Biologically Inspired Algorithms (A4M33BIA)

Optimization: Conventional and Unconventional Optimization Techniques

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Contents

Biologically Inspired Optimization Techniques

What is this subject about?

About **problem solving** by means of **biologically inspired optimization techniques**:

- ✔ Optimization using Evolutionary Algorithms
- ✔ Modelling (classification, regression) using Neural Networks

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- ✔ no low-cost, analytic and complete solution is known

Why are they ‘problematic’?

1. *number of possible solutions* grows very quickly with the problem size
2. the goal is *noisy* or *time dependent*
3. the goal must fulfill some *constraints*
4. *barriers inside the people* solving the problem

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Why are they 'problematic'?

1. *number of possible solutions* grows very quickly with the problem size
   - ✔ complete enumeration impossible
2. the goal is *noisy* or *time dependent*
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1. *number of possible solutions* grows very quickly with the problem size
2. the goal is *noisy* or *time dependent*
   - ✔ the solution process must be repeated over and over
   - ✔ averaging to deal with noise
3. the goal must fulfill some *constraints*
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2. the goal is *noisy* or *time dependent*
3. the goal must fulfill some *constraints*
   - ✔ on one hand, the constraints decrease the number of feasible solutions
   - ✔ on the other hand, they make the problem much more complex, sometimes it is very hard to find *any feasible solution*
4. *barriers inside the people* solving the problem

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4. *barriers inside the people* solving the problem
   - ✔ insufficient equipment (money, knowledge, . . .)
   - ✔ psychological barriers (insufficient abstraction or intuition ability, ‘fossilization’, influence of ideology or religion, . . .)

What are Biologically Inspired Optimization Techniques?

Biologically Inspired Optimization Techniques

- ✔ computational methods inspired by evolution, by nature, and by the brain are being used increasingly to solve complex problems in engineering, computer science, robotics and artificial intelligence.
- ✔ studies, models and analyzes very complex phenomena for which
  - ✘ no low-cost, analytic, or complete solution is known
- ✔ consists especially of:
  - ✘ evolutionary algorithms, swarm intelligence
  - ✘ artificial neural networks
  - ✘ fuzzy systems
  - ✘ probability theory, possibility theory, Bayesian networks
- ✔ tolerance for
  - ✘ imprecision
  - ✘ partial truth
  - ✘ uncertainty
  - ✘ noise

Optimization

Optimization problems

Among all possible objects $x \in \mathcal{F} \subset \mathcal{S}$, we want to determine such an object x_{OPT} that optimizes (minimizes) the function f:

$$x_{\mathrm{OPT}} = \arg \min_{x \in \mathcal{F} \subset \mathcal{S}} f(x) \tag{1}$$

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The space of candidate solutions $\mathcal{S}$ and the objective function f:

1. Representation of the solution
   - ✔ syntactical structure that holds the 'solution'
   - ✔ induces the search space $\mathcal{S}$ and its feasible part $\mathcal{F}$
2. Optimization criterion, objective function, evaluation function f
   - ✔ function that is optimized
   - ✔ 'understands' the solution representation
   - ✔ adds meaning (semantics) to the solution representation
   - ✔ gives us the measure of the solution quality (or, at least, allows us to say that one solution is better than the other)

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Black-box optimization: the inner structure of function f is unknown—it is black box for us (and for the algorithm); the function can be

- ✔ continuous $\times$ discrete
- ✔ differentiable
- ✔ decomposable
- ✔ noisy, time dependent

Neighborhood, local optimum

The **neighborhood** of a point $x \in \mathcal{S}$:

$$N(x,d) = \{y \in \mathcal{S} | dist(x,y) \leq d\} \tag{2}$$

Measure of the **distance between points** x **and** y: $\mathcal{S} \times \mathcal{S} \rightarrow \mathcal{R}$

- ✔ binary space: Hamming distance
- ✔ real space: Euclidean, Manhattan (City-block), Mahalanobis, ...
- ✔ matrices: Amari
- ✔ in general: number of applications of some operator that would transform x into y in $dist(x,y)$ steps

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Local optimum:

- ✔ Point x is local optimum, if $f(x) \leq f(y)$ for all points $y \in N(x, d)$ for some positive d.
- ✔ Small finite neighborhood (or the knowledge of derivatives) allows for validation of local optimality of x.

Conventional optimization methods

Why are there so many of them?

Conventional optimization methods

Why are there so many of them?

- ✔ they are not robust, small change in the problem definition usually requires a completely different method

Classification of optimization algorithms (one of many possible):

1. Constructive algorithms
   - ✔ work with partial solutions, construct full solutions incrementally
   - ✔ not suitable for black-box optimization, must be able to evaluate partial solutions
   - ✔ require discrete search space
   - ✔ based on decomposition, arranging the search space in the form of a tree, . . .
2. Generative algorithms
   - ✔ work with complete candidate solutions, generate them as a whole
   - ✔ suitable for black-box optimization, only complete solutions need to be evaluated
   - ✔ can be interrupted anytime—always have a solution to provide; this solution is usually not optimal (needn't be even locally optimal)

What's next?

1. Review of conventional constructive methods
   - ✔ greedy algorithm, divide and conquer, dynamic programming, branch and bound, A^*
2. Conventional generative methods
   - ✔ Complete enumeration, local search, Nelder-Mead simplex search, gradient methods, linear programming
3. Unconventional methods inspired by nature

Conventional Constructive Methods

Divide and Conquer

1. Problem decomposition
2. Subproblem solutions
3. Combination of partial solutions

Issues:

- ✔ Is the problem decomposable? (If we combine optimal solutions of subproblems, do we get the optimal solution of the problem as a whole?)
- ✔ Is the decomposition worth the work? (Are the expenses for points 1–3 lower than the expenses of solution of the problem as a whole?—Very often yes.)

Suitable for:

- ✔ decomposable problems (huh, surprise!), no matter what is the type of subproblems

Dynamic Programming

Bellman's principle of optimality:

> If the point B lies on the optimal path from point A to point C, then the paths A–B and B–C are optimal as well.

Principle:

✔ Recursivelly solves high number of smaller subproblems

Suitable for:

1. Problem is decomposable on a sequence of decisions on various levels.
2. Several possible states on each level.
3. The decision brings the current state on next level.
4. The price of transition from one state to another is well defined.
5. Optimal decisions on one level are independent of decisions on previous levels.

Dynamic Programming: TSP Example

Traveling Salesperson Problem:

- ✔ Find the shortest path from depot through all the cities back to depot visiting each city only once.
- ✔ NP-complete

Application of DP on TSP:

- ✔ Decomposition to smaller subproblems:
  $f(i, S)$ — length of the shortest path from city i to city 1 through all the cities in S (in any order)
- ✔ $f(4, \{5, 2, 3\})$ — length of the shortes path from city 4 to city 1 through cities 5, 2, and 3
- ✔ TSP solution reduces to finding $f(1, V - \{1\})$ where V is the set of all cities (including the depot 1)
- ✔ Recursive transition from smaller problems to bigger ones:

$$f(i, S) = \min_{j \in S} (dist(i, j) + f(j, S - \{j\})) \tag{3}$$

- ✔ To find the optimal solution, DP often performs complete enumeration!

Best-First Search

- ✔ The search space forms a tree (empty solution in the root node, complete solutions in leaves).
- ✔ Each node x has a value assigned, $f(x)$, that describes our estimate of the quality of the final complete solution using the subsolution of the node x.
- ✔ Maintains two lists of nodes: OPEN and CLOSED.
- ✔ Algorithm:

  1. OPEN = {start}, CLOSED = {}
  2. remove x with best $f(x)$ from OPEN
  3. for all children of x, $y_i \in \text{children}(x)$
     - ✘ $y_i \notin$ OPEN, $y_i \notin$ CLOSED: add y_i to OPEN
     - ✘ $y_i \in$ OPEN: update $f(y_i)$ if it is better then the current one
     - ✘ $y_i \in$ CLOSED: if $f(y_i)$ is better then the current one, remove y_i from CLOSED and put it in OPEN
  4. repeat until OPEN is empty

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Special cases:

- ✔ **Depth-first search**: $f(j) = f(i) - 1$, $j \in \text{children}(i)$, uninformed
- ✔ **Breadth-first search**: $f(j) = f(i) + 1$, $j \in \text{children}(i)$, uninformed
- ✔ **Greedy search**: $f(i) = estimate\_of\_dist(i, target)$, only short-term profit

Branch and Bound

- ✔ Search of the tree structured state spaces
- ✔ During the search, it maintains lower and upper limit on the optimal value of f
- ✔ It does not expand those nodes that do not offer chance for better solution

A and A* Algorithm

A Algorithm

- ✔ Best-first search with function f of special meaning.
- ✔ Function f has the following form:

$$f(i) = g(i) + h(i), \tag{4}$$

where $g(i)$ is the price of the optimal path from root node to node i
$h(i)$ is the price of the optimal path from node i to the goal node

- ✔ Pays attention to future decisions

A* Algorithm

- ✔ Function $h(i)$ in A algorithm expresses the price of future decisions, but they are not known when evaluating node i
- ✔ Function $h(i)$ is approximated with $h^*(i)$ heuristic
- ✔ Function $h^*(i)$ is admissible if it is a non-negative lower estimate of $h(i)$
- ✔ Algorithm A is admissible (always finds the optimal path if it exists) if it uses admissible heuristic function $h^*(i)$ and in such case it is called A* algorithm.

Conventional Generative Methods

Gradient Methods

1. Select initial point $\mathbf{x}_0$.
2. Perform update of point $\mathbf{x}$: $\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k - \alpha_k \cdot \nabla f(\mathbf{x}_k)$
3. Go to 2 until convergence.

Newton's method: special case of gradient method

✔ Iteratively improves an approximation to the root of a real-valued function:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

✔ Finds minimum of quadratic bowl in 1 step

✔ Uses Hessian matrix to compute the update step length:

$$\alpha_k^{-1} = H(f(\mathbf{x}_k)) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 x_D} \\ \frac{\partial^2 f}{\partial x_2 x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x^2 x^D} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_D x_1} & \frac{\partial^2 f}{\partial x_D x_2} & \cdots & \frac{\partial^2 f}{\partial x_D^2} \end{bmatrix} (\mathbf{x}_k) \tag{5}$$

Linear Programming

- ✔ Simplex method (completely different from the Nelder-Mead simplex search)
- ✔ f must be linear
- ✔ Constraints in the form of linear equations and inequations
- ✔ Extremum is found on the boundaries of polyhedra given by the optimized function and the constraints.
- ✔ Unusable in BB optimization, since the function f is generally nonlinear.

Exhaustive, Enumerative Search

- ✔ All possible solutions are generated and evaluated sequentially
- ✔ Often realized using depth-first or breadth-first search
- ✔ Applicable for small discrete search spaces
- ✔ For more complex tasks inappropriate—the number of possible solutions grows usually exponentially
- ✔ Continuous spaces cannot be searched exhaustively!!!

Local Search, Hill-Climbing

Algorithm 1: LS with First-improving Strategy

```
begin
    x ← Initialize()
    while not TerminationCondition() do
        y ← Perturb(x)
        if BetterThan(y, x) then
            x ← y
```

Features:

- ✔ usually stochastic, possibly deterministic, applicable in discrete and continuous spaces

Local Search, Hill-Climbing

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Algorithm 2: LS with Best-improving Strategy

```
begin
    x ← Initialize()
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        y ← BestOfNeighborhood(N(x, D))
        if BetterThan(y, x) then
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```

Features:

- ✔ deterministic, applicable only in discrete spaces, or in descretized real-valued spaces, where $N(x, d)$ is finite and small

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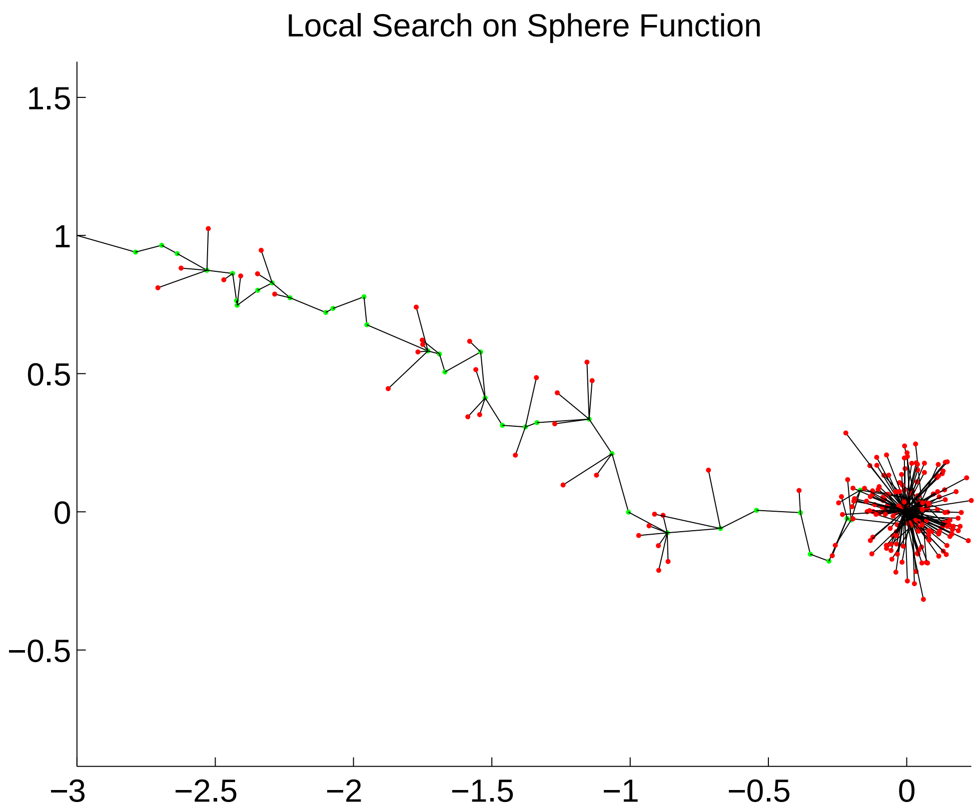
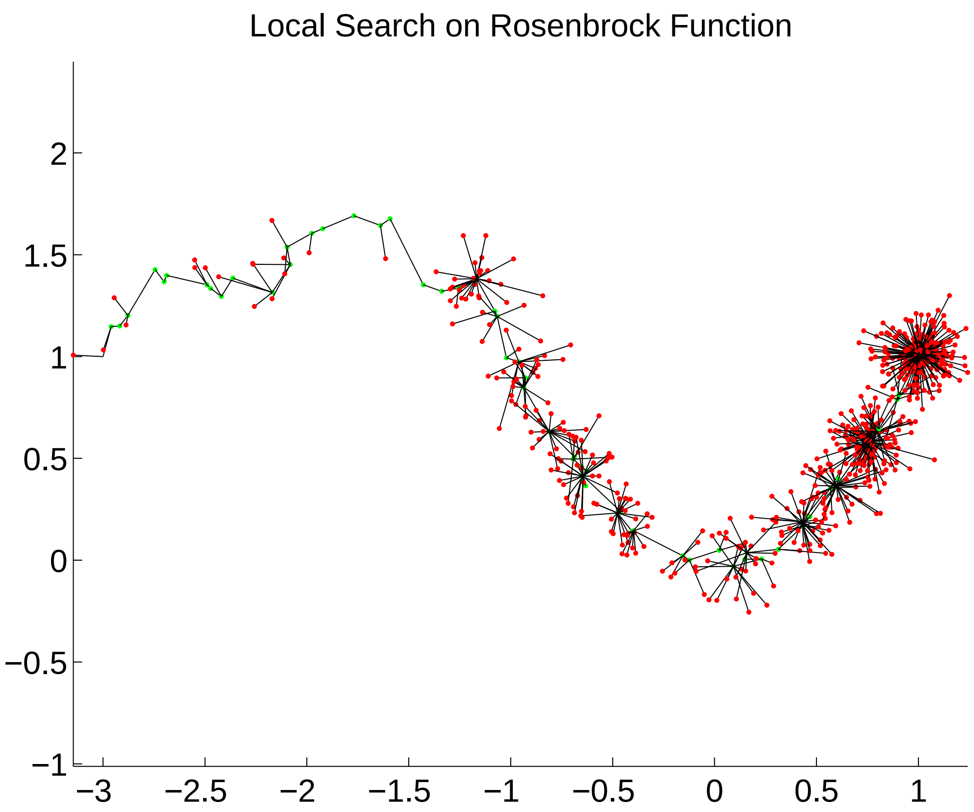
The influence of the neighborhood size:

- ✔ Small neighborhood: fast search, huge risk of getting stuck in local optimum (in zero neghborhood, the same point is generated over and over)
- ✔ Large neighborhood: lower risk of getting stuck in LO, but the efficiency drops. If $N(x,d) = \mathcal{S}$, the search degrades to
  - ✘ random search in case of first-improving strategy, or to
  - ✘ exhaustive search in case of best-improving strategy.

Local Search Demo





Rosenbrock's Optimization Algorithm

Described in [?]:

Algorithm 3: Rosenbrock's Algorithm

Input: $\alpha > 1$, $\beta \in (0,1)$

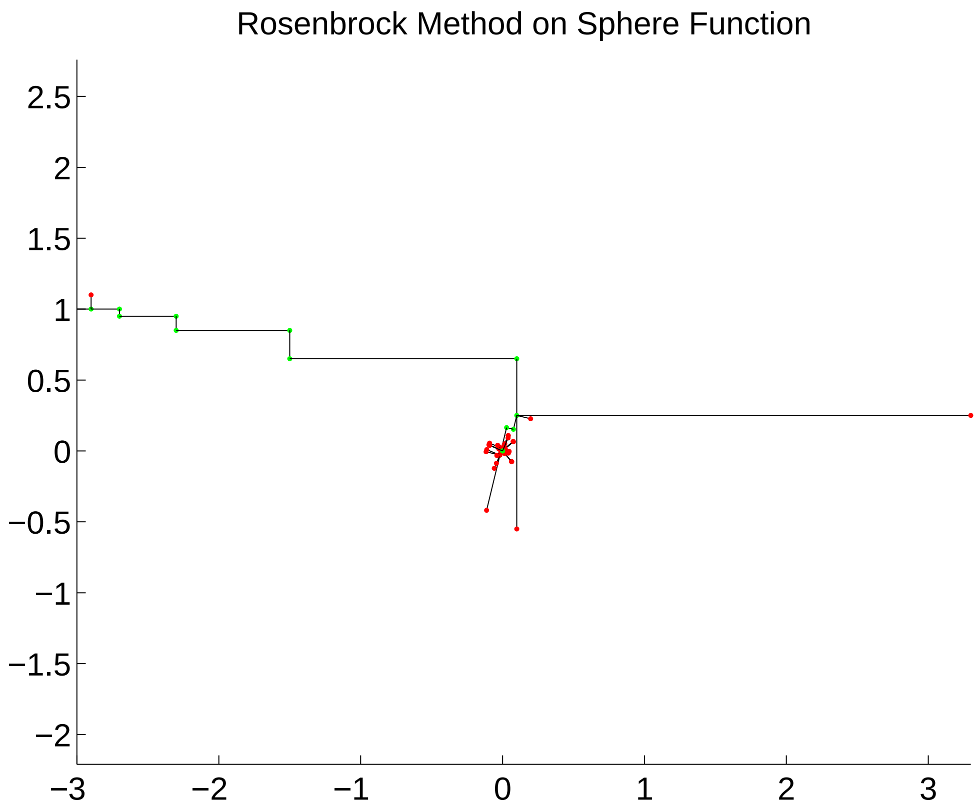
begin
  $\mathbf{x} \leftarrow$ `Initialize()`; $\mathbf{x}_o \leftarrow \mathbf{x}$
  $\{\mathbf{e}_1, \ldots, \mathbf{e}_D\} \leftarrow$ `InitOrtBasis()`
  $\{d_1, \ldots, d_D\} \leftarrow$ `InitMultipliers()`
  while not `TerminationCondition()` **do**
    for i=1 ... D **do**
      $\mathbf{y} \leftarrow \mathbf{x} + d_i \mathbf{e}_i$
      if `BetterThan(`y,x`)` **then**
        $\mathbf{x} \leftarrow \mathbf{y}$
        $d_i \leftarrow \alpha \cdot d_i$
      else
        $d_i \leftarrow -\beta \cdot d_i$
    if `AtLeastOneSuccInAllDirs()` **and** `AtLeastOneFailInAllDirs()` **then**
      $\{\mathbf{e}_1, \ldots, \mathbf{e}_D\} \leftarrow$ `UpdOrtBasis(`$\mathbf{x} - \mathbf{x}_o$`)`
      $\mathbf{x}_o \leftarrow \mathbf{x}$

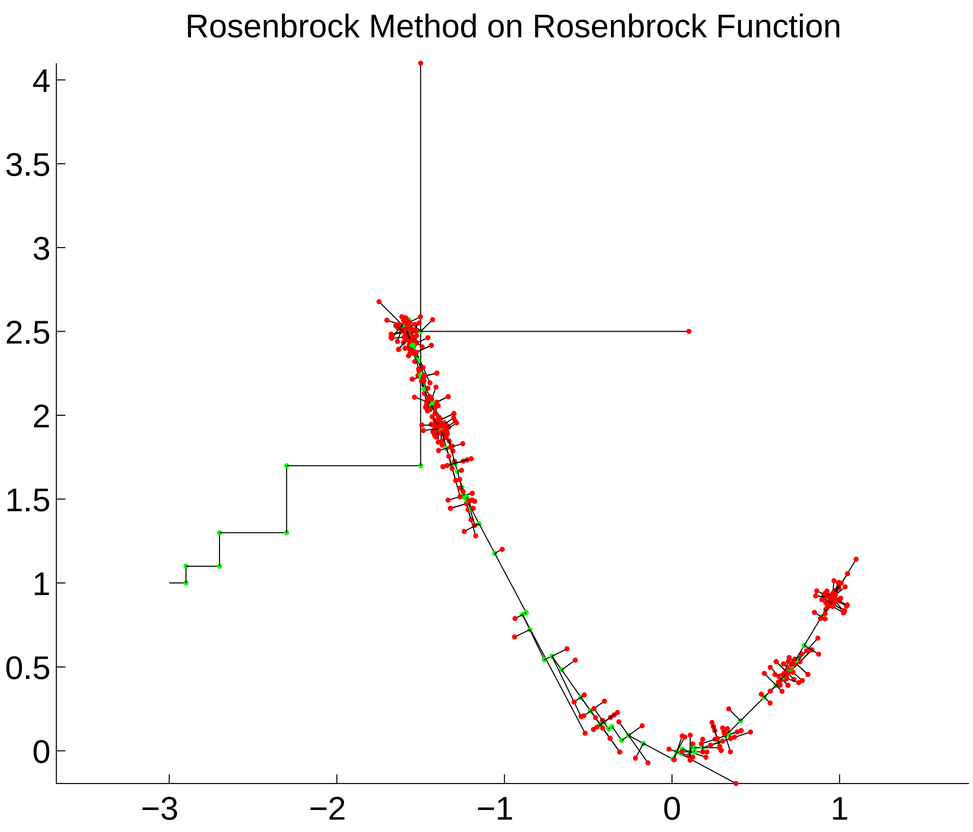
Features:

- ✔ D candidates generated each iteration
- ✔ neighborhood in the form of a pattern
- ✔ adaptive neighborhood parameters
  - ✘ distances
  - ✘ directions

DEMO

Rosenbrock's Algorithm Demo





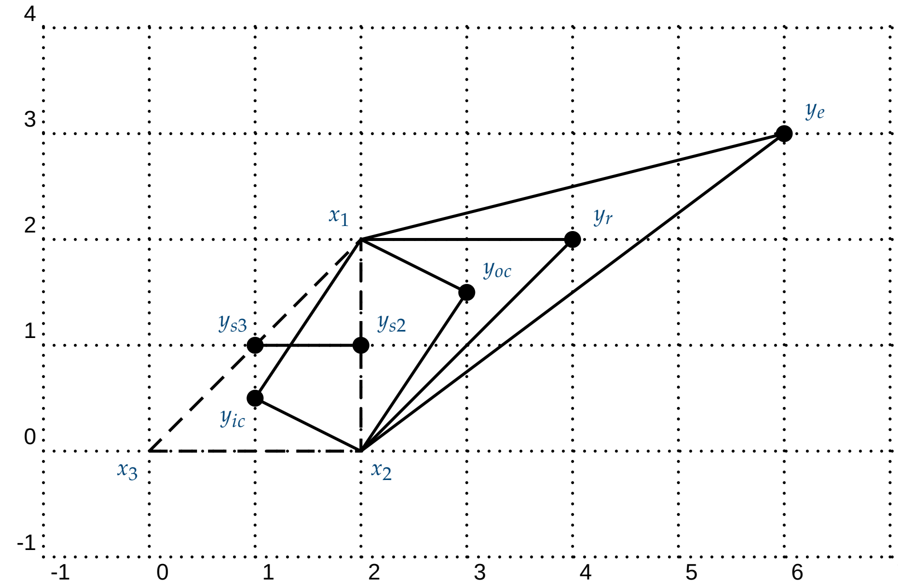
Nelder-Mead Simplex Search

Simplex downhill search (amoeba) [?]:

Algorithm 4: Nelder-Mead Simplex Algorithm

begin
  $(\mathbf{x}_1, \ldots, \mathbf{x}_{D+1}) \leftarrow$ `InitSimplex()`
  `so that` $f(x_1) \leq f(x_2) \leq \ldots \leq f(x_{D+1})$

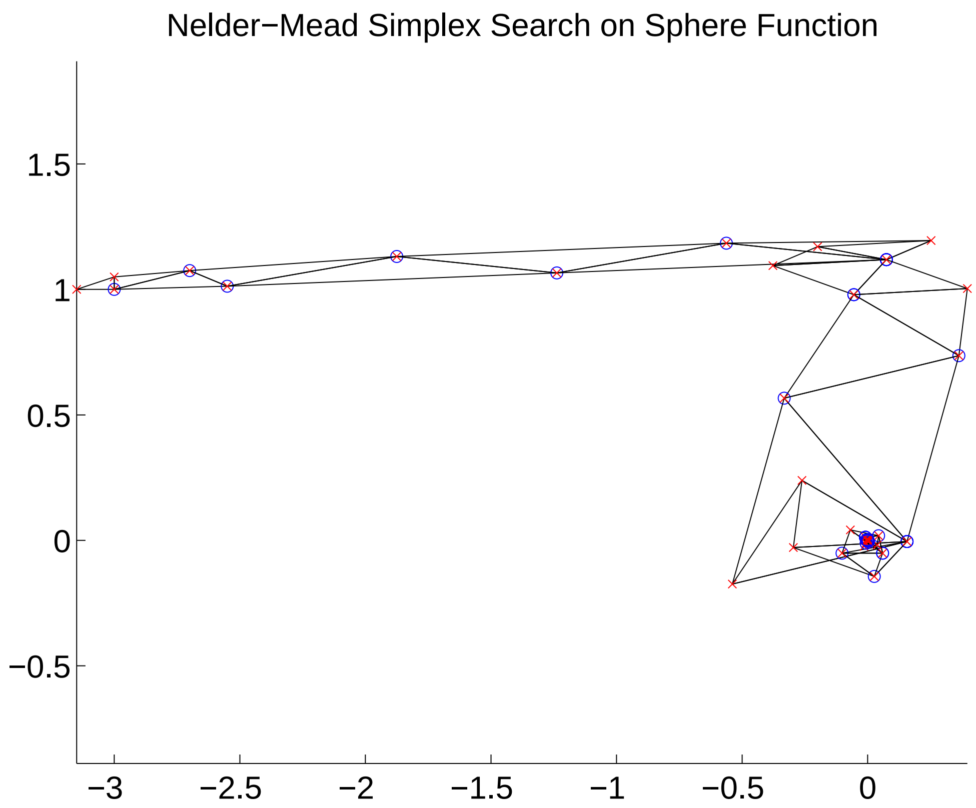
  while not `TerminationCondition()` **do**
    $\bar{\mathbf{x}} \leftarrow \frac{1}{D} \sum_{d=1}^{D} \mathbf{x}_d$
    $\mathbf{y}_r \leftarrow \bar{\mathbf{x}} + \rho(\bar{\mathbf{x}} - \mathbf{x}_{D+1})$
    if `BetterThan(`$\mathbf{y}_r, \mathbf{x}_D$`)` **then** $\mathbf{x}_{D+1} \leftarrow \mathbf{y}_r$
    if `BetterThan(`$\mathbf{y}_r, \mathbf{x}_1$`)` **then**
      $\mathbf{y}_e \leftarrow \bar{\mathbf{x}} + \chi(\mathbf{x}_r - \bar{\mathbf{x}})$
      if `BetterThan(`$\mathbf{y}_e, \mathbf{y}_r$`)` **then** $\mathbf{x}_{D+1} \leftarrow \mathbf{y}_e$;
      `Continue`
    if not `BetterThan(`$\mathbf{y}_r, \mathbf{x}_D$`)` **then**
      if `BetterThan(`$\mathbf{y}_r, \mathbf{x}_{D+1}$`)` **then**
        $\mathbf{y}_{oc} \leftarrow \bar{\mathbf{x}} + \gamma(\mathbf{x}_r - \bar{\mathbf{x}})$
        if `BetterThan(`$\mathbf{y}_{oc}, \mathbf{y}_r$`)` **then**
        $\mathbf{x}_{D+1} \leftarrow \mathbf{y}_{oc}$; `Continue`
      else
        $\mathbf{y}_{ic} \leftarrow \bar{\mathbf{x}} - \gamma(\bar{\mathbf{x}} - \mathbf{x}_{D+1})$
        if `BetterThan(`$\mathbf{y}_{ic}, \mathbf{x}_{D+1}$`)` **then**
        $\mathbf{x}_{D+1} \leftarrow \mathbf{y}_{ic}$; `Continue`

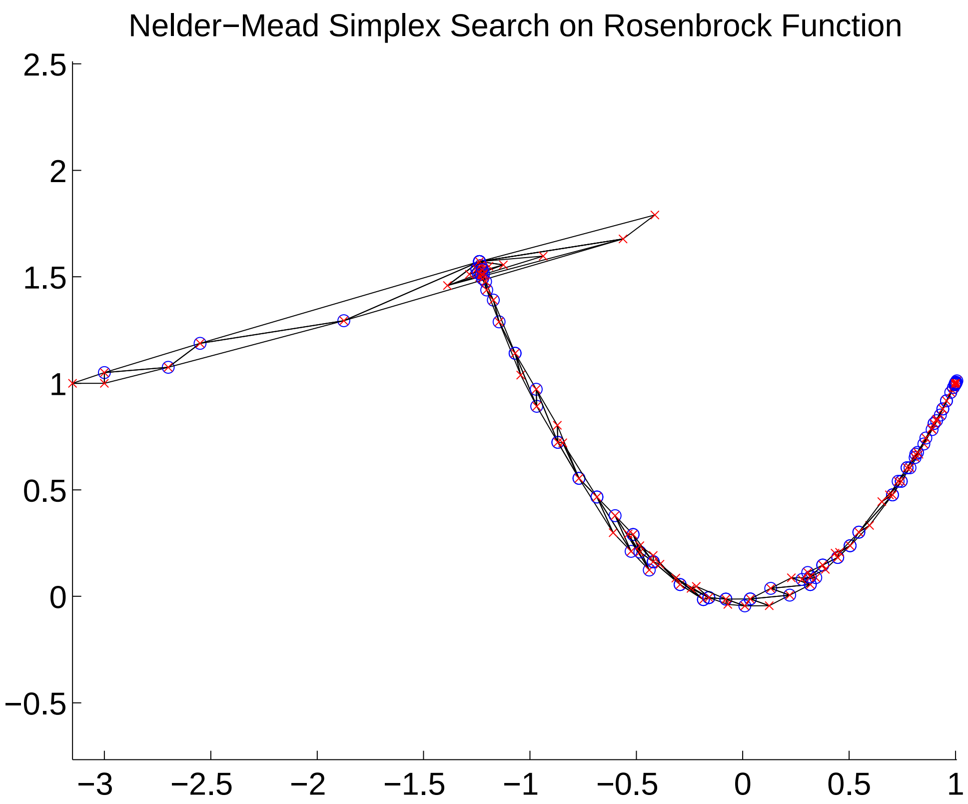


Features:

- ✔ universal algorithm for BBO in real space
- ✔ in $\mathcal{R}^D$ maintains a *simplex* of $D+1$ points
- ✔ neighborhood in the form of a pattern (reflection, extension, contraction, reduction)
- ✔ static neighborhood parameters!
- ✔ adaptivity caused by *changing relationships* among solution vectors!
- ✔ slow convergence, for low D only

Nelder-Mead Simplex Demo





Lessons Learned

- ✔ To *search for the optimum*, the algorithm must *maintain at least one base solution* (fullfiled by all algorithms).
- ✔ To *adapt to the changing position in the environment* during the search, the algorithm must either
  - ✘ *adapt the neighborhood (model)* structure or parameters (as done in Rosenbrock method), or
  - ✘ *adapt more than 1 base solutions* (as done in Nelder-Mead method), or
  - ✘ both of them.
- ✔ The neighborhood
  - ✘ can be *finite* or *infinite*
  - ✘ can have a form of a *pattern* or a *probabilistic distribution*.
- ✔ Candidate solutions can be generated from the neighborhood of
  - ✘ one base vector (LS, Rosenbrock), or
  - ✘ all base vectors (Nelder-Mead), or
  - ✘ some of the base vectors (requires *selection* operator).

Unconventional Methods Inspired by Nature

The Problem of Local Optimum

Goal of these algorithms:

✔ to lower the risk of getting stuck in local optimum.

How can we avoid local optimum?

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1. Run the optimization algorithm from a different initial point.
   - ✔ e.g. iterated hill-climber

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2. Introduce memory and do not stop the search in LO
   ✔ e.g. taboo search

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3. Introduce a probabilistic aspect
   - ✔ stochastic hill-climber
   - ✔ simulated annealing
   - ✔ evolutionary algorithms, swarm intelligence

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   - ✔ e.g. iterated hill-climber
2. Introduce memory and do not stop the search in LO
   - ✔ e.g. taboo search
3. Introduce a probabilistic aspect
   - ✔ stochastic hill-climber
   - ✔ simulated annealing
   - ✔ evolutionary algorithms, swarm intelligence
4. Perform the search in several places in parallel
   - ✔ evolutionary algorithms, swarm intelligence (population-based optimization algorithms)

Taboo Search

Algorithm 5: Taboo Search

```
begin
    x ← Initialize()
    y ← x
    M ← ∅
    while not TerminationCondition() do
        y ← BestOfNeighborhood(N(y, D) − M)
        M ← UpdateMemory(M, y)
        if BetterThan(y, x) then
            x ← y
```

Meaning of symbols:

- ✔ M — memory holding already visited points that become taboo
- ✔ $N(\mathbf{x}, d) \cap M$ — set of states which would arise by taking back some of the previous decisions

Features:

- ✔ canonical version is based on the local search with best-improving strategy
- ✔ first-improving can be used as well
- ✔ difficult use in real domain, usable mainly in discrete spaces

Stochastic Hill-Climber

Assuming minimization:

Algorithm 6: Stochastic Hill-Climber

begin
    x ← `Initialize()`
    while not `TerminationCondition()` **do**
        y ← `Perturb(`x`)`
        $p = \frac{1}{1+e^{\frac{f(\mathbf{y})-f(\mathbf{x})}{T}}}$
        if $rand < p$ **then**
            x ← y

Features:

- ✔ It is possible to move to a worse point *anytime*.
- ✔ T is the algorithm parameter and stays constant during the whole run.
- ✔ When T is low, we get local search with first-improving strategy
- ✔ When T is high, we get random search

Stochastic Hill-Climber

Assuming minimization:

Algorithm 6: Stochastic Hill-Climber

```
begin
    x ← Initialize()
    while not TerminationCondition() do
        y ← Perturb(x)
        p = 1 / (1 + e^((f(y) − f(x)) / T))
        if rand < p then
            x ← y
```

Features:

- ✔ It is possible to move to a worse point *anytime*.
- ✔ T is the algorithm parameter and stays constant during the whole run.
- ✔ When T is low, we get local search with first-improving strategy
- ✔ When T is high, we get random search

Probability of accepting a new point **y** when $f(\mathbf{y}) - f(\mathbf{x}) = -13$:

T	$e^{-\frac{13}{T}}$	p
1	0.000	1.000
5	0.074	0.931
10	0.273	0.786
20	0.522	0.657
50	0.771	0.565
10^{10}	1.000	0.500

Probability of accepting a new point **y** when $T = 10$:

$f(\mathbf{y}) - f(\mathbf{x})$	$e^{\frac{f(\mathbf{y})-f(\mathbf{x})}{10}}$	p
-27	0.067	0.937
-7	0.497	0.668
0	1.000	0.500
13	3.669	0.214
43	73.700	0.013

Simulated Annealing

Algorithm 7: Simulated Annealing

```
begin
    x ← Initialize()
    T ← Initialize()
    while not TerminationCondition() do
        y ← Perturb(x)
        if BetterThan(y,x) then
            x ← y
        else
            p = e^(-(f(y)-f(x))/T)
            if rand < p then
                x ← y
        if InterruptCondition() then
            T ← Cool(T)
```

$$p = e^{-\frac{f(\mathbf{y})-f(\mathbf{x})}{T}}$$

Simulated Annealing

Algorithm 7: Simulated Annealing

```
begin
    x ← Initialize()
    T ← Initialize()
    while not TerminationCondition() do
        y ← Perturb(x)
        if BetterThan(y,x) then
            x ← y
        else
            p = e^(-(f(y)-f(x))/T)
            if rand < p then
                x ← y
        if InterruptCondition() then
            T ← Cool(T)
```

Very similar to stochastic hill-climber

Main differences:

- ✔ If the new point **y** is better, it is *always* accepted.
- ✔ Function `Cool`(T) is the *cooling schedule*.
- ✔ SA changes the value of T during the run:
  - ✘ T is high at beginning: SA behaves like random search
  - ✘ T is low at the end: SA behaves like deterministic hill-climber

Simulated Annealing

Algorithm 7: Simulated Annealing

begin
  x ← `Initialize()`
  T ← `Initialize()`
  while not `TerminationCondition()` **do**
    y ← `Perturb(`x`)`
    if `BetterThan(`y,x`)` **then**
      x ← y
    else
      $p = e^{-\frac{f(\mathbf{y})-f(\mathbf{x})}{T}}$
      if *rand* $< p$ **then**
        x ← y
    if `InterruptCondition()` **then**
      T ← `Cool(`T`)`

Very similar to stochastic hill-climber

Main differences:

- ✔ If the new point **y** is better, it is *always* accepted.
- ✔ Function `Cool`(T) is the *cooling schedule*.
- ✔ SA changes the value of T during the run:
  - ✘ T is high at beginning: SA behaves like random search
  - ✘ T is low at the end: SA behaves like deterministic hill-climber

Issues:

- ✔ How to set up the initial tempereature T and the cooling schedule `Cool`(T)?
- ✔ How to set up the interrupt and termination condition?

SA versus Taboo

Feature	Taboo	SA
When can it accept worse solution?	After visiting LO	Anytime
Deterministic/Stochastic	Usually determininstic (based on best-improving strategy)	Usually stochastic (based on first-improving strategy)
Parameters	Neighborhood size Termination condition Type od memory Memory behaviour (forgetting)	Neighborhood size Termination condition Temperature Cooling schedule

Summary

- ✔ Black-box optimization:
  - ✘ no information about objective function is known
  - ✘ all we can do is ask the objective function to evaluate some candidate solution
- ✔ Constructive vs. generative methods
  - ✘ constructive methods are not suitable for BBO — require ability to evaluate partial solutions
- ✔ 2 sources of adaptivity for generative methods:
  1. definition of local neighborhood
  2. ‘population’ of candidate solutions

Artificial Neural Networks

…next five lectures on Artificial Neural Networks with Jan Drchal.

Thank you for your attention.