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On the Use of Stochastic Optimization in Chemical and Process Engineering

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OUTLINE

1. **STOCHASTIC vs. DETERMNISTIC METHODS of OPTIMIZATION**
2. **ADAPTIVE RANDOM SEARCH**
3. **SIMULATED ANNEALING with SIMPLEX (SA/S)**
4. **GENETIC ALGORITHMS (GA)**
5. **COMPUTER-SOLVER OPTI-STO**
6. **EXAMPLES of APPLICATIONS**
7. **CONCLUSIONS**

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1. DETERMINISTIC vs. STOCHASTIC METHODS of OPTIMIZATION

or *WHY STOCHASTIC METHODS ???*

Because “classical “ deterministic approaches (i.e. mathematical programming) have serious drawbacks (particularly when applied by non-experts)

- **ARE NOT ABLE TO LOCATE the GLOBAL OPTIMUM (in NON-LINEAR PROBLEMS)**
- **REQUIRE SMOOTH FUNCTIONS WITHOUT DISCONTINUITIES and (often) ALSO DIFFERENTIABLE (even twice)**
- **DO NOT PERFORM WELL with MIXED-INTEGER VARIABLES (discrete & continuous – MINLP PROBLEMS)**

Additional troubles with deterministic approaches:

"good" solvers are commercial

- Expensive
- Black-box-like (for non-expert)
- Work in equation mode (in practice external modules of user are very useful)

STOCHASTIC APPROACHES

1) PROVIDE HIGHER PROBABILITY of LOCATING GLOBAL OPTIMUM („GLOBAL” OPIMIZERS)

2) SIMPLE (can be coded by non-experts)

3) DISCONTINUITIES DO NOT CAUSE TROUBLES

4) CAN WORK in EQUATION and MODULAR MODE

BUT

- **LONG COMPUTATION (CPU) TIME**
- **HEURISTIC CONTROL PARAMETERS VALUES (that usually have to be adjusted by error-and-trial procedure)**
- **DIFFICULTIES with EQUALITY CONSTRAINTS**
- **One has to choose from variety of approaches (usually not tested sufficiently)**

- ADAPTIVE RANDOM SEARCH (ARS) - single-point based
- SIMULATED ANNEALING (SA) – single-point based
- GENETIC ALGORITHMS (GA)- population based

2. ARS METHOD

CONCEPT of ADAPTIVE RANDOM SEARCH:

CONCENTRATE GENERATION „AROUND”

CURRENTLY BEST SOLUTION BY SEARCH

REGION CONTRACTION AND / OR THE USE

OF SPECIAL FUNCTION WITH INCREASED

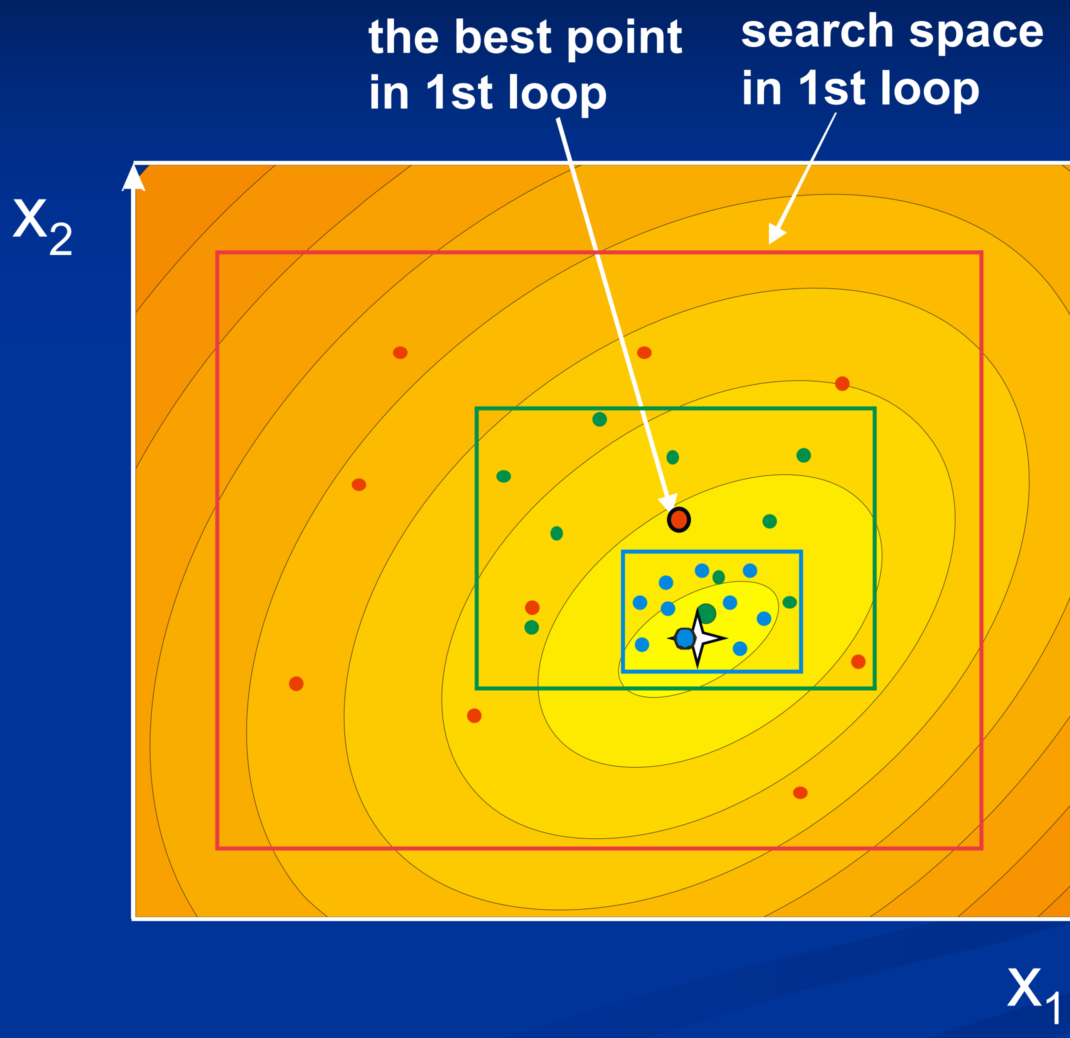
PROBABILITY DENSITY

LUUS - JAAKOLA (LJ) ALGORITHM

IT MAKES SEVERAL SEARCHES WITHIN CURRENT SEARCH REGION without space decrease or density change (EVEN IF THERE IS A „SUCCESS”) WHILE OTHER METHODS (GADDY, SALCEDO,...) INCREASE PROBABILITY DENSITY AND / OR CONTRACT REGION AFTER <u>EACH</u> SUCCESS

⇓

LJ ALGORITHM features resemblance to population-based methods ⇒ should gives higher chance of global optimum (and is very SIMPLE)


the best point
in 1st loop
search space
in 1st loop
x_2
x_1

OUR MAJOR MODIFICATIONS and EXTENSION

1) Adaptation of LJ for MINLP problems (consistent scheme of generating discrete variables)

2) Major changes in the scheme of decreasing the region search sizes:

   a) the decrease is variable dependent (i.e. Region search size decrease varies dependent on a variables),

   b) a rate of region search size decrease is similar to Gauss density distribution → to avoid local optima traps in initial phase.

Illustration of space decrease scheme in original approach

Ad 2b

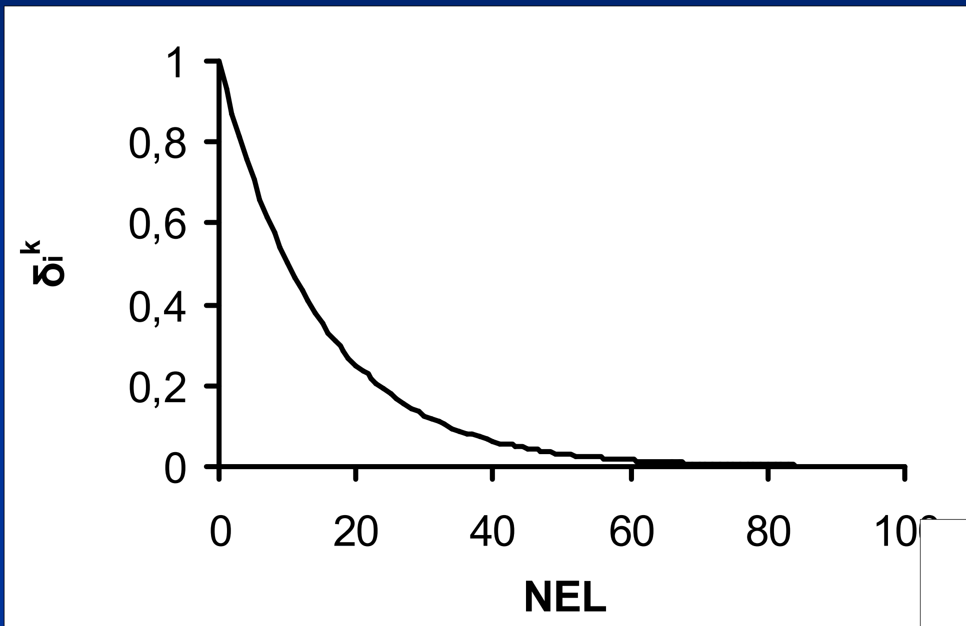
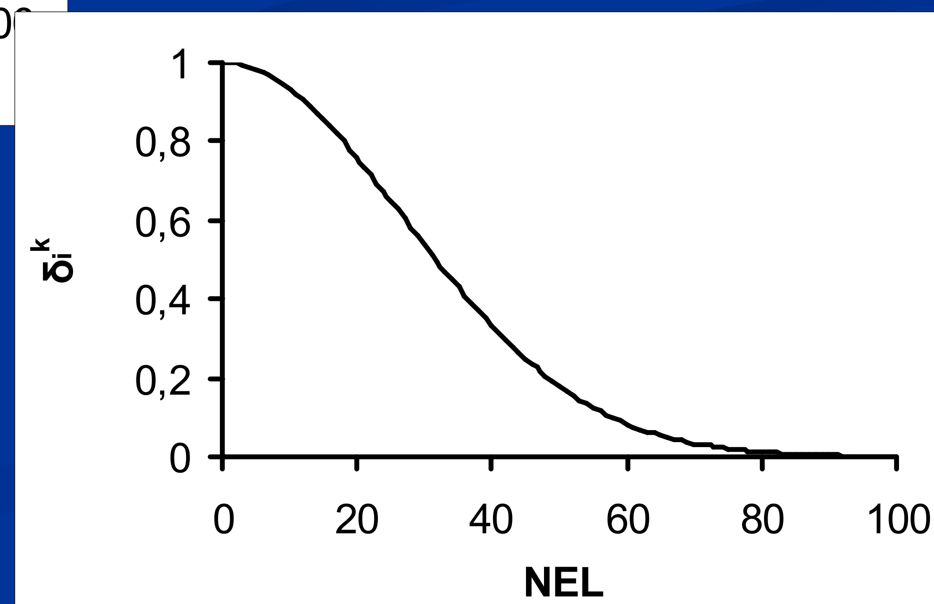


Illustration of space decrease scheme in modified approach



3. SIMULATED ANNEALING

FUNDAMENTAL CONCEPT:
SOLUTION IS ACCEPTED WITH PROBABILITY P

$$P = \begin{cases} 1 & \text{if } \Delta f < 0 \\ \exp(-\Delta f/T) & \text{if } \Delta f \geq 0 \end{cases}$$

where : $\Delta f = f_{i+1} - f_i$

T - temperature

THIS ALLOWS FOR JUMPING OFF OUT OF LOCAL OPTIMA !

GENERAL ALGORITHM

1. Fix T (initial value) and generate X^0
2. Generate X^s (neighboring point), calculate $f(X^s)$ and accept X^s according to P.
3. REPEAT step 2 for decreasing value of T until stopping criteria are met

Remark: X^0 has to be feasible

MODIFICATION of SA for CONTINUOUS (NLP) PROBLEMS

NELDER - MEAD OPTIMIZATION ALGORITHM (SIMPLEX) EMBEDDED INTO SA SCHEME /proposition of Press and Teukolsky ’91/

FUNDAMENTAL CONCEPT:

Each vertex of a simplex is „disturbed” by:

$$P1 = -T \times \ln(z)$$

z - random number from uniform distribution [0,1]

HOW IT WORKS ?

1) P1 is added to each vertex generated by N-M scheme
2) P1 is subtracted from „reflected” vertex of new simplex

⇓

RANDOM MOVEMENTS of SIMPLEX

OUR MODIFICATION

Random movements uphill (for minimization)

AIM:

to give additional randomization for <u>small</u> T values where SA/S performs similarly to Nelder-Mead (i.e. works as deterministic approach)

4. GENETIC ALGORITHMS (GA)

Remark: this is population based approach that is often considered more robust (but also more time consuming)

Specific features of our approach (GEN-COM)

- real coded numbers (not binary coded),
- The use of sub-population consisting with genetically transformed solutions. The solutions from the subpopulation and its parent population compete with each others to create the next parent population $\Rightarrow$ this is to eliminate premature problem, i.e. to escape from local optimum
- 9 mutation and crossover operators that can be used to both continuous and discrete variables
- 3 various mechanisms for dealing with inequality constraints

5. COMPUTER-SOLVER OPTI-STO

Characteristic features:

- coded in C++ with the use of DLL libraries
- can operate under Windows and Linux,
- can operate in equation and equation-modular mode.

Most important:

Has his own generic modeling system (similar to that in GAMS).

Main goal:

easy to use framework for solving equalities

Remark:

equalities are major problems for stochastic approaches, penalty terms, relaxation – are not good solutions

Most efficient is:

solve the equations directly

but

they should be linear ones

SOLUTION SCHEME:

User $\rightarrow$ select decision variables such that equalities become linear in regards to dependent variables

IMPORTANT:

balances involves bilinear terms:

$$X_1 \cdot Y_1 + X_2 \cdot Y_2 + \ldots = 0$$

Choose X1, X2,... decisions variables and.... balances are linear in regards to Y_1, Y_2,....

SOLUTIONS FRAMEWORK:

decision variables (data)

↓

solve equation set no. 1

↓

check set of inequalities

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decision variables (data)

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solve equation set no. 1

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check set of inequalities

SOLUTIONS FRAMEWORK:

decision variables (data)

↓

solve equation set no. 1

↓

check set of inequalities

↓

solve equation set no. 2

↓

⋮

6.1. Mathematical NLP and MINLP problems designed for tests of optimization problems

- about 20 NLP unconstrained functions (highly multimodal)
- more than 10 NLP constrained problems with inequality and/or equality constraints
- some MINLP problems of small scale in regards to no. of discrete variables

Aims of the tests:

1) To evaluate robustness and efficiency of various versions of solution algorithms

2) To find good values of control parameters

3) To get knowledge on properties of the algorithms: for what types of problems, limitations,...

6.2. Small processes engineering problems

- Reaction equilibrium composition
- Alkylation process optimization
- Optimization of reactor train
- Reactor selection from the superstructure
- Multi-product batch train optimization
- Optimal sequence for separating two-component mixture
- Cross-current extraction train with recycles

6.3. Applications for process system engineering problems:

- Optimization of HENs with fixed structure
- Optimization of chromatography
- Retrofitting optimal HENs
- Designing optimal water usage networks

7. CONCLUSIONS

Our experiments (and literature information) show, that stochastic approaches are easy to use, robust methods.

Remember, however, on

„no free lunch theorem”

there is no universal optimization method

One has to:

- **Choose proper approach and adjust parameters**
- **Formulate properly the problem for the chosen method**