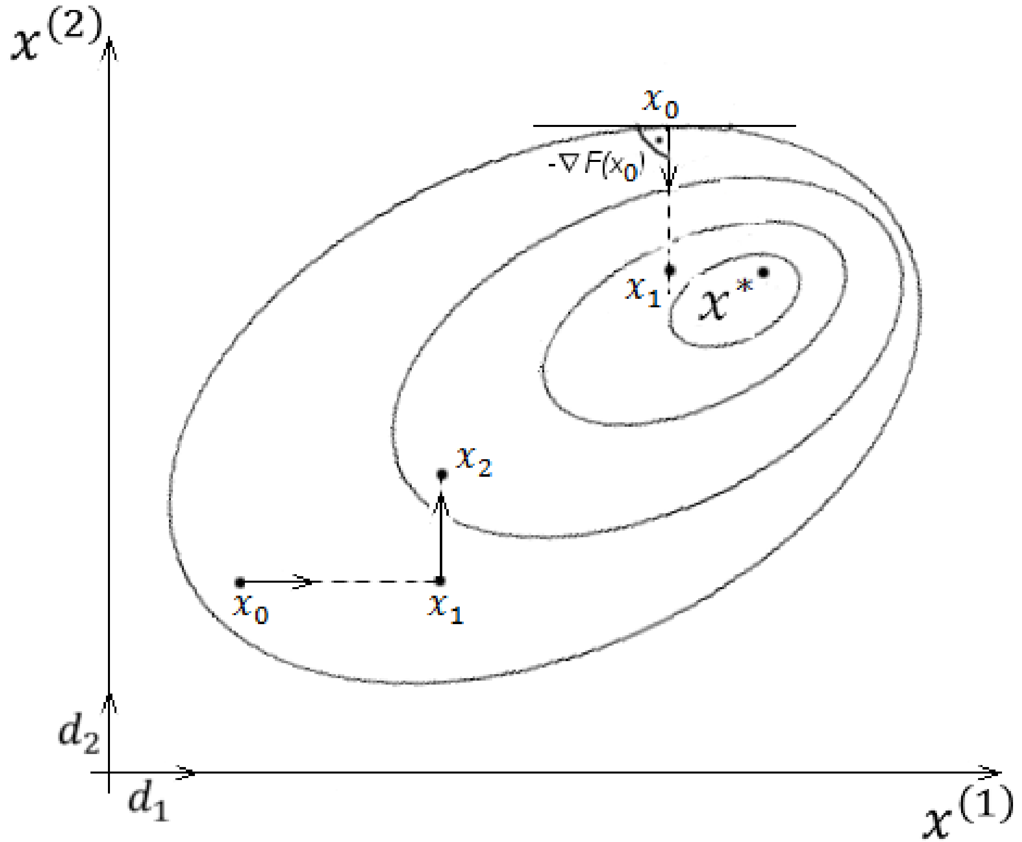
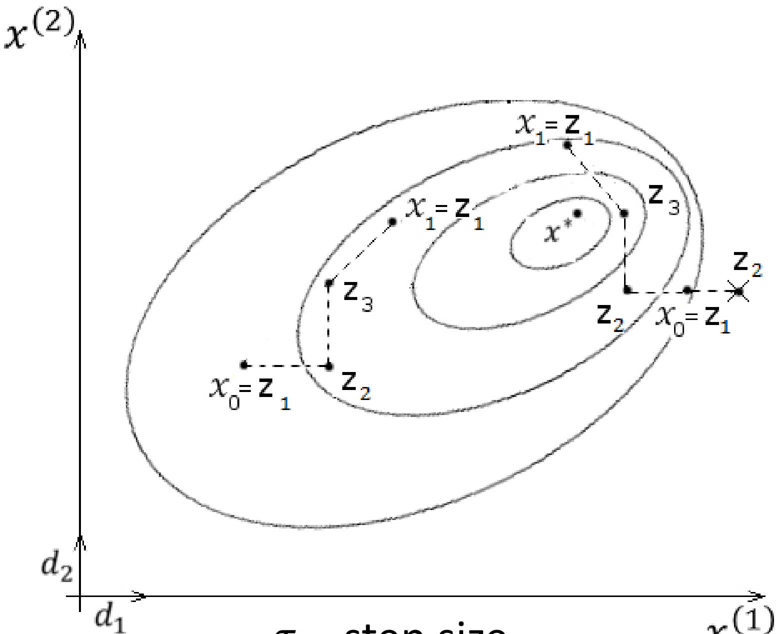
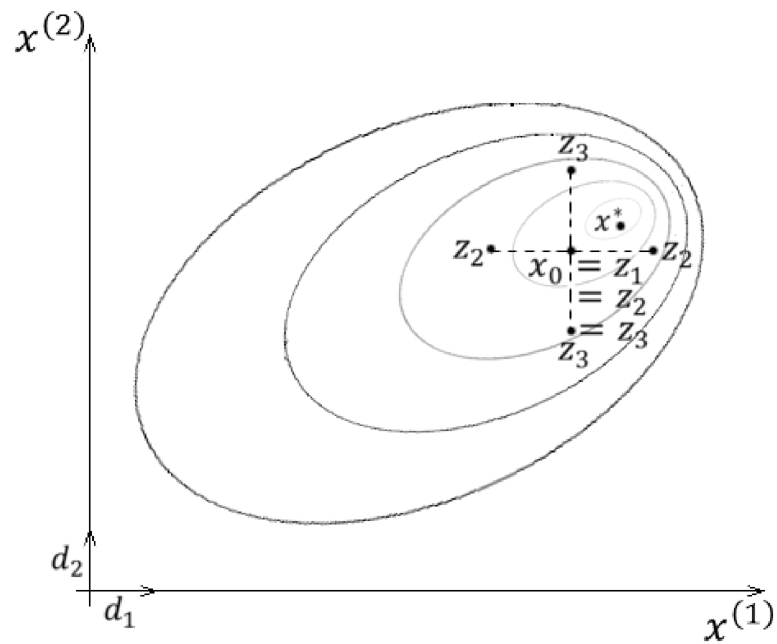
Choice of the search direction



- Basis of search directions – non-gradient methods.
- Search directions based on gradient vectors – gradient-based methods.

Hooke and Jevees Method with discrete steps





τ – step size
$\alpha > 1$ exploratory step size
$\beta \in (0,1)$ acceleration factor
$\tau := \tau\beta$

Hooke and Jevees Method with discrete steps

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

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

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

If $F(z_{s+1}) < F(z_s)$ then go to 2

otherwise $z_{s+1} \coloneqq z_s - \tau d_s$

If $F(z_{s+1}) < F(z_s)$ then go to 2

otherwise $z_{s+1} \coloneqq z_s$

Step 2: If $s < S, \; s \coloneqq s + 1$ then go to 1

otherwise

If $F(z_{S+1}) < F(z_1)$ then go to 3

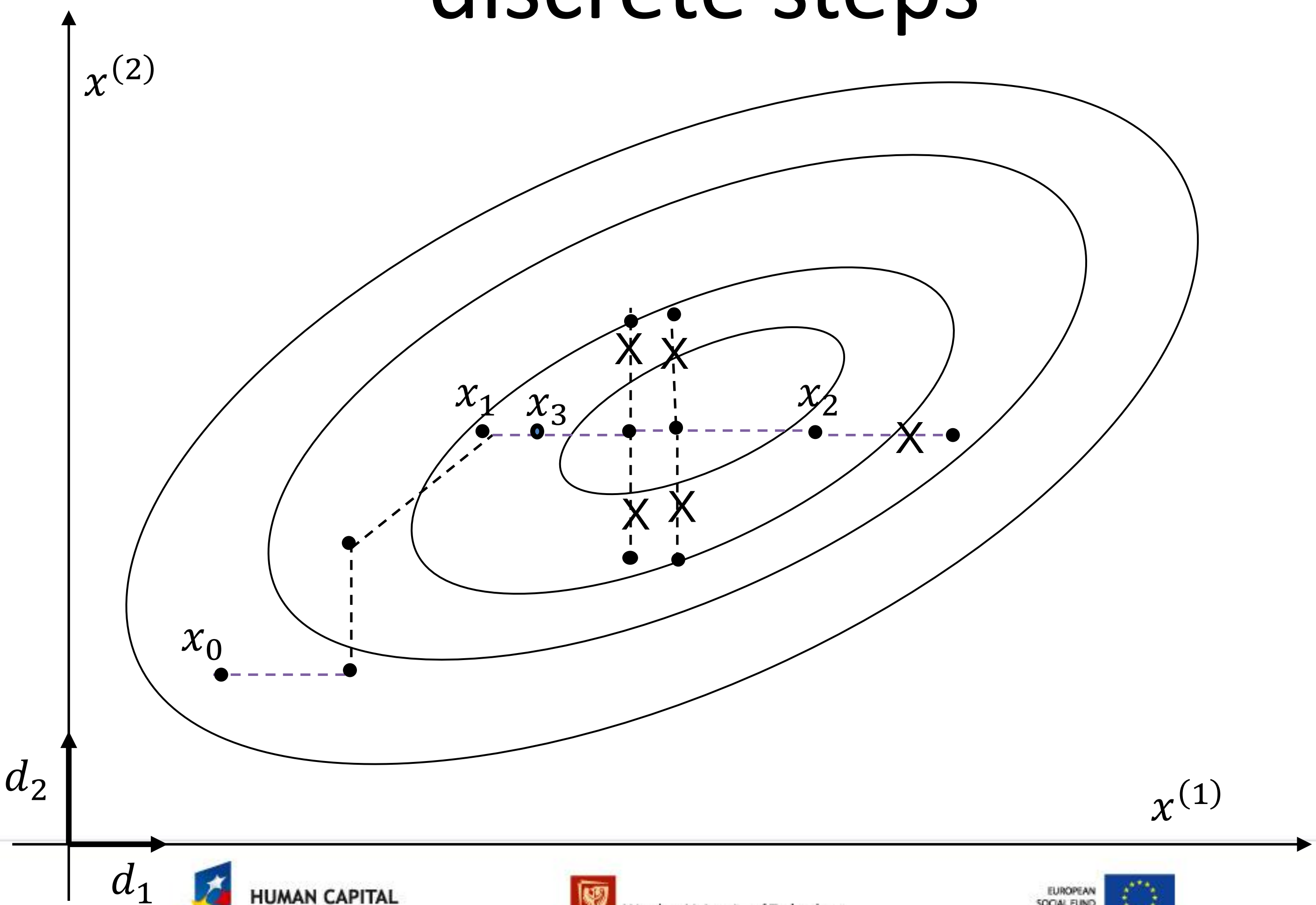
$\tau \coloneqq \tau\beta, x_{n+1} \coloneqq x_n, z_s \coloneqq x_n, n \coloneqq n + 1, s = 1$ then go to 1

Step 3: If $\tau < \varepsilon$, STOP

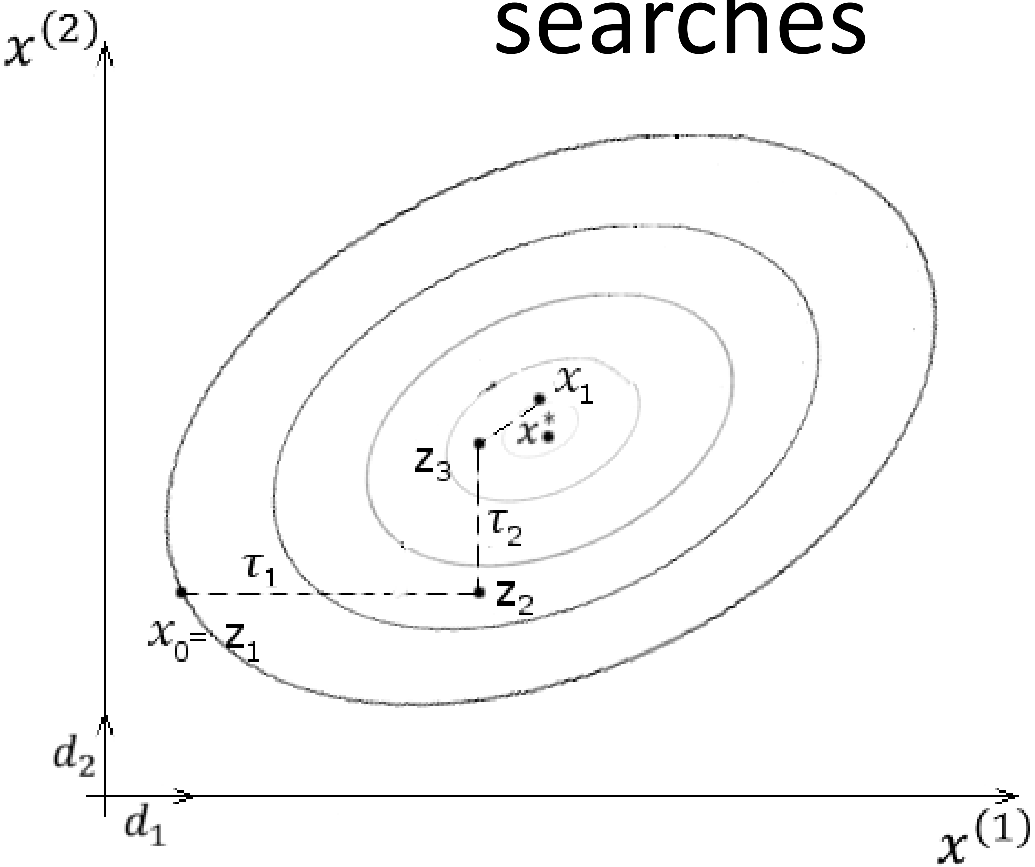
otherwise

$x_{n+1} \coloneqq z_{S+1} + \alpha(z_{S+1} - z_1), n \coloneqq n + 1, s \coloneqq 1$ then go to 1

Hooke and Jevees Method with discrete steps



Hooke and Jeeves Method using line searches



Hooke and Jeeves Method using line searches

Input data: $d_1, d_2, \ldots, d_S, x_0, \varepsilon$

Step 0: $z_s \coloneqq x_0, n = 0, s = 1$

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

τ_s- optimal step size along the direction d_s

Step 2: If $s < S, s = s + 1$ then go to 1

If $\|z_{S+1} - z_1\| < \varepsilon$ - STOP

Step 3: $x_{n+1} \coloneqq z_{S+1} + \tau d$

$\tau \rightarrow$ optimal step size along the direction d

$$d = \frac{z_{S+1} - z_1}{\|z_{S+1} - z_1\|} = \frac{\sum_{S=1}^{S+1} \tau_s d}{\|\sum_{S=1}^{S+1} \tau_s d\|}$$

$n \coloneqq n + 1, s = 1, z_1 = x_n$

GO TO 1

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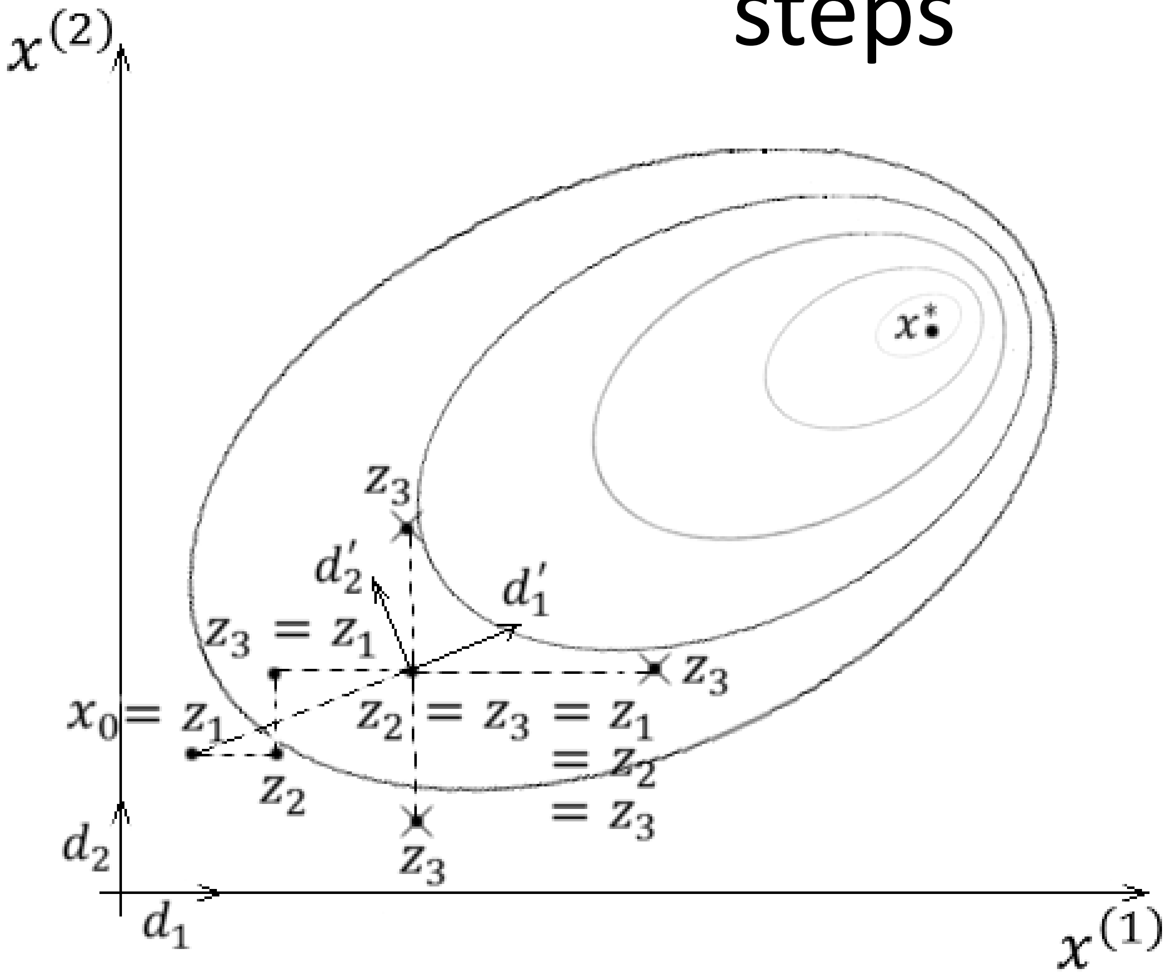
Rosenbrock Method with discrete steps



τ – step size
$\alpha > 1$ – exploratory step size acceleration
$\beta \in (-1, 0)$ – acceleration factor
$\tau_s \coloneqq \tau_s \alpha$
$\tau_s \coloneqq \tau_s \beta$

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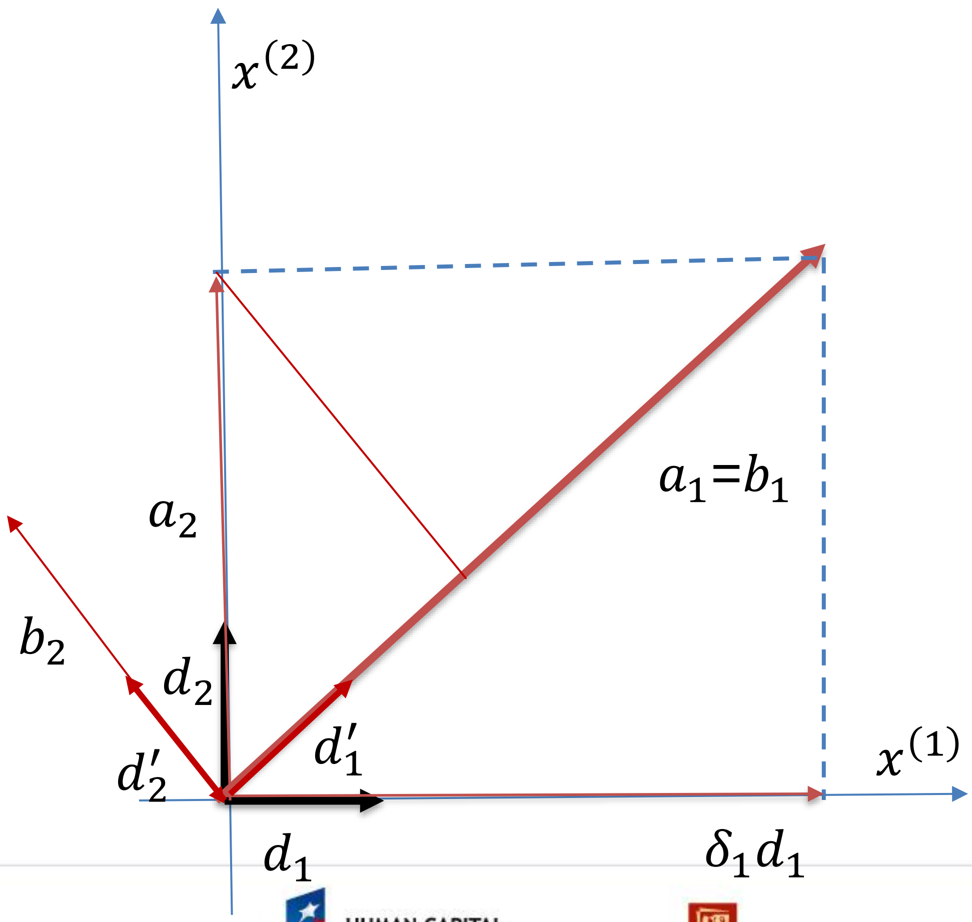
Base rotation
Gram – Schmitd orthogonalisation



$$a_1 = \delta_1 \, d_1 + \delta_2 d_2$$
$$a_2 = \delta_2 \, d_2$$

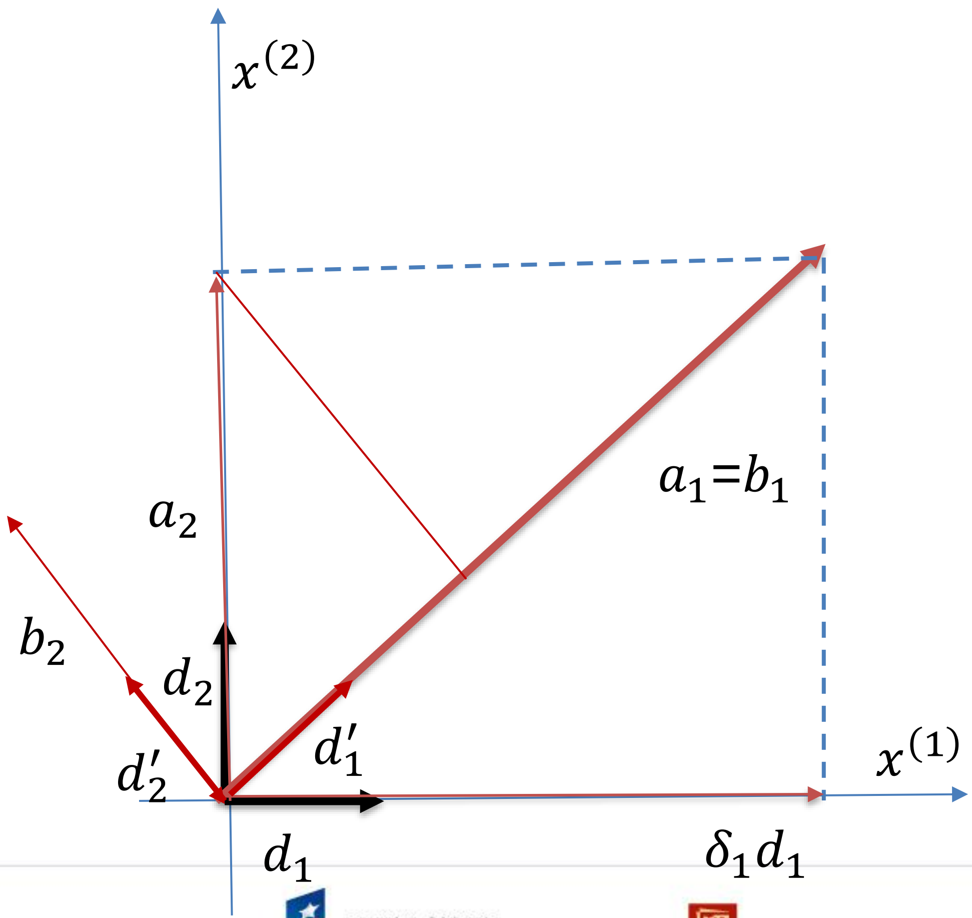
$$b_1 = a_1$$

$$d_1' = \frac{b_1}{\|b_1\|}$$

$$b_2 = a_2 - \left(a_1^T d_1'\right) d_1'$$

$$d_2' = \frac{b_2}{\|b_2\|}$$

Base rotation
Gram – Schmitd orthogonalisation



$$a_s = \begin{cases} d_s & \delta_s = 0 \\ \sum_{j=s}^{S} \delta_j d_j & \delta_s \neq 0 \end{cases}$$

$$b_s = \begin{cases} a_s & s = 1 \\ a_s - \sum_{j=1}^{s-1} \left(a_j^T d_j'\right) d_j' \end{cases}$$

$$d_s' = \frac{b_s}{\|b_s\|} \qquad s = 1,2, \dots, S$$

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Rosenbrock Method with discrete steps

Input data: $d_1, d_2, \dots, d_S, x_0, \tau, \varepsilon, \alpha > 1, \beta \in (-1, 0)$

Step 0: $\tau_1 = \tau_2 = \cdots = \tau_S = \tau,\ \ \delta_1 = \delta_2 = \cdots = \delta_S = 0, \quad z_1 = x_0, \quad n = 0, \quad s = 1$

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

IF $F(z_{s+1}) < F(z_s) \qquad \tau_s \coloneqq \alpha\tau_s$, THEN GO TO 2

ELSE $F(z_{s+1}) \geq F(z_s) \quad \tau_s \coloneqq \beta\tau_s$ THEN GO TO 2

Step 2: IF $s < S \quad s \coloneqq s + 1$ THEN GO TO 1

IF $F(z_{S+1}) < F(z_1) \quad z_1 \coloneqq z_{S+1} \quad s \coloneqq 1$ THEN GO TO 1

IF $F(z_{S+1}) = F(x_n)$

IF $n = 0$ change the initial solution

$x_{n+1} = z_{S+1}$

Step 3: IF STOP? ($\|x_{n+1} - x_n\| < \varepsilon$) STOP

Step 4: Rotation of the basis of search directions

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Base rotation

Krok 4:

$$a_s = \begin{cases} d_s & \delta_s = 0 \\ \sum_{j=s}^{S} \delta_j d_j & \delta_s \neq 0 \end{cases}$$

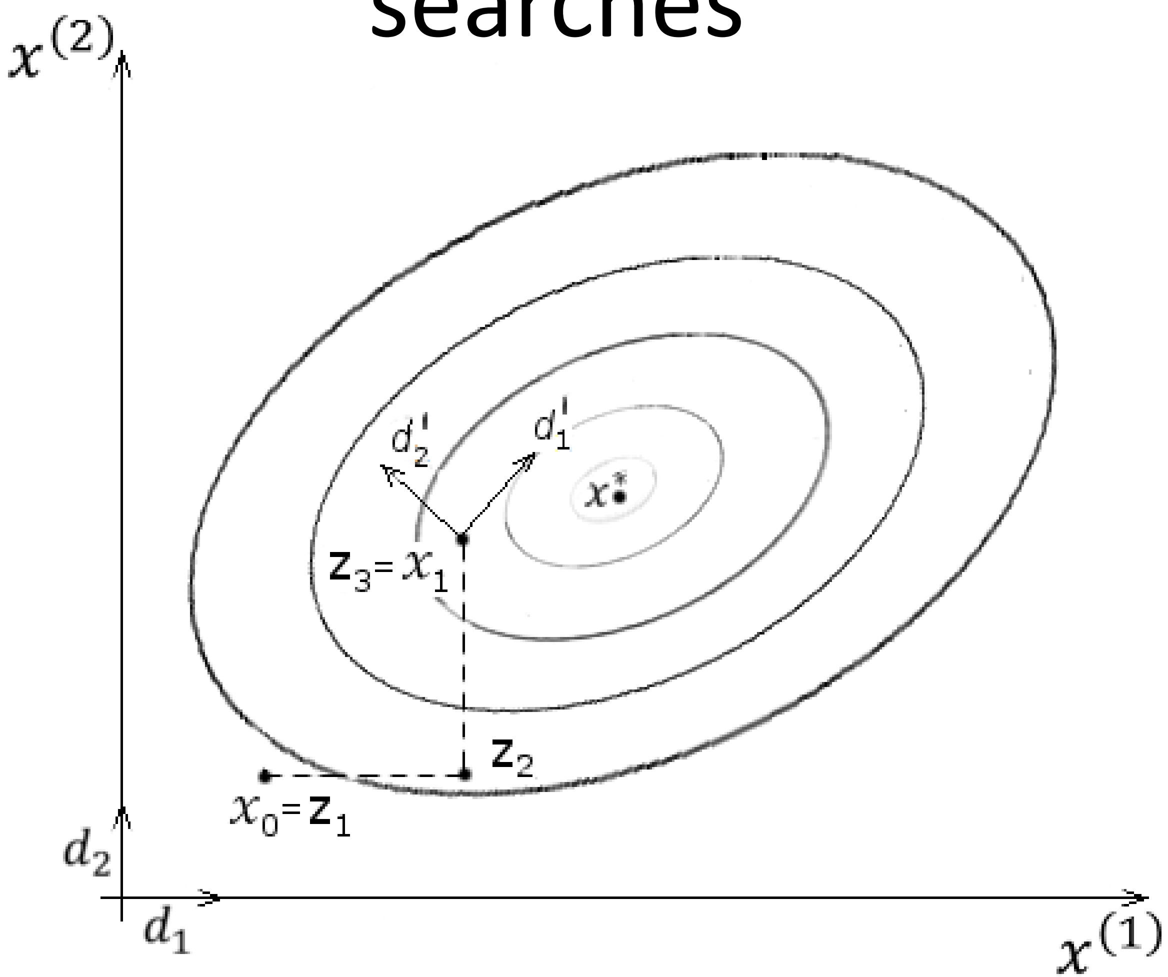
$$b_s = \begin{cases} a_s & s = 1 \\ a_s - \sum_{j=1}^{s-1} (a_j^T d_j') d_j' \end{cases}$$

$$d_s' = \frac{b_s}{\|b_s\|} \qquad s = 1,2,\dots,S$$

$$\tau_1 = \tau_2 = \cdots = \tau_S = \tau,\ \delta_1 = \delta_2 = \cdots = \delta_S = 0,$$

$d_s \coloneqq d_s' \qquad s = 1,2,\dots,S, n \coloneqq n+1, s = 1$ then go to 1

Rosenbrock Method using line searches



Rosenbrock Method using line searches

Input data: $d_1, d_2, \dots, d_S, x_0, \varepsilon$

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

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

τ_s - optimal step size along the direction d_s

Step 2: If $s < S, s \coloneqq s + 1$ then go to 1

If $\|z_{S+1} - z_1\| < \varepsilon$ - STOP

Step 3:

$$a_s = \begin{cases} d_s & \tau_s = 0 \\ \sum_{j=s}^{S} \tau_j d_j & \tau_s \neq 0 \end{cases}$$

$$b_s = \begin{cases} a_s & s = 1 \\ a_s - \sum_{j=1}^{s-1} (a_j^T d_j') d_j' \end{cases}$$

$$d_s' = \frac{b_s}{\|b_s\|} \quad s = 1,2, \dots, S$$

Step 4: $d_s \coloneqq d_s' \quad s = 1,2, \dots, S, n \coloneqq n + 1, s = 1$ then go to 1

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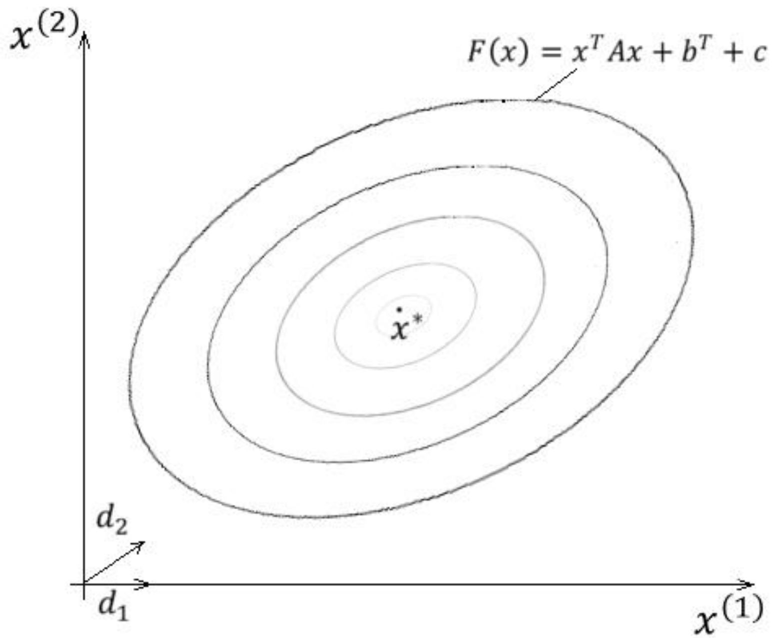
Powell's method – conjugate directions

$d_1, d_2, \dots, d_S$ - conjugated directions,
A – symmetric, positively defined matrix

$$d_i^T A d_j = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$



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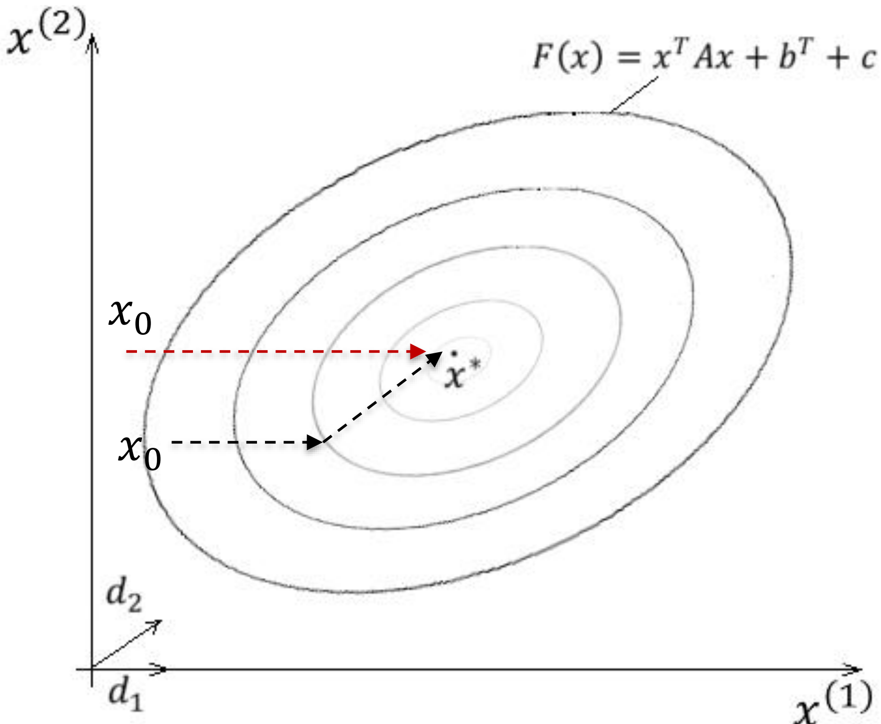
Powell's method – conjugate directions

$F(x) = x^T A x + b^T x + c$, $d_1, d_2, \dots, d_S$ - conjugated directions with respect A

Optimizing along conjugate directions allows to reach solution after at most S steps.



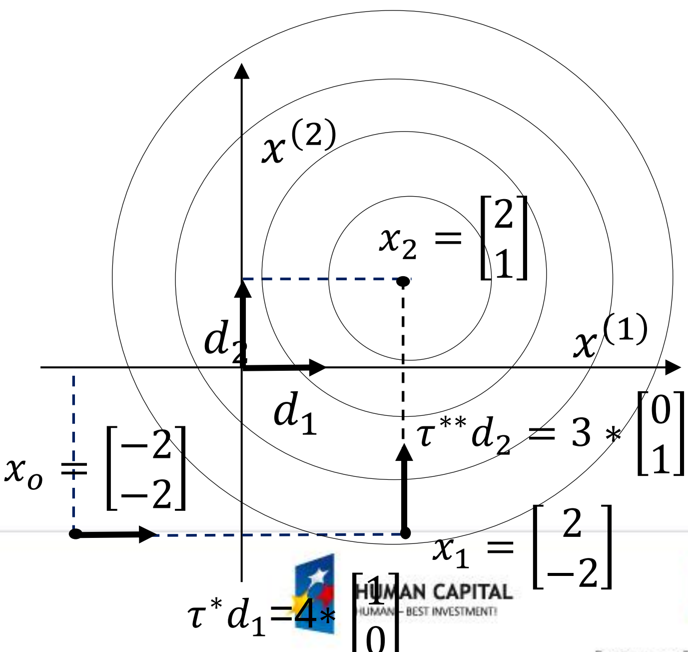
Example

$$F(x) = \left(x^{(1)} - 2\right)^2 + \left(x^{(2)} - 1\right)^2,\ x_0 = \begin{bmatrix} -2 \\ -2 \end{bmatrix}, d_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, d_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad H(x) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

$$d_1^T H d_2 = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0,\ d_1^T H d_1 = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 1,\ d_2^T H d_2 = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 1$$

$$x_1 = x_0 + \tau d_1 = \begin{bmatrix} -2 \\ -2 \end{bmatrix} + \tau \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -2 + 1 * \tau \\ -2 + 0 * \tau \end{bmatrix}$$

$$F(x_0 + \tau d) = (-2 + \tau - 2)^2 + (-2 - 1)^2 = (\tau - 4)^2 + (3)^2 = \tau^2 - 4\tau + 25 \triangleq f_1(\tau)$$



$$f_1'(\tau) = 2\tau^* - 8 = 0 \qquad \tau^* = 4$$

$$x_1 = x_0 + \tau^* d_1 = \begin{bmatrix} -2 \\ -2 \end{bmatrix} + 4 * \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ -2 \end{bmatrix}$$

$$x_2 = x_1 + \tau d_2 = \begin{bmatrix} 2 \\ -2 \end{bmatrix} + \tau \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 2 + 0 * \tau \\ -2 + 1 * \tau \end{bmatrix}$$

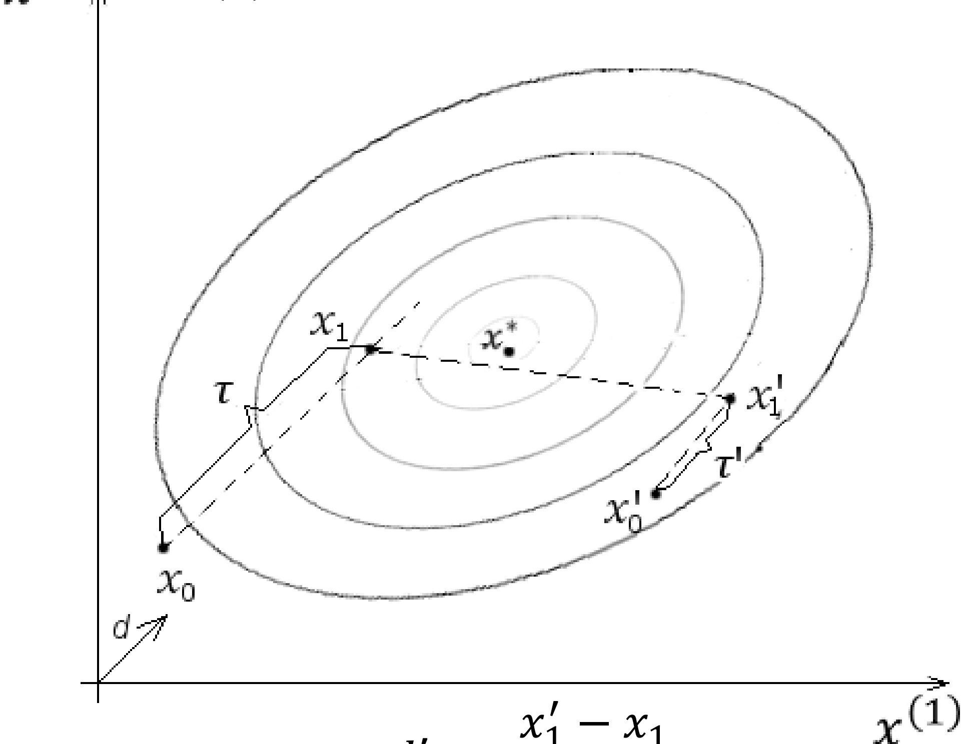
$$F(x_1 + \tau d_2) = (2 - 2)^2 + (-2 + \tau - 1)^2 = 4 + (\tau - 3)^2 \triangleq f_2(\tau)$$

$$f_2'(\tau) = 2\tau^{**} - 6 = 0 \qquad \tau^{**} = 3$$

$$x_2 = x_1 + \tau d_2 = \begin{bmatrix} 2 \\ -2 \end{bmatrix} + 3 \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

Powell's method – conjugate directions

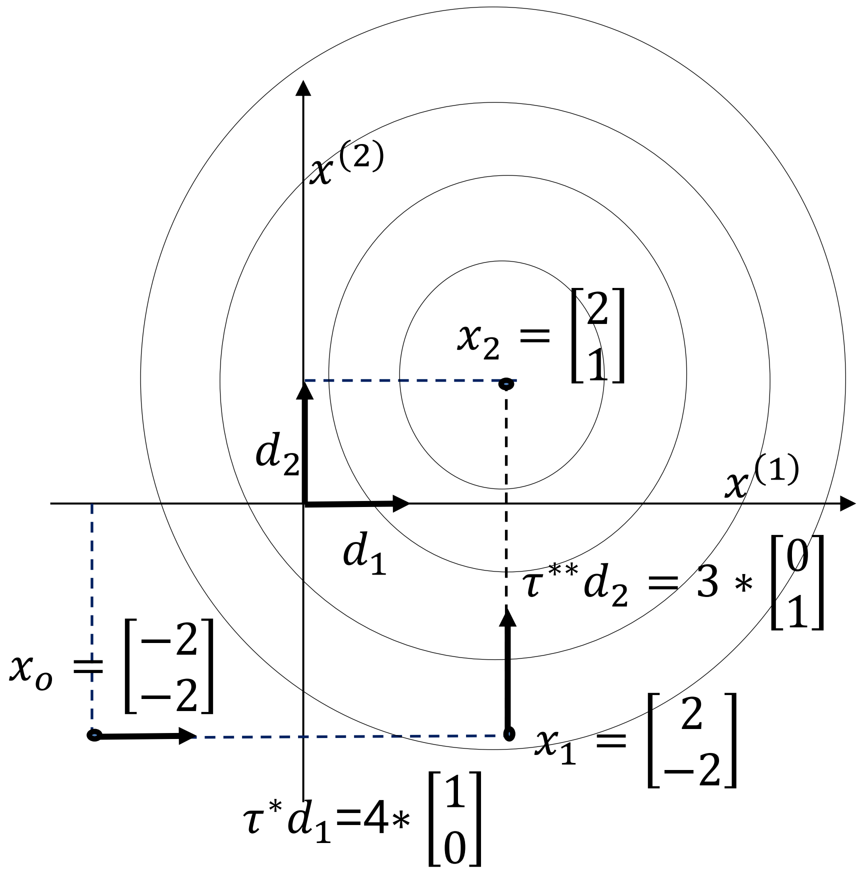
$F(x) = x^T A x + b^T + c$



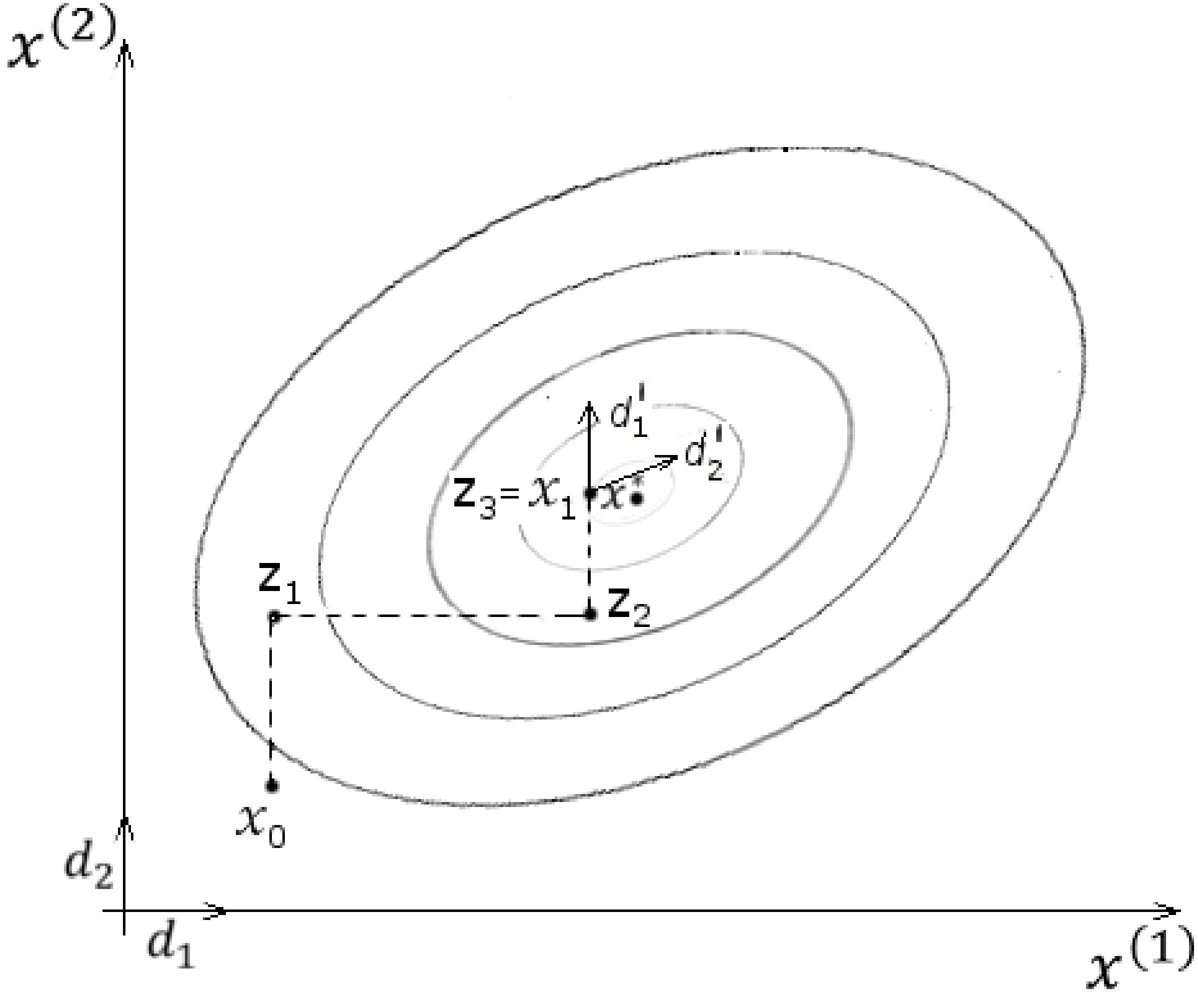
$$d' = \frac{x_1' - x_1}{\|x_1' - x_1\|}$$

$x_1 = x_0 + x^* d$
τ^* - optimal step size along the direction d from x_0
$x_1' = x_0' + \tau^{*\prime} d$
$\tau^{*\prime}$ - optimal step size along the direction d from x_0'

$d^T A d' = 0$
d, d'- conjugated with respect A


$x^{(2)}$
$x_2 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$
d_2
$x^{(1)}$
d_1
$\tau^{**} d_2 = 3 * \begin{bmatrix} 0 \\ 1 \end{bmatrix}$
$x_o = \begin{bmatrix} -2 \\ -2 \end{bmatrix}$
$x_1 = \begin{bmatrix} 2 \\ -2 \end{bmatrix}$
$\tau^{*} d_1 = 4 * \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

Powell's method



Powell's method

Input data: $d_1, d_2, \dots, d_S, x_0, \varepsilon$

Step 0: $z_1 := x_0 + \tau_S d_S, n := 0, \tau_S$ - optimal step size along the direction d_S, s$:= 1$

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

τ_s - optimal step size along the direction d_s

Step 2: If $s < S, s := s + 1$ then go to 1

If $\|z_{S+1} - z_1\| < \varepsilon$ - STOP

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

$d := \frac{z_{S+1} - z_1}{\|z_{S+1} - z_1\|}$

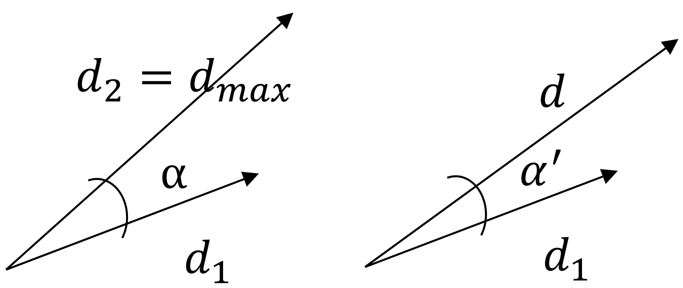
$z_1 := x_{n+1} + \tau d$ $\quad \tau$ – optimal step size along the direction d

$d_s := d_{s+1}$ $\quad s = 1, 2, \dots, S-1$

$d_S := d$

$n = n + 1, s :=$1, go to step 1

Powell's method - modification



$$\Delta = det[d_1\ d_2\ \cdots\ d_S] = \cos\alpha$$

$$\Delta = det[d_1\ d_2\ \cdots d_{max} \cdots d_S\ ] = \cos\alpha$$

$$\uparrow d$$

$$\Delta' = det[d_1\ d_2\ \cdots d \cdots d_S\ ] = \frac{\tau_{max}\Delta}{\|Z_{S+1} - Z_1\|} = \cos\alpha'$$

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

$$d := \frac{Z_{S+1} - Z_1}{\|Z_{S+1} - Z_1\|}$$

$$z_1 := x_{n+1} + \tau d \qquad \tau - \text{min in direction } d$$

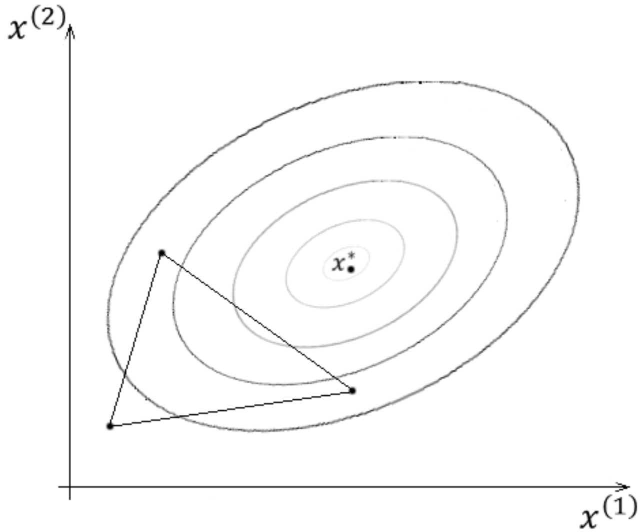
$$\tau_{max} \to \max_{1 \le s \le S} \|z_{s+1} - z_s\| = \max_{1 \le s \le S} \tau_s$$

If $\Delta := \frac{\tau_{max}\Delta}{\|Z_{S+1} - Z_1\|} > 0.8\ d_{max} = d\ , n = n + 1, s := 1$ go to step 1

Else $n = n + 1, s := 1$ go to step 1

Nelder-Mead method

$x_1\ x_2\ \ldots x_{S+1}$ - s-dimensional simplex



$$x_H \to F(x_H) = \max_{1 \le s \le S+1} F(x_s)$$
$$x_L \to F(x_L) = \min_{1 \le s \le S+1} F(x_s)$$
$$\bar{x} = \frac{1}{s} \sum_{s=1, s \ne H}^{S+1} x_s$$

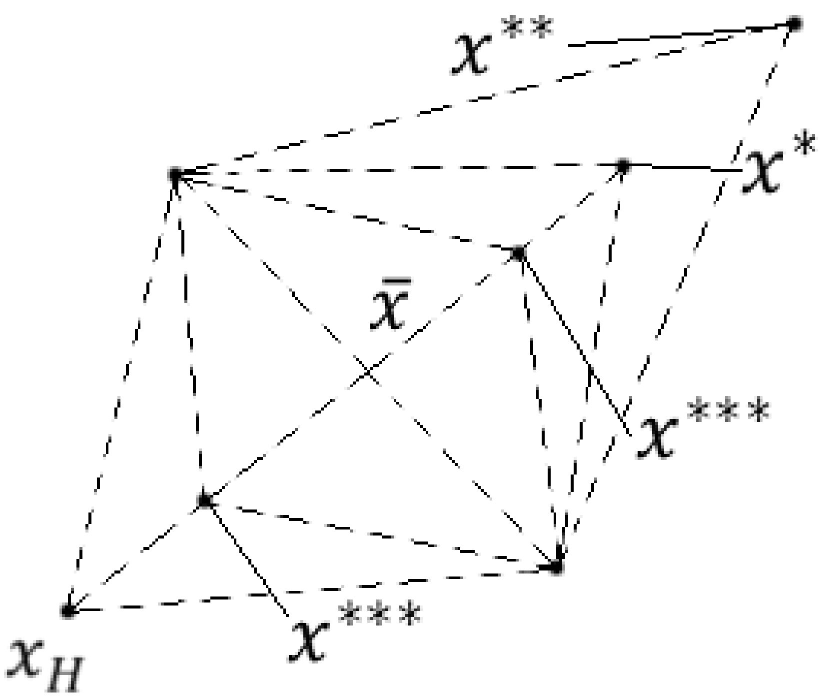
Initial simplex:

x_0, c

$$a = \frac{c}{S\sqrt{2}}(\sqrt{S+1} + \sqrt{2} - 1)$$
$$\mathrm{b} = \frac{c}{S\sqrt{2}}(\sqrt{S+1} - 1)$$

$$d_j = [a\ \ldots a\ b\ a\ \ldots a]$$
$$x_i = x_0 + d_j,\ x_{S+1} = x_0$$

Nelder-Mead method



Reflection

$x^* = \bar{x} + \alpha(\bar{x} - x_H)$

α – reflection coefficient

If $\alpha > 0$

$F(x^*) < F(x_L)$

Expansion

$x^{**} = \bar{x} + \gamma(x^* - \bar{x}) \qquad \gamma > 1$

γ – expansion coefficient

If $F(x^*) > F(x_H)$

Contraction

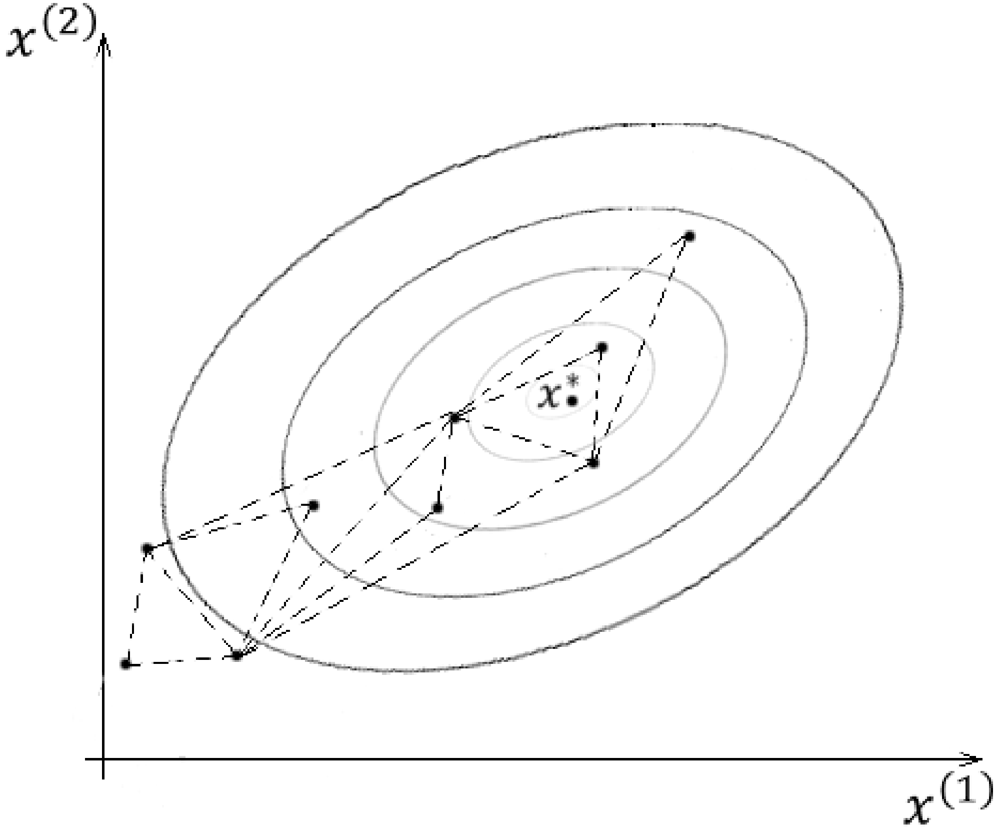
$x^{***} = \bar{x} + \beta(x_H - \bar{x})$

If $F(x^*) > \max\limits_{\substack{1 \le s \le S+1 \\ s \ne H}} F(x_s)$

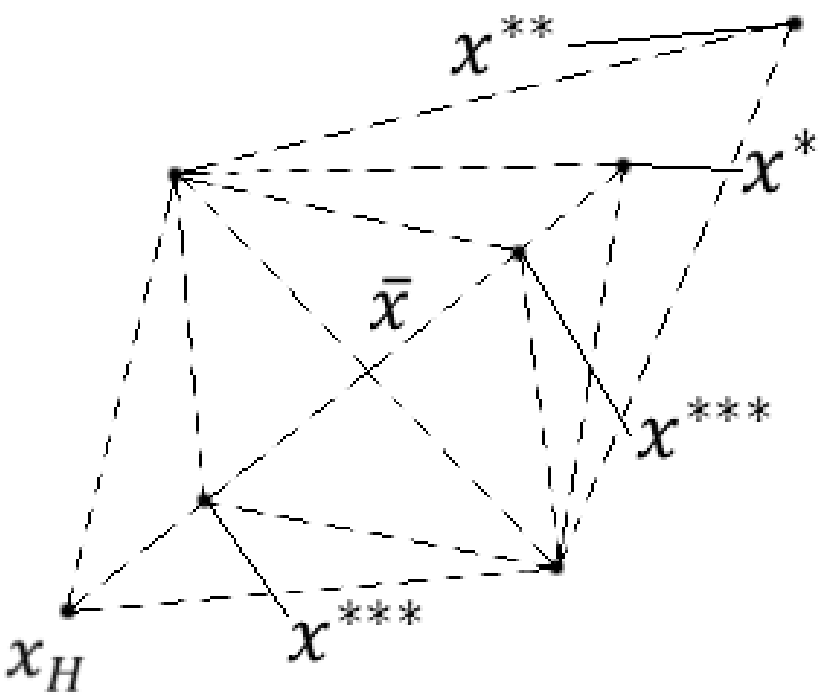
$x^{***} = \bar{x} + \beta(x^* - \bar{x}) \qquad \beta \in (0, 1)$

β – contraction coefficient

Nelder-Mead method



Nelder-Mead method



Reflection

$x^* = \bar{x} + \alpha(\bar{x} - x_H)$

α – reflection coefficient

If $\alpha > 0$

$F(x^*) < F(x_L)$

Expansion

$x^{**} = \bar{x} + \gamma(x^* - \bar{x}) \qquad \gamma > 1$

γ – expansion coefficient

If $F(x^*) > F(x_H)$

Contraction

$x^{***} = \bar{x} + \beta(x_H - \bar{x})$

If $F(x^*) > \max_{\substack{1 \le s \le S+1 \\ s \ne H}} F(x_s)$

$x^{***} = \bar{x} + \beta(x^* - \bar{x}) \qquad \beta \in (0, 1)$

β – contraction coefficient

Nelder-Mead method

Input data: x_0, c, ε

Step 0: $x_1\ x_2\ \dots\ x_{S+1}$ - initial simplex, $n = 0$

Step 1: $x_H \rightarrow F(x_H) = \max_{1 \le s \le S+1} F(x_s), x_L \rightarrow F(x_L) = \min_{1 \le s \le S+1} F(x_s)$

$\bar{x} = \frac{1}{S} \sum_{\substack{s=1 \\ s \neq H}}^{S+1} x_s$

Step 2: $x^* = \bar{x} + \alpha(\bar{x} - x_H)$

If $F(x^*) < F(x_L)$ $\quad x^{**} = \bar{x} + \gamma(x^* - \bar{x})$ then go to 3

otherwise 4

Step 3: If $F(x^{**}) < F(x^*)$ $\quad x_H = x^{**}, n = n + 1$ then go to 1

otherwise $x_H = x^*, n = n + 1$ then go to 1

Step 4: If $F(x^*) < \max_{\substack{1 \le s \le S+1 \\ s \neq H}} F(x_s)$ $\quad x_H = x^*, n = n + 1$

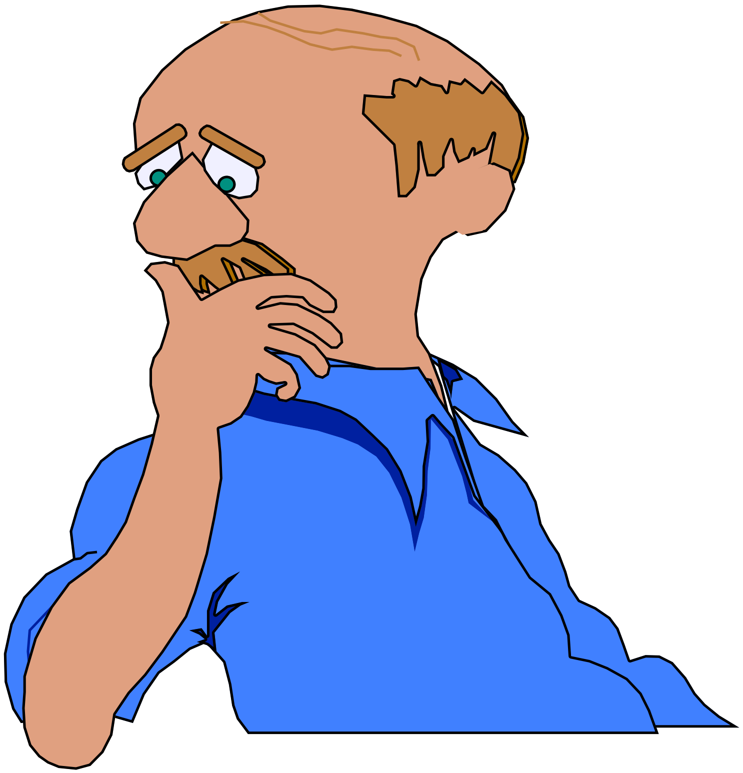
Step 5: $x' - \quad F(x') = \min\{F(x^*), F(x_H)\}$

$x^{***} = \bar{x} + \beta(x' - \bar{x})$

If $F(x^{***}) > F(x')$ $\quad x_j = x_j + \frac{1}{2}(x_L - x_j), j = 1,2, \dots, S + 1$ then go to 1

$x_H = x^{***}, n = n + 1$ then go to 1

Thank you for attention



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