

Scalability of Population-based Stochastic Metaheuristics

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Workshop on "Stochastic Geometry and Big Data" - 24.11.2015

Outline

Motivation

Population-based stochastic metaheuristics

Exploration vs Exploitation. Case Study: Differential Evolution

Cooperative Coevolution

Black box optimization

Example:

- ▶ given a parameterized module for image registration encapsulated in a proprietary software
- ▶ find the parameters values which:
 - ▶ ensure that the registration error is smaller than a given threshold
 - ▶ the running time is as small as possible

Black box optimization

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Characteristics of the black box problems

- ▶ only partial/uncertain apriori knowledge on the influence of parameters on accuracy
- ▶ only objective function values are known, no gradient information

Large scale optimization

Example 1: non-rigid multi-modal image registration¹

- ▶ find the the parameters of a free form deformation model
- ▶ which minimize a similarity measure (e.g. mutual information)
- ▶ **Remarks:**
 - ▶ problem size: for a $8 \times 8 \times 8$ mesh there are 1536 parameters; used optimizer
 - ▶ optimizer: cat swarm optimization

¹Yang et al., Non-rigid Multi-modal Medical Image. Registration by Combining L-BFGS-B with Cat Swarm Optimization, Information Sciences 2015

²Zhang et al., PSO-EM: A Hyperspectral Unmixing Algorithm Based On Normal Compositional Model, TGRS 2014

Large scale optimization

Example 1: non-rigid multi-modal image registration¹

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 - ▶ optimizer: cat swarm optimization

Example 2: (hyper)spectral unmixing²

- ▶ find the abundancy values which maximizes the log-likelihood function from the E-step in an EM framework
- ▶ problem size: number of pixels \times number of endmembers (750 for a 50×50 subimage and 3 endmembers)
- ▶ optimizer: particle swarm optimization

¹Yang et al., Non-rigid Multi-modal Medical Image. Registration by Combining L-BFGS-B with Cat Swarm Optimization, Information Sciences 2015

²Zhang et al., PSO-EM: A Hyperspectral Unmixing Algorithm Based On Normal Compositional Model, TGRS 2014

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Motivation

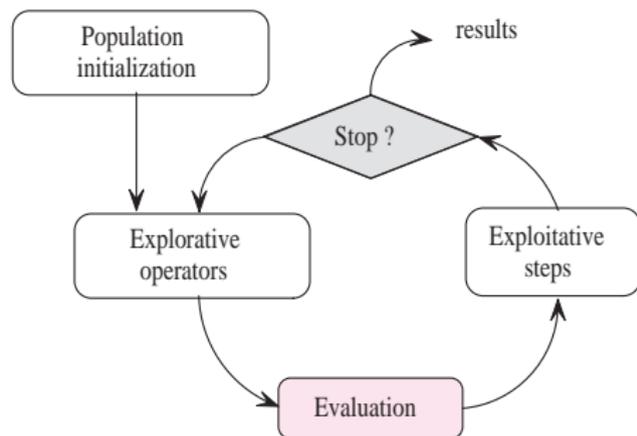
Population-based stochastic metaheuristics

Exploration vs Exploitation. Case Study: Differential Evolution

Cooperative Coevolution

Population-based search

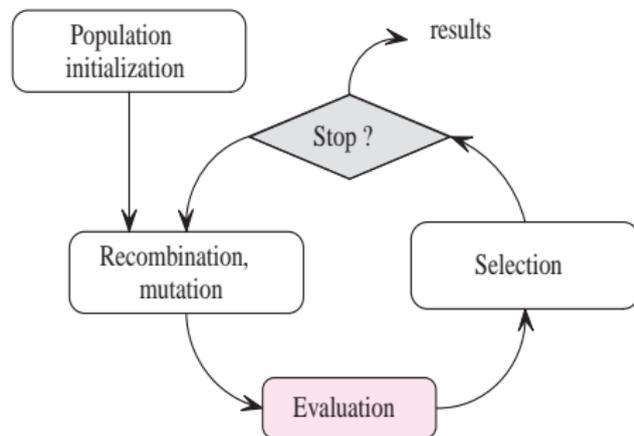
- ▶ an iterative optimization method which uses a population of candidates to search the solutions space
- ▶ it is based on two main mechanisms:
 - ▶ search space **exploration**
 - ▶ **exploitation** of the knowledge collected during the previous search steps



Population Based Iterative Search

Main Components

- ▶ **Mutation**: random perturbation of elements
 - ▶ distribution independent of the current population
 - ▶ **distribution influenced by the current population**
- ▶ **Recombination**: mixing information from several elements
 - ▶ **discrete**
 - ▶ **arithmetical**
- ▶ **Selection**: choice of promising elements
 - ▶ **proportional**
 - ▶ **tournament**



An Evolutionary Algorithm

Outline

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Population-based stochastic metaheuristics

Exploration vs Exploitation. Case Study: Differential Evolution

Cooperative Coevolution

Differential Evolution

... is a simple but rather powerful metaheuristic

- ▶ developed in 1995 by Rainer Storn and Kenneth Price as a continuous optimization method
 - ▶ starting problem: Chebyshev polynomials fitting (33 variables)
 - ▶ initial variant: genetic annealing algorithm developed by Kenneth Price (1994)
- ▶ **main idea**: use a mutation/recombination operator based on **difference(s)** between pairs of elements
- ▶ similarities with older direct search methods:
 - ▶ pattern search (Hooke-Jeeves, 1961)
 - ▶ simplex methods (Nelder-Mead, 1965)
- ▶ other population based methods involving differences:
 - ▶ Particle Swarm Optimization (Kennedy & Eberhart, 1995)

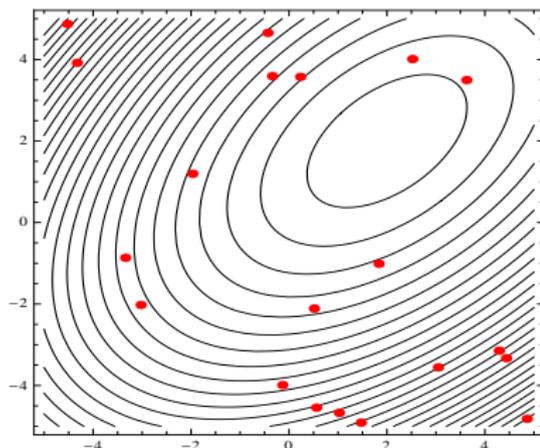
Standard Differential Evolution

Problem to be solved: minimize $f : [a_1, b_1] \times \dots \times [a_n, b_n] \rightarrow \mathbb{R}$

DE in a phrase:

A population of m elements is randomly initialized in $[a_1, b_1] \times \dots \times [a_n, b_n]$ and then iteratively transformed by applying **difference based recombination** and **greedy-like selection**

Initialization: $x_i = U(a_i, b_i)$, $i = \overline{1, m}$



m population size 10/58

Standard Differential Evolution

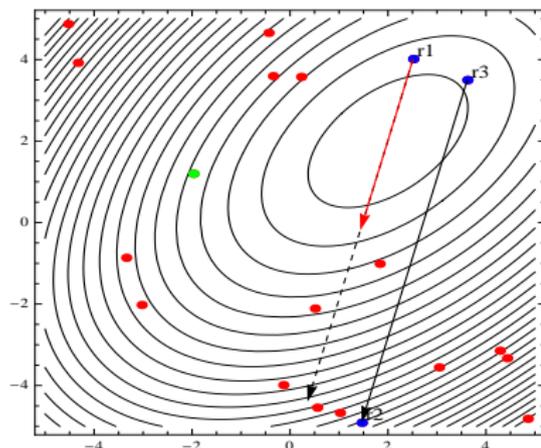
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Initialization: $x_i = U(a_i, b_i)$, $i = \overline{1, m}$

while (NOT termination) do

- **Mutation** - for each element x_i (target or current element) a mutant is constructed:

$$y_i = \underbrace{x_{r_1}}_{\text{base element}} + \underbrace{F \cdot (x_{r_2} - x_{r_3})}_{\text{scaled difference}}$$



m - population size

$F \in (0, 2)$ - scale factor

Standard Differential Evolution

Problem to be solved: minimize $f : [a_1, b_1] \times \dots \times [a_n, b_n] \rightarrow \mathbb{R}$

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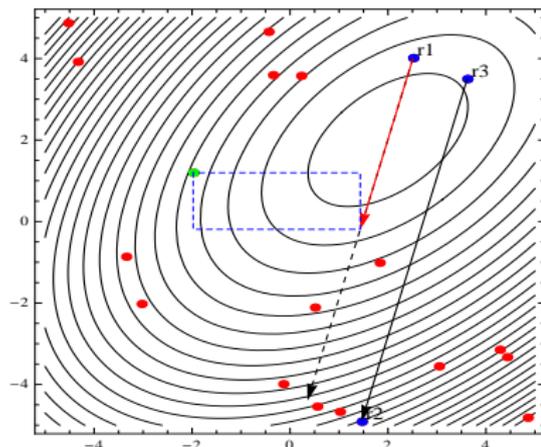
▶ Mutation:

$$y_i = x_{r_1} + F \cdot (x_{r_2} - x_{r_3}), \quad i = \overline{1, m}$$

▶ Crossover:

$$z_i^j = \begin{cases} y_i^j & \text{if } \text{rand}(0, 1) < CR \text{ or } j = j_0 \\ x_i^j & \text{otherwise} \end{cases},$$

$$i = \overline{1, m}, j = \overline{1, n}$$



m - population size

$F \in (0, 2)$ - scale factor

$CR \in [0, 1]$ - crossover rate

j_0 - randomly selected component

Standard Differential Evolution

Problem to be solved: minimize $f : [a_1, b_1] \times \dots \times [a_n, b_n] \rightarrow \mathbb{R}$

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▶ Mutation:

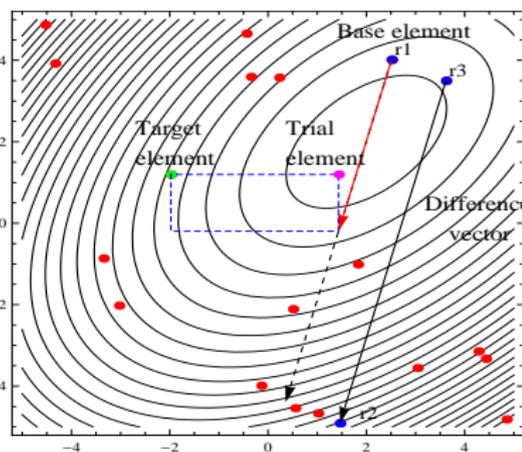
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▶ Selection:

$$x_i(g+1) = \begin{cases} z_i & \text{if } f(z_i) \leq f(x_i(g)) \\ x_i^j & \text{if } f(z_i) > f(x_i(g)) \end{cases}$$



m - population size

$F \in (0, 2)$ - scale factor

$CR \in [0, 1]$ - crossover rate

j_0 - randomly selected component

Differential Evolution Variants

DE taxonomy: DE/ base element/ no. of differences/ crossover type

- ▶ Base element:
 - ▶ random(x_{r_1}): DE/rand/**/*
 - ▶ best (x_*): DE/best/**/*
 - ▶ combination of current and best elements ($\lambda x_* + (1 - \lambda)x_i$): DE/current-to-best/**/*
 - ▶ combination of random and best elements ($\lambda x_* + (1 - \lambda)x_{r_1}$): DE/rand-to-best/**/*
 - ▶ combination of current and random elements ($\lambda x_i + (1 - \lambda)x_{r_1}$): DE/current-to-rand/**/*
- ▶ Number of differences: usually 1 (DE/**/1/**) or 2 (DE/**/2/**)
- ▶ Crossover type: binomial: DE/***/bin, exponential: DE/***/exp)

At least 20 DE variants ...

Mutation variants

- ▶ DE/rand/L/*

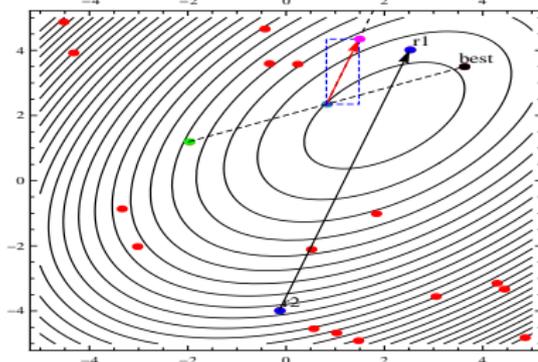
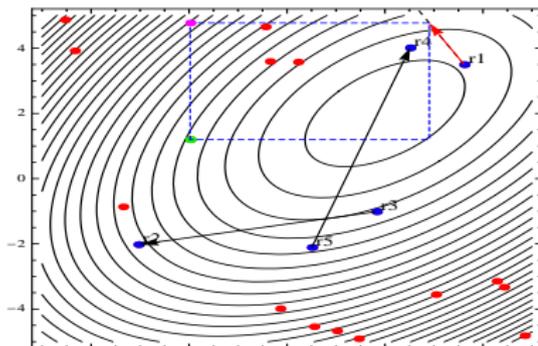
$$y_i = x_{r_1} + \sum_{l=1}^L F_l \cdot (x_{r_1(l)} - x_{r_2(l)})$$

- ▶ Typical variant: $L = 2$
- ▶ Allows to define new mutant directions \Rightarrow stimulates exploration

- ▶ DE/current-to-best/1

$$y_i = (1 - \lambda)x_i + \lambda x_* + F \cdot (x_{r_1} - x_{r_2})$$

- ▶ Introduces a bias toward the currently best element \Rightarrow stimulates exploitation



Crossover variants

- ▶ Binomial (DE/***/bin)

$$z_i^j = \begin{cases} y_i^j & \text{if } \text{rand}(0, 1) < CR \text{ or } j = j_0 \\ x_i^j & \text{otherwise} \end{cases}, \quad i = \overline{1, m}, j = \overline{1, n}$$

- ▶ Exponential (DE/***/exp)

$$z_i^j = \begin{cases} y_i^j & \text{for } j \in \{j_0, \langle j_0 + 1 \rangle_n, \dots, \langle j_0 + K - 1 \rangle_n\} \\ x_i^j & \text{otherwise} \end{cases}, \quad i = \overline{1, m}, j = \overline{1, n}$$

$CR \in [0, 1]$ - crossover rate, $j_0 \sim U(\{1, \dots, m\})$, $K \sim \text{Geom}(CR)$

Other variants

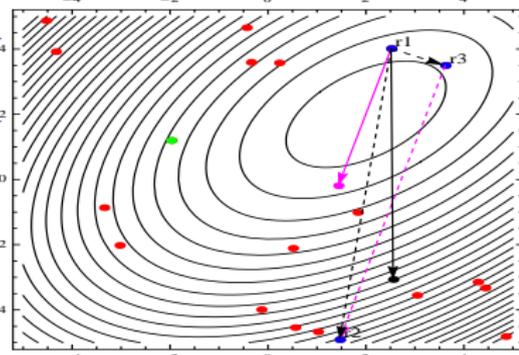
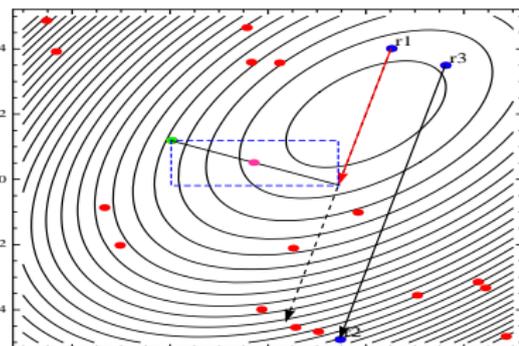
- ▶ Arithmetical (DE/***/arithmetical)

$$z_i = (1-q)x_i + qy_i, \quad i = \overline{1, m}, \quad q \in [0, 1]$$

- ▶ Either mutation or recombination (DE/either-or)

$$z_i = \begin{cases} x_{r_1} + F \cdot (x_{r_2} - x_{r_3}) & \text{if } \text{rand}(0, 1) \leq p_F \\ x_{r_1} + K \cdot (x_{r_2} - x_{r_1}) & \text{if } \text{rand}(0, 1) > p_F \end{cases}$$

- ▶ **Remark:** DE/either-or was created to compensate the lack of rotational invariance of DE involving binomial crossover



Which variant to choose ?

Recommendations

- ▶ no specific knowledge on the problem: use DE/rand/1/*
- ▶ need for an exploitative method: use DE/best/1/*
- ▶ need for a more explorative method: use DE/rand/2/*
- ▶ need for a rotationally invariant method: use DE/either-or

Remark: different variants could be appropriate in different stages of the optimization process \implies need for adaptation

(Self)adaptive variants

Self adaptation

- ▶ use a pool of variants and assign to each element one of these variants
- ▶ record the success/failure information of the variant attached to each element
- ▶ decide which variant to select based on the success/failure information (a probability distribution is usually constructed)
- ▶ self-adaptation of mutation/crossover is usually combined with self-adaptation of parameters
- ▶ Examples: SaDE ³, Competitive DE ⁴, EPSDE ⁵ etc.

³Qin et al., Differential Evolution Algorithm With Strategy Adaptation for Global Numerical Optimization, IEEE TEVC, 2009

⁴Tvrđik, Competitive Differential Evolution, Mendel 2006

⁵[Mallipeddi et al., Differential evolution algorithm with ensemble of parameters and mutation strategies, ASOC 2011]

Searching for Exploration - Exploitation Balance

Usage of differences \Rightarrow implicit adaptation of the amount of change in the population

- ▶ First stage of evolution: large differences \Rightarrow exploration
- ▶ Second stage of evolution: small differences \Rightarrow exploitation
- ▶ There is no clear separation between these stages

Searching for Exploration - Exploitation Balance

Usage of differences \Rightarrow implicit adaptation of the amount of change in the population

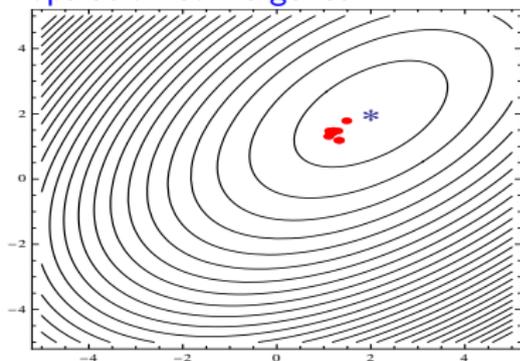
- ▶ First stage of evolution: large differences \Rightarrow exploration
- ▶ Second stage of evolution: small differences \Rightarrow exploitation
- ▶ There is no clear separation between these stages

Main difficulty: find the balance between exploration and exploitation:

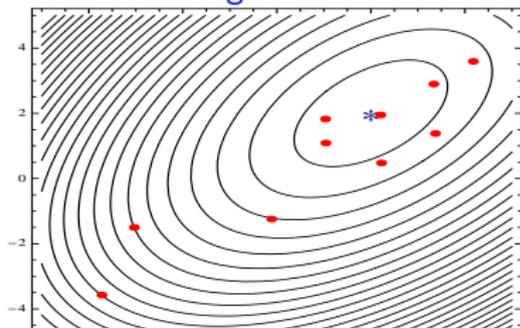
- ▶ less exploration, too much exploitation \Rightarrow premature convergence
- ▶ too much exploration \Rightarrow slow convergence

Searching for Exploration - Exploitation Balance

Population convergence:

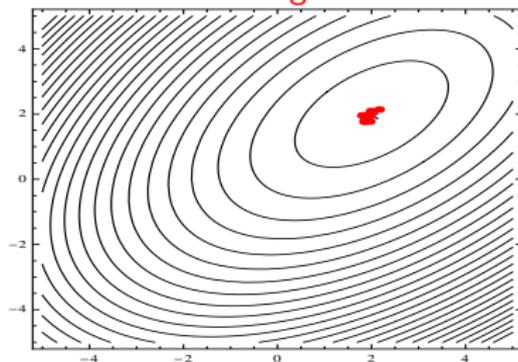


Method convergence:



Ideal situation:

population convergence
is synchronized with
method convergence



Still unclear how to ensure this synchronization ...

Analysis of the DE behavior

Many empirical parameter studies led to statements as:

- ▶ for the same crossover rate (CR), the number of components taken from the mutant is highly depending on the crossover type (binomial vs. exponential) ... **why ?**
- ▶ the control parameters (m , F , CR) influence in an interrelated manner the population diversity ... **how ?**
- ▶ high values of the scale factor, F , are needed to avoid premature convergence ... **does there exist a lower bound ?**

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It would be desirable to have theoretical results which explain such empirical remarks ...

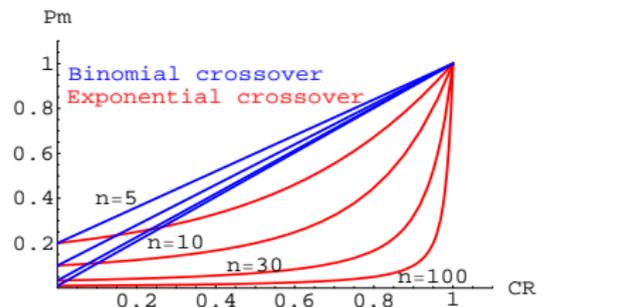
Binomial vs. Exponential Crossover⁶

Binomial crossover:

- ▶ the probability to take a component from the mutant vector is:

$$p_m = CR \left(1 - \frac{1}{n} \right) + \frac{1}{n}$$

- ▶ the number of mutated components: **binomial** distribution



⁶D. Zaharie, Influence of crossover on the behavior of Differential Evolution Algorithms, ASOC 2009

Exponential crossover:

- ▶ the probability to take a component from the mutant vector is:

$$p_m = \frac{1 - CR^n}{n(1 - CR)}$$

- ▶ the number of mutated components: **truncated geometric** distribution

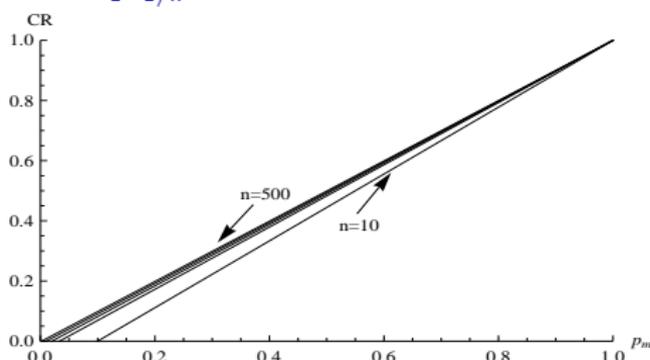
Remark: In the case of exponential crossover larger values of CR should be used in order to have the same number of mutated components as for binomial crossover .

Choice of crossover rate

- ▶ the DE behavior is influenced by the mutation probability, p_m , but the user provide a value for CR
- ▶ what value should have CR in order to ensure a given value for p_m ?

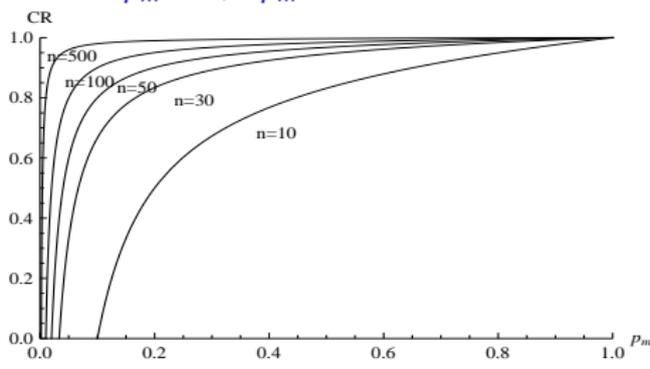
Binomial crossover

$$CR = \frac{p_m - 1/n}{1 - 1/n}$$



Exponential crossover

$$CR^n - np_m CR + np_m - 1 = 0$$

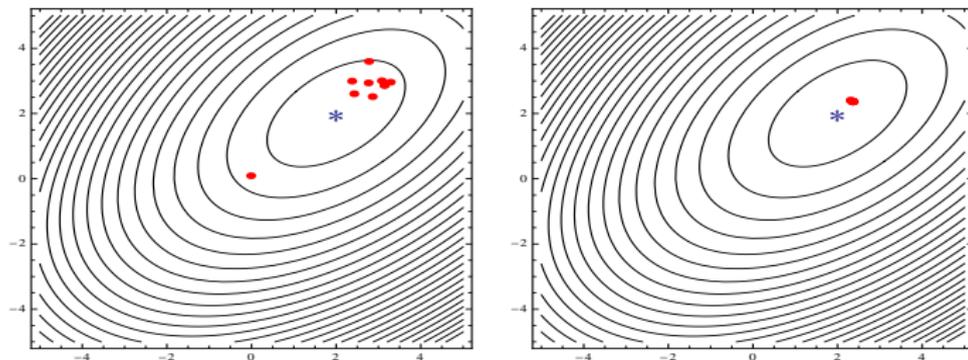


Practical remark: Exponential crossover is more sensitive to the problem size

Population diversity

Importance

- ▶ small diversity in the DE population \Rightarrow small values of the differences \Rightarrow limited progress \Rightarrow premature convergence (all population concentrated in a point which is NOT the optimum)



Question: What is the impact of mutation and crossover on the population diversity ?

Population diversity

Theoretical results ⁷

- ▶ **Diversity measure:** population variance (component level)

$$\text{Var}(X) = \sum_{i=1}^m (x_i - \bar{x}_i)^2 / m$$

- ▶ Notations: $\text{Var}(X)$ = variance of current population;
 $\mathbb{E}(\text{Var}(Z))$ = expected variance of the trial population
- ▶ DE/rand/L/*

$$\mathbb{E}(\text{Var}(Z)) = \left(1 + 2p_m \sum_{l=1}^L F_l^2 - \frac{p_m(2 - p_m)}{m} \right) \text{Var}(X)$$

⁷D. Zaharie, Critical values for the control parameters of differential evolution algorithms, Mendel 2002

Population diversity

Theoretical results⁸

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- ▶ DE/random-to-best/1/*

$$\begin{aligned} \mathbb{E}(\text{Var}(Z)) &= \left(1 + 2p_m F^2 - \frac{p_m(2-p_m)}{m} - \lambda p_m^2 \frac{m-1}{m} \right) \text{Var}(X) \\ &\quad + \lambda^2 \frac{p_m(1-p_m)}{m} \sum_{i=1}^m (x_* - x_i)^2 \end{aligned}$$

⁸D. Zaharie, Statistical Properties of Differential Evolution and Related Random Search Algorithms, CompStat 2008

Population diversity

Theoretical results

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 $\mathbb{E}(\text{Var}(Z))$ =expected variance of the trial population
- ▶ $\text{DE/current-to-rand}/1$ (arithmetical recombination)

$$\mathbb{E}(\text{Var}(Z)) = \left(1 + 2F^2 - 2q + \frac{2m-1}{m} q^2 \right) \text{Var}(X)$$

Population diversity

Theoretical results⁹

- ▶ **Diversity measure:** population variance (component level)
- ▶ Notations: $\text{Var}(X)$ =variance of current population; $\mathbb{E}(\text{Var}(Z))$ =expected variance of the trial population
- ▶ DE/either-or

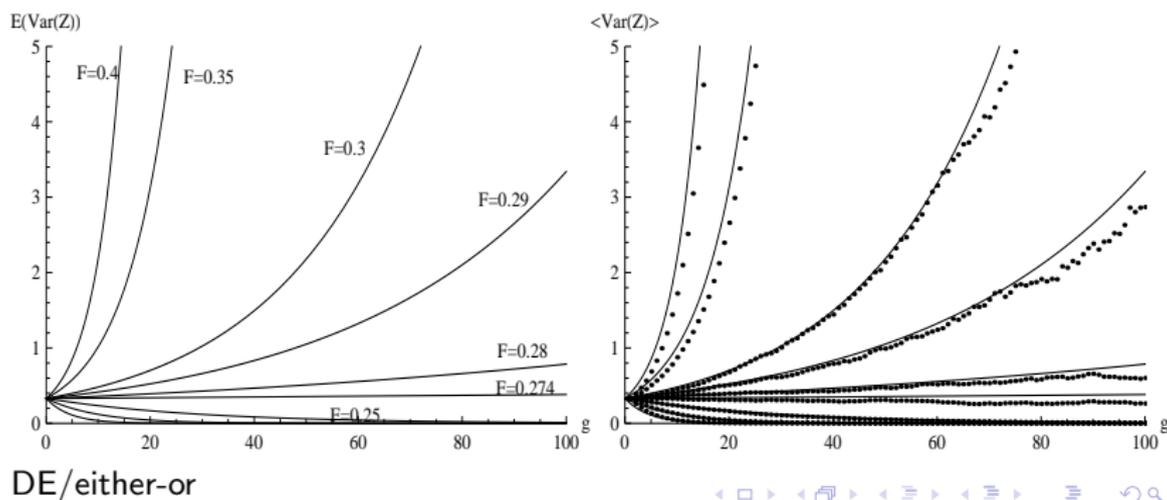
$$\begin{aligned} \mathbb{E}(\text{Var}(Z)) = & \left(p_F^2 \left(1 + 2F^2 - \frac{1}{m} \right) + 2p_F(1 - p_F) \left(\frac{m-1}{m} + F^2 + 3K^2 - 2K \right) \right. \\ & \left. + (1 - p_F)^2 \left(\frac{m-1}{m} + 2 \frac{m-2}{m} (3K^2 - 2K) \right) \right) \text{Var}(X) \end{aligned}$$

⁹D. Zaharie, Differential Evolution. From Theoretical Analysis to Practical Insights, Mendel 2012

Population diversity

Theoretical vs empirical evolution

- ▶ Evolution of population variance after mutation and crossover (no selection)
- ▶ **Practical remark:** the population variance can decrease even in the absence of selection pressure



Population diversity

From theory to practical insights

$$\mathbb{E}(\text{Var}(Z)) = c(F, CR, p_F, q, m, n)\text{Var}(X)$$

Population diversity

From theory to practical insights

$$\mathbb{E}(\text{Var}(Z)) = c(F, CR, p_F, q, m, n)\text{Var}(X)$$

- ▶ if $c(F, CR, p_F, q, m, n) < 1$ the algorithm will probably prematurely converge

Population diversity

From theory to practical insights

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- ▶ if $c(F, CR, p_F, q, m, n) < 1$ the algorithm will probably prematurely converge
- ▶ one can control the impact which mutation and crossover have on the population variance by changing the values of the parameters involved in the factor c

Population diversity

From theory to practical insights

$$\mathbb{E}(\text{Var}(Z)) = c(F, CR, p_F, q, m, n)\text{Var}(X)$$

- ▶ if $c(F, CR, p_F, q, m, n) < 1$ the algorithm will probably prematurely converge
- ▶ one can control the impact which mutation and crossover have on the population variance by changing the values of the parameters involved in the factor c
- ▶ this is a particularity of DE, as in EAs using mutation based on additive perturbation involving an arbitrary distribution:

$$\mathbb{E}(\text{Var}(Z)) = a\text{Var}(X) + b$$

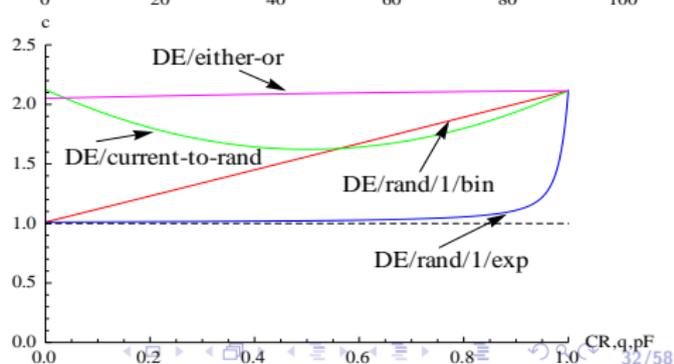
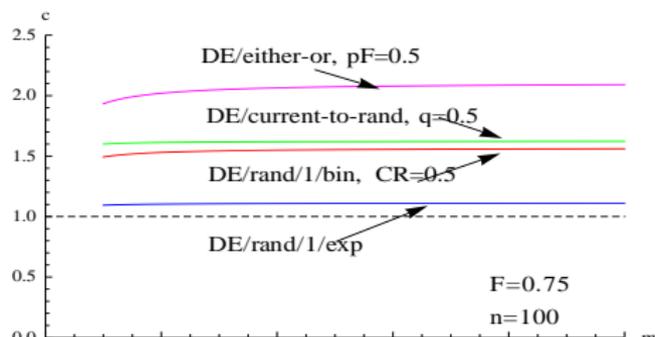
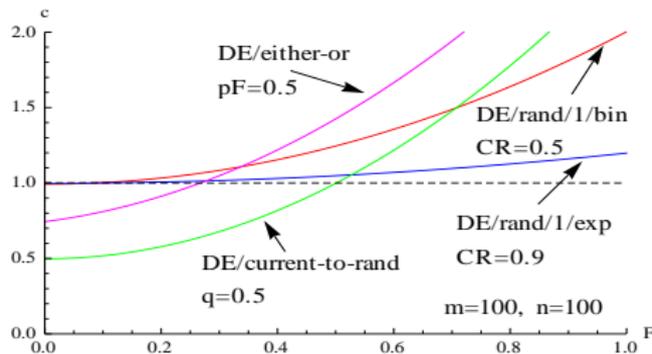
with b not necessarily zero

Population diversity

From theory to practical insights

$$\mathbb{E}(\text{Var}(Z)) = c(F, CR, p_F, q, m, n)\text{Var}(X)$$

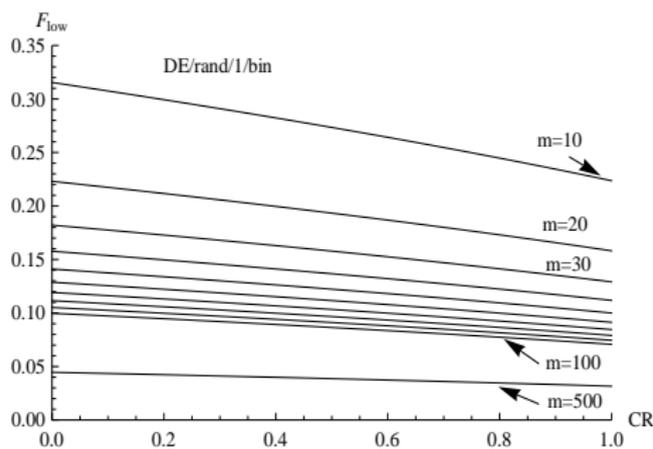
- the value of $c(F, CR, p_F, q, m, n)$ is highly influenced by the type of mutation and crossover



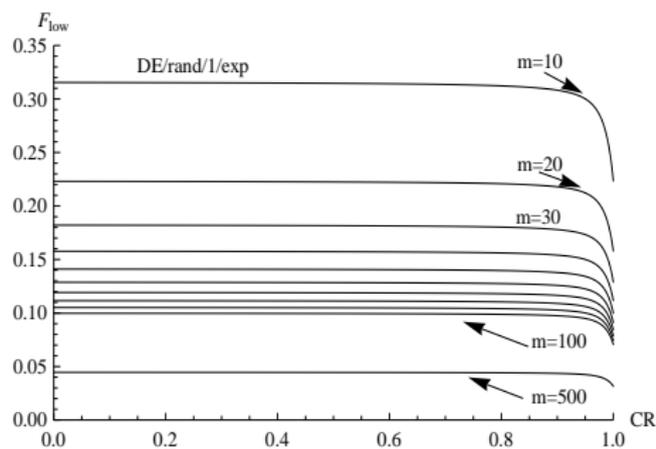
Population diversity

Avoiding premature convergence

- ▶ choose the DE control parameters (F , CR , m etc) such that the population diversity does not decrease too fast ($c(CR, F, q, m, n) > 1$)
- ▶ by solving $c(F, CR, p_F, q, m, n) = 1$ we can find a lower bound for F under which the population variance decreases even in the absence of selection



DE/rand/1/bin

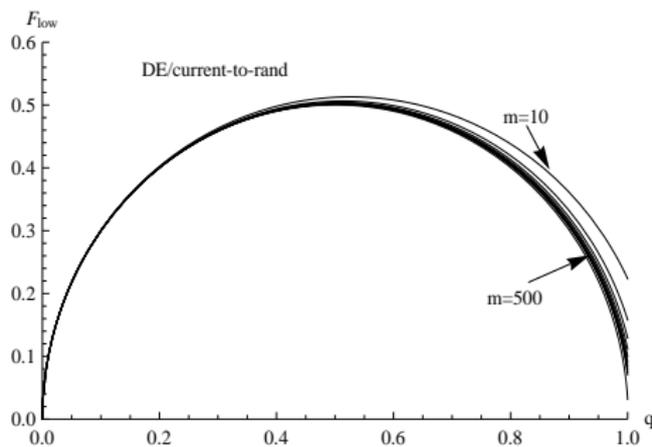


DE/rand/1/exp

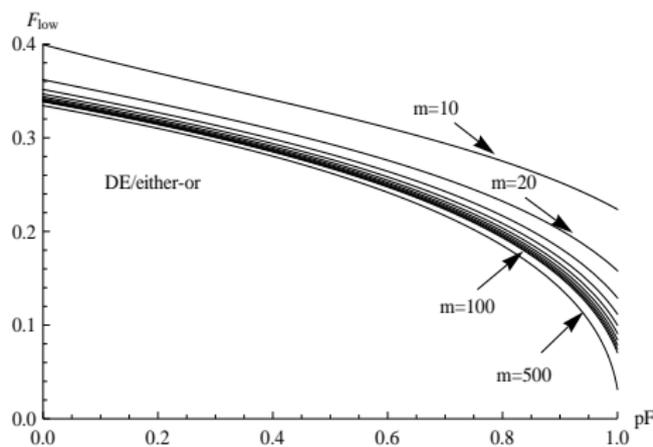
Population diversity

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DE/current-to-rand



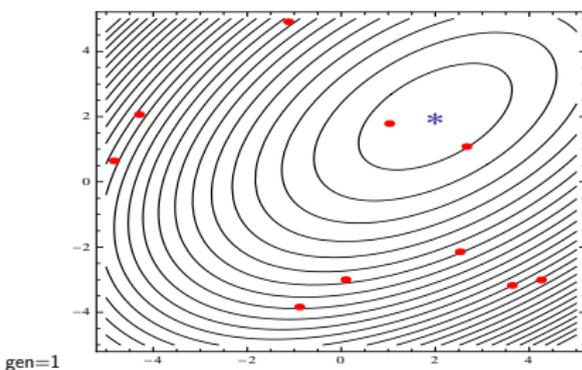
DE/either-or

Population diversity

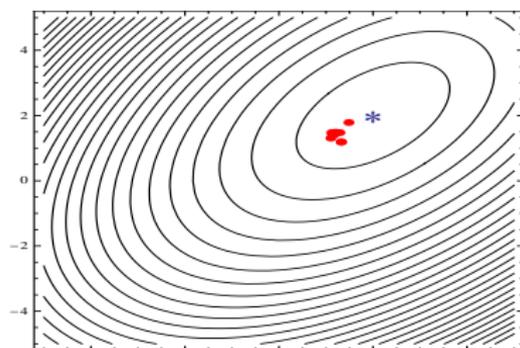
Avoiding premature convergence

Example:

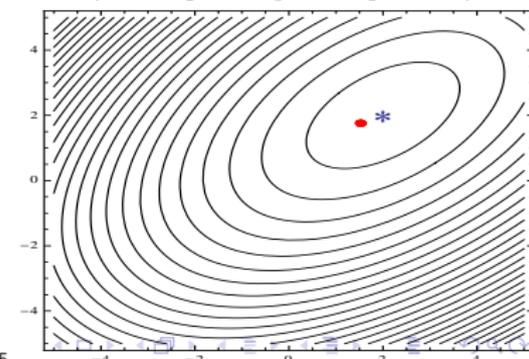
- ▶ DE/rand/1/bin for Neumaier fct,
 $n = 2$
- ▶ $m = 20$, $CR = 0.9$, $F = 0.2$
- ▶ lower bound $F_{low} = 0.23$



gen=1



gen=5



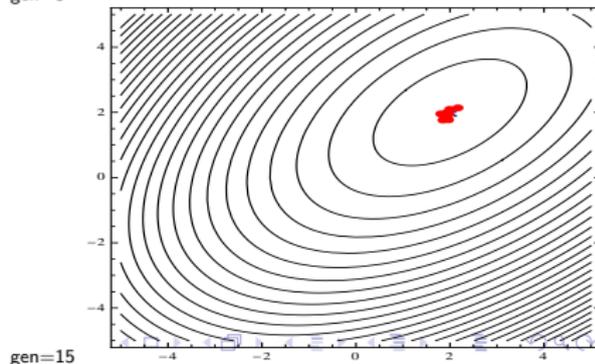
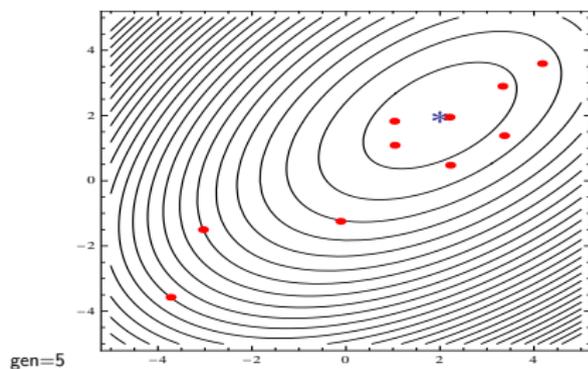
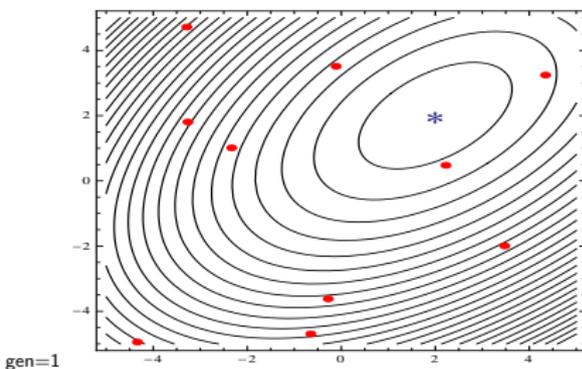
gen=15

Population diversity

Avoiding premature convergence

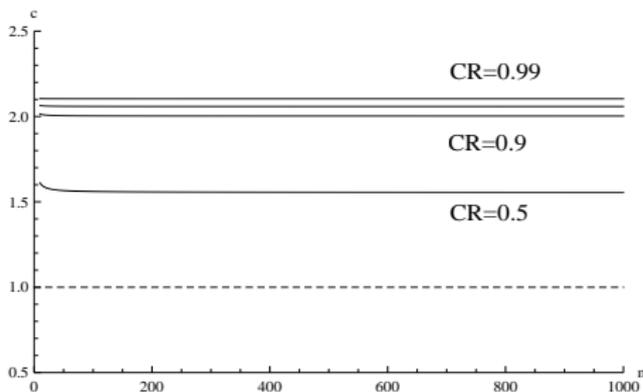
Example:

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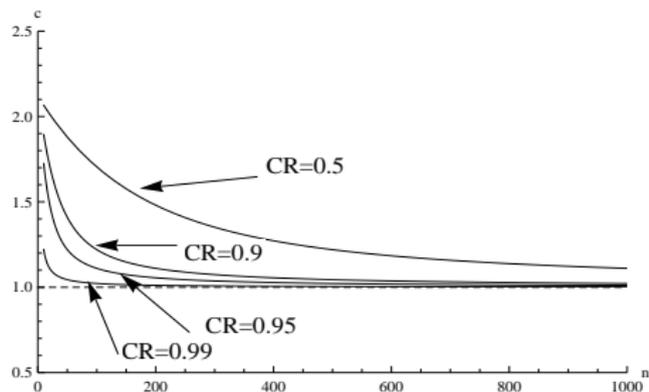


High-dimensional problems

- ▶ The problem size influences directly the relationship between p_m and CR (especially for exponential crossover)
 - ▶ CR values tuned for small size problems are not necessarily good for large size problems



DE/rand/1/bin

 $F = 0.75$ 

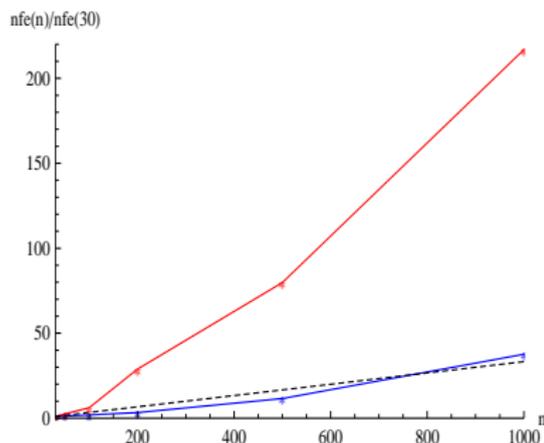
DE/rand/1/exp

Scalability issue

- ▶ a large number of variables means a larger search space
- ▶ asks for a larger volume of resources (larger populations and/or longer evolution time) to reach the same performance
- ▶ the performance of the search method may deteriorate as the problem size increases
- ▶ **Scalable method**: the volume of resources grows (almost) linearly with the problem size

Addressing the scalability issue:

- ▶ design new evolutionary operators and/or control parameter adaptation
- ▶ use a "divide and conquer" approach \implies **cooperative coevolution**



Measure of used resources: number of function evaluations (nfe)

Outline

Motivation

Population-based stochastic metaheuristics

Exploration vs Exploitation. Case Study: Differential Evolution

Cooperative Coevolution

Cooperative coevolution

Main idea: split the problem into smaller sub-problems

- ▶ a potential solution consists of several components
- ▶ evolve independently the population corresponding to each component ([coevolution](#))
- ▶ each component is evaluated in the context of other components ([cooperation](#))

Implementation issues

- ▶ Choosing the components
 - ▶ how many components?
 - ▶ how to assign a variable to a component?
- ▶ Components coevolution
 - ▶ how to construct the evaluation context for each component?
 - ▶ how long should be the evolution of a component in the same context?

Components

- ▶ each solution $x = (x_1, x_2, \dots, x_n)$
- ▶ should be decomposed into components $x = \langle C_1(x), C_2(x), \dots, C_K(x) \rangle$
- ▶ where
 - ▶ K is the number of components
 - ▶ $C(x)$ is a set of variables (not necessarily consecutive in the solution vector)
 - ▶ $\langle \cdot \rangle$ denotes the merging operation

Choosing the components

There are two main decisions to take:

- ▶ choose the number, K , of components
- ▶ define an assignment function of variables to components:
 $c : \{1, \dots, n\} \rightarrow \{1, \dots, K\}$

Variants:

- ▶ **Simplest case**¹⁰:
 $K = n, c(i) = i, C_i(x) = x_i$ (each component corresponds to one variable)
 - ▶ similar to line search techniques; adequate for **separable** problems
 - ▶ the behavior for nonseparable problems can be improved by choosing the adequate context

¹⁰ Potter & deJong, A Cooperative Coevolutionary Approach to Function Optimization, PPSN 1994 

Separability vs. nonseparability

- ▶ A problem is separable if its components do not interact (they are uncorrelated)
- ▶ The relative quality of two values of the same component does not depend on the context:
 - ▶ if $f(x_1, \dots, x_i, \dots, x_n) < f(x_1, \dots, x'_i, \dots, x_n)$ then $f(y_1, \dots, x_i, \dots, y_n) < f(y_1, \dots, x'_i, \dots, y_n)$ for any context y
 - ▶ i.e. if x_i is better than x'_i in a given context then it is better in any context, thus ...
 - ▶ in this case the choice of the context is not critical
- ▶ Example (additively separable): $f(x_1, x_2, \dots, x_n) = \sum_{i=1}^n f_i(x_i)$

Separability vs. nonseparability

- ▶ **Nonseparable functions:** the variables are correlated
- ▶ **Example:** $f(x_1, x_2) = 100(x_1 - x_2)^2 + (1 - x_1)^2$
- ▶ Some simple computations lead to:
 - ▶ $f(1, x_2) < f(2, x_2)$ if $x_2 < 2.501$
 - ▶ $f(1, x_2) > f(2, x_2)$ if $x_2 > 2.501$
- ▶ In this case the relative quality of values 1 and 2 for x_1 depends on the context represented by x_2
- ▶ Thus, the context used to evaluate the quality of a component is important; for this example the variables should be evolved together.
- ▶ Fully nonseparable functions: each variable interacts with at least another variable
- ▶ Real world problems: partially separable

Choosing the components

- ▶ **Ideal case:** each component contains a group of highly interacting variables
 - ▶ difficult to identify the groups of highly correlated variables for black box optimization
- ▶ **Compromise variant:** assign the variables to components in a random manner¹¹
 - ▶ K is randomly chosen
 - ▶ equally sized components: $c(i) = \lfloor \sigma^{-1}(i) \cdot \frac{K}{n} \rfloor + 1$,
 $\sigma = (\sigma(1), \dots, \sigma(n))$ is a random permutation
 - ▶ components with variable size: $c(i) = \text{rand}(\{1, \dots, K\})$

¹¹Yang et al, Large scale evolutionary optimization using cooperative coevolution, Inf. Sci., 2008

Random choice of components (motivation¹²)

The probability of assigning two interacting variables x_i and x_j to the same component in at least g cycles out of the total number of cycles, G :

$$P_g = \sum_{r=g}^G \binom{G}{r} \left(\frac{1}{K}\right)^r \left(1 - \frac{1}{K}\right)^{G-r}$$

Remarks.

- ▶ For $K = 10$ and $G = 50$: $P_1 = 0.9948$, $P_2 = 0.9662$
- ▶ any two variables (correlated or not) have a high chance to belong to the same component at least for a few number of cycles.

¹²Yang et al, Large scale evolutionary optimization using cooperative coevolution, Inf. Sci., 2008

Random choice of components (limits¹³)

The probability of assigning ν interacting variables x_i and x_j to the same component in at least g cycles out of the total number of cycles, G :

$$P_g = \sum_{r=g}^G \binom{G}{r} \left(\frac{1}{K^{\nu-1}}\right)^r \left(1 - \frac{1}{K^{\nu-1}}\right)^{G-r}$$

Remarks.

- ▶ For $K = 10$, $G = 1000$, $\nu = 5$: $P_1 = 0.0951$, $P_2 = 0.0046$
- ▶ the chance of placing more than 4 interacting variables in the same component is small

¹³Omidvar et al., Cooperative Co-evolution for large scale optimization through more frequent random grouping, CEC 2010

Delta grouping¹⁴

Idea:

- ▶ the improvement interval decreases when there are interactions \implies variables with small changes are interacting
- ▶ compute the difference between the population centroids at two consecutive generations: $\Delta = (\delta_1, \delta_2, \dots, \delta_n)$
- ▶ sort Δ and split the set of variables in equally sized components

Disadvantages:

- ▶ the number of components should be specified
- ▶ not appropriate if there is more than one subcomponent of interacting variables

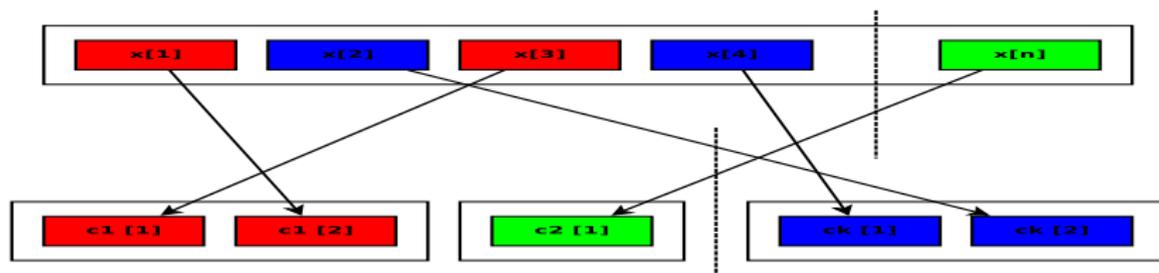
¹⁴M. Omidvar et al., Cooperative co-evolution with delta grouping for large scale for non-separable function optimization, CEC 2010

Differential grouping¹⁵

- ▶ incremental construction of components by identifying pairs of interacting variables
- ▶ two variables i and j satisfying (for an arbitrary selected vector x and arbitrary perturbations δ_i and δ_j)

$$f(\dots, x_i + \delta_i, \dots, x_j + \delta_j, \dots) - f(\dots, x_i + \delta_i, \dots, x_j, \dots) \neq f(\dots, x_i, \dots, x_j + \delta_j, \dots) - f(\dots, x_i, \dots, x_j, \dots)$$

are considered interacting variables



¹⁵M. Omidvar et al., Cooperative Co-evolution with Differential Grouping for Large Scale Optimization, TEVC 2013

Choosing the evaluation context

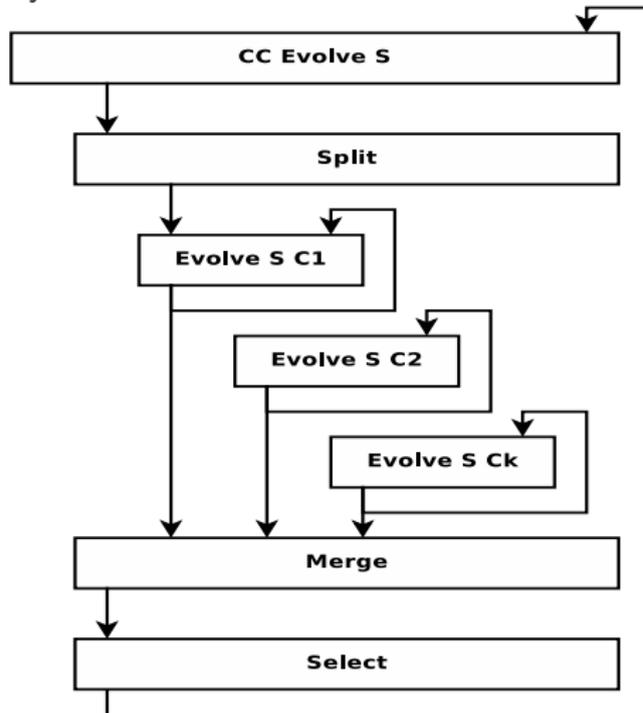
- ▶ to evaluate a component c_k one have to construct a virtual full solution, $\langle c_1, \dots, c_k, \dots, c_K \rangle$, by defining an evaluation context consisting of collaborators c_i provided by the subpopulations corresponding to each other components
- ▶ a collaborator, c_i , can be:
 - ▶ the current **best value of component i** (best individual of the subpopulation corresponding to i th component)
 - ▶ the i th component of the **best individual** in the entire population (it is not necessarily composed of the best components)
 - ▶ the i th component of a **random** individual
 - ▶ the i th component of the **current** individual (that from which the component c_k was evolved)

Implementation issues

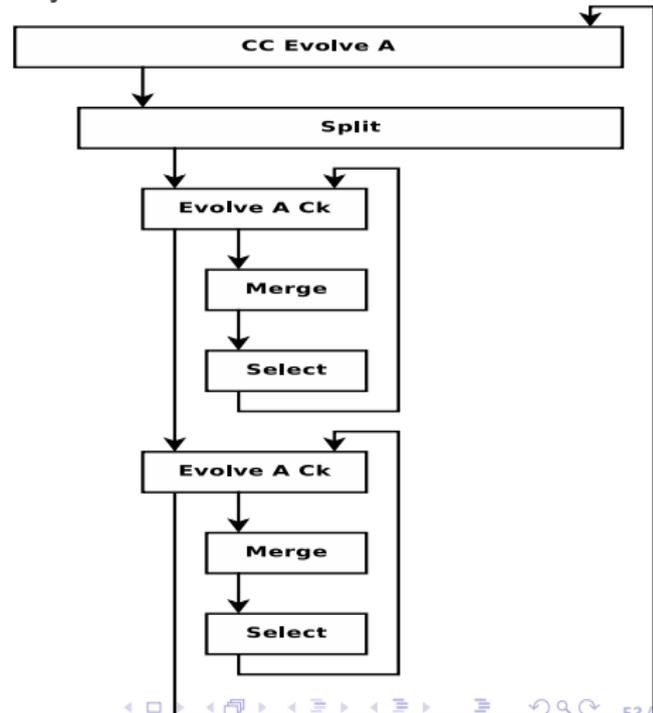
- ▶ most evolutionary algorithms can be
 - ▶ synchronous
 - ▶ asynchronous
- ▶ the same can be said about the Cooperative Coevolution framework
 - ▶ **synchronous**: the population used to provide the context is updated only after all components were evolved
 - ▶ **asynchronous**: the population used to provide the context is updated after the evolution of each component

sCC Synchronous vs Asynchronous

Synchronous



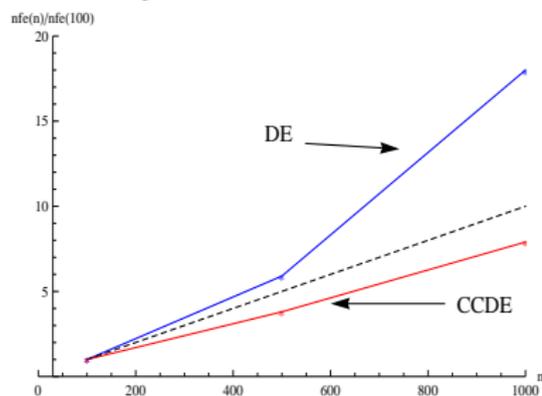
Asynchronous



Results¹⁶

- ▶ analysis approaches:
 - ▶ analyze approximation accuracy for increased computational budget
 $nfe(kn)/nfe(n) = k$
 - ▶ analyze the scalability factor
 $nfe(kn)/nfe(n)$ for a given approximation accuracy (e.g. $\epsilon = 10^{-10}$)

Scalability factor



Results:

- ▶ no significant differences between synchronous and asynchronous approach
- ▶ no critical impact of the context choice (current element context is slightly better)
- ▶ cooperative coevolution enhances the scalability

¹⁶C. Craciun, M. Nicoara, D. Zaharie, Enhancing the scalability of metaheuristics by cooperative coevolution, LSSC'2009

Parallelization models

- ▶ Objective function evaluation \Rightarrow **master-slave model**
 - ▶ the master process executes the iterative process
 - ▶ the slaves only evaluate the population elements (e.g. simulation of a process, costly computations)

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 - ▶ the subpopulations communicate by transferring elements according to a given topology

Parallelization models

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Particularities in the case of coevolution:

- ▶ context broadcasting instead of a topology based migration
- ▶ the communication frequency depends on the sensitivity to the context

Summary

- ▶ DE is an easy to implement, (mostly) effective and an (almost) efficient algorithm for black-box optimization
 - ▶ **important aspect:** choice of the operators and parameters
- ▶ cooperative coevolution is a robust approach for enhancing scalability
 - ▶ **key issue:** choice of the components in accordance with the interaction between variables
- ▶ most of the current results are reported for problem sizes around 1000

Summary: DE-based image processing

▶ Image registration

- ▶ **Aim:** Estimate the parameters of a rigid transformation
- ▶ **Optimization problem:** minimizes the dissimilarity between scene and model images
- ▶ **Method:** DE/rand-to-best/1/exp¹⁷, (DE/rand/1/bin + DE/rand/1/exp)+AIS¹⁸

¹⁷ Salomon et al., 2005

¹⁸ Santamaria et al., 2012

¹⁹ Osuna-Enciso et al., 2013

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- ▶ **Segmentation through multi-level thresholding**
 - ▶ **Aim:** estimate threshold values starting from of a mixture of Gaussians which matches the image histogram
 - ▶ **Optimization problem:** minimizes the Hellinger distance between the mixture of Gaussians and the image histogram
 - ▶ **Population elements:** parameters of each gaussian (mean and standard deviation) and apriori probability of each class¹⁹
 - ▶ **Method:** DE/best/1/bin

¹⁷ Salomon et al., 2005

¹⁸ Santamaria et al., 2012

¹⁹ Osuna-Enciso et al., 2013

Summary: DE-based image processing

- ▶ **Segmentation through deformable models**
 - ▶ **Aim:** Localization of objects in an image
 - ▶ **Optimization problem:** maximizes the similarity between an object and the model or minimizes an energy function
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²⁰ Novo et al., 2012

²¹ Mesejo et al., 2013

²² Das & Kumar, 2009

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 - ▶ **Method:** DE/rand/1/bin
- ▶ **Segmentation through clustering**
 - ▶ **Aim:** Identifying homogeneous regions in the image (the number of regions is not a priori known)
 - ▶ **Optimization problem:** maximizes a clustering validity index
 - ▶ **Population elements:** cluster centroids and cluster activation values ²²
 - ▶ **Method:** DE/rand/1/bin with adaptive parameters

²⁰ Novo et al., 2012

²¹ Mesejo et al., 2013

²² Das & Kumar, 2009



West University of Timisoara, Romania

www.uvt.ro

...in figures

- 11 faculties
- 82 undergraduate programs
- 135 master programs
- 10 doctoral school
- 15000 students

Faculty of Mathematics and Informatics



... in figures

- 1500 students
- 55 teachers
- 2 research centers (Mathematics, Informatics)
- 1 spin-off for research - Institute e-Austria (www.ieat.ro)

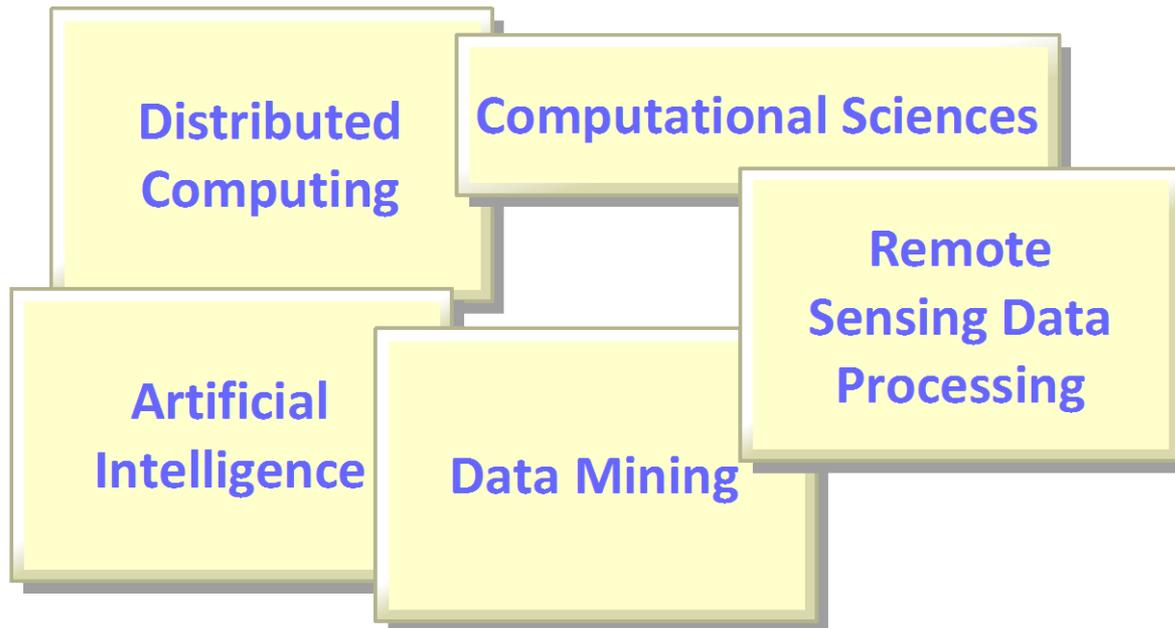


Research Center in Informatics (<http://research.info.uvt.ro>):

- Distributed and Parallel Computing
- Artificial Intelligence
- Theory of Computing
- Computational Mathematics



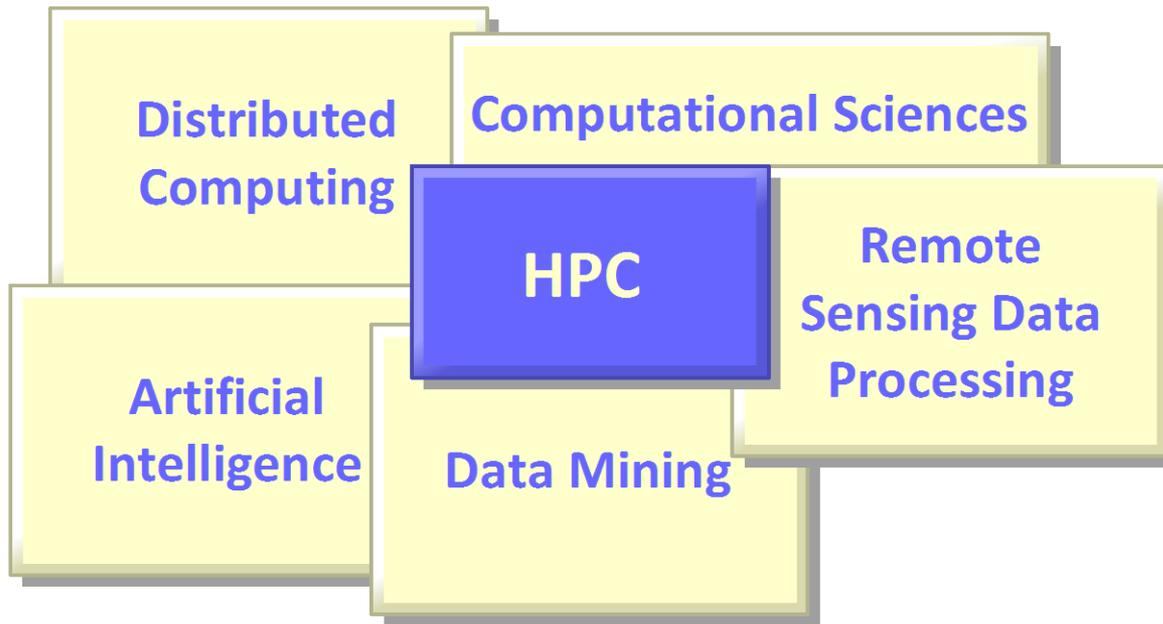
Research Topics Overview



Different topics but similar challenges:

- Large sets of data or large search spaces
- Computationally intensive tasks

Research Topics Overview

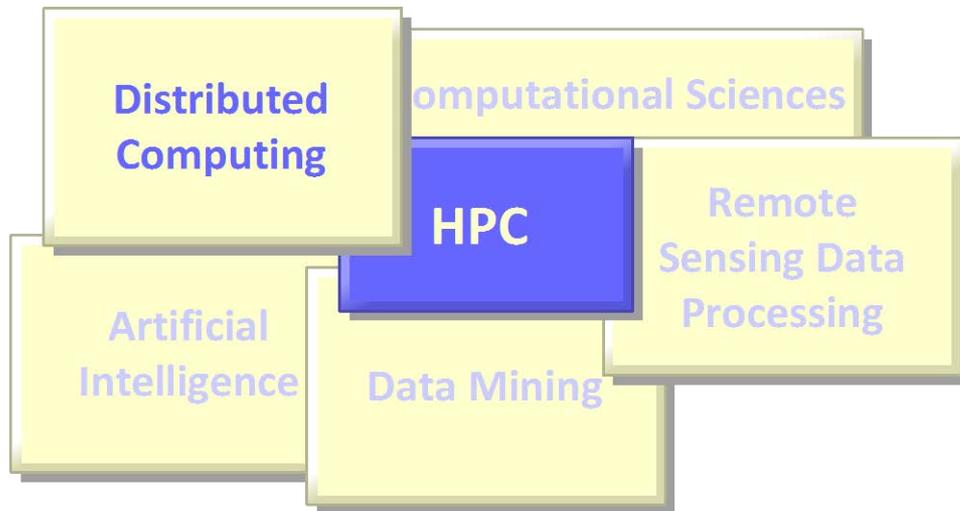


Different topics but similar challenges:

- Large sets of data or large search spaces
- Computationally intensive tasks

... which require high performance solutions

Distributed Computing



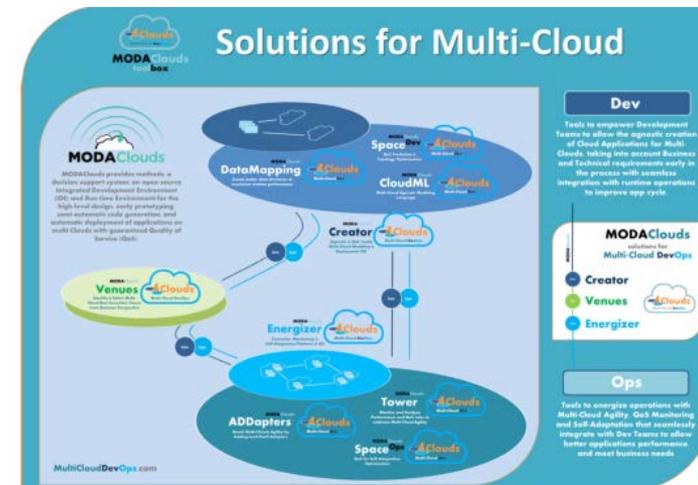
Current research topics:

- Tools for deployment of applications in multiple clouds
- Monitoring tools for data-intensive cloud applications
- Scheduling algorithms for resource provisioning

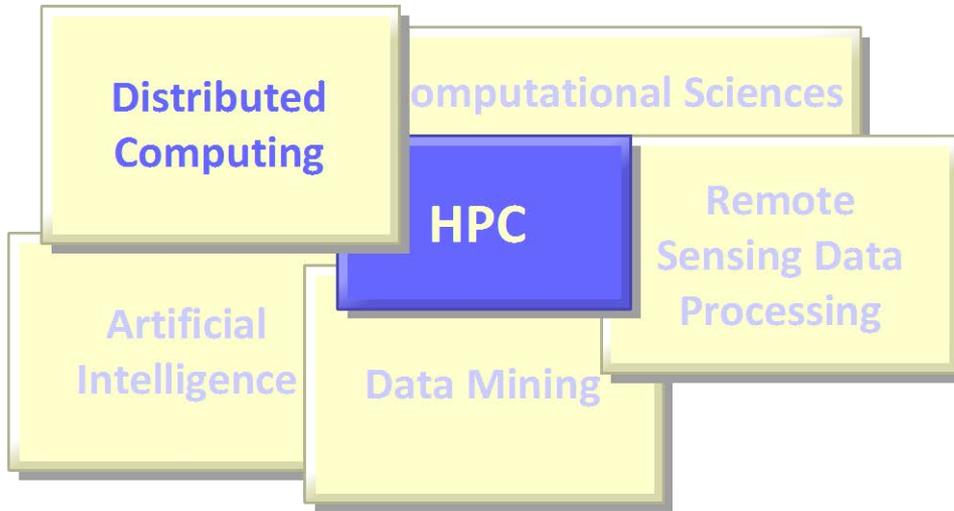
Related projects:

- MODAClouds (www.moda-clouds.eu, FP7 2012-2015)

Results: Multi-cloud toolbox for developers and operators of applications running on multi-clouds



Distributed Computing



Current research topics:

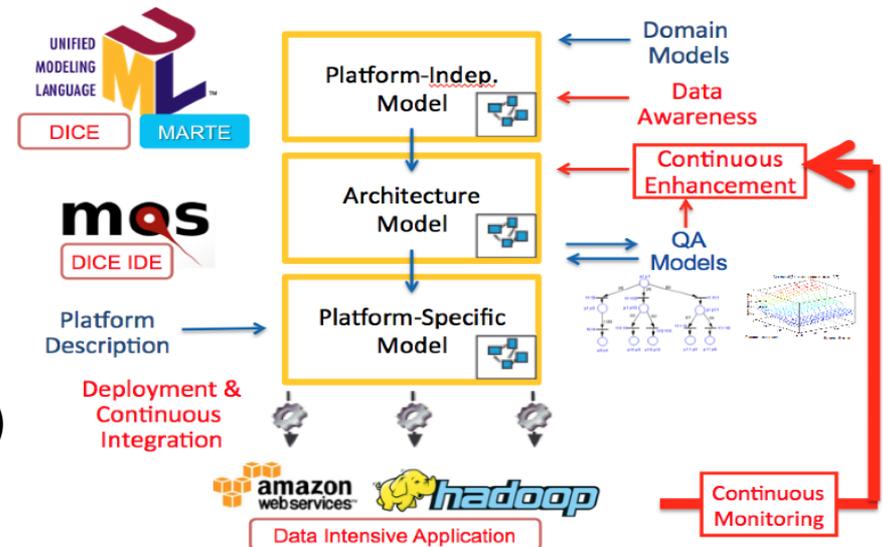
- Tools for deployment of applications in multiple clouds
- Tools for developing data-intensive cloud applications
- Scheduling algorithms for resource provisioning

Related projects:

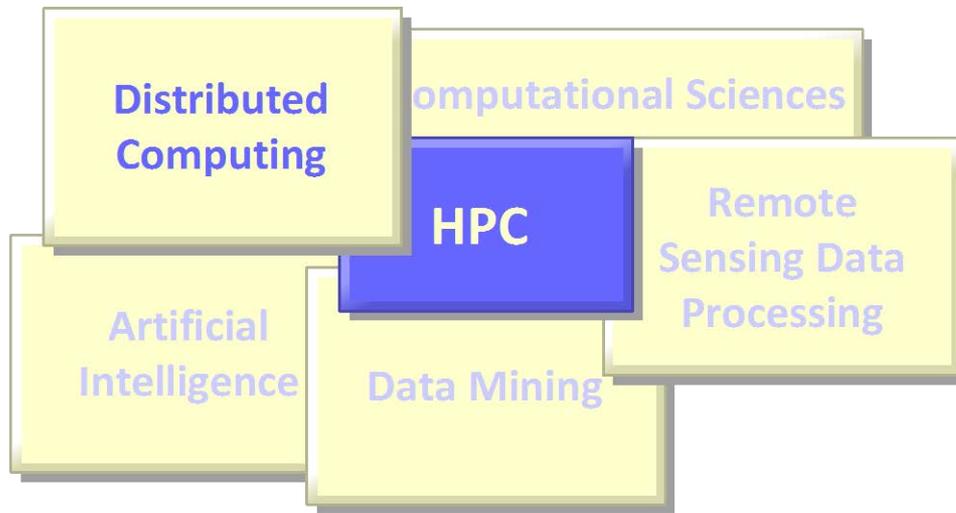
- DICE (www.dice-H2020.eu, 2015-2018)

Aim: develop tool chain containing

- IDE for data-intensive cloud applications
- Tools for quality analysis: monitoring + anomaly detection (using machine learning)



Distributed Computing



Related projects:

- AMICAS - Automated Management in Cloud and Sky Computing Environments (RO 2012-2016)

Current research topics:

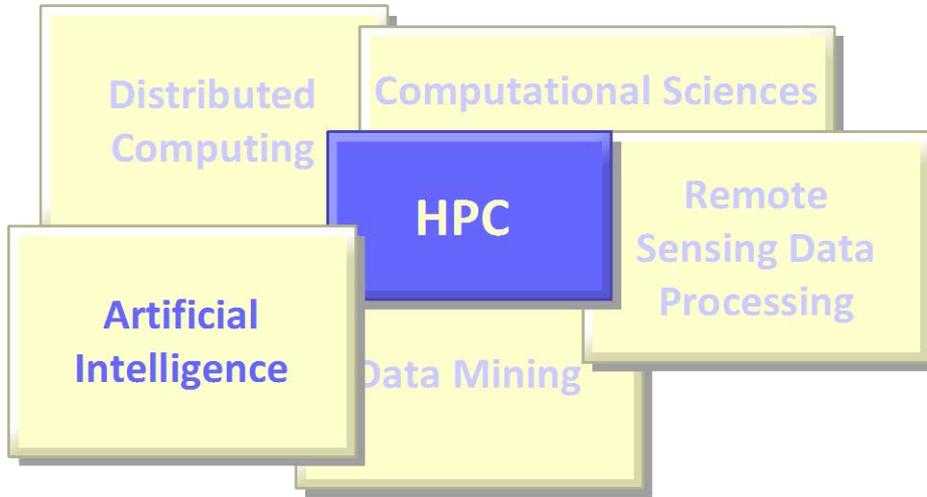
- Tools for deployment of applications in multiple clouds
- Tools for developing data-intensive cloud applications
- Algorithms for scheduling and resource provisioning

Challenges in solving scheduling problems:

- Large search space
- Complex optimization problem (multiple objectives, constraints, dynamic)



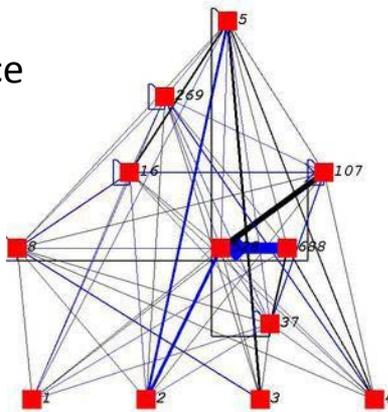
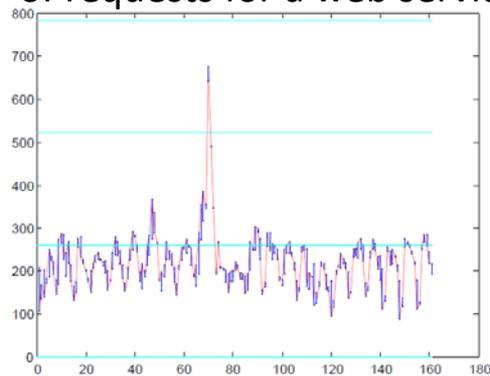
Artificial Intelligence



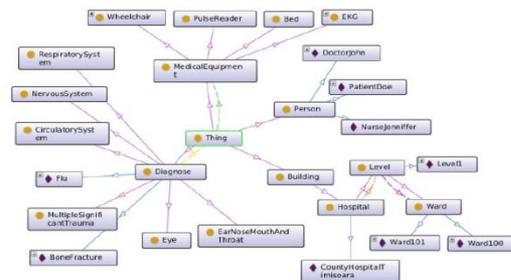
Current research topics:

- Machine learning techniques in:
 - Prediction for auto-scaling of resources in distributed systems
 - Analysis of financial, meteorological, medical data
- Multi-agent approaches in:
 - Stock trading systems
 - Frameworks for strategy games
- Ontologies for
 - Context modelling in IoT
 - Semantic services

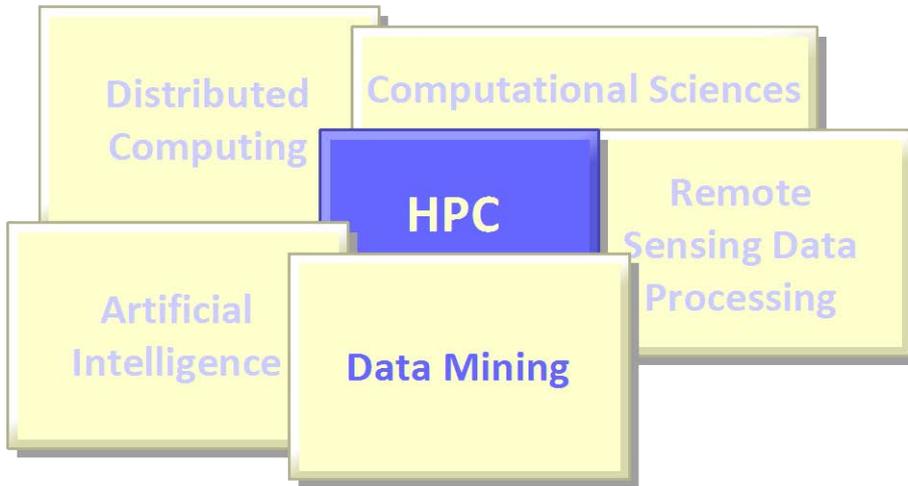
Predicting the number of requests for a web service



Neural networks for game strategy learning



Data Mining



Data mining and machine learning as a Service:

- Access through lightweight web services (REST)
- Access to algorithms' parameters
- User experience enhancements
- Semantic modeling

Research topics:

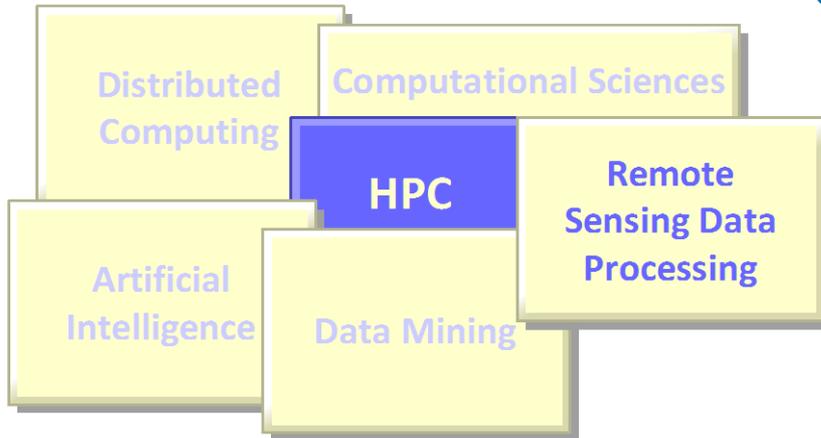
- Distributed architectures for data mining
- Unsupervised classification of distributed data
- Extracting classification/prediction rules from data
- Taxonomy/ ontology based similarity measures for medical data
- Anomaly detection in data

Challenges in data mining:

- Large sets of data
- Response in real-time (prediction models)

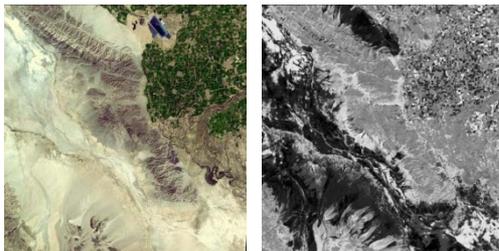


Remote Sensing Data Processing



Research topics:

- Processing multi/hyper spectral images:
 - Identify homogeneous regions
 - Identify reference substances



Challenges:

- Large images (many pixels, many spectral bands)
- Computational intensive image analysis algorithms

Results:

- Parallel/ efficient implementations of
 - spatial variants of fuzzy clustering
 - algorithms for spectral mixture analysis (end-members extraction and abundances estimation)

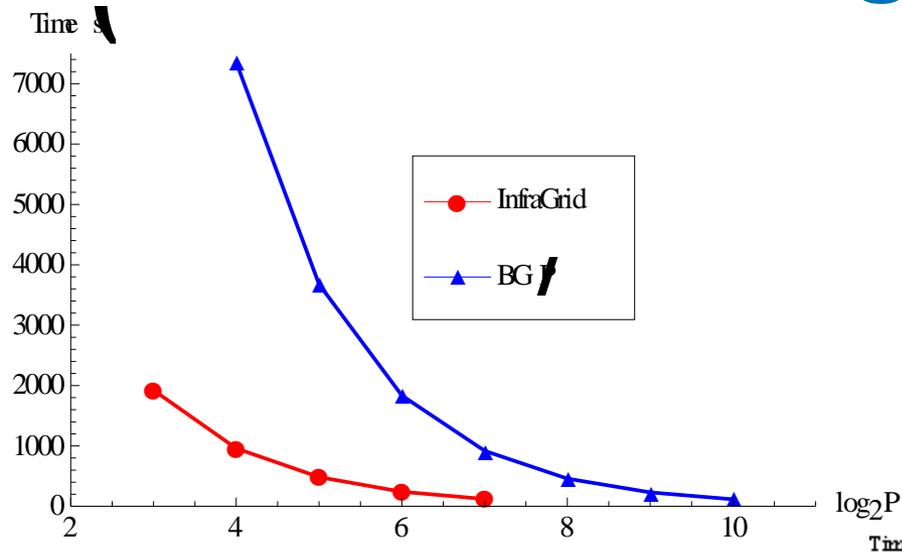
Remote Sensing Data Processing

Efficiency of parallel fuzzy clustering
tested on:

- InfraGrid cluster (400 cores)
- BG/P (1024 CPUs)

Algorithm: Spatial Fuzzy Cmeans

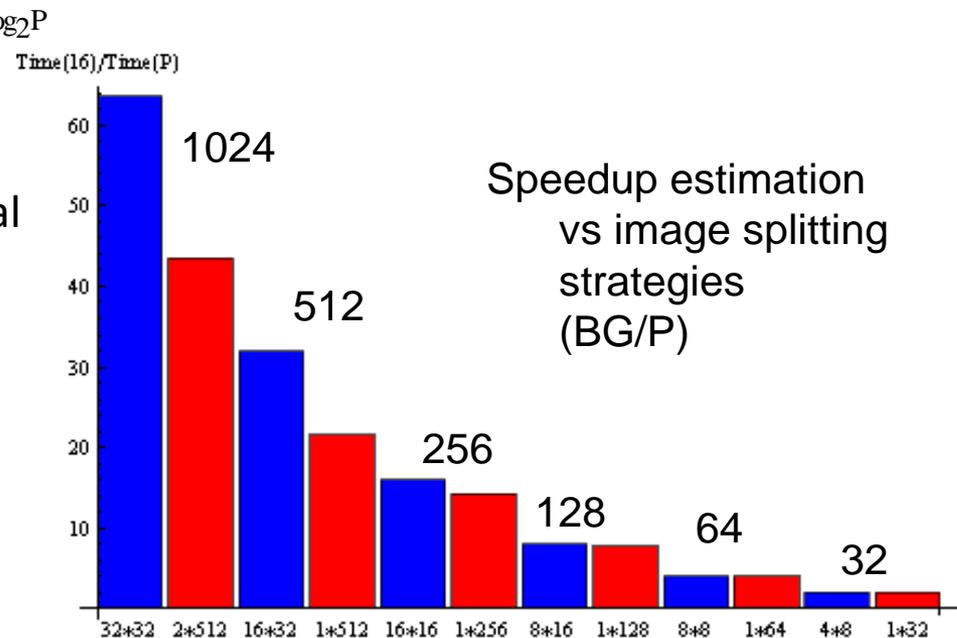
Implementation: C, MPI (MPICH-2)



Test images:

- LANDSAT (7856 x 8786 pixels, 4 spectral bands)
- AVIRIS (1087x614 pixels, 224 spectral bands)

[D.Petcu, D. Zaharie, S. Panica, A. Hussein, A. Sayed, H. El-Shishiny; Fuzzy Clustering of Large Satellite Images using HPC, Proc. SPIE 2011]

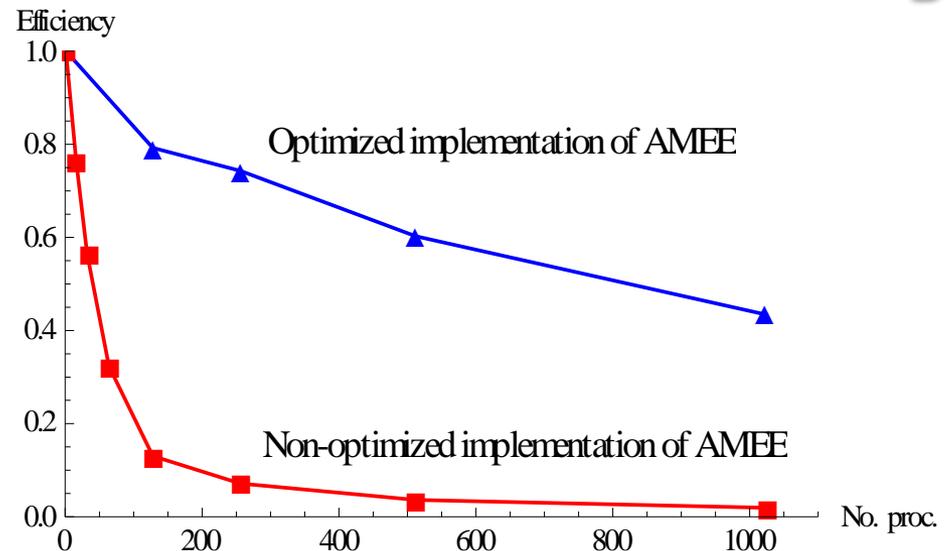


Remote Sensing Data Processing

- Efficient implementation of endmembers extraction algorithms
 - AMEE (Automated Morphological Endmembers Extraction)

AMEE on BG/P

- Split the image + extract local information (local endmembers)
- exploit the structure of spectral angle metric to optimize the paired distances between local endmembers
- avoid a global computation by a particular procedure to merge local sets of endmembers
- control the synchronization among processes in the context of using collective communications (MPIBarrier)



Test image: AVIRIS Cuprite (224 bands, 614x2206 pixels)



Remote Sensing Data Processing

- Efficient implementation of endmembers extraction algorithms
 - MVSA (Minimum Volume Simplex Analysis)

MVSA on GPU

- Sequential implementation (Matlab):
3h
- Parallel implementation:
 - IBM blade with two Intel Xeon quad-core processors and one FermiTesla M2075 GPU, C+CUDA):
 - Time: **2 minutes**

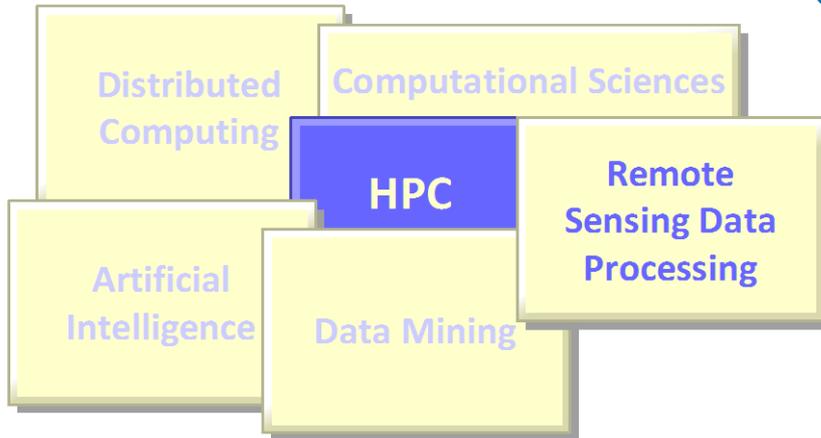
[A. Agathos, J.Li, D. Petcu, A. Plaza; MVSA: Multi-GPU Implementation of MVSA Algorithm for Hyperspectral Unmixing, IEEE JSTARS, 2014]

Fast MVSA

- Sequence of „approximate” constrained quadratic optimization problems solved by interior point method
- Time (for AVIRIS Cuprite data set, 250x190 pixels subscene):
 - Fast MVSA: 3 min
 - Other methods: **7 h** (MVES) or **50 min** (MVC-NMF)

[J.Li, A. Agathos, D. Zaharie, J. Bioucas, A. Plaza, X. Li; MVSA: A Fast Algorithm for Linear Hyperspectral Unmixing, IEEE Trans. Geosci. Rem. Sensing - 2015]

Remote Sensing Data Processing



Collaborations

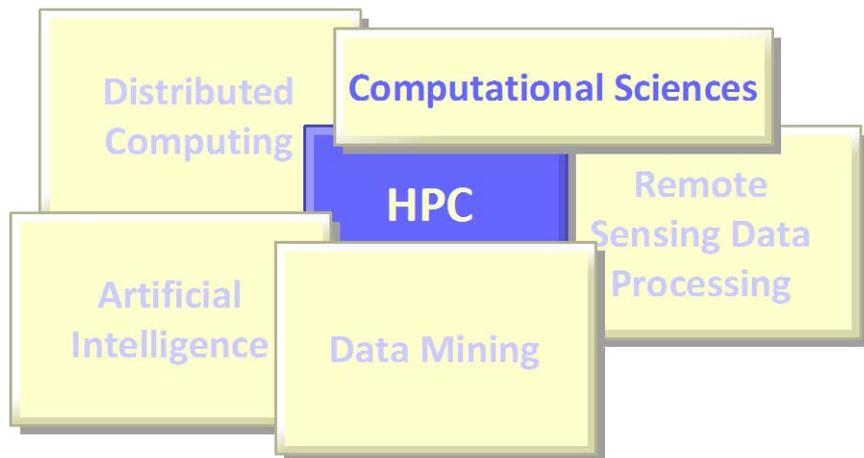
- IBM CAS Cairo, Egypt
- Ain Shams University, Cairo, Egypt
- University of Extremadura, Spain

Related projects:

- IBM OCR – High-Performance Satellite Multi/Hyperspectral Image Processing (2010-2011)
- GiSHEO - On demand Grid services for high education and training in Earth observation (ESA-PECS, 2008-2010)
- HPC-SEE - High-Performance Computing Infrastructure for South East Europe's Research Communities (FP7-Infrastructures, 2010-2013)
- HOST – HPC Service Center (FP7-REGPOT, 2012-2014)



Computational Sciences



Related projects:

- Analysis of some mathematical physics problems occurring in the sound attenuation in an acoustically lined duct carrying gas flow (RO PN-II-ID-PCE, 2011-2013)
- SIMTIM -Modeling and simulation of the dynamics of thymocyte populations and cells of the thymus medulla under normal and pathological situations (RO PN-II-ID-PCE, 2012-2016)

Computational Mathematics:

- Efficient methods for solving large systems of equations
- Preconditioning through bandwidth reduction

Computational Physics:

- Efficient computational methods in nanoscale optics
- Simulation of crystallization processes, transport phenomena, acoustic lining

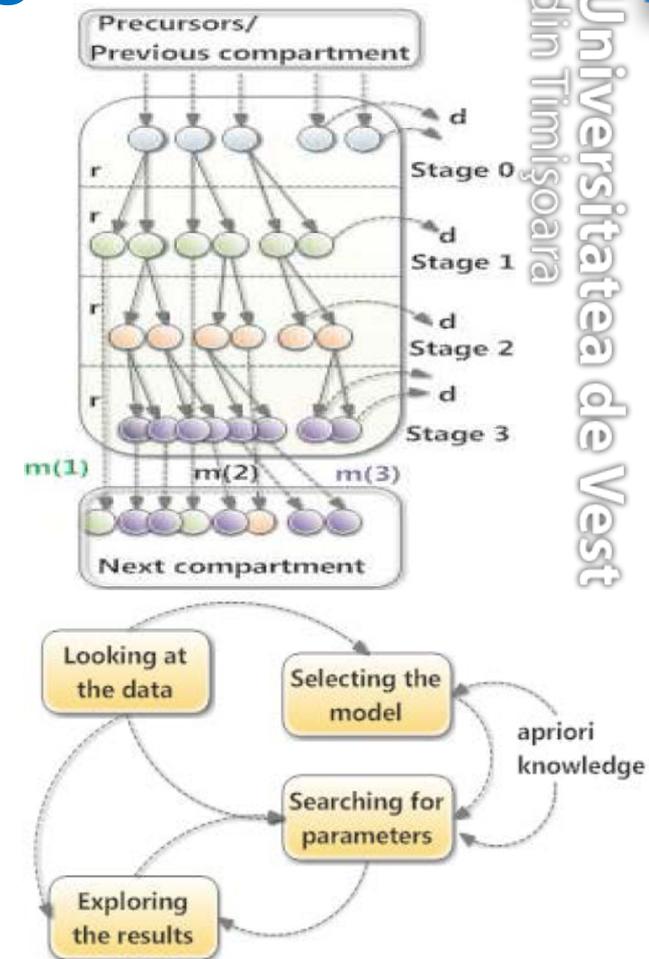
Computational Biology :

- Simulating the dynamics of thymus cells populations based on experimental data

Computational Sciences

Computational Biology :

- Multi-compartmental models :
 - Systems of (non)linear differential equations (from 4 to more than 20)
 - Various models for biological processes (proliferation, transfer, death)
 - Many parameters to estimate (from 30 to 55)
- Challenges for parameter estimation
 - no explicit relationship between objective function and parameters („semi-transparent” model)
 - parameter (non)identifiability
 - hard to check constraints
- Approach:
 - use of population-based metaheuristics



[D. Zaharie, L. Moleriu, V. Negru, Evolutionary Parameter Estimation in Multi-stage Compartmental Models of Thymocyte Dynamics, Proc. GECCO 2013]

[D. Moleriu, D. Zaharie et al, Insights into the mechanisms of thymus involution ... , J. Theor. Biol., 2014]