Automatic and Interactive Tuning of Algorithms

Agenda

Thomas	s Bartz-Beielstein ¹ Mike F	Preuss ²			 Introduction Why Experimentation 	ı?	SPO Toolbox (SPOT) Toolbox		
¹ Faculty	of Computer Science and Engineering Cologne University of Applied Sciences	Science			Computer Science Ex Why Algorithm Tuning	xperiments g?	SPOT Case Studies Settings		
	² Department of Computer Science TU Dortmund				2 Tuning: Goals and Prob Goals	olems	Automated versus Int Tuning	eractive	
	July 2011				Factors Settings Tuning Outcome Experimental Primer Performance Measuri Visualization & Repor	ing rting	 6 Extensions and Further Approaches 7 Problems and Developr What can go Wrong? Tuning Efficiency 8 Suggested Readings 	nent	
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Instructor Biographies

intro

- Dr. Thomas Bartz-Beielstein is a professor for Applied Mathematics at Cologne University of Applied Sciences. He has published more than several dozen research papers, presented tutorials about tuning, and has edited several books in the field of Computational Intelligence. His research interests include optimization, simulation, and statistical analysis of complex real-world problems
- Mike Preuss is research associate at the Computer Science Department, TU Dortmund. His main fields of activity are EAs for real-valued problems and their application in numerous engineering domains, the development of the experimental methodology for stochastic optimization, and Computational Intelligence techniques in computer games (see DETA track).
- Prof. Bartz-Beielstein and Mike Preuss invented the sequential parameter optimization, which was applied as a tuner for numerous optimization algorithms such as evolution strategies, differential evolution, or particle swarm optimization

Objectives of the Tutorial

intro

- (O-1) *Tuning*. Making your algorithms faster (and more reliable)
- (O-2) Understanding and Learning. Helping you to understand your algorithms (so that forthcoming versions will run even much faster)
- (O-3) Provide Experimental Guidelines. Enables you to perform solid experiments one can learn from where theory is not applicable
- (O-3) Pros and Cons. Consider benefits and disadvantages of state-of-the-art tuning approaches
- (O-4) Networking. Meet and get into contact with others who are interested in tuning. Discuss open issues and interesting research projects in experimental research

Bartz

Why Do We Need Experimentation?

why experimentation?

- Practitioners need so solve problems, even if theory is not developed far enough
- Counterargument of practitioners: Tried that once, didn't work (expertise needed to apply convincingly)
- We need to establish guidelines how to adapt the algorithms to practical problems (or let them Self*)
- Helps theoreticians to find exploitable (parameter/problem) relations

Experimental methodology is improving, we are leaving the phase of

- a) Funny but useless performance figures
- b) Lots of better and better algorithms that soon disappear again

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Why Do We Need Experimentation?

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- Helps theoreticians to find exploitable (parameter/problem) relations

Instead, we converge to

a) Deliberate and justified choice of parameters, problems, performance criteria—no more arbitrariness

Algorithm Engineering How Theoreticians Handle it...(Recently)

b) Better generalizability (not quite resolved, but targetted)

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	intro	why experimentation?				intro	experimentation in comp	uter science		

Are We Alone (With This Problem)?

In natural sciences, experimentation is not in question

- Many inventions (batteries, x-rays, ...) made by experimentation, sometimes unintentional
- Experimentation leads to theory, theory has to be *useful* (can we do predictions?)

In computer science, the situation seems different

- 2 widespread stereotypes influence our view of computer experiments:
- a) Programs do (exactly) what algorithms specify
- b) Computers (programs) are deterministic, so why statistics?



This is an experiment



Is this an experiment?

- Algorithm Engineering is theory + real data + concrete implementations + experiments
- Principal reason for experiments: Test validity of theoretical claims
- Are there important factors in practice that did not go into theory?
- Approach also makes sense for metaheuristics, but we start with no or little theory
- Measuring (counting evaluations) usually no problem for us



algorithm engineerir	realistic models 1 design falsifiable	
analysis	3 hypotheses 5 experiments	è
deduction	induction 4	G
perf	implementation	Ű
guarantees	algorithm- libraries	

intro experimentation in computer science

frequency

So What About Statistics?

Are the methods all there? Some are, but:

- Our data is usually not normal
- We can most often have lots of data
- This holds for algorithmics, also!
- These are not the conditions statisticians are used to
- In some situations, there is just no suitable test procedure

Best of run distribution ES 100-peaks problem 10



log(best fitness)

 \Rightarrow There is a need for more statistics and more statistical methods.

Catherine McGeogh:

Our problems are unfortunately not sexy enough for the Statisticians...

Algorithms, Parameters and the Reasoning for Tuning

- We have learned to think in parameters where others hide these as constants
- Consequently, we include (generic!) adaptability of algorithms to problems in the algorithm design
- Knowledge about parameter interactions helps us to understand algorithms and problems
- This helps us to approach the final question: Which algorithm (or which parameter set) do I apply for my problem ?

But:

- How do we do it?
- Tuning is expensive, cannot be applied in all situations
- \Rightarrow Experimental methodology and reliable tuning methods needed

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	tuning goals & problems goals				tuning goals & problems	factors			
	Tuning: Goals			First step	: Archeolo	gy—Dete	ect Factors		

- (TG-1) Performance. Important parameters; what should be optimized?
- (TG-2) Comparison. Comparing the performance of heuristics
- (TG-3) Conjecture. Good: demonstrate performance. Better: explain and understand performance Needed: Looking at the behavior of the algorithms, not only results
- (TG-4) Quality. Robustness (includes insensitivity to exogenous factors, minimization of the variability) [Mon01] Invariance properties (e.g., CMA-ES): Find out, for what (problem, parameter, measure) spaces our results hold



Figure: Schliemann in Troja

 \Rightarrow We have (beside others) a parameter problem, many EAs highly depend on choosing them 'right'

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

algorithm problem

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Components of an Experiment in Metaheuristics



Classification



- Problem design
 - Search space dimension
 - Starting point
 - Objective function
- Vary problem design \implies effectivity (robustness)
- Vary algorithm design \implies efficiency (tuning)

- July 2011 13 / 58 Bartz-Beielstein, Preuss (Cologne, Dortmund) Automatic and Interactive Tuning July 2011 12/58 Bartz-Beielstein, Preuss (Cologne, Dortmund) Automatic and Interactive Tuning tuning goals & problems tuning goals & problems factor factors Factor Effects Factors: Overview
 - Important question: Does a factor influence the algorithm's performance?
 - How to measure effects?
 - First model:

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

where

- $\vec{X} = (X_a, X_p)$, where X_a and X_p denote factors from the algorithm and problem design, respectively and
- Y denotes some output (i.e., best function value from 1000 generations)
- Uncertainty analysis: compute average output, standard deviation, outliers \Rightarrow related to Y
- Sensitivity analysis: which of the factors are more important in influencing the variance in the model output $Y? \Rightarrow$ related to the relationship between X_a, X_p and Y



Problems and Algorithms

SASP – Single Algorithm, Single Problem

Tuning can be performed for

(SASP) One single algorithm and one single problem instance

(SAMP) One single Algorithm and multiple problems instances

(MASP) Multiple algorithms and one single problem instance

(MAMS) Multiple algorithms and multiple problem instances

- How to perform comparisons?
- Adequate statistics?

- Typical real-world setting
- Determine important factors
- Optimization
- Crucial: number of function evaluations
- Benefit:
 - \$\$\$

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SAMP – Sin	gle Algorithm, Multi	ple Problems		MASP – Mu	Itiple Algo	rithms, Si	ingle Problem	

- Algorithm development
- Determine important factors
- Optimization
- Robustness
- Benefit:
 - Determine important factors
 - Understanding

- Research (beginner's paper \Rightarrow rejected)
- Optimization
- Note: multiple algorithms \sim one algorithm with different parameters
- Tuning and comparison
- Benefit:
 - · Similarities between algorithms
 - Understanding

MAMP – Multiple Algorithms, Multiple Problems

settings

tuning goals & problems

- Research (expert paper \Rightarrow accepted)
- Comparison
- Huge complexity
- Benefit:
 - Accepted paper

- A best configuration from {*perf*(*alg*(*arg*^{exo}_t))|1 ≤ t ≤ T} for T tested configurations
- A spectrum of configurations, each containing a set of single run results
- Detect unsuitable parameter configurations



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	tuning goals & problems tuning outcome				tuning goals & problems	tuning outcome		

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Bartz-Beielstein, Preuss (Cologne, Dortmund)

A Simple, Visual Approach: Sample Spectra







- Large variances originate from averaging
- The τ₀ and especially τ₁ plots show different behavior on extreme values (see error bars), probably distinct (averaged) effects/interactions

Automatic and Interactive Tuning

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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

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Research Question

- Not trivial \Rightarrow many papers are not focused
- The (real) question is not: Is my algorithm faster than others on a set of benchmark functions?
- What is the added value? Difficult in Metaheuristics.
 - Wide variance of treated problems
 - Usually (nearly) black-box: Little is known

Horse racing: set up, run, comment...

Explaining observations leads to new questions:

- Multi-step process appropriate (also for tuning)
- Conjectures obtained from results shall itself be tested experimentally
- Range of validity shall be explored (problems, parameters, etc.)



Einstein thinking

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	experimental primer				experimental primer			
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Research Question

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Horse racing: set up, run, comment...NO!

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Einstein thinking

How to Set Up Research Questions?

It is tempting to create a new algorithm, but

- There are many existing algorithms not really understood well
- We shall try to aim at improving our knowledge about the 'working set'
- When comparing, always ask if any difference is meaningful in practice

Usually, we do not know the 'perfect question' from the start

- An inherent problem with experimentation is that we do (should) not know the outcome in advance
- But it may lead to new, better questions
- Try small steps, expect the unexpected





experimental primer performance measuring

"Traditional" Measuring in EC

• 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?



Aggregated Measures

Especially Useful for Restart Strategies

Success Performances:

SP1 [HK04] for equal expected lengths of successful and unsuccessful runs 𝔅(𝔅^s) = 𝔅(𝔅^{us}):

$$SP1 = \frac{\mathbb{E}(T_A^s)}{\rho_s} \tag{1}$$

 ERT(*f_{target}*) as used in the BBOB setup for different expected lengths, unsuccessful runs are stopped at *FE_{max}*:

$$ERT(f_{target}) = \frac{\#FEs(f_{best} \ge f_{target})}{\#succ}$$
(2)

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

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	experimental primer performance measuri	na		experimental primer performance measuring	

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 (horizontal)
- Or tasks reachable with short runs (vertical)

Selecting a performance measure is a very important step

Convergence of Measuring Perspectives



(Thomas Bartz-Beielstein)

(Anne Auger/Nikolaus Hansen)

- · Vertical: Probably nearer to real-world situation
- Horizontal: Easier to interpret (BBOB'09), but targets must be fixed
- However, we have still distributions! Mean or median may be insufficient!
- Carlos Fonseca: Attainment surfaces?

Diagrams Instead of Tables

Reporting and Keeping Track of Experiments



Around 40 years of experimental tradition in EC, but:

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

Keeping experimental journals helps:

- Record context and rough idea
- Report each experiment
- Running where (machine)
- Finished when (date/time), link to result file(s)

 \Rightarrow We suggest a 7-part reporting scheme (also well suited for tuning experiments)

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	experimental primer	visualization&reporting				spot	sequential parameter opt	timization toolbox		
Sua	pested Re	eport Strue	cture			SP	OT			

- ER-1: Focus/Title 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 SPO experiments (but not only)

- Sequential parameter optimization toolbox (SPOT)
- Developed over recent years by Thomas Bartz-Beielstein, Christian Lasarczyk, and Mike Preuss [BBLP05]
- Main goals of SPOT
 - Determination of improved parameter settings for optimization algorithms
 - Provide statistical tools for analyzing and understanding their performance

Use information from the exploration of the search space to

guide the search by building one or several meta models

Choose new design points based on predictions from the

• Refine the meta model(s) stepwise to improve knowledge

SPOT: Definition

SPOT-1 Use the available budget (e.g., simulator runs, number of

SPOT-2 If necessary, try to cope with *noise* by improving confidence.

Guarantee comparable confidence for search points

SPOT-3 Collect information to *learn* from this tuning process, e.g., apply

SPOT-4 Provide mechanisms both for *interactive* and *automated tuning*

Definition (Sequential Parameter Optimization Toolbox)

meta model(s)

explorative data analysis

function evaluations) sequentially:

about the search space

sequential parameter optimization toolbox

SPOT Applications

- SPOT was successfully applied in the fields of
 - bioinformatics [Vol06, FMKH09]
 - environmental engineering [KZBB09, FBBD⁺10]
 - fuzzy logic [Yi08]
 - multimodal optimization [PRT07]
 - statistical analysis of algorithms [Las07, TM09]
 - multicriteria optimization [BBNWW09]
 - genetic programming [LB05]
 - particle swarm optimization [BBPV04, KGG07]
 - automated and manual parameter tuning [Fob06, SE09, HBBH⁺09, HHLBM10]
 - graph drawing [Tos06, Pot07]
 - aerospace and shipbuilding industry [NQBB06, RPQ09]
 - mechanical engineering [MMLBB07]
 - chemical engineering [HBK⁺08]
 - Bartz-Beielstein [BB10] collects publications related to the sequential parameter optimization

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	spot sequential parameter op	timization toolbox			spot	sequential parameter or	ptimization toolbox		
	SPOT Tasks			Factor	s. Desian	s and Pre	dictors		

- SPOT provides tools to perform the following tasks:
 - Initialize. Generate an initial design: parameter region and constant algorithm parameters
 - Run. Start optimization algorithm with configurations of the generated design. The algorithm provides the results to SPOT
 - Sequential step. Generate a new design, based on information from the algorithms result. A prediction model is used in this step. Several generic prediction models are available in SPOT already. User-specified prediction models can easily be integrated
 - · Report. Generate an analysis, based on information from the results. SPOT contains some scripts to perform a basic regression analysis and plots such as histograms, scatter plots, plots of the residuals, etc.
 - Automatic mode. In the automatic mode, the steps run and sequential are performed after an initialization for a predetermined number of times.

- Factors
 - Numerical
 - Categorical (ordered and unordered)
- Designs
 - Classical fractional factorial designs
 - Space-filling designs, e.g., Latin hypercube designs
- Predictors
 - Linear regression
 - Regression trees
 - Tree based Gaussian process

Factors, Designs and Predictors

spot sequential parameter optimization toolbox

Predictors

btgpllm z Improv stats (g=1)

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		case studies settings					C
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					137	1	

case studies settings

SPOT Applications



• Box plots • Trellis plots • Design plots

Plotted against TAU

TAU1

• ...

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	case studies settings				case studies settings		
SPC	DT: Sensitivity Anal	ysis			SPOT: EDA		

btgpllm z mean

SPOT: EDA



Automated versus Interactive Tuning





RESTARTS effect plot

IPSF effect plot

- Interactive
 - Expert knowledge
 - · Simple models and designs, e.g., classical fractional factorial designs and response surface
 - Insight
 - Understanding
- Automated
 - Time consuming
 - · Complex models, e.g., (tree based) Gaussian process
 - Limited insight

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	further approaches				further approaches			
S	SPOT is not alone			SF	POT Open (Questions		
 Tuning methods are an ac Comparison of algori unsuitable algorithms Tuning reveals param 	ctive research area: thms without parameter tur s neter relevance and interact	ing is comparing ions		 Models? (Linear) Regress Stochastic procession Designs? Space filling Factorial 	sion models ess models	 SPOT Community: Provide SPOT ini important optimiz algorithms Simple and open specification 	erfaces fo ation	ſ

Recent methods:

- F-Race (Birattari, Stützle): Iterative bad parameter elimination
- REVAC (Nannen, Eiben, Smit): Meta-EDA
- Probably more to come...

- Factorial
- Statistical tools
- Significance
- Standards
- SPO is a methodology more than just an optimization algorithm (Synthese)
- Recent trend: SPOT used as an optimizer

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• Currently available for

several algorithms, more

than a dozen applications

problems & development what can go wrong?

problems & development what can go wrong?

A Famous Example: The Rosenberg Study

Automatic and Interactive Tuning

A Famous Example: The Rosenberg Study

Automatic and Interactive Tuning

• Problem:

· Jobs build binary tree

- Parallel computer with ring topology
- 2 algorithms:

Bartz-Beielstein, Preuss (Cologne, Dortmund)

Keep One, Send One (KOSO) to my right neighbor Balanced strategy KOSO*: Send to neighbor with lower load only

• Is KOSO* better than KOSO?

1

- Problem:
 - Jobs build binary tree
 - Parallel computer with ring topology
- 2 algorithms:

Bartz-Beielstein, Preuss (Cologne, Dortmund)

Keep One, Send One (KOSO) to my right neighbor Balanced strategy KOSO*: Send to neighbor with lower load only

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problems & development what can go wrong?	problems & development what can go wrong?
A Famous Example: The Rosenberg Study	A Famous Example: The Rosenberg Study
 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? 	 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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problems & development what can go wrong?	problems & development what can go wrong?
A Famous Example: The Rosenberg Study	Experimental Analysis: What is the Problem?
	 Hypothesis: Algorithms influence running time
	 But: Analysis reveals
 Jobs build binary tree	# Processors und # Jobs explain 74 % of the variance of the running time
 Parallel computer with ring topology 	Algorithms explain nearly nothing
2 algorithms:	• Why?
Keep One, Send One (KOSO) to my right neighbor Balanced strategy KOSO*: Send	Load balancing has no effect, as long as no processor starves. But: Experimental setup produces many situations in which processors do not starve
to neighbor with lower load only Is KOSO* better than KOSO?	 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

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	problems & development	what can go wrong?				problems & development	what can go wrong?		
Flo	or and Co	eilina Effe	ects			Confound	ed Effects		

Floor and Ceiling Effects

- Floor effect: Compared algorithms attain set task very rarely \Rightarrow Problem is too hard
- Ceiling effect: Algorithms nearly always reach given task
 ⇒ Problem is too easy

If problem is too hard or too easy, nothing is shown. Tuning processes will fail because of insufficient feedback!

- Pre-experimentation is necessary to obtain reasonable tasks
- If task is reasonable (e.g. practical requirements), then algorithms are unsuitable (floor) or all good enough (ceiling), statistical testing does not provide more information
- Arguing on minimal differences is statistically unsupported and scientifically meaningless

Two or more effects or helper algorithms are merged into a new technique, which is improved

• Where does the improvement come from?

experimental studies

- It is necessary to test both single effects/algorithms, too
- Either the combination helps, or only one of them
- Knowing that is useful for other researchers!



complex machinery

Underestimated Randomness

-220

-300

ean(-HV)

-332

min(-HV)

-324

- Idea: Find Pareto front of two tuning criteria
- Parameter changes not interpretable
- Validation failed
- Reason: Deviations much too high!



More difficulties: See also papers of the GECCO'09 workshop Learning from Failures in Evolutionary Computation (LFFEC)

There Is a Problem With the Experiment

After all data is in, we realize that something was wrong (code, parameters, environment?), what to do?

- Current approach: Either do not mention it, or redo everything
- If redoing is easy, nothing is lost
- If it is not, we must either:
 - · Let people know about it, explaining why it probably does not change results
 - Or do validation on a smaller subset: How large is the difference (e.g. statistically significant)?
- Do not worry, this situation is rather normal
- Thomke: There is nearly always a problem with an experiment
- Early experimentation reduces the danger of something going completely wrong

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	problems & development tuning efficiency				problems & development tuning efficiency		

Efficiency vs. Adaptability

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

- Adaptability (how expensive is it to adapt the algorithm) to a problem is usually not measured, although
- It is known as one of the important advantages of EAs (this is all tuning is about!)
- Measure suggested in [Pre09]
- Adaptability is the hardness of the tuning problem

Interesting, previously neglected aspects:

- Interplay between adaptability and efficiency?
- What is the problem spectrum an algorithm performs well on?
- Systematic investigation may reveal inner logic of algorithm parts (operators, parameters, etc.)

How to Tune On Real-World Problems?

Idea: We build a surrogate model of the problem and use it for algorithm tuning, then apply tuned algorithm to original problem



- Possible solution for expensive problems, but can this work?
- Yes, but we need enough points to capture the local structure of the problem
- ${\tt 1375}$ \Rightarrow First successful study (Preuss/Rudolph/Wessing) GECCO'10

problems & development tuning efficiency

Realtime Tuning

(Wessing/Preuss/Rudolph), GECCO'11

Idea: Modern EA's as the CMA-ES need many restarts, why not do these with (slightly) different parameters?



• On non-trivial problem instances, this is nearly always an advantage

• Does not help on trivial or very hard instances (floor/ceiling effects)

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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