Experimental Research in Evolutionary Computation

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Overview

Goals in Evolutionary Computation

(RG-1) *Investigation.* Specifying optimization problems, analyzing algorithms. Important parameters; what should be optimized?

(RG-2) *Comparison.* Comparing the performance of heuristics

(RG-3) *Conjecture.* Good: demonstrate performance. Better: explain and understand performance

(RG-4) *Quality.* Robustness (includes insensitivity to exogenous factors, minimization of the variability) [Mon01]

What happend so far?

- Presentations at MIC, HM, PPSN, CEC, GECCO, . . .
- More than a dozen talks, workshops and tutorials
- A few tens publications
- Next steps?

Next steps

- Learning from history
- Some ideas presented today

A Totally Subjective History of Experimentation in Evolutionary Computation

- Palaeolithic: Mean values
- Yesterday: Mean values and simple statistics
- Today: Correct statistics, statistically meaningful conclusions
- Tomorrow: Scientific meaningful conclusions

Some myth

- GAs are better than other algorithms (on average)
- Comparisons based on the mean
- One-algorithm, one-problem paper
- Everything is normal
- 10 (100) is a nice number
- One-max, Sphere, Ackley

Today: Based on Correct Statistics

Example (Good practice?)

- Authors used
  - Pre-defined number of evaluations set to 200,000
  - 50 runs for each algorithm
  - Population sizes 20 and 200
  - Crossover rate 0.1 in algorithm *A*, but 1.0 in *B*
  - *A* outperforms *B* significantly in f_6 to f_{10}

- We need tools to
  - Determine adequate number of function evaluations to avoid floor or ceiling effects
  - Determine the correct number of repeats
  - Determine suitable parameter settings for comparison
  - Determine suitable parameter settings to get working algorithms
  - Draw meaningful conclusions

- Problems of today:
  Adequate statistical methods, but wrong scientific conclusions

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High-Quality Statistics

- Fantastic tools to generate statistics: R, S-Plus, Matlab, Mathematica, SAS, ec.
- Nearly no tools to interpret scientific significance
- Fundamental problem in every experimental analysis: Is the observed value, e.g., difference, meaningful?
- Standard statistic: p-value
- Problems related to the p-value

High-Quality Statistics

- Fundamental to all comparisons - even to high-level procedures
- The basic procedure reads:

  Select test problem (instance) P
  Run algorithm A, say n times
  Obtain n fitness values: $x_{A,i}$
  Run algorithm B, say n times
  Obtain n fitness values: $x_{B,i}$

R-demo

- ```
  > n=100
  > run.algorithm1(n)
    [1]  99.53952  99.86982 101.65871...
  > run.algorithm2(n)
    [1]  99.43952  99.76982 101.55871...
  ```
- Now we have generated a plethora of important data - what is the next step?
- Select a test (statistic), e.g., the mean
- Set up a hypothesis, e.g., there is no difference
  ```

R-demo. Analysis

- Minimization problem
- For reasons of simplicity: Assume known standard deviation $\sigma = 1$
- Compare difference in means:

$$d(A, B, P, n) = \frac{1}{n}\sum_{i=1}^{n}(x_{A,i} - x_{B,i})$$

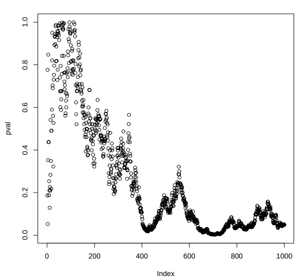
- Formulate hypotheses:

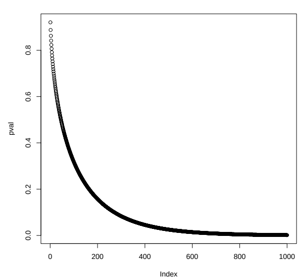
  H_0: $d <= 0$ there is no difference in means vs.
  H_1: $d > 0$ there is a difference (B is better than A)

R-demo. Analysis

- ```
  > n=5
  > run.comparison(n)
  [1] 0.8230633
  ```
- Hmmm, that does not look very nice. Maybe I should perform more comparisons, say $n = 10$
- ```
  > n=10
  > run.comparison(n)
  [1] 0.7518296
  ```
- Hmmm, looks only slightly better. Maybe I should perform more comparisons, say $n = 100$
- ```
  > n=100
  > run.comparison(n)
  [1] 0.3173105
  ```
- I am on the right way. A little bit more CPU-time and I have the expected results.
  ```
  > n=1000
  > run.comparison(n)
  [1] 0.001565402
  ```
- Wow, this fits perfectly.

Large n problem





Scientific?

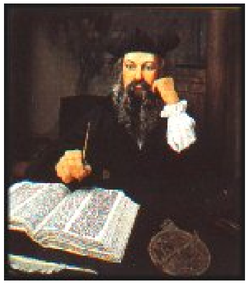
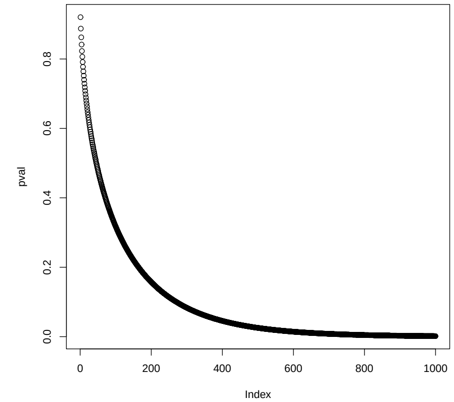


Figure: Nostradamus


  ```

Tomorrow: Correct Statistics and Correct Conclusions

- Tomorrow:
  - Consider scientific meaning
  - Severe testing as a basic concept
  - First Symposium on Philosophy, History, and Methodology of Error, June 2006
- To discover the scientific meaning of a result, it is necessary to pose the right question in the beginning
- In the beginning: before we perform experiments

Why are we performing experiments?

- Why are we interested in improving the algorithm's performance?
  - Because it does not find any feasible solution or
  - Because it has to be competitive to the best known algorithm
- How do we define importance or significance?
- Many statistics available
- Each measure will produce its own ranking
- Planning of experiments

First step: Archeology—Detect factors

Figure: Schliemann in Troja

- "Playing trumpet to tulips" or "experimenter's socks"
- In contrast to field studies: Computer scientists have all the information at hand
- First classification:

  algorithm
  problem

Classification

- Algorithm design
  - Population size
  - Selection strength
- Problem design
  - Search space dimension
  - Starting point
  - Objective function
- Vary problem design $\Longrightarrow$ effectivity (robustness)
- Vary algorithm design $\Longrightarrow$ efficiency (tuning)

Efficiency

- Tuning
- Problems
  - Many factors
  - Real–world problem: complex objective function (simulation) and only small number of function evaluations
  - Theoretical investigations: simple objective function and many function evaluations
- Screening to detect most influential factors

Factor effects

- Important question: Does a factor influence the algorithm's performance?
- How to measure effects?
- First model:

$$Y = f(\vec{X}),$$

  where
  - $\vec{X} = (X_1, X_2, \dots, X_r)$ denote r factors from the algorithm design and
  - Y denotes some output (i.e., best function value from 1000 generations)
- Problem design remains unchanged

Measures for factor effects

- Overview

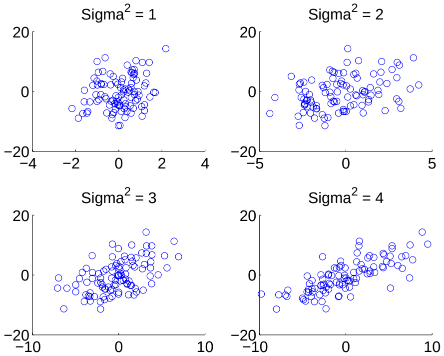
  Statistics: Variance (V's)
  Calculus: Derivation (∂'s)
  DoE: Regression coefficients (β's)
  DACE: Coefficients (θ's)
  Graphics: Visualizations

Measures: Variance

Example (Toy problem)

$$Y = f(\vec{X}) = \sum_{i=1}^{r} \alpha X_i$$

- $X_i \sim N(0, \sigma_i^2)$
- $r = 4$, $\sigma_i^2 = i$



Measures: Variance

Example (Toy problem)

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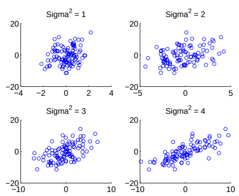


- Effect should produce shape or pattern
- Effect of factor

$$\frac{V_i(E_{-i}(Y|X_i))}{V(Y)}$$

Measures: Variance

Example (Summary: Toy problem)

- $Y = f(\vec{X}) = \sum_{i=1}^{r} \alpha X_i$ far too simple
- Which of the factors can be fixed without affecting Y
- Detect important less important factors
- Interactions

Measures: Derivation based

- Evaluate the function at a set of different points in the problem domain
- Define the *effect* of the ith factor as incremental ratio

$$\frac{f(X_1, X_2, \ldots, X_i + \Delta, \ldots, X_r) - f(X_1, \ldots X_r)}{\Delta}$$

Measures: regression based

- Regression based measures
- Relate the *effect* of the ith factor to its regression coefficient

$$Y = \beta_0 + \sum_{i=1}^{r} \beta_i X_i$$

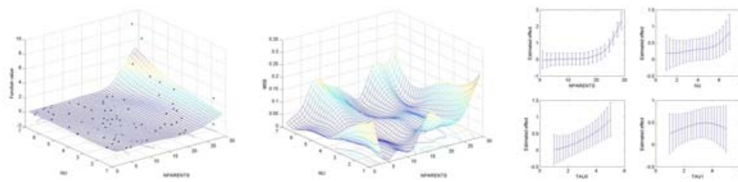
- Related: Kriging based measures

Screening Evolution Strategies

- Detect important factors
- CMA-ES [HO01]
- Screening uses tools from SPOT

SPO in Action

- Sequential Parameter Optimization Toolbox (SPOT)
- Introduced in [BB06]



- Software can be downloaded from `http://www.gm.fh-koeln.de/~bartz/experimentalresearch/spot.zip`

SPO Installation

- Create a new directory, e.g., `g:\myspot`
- Unzip SPO toolbox
- Unzip MATLAB DACE toolbox: `http://www2.imm.dtu.dk/~hbn/dace/`
- Unzip CM-ES package from Nikolas Hansen's WWW-page.
- Start MATLAB
- Add `g:\myspot` to MATLAB path
- Run `spotdriver('demo1000')`

SPO Region of Interest (ROI)

- *Region of interest* (ROI) files specify the region, over which the algorithm parameters are tuned

```
name low high isint pretty
NPARENTS 1 10 TRUE 'NPARENTS'
NU 1 5 FALSE 'NU'
TAU1 1 3 FALSE 'TAU1'
```

Figure: demo1000.roi

SPO Configuration file

- *Configuration* files (CONF) specify SPO specific parameters, such as the regression model

```
new=0
defaulttheta=1
loval=1E-3
upval=100
spotrmodel='regpoly2'
spotcmodel='corrgauss'
isotropic=0
repeats=3
...
```

Figure: demo1000.m

SPO Output file

- *Design* files (DES) specify algorithm designs
- Generated by SPO
- Read by optimization algorithms

```
TAU1 NPARENTS NU TAU0 REPEATS CONFIG SEED STEP
0.210507 4.19275 1.65448 1.81056 3 1 0 1
0.416435 7.61259 2.91134 1.60112 3 2 0 1
0.130897 9.01273 3.62871 2.69631 3 3 0 1
1.65084 2.99562 3.52128 1.67204 3 4 0 1
0.621441 5.18102 2.69873 1.01597 3 5 0 1
1.42469 4.83822 1.72017 2.17814 3 6 0 1
1.87235 6.78741 1.17863 1.90036 3 7 0 1
0.372586 3.08746 3.12703 1.76648 3 8 0 1
2.8292 5.85851 2.29289 2.28194 3 9 0 1
...
```

Figure: demo1000.des

Algorithm: Result File

- Algorithm run with settings from design file
- Algorithm writes *result file* (RES)
- RES files provide basis for many statistical evaluations/visualizations
- RES files read by SPO to generate stochastic process models

```
Y NPARENTS FNAME ITER NU TAU0 TAU1 KAPPA NSIGMA RHO DIM CONFIG SEED
3809.15 1 Sphere  500 1.19954 0 1.29436 Inf 1 2 2  1 1
0.00121541  1 Sphere  500 1.19954 0 1.29436 Inf 1 2 2 1 2
842.939 1 Sphere 500 1.19954 0 1.29436 Inf 1 2 2  1 3
2.0174e-005 4 Sphere 500 4.98664 0 1.75367 Inf 1 2 2  2 1
0.000234033 4 Sphere 500 4.98664 0 1.75367 Inf 1 2 2  2 2
1.20205e-007  4 Sphere 500 4.98664 0 1.75367 Inf 1 2 2  2 3
...
```

Figure: demo1000.res

Summary: SPO Interfaces

- SPO requires CONF and ROI files
- SPO generates DES file
- Algorithm run with settings from DES
- Algorithm writes *result file* (RES)
- RES files read by SPO to generate stochastic process models
- RES files provide basis for many statistical evaluations/visualizations (EDA)

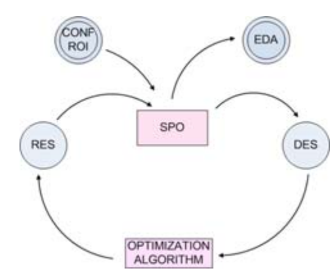
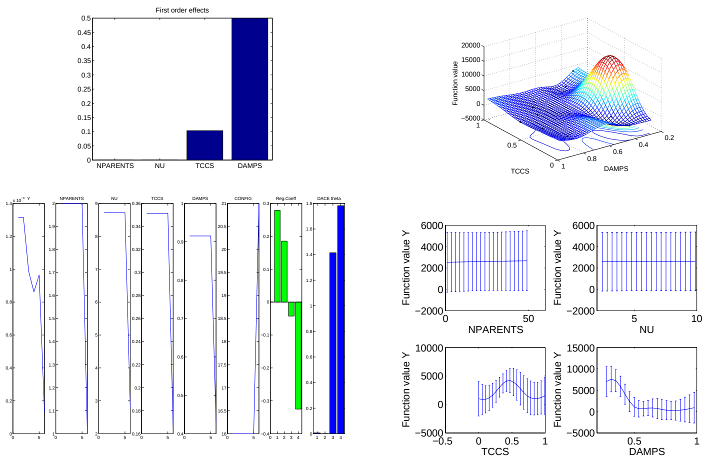


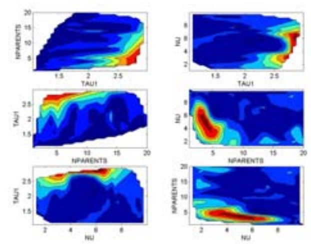
Figure: SPO Interfaces

SPO live demo: some impressions

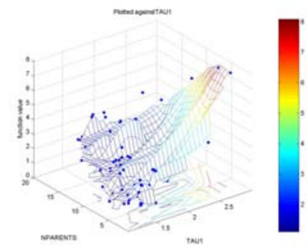


SPO and EDA

- Interaction plots
- Main effect plots
- Regression trees
- Scatter plots



- Box plots
- Trellis plots
- Design plots
- ...



SPO Open Questions

- Models?
  - (Linear) Regression models
  - Stochastic process models
  - Tree-based models
- Designs?
  - Space filling
  - Factorial
  - Combinations
- Statistical tools
- Significance
- Standards

- TBD
  - Provide SPOT interfaces for important optimization algorithms
  - Tools to derive meta-statistical rules
  - Other tools needed, because *p* value is not sufficient

The Art of Comparison

Orientation

The NFL[1] told us things we already suspected:

- We cannot hope for the one-beats-all algorithm (solving the general nonlinear programming problem)
- Efficiency of an algorithm heavily depends on the problem(s) to solve and the exogenous conditions (termination etc.)

In consequence, this means:

- The posed question is of extreme importance for the relevance of obtained results
- The focus of comparisons has to change from:
  - *Which algorithm is better?* to questions like
  - *What exactly is the algorithm good for?*
    How can we generalize the behavior of an algorithm?
    $\Rightarrow$ *Rules of thumb, finally theory?*

[1] no free lunch theorem

The Art of Comparison

Efficiency vs. Adaptability

Most existing experimental studies focus on the efficiency of optimization algorithms, but:

- Adaptability to a problem is not measured, although
- It is known as one of the important advantages of EAs

Interesting, previously neglected aspects:

- Interplay between adaptability and efficiency?
- How much effort does adaptation to a problem take for different algorithms?
- What is the problem spectrum an algorithm performs well on?
- Systematic investigation may reveal inner logic of algorithm parts (operators, parameters, etc.)

What is the Meaning of Parameters?

Are Parameters “Bad”?

Cons:

- Multitude of parameters dismays potential users
- It is often not trivial to understand parameter-problem or parameter-parameter interactions

  ⇒ Parameters complicate evaluating algorithm performances

But:

- Parameters are simple handles to modify (adapt) algorithms
- Many of the most successful EAs have lots of parameters
- New theoretical approaches: Parametrized algorithms / parametrized complexity, (“two-dimensional” complexity theory)

Possible Alternatives?

Parameterless EAs:

- Easy to apply, but what about performance and robustness?
- Where did the parameters go?

Usually a mix of:

- Default values, sacrificing top performance for good robustness
- Heuristic rules, applicable to *many* but not *all* situations; probably not working well for completely new applications
- (Self-)Adaptation techniques, these cannot learn too many parameter values at once, and not necessarily reduce the number of parameters

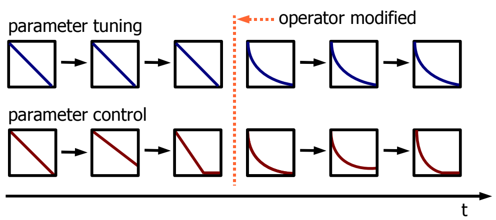
⇒ We can reduce number of parameters, but usually at the cost of either performance or robustness

Parameter Control or Parameter Tuning?

The time factor:

- Parameter control: during algorithm run
- Parameter tuning: before an algorithm is run

But: Recurring tasks, restarts, or adaptation (to a problem) blur this distinction

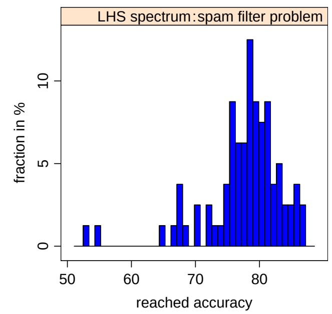


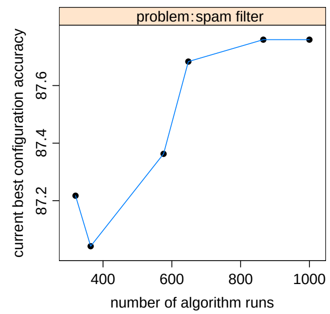
And: How to find meta-parameter values for parameter control?
⇒ Parameter control *and* parameter tuning

Tuning and Comparison

What do Tuning Methods (e.g. SPO) Deliver?

- A best configuration from $\{perf(alg(arg_t^{exo}))|1 \leq t \leq T\}$ for T tested configurations
- A spectrum of configurations, each containing a set of single run results
- A progression of current best tuning results





How do Tuning Results Help?

...or Hint to new Questions

What we get:

- A near optimal configuration, permitting top performance comparison
- An estimation of how good any (manually) found configuration is
- A (rough) idea how hard it is to get even better

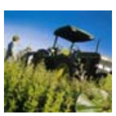
No excuse: A first impression may be attained by simply doing an LHS

Yet unsolved problems:

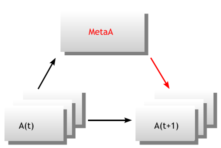
- How much amount to put into tuning (fixed budget, until stagnation)?
- Where shall we be on the spectrum when we compare?
- Can we compare spectra ($\Rightarrow$ adaptability)?

Similarities and Differences to Existing Approaches

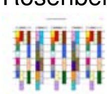
- Agriculture, industry: Design of Experiments (DoE)



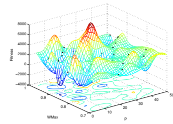
- Evolutionary algorithms: Meta-algorithms



- Algorithm engineering: Rosenberg Study (ANOVA)



- Statistics: Design and Analysis of Computer Experiments (DACE)



Empirical Analysis: Algorithms for Scheduling Problems

1

- Problem:
  - Jobs build binary tree
  - Parallel computer with ring topology
- 2 algorithms:
  - Keep One, Send One (KOSO) to my right neighbor
  - Balanced strategy KOSO*: Send to neighbor with lower load only
- Is KOSO* better than KOSO?

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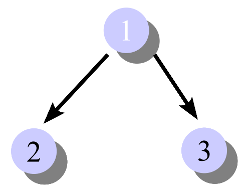

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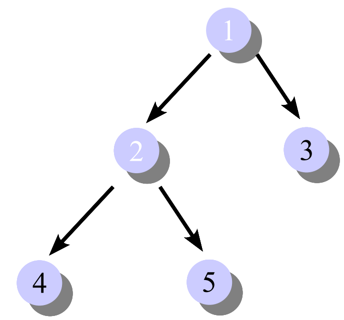

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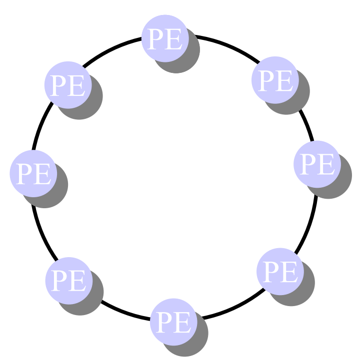

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Empirical Analysis: Algorithms for Scheduling Problems

- Hypothesis: Algorithms influence running time
- But: Analysis reveals
  - # Processors und # Jobs explain 74 % of the variance of the running time
  - Algorithms explain nearly nothing
- Why?
  - Load balancing has no effect, as long as no processor starves.
  - But: Experimental setup produces many situations in which processors do not starve
- Furthermore: Comparison based on the optimal running time (not the average) makes differences between KOSO und KOSO*.
- Summary: Problem definitions and performance measures (specified as algorithm and problem design) have significant impact on the result of experimental studies

Designs

- Sequential Parameter Optimization based on
  - Design of Experiments (DOE)
  - Design and Analysis of Computer Experiments (DACE)
- Optimization run = experiment
- Parameters = design variables or factors
- Endogenous factors: modified during the algorithm run
- Exogenous factors: kept constant during the algorithm run
  - Problem specific
  - Algorithm specific

SPO Overview

1. Pre-experimental planning
2. Scientific thesis
3. Statistical hypothesis
4. Experimental design: Problem, constraints, start-/termination criteria, performance measure, algorithm parameters
5. Experiments
6. Statistical model and prediction (DACE, Regression trees, etc.). Evaluation and visualization
7. Solution good enough?
   - Yes: Goto step 8
   - No: Improve the design (optimization). Goto step 5
8. Acceptance/rejection of the statistical hypothesis
9. Objective interpretation of the results from the previous step: severity etc.

Statistical Model Building and Prediction

Design and Analysis of Computer Experiments (DACE)

- Response Y: Regression model and random process
- Model:

$$Y(x) = \sum_h \beta_h f_h(x) + Z(x)$$

  - $Z(\cdot)$ correlated random variable
  - Stochastic process.
  - DACE stochastic process model
- Until now: DACE for deterministic functions, e.g. [SWN03]
- New: DACE for stochastic functions

Expected Model Improvement

Design and Analysis of Computer Experiments (DACE)

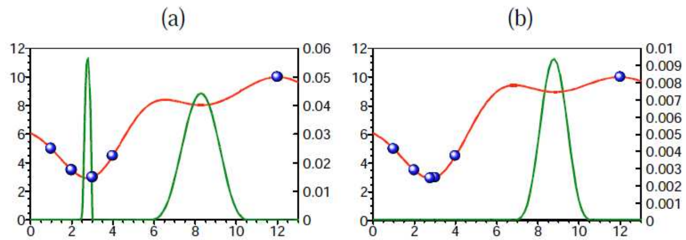


Figure: Axis labels left: function value, right: expected improvement. Source: [JSW98]

(a) Expected improvement: 5 sample points
(b) Another sample point $x = 2.8$ was added

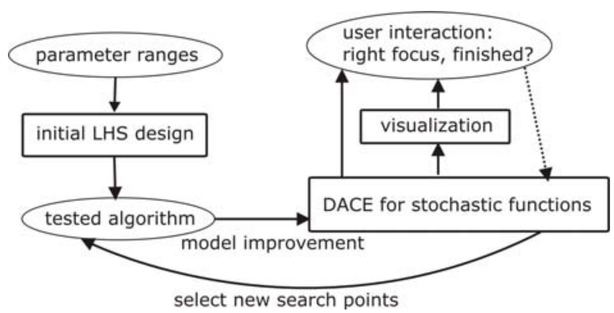
Heuristic for Stochastically Disturbed Function Values

- Latin hypercube sampling (LHS) design: Maximum spread of starting points, small number of evaluations
- Sequential enhancement, guided by DACE model
- Expected improvement: Compromise between optimization (min Y) and model exactness (min MSE)
- Budget-concept: Best search points are re-evaluated
- Fairness: Evaluate new candidates as often as the best one

Table: SPO. Algorithm design of the best search points

Y	s	c_1	c_2	w_{max}	w_{scale}	w_{iter}	v_{max}	Conf.	n
0.055	32	1.8	2.1	0.8	0.4	0.5	9.6	41	2
0.063	24	1.4	2.5	0.9	0.4	0.7	481.9	67	4
0.061	32	1.8	2.1	0.8	0.4	0.5	9.6	41	4
0.058	32	1.8	2.1	0.8	0.4	0.5	9.6	41	8

Data Flow and User Interaction



- User provides parameter ranges and tested algorithm
- Results from an LHS design are used to build model
- Model is improved incrementally with new search points
- User decides if parameter/model quality is sufficient to stop

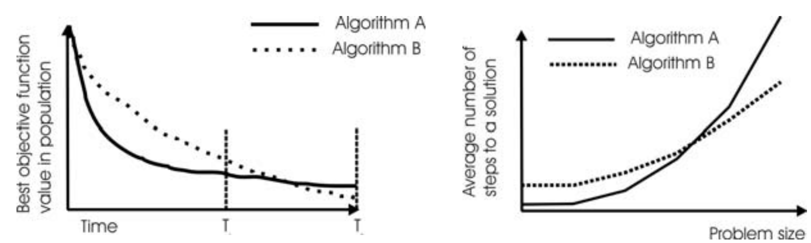
□

"Traditional" Measuring in EC

Simple Measures

- MBF: mean best fitness
- AES: average evaluations to solution
- SR: success rates, SR(t) $\Rightarrow$ run-length distributions (RLD)
- best-of-n: best fitness of n runs

But, even with all measures given: Which algorithm is better?



(figures provided by Gusz Eiben)

Aggregated Measures

Especially Useful for Restart Strategies

Success Performances:

- SP1 [HK04] for equal expected lengths of successful and unsuccessful runs $\mathbb{E}(T^s) = \mathbb{E}(T^{us})$:
$$SP1 = \frac{\mathbb{E}(T_A^s)}{p_s} \quad (1)$$
- SP2 [AH05] for different expected lengths, unsuccessful runs are stopped at FE_{max}:
$$SP2 = \frac{1 - p_s}{p_s} FE_{max} + \mathbb{E}(T_A^s) \quad (2)$$

Probably still more aggregated measures needed (parameter tuning depends on the applied measure)

Choose the Appropriate Measure

- Design problem: Only best-of-n fitness values are of interest
- Recurring problem or problem class: Mean values hint to quality on a number of instances
- Cheap (scientific) evaluation functions: exploring limit behavior is tempting, but is not always related to real-world situations

In real-world optimization, 10^4 evaluations is a lot, sometimes only 10^3 or less is possible:

- We are relieved from choosing termination criteria
- Substitute models may help (Algorithm based validation)
- We encourage more research on short runs

Selecting a performance measure is a *very* important step

Current “State of the Art”

Around 40 years of empirical tradition in EC, but:

- No standard scheme for reporting experiments
- Instead: one (“Experiments”) or two (“Experimental Setup” and “Results”) sections in papers, providing a bunch of largely unordered information
- Affects readability and impairs reproducibility

Other sciences have more structured ways to report experiments, although usually not presented in full in papers. Why?

- Natural sciences: Long tradition, setup often relatively fast, experiment itself takes time
- Computer science: Short tradition, setup (implementation) takes time, experiment itself relatively fast

⇒ We suggest a 7-part reporting scheme

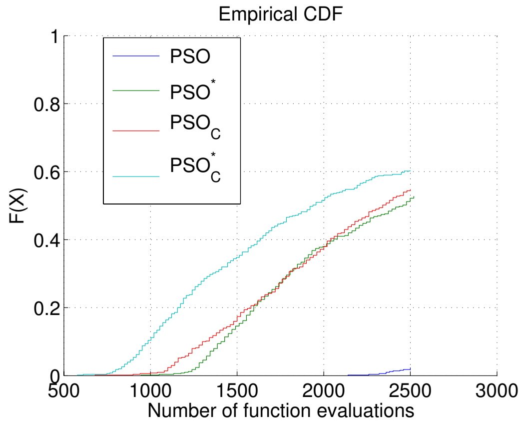
Suggested Report Structure

ER-1: **Research Question** the matter dealt with
ER-2: **Pre-experimental planning** first—possibly explorative—program runs, leading to task and setup
ER-3: **Task** main question and scientific and derived statistical hypotheses to test
ER-4: **Setup** problem and algorithm designs, sufficient to replicate an experiment
ER-5: **Results/Visualization** raw or produced (filtered) data and basic visualizations
ER-6: **Observations** exceptions from the expected, or unusual patterns noticed, plus additional visualizations, no subjective assessment
ER-7: **Discussion** test results and necessarily subjective interpretations for data and especially observations

This scheme is well suited to report 12-step SPO experiments

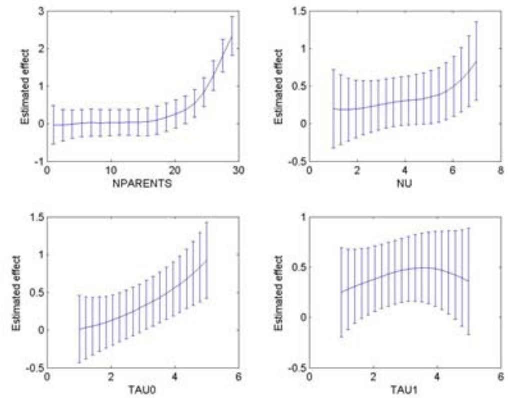
Objective Interpretation of the Results

Comparison. Run-length distribution



(Single) Effect Plots

Useful, but not Perfect

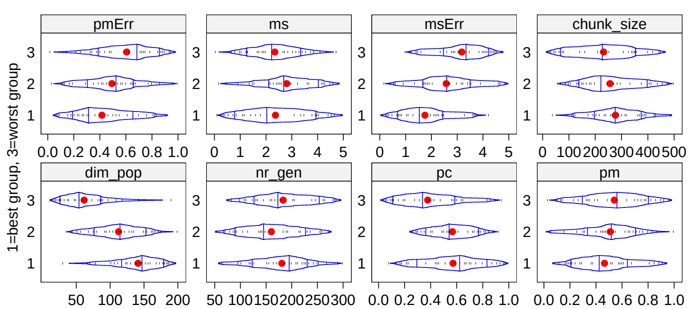


- Large variances originate from averaging
- The τ_0 and especially τ_1 plots show different behavior on extreme values (see error bars), probably distinct (averaged) effects/interactions

One-Parameter Effect Investigation

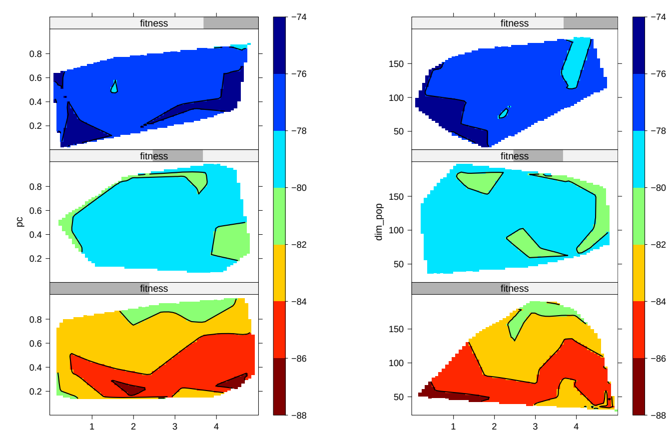
Effect Split Plots: Effect Strengths

- Sample set partitioned into 3 subsets (here of equal size)
- Enables detecting more important parameters visually
- Nonlinear progression 1–2–3 hints to interactions or multimodality



Two-Parameter Effect Investigation

Interaction Split Plots: Detect Leveled Effects



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Updates

- Please check
  `http://www.gm.fh-koeln.de/~bartz/experimentalresearch/ExperimentalResearch.html`
  for updates, software, etc.

Discussion

- SPO is not the final solution—it is one possible (but not necessarily the best) solution
- Goal: continue a discussion in EC, transfer results from statistics and the philosophy of science to computer science
- Standards for good experimental research
- Review process
- Research grants
- Meetings
- Building a community
- Teaching
- ...

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