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Global optimisation techniques in water resources management

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Parts of the presentation

- Water resources engineering and global optimization
- The nonlinear unconstrained optimization problem
- An overview of nonlinear optimization techniques
  - ✓ The downhill simplex method
  - ✓ Genetic algorithms
  - ✓ The shuffled complex evolution method
  - ✓ An evolutionary annealing-simplex algorithm
- Evaluation of global optimisation algorithms
  - ✓ Application in mathematical problems
  - ✓ Application in real-world problems
- Conclusive remarks

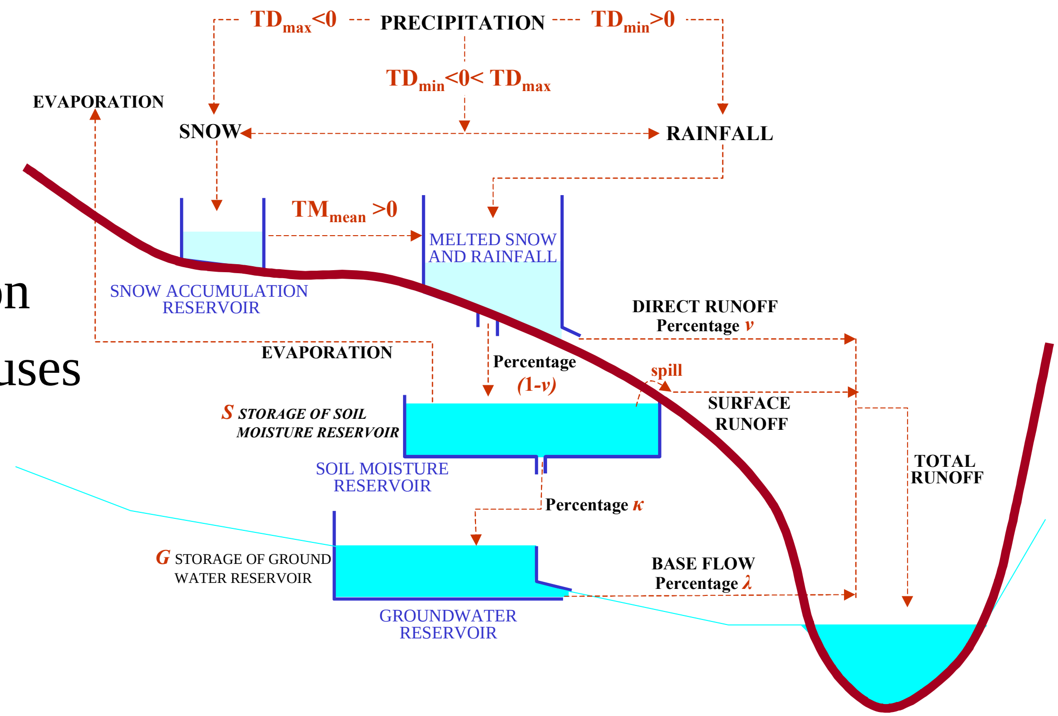
Global optimisation and water resources –
Example 1: Hydrological models calibration

Input data:

- Precipitation
- Temperature (average, minimum, maximum)
- Potential evapotranspiration
- Geomorphology and land uses

Output data:

- Soil and ground storage
- Real evapotranspiration
- Total runoff



Problem formulation:
Identify the values of model parameters by minimising the deviation between the computed output variables and the outputs measured in the physical system.

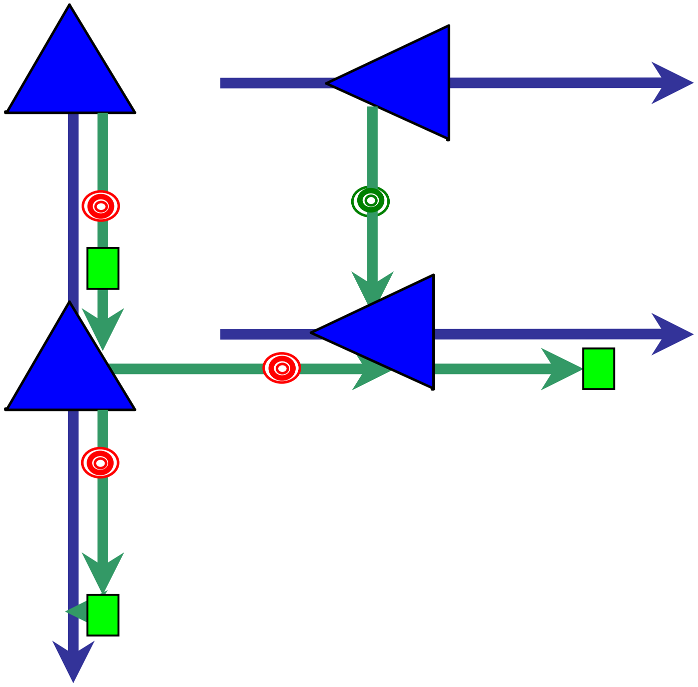
Global optimisation and water resources –
Example 2: Hydrosystems control and management

Hydrosystem components:

- Surface and groundwater resources.
- Water conveyance systems.
- Power generators (hydroelectric stations) or consummators (pumps).

Mathematical model inputs:

- Network topology.
- Physical constraints, due to project attributes (e.g., storage capacity).
- Inflow data (historic, synthetic).
- Targets, specified from the manager of the hydrosystem (e.g., water supply, flood control, environmental protection, power production).



Problem formulation:
Maximise the performance measure of the system (expressed in terms of yield, reliability or profit), which is evaluated via stochastic simulation.

Global optimisation and water resources –
Example 3: Parameters estimation of stochastic models

- In linear multivariate stochastic models of the form:

$$\mathbf{Y} = \mathbf{a}\,\mathbf{Z} + \mathbf{b}\,\mathbf{V}$$

the problem of estimating the elements of parameter matrix **b** arises.

- Matrix **b** is given from an equation of the form:

$$\mathbf{c} = \mathbf{b}\,\mathbf{b}^T$$

where **c** is a covariance matrix.

- If **c** is positive definite, the problem has infinite solutions; otherwise there are no feasible solutions (inconsistent **c**).
- The skewness of noise variables **V** depends on **b**, i.e. $\mu_3[\mathbf{V}] = \boldsymbol{\xi}(\mathbf{b})$. If some element of $\boldsymbol{\xi}$ is too high, $\mu_3[\mathbf{V}]$ cannot be preserved.

Problem formulation:
Determine **b** from the known $\mathbf{c} = \mathbf{b}\,\mathbf{b}^T$ so that the coefficients of skewness of noise variables **V** be as small as possible.

For more details about decomposition of covariance matrices see: Koutsoyiannis, 1999

The nonlinear unconstrained optimization problem

Find an optimiser $\mathbf{x}^*$ such that:

$$f(\mathbf{x}^*) = \min f(\mathbf{x}),\ \mathbf{a} < \mathbf{x} < \mathbf{b}$$

Main assumptions:

- The control variables are continuous and bounded.
- All constraints are handled either using penalty functions or via simulation.

Typical handicaps:

- Due to non-convexity, *f* may have many local optima.
- The partial derivatives of *f* may not be calculable and a numerical approximation of them is usually impractical.
- An analytical expression of *f* may not be available.
- The evaluation of *f* may be very expensive or time-consuming.

In real-world applications, a highly accurate solution is neither *possible* (due to uncertainties and errors in the underlying model or data) nor *feasible* (because of the unacceptably high computational effort).

An overview of nonlinear optimization techniques

Deterministic local optimisation methods:

- Gradient methods (e.g., steepest descend, conjugate gradient, quasi-Newton or variable metric methods).
- Direct search methods (e.g., downhill simplex, rotating directions).

Global optimization methods:

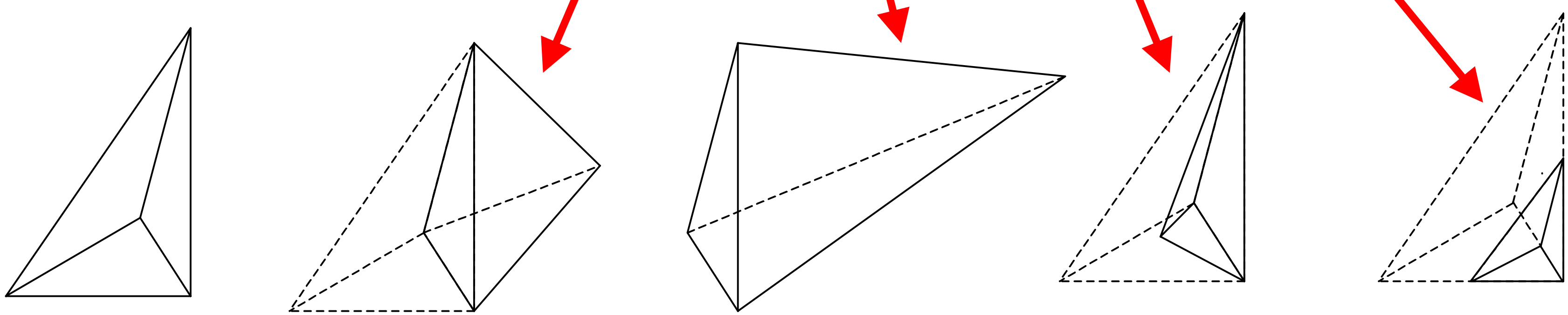
- Set covering techniques.
- Pure random search.
- Adaptive & controlled random search.
- Multiple local search.
- Evolutionary & genetic algorithms.
- Simulated annealing.
- Tabu search.
- Combined algorithms (e.g., shuffled complex evolution, simplex-annealing).

Global optimisation algorithms involve the evaluation of the function usually at a *random sample* of points in the feasible parameter space, followed by subsequent manipulations of the sample using a combination of *deterministic* and *probabilistic* rules. They guarantee *asymptotic convergence* to the global optimum.

The downhill simplex method
(Nelder and Mead, 1965)

Description of the algorithm:

- A set of $n + 1$ points (a *simplex*) is generated in the n-dimensional space.
- At each iteration, the simplex is *reflected* from the worst vertex.
- When it can do so, the simplex is *expanded* to take larger steps.
- When the simplex reaches a valley floor, it is *contracted* in the transverse direction and tries to ooze down the valley.
- If the simplex tries to pass through the eye of the needle, it *shrinks* in all directions, pulling itself around the best vertex.



Although the downhill simplex is not a global optimisation method, its principles are commonly applied in several global optimisation algorithms.

Genetic algorithms

Main concepts:

- Inspired from the process of natural selection of biological organisms.
- Representation of control variables on a chromosome-like (usually binary string) structure.
- Search through a population of points (individuals), not a single point.
- A fitness value is assigned to each solution, expressing its quality measure.
- Genetic operators are applied in order to create new generations.

Genetic operators:

- **Selection**: Chooses the fittest individual strings to be recombined in order to produce better offsprings; a probabilistic mechanism (i.e., a roulette wheel) is used, allocating greater survival to best individuals.
- **Crossover**: Recombines (exchanges) genes of randomly selected pairs of individuals with a certain probability.
- **Mutation**: Randomly changes genes in the chromosomes with a certain (small) probability, thus keeping the population diverse and preventing form premature convergence onto a local optimum.

The shuffled complex evolution method (Duan et al., 1992)

Main concepts:

- Combination of probabilistic and deterministic approaches.
- Systematic evolution of a complex of points spanning the parameter space.
- Competitive evolution.
- Complex shuffling.

Description of the algorithm:

- A random set of points (a "population") is sampled and partitioned into a number of *complexes*.
- Each of the complexes is allowed to evolve in the direction of global improvement, using *competitive evolution* techniques that are based on the downhill simplex method.
- At periodic stages in the evolution, the entire set of points is *shuffled* and reassigned to new complexes to enable information sharing.

Simulated annealing

Principles of the annealing process in thermodynamics:

- For *slowly cooled* thermodynamical systems (e.g., metals) nature is able to find the minimum energy state, while the system may end in an amorphous state having a higher energy if it is cooled quickly.
- Nature's minimisation strategy is to allow the system sometimes to go *uphill* as well as downhill, so that it has a chance to escape from a local energy minimum in favor of finding a better, more global minimum.
- For a system at a given temperature T, its energy is probabilistically distributed among all energy states E according to the Bolzmann function:

$$\text{Prob}(E) \sim \exp\left(- E / k\, T\right)$$

- The lower the temperature, the less likely is any significant uphill step.

Necessary components of a simulated annealing algorithm:

- A generator of random changes in the configuration of the system.
- An objective function (analogue of energy) to be minimised.
- A control parameter T (analogue of temperature) and an annealing cooling schedule, which describes the gradual reduction of T.

An evolutionary annealing-simplex algorithm

Main concepts:

- Combination of the robustness of simulated annealing in rugged problems with the efficiency of local optimisation methods in simple search spaces.
- Generalisation of the simplex method to be competitive and stochastic.
- Introduction of follow-up strategies to escape from local optima.

Description of the algorithm:

- An initial population P is randomly generated into the feasible space.
- At each iteration a simplex is formulated, by choosing $n + 1$ points from P.
- The simplex is reflected from a randomised “worst” vertex $\mathbf{x}_w$.
- If the reflection point $\mathbf{x}_r$ is either not accepted or $f(\mathbf{x}_r) < f(\mathbf{x}_w)$, the simplex is moved downhill according to the Nelder-Mead criteria performing randomised expansion, contraction or shrinkage steps.
- If $\mathbf{x}_r$ is accepted albeit being worse than $\mathbf{x}_w$, trial expansion steps are taken along the uphill direction in order to “climb” the hill and explore the neighboring area. If any trial step success, a random point is generated far from the population and replaces $\mathbf{x}_r$ according to a mutation probability.

Evaluation and comparison of optimisation methods

General methodology:

- Multiple runs of each problem, starting from stochastically independent initial conditions (e.g., different initial population).
- Evaluation of the *effectiveness* (i.e., probability of locating the global optimum) and *efficiency* (i.e., convergence speed) of each algorithm.

Differences between real-world and mathematical applications:

- The properties of the response surface as well as the citation of the global optimum are not known a priori.
- Due to the computational effort for each function evaluation, it is likely to stop the optimisation procedure before convergence criteria are satisfied.

Algorithms examined:

- Downhill simplex (source code adapted from Press et al., 1992).
- Simple genetic algorithm (source code adapted from Goldberg, 1989).
- Shuffled complex evolution (source code adapted from Duan et al., 1994).
- Evolutionary annealing-simplex (original code).

Mathematical applications

Function name	*n*	Number of optima	Downhill simplex	Genetic algorithm	SCE-UA	Annealing-simplex
Sphere	10	1	93 (212)	100 (45463)	100 (5159)	100 (4128)
Hozaki	2	2	4 (18205)	81 (26731)	100 (296)	100 (324)
Goldestein-Price	2	4	49 (5028)	96 (26731)	99 (449)	100 (552)
Rozenbrock	2	1	85 (6560)	65 (27374)	100 (1191)	100 (619)
Rozenbrock	10	1	0 (372)	0 (45463)	99 (11105)	26 (10847)
Griewank	10	> 1000	73 (603)	89 (52853)	100 (5574)	91 (2768)
Michalewicz	2	unknown	2 (27518)	31 (27048)	44 (438)	51 (1409)
Integer step	10	1	0 (48011)	4 (45463)	1 (2350)	100 (3324)
Average			**38.3**	**58.3**	**80.0**	**83.5**

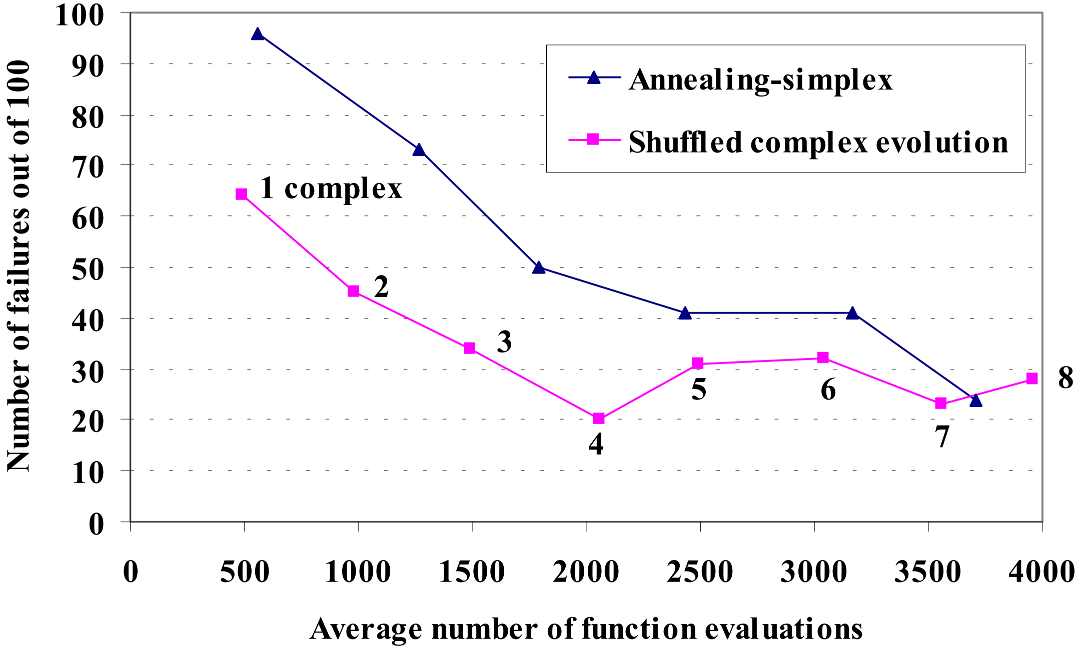
Effectiveness index (number of successes out of 100 stochastically independent trials)

Efficiency index (average number of function evaluations required)

Real-world applications (1)

Calibration of a simple water balance model

- Model parameters (6 in total):
  - ✓ percentage of imperviousness surface
  - ✓ storage capacity of soil moisture reservoir
  - ✓ recession coefficient of soil moisture and ground water
  - ✓ initial values of soil and ground storage
- Calibration period: October 1980 – June 1988

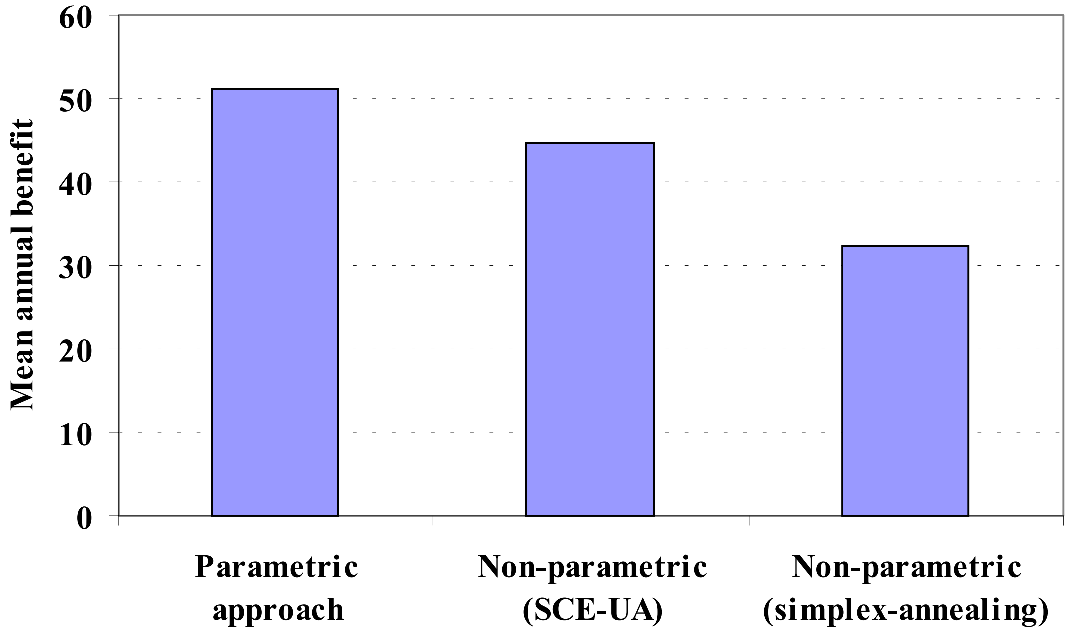


Even for the simple hydrologic model with only 6 parameters, a large number of function evaluations is required in order to achieve a relatively acceptable failure rate.

Real-world applications (2)

Maximisation of benefit from energy production

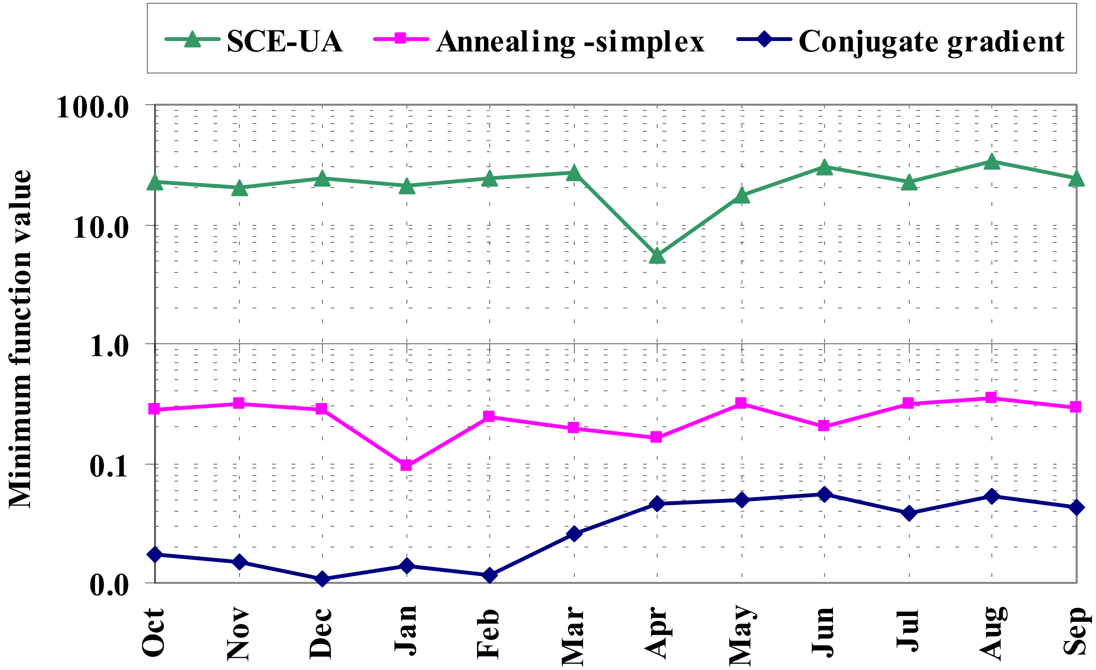
- The system consists of two hypothetical parallel hydroelectric reservoirs.
- A 16-year (192 months) synthetic inflow data is used.
- Reservoir target releases are assumed as control variables of the model; thus the total number of parameters is $2 \times 192 = 384$.
- Results are compared to those of a low-dimensional methodology, where parametric operation rules are used (Nalbantis and Koutsoyiannis, 1997).



Real-world applications (3)

Decomposition of covariance matrices of a PAR(1) model

- The objective function consists of 3 components, for the preservation (or approximation) of covariances, variances and skewness, respectively.
- The derivative of the function has an analytical expression, thus enabling the usage of a fast and accurate gradient-based optimisation method.
- Model parameters are $8^2 = 64$ (monthly rainfall and runoff in 4 locations).



Unable to preserve any of historical sample statistics.

Satisfactory approximation of historical statistics.

Almost exact preservation of historical statistics.

Concluding remarks

- The current trend in global optimisation research is the *combination* of strategies obtained from diverse methodological approaches (including classical mathematics), in order to develop more robust search schemes.
- After comparing three representative algorithms, the main conclusions are:
  - ✓ In most cases, the the simple, binary-coded genetic algorithm is neither effective nor efficient enough.
  - ✓ The shuffled complex evolution method is obviously robust and efficient and should be preferred, especially when the fast location of a good solution is desired.
  - ✓ The evolutionary annealing-simplex scheme, although not very fast, seems to be the most appropriate for hard optimisation problems with pathogenic characteristics (e.g., many local optima).
- The performance of all methods depends, less or more, on the algorithmic input arguments (e.g., population size), usually calibrated experimentally.
- In spite of the development of robust and fast optimisation techniques, the *parsimony of parameters* still remains a significant requirement of the mathematical models building.

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