# Optimization for Machine Learning

## Lecture 3: Continuous Optimization II

October 25, 2021

TC2 - Optimisation

Université Paris-Saclay

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# Course Overview

| Date | | Topic |
|---|---|---|
| Thu, 4.11.2021 | DB | Introduction |
| Thu, 11.11.2021 | | no lecture |
| Thu, 18.11.2021 | AA | Continuous Optimization I: differentiability, gradients, convexity, optimality conditions |
| Thu, 25.11.2021 | AA | Continuous Optimization II: constrained optimization, gradient-based algorithms, stochastic gradient [written test / « contrôle continue »] |
| Thu, 2.12.2021 | AA | Continuous Optimization III: stochastic algorithms, derivative-free optimization |
| Thu, 9.12.2021 | DB | Discrete Optimization: greedy algorithms, dynamic programming [2nd written test / « contrôle continue »] |
| Thu 16.12.2021 | DB | Written exam |
| | | |
| | | always 13h30 till 16h00 |

# Constrained Optimization

# Reminder: Equality Constraint

**Objective:**

Generalize the necessary condition of $\nabla f(x) = 0$ at the optima of f

*when $f$ is in $\mathcal{C}^1$, i.e. is differentiable and its differential is continuous*

**Theorem:**

Be $U$ an open set of $(E, \|\ \|)$, and $f: U \to \mathbb{R}$, $g: U \to \mathbb{R}$ in $\mathcal{C}^1$.

Let $a \in E$ satisfy

$$\begin{cases} f(a) = \inf \{f(x) \mid x \in \mathbb{R}^n, g(x) = 0\} \\ g(a) = 0 \end{cases}$$

i.e. $a$ is optimum of the problem

If $\nabla g(a) \neq 0$, then there exists a constant $\lambda \in \mathbb{R}$ called *Lagrange multiplier*, such that

$$\underbrace{\nabla f(a) + \lambda \nabla g(a) = 0}\quad \text{Euler} - \text{Lagrange equation}$$

i.e. gradients of $f$ and $g$ in $a$ are colinear

# Geometrical Interpretation Using an Example

**Exercise:**

Consider the problem

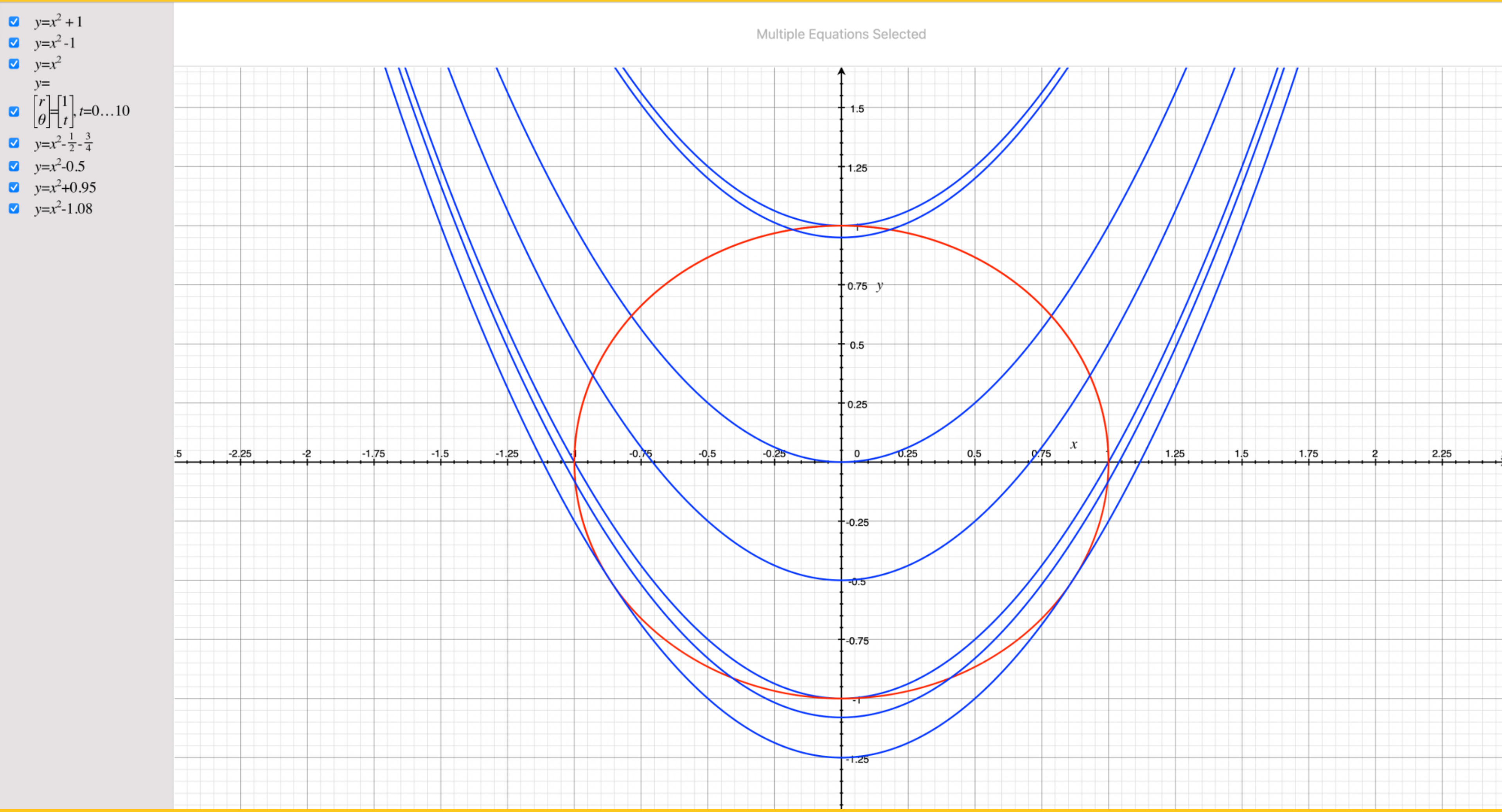
$$\inf \{ f(x, y) \mid (x, y) \in \mathbb{R}^2, g(x, y) = 0\}$$

$f(x, y) = y - x^2 \qquad g(x, y) = x^2 + y^2 - 1 = 0$

1) Plot the level sets of $f$, plot $g = 0$
2) Compute $\nabla f$ and $\nabla g$
3) Find the solutions with $\nabla f + \lambda \nabla g = 0$

   *equation solving with 3 unknowns $(x, y, \lambda)$*
4) Plot the solutions of 3) on top of the level set graph of 1)

# Visual Solution



# Answer

- $(x_1, y_1, \lambda_1) = \left(0, 1, -\frac{1}{2}\right)$ [max local]
- $= \left(0, -1, \frac{1}{2}\right)$ [max local]
- $= \left(\sqrt{\frac{3}{4}}, -\frac{1}{2}, 1\right)$ [min global]
- $= \left(-\sqrt{\frac{3}{4}}, -\frac{1}{2}, 1\right)$ [min global]

**Note:**

Here we see clearly that the previous conditions are necessary conditions but not sufficient conditions.

# Interpretation of Euler-Lagrange Equation

Intuitive way to retrieve the Euler-Lagrange equation:

- In a local minimum $a$ of a constrained problem, the hypersurfaces (or level sets) $f = f(a)$ and $g = 0$ are necessarily tangent (otherwise we could decrease $f$ by moving along $g = 0$).
- Since the gradients $\nabla f(a)$ and $\nabla g(a)$ are orthogonal to the level sets $f = f(a)$ and $g = 0$, it follows that $\nabla f(a)$ and $\nabla g(a)$ are colinear.

# Generalization to More than One Constraint

**Theorem**

- Assume $f: U \to \mathbb{R}$ and $g_k: U \to \mathbb{R}$ $(1 \leq k \leq p)$ are $\mathcal{C}^1$.
- Let $a$ be such that

$$\begin{cases} f(a) = \inf \{ f(x) \mid x \in \mathbb{R}^n, \quad g_k(x) = 0, \quad 1 \leq k \leq p \} \\ g_k(a) = 0 \ \text{ for all } 1 \leq k \leq p \end{cases}$$

- If $\left(\nabla g_k(a)\right)_{1 \leq k \leq p}$ are linearly independent, then there exist $p$ real constants $(\lambda_k)_{1 \leq k \leq p}$ such that

$$\nabla f(a) + \sum_{k=1}^{p} \lambda_k \nabla g_k(a) = 0$$

↑

Lagrange multiplier

again: $a$ does not need to be global but local minimum

# The Lagrangian

- Define the Lagrangian on $\mathbb{R}^n \times \mathbb{R}^p$ as

$$\mathcal{L}(x, \{\lambda_k\}) = f(x) + \sum_{k=1}^{p} \lambda_k g_k(x)$$

- To find optimal solutions, we can solve the optimality system

$$\begin{cases} \text{Find } (x, \{\lambda_k\}) \in \mathbb{R}^n \times \mathbb{R}^p \text{ such that } \nabla f(x) + \sum_{k=1}^{p} \lambda_k \nabla g_k(x) = 0 \\ g_k(x) = 0 \ \text{ for all } 1 \leq k \leq p \end{cases}$$

$$\Leftrightarrow \begin{cases} \text{Find } (x, \{\lambda_k\}) \in \mathbb{R}^n \times \mathbb{R}^p \text{ such that } \nabla_x \mathcal{L}(x, \{\lambda_k\}) = 0 \\ \nabla_{\lambda_k} \mathcal{L}(x, \{\lambda_k\})(x) = 0 \ \text{ for all } 1 \leq k \leq p \end{cases}$$

# Inequality Constraint: Definitions

Let $\mathcal{U} = \{x \in \mathbb{R}^n \mid g_k(x) = 0 \text{ (for } k \in E), \; g_k(x) \leq 0 \text{ (for } k \in I)\}$.

**Definition:**

The points in $\mathbb{R}^n$ that satisfy the constraints are also called *feasible* points.

**Definition:**

Let $a \in \mathcal{U}$, we say that the constraint $g_k(x) \leq 0$ (for $k \in I$) is *active* in $a$ if $g_k(a) = 0$.

**Theorem (Karush-Kuhn-Tucker, KKT):**

Let $U$ be an open set of $(\mathbb{R}^n, || \, ||)$ and $f: U \to \mathbb{R}$, $g_k: U \to \mathbb{R}$, all $\mathcal{C}^1$

Furthermore, let $a \in U$ satisfy

$$\begin{cases} f(a) = \inf(f(x) \mid x \in \mathbb{R}^n, g_k(x) = 0 \ (\text{for } k \in E), g_k(x) \leq 0 \ (\text{for } k \in \mathrm{I}) \\ g_k(a) = 0 \ (\text{for } k \in E) \\ g_k(a) \leq 0 \ (\text{for } k \in I) \end{cases}$$

also works again for $a$ being a local minimum

Let $I_a^0$ be the set of constraints that are active in $a$. Assume that $\left(\nabla g_k(a)\right)_{k \in E \cup I_a^0}$ are linearly independent.

Then there exist $(\lambda_k)_{1 \leq k \leq p}$ that satisfy

$$\begin{cases} \nabla f(a) + \sum_{k=1}^{p} \lambda_k \nabla g_k(a) = 0 \\ g_k(a) = 0 \ (\text{for } k \in E) \\ g_k(a) \leq 0 \ (\text{for } k \in I) \\ \lambda_k \geq 0 \ (\text{for } k \in I_a^0) \\ \lambda_k g_k(a) = 0 \ (\text{for } k \in E \cup I) \end{cases}$$

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either active constraint or $\lambda_k = 0$

# Descent Methods

# Descent Methods

## General principle

❶ choose an initial point $\boldsymbol{x}_0$, set $t = 0$

❷ while not happy

- choose a descent direction $\boldsymbol{d}_t \neq 0$
- line search:
  - choose a step size $\sigma_t > 0$
  - set $\boldsymbol{x}_{t+1} = \boldsymbol{x}_t + \sigma_t \boldsymbol{d}_t$
- set $t = t + 1$

## Remaining questions

- how to choose $\boldsymbol{d}_t$?
- how to choose $\sigma_t$?

# Gradient Descent

**Rationale:** $\boldsymbol{d}_t = -\nabla f(\boldsymbol{x}_t)$ is a descent direction

indeed for $f$ differentiable

$$f\big(x - \sigma\nabla f(x)\big) = f(x) - \sigma||\nabla f(x)||^2 + o(\sigma||\nabla f(x)||)$$

$< f(x)$ for $\sigma$ small enough

## Step-size

- optimal step-size: $\sigma_t = \underset{\sigma}{\operatorname{argmin}} f(\boldsymbol{x}_t - \sigma\nabla f(\boldsymbol{x}_t))$
- **Line Search:** total or partial optimization w.r.t. $\sigma$
  Total is however often too "expensive" (needs to be performed at each iteration step)
  Partial optimization: execute a limited number of trial steps until a loose approximation of the optimum is found. Typical rule for partial optimization: Armijo rule (see next slides)

## Typical stopping criterium:

norm of gradient smaller than $\epsilon$

# The Armijo-Goldstein Rule

## Choosing the step size:

- Only to decrease $f$-value not enough to converge (quickly)
- Want to have a reasonably large decrease in $f$

## Armijo-Goldstein rule:

- also known as backtracking line search
- starts with a (too) large estimate of $\sigma$ and reduces it until $f$ is reduced enough
- what is enough?
  - assuming a linear $f$ e.g. $m_k(x) = f(x_k) + \nabla f(x_k)^T(x - x_k)$
  - expected decrease if step of $\sigma_k$ is done in direction $\boldsymbol{d}$: $\sigma_k \nabla f(x_k)^T \boldsymbol{d}$
  - actual decrease: $f(x_k) - f(x_k + \sigma_k \boldsymbol{d})$
  - stop if actual decrease is at least constant times expected decrease (constant typically chosen in [0, 1])

## The Actual Algorithm:

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**Input:** descent direction $\mathbf{d}$, point $\mathbf{x}$, objective function $f(\mathbf{x})$ and its gradient $\nabla f(\mathbf{x})$, parameters $\sigma_0 = 10$, $\theta \in [0,1]$ and $\beta \in (0,1)$
**Output:** step-size $\sigma$

Initialize $\sigma$: $\sigma \leftarrow \sigma_0$
**while** $f(\mathbf{x} + \sigma\mathbf{d}) > f(\mathbf{x}) + \theta\sigma\nabla f(\mathbf{x})^T\mathbf{d}$ **do**
    $\sigma \leftarrow \beta\sigma$
**end while**

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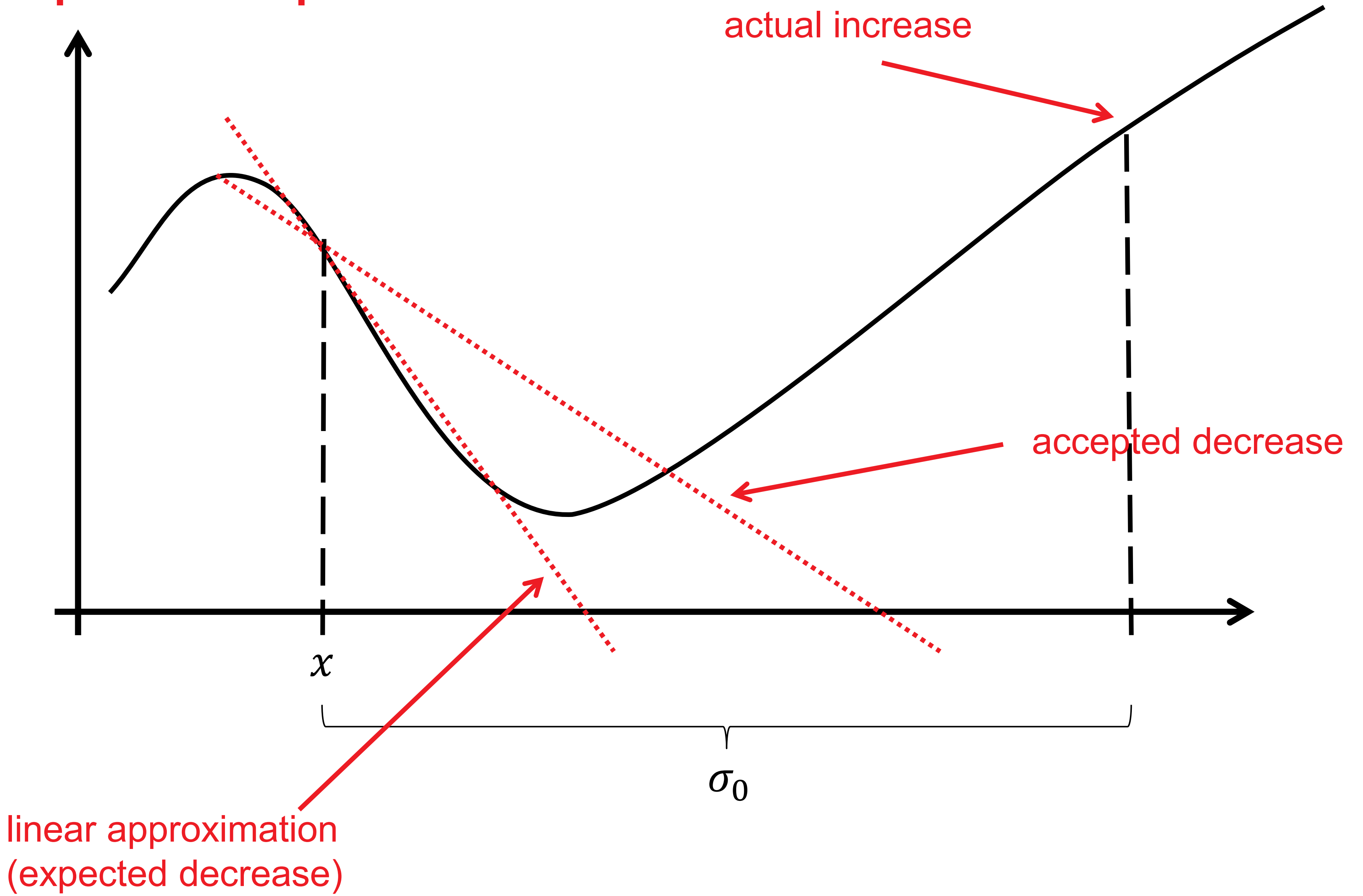
Armijo, in his original publication chose $\beta = \theta = 0.5$.
Choosing $\theta = 0$ means the algorithm accepts any decrease.

## Graphical Interpretation



# The Armijo-Goldstein Rule

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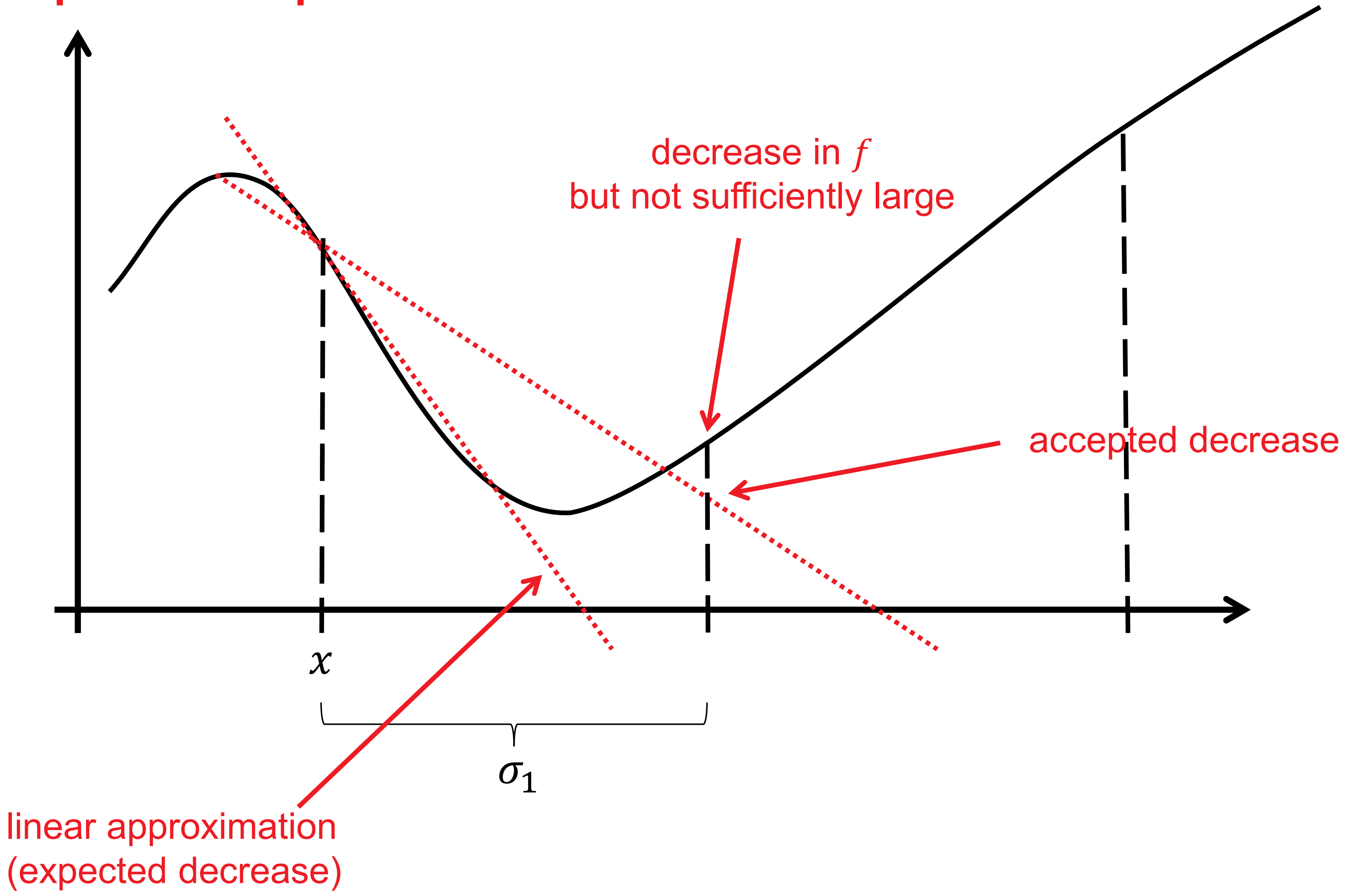

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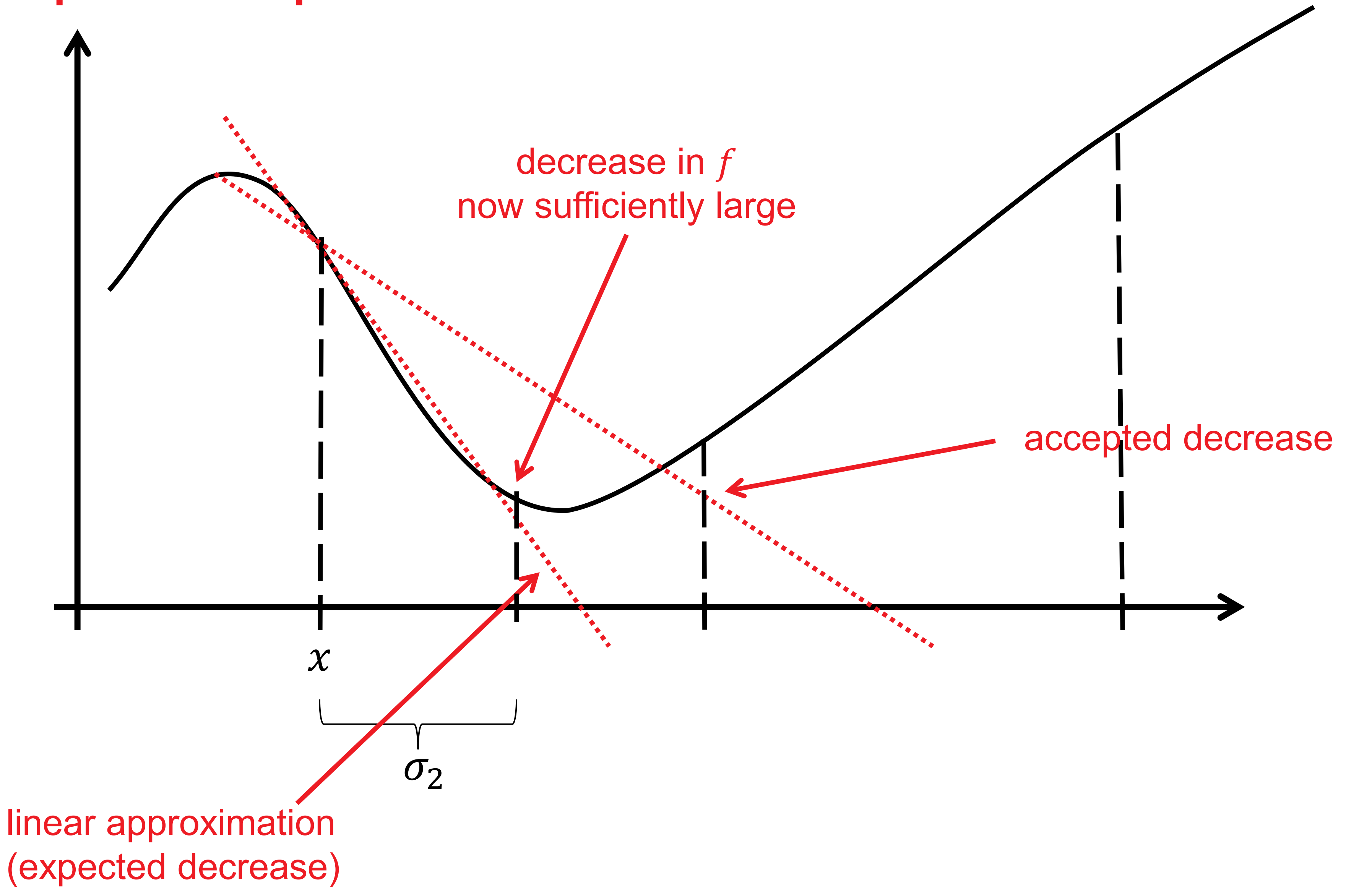

# Newton Algorithm

## Newton Method

- descent direction: $-[\nabla^2 f(x_k)]^{-1}\nabla f(x_k)$ [so-called Newton direction]
- The Newton direction:
  - minimizes the best (locally) quadratic approximation of $f$:
    $\tilde{f}(x+\Delta x) = f(x) + \nabla f(x)^T \Delta x + \frac{1}{2}(\Delta x)^T \nabla^2 f(x) \Delta x$
  - points towards the optimum on $f(x) = (x - x^*)^T A (x - x^*)$
- however, Hessian matrix is expensive to compute in general and its inversion is also not easy

*quadratic convergence*

(i.e. $\lim_{k\to\infty} \frac{|x_{k+1}-x^*|}{|x_k - x^*|^2} = \mu > 0$)

# Remark: Affine Invariance

**Affine Invariance:** same behavior on $f(x)$ and $f(Ax+b)$ for $A \in \mathrm{GLn}(\mathbb{R})$ = set of all invertible $n \times n$ matrices over $\mathbb{R}$

- Newton method is affine invariant

  see **`http://users.ece.utexas.edu/~cmcaram/EE381V_2012F/Lecture_6_Scribe_Notes.final.pdf`**

- same convergence rate on all convex-quadratic functions
- Gradient method not affine invariant

# Quasi-Newton Method: BFGS

$x_{t+1} = x_t - \sigma_t H_t \nabla f(x_t)$ where $H_t$ is an approximation of the inverse Hessian

**Key idea of Quasi Newton:**

successive iterates $x_t$, $x_{t+1}$ and gradients $\nabla f(x_t)$, $\nabla f(x_{t+1})$ yield second order information

$$q_t \approx \nabla^2 f(x_{t+1}) p_t$$

where $p_t = x_{t+1} - x_t$ and $q_t = \nabla f(x_{t+1}) - \nabla f(x_t)$

Most popular implementation of this idea: Broyden-Fletcher-Goldfarb-Shanno (BFGS)

- default in MATLAB's **`fminunc`** and python's **`scipy.optimize.minimize`**

# Conclusions

I hope it became clear...

...what are the difficulties to cope with when solving numerical optimization problems

*in particular dimensionality, non-separability and ill-conditioning*

...what are gradient and Hessian

...what is the difference between gradient and Newton direction

...and that adapting the step size in descent algorithms is crucial.

# Derivative-Free Optimization

# Derivative-Free Optimization (DFO)

## DFO = blackbox optimization


## Why blackbox scenario?

- gradients are not always available (binary code, no analytical model, ...)
- or not useful (noise, non-smooth, ...)

- problem domain specific knowledge is used only within the black box, e.g. within an appropriate encoding
- some algorithms are furthermore function-value-free, i.e. *invariant* wrt. monotonous transformations of $f$.

# Derivative-Free Optimization Algorithms

- (gradient-based algorithms which approximate the gradient by finite differences)

- coordinate descent
- pattern search methods, e.g. Nelder-Mead
- surrogate-assisted algorithms, e.g. NEWUOA or other trust-region methods
- other function-value-free algorithms
  - typically stochastic
  - evolution strategies (ESs) and Covariance Matrix Adaptation Evolution Strategy (CMA-ES)
  - differential evolution
  - particle swarm optimization
  - simulated annealing
  - ...

# Downhill Simplex Method by Nelder and Mead

While not happy do:

[assuming minimization of $f$ and that $x_1, \dots, x_{n+1} \in \mathbb{R}^n$ form a simplex]

**1) Order** according to the values at the vertices: $f(x_1) \leq f(x_2) \leq \cdots \leq f(x_{n+1})$

**2)** Calculate $x_o$, the centroid of all points except $x_{n+1}$.

**3) Reflection**

Compute reflected point $x_r = x_o + \alpha (x_o - x_{n+1})$ $(\alpha > 0)$

If $x_r$ better than second worst, but not better than best: $x_{n+1} := x_r$ , and go to 1)

**4) Expansion**

If $x_r$ is the best point so far: compute the expanded point

$$x_e = x_o + \gamma (x_r - x_o) (\gamma > 0)$$

If $x_e$ better than $x_r$ then $x_{n+1} := x_e$ and go to 1)

Else $x_{n+1} := x_r$ and go to 1)

Else (i.e. reflected point is not better than second worst) continue with 5)

**5) Contraction** (here: $f(x_r) \geq f(x_n)$)

Compute contracted point $x_c = x_o + \rho(x_{n+1} - x_o)$ $(0 < \rho \leq 0.5)$

If $f(x_c) < f(x_{n+1})$: $x_{n+1} := x_c$ and go to 1)

Else go to 6)

**6) Shrink**

$x_i = x_1 + \sigma(x_i - x_1)$ for all $i \in \{2, \dots, n+1\}$ $(\sigma < 1)$ and go to 1)

*J. A Nelder and R. Mead (1965). "A simplex method for function minimization". Computer Journal.* ***7****: 308–313. doi:10.1093/comjnl/7.4.308*

# Nelder-Mead: Reflection

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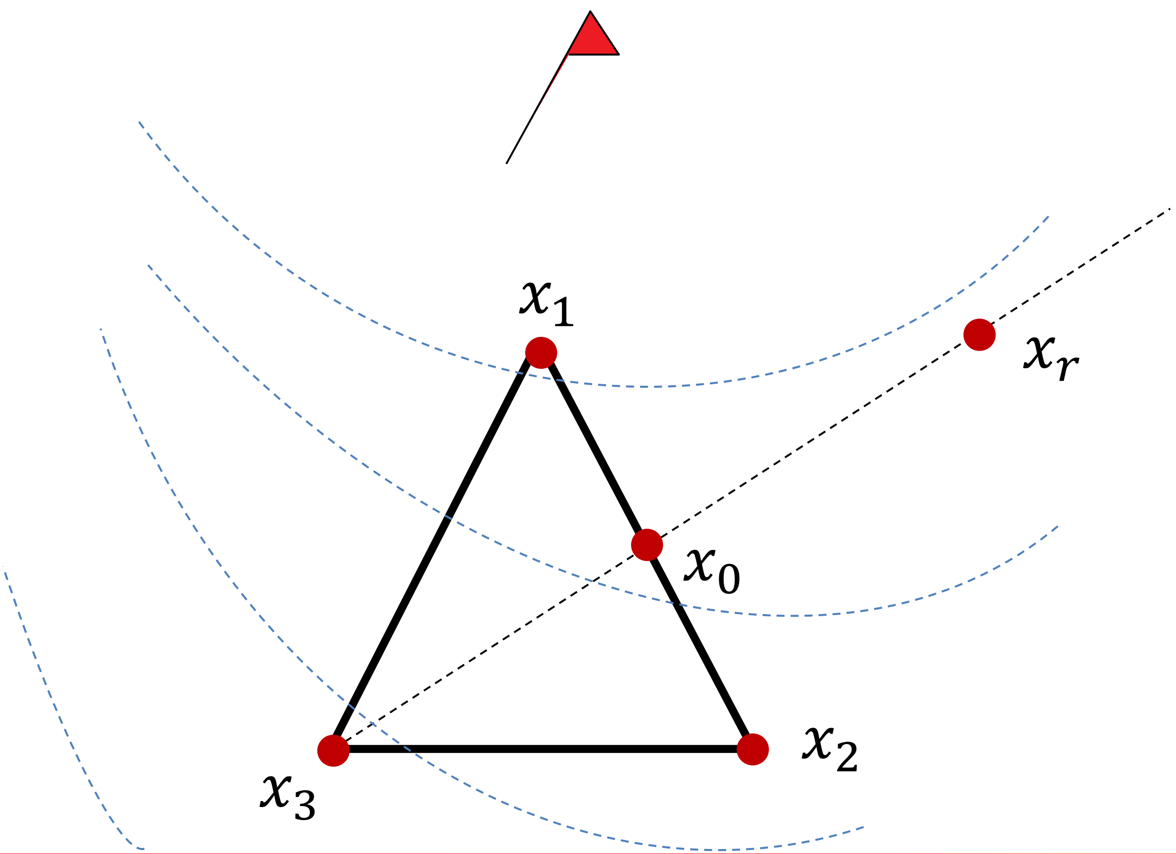

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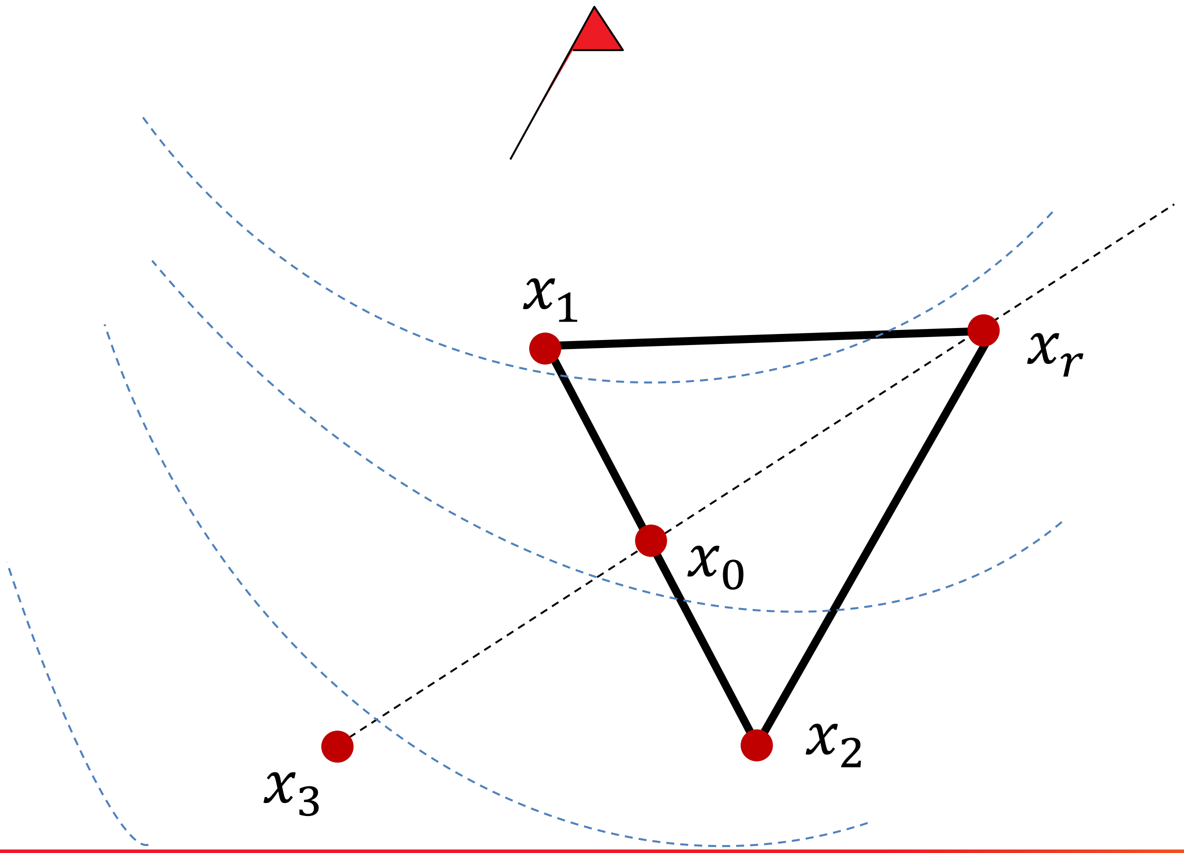

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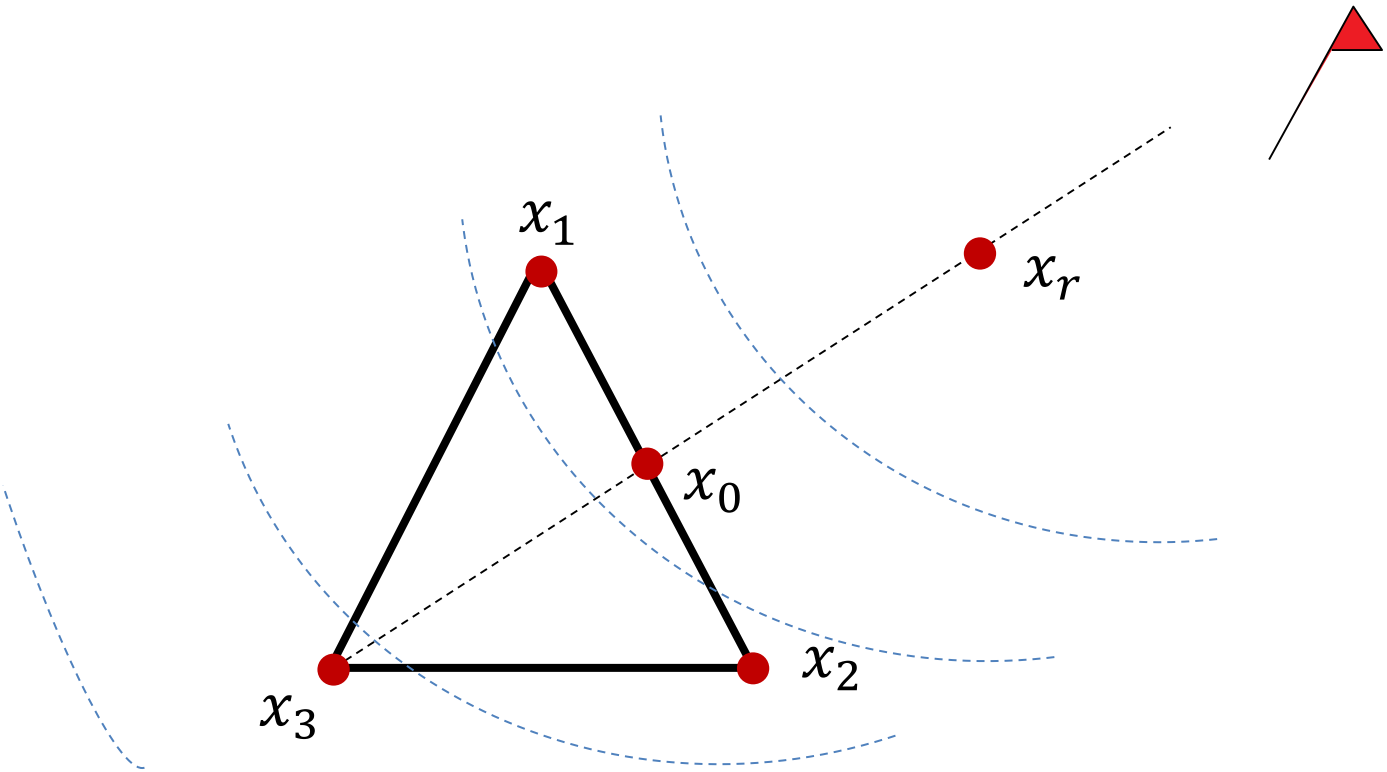

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**2)** Calculate $x_o$, the centroid of all points except $x_{n+1}$.

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$$x_e = x_o + \gamma\,(x_r - x_o)(\gamma > 0)$$

If $x_e$ better than $x_r$ then $x_{n+1} \coloneqq x_e$ and go to 1)

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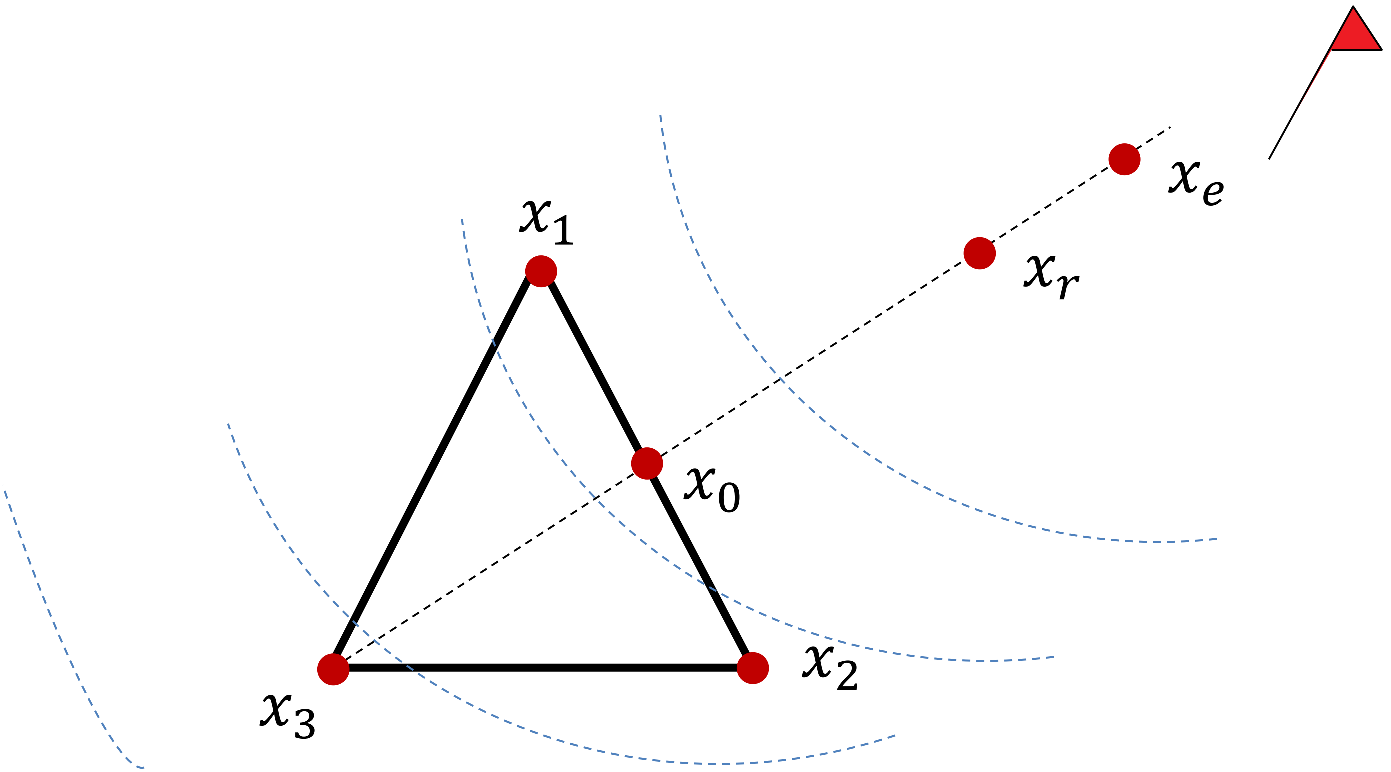

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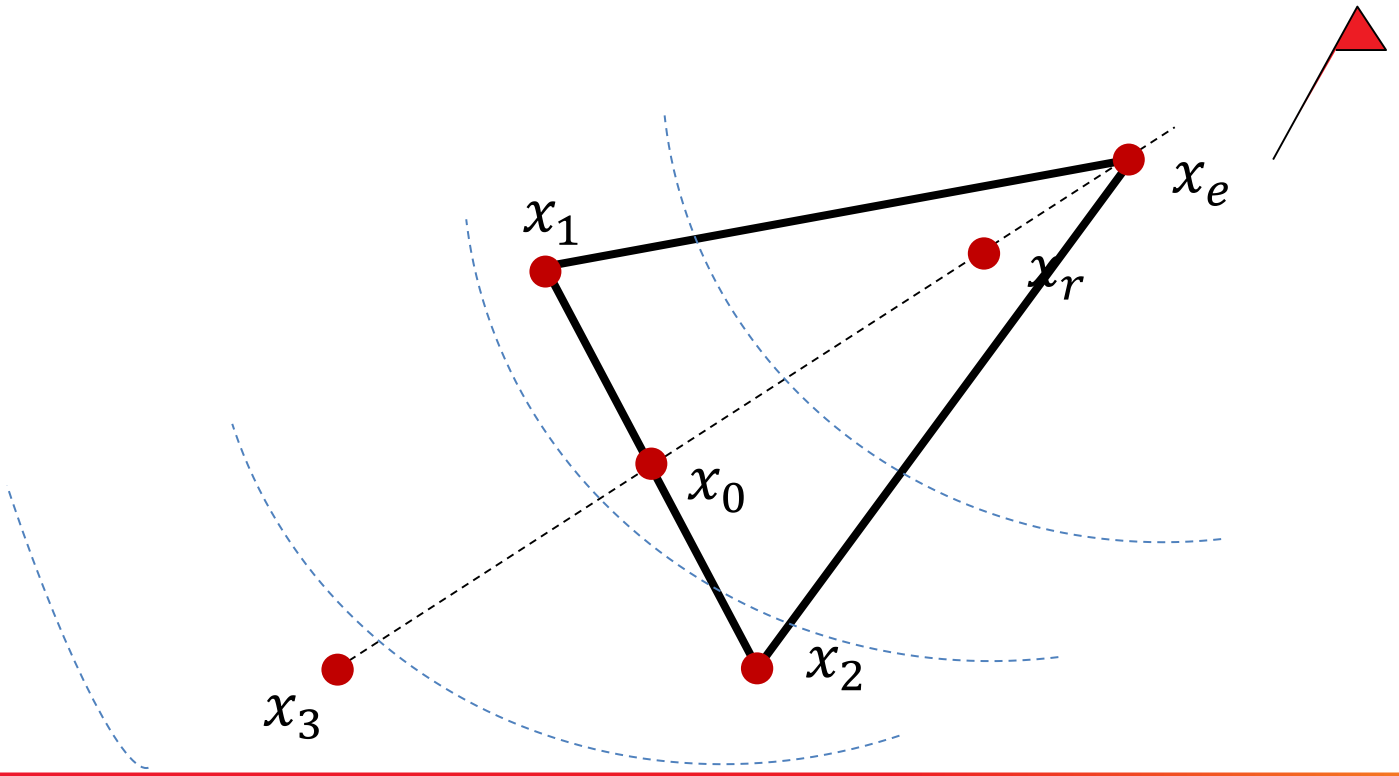

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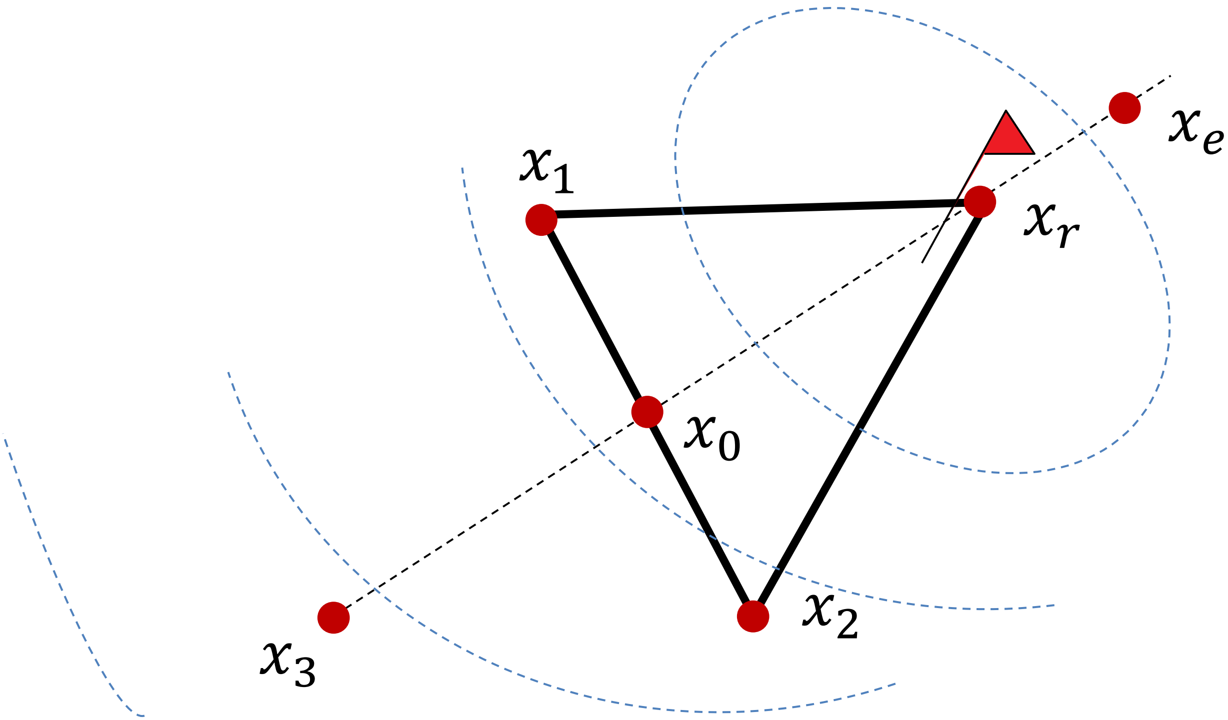

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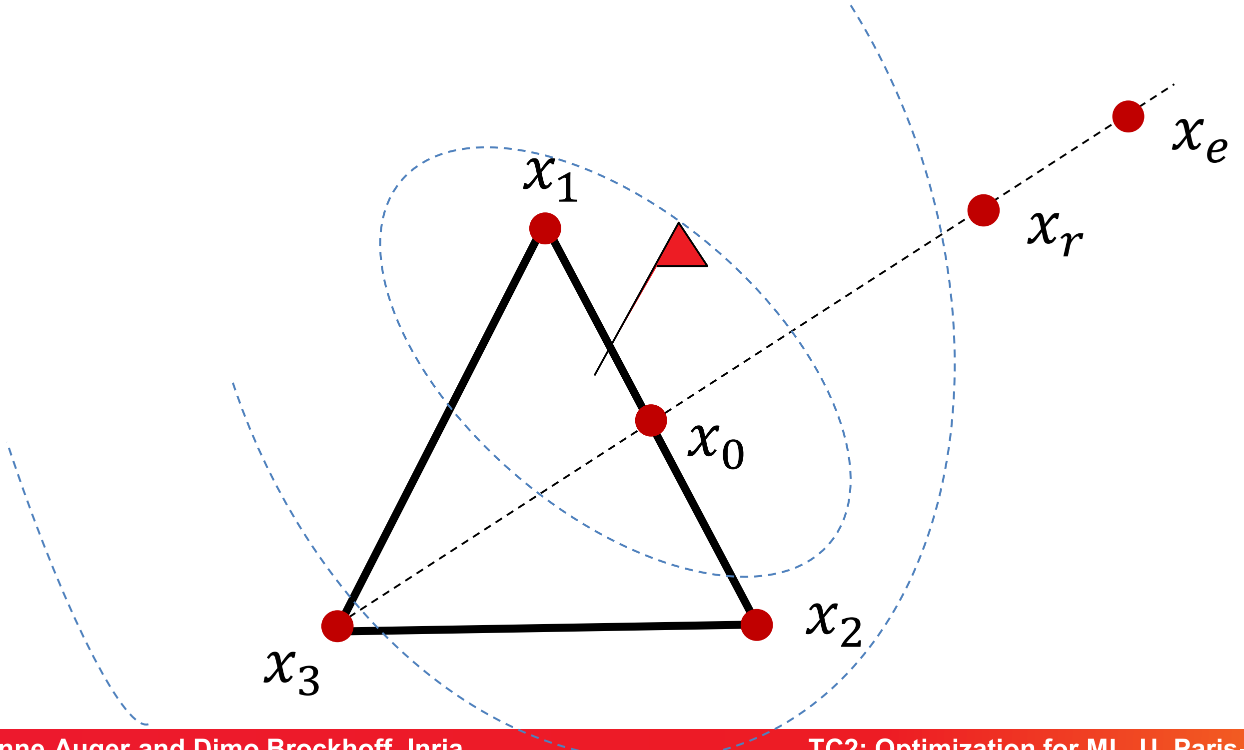

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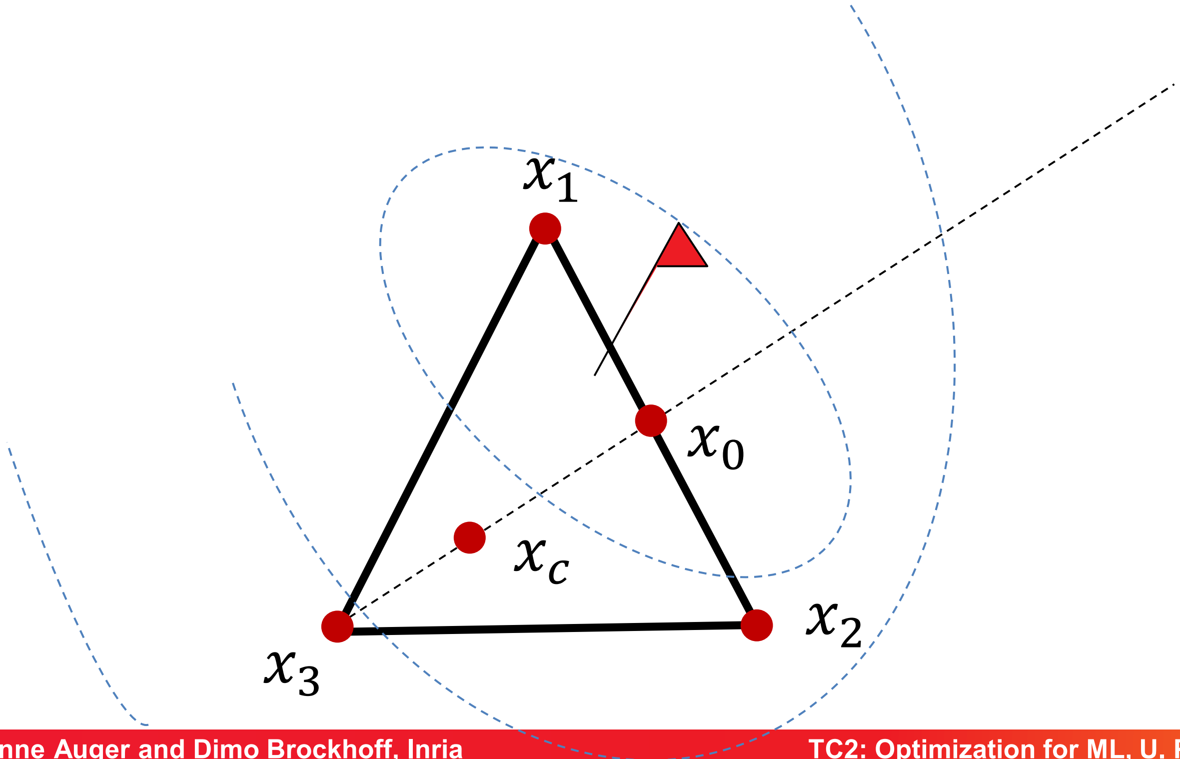

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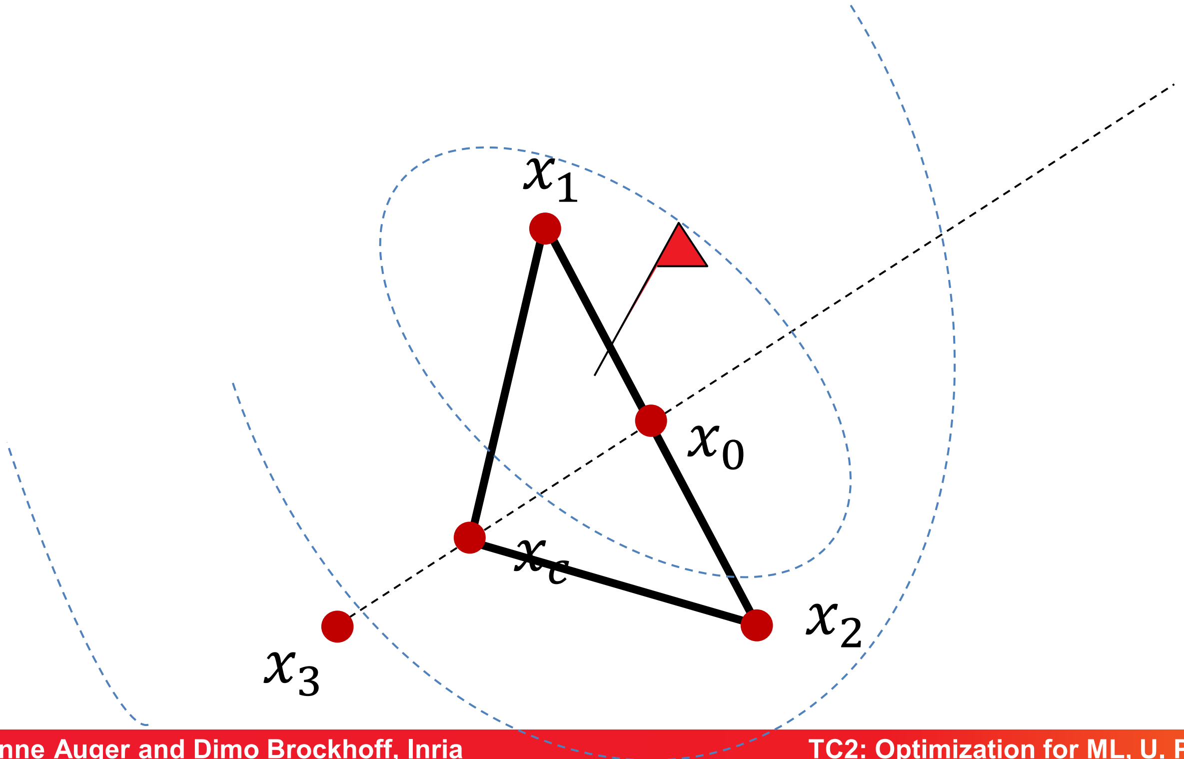

# Nelder-Mead: Expansion

**2)** Calculate $x_o$, the centroid of all points except $x_{n+1}$.

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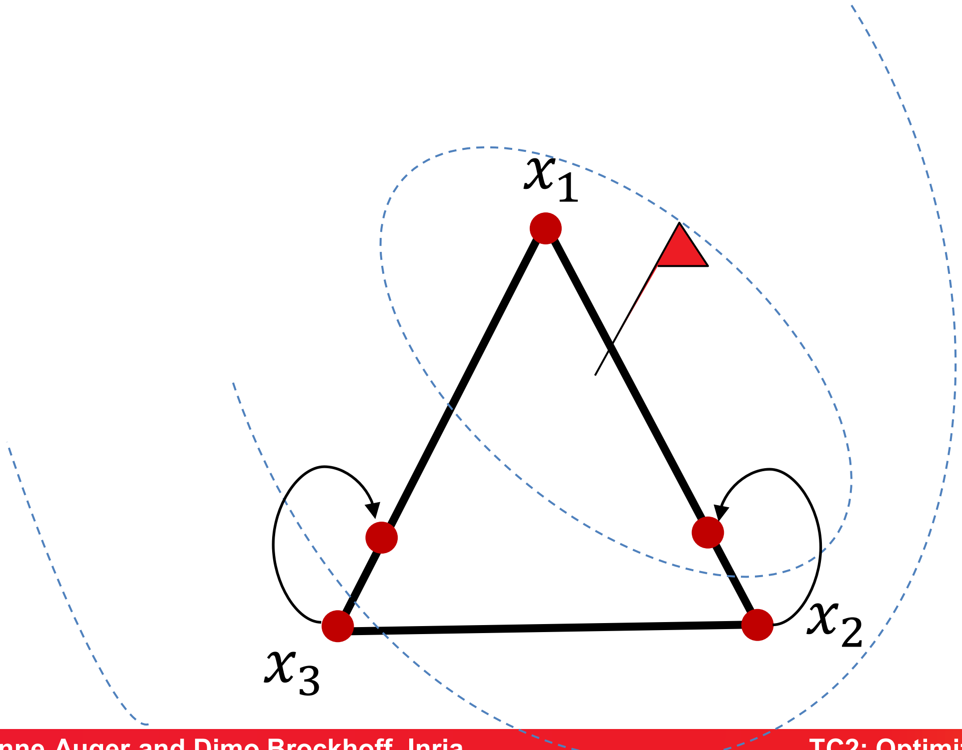
$x_i = x_1 + \sigma(x_i - x_1)$ for all $i \in \{2, \ldots, n+1\}$ and go to 1)



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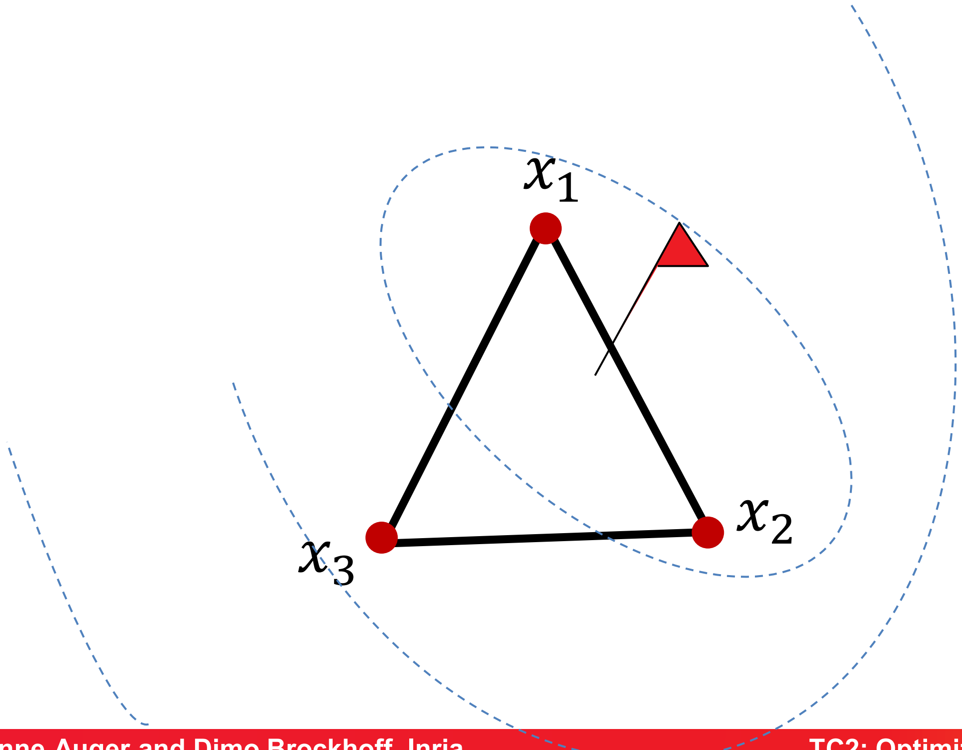


# Nelder-Mead: Standard Parameters

- reflection parameter : $\alpha = 1$
- expansion parameter: $\gamma = 2$
- contraction parameter: $\rho = \frac{1}{2}$
- shrink parameter: $\sigma = \frac{1}{2}$

some visualizations of example runs can be found here:
https://en.wikipedia.org/wiki/Nelder%E2%80%93Mead_method

# stochastic algorithms

# Stochastic Search Template

**A stochastic blackbox search template to minimize $f: \mathbb{R}^n \to \mathbb{R}$**

Initialize distribution parameters $\theta$, set population size $\lambda \in \mathbb{N}$

While happy do:

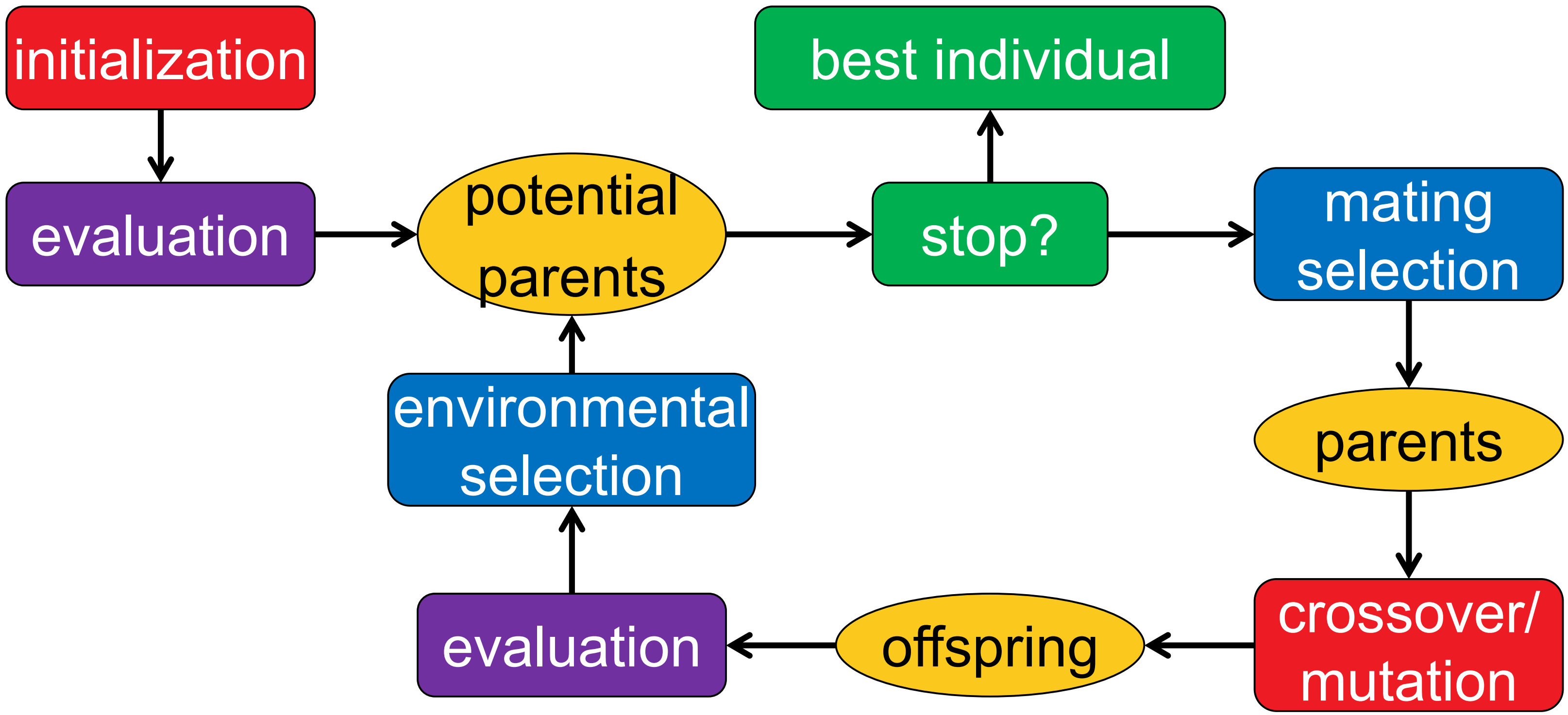
- Sample distribution $P(\boldsymbol{x}|\theta) \to \boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda \in \mathbb{R}^n$
- Evaluate $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda$ on $f$
- Update parameters $\theta \leftarrow F_\theta(\theta, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda, f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_\lambda))$

- All depends on the choice of $P$ and $F_\theta$

*deterministic algorithms are covered as well*

- In Evolutionary Algorithms, $P$ and $F_\theta$ are often defined implicitly via their operators.

# Generic Framework of an Evolutionary Algorithm




stochastic operators

"Darwinism"

stopping criteria

Nothing else: just interpretation change

## The CMA-ES

Input: $\boldsymbol{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\lambda$
Initialize: $\mathbf{C} = \mathbf{I}$, and $p_c = \mathbf{0}$, $p_\sigma = \mathbf{0}$,
Set: $c_c \approx 4/n$, $c_\sigma \approx 4/n$, $c_1 \approx 2/n^2$, $c_\mu \approx \mu_w/n^2$, $c_1 + c_\mu \leq 1$, $d_\sigma \approx 1 + \sqrt{\frac{\mu_w}{n}}$,
and $w_{i=1\ldots\lambda}$ such that $\mu_w = \frac{1}{\sum_{i=1}^{\mu} {w_i}^2} \approx 0.3\,\lambda$

While not terminate

$\boldsymbol{x}_i = \boldsymbol{m} + \sigma \boldsymbol{y}_i, \quad \boldsymbol{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$, for $i = 1, \ldots, \lambda$ — sampling

$\boldsymbol{m} \leftarrow \sum_{i=1}^{\mu} w_i \boldsymbol{x}_{i:\lambda} = \boldsymbol{m} + \sigma \boldsymbol{y}_w$ where $\boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}$ — update mean

$p_c \leftarrow (1 - c_c)\, p_c + \mathbb{1}_{\{\|p_\sigma\| < 1.5\sqrt{n}\}} \sqrt{1 - (1 - c_c)^2} \sqrt{\mu_w}\, \boldsymbol{y}_w$ — cumulation for $\mathbf{C}$

$p_\sigma \leftarrow (1 - c_\sigma)\, p_\sigma + \sqrt{1 - (1 - c_\sigma)^2} \sqrt{\mu_w}\, \mathbf{C}^{-\frac{1}{2}} \boldsymbol{y}_w$ — cumulation for $\sigma$

$\mathbf{C} \leftarrow (1 - c_1 - c_\mu)\, \mathbf{C} + c_1\, p_c {p_c}^{\mathrm{T}} + c_\mu \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda} \boldsymbol{y}_{i:\lambda}^{\mathrm{T}}$ — update $\mathbf{C}$

$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|p_\sigma\|}{\mathrm{E}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|} - 1\right)\right)$ — update of $\sigma$

Not covered on this slide: termination, restarts, useful output, boundaries and encoding