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Meaningful Problem Instances and Generalizable Results

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Abstract

Computational intelligence methods have gained importance in several real-world domains such as process optimization, system identification, data mining, or statistical quality control. Tools are missing, which determine the applicability of computational intelligence methods in these application domains in an objective manner. Statistics provide methods for comparing algorithms on certain data sets. In the past, several test suites were presented and considered as state of the art. However, there are several drawbacks of these test suites, namely: (i) problem instances are somehow artificial and have no direct link to real-world settings; (ii) since there is a fixed number of test instances, algorithms can be fitted or tuned to this specific and very limited set of test functions; (iii) statistical tools for comparisons of several algorithms on several test problem instances are relatively complex and not easily to analyze. We propose a methodology to overcome these difficulties. It is based on standard ideas from statistics: analysis of variance and its extension to mixed models. This chapter combines essential ideas from two approaches: problem generation and statistical analysis of computer experiments.

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1 Introduction

Computational intelligence (CI) methods have gained importance in several real-world domains such as process optimization, system identification, data mining, or statistical quality control. Tools are missing, which determine the applicability of CI methods in these application domains in an objective manner. Statistics provide methods for comparing algorithms on certain data sets. In the past, several test suites were presented and considered as state of the art. However, there are several drawbacks of these test suites, namely:

- problem instances are mostly artificial and have no direct link to real-world settings;
- since there is a fixed number of test instances, algorithms can be fitted or tuned to this specific and very limited set of test functions. As a consequence, studies (benchmarks) provide insight how these algorithms perform on this specific set of test instances, but no insight on how they perform in general;
- statistical tools for comparisons of several algorithms on several test problem instances are relatively complex and not easy to analyze.

We propose a methodology to overcome these difficulties. This methodology, which generates problem classes rather than uses one instance, is constructed as follows.

1. First, we pre-process the underlying real-world data.

2. In a second step, features from these data are extracted. This extraction relies on the assumption that mathematical variables can be used to represent real-world features. For example, decomposition techniques can be applied to model the underlying data structures, if we are using time-series data. The original time series is deconstructed into a number of component series, where each of these reflects a certain type of behavior, e.g., a trend or seasonality[9]. We obtain an analytic model of the data.

3. Then, we parametrize this model. Based on this parametrization and randomization, we can generate infinitely many new problem instances.

4. If no real-world data are available, problem instances can be generated using test-problem generators. The generation of test problems, which are well-founded and have practical relevance, is an on-going field of research for several decades.

5. From this infinite set, we can draw a limited number of problem instances which will be used for the comparison.

6. Since problem instances are selected randomly, we apply random and mixed models for the analysis [15]. Mixed models include fixed and random effects. A fixed effect is an unknown constant. Its estimation from the data is a common practice in analysis of variance (ANOVA) or regression. A random effect is a random variable. We are estimating the

parameters that describe its distribution, because—in contrast to fixed effects—it makes no sense to estimate the random effect itself.

This chapter combines ideas from two approaches: problem generation and statistical analysis of computer experiments. The work presented by Chiarandini and Goegebeur [11] provides the basis of our statistical analysis. They present a systematic and well-developed framework for mixed models. Related modeling approaches were suggested by McGeoch[14] and Birattari [7]. Gallagher and Yuan [13] present a problem instance (landscape) generator that is parameterized by a small number of parameters, and the values of these parameters have a direct and intuitive interpretation in terms of the geometric features of the landscapes that they produce. Castiñeiras, Cauwer, and O'Sullivan [10] present a parametrizable benchmark generator for bin packing instances based on the well-known Weibull distribution. Using the shape and scale parameters of the Weibull distribution, the authors generate benchmarks that contain a variety of item size distributions. They report that for all bin capacities, the number of bins required in an optimal solution increases as the Weibull shape parameter increases. Using this feature, scalability is enabled.

Basically, this chapter tries to find answers for the following fundamental questions in experimental research.

(Q-1) How to generate problem instances?

(Q-2) How to generalize experimental results?

The chapter is structured as follows. Section 2 introduces real-world and artificial optimization problems. Algorithms are described in Sect. 3. Objective functions and statistical models are introduced in Sect. 4. These models take problem and algorithm features into consideration. Section 5 presents case studies, which illustrate our methodology. This chapter closes with a summary and an outlook.

2 Features of Optimization Problems

2.1 Problem Classes and Instances

Nowadays, it is a common practice in optimization to choose a *fixed* set of problem instances in advance and to apply classical ANOVA or regression analysis. In many experimental studies a few problem instances π_i $(i = 1, 2, \ldots, q)$ are used and results of some runs of the algorithms α_j $(j = 1, 2, \ldots, h)$ on these instances are collected. The instances can be treated as *blocks* and all algorithms are run on each single instance. Results are grouped per instance π_i. Analyses of these experiments shed some light on the performance of the algorithms on those specific instances. However, the interest of the researcher should not be just the performance of the algorithms on those specific instances chosen, but rather on the generalization of the results to the entire class Π. Generalizations

about the algorithm's performance on new problem instances are difficult or impossible in this setting.

Based on ideas from Chiarandini and Goegebeur [11], to overcome this difficulty, we propose the following approach: A small set of problem instances $\{\pi_i \in \Pi | i = 1, 2, \ldots, q\}$ is chosen at random from a large set, or class Π, of possible instances of the problem. Problem instances are considered as factor levels. However, this factor is of a different nature from the fixed algorithmic factors in the classical ANOVA setting. Indeed, the levels are chosen at random and the interest is not in these specific levels but in the problem class Π from which they are sampled. Therefore, the levels and the factor are *random*. Consequently, our results are not based on a limited, fixed number of problem instances. They are randomly drawn from an infinite set, which enables generalization.

2.2 Feature Extraction and Instance Generation

A problem class Π can be generated in different manners. We will consider *artificial* and *natural* problem class generators. Artificially generated problems allow feature generation based on some predefined characteristics. They are basically theory driven, i.e., the researcher defines certain features such as linearity or multi modality. Based on these features, a model (formula) is constructed. By integrating parameters into this formula, many problem instances can be generated by parameter variation. We will exemplify this approach in the following paragraph. The second way, which will generate natural problem classes, uses a three-stage approach. First, the real-word system and its components are described. Then, features are extracted from a real-world system. Based on this feature set, a model is defined. Adding parameters to this model, new problem instances can be generated. There is also a third way to "generate" test instances: if we are lucky, many data are available. In this case, we can sample a limited number of problem instances from the larger set of real-world data. The statistical analysis is similar for these three cases.

2.2.1 Artificial Test Functions

Several problem instance generators have been proposed over the last years. For example, Gallagher and Yuan present a landscape test generator, which can be used to set up problem instances for continuous, bound-constrained optimization problems [13]. The *Max-Set of Gaussian Landscape Generator* (MSG) uses the maximum of m weighted Gaussian functions

$$G(x) = \max_{i \in 1,2,\ldots,m} (w_i g_i(x)),$$

where $g : \mathbb{R}^n \to \mathbb{R}$ denotes an n-dimensional Gaussian function

$$g(x) = \left(\frac{\exp\left(-\frac{1}{2}(x-\mu)\Sigma^{-1}(x-\mu)^T\right)}{(2\pi)^{n/2}|\Sigma|^{1/2}} \right)^{1/n},$$

μ is an n-dimensional vector of means, and Σ is an $(n \times n)$ covariance matrix. The mean of each Gaussian corresponds to an optimum on the landscape and the location of all optima is known. The global optimum is the one with the largest value. We will use the MSG problem instance generator in Sect. 5 to demonstrate our approach.

2.2.2 Natural Problem Classes

This section exemplifies the three fundamental steps for generating real-world problem instances, namely

1. Describing the real-world system and its data
2. Feature extraction and model construction
3. Instance generation.

We will illustrate this procedure by using the classic Box and Jenkins airline data [8]. These data contain the monthly totals of international airline passengers from 1949 to 1961. The feature extraction is based on methods from time-series analysis. Because of its simplicity the Holt-Winters method is popular in many application domains. It is able to adapt to changes in trends and seasonal patterns. The Holt-Winters prediction function requires the estimation of three parameters, i.e., α, β and γ, which can be estimated from original time-series data. Their optimal values are determined by minimizing the squared one-step prediction error. To generate new problem instances, these parameters can be slightly modified. Based on these modified values, the model is re-fitted. Finally, we can extract the new time series. One typical result from this instance generation is shown in Fig. 1. Bartz-Beielstein [2] describes this procedure in detail.

To illustrate the wide applicability of this approach, we will list further real-work problem domains, which are subject of our current research.

Smart Metering. The development of accurate forecasting methods for electrical energy consumption profiles is an important task. We consider time series collected from a manufacturing process. Each time series contains quarter-hourly samples of the energy consumption of a bakery. A detailed data description can be found in [3].

Water Industry. CANARY is a software developed by the *United States Environmental Protection Agency* (US EPA) and Sandia National Laboratories. Its purpose is to detect events in the context of water contamination. An event is in this context defined as a certain time period where a contaminant significantly deteriorates the water quality. Distinguishing events from (i) background changes, (ii) maintenance and modification due to operation, and (iii) outliers is an essential task, which was implemented in the CANARY software. Therefore, deviations are compared to regular patterns and short term changes. The corresponding data contains multivariate time-series data. It is a selection from a larger dataset shipped with the open source event-detection software CANARY developed by US EPA and Sandia National Laboratories [19].

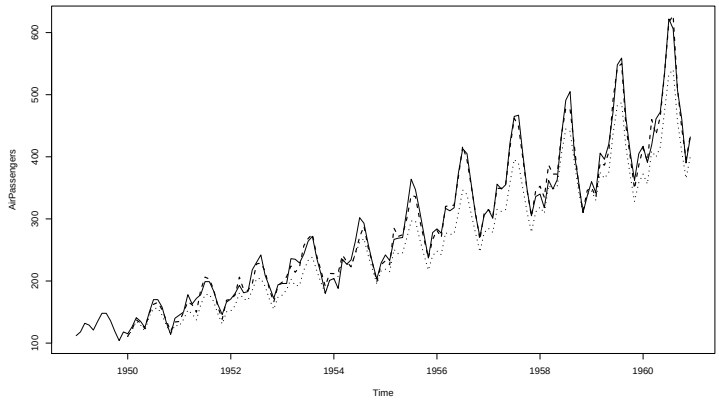

Figure 1: Holt-Winters problem instance generator. The *solid* line represents the real data, the *dotted* line predictions from the Holt-Winters model and the *fine dotted* line modified predictions, respectively.

Finance. The data are real-world data from intraday *foreign exchange* (FX) trading. The FX market is a financial market for trading currencies to enable international trade and investment. It is the largest and most liquid financial market in the world. Currencies can be traded via a wide variety of different financial instruments, ranging from simple spot trades over to highly complex derivatives. We are using three foreign exchange (currency rate) time series collected from Bloomberg. Each time series contains hourly samples of the change in currency exchange rate [12].

One typical goal in forecasting is the minimization of the forecast errors or the differences between real (observed) values, say y_i, and predicted values, say $\hat{y}_i$. This goal can be considered as an optimization problem.

As stated in Sect. 2.2, the statistical analysis is similar for artificial and natural problem classes. Our goal can be stated as follows: For a given problem class Π, which can be artificial or natural, we are trying to determine if an optimization algorithm α or several algorithm instances α_i show similar behavior on randomly selected problem instances $\pi_i \in \Pi$. This question will be formulated as a statistical hypothesis. Based on the related statistical framework, we can determine confidence intervals for the performance of the algorithm on unseen problem instances.

3 Algorithm Features

3.1 Factors and Levels

Evolutionary algorithms (EA) belong to the large class of bio-inspired search heuristics. They combine specific components, which may be *qualitative*, like the recombination operator or *quantitative*, like the population size. Our interest is in understanding the contribution of these components. In statistical terms, these components are called *factors*. The interest is in the effects of the specific *levels* chosen for these factors. Hence, we say that the levels and consequently the factors are *fixed*. Although modern search techniques like sequential parameter optimization or Pareto genetic programming [18] allow multi-objective performance measures (solution quality versus variability or description length), we restrict ourselves to analyze the effect of these factors on a univariate measure of performance. We will use the quality of the solutions returned by the algorithm at termination as the performance measure.

3.2 Example: Evolution Strategy

Evolution strategies (ES) are prominent representatives of evolutionary algorithms, which includes genetic algorithms and genetic programming as well [17]. They can be classified as generic population-based metaheuristic optimization algorithms for global optimization that in some sense mimics the natural evolution. Evolution strategies are applied to hard real-valued optimization problems. Mutation is performed by adding a normally distributed random value to each vector component. The standard deviation of these random values is modified by self-adaptation. Evolution strategies can use a population of several solutions. Each solution is considered as as individual and consists of object and strategy variables. Object variables represent the position in the search space, whereas strategy variables store the step sizes, i.e., the standard deviations for the mutation. We are analyzing the ES basic variant, which has been proposed in [6].

Mutation means neighborhood-based movement in search space that includes the exploration of the "outer space" currently not covered by a population, whereas recombination rearranges existing information and so focuses on the "inner space". Selection is meant to introduce a bias towards better fitness values. A concrete ES may contain specific mutation, recombination, or selection operators, or call them only with a certain probability, but the control flow is usually left unchanged. Each of the consecutive cycles is termed a *generation*. The control flow is shown in Fig. 2. Concerning the representation, it should be noted that most empiric studies are based on canonical forms as binary strings or real-valued vectors, whereas many real-world applications require specialized, problem dependent ones. Table 1 summarizes important ES parameters. This chapter presents two case studies. The first case study is based on a fixed ES parameter setting, whereas the second case study modifies the recombination operator for object variables. We are convinced that the applicability of the

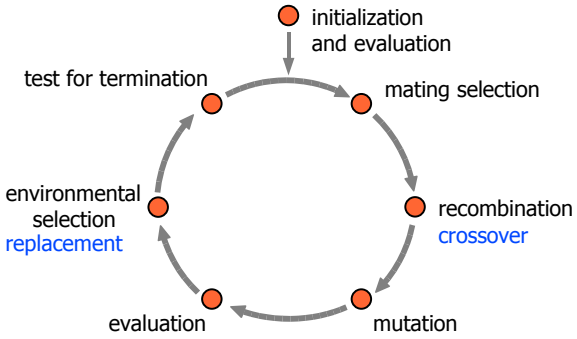

Figure 2: The evolutionary cycle, basic working scheme of all ES and EA. Terms common for describing evolution strategies are used, alternative terms are added below in blue.

methods presented in this chapter goes far beyond the simplified case studies. Our main contribution is a framework, which allows conclusions that are not limited to a small number of problem instances but to problem classes.

4 Objective Functions

We will use the following optimization framework: An ES is applied as a minimizer on the test function $f(x)$. Formally speaking, let S denote some set, e.g., $S \subseteq \mathbb{R}^n$. We are seeking for values f^* and x^*, such that $\min_{x \in S} f(x)$ with $f^* = \min_{x \in S} f(x)$ and $x^* = \arg\min f(x)$. This approach can be extended in many ways. For example, if S denotes times-series data, then an optimization algorithm can be applied to minimize the empirical mean squared prediction error.

Test problem instances will be drawn from Gallagher's and Yuan's MSG test function generator. The following parameters can be used to specify the MSG generator.

- The number of Gaussian components m.
- The mean vector μ of each component.
- The covariance matrix Σ of each component.
- The weight of each component w_i.
- A maximum threshold $t \in [0; 1]$ can be specified for local optima and the fitness value of the global optimum G^*. Local optima are randomly generated within $[0; t \times G^*]$.

Table 1: Settings of exogenous parameters of an ES. Recombination operators are labeled as follows: 1=no, 2=dominant, 3=intermediate, 4=intermediate as in [6]. Mutation uses the following encoding: 1 = no mutation, 2 = self adaptive mutation.

Parameter	Symbol	Name	Range	Value
mue	μ	Number of parent individuals	$\mathbb{N}$	5
nu	$\nu = \lambda/\mu$	Offspring-parent ratio	$\mathbb{R}_+$	2.0
sigmaInit	$\sigma_i^{(0)}$	Initial standard deviations	$\mathbb{R}_+$	1.0
nSigma	n_σ	Number of standard deviations. d denotes the problem dimension	$\{1, d\}$	1
	c_τ	Multiplier for individual and global mutation parameters	$\mathbb{R}_+$	1.0
tau0			$\mathbb{R}_+$	0.0
tau			$\mathbb{R}_+$	1.0
rho	ρ	Mixing number	$\{1, \mu\}$	2
sel	κ	Maximum age	$\mathbb{R}_+$	1.0
mutation		Mutation	$\{1, 2\}$	2
sreco	r_σ	Recombination operator for strategy variables	$\{1, 2, 3, 4\}$	3
oreco	r_x	Recombination operator for object variables	$\{1, 2, 3, 4\}$	2

The following tuple can be used to specify an MSG generator:

$$\Pi := ([-c, c]^n, n, m, D_\mu, \{D_\Sigma\}, \{t, G^*\}), \tag{1}$$

where $c \in \mathbb{R}$ defines the boundary constraints of the search space, n the search space dimensionality, m the number of Gaussian components, D_μ the distribution used to generate the mean vectors of components, D_Σ the distribution or procedures used to generate covariances of components, $t \in [0; 1]$ the threshold for local optima, and G^* the function value of the global optimum.

Based on Eq. (1), we have specified the following MSG landscape generator for our experiments:

$$\begin{aligned}\Pi_{\text{MSG}} := \big([-1; 1]^2, 2, 10, &\mathcal{U}[-1; 1], \{\mathcal{U}[0.05; 0.15], \\ &\mathcal{U}[-\pi/4, \pi/4]\}, \{0.8, 1\}\big)\,.\end{aligned} \tag{2}$$

With this setting, the mean vector of each component is generated randomly within $[-1, 1]^2$. The covariance matrix of each component is generated with the procedure D_Σ in three steps:

1. A diagonal matrix S with eigenvalues is generated.
2. An orthogonal matrix T is generated through $n(n-1)/2$ rotations with random angles between $[-\pi/4, \pi/4]$.
3. The covariance matrix is generated as $T^T S T$.

The weight w_i of the component corresponding to the global optimum is set to 1 while other weights are randomly generated within $[0; 0.8]$. The nine problem instances, $\pi_i \in \Pi_{\text{MSG}}$, $(i = 1, \ldots, 9)$ from Fig. 3 were generated with this parametrization.

Note, we are using the distance to the optimum as an objective function in our experiments. Our objective function reads $G^* - f(x)$, because we are considering minimization problems. Other measures of interest might be the *gap percent of optimality* $(G^* - f(x))/G^* \times 100$, or computation time etc., see, e.g. [1].

5 Case Studies

Bartz-Beielstein introduced the acronyms

- 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

for classifying optimization designs [4].

5.1 Single Problem Designs: SASP and MASP

In SASP we are analyzing the performance of an *optimization algorithm* α on a single problem instance π. An optimization problem has a set of input data which instantiate the problem. This might be a function in continuous optimization or the location and distances between cities in a traveling salesman problem. In the following, we will use Y to denote the random performance measure obtained by r runs of algorithm α on problem instance π. Because many optimization algorithms such as evolutionary algorithms are randomized, their performance Y on one instance is a random variable. It might be described by a probability density/mass function $p(y|\pi)$. Running the algorithm with different random seeds on one problem instance, we collect sample data $y_1, \ldots, y_r$, which are *independent and identically distributed* (i.i.d.).

There are situations, in which SASP is the method of first choice. Real-world problems, which have to be solved only once in a very limited time, are good examples for using SASP optimizations. MASP shares several characteristics with SASP. Because of their limited capacities for generalization, SASP and MASP will not be further investigated in this study.

5.2 SAMP: Single Algorithm, Multiple Problems

5.2.1 Fixed-effects Models

This setup is commonly used for testing an algorithm on a given (fixed) set of problem instances. Standard assumptions from *analysis of variance* (ANOVA) lead us to propose the following *fixed-effects model* [15]:

$$Y_{ij} = \mu + \tau_i + \varepsilon_{ij}, \tag{3}$$

where μ is an overall mean, τ_i is a parameter unique to the ith treatment (problem instance factor), and ε_{ij} is a random error term for replication j on problem instance i. Usually, the model errors ε_{ij} are assumed to be normally and independently distributed with mean zero and variance σ^2. If problem instance factors are considered fixed, i.e., non random, the stochastic behavior of the response variable originates from the algorithm. This implies the experimental results

$$Y_{ij} \sim N(\mu + \tau_i, \sigma^2), \quad i = 1, \ldots, q,\ j = 1, \ldots, r, \tag{4}$$

and that the Y_{ij} are mutually independent. Results from statistical analyses remain valid only on the specific instances. Furthermore, SAMP with a fixed set of problem instances is subject to criticism, e.g., that algorithms are trained for this specific set up test instances (over fitting).

In order to make the results of the analysis independent on the specific instances and dependent instead on the class of instances from which the specific instances are drawn, Chiarandini and Goegebeur propose randomized and mixed models for the experimental analysis of optimization algorithms as an extension of (3) [11]. In contrast to model (3), these models allow generalizations of results to the whole class of instances.

5.2.2 Randomized Models

In the following, we consider a population or *class* of instances Π. The class Π consists of a large, possibly an infinite, number of problem instances $\pi_i, i = 1, 2, 3, \ldots$ Let $p(\pi)$ denote the probability of sampling instance π. The performance Y of the algorithm α on the class Π is described by the probability function

$$p(y) = \sum_{\pi \in \Pi} p(y|\pi)p(\pi). \tag{5}$$

If we ran an algorithm α r times on instance π, then we receive r replicates of α's performance, denoted by $Y_1, \ldots, Y_r$. These r observations are i.i.d., i.e.,

$$p(y_1, \ldots, y_r|\pi) = \prod_{j=1}^{r} p(y_j|\pi). \tag{6}$$

So far, we have considered r replicates of the performance measure Y on *one* problem instance π. Now consider *several*, randomly sampled problem instances. Over all the instances the joint probability distribution of the observed performance measures is obtained by marginalizing over all instances:

$$p(y_1, \ldots, y_r) = \sum_{\pi \in \Pi} p(y_1, \ldots, y_r|\pi)p(\pi). \tag{7}$$

Extending the model (7) to the case where one algorithm with several parameter settings or several algorithms are analyzed leads to mixed models, which will be discussed in Sec. 5.3.

5.2.3 Example SAMP: ES on Π_1 (Random-Effects Design)

The simplest random-effects experiment is performed as follows. For $i = 1, \ldots, q$ a problem instance π_i is drawn randomly from the class of problem instances Π. On each of the sampled π_i, the algorithm α is run r times using different seeds for α. Due to α's stochastic nature, we obtain, *conditionally on the sampled instance*, r replications of the performance measure that are i.i.d.

Let Y_{ij} $(i = 1, \ldots, q;\ j = 1, \ldots, r)$ denote the random performance measure obtained in the jth replication of α on π_i. We are interested in drawing conclusions about α's performance on a larger set of problem instances from Π, and not just on those q problem instances included in the experiment. A systematic approach to accomplish this task comprehends the following steps.

SAMP-1 Algorithm and Problem Instances
SAMP-2 ANOVA and REML Model Building
SAMP-3 Validation of the Model Assumptions
SAMP-4 Hypothesis Testing
SAMP-5 Confidence Intervals and Prediction

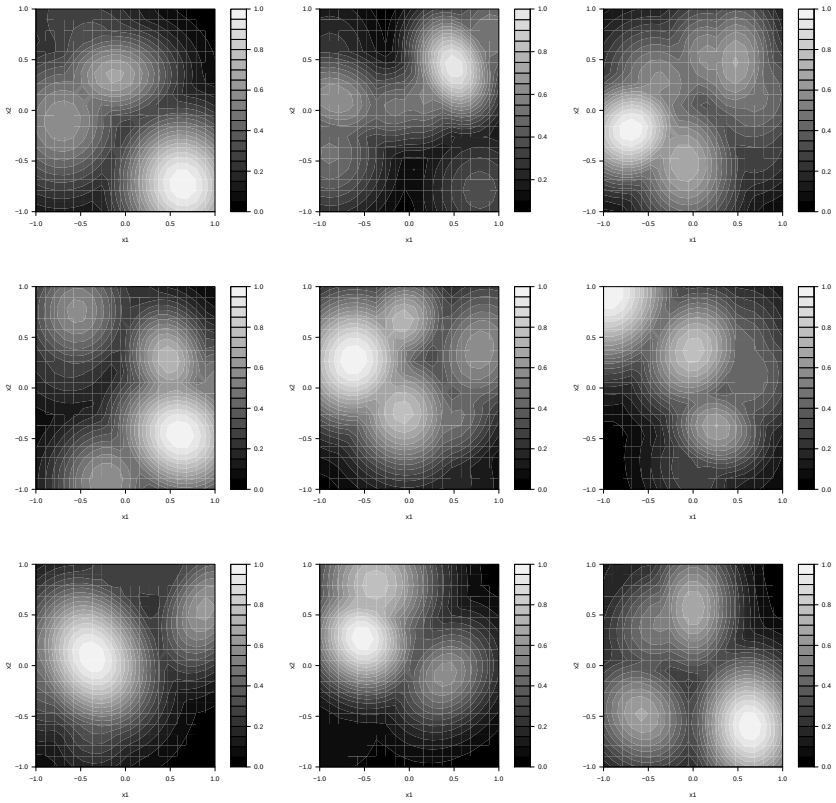

Figure 3: Nine test problem instances from Π_{MSG}, which were generated with the MSG landscape generator as specified in Eq. 2.

SAMP-1 Algorithm and Problem Instances The goal of this case study is to analyze if one algorithm shows a similar performance on a class of problem instances, say Π_{MSG}. A random-effects design will be used to model the results. We illustrate the decomposition of the variance of the response values in (i) the variance due to problem instance and (ii) the variance due to the algorithm and derive results, which are based on hypotheses testing as introduced in (12).

We consider one algorithm, an ES, which is run $r = 10$ times on a set of randomly generated problem instances. The ES is parametrized with the default setting from Table 1. These parameters are kept constant during the experiment. Nine instances are drawn from the set of problem instances Π_{MSG}. Problem instances were generated with the MSG landscape generator as specified in Eq. 2. The corresponding problem instances are shown in Fig. 3.

The null hypothesis reads "There is no instance effect". Since we are considering the SAMP case, our experiments is based on one ES instance only. There are 90 observations, because 10 repeats were performed on 9 problem instances.

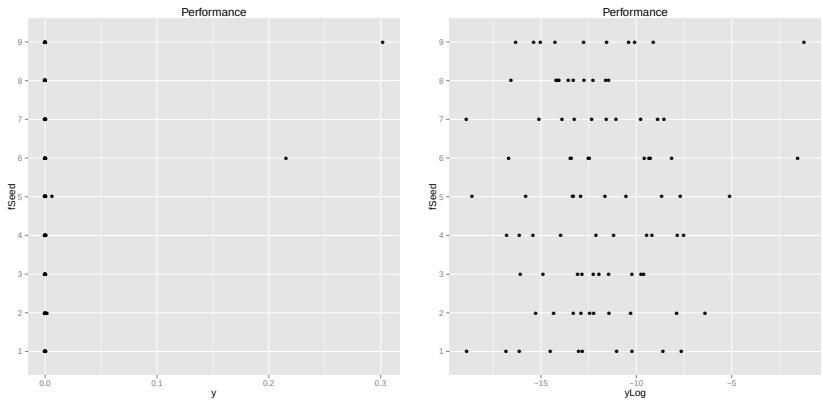

Figure 4: Performance of the ES on nine test problem instances. *Left:* Problem instances plotted versus algorithm performance. *Right:* Problem instances plotted against logarithmic performance. Smaller values are better.

Figure 4 shows the performance of the ES on these nine instances. The variable `fSeed` is used to denote the problem instance number π_i.

SAMP-2 ANOVA and REML Model Building

ANOVA Model Building. The following analysis is based on the linear statistical model

$$Y_{ij} = \mu + \tau_i + \varepsilon_{ij} \left\{ \begin{array}{l} i = 1, \ldots, q \\ j = 1, \ldots, r \end{array} \right. \tag{8}$$

where μ is an overall mean and ε_{ij} is a random error term for replication j on instance i. Note, in contrast to the fixed-effects model from (3), τ_i is a random variable representing the effect of instance i. The stochastic behavior of the response variable originates from both the instance and the algorithm. This is reflected in (8), where both τ_i and ϵ_{ij} are random variables. The model (8) is the so-called *random-effects model*, cf. [15] or [11].

We assume that $\tau_1, \ldots, \tau_q$ are i.i.d. $\mathcal{N}(0, \sigma_\tau^2)$ and ε_{ij}, $i = 1, \ldots, q$, $j = 1, \ldots, r$, are i.i.d. $\mathcal{N}(0, \sigma^2)$. If τ_i is independent of ϵ_{ij} and has variance $\mathrm{V}(\tau_i) = \sigma_\tau^2$, the variance of any observation is $\mathrm{V}(Y_{ij}) = \sigma^2 + \sigma_\tau^2$. Similar to the partition in classical ANOVA, the variability in the observations can be partitioned into a component that measures the variation between treatments and a component that measures the variation within treatments. Based on the fundamental ANOVA identity $\mathrm{SS}_{\mathrm{total}} = \mathrm{SS}_{\mathrm{treat}} + \mathrm{SS}_{\mathrm{err}}$, we define

$$\mathrm{MS}_{\mathrm{treat}} = \frac{\mathrm{SS}_{\mathrm{treat}}}{q-1} = \frac{r \sum_{i=1}^{q} (\bar{Y}_{i.} - \bar{Y}_{..})^2}{q-1},$$

Table 2: ANOVA table for a one-factor fixed and random effects models

Source of Variation	Sum of Squares	Degrees of freedom	Mean Square	EMS Fixed	EMS Random
Treatment	$\mathrm{SS}_{\mathrm{treat}}$	$q-1$	$\mathrm{MS}_{\mathrm{treat}}$	$\sigma^2 + r\frac{\sum_{i=1}^{q}\tau_i^2}{q-1}$	$\sigma^2 + r\sigma_\tau^2$
Error	$\mathrm{SS}_{\mathrm{err}}$	$q(r-1)$	$\mathrm{MS}_{\mathrm{err}}$	σ^2	σ^2
Total	$\mathrm{SS}_{\mathrm{total}}$	$qr-1$			

and

$$\mathrm{MS}_{\mathrm{err}} = \frac{\mathrm{SS}_{\mathrm{err}}}{q(r-1)} = \frac{\sum_{i=1}^{q}\sum_{j=1}^{r}(Y_{ij} - \bar{Y}_{i\cdot})^2}{q(r-1)}.$$

It can be shown that

$$E(\mathrm{MS}_{\mathrm{treat}}) = \sigma^2 + r\sigma_\tau^2 \quad \text{and} \quad E(\mathrm{MS}_{\mathrm{err}}) = \sigma^2, \tag{9}$$

cf. [15]. Therefore, the estimators of the variance components are

$$\hat{\sigma}^2 = \mathrm{MS}_{\mathrm{err}}, \tag{10}$$

$$\hat{\sigma_\tau^2} = \frac{\mathrm{MS}_{\mathrm{treat}} - \mathrm{MS}_{\mathrm{err}}}{r}. \tag{11}$$

The corresponding ANOVA table is shown in Table 2.

Based on ANOVA calculations, we obtain with (10) an estimator of the first variance component $\hat{\sigma}^2 = -0.4848257$, and from (11), we obtain the second component $\hat{\sigma}_\tau^2 = 11.32854$. The model variance can be determined as $\hat{\sigma}^2 + \hat{\sigma}_\tau^2 = 10.84372$. The mean $\mu = -12.05554$ from (8) can be extracted. Finally, the p value in the ANOVA table is calculated as 0.7979083.

Note, that we have obtained a negative variance. Since negative variances are not feasible, we can proceed by setting their values to zero and proceed with this modified values. A more elegant way is presented in the following.

Restricted maximum likelihood. In some cases, the standard ANOVA, which was used in our example, produces a negative estimate of a variance component. This can be seen in (11): If $\mathrm{MS}_{\mathrm{err}} > \mathrm{MS}_{\mathrm{treat}}$, negative values occur. By definition, variance components are positive. Methods, which always yield positive variance components have been developed. Here, we will use *restricted maximum likelihood estimators* (REML). The ANOVA method of variance component estimation, which is a method of moments procedure, and REML estimation may lead to different results. Output from an `R`-based analysis with the function `lme` from the package `lme4` reads as follows (`fSeed` denotes the problem instance) [16]:

```
Linear mixed model fit by REML
Formula: yLog ~ 1 + (1 | fSeed)
   Data: samp.df
```

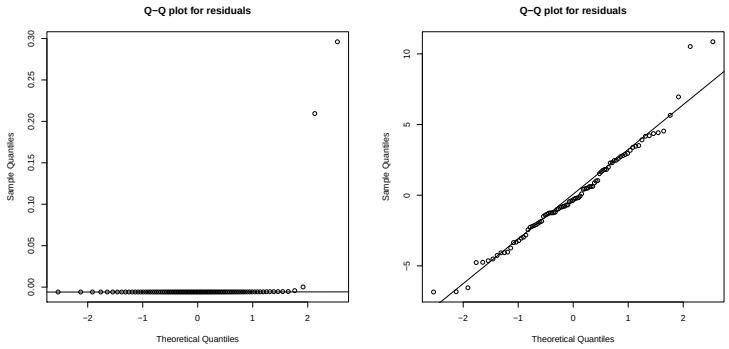

Figure 5: *Left*: Q-Q plot of the residuals for raw data. *Left*: Q-Q plot for the log-transformed responses.

```
   AIC   BIC logLik deviance REMLdev
 475.6 483.1 -234.8    469.3   469.6
Random effects:
 Groups   Name        Variance Std.Dev.
 fSeed    (Intercept)  0.000   0.0000
 Residual             10.893   3.3004
Number of obs: 90, groups: fSeed, 9

Fixed effects:
            Estimate Std. Error t value
(Intercept) -12.0555     0.3479  -34.65
```

Compared to the ANOVA setting, different values for $\hat{\sigma}^2$, $\hat{\sigma}_\tau^2$, and μ were obtained. However, the REML based analysis also shows that the variability in the response observations can be attributed to the variability of the algorithm.

SAMP-3 Validation of the Model Assumptions Before performing hypothesis testing based on the models introduced in SAMP-2, the validity of the model assumptions has to be investigated. If the model is adequate, the residuals should exhibit no structure. Residuals are plotted against fitted values to check the assumption of homoscedasticity and quantile-quantile (Q-Q) plots are used to check if residuals meet the normality assumption. Quantile-quantile plots of the residuals is shown in Fig. 5 for the raw and the log-transformed responses. These plots provide a good way to compare the the distribution of a sample with a distribution. Large deviations from the line indicate non-normality of the sample data. These Q-Q plots indicate that a log transformation of the response might be useful in our setting.

SAMP-4 Hypothesis Testing Testing hypotheses about individual treatments (instances) is useless, because the problem instances π_i are here consid-

ered as samples from some larger population of instances Π. We test hypotheses about the variance component σ_τ^2, i.e., the null hypothesis

$$H_0 : \sigma_\tau^2 = 0 \text{ versus } H_1 : \sigma_\tau^2 > 0. \tag{12}$$

Under H_0, the algorithm performance is identical on all problem instances ("all treatments are identical"), i.e., $r\sigma_\tau^2$ is very small. Based on (9), we conclude that $E(\mathrm{MS}_{\mathrm{treat}}) = \sigma^2 + r\sigma_\tau^2$ and $E(\mathrm{MS}_{\mathrm{err}}) = \sigma^2$ are similar. Under the alternative, variability exists between treatments. Standard analysis shows that $\mathrm{SS}_{\mathrm{err}}/\sigma^2$ is distributed as chi-square with $q(r-1)$ degrees of freedom. Let $F_{u,v}$ denote the F distribution with u numerator and v denominator degrees of freedom. Under H_0, the ratio

$$F_0 = \frac{\frac{\mathrm{SS}_{\mathrm{treat}}}{q-1}}{\frac{\mathrm{SS}_{\mathrm{err}}}{q(r-1)}} = \frac{\mathrm{MS}_{\mathrm{treat}}}{\mathrm{MS}_{\mathrm{err}}}$$

is distributed as $F_{q-1,q(r-1)}$. To test hypotheses in (8), we require that $\tau_1, \ldots, \tau_q$ are i.i.d. $\mathcal{N}(0, \sigma_\tau^2)$, ε_{ij}, $i = 1, \ldots, q$, $j = 1, \ldots, r$, are i.i.d. $\mathcal{N}(0, \sigma^2)$, and all τ_i and ε_{ij} are independent of each other. These considerations lead to the decision rule to reject H_0 at the significance level α if

$$f_0 > F(1-\alpha; q-1, q(r-1)), \tag{13}$$

where f_0 is the realization of F_0 from the observed data. An intuitive motivation for the form of statistic F_0 can be obtained from the expected mean squares. Under H_0 both $\mathrm{MS}_{\mathrm{treat}}$ and $\mathrm{MS}_{\mathrm{err}}$ estimate σ^2 in an unbiased way, and F_0 can be expected to be close to one. On the other hand, large values of F_0 give evidence against H_0.

Regarding the SAMP case, we obtain the following values: Based on (9) and (13), we can determine the F statistic and the p value. We get $\mathrm{MS}_{\mathrm{treat}} = \mathrm{MS}_{\mathrm{err}} = 10.89275$ and $f_0 = 1$, which results a large p value: 0.4426363. The null hypothesis $H_0 : \sigma_\tau^2 = 0$ from (12) can not be rejected, i.e., we conclude that there is no instance effect. A similar conclusion was obtained from the ANOVA method of variance component estimation as introduced in Table 2.

SAMP-5 Confidence Intervals and Prediction An unbiased estimator of the overall mean μ is

$$\hat{\mu} = \bar{y}_{\cdot\cdot} = \sum_{i=1}^{q} \sum_{j=1}^{r} y_{ij}/(qr).$$

Its variance is given by

$$\mathrm{V}(\bar{y}_{\cdot\cdot}) = \mathrm{V}\left(\sum_{i=1}^{q} \sum_{j=1}^{r} y_{ij}/(qr) \right) = \frac{r\sigma_\tau^2 + \sigma^2}{qr}.$$

With (9) and (10), we obtain an estimator of the variance of the overall mean μ as

$$\hat{\mathrm{V}}(\bar{y}_{\cdot\cdot}) = \mathrm{MS}_{\mathrm{treat}}/qr.$$

Since

$$\frac{\bar{Y}_{..} - \mu}{\sqrt{\mathrm{MS}_{\mathrm{treat}}/qr}} \sim t_{q(r-1)},$$

the confidence limits for μ can be derived as

$$\bar{y}_{..} \pm t_{1-\alpha/2;q(r-1)} \sqrt{\mathrm{MS}_{\mathrm{treat}}/qr}. \tag{14}$$

We conclude the SAMP case study with prediction of the algorithm's performance on a new instance from the same class. Based on (14), we obtain the following 95% confidence interval: $[2.6773e-06; 1.262e-05]$. Again, confidence intervals from the REML and ANOVA methods are very similar. Summarizing, we can conclude that the ES performs similar on instances from Π_{MSG}, which were generated with Eq. 2.

5.3 MAMP: Multiple Algorithms, Multiple Problems

In the MAMP case study, fixed effects are included in the conditional structure of (6), which leads to a mixed model. Instead of one fixed algorithm as in the SAMP case, we consider either several algorithms or algorithms with several parameters. Both situations can be treated while considering algorithms as levels of a fixed factor, whereas problem instances are drawn randomly from the population of instances Π_{MSG}.

MAMP-1 Algorithm and Problem Instances
MAMP-2 ANOVA and REML Model Building
MAMP-3 Validation of the Model Assumptions
MAMP-4 Hypothesis Testing
  a) Random effects
  b) Fixed effects
MAMP-5 Confidence Intervals and Prediction

MAMP-1 Algorithm and Problem Instances We aim at comparing the performance of the ES with different recombination operators over an instance class. More precisely, we have four ES instances using recombination operators $\{1, 2, 3, 4\}$ and nine instances randomly sampled from the class Π_{MSG} as illustrated in Fig. 3. Each run is repeated ten times. In this study $4 \times 9 \times 10 = 360$ data were used. We are interested in the following questions:

- Is there an instance effect?
- Do the mean performances of the ES with different recombination operators differ?
- Do the instance-algorithm interactions contribute to the variability of the response?

A first visual inspection, which plots the performance of the algorithm within each problem instance, is shown in Fig. 6. In eight of the nine instances the linear regression line does have a negative slope and the intercepts do not differ very much. This indicates that there is no significant interaction between the fixed and the random factors.

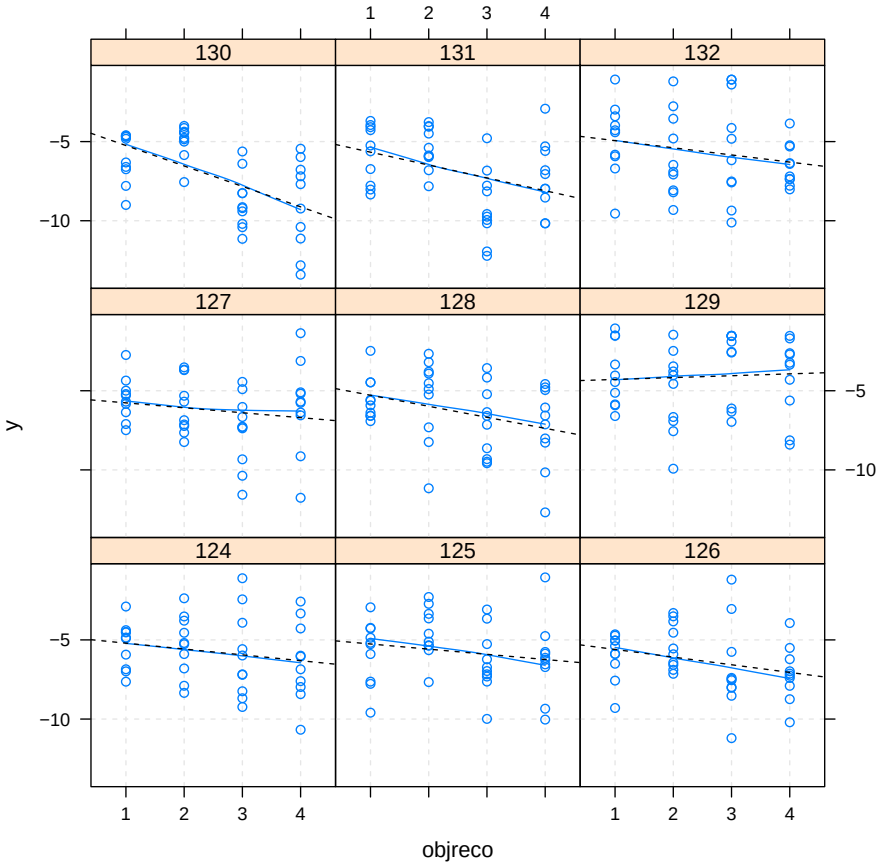

Figure 6: Four algorithms (ES with modified recombination operators) on nine test problem instances. Each panel represents one problem instance and problem instances are labeled from 124 to 130. Performance is plotted against the level of the recombination operator.

MAMP-2 ANOVA and REML Model Building The variability in the performance measure can be decomposed according to the following *mixed-effects ANOVA model*:

$$Y_{ijk} = \mu + \alpha_j + \tau_i + \gamma_{ij} + \varepsilon_{ijk}, \tag{15}$$

where μ is an overall performance level common to all observations, α_j is a fixed effect due to the algorithm j, τ_i is a random effect associated with instance i, γ_{ij} is a random interaction between instance i and algorithm j, and ε_{ijk} is a random error for replication k of algorithm j on instance i. We assume that the α_j's are fixed effects such that $\sum_{j=1}^{h} \alpha_j = 0$ and that the random elements are τ_i are i.i.d. $\mathcal{N}(0, \sigma_\tau^2)$, γ_{ij} are i.i.d. $\mathcal{N}(0, \sigma_\gamma^2)$, ε_{ijk} are i.i.d. $\mathcal{N}(0, \sigma^2)$, and τ_i, γ_{ij} and ε_{ijk} are mutually independent random variables. Similar to (6) the conditional distribution of the performance measure given the instance and the instance–algorithm interaction is given by

$$Y_{ijk} | \tau_i, \gamma_{ij} \sim \mathcal{N}(\mu + \alpha_j + \tau_i + \gamma_{ij}, \sigma^2), \tag{16}$$

with $i = 1, \ldots, q$, $j = 1, \ldots, h$, and $k = 1, \ldots, r$. The marginal model reads (after integrating out the random effects τ_i and γ_{ij}):

$$Y_{ijk} \sim \mathcal{N}(\mu + \alpha_j, \sigma^2 + \sigma_\tau^2 + \sigma_\gamma^2). \tag{17}$$

Based on these statistical assumptions, hypothesis tests can be performed about fixed and random factor effects. Using the mixed model (16), we are interested in testing whether there is a difference between the factor level means $\mu + \alpha_j$ ($j = 1, \ldots, h$). The hypotheses for testing the fixed effects can be formulated as

$$H_0 : \alpha_i = 0 \, \forall i \quad \text{against} \quad H_1 : \exists \, \alpha_j \neq 0 \tag{18}$$

Regarding random effects, tests about particular levels are useless. This is similar to the random-effects model (8). Again, we perform tests about the variance components σ_τ^2 and σ_γ^2 instead. These can be formulated as follows:

$$\begin{array}{rcl@{\qquad}rcl} H_0 & : & \sigma_\tau^2 = 0, & \text{and} & H_0 & : & \sigma_\gamma^2 = 0, \\ H_1 & : & \sigma_\tau^2 > 0, & & H_1 & : & \sigma_\gamma^2 > 0, \end{array} \tag{19}$$

respectively. If all treatment (problem instances) combinations have the same number of observations, i.e., if the design is balanced, the test statistics for these hypotheses are ratios of mean squares that are chosen such that the expected mean squares of the numerator differs from the expected mean squares of the denominator only by the variance components of the random factor under test. Chiarandini and Goegebeur [11] present the resulting analysis of variance, which is shown in Table 3.

ANOVA Model Building. The ANOVA table for the experiments from the MAMP case study is shown in Table 4. Equating the observed mean squares

Table 3: Expected mean squares and consequent appropriate test statistics for a mixed two-factor model with h fixed factors, q random factors, and r repeats. From [11].

Effects	Mean squares	df	Expected mean squares	Test statistics
Fixed factor	MSA	$h-1$	$\sigma^2+r\sigma^2_\gamma+rq\frac{\sum_{j=1}^{h}\alpha_j^2}{h-1}$	MSA/MSAB
Random factor	MSB	$q-1$	$\sigma^2+r\sigma^2_\gamma+rh\sigma^2_\tau$	MSB/MSAB
Interaction	MSAB	$(h-1)(q-1)$	$\sigma^2+r\sigma^2_\gamma$	MSAB/MSE
Error	MSE	$hq(r-1)$	σ^2	

Table 4: ANOVA for the MAMP case

Mean squares	Factors	Df	Sum Sq	Mean Sq	F value	Pr(>F)
MSA	objreco	3	154.59	51.53	11.05	0.0000
MSB	fSeed	8	251.79	31.47	6.75	0.0000
MSAB	objreco:fSeed	24	185.60	7.73	1.66	0.0288
MSE	Residuals	324	1511.27	4.66		

in the lines of the ANOVA table to their expected values and solving for the variance components leads to the following equations[15]:

$$\hat{\sigma}_\tau^2 = \frac{MSB - MSAB}{hr} = 0.593502$$
$$\hat{\sigma}_\gamma^2 = \frac{MSAB - MSE}{r} = 0.306907$$
$$\hat{\sigma}^2 = MSE = 4.664423$$

Next, we will compare these results to the REML based analysis of the mixed model.

REML Model Building. We have specified sum contrasts instead of the default treatment contrasts used in `lmer()`. Again, `fSeed` represents the problem instance, whereas the algorithm instance α_j, $j = 1, \ldots, 4$, is represented by `objreco`.

```
Linear mixed model fit by REML
Formula: yLog ~ objreco + (1 | fSeed)
               + (1 | fSeed:objreco)

Random effects:
 Groups        Name        Variance Std.Dev.
 fSeed:objreco (Intercept) 0.30691  0.55399
 fSeed         (Intercept) 0.59351  0.77039
 Residual                  4.66442  2.15973
Number of obs: 360,
groups: fSeed:objreco, 36; fSeed, 9

Fixed effects:
            Estimate Std. Error t value
(Intercept)  -6.0222     0.2956 -20.370
objreco1      0.6176     0.2539   2.433
objreco2      0.6918     0.2539   2.725
objreco3     -0.6671     0.2539  -2.628
```

As can be seen from the `Random effects` section of the REML model output, the estimated variances for the problem instance and the instance-interaction random effects are $\hat{\sigma}_\tau^2 = 0.59351$ and $\hat{\sigma}_\gamma^2 = 0.30691$, respectively. The `Random effects` section presents the estimates of the fixed effects model parameters, i.e., `objreco`.

MAMP-3 Validation of the Model Assumptions Again, the check of the diagnostic plots (Fig. 7) reveals that a log transformation of the response improves the model adequacy.

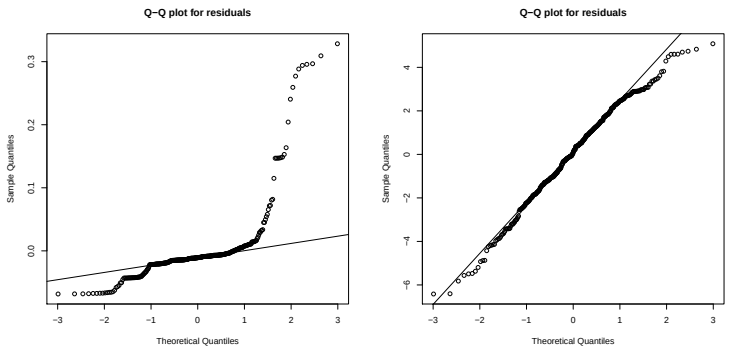

Figure 7: *Left*: Q-Q plot of the residuals for raw data. *Left*: Q-Q plot for the log-transformed responses.

MAMP-4a Hypothesis Testing: Random Effects We will consider random effects first. Regarding problem instances, test about levels are meaningless. Hence, we perform tests about the variance components σ_τ^2 and σ_γ^2, which were presented in (19). First, we are testing the null hypothesis, which states that the components of the random effects are zero. Based on the ANOVA from Table 3, we obtain the values for the MAMP case that are shown in Table 4. The values reveal that there are main factor effects (fixed and random), but no significant interaction effects.

Alternatively, we can compute the likelihood ratios of models with and without the factors under observation.

```
Data: mamp.df
Models:
mamp.lmer2: yLog ~ objreco + (1 | fSeed)
mamp.lmer3: yLog ~ objreco + (1 | fSeed)
            + (1 | fSeed:objreco)
           Df    AIC    BIC  logLik
mamp.lmer2  6 1616.7 1640.0 -802.35
mamp.lmer3  7 1616.6 1643.8 -801.31
   Chisq Chi Df Pr(>Chisq)
   2.0929      1      0.148
```

These tests indicate that there are also no significant instance-algorithm interactions. Additional likelihood-ratio test show that the fixed factor and random factor effects are significant.

MAMP-4b Hypothesis Testing: Fixed Factor Effects Regarding fixed factors, we are interested in testing for differences in the factor level means $\mu + \alpha_i$. These tests were formulated in (18), i.e., we are testing H_0: all α_i are equal to 0 versus H_1: at least one $\alpha_j \neq 0$. Here, we are using the test

statistic from [15, p. 523] for testing that the means of the fixed factor effects are equal. The appropriate test statistic for testing that the means of the fixed factor effects are equal, i.e., H_0 is true, is

$$F_0 = \frac{MSA}{MSAB} = \frac{154.59/3}{185.6/24} = 6.663362,$$

with values taken from Table 4. The reference distribution is $F_{n-1,(n-1)(q-1)}$. We calculate the p value for the test on the fixed-effect term. The obtained p value is 0.002, hence the results collected indicate that the factor recombination (`objreco`) has a statistically significant impact on the performance of the algorithm. Using sum of contrasts implies that $\sum \alpha_j = 0$. The point estimates for the mean algorithm performance with the jth fixed factor setting can be obtained by $\mu_{\cdot j} = \mu + \alpha_j$. The fixed factor effects can be estimated in the mixed model as

$$\hat{\mu} = \overline{y}_{\cdots}$$
$$\hat{\alpha}_j = \overline{y}_{j\cdot} - \overline{y}_{\cdots},$$

which results in the following estimates: $\hat{\alpha}_1 = 0.6175519$, $\hat{\alpha}_2 = 0.6918047$, $\hat{\alpha}_3 = -0.6671266$, and $\hat{\alpha}_4 = -0.6423659$.

The same estimates were obtained with the REML analysis as can be seen from the REML model output on page 22. The corresponding fixed effects are shown in the `Fixed effects` section of the REML output. For example, we obtain the following value: `objreco1` $= \hat{\alpha}_1 = 0.6176$.

MAMP-5 Confidence Intervals and Prediction We generate paired comparisons plots, which are based on confidence intervals. The wrapper function `intervals()` from Chiarandini and Goegebeur [11] was used for visualizing these confidence intervals as shown in Fig. 8. When intervals overlap we conclude that there is no significant difference. Here, we can conclude that the recombination operators `(1)` and `(2)` show a similar performance, whereas performances between `(3)` and `(2)` are different. *Intermediate* recombination of the object variables, i.e., `(3)` and `(4)`, results in a significant improvement of the performance.

6 Summary and Outlook

In order to answer question (Q-1), we propose an approach to generate natural problem classes, which are based on real-world data. If no such data are available, artificial problem generators such as MSG can be used. Since our approach uses a model, say M, to generate new problem instances, one conceptual problem arises: This approach is not applicable, if the final goal is the determination of a model for the data, because M is per definition the best model in this case and the search for good models will result in M. But there is a simple solution to this problem. In this case, the feature extraction and

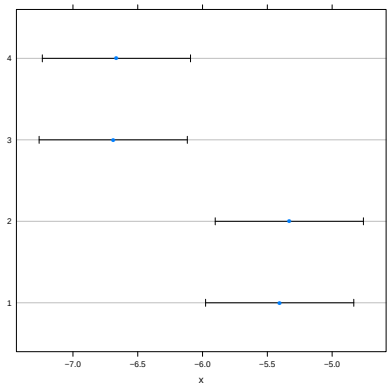

Figure 8: Paired comparison plots. Results from four ES instances with different recombination operators are shown in this plot.

model generation should be skipped and the original data should be modified by adding some noise or performing transformations on the data. However, if applicable, the model-based approach is preferred, because it sheds some light on the underlying problem structure.

The model-based approach can be used to generate infinitely many test-problem instances. Instead of using a fixed number of problem instances, we propose

1. using randomly generated problem instances and
2. treating the problem instance as a random factor.

Algorithms with different parameterizations are tested on this set of randomly generated problem instances. This experimental setup requires modified statistics, so-called random-effects models or mixed models. This approach may lead to objective evaluations and comparisons. If normality assumptions are met, confidence intervals can be determined, which "forecast" the behavior of an algorithm on unseen problem instances. Furthermore, results can be generalized in real-world settings. This gives an answer to question (Q-2).

In order to demonstrate the applicability of our approach, the performance of an evolution strategy was analyzed. The first SAMP example illustrates that the selection of the problem instance from the problem class Π_{MSG} has no significant impact on the performance of the optimization algorithm. Furthermore, confidence intervals, which can be used the predict the performance of the algorithm on a problem class, were determined. The MAMP case exemplifies how to analyze the effect of different algorithm parameter settings on the performance. Four variants of the recombination operator and nine problem instances were used. The analysis reveals that the choice of the recombination operator has a significant effect on the algorithm's performance: the performance of the algorithm differs with different recombination operators. Intermediate

recombination of the object variables results in an performance improvement. We demonstrated that the problem instances contribute significantly to the variability in the response and that there is no significant instance-algorithm interaction.

The software, which was used in this study, will be integrated into the `R` package SPOT [5].

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In addition, the paper and the corresponding `R` code is based on Chiarandini's and Goegebeur's publication *Mixed Models for the Analysis of Optimization Algorithms* [11].

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