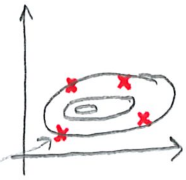
The Complex Method

* Use $k > n+1$ points. Box suggested $k = 2 \cdot n$
  (n: no. of design variables)

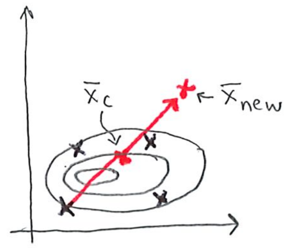
* The figure in $\mathbb{R}^n$ with $k > n+1$ points is called a Complex

Step 0: Generate k points at random locations in the design space



Step 1: Identify the worst point

Step 2: Reflect the worst point through the center of the remaining points with a reflection factor α.
Box suggested $\alpha = 1.3$



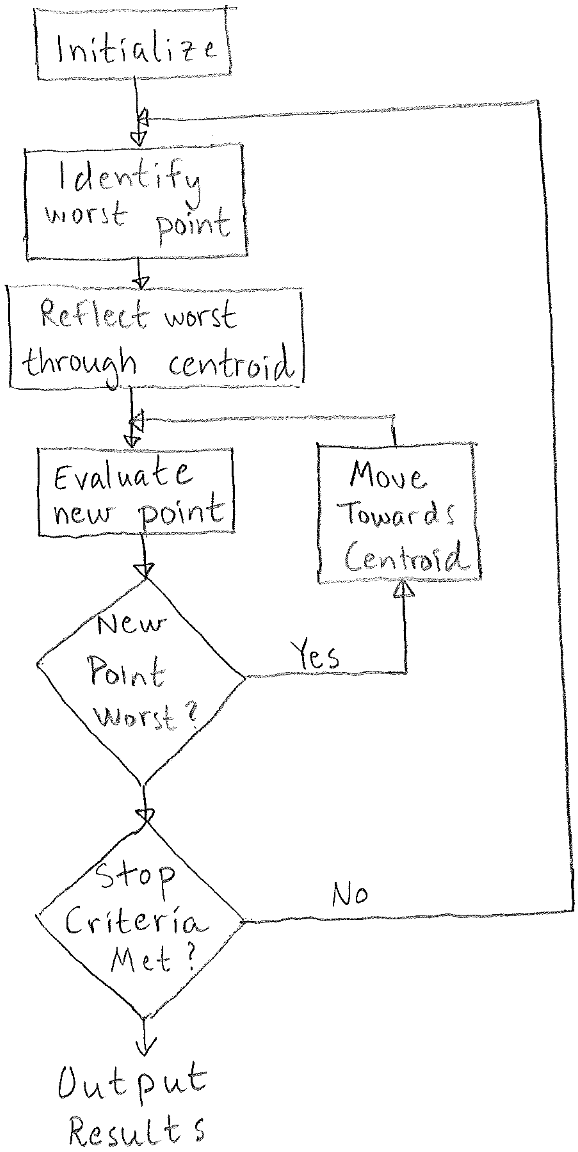
$$\underbrace{x_{c,j}}_{\text{design variable } j} = \frac{1}{k-1}\left(\underbrace{\sum_{i=1}^{k} x_{ij}}_{\text{sum of all points}} - \underbrace{x_{worst,j}}_{\text{remove worst}}\right), \quad j = 1, \ldots, n$$

new point $= \bar{x}_{new} = \bar{x}_c + \alpha(\bar{x}_c - \bar{x}_{worst})$

Step 3: Evaluate the objective function of the new point

Step 4: If the point is still the worst one, move it towards the centroid and go to step 3.
Otherwise, go to step 5.

Step 5: Check termination criteria. If not fulfilled, increase iteration counter and go to step 1



Termination Criteria

* Convergence in function values

$$\max_{i=1,\dots,k}\left(f(\bar{x}_i)\right) - \min_{i=1,\dots,k}\left(f(\bar{x}_i)\right) \leq \varepsilon_f \qquad (1)$$

(The spread in function values is smaller than ε_f)

* Convergence in optimization variables

$$\max_{j=1,\dots,n}\left(\max_{i=1,\dots,k}(x_{ij}) - \min_{i=1,\dots,k}(x_{ij})\right) \leq \varepsilon_v \qquad (2)$$

(The spread of the design variables is smaller than ε_v)

* Max number of evaluations

no evaluations $\geq$ Max number of evaluations

Example of spread calculation:

Assume $0 \le x_i \le 4$ (design space)

Consider a Complex with the following 4 points:

k	x_1	x_2	f
1	2.0	1.0	4
2	2.2	0.8	3.8
3	1.8	1.5	4.2
4	1.9	1.1	4.1

The spread in function values according to (1)

$$spread\_f = 4,2 - 3.8 = 0,4$$

This number could be normalized

$$spread\_f = \frac{\max(f(x_i)) - \min(f(x_i))}{\min(f(x_i))} = \frac{4.2 - 3.8}{3,8} = 0.105$$

The spread in variable space according to (2)

$$spread\_x = \max(\underbrace{2.2 - 1.8}_{x_1}, \underbrace{1.5 - 0.8}_{x_2}) = \max(0.4, 0.7) = 0.7$$

This number could be normalized by dividing with the variable range

$$spread\_v = \max_{j=1,..,n} \left(\frac{\max_{i=1,..,k}(x_{ij}) - \min_{i=1,..,k}(x_{ij})}{x_{up,j} - x_{low,j}} \right)$$

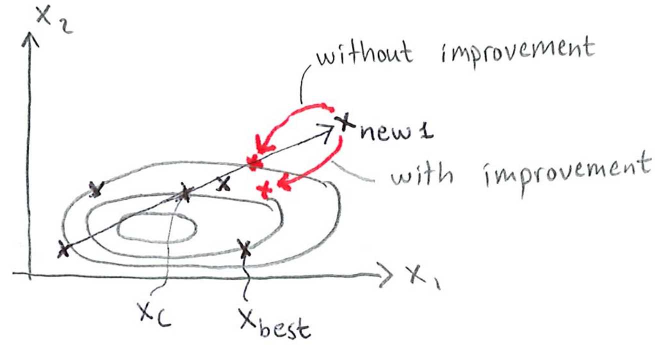
In this case

$$\max\left(\underbrace{\frac{2.2 - 1.8}{4 - 0}}_{x_1}, \underbrace{\frac{1.5 - 0.8}{4 - 0}}_{x_2}\right) = \max\left(\frac{0.4}{4}, \frac{0.7}{4}\right) = 0.175$$

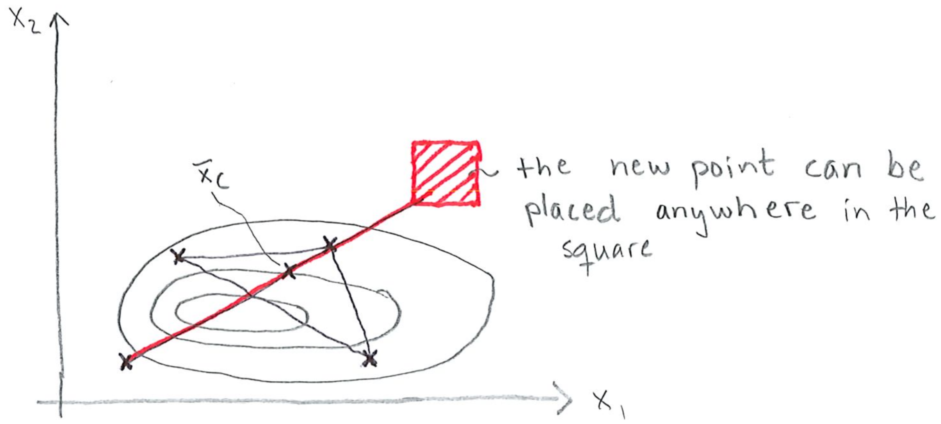
Complex Improvements

* Move the new point gradually towards the best when it is moved inward, towards the centroid

  Otherwise, the Complex might collapse if there is a local maximum at the centroid

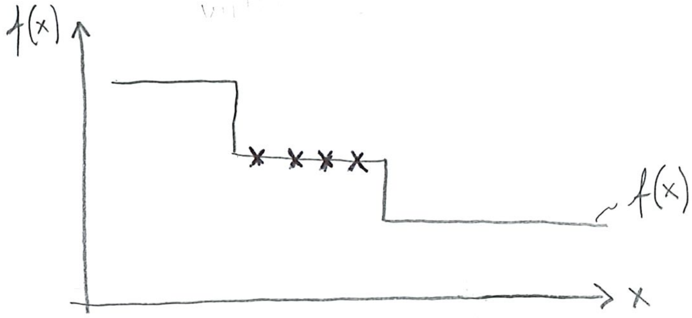


* Add noise to the new point so that the Complex does not converge to a local optimum



* Add forgetting factor so that all points become slightly worse in each iteration

⇒ Old objective function values are not as reliable as new ones



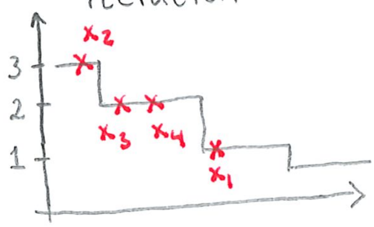
Without forgetting factor: The algorithm stops when all points have the same value ($f(x)$)

with forgetting factor:

Iteration 0

i	$f(x_i)$
1	3
2	3
3	2
4	2

Iteration 1

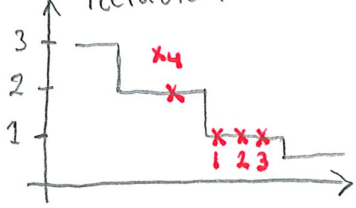


i	$f(x_i)$
1	1
2	3.0001
3	2.0001
4	2.0001

Iteration 2

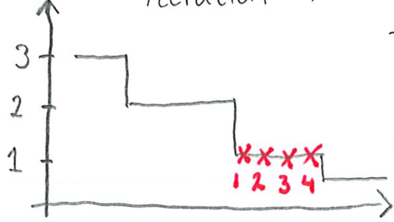
i	$f(x_i)$
1	1.0001
2	1
3	2.0002
4	2.0002

Iteration 3



i	$f(x_i)$
1	1.0002
2	1.0001
3	1
4	2.0003

Iteration 4



i	$f(x_i)$
1	1.0003
2	1.0002
3	1.0001
4	1

Exemplification of the Complex method

$$\min f(x) = (x_1-5)^2 + (x_2-5)^2 + 0{,}1\, x_1 \cdot x_2$$

$$0 \leq x_i \leq 10$$

We have two optimization variables.
⇒ Use a Complex of 4 points, $k=4$.

* Generate starting points randomly. Say

$\bar{X}_1 = (1, 1)$, $f(\bar{X}_1) = 32{,}1$
$\bar{X}_2 = (1, 2)$ $f(\bar{X}_2) = 25{,}2$
$\bar{X}_3 = (3, 1)$ $f(\bar{X}_3) = 20{,}3$
$\bar{X}_4 = (3, 2)$ $f(\bar{X}_4) = 13{,}6$

* Identify the worst point.

$\bar{X}_1$ is the worst ($f(\bar{X}_1)$ is the highest obj. func. value of the points in the complex)

* Calculate the centroid of the remaining points

$$X_{c,j} = \frac{1}{k-1}\left[\sum_{i=1}^{k} X_{i,j} - X_{w,j}\right], \quad j = 1..n$$

$$X_{c,1} = \frac{1}{4-1}\cdot\left[(1+3+1+3)-1\right] = 2{,}33$$

$$X_{c,2} = \frac{1}{4-1}\cdot\left[(1+1+2+2)-1\right] = 1{,}667$$

* Reflect the worst point through the centroid

$$X_{new,1} = X_{c,1} + \alpha^{1,3} \cdot (X_{c,1} - X_{w,1}) = 2,33 + 1,3\,(2,33 - 1) = 4,066$$

$$X_{new,2} = 1,667 + 1,3 \cdot (1,667 - 1) = 2,53$$

* Evaluate the objective function in the new point.

$$f(4,066; 3,3) = 0,0$$

* Identify the worst point.

$$X_W = (1,2)$$

* Calculate the centroid

$$X_{c,1} = \frac{1}{3}(3 + 1 + 3 + 4,066 - 1) = 3,36$$

$$X_{c,2} = \frac{1}{3}(1 + 2 + 2 + 2,53 - 2) = 1,84$$

* Reflect the worst point through the centroid

$$X_{new,1} = 3,36 + 1,3\,(3,36 - 1) = 6,42$$

$$f(6,42\,,\,1,63) = 14,41$$

$$X_{new,2} = 1,84 + 1,3\,(1,84 - 2) = 1,63$$