Evolutionary Optimization Algorithms (EOAs): Comparison, Selection and Application

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October 19th 2010

EOA: A First Glance

Computer science

→ Artificial intelligence → Computational intelligence → Evolutionary computation→ EOA

Research forums

- Journals
 - <u>Evolutionary Computation</u> (2009 SCI impact factor: 3.103)
 - * <u>IEEE Transactions on Evolutionary Computation</u> (2009 SCI impact factor: 4.589)

At the 2nd among 130 "Computer Science, Artificial Intelligence" journals, the 3rd among 91 "Computer Science, Theory & Methods" journals, and the 4th among all 426 Computer Science journals. According to the 5 year impact factor (7.621), IEEE TEVC was ranked the 2nd, 2nd and 4th, respectively, in the above categories.

- * <u>Genetic Programming and Evolvable Machines</u> (2009 SCI impact factor: 1.091)
- Conferences
 - * The Genetic and Evolutionary Computation Conference (GECCO)
 - * IEEE Congress on Evolutionary Computation (CEC)
 - The Evo* conference (the main European events on evolutionary computation)

Most cited literature

Goldberg, David E. (1989) Genetic Algorithms in Search Optimization and Machine Learning Google scholar citation: 35919 (till 2010.10.18)

EOA: Applications

Computer vision

- > Image enhancement
- > Image reconstruction
- Image registration
- Image segmentation
- Image classification
- > Texture synthesis
- > Calibration
- Tracking

D Pattern Recognition

- Evolutionary clustering
- Evolutionary classification
 - Evolutionary parameter estimation
 - Evolving neural networks
 - Learning classifier systems

D Statistical modeling

> Evolutionary parameter estimation

Bioinformatics

- Alignment and comparison of DNA, RNA, and protein sequences
- > Gene mapping on chromosomes
- Gene finding and promoter identification from DNA sequences
- Gene selection from microarray gene expression data
- Gene regulatory network identification
- Construction of phylogenetic trees for studying evolutionary relationship
- > DNA/RNA structure prediction
- Protein structure prediction and classification
- Molecular design and molecular docking

Outline

Part I: Introduction of EOAs

- **Basic ideas**
- **Generic paradigm and core components**
- **Historical perspective**
- **Categorization**

- **Canonical EOAs**
- **State-of-the-art EOAs**
- **Benchmarking testbeds**
- Challenges in practice

Part II: Two advanced EOAs: CLPSO and SaDE

- **Particle swarm optimization (PSO)**
- **My previous work: comprehensive learning PSO (CLPSO)**
- **Differential evolution (DE)**
- **My previous work: self-adaptive DE (SaDE)**

Part III: Research plan discussion

- **Statistical comparison and interactive selection of EOAs**
- **Development of novel EOAs**
- **D** Applications

Evolutionary Optimization Algorithms (EOAs)

Part I: General Introduction of EOAs

- Basic ideas
- □ Generic paradigm and core components
- Historical perspective
- **Categorization**
- Canonical EOAs
- **State-of-the-art EOAs**
- Benchmarking testbeds
- Challenges in practice

Optimization

- **Optimization** seeks to improve performance towards some optimal point(s).
 - Destination (theoretical view point)
 - Improvement (practical viewpoint)
- **Optimization problem** aims at minimizing (or maximizing) a real-valued objective function by choosing the values of decision variables from within an allowed set.

Maximize (or minimize) $f(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_M(\mathbf{x}))$ w.r.t. $\mathbf{x} = (x_1, \dots, x_D), f: \Omega^D \to \Re^M$ s.t. $\mathbf{x} \in [\mathbf{x}_{\min}, \mathbf{x}_{\max}]; g_j(\mathbf{x}) \le 0, j = 1, \dots, J; h_k(\mathbf{x}) = 0, k = 1, \dots, K$

- A large number of scientific and engineering problems can be formulated as optimization problems, and solved by some computational methods called **optimization algorithms**.
- Categorization of optimization algorithms
 - > As per problem properties
 - Decision variables: discrete vs. continuous vs. mixed; constrained vs. unconstrained
 - Objective function: single-objective vs. multi-objective
 - Fitness landscape: unimodal vs. multimodal; noise-free vs. noisy; static vs. dynamic
 - > As per algorithm characteristics
 - Deterministic vs. stochastic

EOA: Basic Ideas

- Evolutionary optimization algorithms (EOAs) are computational methods inspired by natural evolution process characterized by Darwin's *survival of the fittest* principle.
- The key idea of EOAs is to identify and capture computationally useful aspects of natural evolution processes instead of faithfully (or even plausibly) modeling of biological processes.
- EOAs are meta-heuristic, stochastic search techniques, effective for solving complex optimization problems with multi-modal, static/dynamic multi-dimensional search space in the black-box manner, i.e., the landscape model of the search space is not required in advance.
- EOAs iteratively evolve populations of candidate solutions using parallel guided random search to achieve the desired end.
- Major characteristics of an EOA
 - > Populations of candidate solutions
 - > Fitness-guided random population changing during the course of search
 - Variation with inheritance
 - ✤ Replacement

EOA: Generic Paradigm



EOA: Core Components

Problem aspects:

Golution representation

- > Data structures that computer uses to represent solutions
- > Genotype vs. phenotype
- > Batch vs. sequential
- > Individual vs. collective

D Objective function evaluation

- > Known vs. unknown function
- > Time-expensive evaluation

Algorithm aspects:

Initialization

- > Known vs. unknown search range
- Prior knowledge
- Sampling method

Reproduction

- > Parent selection: sexual vs. asexual
- > Reproduction operators: recombination vs. mutation

Generation

- > Evolving population over generations (time)
- > Darwinian *survival of the fittest* principle
- > Selection pressure

EOA: Historical Perspective

1930s~1950s: early algorithmic views

- > Viewing an evolutionary system as an optimization process
- > Viewing an evolutionary system as a complex adaptive controller

1960s: three canonical EOAs developed independently

- ► Genetic Algorithm (GA) Holland, USA, 1962, 1967
- Evolutionary Strategy (ES)Rechenberg and Schwefel, Gemany, 1965
- > Evolutionary Programming (EP) Fogel, USA, 1966
- **1970s~1980s: exploitation and exploration**
- **1990s: unified field as evolutionary computation**
- **1990s~2000s: boosting**
 - > Swarm intelligence
 - > Differential evolution
 - > Estimation of distribution
 - Harmonic search

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EOA: Categorization

As per problem properties

- > Discrete vs. continuous vs. mixed vs. structural
- > Constrained vs. unconstrained
- > Single-objective vs. multi-objective
- > Noiseless vs. noisy
- > Static vs. dynamic

• As per algorithmic operators

- Genetic algorithms
- > Genetic programming
- Evolutionary strategies/programming
- Swarm intelligence
- > Estimation of distribution algorithms
- > Differential evolution
- > Artificial immune system
- > Harmonic search
- > Culture algorithm
- > Memetic algorithm

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Canonical EOAs: Genetic Algorithm

- **Basic concepts**
 - Chromosome
 - > Gene, locus and allele
 - Genotype and phenotype
- **A simple GA**
 - Encoding
 - Initialization
 - Reproduction
 - Parents selection
 - Crossover (recombination)
 - Mutation
 - > Selection of survivals
- **Implicit parallelism explained by schema theory** (a specified string of length l contains 2^l schema) 011: 011, *11, 0*1, 01*, **1, *1*, 0**, ***
- **Advanced GA**
 - > Real-parameter GA
 - > Arithmetic crossover and mutation
 - > Probabilistic model building GA
 - Niching based GA

| Γ | String | Initial | x | f(x) | % of | No. | Mating | Mate | C'over | New | x | f(x) |
|---|---------|---------|----|------|-------|------|--------|------|--------|-------|----|------|
| | No. | Popn. | | | Total | Sel. | Pool | | Site | Popn. | | |
| | 1 | 01101 | 13 | 169 | 14.4 | 1 | 01101 | 2 | 4 | 01100 | 12 | 144 |
| | 2 | 11000 | 24 | 576 | 49.2 | 2 | 11000 | 1 | 4 | 11001 | 25 | 625 |
| | 3 | 01000 | 8 | 64 | 5.5 | 0 | 11000 | 4 | 2 | 11011 | 27 | 729 |
| L | 4 | 10011 | 19 | 361 | 30.9 | 1 | 10011 | 3 | 2 | 10000 | 16 | 256 |
| | Sum | | | 1170 | 100.0 | 4 | | | | | | 1754 |
| 1 | Average | | | 293 | | | | | | | | 439 |

Canonical EOAs: Evolutionary Strategy

Evolutionary strategy vs. evolutionary programming

- **A simple ES**
 - Initialization
 - Reproduction
 - * Parents selection
 - Mutation
 - > Selection of survivals

D Mutation strategies

- \succ (u, v) and (u+v)
- > Gaussian mutation

Relation to GA

- > No need to encoding
- No crossover

Advanced ES

- Crossover added
- **Fast evolutionary programming**
- > Covariance matrix adaptation ES (CMA-ES)

State-of-the-art EOAs

Advanced GA

- > Real-parameter GA
- Probabilistic model building GA

Advanced ES

- Fast evolutionary programming
- Covariance matrix adaption ES
- **Genetic programming**
- **Swarm intelligence**
 - Particle swarm optimization
 - > Ant colony optimization
 - Bee colony optimization
 - Cuckoo search
 - Bat algorithm

Differential evolution

 Estimation of distribution algorithms

- Population-based incremental learning
- Estimation of multivariate normal algorithm
- Bayesian optimization algorithm
- **Artificial immune system**
- **Harmonic search**
- **D** Memetic algorithm
- **Culture algorithm**

...

EOA: Benchmarking Testbeds

Benchmark test problems

- > Numerical functions
 - Discrete vs. continuous vs. mixed vs. structural
 - Constrained vs. unconstrained (CEC'06, CEC'10)
 - Single-objective (CEC'05, GECCO'09, GECCO'10) vs. multi-objective (CEC'07, CEC'09)
 - Noiseless vs. noisy (GECCO'09, GECCO'10)
 - Static vs. dynamic (CEC'09)
- > (Simulated) real problems
- > Problem scale (CEC'08, CEC'10)

D Performance measurement

- Convergence map
- > Average objective function values
- > Success rate with the average number of objective function evaluations
- > Expected running time
- Bootstrapping based dispersion measure
- > Empirical cumulative distribution
- > Time complexity

Comparison methods

- > Numerical values
- > Hypothesis testing

EOA: Challenges in Practice

- **Problem formulation**
 - > Solution representation
 - > Objective function

Algorithm comparison

- > Which performance measures to choose?
- > Whether algorithms are statistically significantly different?
- > How to make comparison conclusions?

Algorithm selection

- > Problem-dependent
- > Requirement-dependent
- > User-dependent
- > Statistical data mining is needed!
- Parameter and operator selection
 - > Many parameters: are they equally sensitive?
 - > Many operators: are they significantly influential?
- **Computational cost**
 - > Expensive objective function evaluation
 - > Sequential algorithmic structure







Evolutionary Optimization Algorithms (EOAs)

Part II: Two Advanced EOAs

- Particle swarm optimization (PSO)
- □ My previous work: comprehensive learning PSO (CLPSO)

J. J. Liang, A. K. Qin, P. N. Suganthan and S. Baskar, "Comprehensive learning particle swarm optimizer for global optimization of multimodal functions," *IEEE Transactions on Evolutionary Computation*, 10(3): 281-295, 2006. (Google scholar: 298)

Differential evolution (DE)

■ My previous work: self-adaptive DE (SaDE)

A. K. Qin and P. N. Suganthan, "Self-adaptive differential evolution algorithm for numerical optimization," *Proc. of the 2005 IEEE Congress on Evolutionary Computation (CEC'05)*, Edinburgh, UK, September 2005. (Google scholar: 158)

A. K. Qin, V. L. Huang and P. N. Suganthan, "Differential evolution with strategy adaptation for global numerical optimization," *IEEE Transactions on Evolutionary Computation*, 13(2): 398-417, 2009. (Google scholar: 72)

Particle swarm optimization (PSO)



- □ Introduced by Eberhart and Kennedy in 1995.
- Emulate social behavior of bird flocking or fish schooling to solve optimization problems.
- Each potential solution is represented as a particle.
- **Each** particle is associated with the objective function value and the velocity.

Notations in PSO

- $\mathbf{x}_i = (x_i^1, x_i^2, ..., x_i^D)$ represents the position of the *i*th particle.
- $\mathbf{v}_i = (v_i^1, v_i^2, ..., v_i^D)$ represents the position changing rate (velocity) of the *i*th particle.
- □ **pbest**_{*i*} = (*pbest*_{*i*}¹, *pbest*_{*i*}²,..., *pbest*_{*i*}^{*D*}) represents the best previous position (the position associated with the best objective function value) of the *i*th particle.
- **gbest** = $(gbest^1, gbest^2, ..., gbest^D)$ represents the best previous position of the whole swarm.
- □ **Ibest**_{*i*} = (*lbest*_{*i*}¹, *lbest*_{*i*}²,..., *lbest*_{*i*}^D) represents the best previous position achieved by those particles within the neighborhood of the i^{th} particle.

Basic PSO formula

- **Two basic versions of PSO**
 - Global version: each particle learns from its own previous best position (pbest) and the best position found by the whole swarm (gbest).

$$v_i^{d} \leftarrow v_i^{d} + c_1 \times rand 1_i^{d} \times (pbest_i^{d} - x_i^{d}) + c_2 \times rand 2_i^{d} \times (gbest^{d} - x_i^{d})$$
$$x_i^{d} \leftarrow x_i^{d} + v_i^{d} \qquad i - \text{particle index}, \ d - \text{dimension index}$$
$$c_1, c_2 - \text{accelerating constants}$$

► Local version: each particle learns from its **pbest** and the best position found by particles within its certain neighborhood (**lbest**).

$$v_i^{d} \leftarrow v_i^{d} + c_1 \times rand 1_i^{d} \times (pbest_i^{d} - x_i^{d}) + c_2 \times rand 2_i^{d} \times (lbest_i^{d} - x_i^{d})$$
$$x_i^{d} \leftarrow x_i^{d} + v_i^{d}$$

□ The random numbers $(rand1_i^d \text{ and } rand2_i^d)$ should be generated for per dimension of each particle in every iteration.

PSO variants

- Controlling velocities
 - > Inertia weight ω
 - > Constriction coefficient
 - > Time varying acceleration coefficients
 - Linearly decreasing the upper bound of velocity
- **Introducing neighborhood topologies**
 - > Extensive experimental studies
 - > Dynamic neighborhood
 - > Combine the global version and the local version, named as unified PSO (UPSO)
 - Fully informed PSO (FIPS)
- **u** Hybrid PSO
 - > PSO + selection operator
 - \rightarrow PSO + crossover operator
 - > PSO + mutation operator
 - > PSO + co-operative approach
- Others
 - Binary optimization
 - > Constrained optimization
 - > Multi-objective optimization
 - > Dynamic optimization

Comprehensive learning PSO (CLPSO)

- **•** Motivation
 - > Premature convergence due to the social learning aspect.
 - Every particle's **pbest** may involve some beneficial components deserved to be learn by other particles.
- Comprehensive learning strategy in CLPSO:

$$v_i^d \leftarrow w \times v_i^d + c \times rand_i^d \times \left(pbest_{f_i(d)}^d - x_i^d\right)$$
$$x_i^d \leftarrow x_i^d + v_i^d$$

• $f_i = [f_i(1), f_i(2), ..., f_i(D)]$ denotes a set of particle indices with respect to each dimension of the particle *i*. **pbest**_{f_i} represents a comprehensive exemplar with each dimension taking on the value from the corresponding dimension of the *pbest* of particle $f_i(d)$. These indices take the value *i* itself with the probability Pc_i , referred to as the learning probability, which takes different values with respect to different particles.



Flow chart: the procedure of obtaining $pbest_{f_i}$ for the *i*th particle in the swarm with respect to certain generation



CLPSO

- A particle learns from its comprehensive exemplar until stopping to improve for a certain number of generations, called the refreshing gap *m*. After that, the comprehensive exemplar is re-chosen.
- **CLPSO** vs. conventional PSO
 - Instead of using particle's **pbest** and **gbest** as the exemplars, all particles' **pbests** can be used to guide a particle's flying direction.
 - Instead of learning from the same exemplar for all dimensions, different dimensions of a particle may learn from different exemplars. In other words, at one iteration, different dimensions of a particle may learn from different particle's **pbests** at the corresponding dimension.
 - Instead of learning from two exemplars (pbest and gbest) in every generation, each dimension of a particle in CLPSO learns from just one comprehensive exemplar.
- Search behavior: diversity is much increased!

- Parameter sensitivity analysis:
 - > Learning probability Pc_i

$$Pc_i = 0.05 + 0.45 * \frac{\left(\exp\left(\frac{10(i-1)}{ps-1}\right) - 1\right)}{(\exp(10) - 1)}$$

> Refreshing gap *m*





Searching boundary problem

No re-initialization, not fixed at boundary point, but NOT evaluate!

- **D** Performance comparison
 - > 9 methods in comparison
 - PSO with inertia weight (PSO-w)
 - PSO with constriction factor (PSO-cf)
 - Local version of PSO with inertia weight (PSO-w-local);
 - Local version of PSO with constriction factor (PSO-cflocal)
 - UPSO
 - · Fully informed particle swarm (FIPS)
 - FDR-PSO
 - CPSO-H
 - CLPSO
 - I6 numerical test functions of 10D and 30D in 4 groups with different complexity
 - > 30 independent runs for each algorithm
 - Computational budgets: 30,000 FEs for 10D; 200, 000 FEs for 30D
 - > Performance measures
 - Table: means and stds of objective functions values over 30 runs for each individual algorithm
 - Convergence map: median objective function value within 30 runs vs. FEs

| Func | Group C | Group C | Group D | Group D |
|--------------|-------------------------------|-----------------------|---|-----------------------|
| PSOs | 13 | 14 | 15 | 16 |
| PSO-w | $1.02e+001 \pm 3.58e+000$ | 5.69e+002 ± 2.16e+002 | $1.20e+002 \pm 8.94e+001$ | 1.38e+002 ± 1.80e+002 |
| PSO-cf | $1.53e{+}001\pm 6.38e{+}000$ | 1.19e+003 ± 4.23e+002 | $1.60\text{e}{+}002 \pm 1.64\text{e}{+}002$ | 2.31e+002 ± 1.93e+002 |
| PSO-w-local | $1.09e{+}001 \pm 4.08e{+}000$ | 4.72e+002 ± 3.07e+002 | $4.00e{+}001\pm5.98e{+}001$ | 1.53e+002 ± 1.53e+002 |
| PSO-cf-local | $1.07e{+}001\pm2.81e{+}000$ | 9.09e+002 ± 3.25e+002 | $9.00e{+}001\pm8.52e{+}001$ | 1.34e+002 ± 1.71e+002 |
| UPSO | $1.47e+001 \pm 6.53e+000$ | 1.27e+003 ± 2.29e+002 | $8.00e{+}001\pm8.34e{+}001$ | 1.79e+002 ± 1.56e+002 |
| FDR | $1.07e{+}001 \pm 3.86e{+}000$ | 1.07e+003 ± 2.23e+002 | $1.00e{+}002 \pm 9.73e{+}001$ | 1.53e+002 ± 2.01e+002 |
| FIPS | $8.84e+000 \pm 3.27e+000$ | 2.89e+002 ± 2.00e+002 | $6.00\text{e}{+}001 \pm 5.16\text{e}{+}001$ | 4.21e+001 ± 6.37e+001 |
| CPSO-H | $1.90e{+}001 \pm 9.05e{+}000$ | 9.67e+002 ± 3.67e+002 | $1.65e{+}002 \pm 1.42e{+}002$ | 2.46e+002 ± 2.18e+002 |
| CLPSO | 5.44e+000 ± 1.39e+000 | 1.14e+002 ± 1.28e+002 | 1.64e+001 ± 3.63e+001 | 1.98e+001 ± 2.93e+001 |
| h | 1 | 1 | 1 | 1 |



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- General conclusions
 - CLPSO shows slower convergence speed on unimodal and simple multimodal problems.
 - CLPSO achieves much better optimization performance on multimodal problems, especially on the most complex composition functions.
 - CLPSO is more effective in solving problems with less linkage due to the dimension-wise updating rule.

Differential evolution (DE)

- DE, proposed by Price and Storn in 1995, was motivated by an attempt to using Genetic Annealing to solve the Chebychev polynomial fitting problem.
- Genetic annealing is a population-based, combinatorial optimization algorithm.
- Price modified genetic annealing by using floating-point encoding instead of bit-string one, arithmetic operations instead of logical ones, population-driven differential mutation instead of bit-inversion mutation and removed the annealing criterion. Storn suggested creating separate parent and children populations.
- DE is closely related to many other multi-point derivative free search methods.

DE at a glance

Characteristics

- Population-based stochastic direct search
- Self-referential mutation
- Simple but powerful
- Reliable, robust and efficient
- Easy parallelization
- Floating-point encoding

Basic components

- Initialization
- Trial vector generation
 - Mutation
 - Recombination
- > Replacement
- **- Feats**
 - > DE demonstrated promising performance in 1st and 2nd ICEO

Insight into classic DE (DE/rand/1/bin)

Initialization

A population $P_{x,0}$ of *Np D*-dimensional parameter vectors $\mathbf{x}_{i,0} = [x_{1,i,0}, \dots, x_{D,i,0}]$, *i*=1,...,*Np* is randomly generated within the prescribed lower and upper bound $\mathbf{b}_{L} = [\mathbf{b}_{1,L}, \dots, \mathbf{b}_{D,L}]$ and $\mathbf{b}_{U} = [\mathbf{b}_{1,U}, \dots, \mathbf{b}_{D,U}]$

Example: the initial value (at generation g=0) of the j^{th} parameter of the i^{th} vector is generated by: $x_{j,i,0} = \operatorname{rand}_{j}[0,1] \cdot (b_{j,U}-b_{j,L}) + b_{j,L}, j=1,...,D, i=1,...,Np$

Trial vector generation

At the g^{th} generation, a trial population $P_{u,g}$ consisting of *Np D*-dimensional trial vectors $\mathbf{v}_{i,g} = [v_{1,i,g}, \dots, v_{D,i,g}]$ is generated via mutation and recombination operations applied to the current population $P_{x,g}$

Differential mutation: with respect to each vector $\mathbf{x}_{i,g}$ in the current population, called target vector, a mutant vector $\mathbf{v}_{i,g}$ is generated by adding a scaled, randomly sampled, vector difference to a basis vector randomly selected from the current population

Insight into classic DE (DE/rand/1/bin)

Example: at the *g*th generation, the *i*th mutant vector $\mathbf{v}_{i,g}$ with respect to *i*th target vector $\mathbf{x}_{i,g}$ in the current population is generated by $\mathbf{v}_{i,g} = \mathbf{x}_{r0,g} + F \cdot (\mathbf{x}_{r1,g} - \mathbf{x}_{r2,g})$, $i \neq r0 \neq r1 \neq r2$, mutation scale factor $F \in (0, 1+)$

Discrete recombination: with respect to each target vector $\mathbf{x}_{i,g}$ in the current population, a trial vector $\mathbf{u}_{i,g}$ is generated by crossing the target vector $\mathbf{x}_{i,g}$ with the corresponding mutant vector $\mathbf{v}_{i,g}$ under a pre-specified crossover rate $Cr \in [0,1]$

Example: at the g^{th} generation, the i^{th} trial vector $\mathbf{u}_{i,g}$ with respect to i^{th} target vector $\mathbf{x}_{i,g}$ in the current population is generated by:

$$u_{j,i,g} = \begin{cases} v_{j,i,g} & \text{if } \operatorname{rand}_{j}[0,1] \leq Cr \text{ or } j = j_{\text{rand}} \\ x_{j,i,g} & \text{otherwise} \end{cases}$$

Replacement

If the trial vector $\mathbf{u}_{i,g}$ has the better objective function value than that of its corresponding target vector $\mathbf{x}_{i,g}$, it replaces the target vector in the $(g+1)^{\text{th}}$ generation; otherwise the target vector remains in the $(g+1)^{\text{th}}$ generation



Illustration of classic DE



Illustration of classic DE



Four operating vectors in 2D continuous space



Mutation
Illustration of classic DE



Crossover

Illustration of classic DE



Replacement

Differentiation

Intelligent use of differences between individuals resulted in a simple linear operator, so-called differentiation, makes differential evolution unique.

Most important characteristics of DE: self-referential mutation!

Step size is adapted intrinsically along evolution process: large step size at beginning, small step size when converging.

Randomness of search direction and base vector retards convergence.

Modification of different components of DE can result in many DE variants:

Initialization

Uniform distribution, Gaussian distribution

Opposition-based initialization (Hamid R. Tizhoosh)

$$OP_{\mathbf{x},0}(j) = b_{j,U} + b_{j,L} - P_{\mathbf{x},0}(j), j = 1,...,D$$

Trial vector generation

- Base vector selection
 - > Random selection without replacement: $r_0 = \text{ceil}(\text{rand}_i[0,1] \cdot Np)$
 - > Permutation selection: r₀=permute[i]
 - > Random offset selection: $r_0 = (i + r_g) \% Np$ (e.g. $r_g = 2$)
 - > Biased selection: global best, local best and better

Differential mutation

- > One difference vector: $F \cdot (\mathbf{x}_{r1} \mathbf{x}_{r2})$
- > Two difference vector: $F \cdot (\mathbf{x}_{r1} \mathbf{x}_{r2}) + F \cdot (\mathbf{x}_{r3} \mathbf{x}_{r4})$
- > Mutation scale factor *F*
 - Crucial role: balance exploration and exploitation

Dimension dependence: *jitter* (rotation variant) and *dither* (rotation invariant)

* Randomization: different distributions of F

DE/rand/1:
$$\mathbf{V}_{i,G} = \mathbf{X}_{r_1,G} + F \cdot \left(\mathbf{X}_{r_2,G} - \mathbf{X}_{r_3,G}\right)$$

DE/best/1:
$$\mathbf{V}_{i,G} = \mathbf{X}_{best,G} + F \cdot \left(\mathbf{X}_{r_1,G} - \mathbf{X}_{r_2,G}\right)$$

DE/current-to-best/1:
$$\mathbf{V}_{i,G} = \mathbf{X}_{i,G} + F \cdot \left(\mathbf{X}_{best,G} - \mathbf{X}_{i,G}\right) + F \cdot \left(\mathbf{X}_{r_1,G} - \mathbf{X}_{r_2,G}\right)$$

DE/rand/2:
$$\mathbf{V}_{i,G} = \mathbf{X}_{r_1,G} + F \cdot \left(\mathbf{X}_{r_2,G} - \mathbf{X}_{r_3,G} + \mathbf{X}_{r_4,G} - \mathbf{X}_{r_5,G}\right)$$

DE/best/2:
$$\mathbf{V}_{i,G} = \mathbf{X}_{best,G} + F \cdot \left(\mathbf{X}_{r_1,G} - \mathbf{X}_{r_2,G} + \mathbf{X}_{r_3,G} - \mathbf{X}_{r_4,G}\right)$$

- Recombination
 - Discrete recombination (crossover) (rotation variant)
 - One point and multi-point
 - Exponential
 - Binominal (uniform)
 - > Arithmetic recombination
 - Line recombination (rotation invariant)
 - Intermediate recombination (rotation variant)
 - Extended intermediate recombination (rotation variant)



> Crossover rate $CR \in [0,1]$

Decomposable (small *CR*) and indecomposable functions (large *CR*)

Degenerate cases in the trial vector generation

For example, in classic DE, $r_1=r_2$, $r_0=r_1$, $r_0=r_2$, $i=r_0$, $i=r_1$, $i=r_2$

Better to generate mutually exclusive indices for target vector, base vector and vectors constituting the difference vector

Replacement

- One-to-one replacement
- Neighborhood replacement

Motivation for self-adaptation in DE

- The performance of DE on different problems mainly depends on:
- Population size
- **Strategy** and the associated parameter setting to generate trial vectors
- □ Replacement scheme

It is hard to choose a unique combination to successfully solve any problem at hand

- □ Population size usually depends on the problem scale and complexity
- During evolution, different strategies coupled with specific parameter settings may favor different search stages
- **□** Replacement schemes influence the population diversity
- □ Trial and error scheme may take excessive computational time & resources

Automatically adapt the configuration in DE so as to generate promising trial vectors during evolution

Related works

Practical guideline: for example, $Np \in [5D, 10D]$; Initial choice of F=0.5 and CR=0.1/0.9; Increase NP and/or F if premature convergence happens. Conflicting conclusions with respect to different test functions.

Fuzzy adaptive DE: use fuzzy logical controllers whose inputs incorporate the relative function values and individuals of successive generations to adapt the mutation and crossover parameters.

Self-adaptive Pareto DE: encode crossover rate in each individual, which is simultaneously evolved with other parameters. Mutation scale factor is generated for each variable according to Gaussian distribution N(0,1).

Zaharie: theoretically study the DE behavior so as to adapt the control parameters of DE according to the evolution of population diversity.

Self-adaptive DE (1): encode mutation scale factor in each individual, which is simultaneously evolved with other parameters. Crossover rate is generated for each variable according to Gaussian distribution N(0.5, 0.15).

DE with self-adaptive population: population size, mutation scale factor and crossover rate are all encoded into each individual.

Self-adaptive DE (2): encode mutation scale factor and crossover rate in each individual, which are reinitialized according to two new probability variables.

DE with strategy and parameter self-adaptation

Strategy adaptation: select one strategy from a pool of candidate strategies with the probability proportional to its previous successful experience to generate promising trial vectors within a certain learning period

Steps:

- □ Initialize selection probability $p_i = 1/num_st$, $i=1,...,num_st$ for every strategy
- According to the current probabilities, we employ *stochastic universal selection* to assign one strategy to each target vector in the current population
- □ For each strategy, we define $ns_{i,g}$ and $nf_{i,g}$, $i=1,...num_st$ to store the number of trial vectors successfully entering the next generation or discarded by applying this strategy, respectively, at the generation g.

- □ Success and failure memories are created to store those numbers within a specified number of previous generations, called "learning period (LP)".
- □ When the memories overflow, the first record of the earliest generation will be removed and the latest record will enter the memory.



• The selection probability p_i is updated by:

$$p_{k,G} = \frac{S_{k,G}}{\sum_{k=1}^{K} S_{k,G}} \qquad S_{k,G} = \frac{\sum_{g=G-LP}^{G-1} ns_{k,g}}{\sum_{g=G-LP}^{G-1} ns_{k,g} + \sum_{g=G-LP}^{G-1} nf_{k,g}} + \varepsilon \quad (k=1,2,..,num_st; G>LP)$$

• 4 strategies involved in the candidate pool:

DE/rand/1/bin: $\mathbf{V}_{i,G} = \mathbf{X}_{r_1,G} + F \cdot \left(\mathbf{X}_{r_2,G} - \mathbf{X}_{r_3,G}\right)$ DE/rand/2/bin: $\mathbf{V}_{i,G} = \mathbf{X}_{r_1,G} + F \cdot \left(\mathbf{X}_{r_2,G} - \mathbf{X}_{r_3,G} + \mathbf{X}_{r_4,G} - \mathbf{X}_{r_5,G}\right)$ DE/current-to-best/2/bin: $\mathbf{V}_{i,G} = \mathbf{X}_{i,G} + F \cdot \left(\mathbf{X}_{bestG} - \mathbf{X}_{i,G}\right) + F \cdot \left(\mathbf{X}_{r_1,G} - \mathbf{X}_{r_2,G} + \mathbf{X}_{r_3,G} - \mathbf{X}_{r_4,G}\right)$ DE/current-to-rand/1: $\mathbf{V}_{i,G} = \mathbf{X}_{i,G} + rand(0,1) \cdot \left(\mathbf{X}_{r_1,G} - \mathbf{X}_{i,G}\right) + F \cdot \left(\mathbf{X}_{r_2,G} - \mathbf{X}_{r_3,G}\right)$

Parameter adaptation

Mutation scale factor (*F*): for each target vector in the current population, we randomly generate *F* value according to a normal distribution N(0.5,0.3). Therefore, 99% *F* values fall within the range of [-0.4,1.4].

Crossover rate (CR_j) : when applying strategy *j* to a target vector, the corresponding CR_j value is generated according to an assumed distribution. We hereby assume that each CR_j , $j=1,...,num_st$ is normally distributed with its mean and standard deviation initialized to 0.5 and 0.1, respectively. Those CR_j values that had generated trial vectors successfully entering the next generation over previous generations are stored in a memory of size LP. The mean of CR_j normal distribution is updated at every generation after initial LP generations by using the median value in the memory.



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0.) 0.6

•3

82

0.1

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200

600

800

1000

Rastrigin function

Generation

1200

1800 2000

400

통 85 8.1

. and/2

Self-adaptation of crossover probability



Self-adaptation of trial vector generation strategy



- Performance comparison
 - > 10 methods in comparison
 - DE /rand/1/bin, F=0.9, CR=0.1
 - DE /rand/1/bin, F=0.9, CR=0.9
 - DE/rand/1/bin, F=0.5, CR=0.3
 - DE/rand-to-best/1/bin F=0.5, CR=0.3
 - DE/rand-to-best/2/ bin with F=0.5, CR=0.3

- Adaptive DE
- SDE
- *j*DE
- FADE
- SaDE
- > 26 numerical test functions: $f_1 \sim f_{14}$ (10D and 30D), $f_{15} \sim f_{26}$ (specified)
- > 30 independent runs for each algorithm
- Computational budgets: $f_1 \sim f_{14}$ (10D: 100,000 FEs; 30D: 300, 000 FEs); $f_{15} \sim f_{26}$ (500,000FEs)
- > Performance measures
 - Table: means & stds of objective functions values as well as the successful rate for $f_1 \sim f_{14}$; means of FEs for $f_{15} \sim f_{26}$ over 30 runs
 - Convergence map: median objective function value within 30 runs vs. FEs
 - Empirical distribution of normalized success performance

- General conclusions
 - In comparison with conventional DE, SaDE achieves smaller mean function values and higher success rates for all problems, while the convergence speed is faster for most problems.
 - In comparison with other adaptive DE variants, SaDE compares favorably with others.
 - Overall comparison: SaDE outperforms other algorithms in terms of empirical distribution of normalized success performance.

Evolutionary Optimization Algorithms (EOAs)

Part III: Research Plan Discussion

- **Statistical comparison and interactive selection of EOAs**
- Development of novel EOAs
- Applications
 - Computer vision and pattern recognition
 - Statistical modeling
 - > Bioinformatics

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Statistical Comparison of EOAs

D Motivations

- Many algorithms
- > Many operators
- > Many parameters
- **Objectives:** statistical comparison, grouping and ranking of EOAs

Challenges

- > Problem dependent
- Choose suitable performance measures
- Choose statistically sound comparison methods

D Pre-requisites

- Survey of existing benchmarking test problems
- Survey of existing performance measures
- Survey of existing comparison method

Research directions

- > Survey of existing benchmarking testbeds and comparison methods
- Investigation of inferential statistical tests
 - Symmetric hypothesis test
 - Random process
 - Factorial analysis of variance
- > Statistical comparison, grouping and ranking state-of-the-art PSO and DE

Interactive Selection of EOAs

D Motivations

- > Problem dependent
- > Requirement dependent
- > User dependent
- **Objectives:** user-friendly interactive selection software
- **Challenges**
 - Less known problem properties in practice

D Pre-requisite

> Statistical comparison, grouping and ranking of EOAs

Research plans

- > Iterative selection pipeline
- > Test on real applications
- > Online selection website

Development of Novel EOAs

- **Novel ensemble EOAs framework**
- **GMM**, extreme value theory and copula theory with EOAs
- **High-dimensional EOAs**
- **Common PC based parallel EOAs**

Applications

- Computer vision and pattern recognition
- Statistical modeling
 - > Any helps on model parameter estimation?
- **Bioinformatics**
 - Gene regulatory network model inference?
 - ► Gene selection?
 - > Any others?
- Other potential applications

Thanks

