Advanced computational statistics, lecture 3

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LINKÖPING UNIVERSITY

Course schedule

- Topic 1: **Gradient based optimisation**
- Topic 2: **Stochastic gradient based optimisation**
- Topic 3: **Gradient free optimisation**
- Topic 4: **Optimisation with constraints**
- Topic 5: **EM algorithm and bootstrap**
- Topic 6: **Simulation of random variables**
- Topic 7: **Importance sampling**

Course homepage:
http://www.adoptdesign.de/frankmillereu/adcompstat2025.html

Includes schedule, reading material, lecture notes, assignments

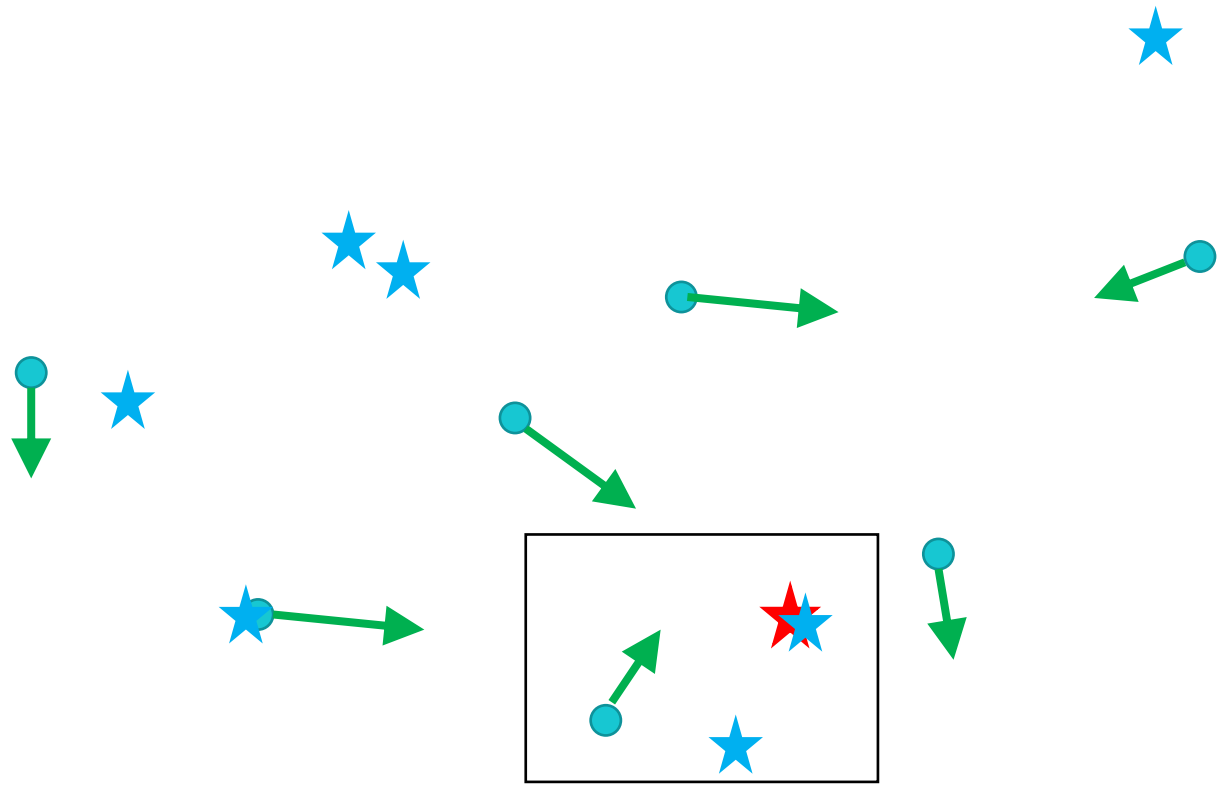
Today's schedule: gradient free methods

- **Particle swarm optimisation** (PSO)
  - Idea
  - Different versions
  - Theoretical investigations
- **Simulated annealing**
  - Idea (for the generic optimisation problem)
  - Simulated annealing for combinatorial optimisation
  - Theoretical basis
- To compare algorithms or hyperparameter choices by empirical studies
- **Nelder-Mead algorithm**

Particle swarm optimization (PSO)

Particle swarm optimisation

- Swarm of s particles
  - Position of particle i at iteration $t + 1$: $\boldsymbol{x}_i^{(t+1)}$
  - Velocity of particle i at iteration $t + 1$: $\boldsymbol{v}_i^{(t+1)}$
- Best positions found so far:
  - Best location found by particle i: $\boldsymbol{p}_{\text{best},\,i}^{(t)}$
  - Global best solution found: $\boldsymbol{g}_{\text{best}}^{(t)}$

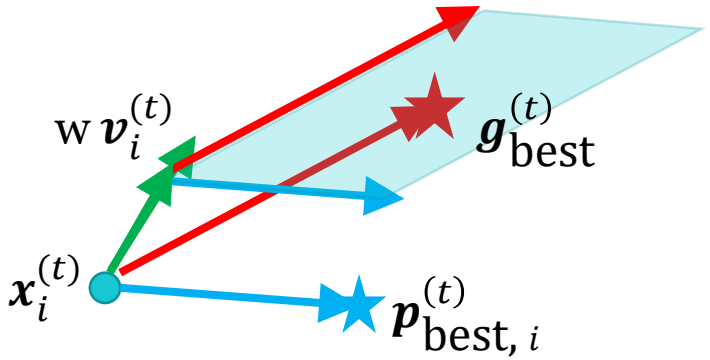


Particle swarm optimisation

- Movement of particle i at iteration $t + 1$:
  - $\boldsymbol{x}_i^{(t+1)} = \boldsymbol{x}_i^{(t)} + \boldsymbol{v}_i^{(t+1)}$
  - $\boldsymbol{v}_i^{(t+1)} = w\boldsymbol{v}_i^{(t)} + c_1 R_1^{(t+1)} (\boldsymbol{p}_{\text{best},\, i}^{(t)} - \boldsymbol{x}_i^{(t)}) + c_2 R_2^{(t+1)} (\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}_i^{(t)})$

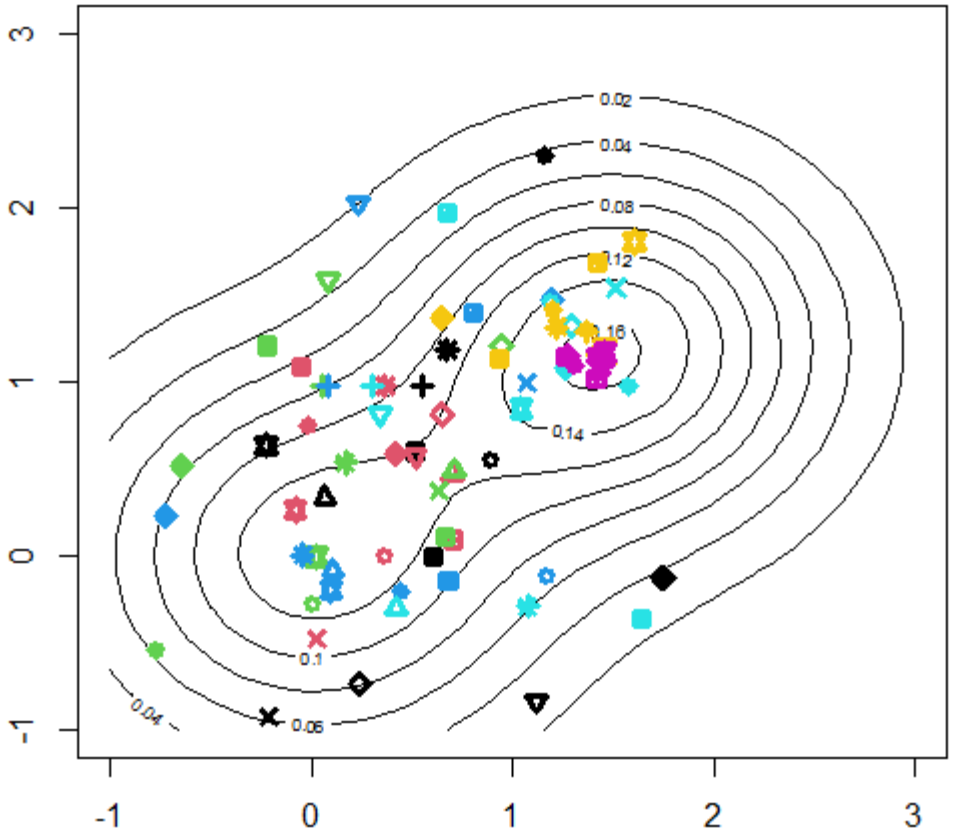
inertia weight — cognitive component — social component

- $R_1^{(t+1)}$ and $R_2^{(t+1)}$ are uniformly distributed, **`runif()`**



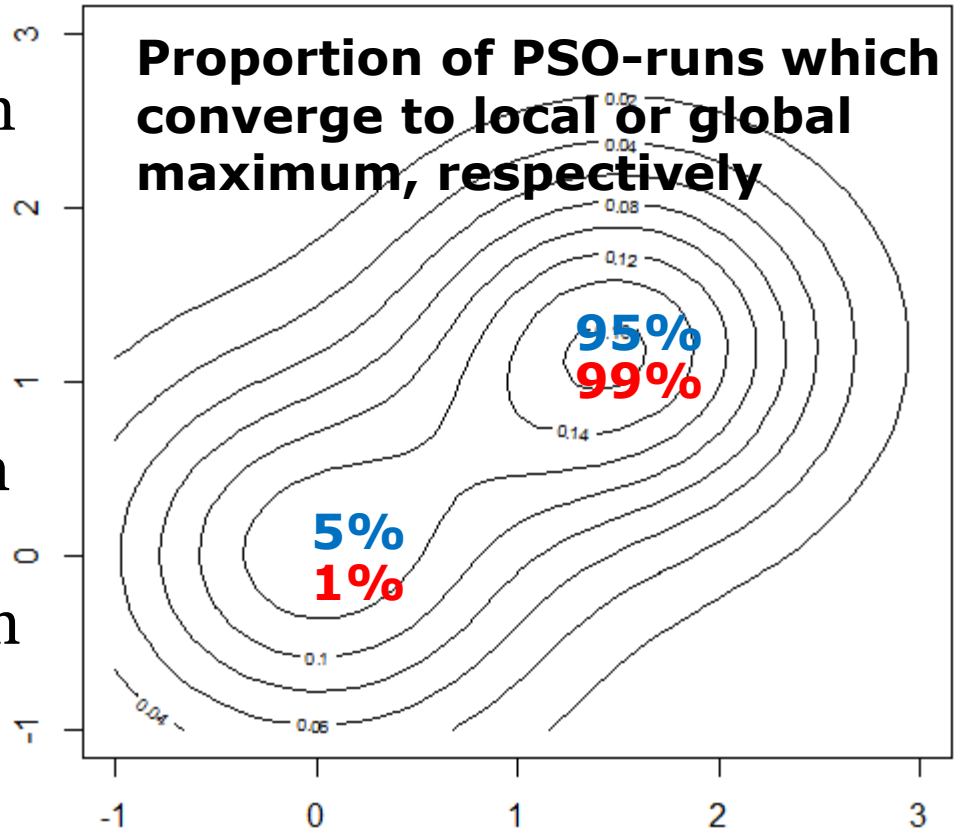
Particle swarm optimisation

- Bimodal normal mixture example from Lecture 1
- PSO with $s = 12$ particles using **`psoptim`** (in **`R`**-package **`pso`**)
  - Iteration 1
  - Iteration 2
  - Iteration 3
  - Iteration 4
  - Iteration 5
  - Iteration 20
  - Iteration 40



Particle swarm optimisation

- Bimodal normal mixture example from Lecture 1
- In some runs, the local maximum is identified as global maximum
- Risk to remain at a local maximum can be reduced if not all particles are informed about the global best solution
- Option `control=list(p= )` controls proportion informed; default `1-(11/12)^3=0.23`.



Particle swarm optimisation

- Example call:
-
```
pso <- psoptim(par=rep(NA,2),
               fn=g,
               lower=-1, upper=3,
               control=list(
                  fnscale=-1,
                  maxit=1000,
                  p=0.23,
                  s=12
               ))
```

Dimension of problem

Function to optimise

Search space
(using vectors as limits enables different limits for the dimensions)

For maximisation

Iteration number; *default can be too large in many situations*

Proportion informed

Swarm size; *default can be too low in some situations*

Running time roughly linear in each of these two parameters

- Some further options: **c.p=** c_1 (cognitive comp.), **c.g=** c_2 (social comp.), **w=** w (inertia weight/exploitation const.), **trace=1** (output of tracing info)

Particle swarm optimisation – versions

- PSO first suggested: 1995 by Kennedy and Eberhart
- Clerc (2016) distinguishes following (main) versions:
  - 1998. A basic version
  - SPSO 2007 (”Standard PSO”)
  - SPSO 2011

Particle swarm optimisation – inertia weight

- Movement of particle i at iteration $t + 1$:
  - $\boldsymbol{x}_i^{(t+1)} = \boldsymbol{x}_i^{(t)} + \boldsymbol{v}_i^{(t+1)}$
  - $\boldsymbol{v}_i^{(t+1)} = w\boldsymbol{v}_i^{(t)} + c_1 R_1^{(t+1)} (\boldsymbol{p}_{\text{best},\, i}^{(t)} - \boldsymbol{x}_i^{(t)}) + c_2 R_2^{(t+1)} (\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}_i^{(t)})$
- In the first version from 1995, the inertia weight w was not included
- Particle swarm might “explode”
- Explosion can be prevented by introducing maximum velocity
- Alternatively, inertia weight $w < 1$ can prevent explosion
- Included in basic version from 1998

Particle swarm optimisation – dimensions

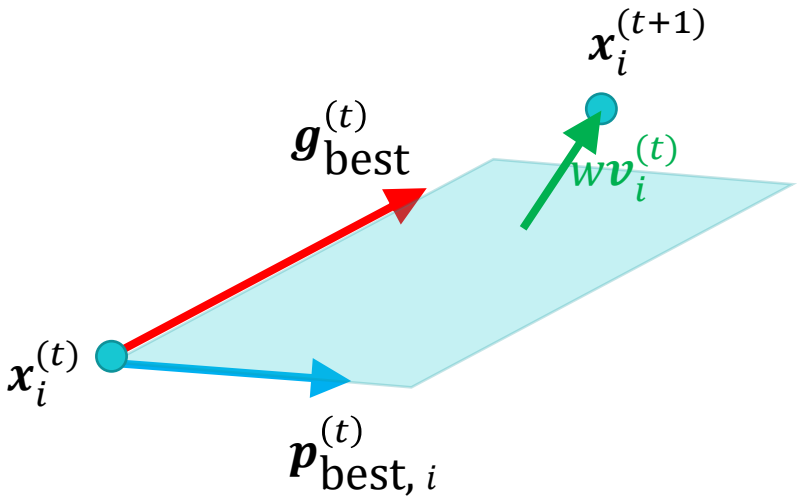
- In first versions including 1998-basic version and SPSO 2007, random variables applied for each dimension separately:
  - $\boldsymbol{v}_i^{(t+1)} = w\boldsymbol{v}_i^{(t)} + c_1\boldsymbol{R}_1^{(t+1)} \otimes \left(\boldsymbol{p}_{\text{best},\,i}^{(t)} - \boldsymbol{x}_i^{(t)}\right) + c_2\boldsymbol{R}_2^{(t+1)} \otimes \left(\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}_i^{(t)}\right)$

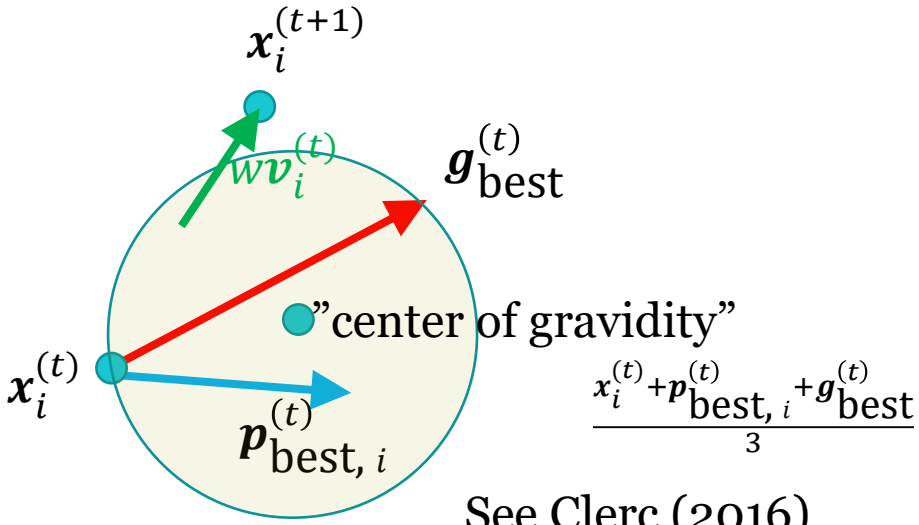
    where $\otimes$ is componentwise multiplication and $\boldsymbol{R}_k^{(t+1)}$ are vectors
- `v[i] <- w*v[i] + c1*runif(p)*(pbest[i]-x[i]) + c2*runif(p)*(gbest-x[i])`

  where `v[i], x[i], pbest[i], gbest` vectors for each particle `i`
- In SPSO 2011, same random variable used for all dimensions leading to movement in hyperspheres:
  - $\boldsymbol{v}_i^{(t+1)} = w\boldsymbol{v}_i^{(t)} + c_1 R_1^{(t+1)} (\boldsymbol{p}_{\text{best},\,i}^{(t)} - \boldsymbol{x}_i^{(t)}) + c_2 R_2^{(t+1)} (\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}_i^{(t)})$
- `v[i] <- w*v[i] + c1*runif(1)*(pbest[i]-x[i]) + c2*runif(1)*(gbest-x[i])`

Particle swarm optimisation – dimensions

- Velocity of particle i at iteration $t + 1$:
  - $\boldsymbol{v}_i^{(t+1)} = w\boldsymbol{v}_i^{(t)} + c_1 R_1^{(t+1)} (\boldsymbol{p}_{\text{best},\, i}^{(t)} - \boldsymbol{x}_i^{(t)}) + c_2 R_2^{(t+1)} (\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}_i^{(t)})$
- In SPSO 2011, same random variable used for all dimensions leading to movement in hyperspheres





See Clerc (2016)

Particle swarm optimisation – dimensions

- In version SPSO 2011, particles can move only in hyperspace spanned by starting particles
- Disadvantages:
  - If dimension of problem p is large in relation to swarm size s, e.g. $p > s$, optimisation done only in a subspace and high risk that optimum is missed
  - Even if starting particles well distributed, they might become close to a hyperspace after some iterations
- Advantages:
  - Problem with dependence on coordinate system and with “biased search” is reduced; finds optima along axes and diagonal easier (Clerc, 2016)
  - Linearly constrained problems can easily be handled (see L4)

PSO – choice of hyperparameters

- Velocity of particle i at iteration $t + 1$:
  - $\boldsymbol{v}_i^{(t+1)} = w\boldsymbol{v}_i^{(t)} + c_1 R_1^{(t+1)} (\boldsymbol{p}_{\text{best},\, i}^{(t)} - \boldsymbol{x}_i^{(t)}) + c_2 R_2^{(t+1)} (\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}_i^{(t)})$
- Hyperparameters to choose: w, c_1, c_2
- Particles should not diverge
- "Stability analyses" had been done – these are simplified analytical computations, **for example**:
  - Assume one-dimensional case,
  - Assume static $\boldsymbol{p}_{\text{best},\, i}^{(t)} = \boldsymbol{p}_{\text{best},\, i}$ and $\boldsymbol{g}_{\text{best}}^{(t)} = \boldsymbol{g}_{\text{best}}$ ("stagnation assumption")
  - Ignore randomness (replace $R_k^{(t+1)}$ by expected value ½)
- Derive requirements for w, c_1, c_2 such that $\boldsymbol{x}_i^{(t)}$ "converges"

PSO – choice of hyperparameters

- Velocity of particle i at iteration $t+1$:
  - $\boldsymbol{v}_i^{(t+1)} = w\boldsymbol{v}_i^{(t)} + c_1 R_1^{(t+1)} (\boldsymbol{p}_{\text{best},\, i}^{(t)} - \boldsymbol{x}_i^{(t)}) + c_2 R_2^{(t+1)} (\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}_i^{(t)})$
- Standard choice in SPSO 2007, based originally on stability analyses from Clerc and Kennedy (2002):
  - $w = \frac{1}{2\ln(2)} = 0.721,$
  - $c_1 = c_2 = \frac{1}{2} + \ln(2) = 1.193$
- Since deterministic $R_k^{(t+1)} = \frac{1}{2}$ and static $\boldsymbol{p}_{\text{best}}$, $\boldsymbol{g}_{\text{best}}$ are used in stability analyses, no distinctive requirements for c_1 and c_2 are obtained and a default is often just $c_1 = c_2$
- Write now $C_k^{(t+1)} = c_k R_k^{(t+1)} \sim Unif[0, c_k], k = 1,2.$

Particle swarm optimisation – stability analyses

- Movement of specific particle at iteration $t+1$ (drop index i):
  - $\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} + \boldsymbol{v}^{(t+1)}$
  - $\boldsymbol{v}^{(t+1)} = w\boldsymbol{v}^{(t)} + C_1^{(t+1)}(\boldsymbol{p}_{\text{best}}^{(t)} - \boldsymbol{x}^{(t)}) + C_2^{(t+1)}(\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}^{(t)})$
- Focusing on particle locations, we can describe PSO as:

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} + \boldsymbol{v}^{(t+1)}$$
$$= \boldsymbol{x}^{(t)} + w\boldsymbol{v}^{(t)} + C_1^{(t+1)}\left(\boldsymbol{p}_{\text{best}}^{(t)} - \boldsymbol{x}^{(t)}\right) + C_2^{(t+1)}\left(\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}^{(t)}\right)$$
$$= \boldsymbol{x}^{(t)} + w\left(\boldsymbol{x}^{(t)} - \boldsymbol{x}^{(t-1)}\right) + C_1^{(t+1)}\left(\boldsymbol{p}_{\text{best}}^{(t)} - \boldsymbol{x}^{(t)}\right) + C_2^{(t+1)}\left(\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}^{(t)}\right)$$
$$= \boldsymbol{x}^{(t)}\left(1 + w - C_1^{(t+1)} - C_2^{(t+1)}\right) - w\boldsymbol{x}^{(t-1)} + C_1^{(t+1)}\boldsymbol{p}_{\text{best}}^{(t)} + C_2^{(t+1)}\boldsymbol{g}_{\text{best}}^{(t)}$$

$\boldsymbol{x}^{(t)} = \boldsymbol{x}^{(t-1)} + \boldsymbol{v}^{(t)}$

- Therefore, a single equation is sufficient to describe the PSO iterations ($\boldsymbol{x}^{(t+1)}$ depends then on both $\boldsymbol{x}^{(t)}$ and $\boldsymbol{x}^{(t-1)}$)

Particle swarm optimisation – stability analyses

- Movement of specific particle at iteration $t + 1$ with PSO:

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)}\left(1 + w - C_1^{(t+1)} - C_2^{(t+1)}\right) - \mathrm{w}\boldsymbol{x}^{(t-1)} + C_1^{(t+1)}\boldsymbol{p}_{\text{best}}^{(t)} + C_2^{(t+1)}\boldsymbol{g}_{\text{best}}^{(t)}$$

- Stability analyses were improved during the two previous decades, see Bonyadi and Michalewicz (2016) and Cleghorn and Engelbrecht (2018); definitions below follow the latter
- Order-1 stability
  A sequence $(\boldsymbol{x}^{(t)})$ of p-dimensional random variables is called *order-1 stable* if $\mathrm{E}\left[\boldsymbol{x}^{(t)}\right] \to \boldsymbol{x}_E$ for some $\boldsymbol{x}_E$
- Order-2 stability
  A sequence $(\boldsymbol{x}^{(t)})$ of p-dimensional random variables is called *order-2 stable* if $\mathrm{Var}\left[\boldsymbol{x}^{(t)}\right] \to \boldsymbol{x}_V$ for some $\boldsymbol{x}_V$

Particle swarm optimisation – stability analyses

- Movement of specific particle at iteration $t+1$ with PSO:

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)}\left(1 + w - C_1^{(t+1)} - C_2^{(t+1)}\right) - w\boldsymbol{x}^{(t-1)} + C_1^{(t+1)}\boldsymbol{p}_{\text{best}}^{(t)} + C_2^{(t+1)}\boldsymbol{g}_{\text{best}}^{(t)}$$

- Bonyadi and Michalewicz (2016) interpret each of $C_1^{(t+1)}, C_2^{(t+1)}, \boldsymbol{p}_{\text{best}}^{(t)}, \boldsymbol{g}_{\text{best}}^{(t)}$ as iid random variables
- This generalises assumptions that these values are fixed values; it weakens the stagnation assumption
- The iid assumption for $\boldsymbol{p}_{\text{best}}^{(t)}, t = 1, \ldots$ and for $\boldsymbol{g}_{\text{best}}^{(t)}, t = 1, \ldots$ still need to be seen as approximations

Particle swarm optimisation – stability analyses

- We consider the one-dimensional case ($p = 1$) now
- Movement of specific particle at iteration $t + 1$ with PSO:

$$x^{(t+1)} = x^{(t)}\left(1 + w - C_1^{(t+1)} - C_2^{(t+1)}\right) - \mathrm{w}x^{(t-1)} + C_1^{(t+1)} p_{\text{best}}^{(t)} + C_2^{(t+1)} g_{\text{best}}^{(t)}$$

- To write the iterations as a linear one-step relation, we write

$$\boldsymbol{z}^{(t+1)} = (x^{(t+1)}, x^{(t)})^T, \qquad U = 1 + w - C_1^{(t+1)} - C_2^{(t+1)},$$

and

$$\boldsymbol{z}^{(t+1)} = \begin{pmatrix} U & -w \\ 1 & 0 \end{pmatrix} \boldsymbol{z}^{(t)} + \begin{pmatrix} C_1^{(t+1)} p_{\text{best}}^{(t)} + C_2^{(t+1)} g_{\text{best}}^{(t)} \\ 0 \end{pmatrix}$$

- Since U and $\boldsymbol{z}^{(t)}$ are independent, we have

$$E\boldsymbol{z}^{(t+1)} = \begin{pmatrix} EU & -w \\ 1 & 0 \end{pmatrix} E\boldsymbol{z}^{(t)} + \begin{pmatrix} E\left[C_1^{(t+1)} p_{\text{best}}^{(t)}\right] + E\left[C_2^{(t+1)} g_{\text{best}}^{(t)}\right] \\ 0 \end{pmatrix}$$

➢ Sequence $E\boldsymbol{z}^{(t+1)}$ is of form $E\boldsymbol{z}^{(t+1)} = \boldsymbol{M}E\boldsymbol{z}^{(t)} + \boldsymbol{b}$

Particle swarm optimisation - stability analyses

- Sequence $E\boldsymbol{z}^{(t+1)}$ is of form $E\boldsymbol{z}^{(t+1)} = \boldsymbol{M}E\boldsymbol{z}^{(t)} + \boldsymbol{b}$
- Functional analysis says that $E\boldsymbol{z}^{(t)}$ converges if spectral radius of $\boldsymbol{M}$ is <1, see Bonyadi and Michalewicz (2016)'s Lemma 1
- Spectral radius $\rho(\boldsymbol{M})$ of $\boldsymbol{M} \in \mathbb{R}^{p\times p}$ is $\rho(\boldsymbol{M}) = \max\{|\lambda_1|, \ldots, |\lambda_p|\}$ where λ_j are the p (real or complex) eigenvalues of $\boldsymbol{M}$
- Recall that a non-symmetric $\mathbb{R}^{p\times p}$ matrix still has p eigenvalues as long as we allow for complex eigenvalues
- If $\lambda = r + c\mathrm{i}$ then $|\lambda| = \sqrt{r^2 + c^2}$; **R** can cope with this easily:

```
> M <- matrix(c(-0.66, 1, -0.72, 0), ncol=2)
> eigen(M)$values
[1] -0.33+0.7817289i -0.33-0.7817289i
> max(abs(eigen(M)$values))  # spectral radius
[1] 0.8485281
```

Particle swarm optimisation - stability analyses

- We have

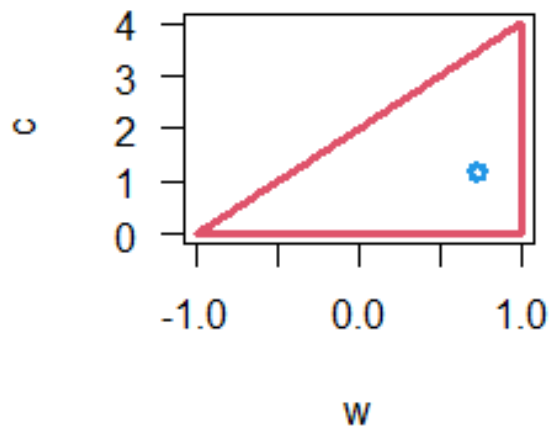
$$E\boldsymbol{z}^{(t+1)} = \begin{pmatrix} EU & -w \\ 1 & 0 \end{pmatrix} E\boldsymbol{z}^{(t)} + \begin{pmatrix} E\left[C_1^{(t+1)} p_{\text{best}}^{(t)}\right] + E\left[C_2^{(t+1)} g_{\text{best}}^{(t)}\right) \\ 0 \end{pmatrix}$$

- Compute spectral radius of $\begin{pmatrix} EU & -w \\ 1 & 0 \end{pmatrix}$
- Eigenvalues: $0 = \det\begin{pmatrix} \lambda - EU & w \\ -1 & \lambda \end{pmatrix} = \lambda^2 - \lambda EU + w \quad \Rightarrow \quad \lambda_{1,2} = \frac{EU \pm \sqrt{EU^2 - 4w}}{2}$
- $EU = 1 + w - EC_1^{(t+1)} - EC_2^{(t+1)} = 1 + w - \frac{c_1 + c_2}{2}$
- One can show:

$$\rho(M) = \max\left\{\frac{\left|EU + \sqrt{EU^2 - 4w}\right|}{2}, \frac{\left|EU - \sqrt{EU^2 - 4w}\right|}{2}\right\} < 1 \text{ iff}$$

$$-1 < w < 1 \text{ and } 0 < \frac{c_1 + c_2}{2} < 2(w + 1)$$

- Assume $c = c_1 = c_2$

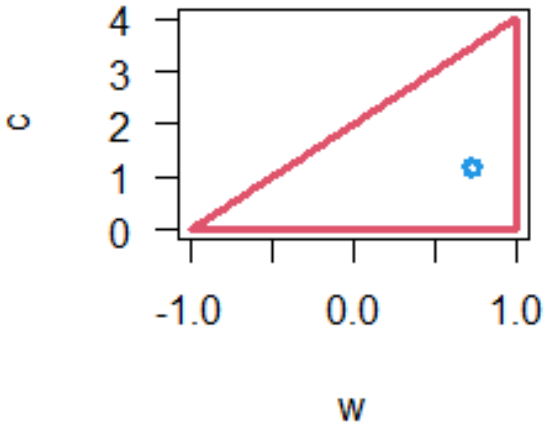


Particle swarm optimisation - stability analyses

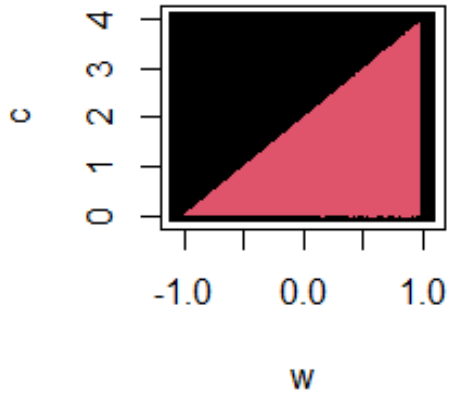
- Assume $c = c_1 = c_2$. $EU = 1 + w - c$
- One can show:

$$\rho(M) = \max\left\{\frac{|EU+\sqrt{EU^2-4w}|}{2}, \frac{|EU-\sqrt{EU^2-4w}|}{2}\right\} < 1 \text{ iff}$$

$$-1 < w < 1 \text{ and } 0 < c < 2(w+1)$$



- If it would be too difficult to show the above, one could calculate the maximum eigenvalue for a grid of (w, c)-pairs and plot the cases when it is <1 (see **R** code on homepage)



Particle swarm optimisation – stability analyses

- To do stability analyses for order-2 stability (about the limit of the variance $\mathrm{Var}(\boldsymbol{z}^{(t+1)})$), we can investigate

$$\boldsymbol{z}^{(t+1)} = (x^{(t+1)}, x^{(t)}, \left(x^{(t+1)}\right)^2, \left(x^{(t)}\right)^2, x^{(t+1)} x^{(t)})^T$$

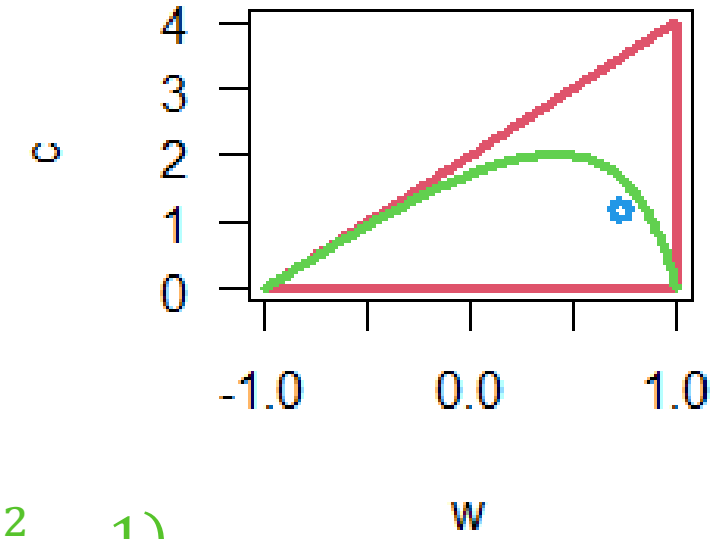
- The iterations can be written as system

$$E\boldsymbol{z}^{(t+1)} = \begin{pmatrix} EU & -w & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 2E[UP] & -2wEP & E[U^2] & w^2 & -2wEU \\ 0 & 0 & 1 & 0 & 0 \\ EP & 0 & EU & 0 & -w \end{pmatrix} E\boldsymbol{z}^{(t)} + \boldsymbol{b}$$

where $P = C_1^{(t+1)} p_{\text{best}}^{(t)} + C_2^{(t+1)} g_{\text{best}}^{(t)}$

Particle swarm optimisation – stability analyses

- $c = c_1 = c_2$
- $-1 < w < 1$ and
  $0 < c < 2(w + 1)$



- Sequence $\left(\boldsymbol{z}^{(t+1)}\right)$ is order-2 stable if:
  $-1 < w < 1$ and

$$0 < c < \frac{12(w^2 - 1)}{5w - 7}$$

- Default in **R**–package **pso** based on Clerc and Kennedy (2002):
  $w = \frac{1}{2\ln(2)} = 0.721, c = c_1 = c_2 = \frac{1}{2} + \ln(2) = 1.193$

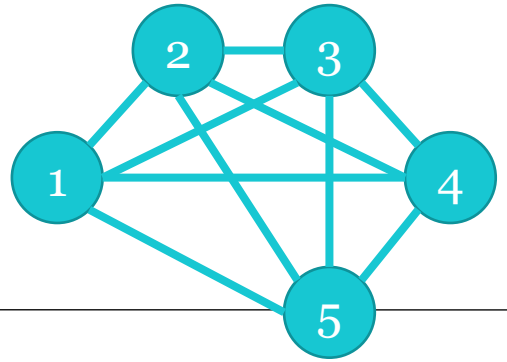
PSO – choice of hyperparameters

- Based on stability analysis, choose w, c_1, c_2 respecting $-1 < w < 1$ and $0 < c_1 + c_2 < \frac{24(w^2-1)}{5w-7}$
- $w > 0$ is in spirit of the algorithm's idea

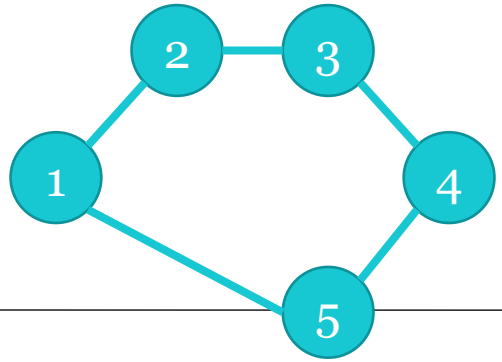
- Another hyperparameter to be chosen: swarm size s
- Swarm size motivated by empirical studies based on standard optimisation problems
- SPSO 2007: $s = 10 + \lceil 2\sqrt{p} \rceil$
- Clerc (2012) shows with 12 standard optimisation problems:
  - usually swarm sizes $s > 10 + \lceil 2\sqrt{p} \rceil$ better,
  - dependence on dimension p is weak
- SPSO 2011: choice of user; suggested: 40

PSO – topologies for particles

- Particles ”inform” other particles about their results
- In the original PSO, each particle informs all others
- To ensure that not all particles are attracted prematurely by particle at a local optimum, do not inform all particles
- The structure how information flows is specified in ”topologies”
- Global top. (all inform all)



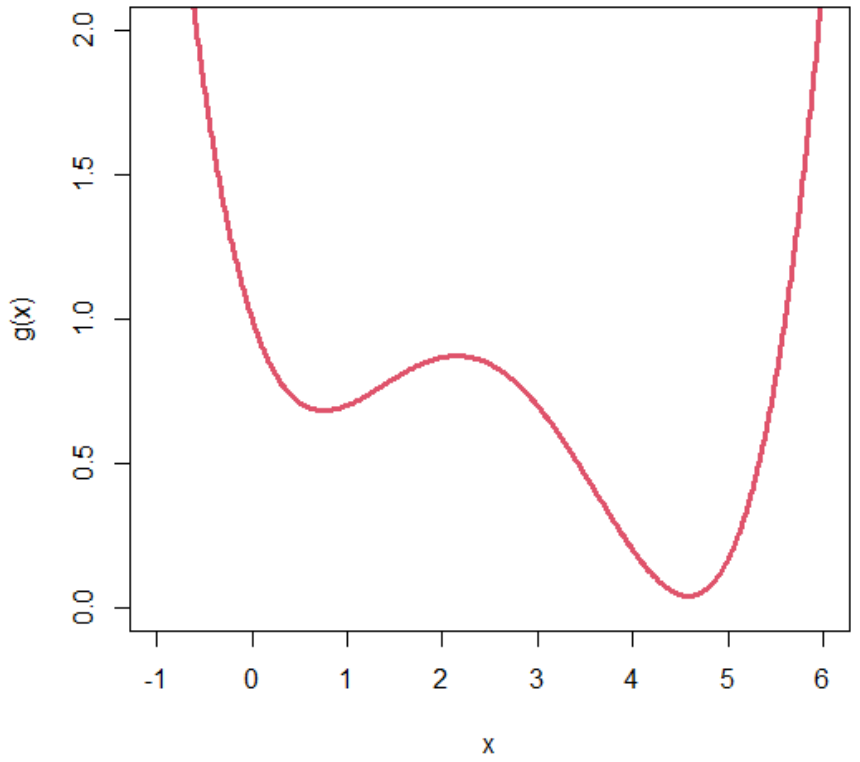
Ring top. (all inform their two ”neighbours”)



PSO – exploration versus exploitation

- Exploration of the search space
- Exploitation around a promising position
- The topology: A sparce topology (e.g. ring top.) ensures more exploration compared to a dense one (e.g. global top.)
- Parameter w: Larger w leads to more exploration
- Parameters c_1 and c_2: Smaller c_2 (and c_1) lead to more exploration
- Clerc (2016; Section 8.6.4.1): The experimental evidence for such dependencies [on w, c_1, c_2] is weak

Simulated annealing



AlphaOpt (2017). Introduction To Optimization: Gradient Free Algorithms (2/2) – Simulated Annealing, Nelder-Mead (0:15-1:35)

Simulated annealing

- Start value $\boldsymbol{x}^{(0)}$; stage $j = 0, 1, 2, \ldots$ has m_j iterations; initial temperature τ_0; set $j = 0$
- Given iteration $\boldsymbol{x}^{(t)}$, generate $\boldsymbol{x}^{(t+1)}$ as follows:

1. Sample a candidate $\boldsymbol{x}^*$ from a proposal distribution $p(\cdot\,|\boldsymbol{x}^{(t)})$
2. Compute $h\left(\boldsymbol{x}^{(t)}, \boldsymbol{x}^*\right) = \exp\left(\frac{g(\boldsymbol{x}^*) - g\left(\boldsymbol{x}^{(t)}\right)}{\tau_j}\right)$
3. Define next iteration $\boldsymbol{x}^{(t+1)}$ according to

$$\boldsymbol{x}^{(t+1)} = \begin{cases} \boldsymbol{x}^*, \text{with probability } \min\{h\left(\boldsymbol{x}^{(t)}, \boldsymbol{x}^*\right), 1\} \\ \boldsymbol{x}^{(t)}, \text{otherwise} \end{cases}$$

4. Set `t <- t+1` and repeat 1.-3. m_j times
5. Update $\tau_j = \alpha(\tau_{j-1})$ and $m_j = \beta(m_{j-1})$; set `j <- j+1`; go to 1

$g\left(\boldsymbol{x}^{(t)}\right) - g(\boldsymbol{x}^*)$ for minimisation

τ_j is temperature; function α should slowly decrease it; function β should be increasing

Simulated annealing

- Initially, also “bad” proposals are accepted
- With decreasing temperature, accept only improvements
- This helps to explore first and avoids convergence to a local maximum too early
- Algorithm which has therefore chances to find the global optimum in presence of multiple local optima

- **`method="SANN"`** of R function **`optim`** is “a variant of simulated annealing” (documentation of **`optim`**)
  - Initial temperature can be important choice (can be changed e.g. by **`control=list(temp=0.01)`**; default 10 might be bad)

Simulated annealing: proposal distribution

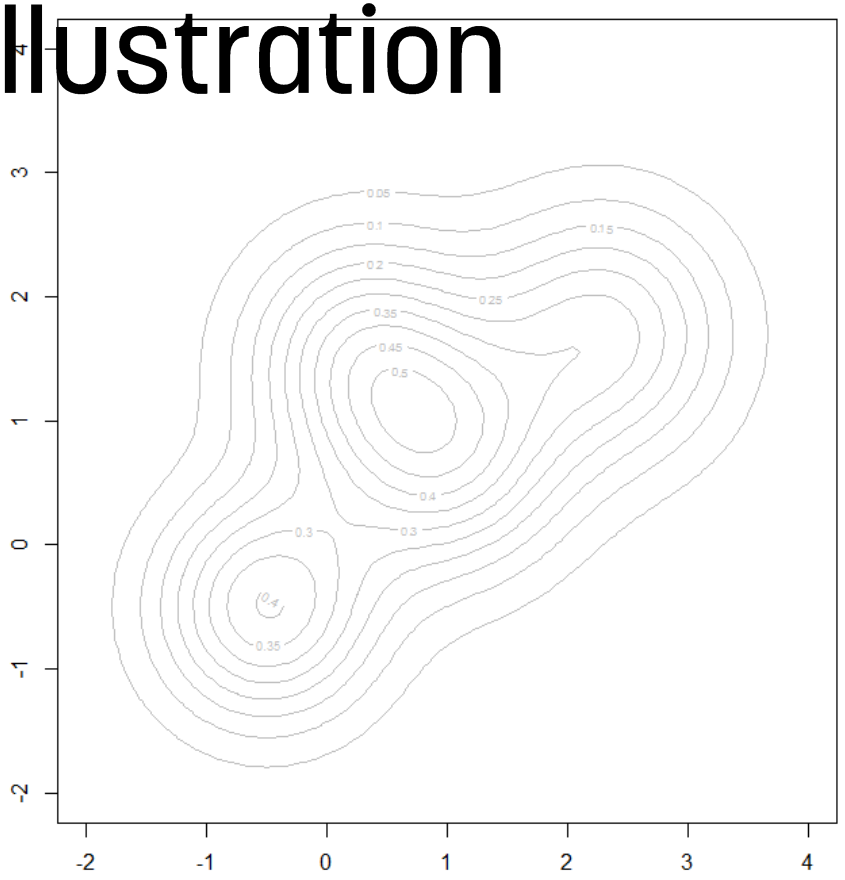
- Step 1 in simulated annealing iteration rule:

1. Sample a candidate $\boldsymbol{x}^*$ from a proposal distribution $p(\cdot\,|\boldsymbol{x}^{(t)})$

- Proposal distribution could be uniform distribution on a **neighbourhood** of $x^{(t)}$; for a unidimensional optimisation problem:
  `xs <- xt + runif(n=1, min=-1, max=1)`
- Instead of Unif[-1,1], a distribution on a smaller or larger neighbourhood can be used
- But also, normal distribution $N(0, \sigma^2)$ or other **symmetric** distribution around 0 might be added to $x^{(t)}$ instead
- For multidimensional cases, one could use iid components, a uniform distribution on a ball around $\boldsymbol{x}^{(t)}$ or a multivariate normal distribution with mean $\boldsymbol{x}^{(t)}$

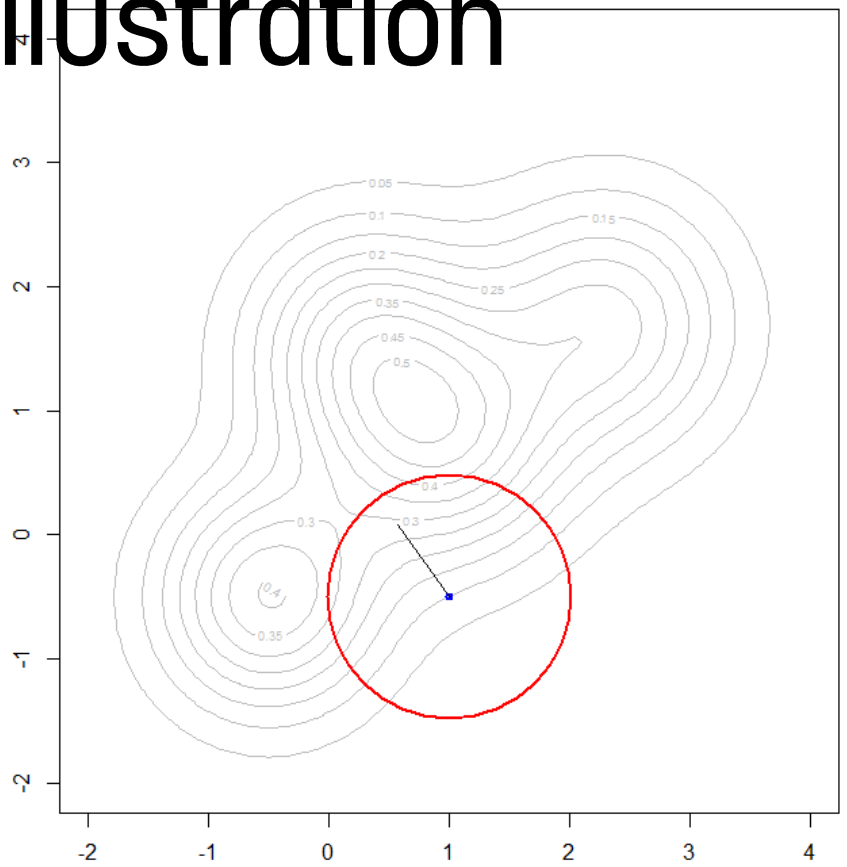
Simulated annealing – Illustration

- For illustration, we consider two-dimensional function g according to contour lines in figure (one global and one local maximum) and fixed temperature τ
- Proposal distribution
  $p(\boldsymbol{x}^*|\boldsymbol{x}^{(t)}) = p(\boldsymbol{x}^{(t)}|\boldsymbol{x}^*)$
  $= \frac{1}{\pi r^2}\mathbf{1}\{\|\boldsymbol{x}^{(t)} - \boldsymbol{x}^*\| < r\}$
  for some constant r (here=1)



Simulated annealing – Illustration

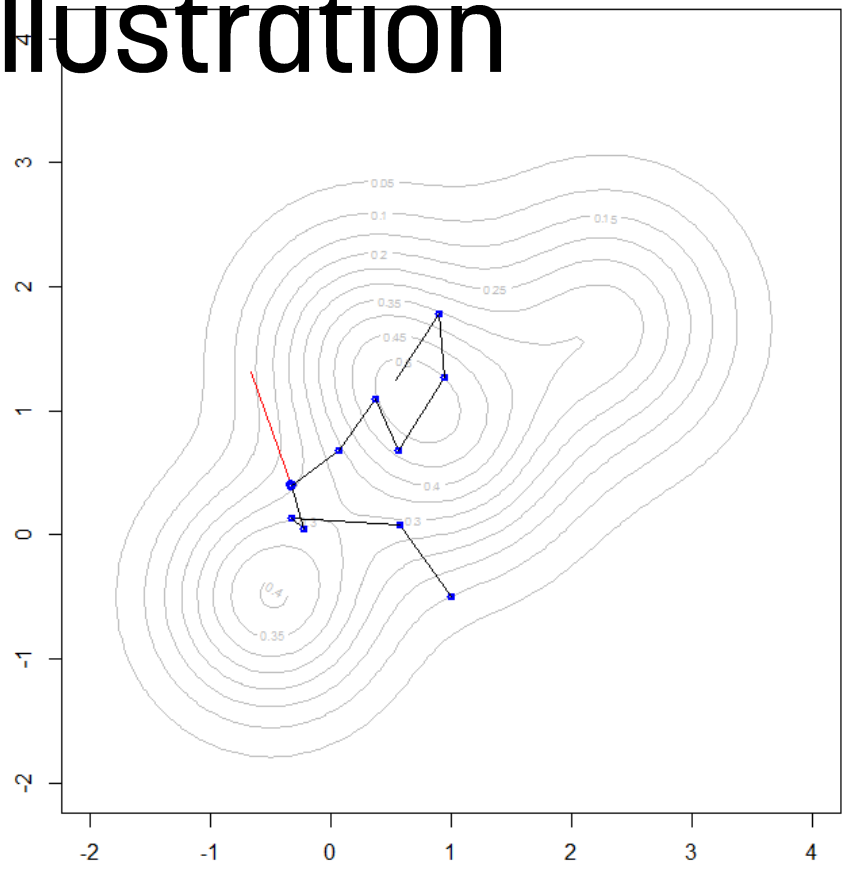
- Proposal distribution
  $p(\boldsymbol{x}^*|\boldsymbol{x}^{(t)}) = p(\boldsymbol{x}^{(t)}|\boldsymbol{x}^*)$
  $= \frac{1}{\pi r^2}\mathbf{1}\{\|\boldsymbol{x}^{(t)} - \boldsymbol{x}^*\| < r\}$
  for some constant r (here=1)
- Start here with $\boldsymbol{x}^{(0)} = (1, -0.5)$
- Randomize uniformly on unit circle around $\boldsymbol{x}^{(0)}$ (proposal distribution); result $\boldsymbol{x}^* = (0.58, 0.08)$



- $g(\boldsymbol{x}^*) = 0.296 > g(\boldsymbol{x}^{(0)}) = 0.098$; so, this was an uphill step and is automatically accepted ($h(\boldsymbol{x}^{(t)}, \boldsymbol{x}^*) > 1$)

Simulated annealing – Illustration

- $\boldsymbol{x}^{(0)} = (1, -0.5)$
- Uphill steps: $\boldsymbol{x}^{(1)} = (0.58, 0.08)$
- $\boldsymbol{x}^{(2)} = (-0.33, 0.13)$
- $\boldsymbol{x}^{(3)} = (-0.23, 0.05)$
- Then downhill step proposed:
  $\boldsymbol{x}^{*} = (-0.32, 0.4)$, $h\left(\boldsymbol{x}^{(t)}, \boldsymbol{x}^{*}\right) = 0.774$
- Random Unif(0,1) generated: 0.573
  and since this is smaller than $R = 0.774$,
  $\boldsymbol{x}^{(4)} = \boldsymbol{x}^{*} = (-0.32, 0.4)$ is accepted



- Again downhill step proposed: $\boldsymbol{x}^{*} = (-0.67, 1.31)$,
  $h\left(\boldsymbol{x}^{(t)}, \boldsymbol{x}^{*}\right) = 0.560$; random Unif(0,1): 0.890 and rejection of $\boldsymbol{x}^{*}$
- $\boldsymbol{x}^{(5)} = \boldsymbol{x}^{(4)} = (-0.32, 0.4)$

Combinatorial optimisation

- Generic optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$

- Now, we consider also optimisation problems which cannot exactly be formulated according to the generic one
- Especially, function g might be defined on another space than $\mathbb{R}^p$

- Generalized optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{S} \to \mathbb{R}$ function for some set $\mathbb{S}$
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$

Example: Multiple linear regression

- Generalized optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{S} \to \mathbb{R}$ function for some set $\mathbb{S}$
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$

- Multiple linear regression with q predictors
- Desired to choose best model based on criterion like AIC
- There are 2^q possible models
- If q small, AIC of all models can be computed (exhaustive search); for q larger, this is impossible (e.g. q=50, $1ms$ to compute an AIC → more than 35 000 years needed!)
- One model can be represented as element of $\mathbb{S} = \{0, 1\}^q$ (1=predictor included in model, 0 otherwise)

Example: Multiple linear regression

- Generalized optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{S} \to \mathbb{R}$ function for some set $\mathbb{S}$
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
- Optimisation problem: Which model gives best AIC?
- Model 1: (1, 0, 0, 0, 1, 1, 0, 1, ...)
  Model 2: (1, 1, 1, 0, 1, 1, 0, 0, ...)
- Which models are ”close” to each other? (Need metric on $\mathbb{S} = \{0, 1\}^q$)
  What is a neighbourhood of a model?

- Apply simulated annealing e.g. with neighbourhood being all models which differ by one predictor (for proposal dist.)
- Uniform distribution on neighbourhood can be used

Example: Multiple linear regression

- Generalized optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{S} \to \mathbb{R}$ function for some set $\mathbb{S}$
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$

- Arbitrary starting model generated (e.g. uniform distribution on $\mathbb{S} = \{0, 1\}^q$, `xs <- rbinom(q, size=1, prob=0.5)`)

- See example in Givens and Hoeting (2013), Section 3.3, with 27 predictors

Recall from L1: Maximising information of experimental designs

- Regression model $\boldsymbol{y} = \boldsymbol{X\beta} + \boldsymbol{\varepsilon}$ (where $\boldsymbol{\varepsilon}$ has iid components)
- $\boldsymbol{X}$ design matrix (depends on choice of observational points)
- Covariance matrix of Least Squares estimate $\widehat{\boldsymbol{\beta}}$ is

$$\mathrm{Cov}\left(\widehat{\boldsymbol{\beta}}\right) = (\boldsymbol{X^T X})^{-1} \cdot const$$

- Choose design of an experiment such that $\boldsymbol{X^T X}$ “large”
- D-optimality: $g(\text{"}\mathbf{design}\text{"}) = \det(\boldsymbol{X^T X})$
- We search $\mathbf{design}^*$ with $g(\mathbf{design}^*) = \max g(\mathbf{design})$

Ex: Maximising information of experimental designs

- Regression model $\boldsymbol{y} = \boldsymbol{X\beta} + \boldsymbol{\varepsilon}$, $\mathrm{Cov}(\widehat{\boldsymbol{\beta}}) = (\boldsymbol{X^T X})^{-1} \cdot const$
- We search $\mathbf{design}^*$ with $g(\mathbf{design}^*) = \max g(\mathbf{design})$
- Example: cubic regression, $y = \beta_0 + \beta_1 w + \beta_2 w^2 + \beta_3 w^3 + \varepsilon$,
  w can be chosen in [-1, 1], but practical circumstances require here a distance between design points of 0.05
- Therefore, we allow design points {-1, -0.95, -0.9, …, 1} and at most one observation can be done at each point
- Each observation has a cost; and we want to minimise the penalized D-optimality
  $\#\text{observations} * 0.2 - \log\left(\det\left(\boldsymbol{X^T X}\right)\right)$
- $$\boldsymbol{X} = \begin{pmatrix} 1 & w_1 & w_1^2 & w_1^3 \\ 1 & w_2 & w_2^2 & w_2^3 \\ \dots & \dots & \dots & \dots \\ 1 & w_n & w_n^2 & w_n^3 \end{pmatrix}$$

Ex: Maximising information of experimental designs

- Example: cubic regression, $y = \beta_0 + \beta_1 w + \beta_2 w^2 + \beta_3 w^3 + \varepsilon$,
  w can be chosen in [-1, 1], but practical circumstances require here a distance between design points of 0.05
- Therefore, we allow design points {-1, -0.95, -0.9, …, 1} and at most one observation can be done at each point
- A design can be represented by a vector in $\mathbb{S} = \{0, 1\}^{41}$ where 0 means that no observation is done at a design point and 1 means that one observation is made there
- How can a reasonable neighbourhood on $\mathbb{S}$ look like here?

Simulated annealing

- Start value $\boldsymbol{x}^{(0)}$; stage $j = 0, 1, 2, \ldots$ has m_j iterations; initial temperature τ_0; set $j = 0$
- Given iteration $\boldsymbol{x}^{(t)}$, generate $\boldsymbol{x}^{(t+1)}$ as follows:

1. Sample a candidate $\boldsymbol{x}^*$ from a proposal distribution $p(\cdot\,|\boldsymbol{x}^{(t)})$
2. Compute $h\left(\boldsymbol{x}^{(t)}, \boldsymbol{x}^*\right) = \exp\left(\frac{g(\boldsymbol{x}^*) - g\left(\boldsymbol{x}^{(t)}\right)}{\tau_j}\right)$

$g\left(\boldsymbol{x}^{(t)}\right) - g(\boldsymbol{x}^*)$ for minimisation

3. Define next iteration $\boldsymbol{x}^{(t+1)}$ according to

$$\boldsymbol{x}^{(t+1)} = \begin{cases} \boldsymbol{x}^*, \text{with probability } \min\{h\left(\boldsymbol{x}^{(t)}, \boldsymbol{x}^*\right), 1\} \\ \boldsymbol{x}^{(t)}, \text{otherwise} \end{cases}$$

4. Set `t <- t+1` and repeat 1.-3. m_j times
5. Update $\tau_j = \alpha(\tau_{j-1})$ and $m_j = \beta(m_{j-1})$; set `j <- j+1`; go to 1

τ_j is temperature; function α should slowly decrease it; function β should be increasing

Markov Chain Monte Carlo – Metropolis algorithm

(Metropolis et al., 1953)

- Given a density $f(\boldsymbol{x})$ and aim is to generate a sample following f
- A starting value $\boldsymbol{x}^{(0)}$ is generated from some starting distribution
- Given observation $\boldsymbol{x}^{(t)}$, generate $\boldsymbol{x}^{(t+1)}$ as follows:

1. Sample candidate $\boldsymbol{x}^*$ from symmetric proposal dist. $p(\cdot\,|\boldsymbol{x}^{(t)})$
2. Compute ratio $R\left(\boldsymbol{x}^{(t)}, \boldsymbol{x}^*\right) = \frac{f(\boldsymbol{x}^*)}{f\left(\boldsymbol{x}^{(t)}\right)}$
3. Sample $\boldsymbol{x}^{(t+1)}$ according to

$$\boldsymbol{x}^{(t+1)} = \begin{cases} \boldsymbol{x}^*, \text{with probability } \min\{R\left(\boldsymbol{x}^{(t)}, \boldsymbol{x}^*\right), 1\} \\ \boldsymbol{x}^{(t)}, \text{otherwise} \end{cases}$$

4. If more observations needed, set `t <- t+1`; go to 1

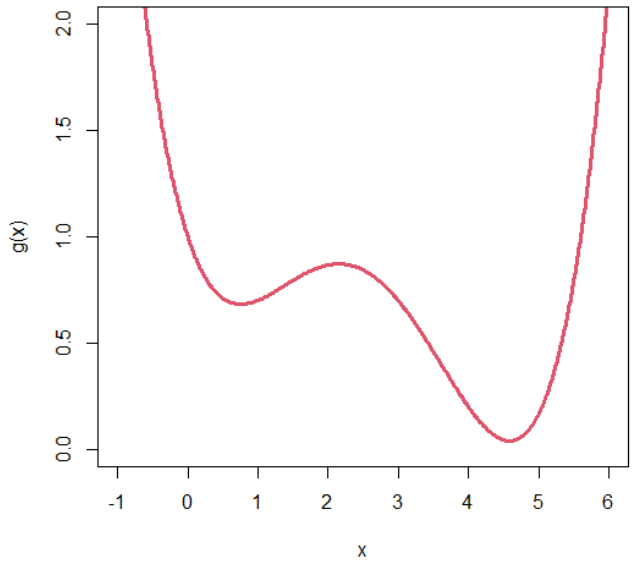
symmetric proposal:
$p\left(\boldsymbol{x}^{(t)}|\boldsymbol{x}^*\right) = p\left(\boldsymbol{x}^*|\boldsymbol{x}^{(t)}\right)$

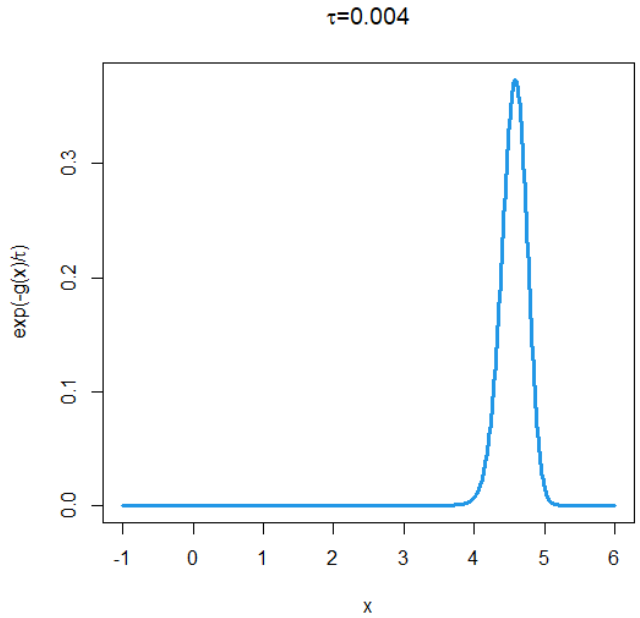
Simulated annealing and Metropolis algorithm

- For fixed temperature τ, simulated annealing algorithm is a Metropolis algorithm
- Kirkpatrick et al. (1983) proposed name simulated annealing for using it as optimisation method
- $h\left(\boldsymbol{x}^{(t)}, \boldsymbol{x}^{*}\right) = \exp\left(\frac{g\left(\boldsymbol{x}^{(t)}\right) - g(\boldsymbol{x}^{*})}{\tau_j}\right) = \frac{\exp\left(-\frac{g(\boldsymbol{x}^{*})}{\tau_j}\right)}{\exp\left(-\frac{g\left(\boldsymbol{x}^{(t)}\right)}{\tau_j}\right)} = \frac{f(\boldsymbol{x}^{*})}{f\left(\boldsymbol{x}^{(t)}\right)} = R(\boldsymbol{x}^{(t)}, \boldsymbol{x}^{*})$
- Key ingredient of Metropolis and simulated annealing alg.: Markov chain $\boldsymbol{x}^{(t)}$ **has limiting stationary distribution $\boldsymbol{f}$**; for a proof see e.g. Koski (2009)
- Requirement for all: $\boldsymbol{x}^{(t)}$ irreducible and aperiodic chain

Simulated annealing: stationary distribution for fixed temperature τ

- Fixed temperature τ: Markov chain $x^{(t)}$ has limiting stationary distribution with density proportional to $f(x) = \exp\left(-\frac{g(x)}{\tau}\right)$





Convergence of simulated annealing

- Convergence proofs see generated sequence either as sequence of homogeneous Markov chains (one for each τ) or as one inhomogeneous Markov chain
- For discrete $\mathbb{S} = \{x_1, x_2, x_3, \dots\}$ and g having a finite set M of global minima, simulated annealing converges with probability $1/|M|$ to each of the M global minima (references for proofs in Givens and Hoeting, 2013); main idea:
- Stationary distribution proportional to: $\exp\left(-\frac{g(x)}{\tau}\right)$ or to $\exp\left(-\frac{g(x)-g_{min}}{\tau}\right)$ with $g_{min} = \min\{g(x)\}$
- Therefore, if P is distribution according to stationary distribution,

$$P(x_i) = \exp\left(-\frac{g(x_i)-g_{min}}{\tau}\right) / \{|M| + \sum_{x_j \notin M} \exp\left(-\frac{g(x_j)-g_{min}}{\tau}\right)\} \to \frac{1}{|M|} \; (x_i \in M)$$

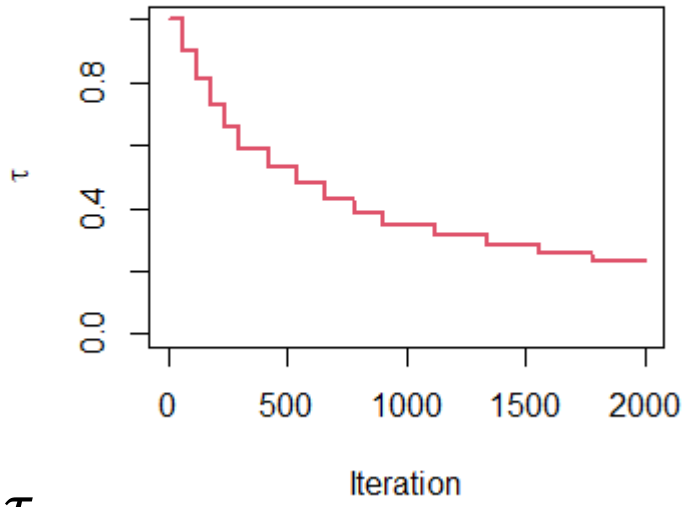
$\tau \to 0$:

$\to 0$ for $x_i \notin M$,
$= 1$ for $x_i \in M$

$\to 0$

Convergence of simulated annealing

- To achieve convergence to a global optimum (possibly in presence of local optima) in practise, one needs:
  - Run iterations for each fixed temperature long enough such that convergence to stationary distribution achieved
  - Cool temperature slowly enough such that iterations have time to escape from local optima
- Example from Givens and Hoeting (2013; p.73):
  - 5 stages with 60 iterations, then
  - 5 stages with 120 iterations, then
  - 5 stages with 220 iterations
  - From one stage to the next, τ is decreased by 10%, `tau <- 0.9*tau`; final τ is $0.9^{15} = 0.206$*initial τ



Simulated annealing: + and –

+ Very easy to implement
+ Theoretical property is good: theoretically, we can guarantee convergence to a global optimum even in the presence of local optima
+ Can even handle some non-standard optimisation problems
– In practice, convergence can be “maddeningly slow”
– One needs to play around with cooling schedule to ensure convergence in practice
  - We need to run the algorithm “long enough” at each temperature (to ensure stationary distribution)
  - We need to cool the temperature slowly enough (to allow escaping from local optima)

Comparisons of algorithms or hyperparameter choices based on empirical studies

- We have several options for optimisation algorithms
- Or – within one algorithm – we can choose some hyperparameters
- A possibility is to compare the options by running them on an example problem. Better, one might want to compare options for a set of easy and difficult optimisation problems
- For comparability, often ”standard optimisation problems” used; see e.g. Liang et al. (2013)
- Can be mathematical functions or statistical optimisation problems

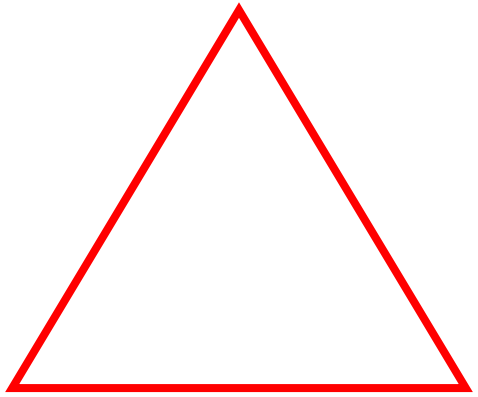
Comparisons of algorithms or hyperparameter choices based on empirical studies

- After choosing some standard optimisation problems, one needs to define a success criterion (example in Clerk, 2016)
- Possibility: count runs of algorithm leading to a solution $\boldsymbol{x}_s$ with $g(\boldsymbol{x}_s) > g(\boldsymbol{x}^*) - \delta$; here $\boldsymbol{x}^*$ true position of global maximum, and δ small (ideally $\delta < g(\boldsymbol{x}^*) - g(\boldsymbol{x}_L)$ for any local maximum $\boldsymbol{x}_L$)
- If true success rate for an algorithm is p, we observe a $\mathrm{Bin}(1, p)$-random variable in each run

➢ Success rate has sd $\sqrt{\frac{p(1-p)}{n}}$ when doing n runs and you can do informed choice of n

- E.g. $p = 0.8, n = 100 \rightarrow \ \mathrm{sd} = 0.04$.

Nelder-Mead algorithm



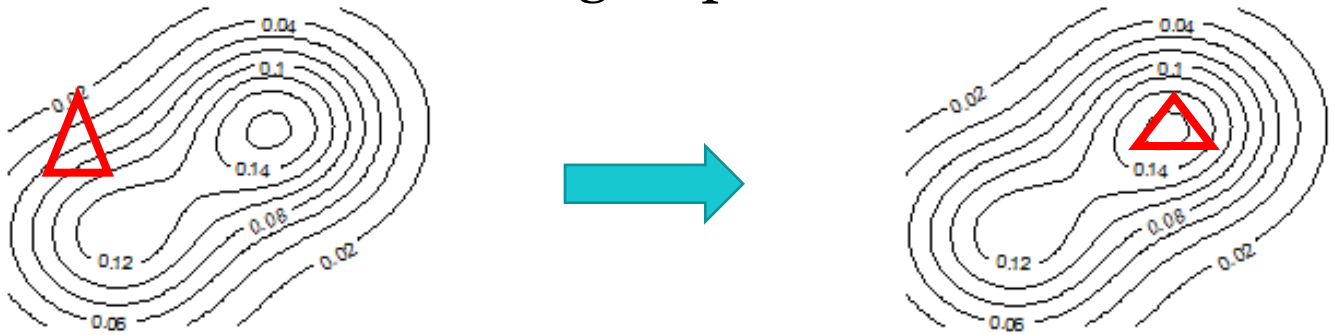
Nelder-Mead

- $\boldsymbol{x}$ $p-$dimensional vector, g: $\mathbb{R}^p \rightarrow \mathbb{R}$ function
- We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$

- Nelder-Mead method is heuristic method for p-dimensional optimisation problem (default in **R**-function **optim**)
- Positive:
  +No computation of derivatives necessary
- Negative:
  - No theoretical guarantee for converge (counter examples exist)
  - Might be slow
- Works often well, especially if p not too large

Nelder-Mead

- Idea: Work with simplex of p+1 points; i.e. for two-dimensional optimisation: work with triangle
- Aim that triangle includes maximum
- Choose arbitrary starting triangle
- Change vertices to ”move the triangle upwards”



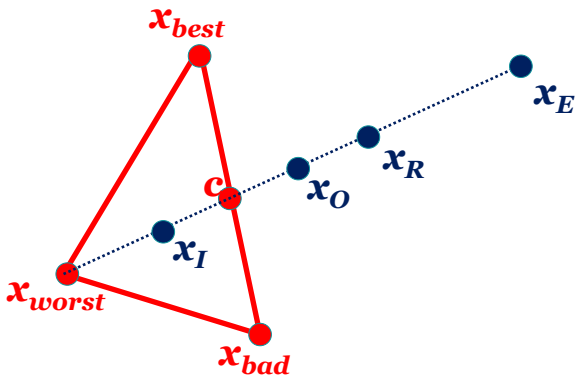
- Two animations:
  - https://upload.wikimedia.org/wikipedia/commons/9/96/Nelder_Mead2.gif
  - https://www.youtube.com/watch?v=KEGSLQ6TlBM

Nelder-Mead

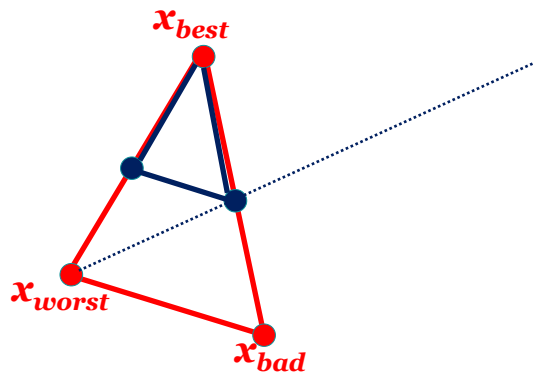
- Identify worst vertex $\boldsymbol{x_{worst}}$ ($g(\boldsymbol{x_{worst}})$ minimal among all vertices) and compute average $\boldsymbol{c}$ of remaining vertices
- Let $\boldsymbol{x_{best}}$ be best and $\boldsymbol{x_{bad}}$ be second worst vertex
- Rules for
  - Reflection
  - Expansion
  - Outer contraction
  - Inner contraction
  - Shrinkage

Nelder-Mead

- Replace $\boldsymbol{x_{worst}}$ with one of $\boldsymbol{x_I}$, $\boldsymbol{x_O}$, $\boldsymbol{x_R}$, $\boldsymbol{x_E}$ (rule depends on values for $g(\boldsymbol{x_{worst}})$, $g(\boldsymbol{x_{bad}})$, $g(\boldsymbol{x_{best}})$, $g(\boldsymbol{x_I})$, $g(\boldsymbol{x_O})$, $g(\boldsymbol{x_R})$, $g(\boldsymbol{x_E})$; see Givens and Hoeting, page 47-48) and create new simplex/triangle



- Or in specific cases: Shrink (keep $\boldsymbol{x_{best}}$ and move all other vertices towards it)



Nelder-Mead

- Nelder-Mead algorithm is quite old, but still popular
- Research is ongoing e.g. about convergence results and variants of Nelder-Mead

- Note that Nelder-Mead can be used for dimension $p = 1$ as well
- However, there exist better gradient free algorithms for $p = 1$
  - **R**-function **`optimize`** uses gradient free algorithm with convergence order $q = 1.324$ (some requirements to function g necessary)

Solution x of $0 = x^3 - x - 1$; (Brent, 1973)

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