Metaheuristic algorithms.

Lab 1: Optimization problems
Introduction into Scilab

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1. Optimization problems

The optimization problems represent one of the most frequently encountered class of problems arising in applications which require:

- *Planning* (scheduling and/or establishing the execution order of some activities, resource allocation, timetabling etc)
- *Modelling* (constructing a model which fits well some experimental data)
- *Adaptation* (changing the behavior of a system by training based on some training data)

All optimization problems are characterized by: solution search space, optimization criterion (objective function) and constraints.

1.1. ***Solution search space.*** There are two main cases:

- Discrete search space (usually a finite but of large size set).
- Continuous search space

Depending on the search space there are two main classes of optimization problems:

- Combinatorial optimization problems
  - Assignment/allocation/selection problems (e.g. knapsack problem, bin packing problem)
  - Routing problems (e.g. travelling salesman problem)
- Continuous optimization problems
  - Parameter estimation (e.g. neural networks training, find cluster prototypes in data clustering)

1.2. ***Optimization criterion (objective function).*** It represents the value which should be maximized (minimized or maximized). Depending on the number of optimization criteria there are:

- Single-objective optimization
- Multi-objective optimization

Depending on the information which are available on the objective function the optimization problems can be:

- *White-box:* the objective function is explicitly and its properties can be analyzed and exploited (linear/non-linear, continuous/discontinuous, smoothness etc).
- *Black-box:* the objective function is not explicitly known – it can be only evaluated (e.g. in the case of objective functions which are based one simulation).

1.3 ***Constraints.*** The constraints define the space of feasible solutions and can be of several types

- Bound constraints: a<=x<=b
- Equality constraints: g(x)=a
- Inequality constraints: h(x)<=b

Depending on their importance, the constraints can be:

- hard: they have to be satisfied
- soft: it is preferable that they are satisfied but they are not mandatory

2. Steps in solving optimization problems

Step 1: problem analysis and identification of the following elements:

- Structure (encoding) of candidate solutions; this allows to establish the properties and the size of the search. The problem can be of one of the following classes:
    - Combinatorial optimization
    - Continuous optimization

  of size
    - small (less than 10 variabile)
    - medium (between 10 and 100 variables)
    - large (more than 100 de variables)

- Constraints
- Objective function and its properties:
    - Linear, quadratic, arbitrary
    - continuous/discontinuous, differentiable/nondifferentiable
    - one objective function/ several objective functions, unimodal/multimodal
    -

Step 2: Method selection:

- Methods for objective functions/constraints which are linear/ quadratic
- Derivatives-based local optimization
- Derivatives-free local optimization
- Global optimization
- Multi-objective optimization

Appendix 1: Scilab - Open source software for numerical computation (http://www.scilab.org/)

Scilab is an interpreted programming language which offers support for computational tasks arising in linear algebra, polynomials operations, interpolation and approximation, linear and quadratic optimization, differential equations, signal processing, statistics and graphics.

In Scilab the basic object is the matrix, both the vectors and the scalars being particular cases of matrices.

Some general aspects:

- Scilab is case-sensitive
- Being an interpreter, the variables do not have to be declared but they should have a value assigned; the assignment operator is =
- The predefined constants have names with the prefix % (e.g. %pi, %i, %e, %t (true), %f (false))
- The relational operators are: == (equal), ~= or <> (unequal), <=, >=
- The logical operators are: ~ (not), & (and), | (or)
- The result of an evaluation which is not explicitly assigned to a variable is implicitly assigned to the object ans which can be used in the following command
- The commands specified on the same line should be separated by ; (this separator has also the effect of inhibiting the visualization of the last evaluation result).
- The strings are specified using doubl quotes (") and their concatenation can be realized using +
- The line comments can be specified by //

Specifying matrices:

- Explicitly, by specifying all elements (the elements on the same row should be separated by , or space and the rows should be separated by ; or enter):
  A=[a11,a12,…a1n; a21,a22,…,a2n; …;am1, am2,…,amn]

- Implicitly, by using functions which generate matrices:
  - zeros(m,n) : matrix with m rows and n columns and elements equal to 0
  - ones(m,n): matrix with m rows and n columns and elements equal to 1
  - rand(m,n): matrix with m rows and n columns and elements randomly generated in (0,1)

Operations with matrices.

- Finding the size: size(mat) returns [nr rows, nr columns]
- Reorganizing a matrix: matrix(mat, nr rows, nr columns) returns a matrix with the specified size and elements taken row by row from the object specified as the first parameter
- Accessing the elements: mat(row index,column index).
  Obs: the indices can be individual values or ranges specified as inf:sup. The last index of a row or column can be specified by $. For instance mat($,$-1) specifies the element on the last row and the column before the last one.
  Obs: the indices start with 1
- Changing a matrix:
  - Change an element: mat(i,j)=val

    - Add a row: mat=[mat; el1, el2,…,eln]
    - Add a column: mat=[mat’; el1, el2,…,elm]’   (the operator ‘ denotes the transpose)
    - Remove a row: mat(i,:)=[]
    - Remove a column: mat(:,j)=[]
- Arithmetical operations: all arithmetical operations are vectorized; in order to specify operations at the level of elements the operators should be prefixed by . (dot). For instance, A*B returns the algebraic product of matrices A and B ans A.*B returns the matrix which is obtained by multiplying the corresponding elements from the matrices.

Other types of objects in Scilav:

- Structures:
    - struct(fieldname1,value1, fieldname2,value2,…., fieldnamen,valuen)
    - Example: date=struct(‘day’,3,’month’,’october’,’year’,2014)
    - Element specification: StructureName.Fieldname(e.g.: date.day is 3)

- Heterogeneous lists:
    - Simple list: list(Element1,Element2,…,Elementn)
      Remark: the elements are specified using indices
    - Typed list: tlist(Names,Element1,Element2,…,Elementn) ;
      Example: d=tlist([‘date’,’day’,’month’,’year’],3,’october’,2014)
      Remark: the elements can be specified both by indexing abd by qualification: d(2) is identical to d.day

Instructions

- **If statement:**

```
if (condition) then
        <statements 1>
else
        < statements 2>
end
```

  Variant:

```
if (condition1) then
        < statements 1>
elseif (condition 2)
        < statements 2>
else
        < statements 3>
end
```

- **Select statement:**

```
select < selector>
case < val 1>
        < statements 1>
case <val 2>
```

```
        < statements 2>
…
case <val n>
        < statements n>
else
        <other statements >
end
```

- **for statement**

  ```
  for contor=inf:step:sup
          < statements >
  end
  ```

  Remark: If step is 1 the it can be ommitted. The value of the step can be less than 0. The iteration can be done over the elements of a vector (one row matrix):

  ```
  for contor=vector
          < statements >
  end
  ```

- **while statement**

  ```
  while(conditie)
          < statements >
  end
  ```

Functions

Scilab functions can be used to compute several results (specified by output variables in the function header):

```
function [output1, …,outputm]=functionName(input1,…,inputn)
        <function body>
endfunction
```

Graphics

Several graphics functions:
- plot - one-dimensional functions
- fplot3d and contour - surfaces
- paramfplot2d – curves given by parametric equations
- polarplot – polar coordinates representation

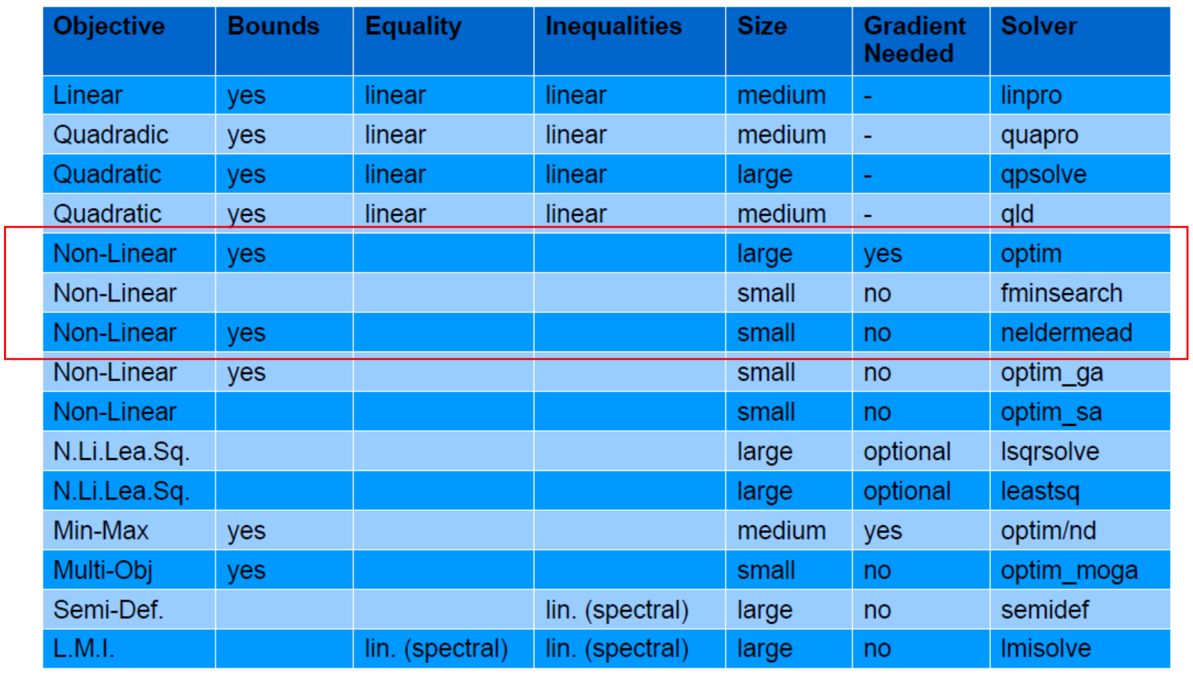
Example:

```
// one-dimensional function to be plotted
function y=f(x)
    y=x*x/10+sin(x)
endfunction

x=-2*%pi:0.1:2*%pi
clf
plot(x,f)

// surface
function y=f2arg(x1, x2) // function with 2 arguments
    y = x1 **2 + x2 **2;
endfunction
x1data = linspace ( -1 , 1 , 100 ); // this is equivalent with x1data = -1:0.1:1;
x2data = linspace ( -1 , 1 , 100 );
contour ( x1data , x2data , f2arg , 10)  // contour plot
pause
clf                                   // clean the screen
fplot3d( x1data , x2data , f2arg)       // surface plot
```

Optimization in SciLab



Objective	Bounds	Equality	Inequalities	Size	Gradient Needed	Solver
Linear	yes	linear	linear	medium	-	linpro
Quadradic	yes	linear	linear	medium	-	quapro
Quadratic	yes	linear	linear	large	-	qpsolve
Quadratic	yes	linear	linear	medium	-	qld
Non-Linear	yes			large	yes	optim
Non-Linear				small	no	fminsearch
Non-Linear	yes			small	no	neldermead
Non-Linear	yes			small	no	optim_ga
Non-Linear				small	no	optim_sa
N.Li.Lea.Sq.				large	optional	lsqrsolve
N.Li.Lea.Sq.				large	optional	leastsq
Min-Max	yes			medium	yes	optim/nd
Multi-Obj	yes			small	no	optim_moga
Semi-Def.			lin. (spectral)	large	no	semidef
L.M.I.		lin. (spectral)	lin. (spectral)	large	no	lmisolve

SciLab functions for different optimization problems [M. Baudin, V. Couvert, Optimization with SciLab, 2011]

2.1. Optimization using optim

Types of problems which can be solved: unconstrained nonlinear optimization problems.

Methods: quasi-Newton (local methods which require an initial approximation and the gradient)

Calls:
```
[xopt,fopt]=optim(objfct, x0)      // x0 = initial approximation
[xopt,fopt]=optim(objfct,"b",liminf,limsup, x0)   // liminf, limsup = bounding vectors

[xopt,fopt]=optim(objfct,x0, alg)   //alg=algorihtm
              //"qn": quasi-Newton (default) based on BFGS (Broyden-Fletcher-Goldfarb-Shanno)
              //"gc": BFGS with limited memory (for a large number of variables)
              //"nd": for non-differentiable objective functions
```

Remark: the SciLab function which implements the objective function should return both the objective function and its gradient.

Example: Find an optimum of the function, f:RxR->R, in the neighborhood of (-1,1.5).

$f(x1,x2)=100*(x2-x1^2)^2 +(1-x1)^2$

(the function is known as Rosenbrock function and is considered difficult to be optimized in the case of a large number of variables)

Scilab:
```
function [f, g, ind]=rosenbrock(x, ind)
  f = 100*(x(2)-x(1)^2)^2 + (1-x(1))^2         // objective function
  g(1) = - 400*(x(2)-x(1)^2)*x(1) - 2*(1-x(1)) // gradient
                                               //components
  g(2) = 200*(x(2)-x(1)^2)
endfunction
x0 = [-1.0 1.5];    // initial approximation
[ fopt , xopt ] = optim ( rosenbrock , x0)
```

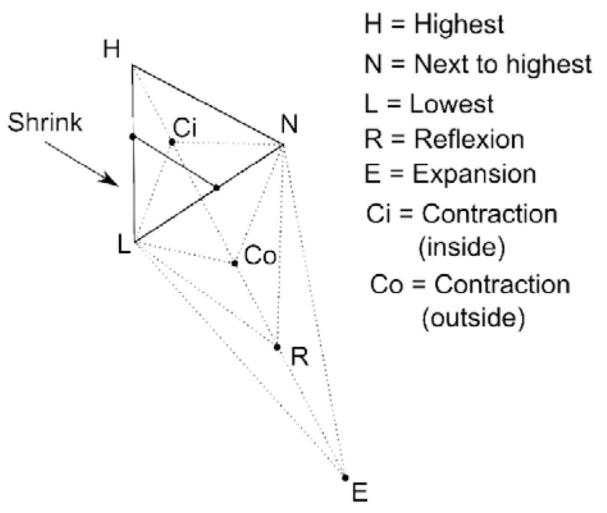
Exercise 1.

a) Estimat the optimum of the Griewank function using various methods ("qn", "gc", "nd") and compare the results
b) Analyze the case when the derivatives are not computed analytically but numerically: g=numderivative(rosebrockF,x)
   In the call of the function numderivative, the parameter rosenbrockF denotes a function which returns only the value (it does not provide the gradient)
c) Change the function in order to work for more than two variables.

2.2. Optimization using fminsearch

Types of problems which can be solved: unconstrained nonlinear optimization problems for non-differentiable objective functions.

Methods: Nelder-Mead (the search is based on the construction of new solutions using a simplex structure and a set of transformations – see the following figure and Lecture 2)



Call:

```
[xopt,fopt]=fminsearch(objfct, x0)      // x0 = initial approximation
[xopt,fopt]=fminsearch(objfct, x0, options)
```

The options are set using optimset: `options= optimset(OptionName,OptionValue)`

Types of optiona:

- MaxIter - maximal number of iterations (default: 200*number of variables)
- MaxFunEvals – maximal number of objective function evaluations (default: 200*number of variables)
- TolFun – tolerance on the objective function value (implicit: 0.0001)
- TolX – tolerance on the variables (implicit: 0.0001)
- PlotFcns – plot of the objective function value vs the number of iterations (default: empty – no visualization)

Examplu: Rosenbrock function

SciLab:

```
function f=rosenbrockF(x)
  f = 100*(x(2)-x(1)^2)^2 + (1-x(1))^2         // objective function

endfunction
x0 = [-1.0 1.5];    // initial approximation
[ fopt , xopt ] = fminsearch ( rosenbrockF , x0)
```

Exercise 2. Implement and test the following variants:

a) Visualization of the minimization process:

```
optiuni = optimset ( "PlotFcns" , optimplotfval )
x0=[-1,1.5]
[ fopt , xopt ] = fminsearch ( rosenbrockF , x0, options)
```

b) Output of the transformations applied at each iteration:

```
optiuni = optimset ( "Display" , iter )
x0=[-1,1.5]
[ fopt , xopt ] = fminsearch ( rosenbrockF , x0, options)
```

c) Test the case with a larger number of variables