Mallows, Black-box combinatorial optimization, limited budget, ???

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Abstract. Black-box combinatorial optimization problems arise in practice when the objective function is evaluated by means of a simulator or a real-world experiment. In such cases, classical techniques such as mixed-integer programming and local search cannot be applied. Moreover, often each solution evaluation is expensive in terms of time or resources, thus only a limited number of evaluations is possible, typically several order of magnitude smaller than in white-box optimization problems. In the continuous case, Bayesian optimization, in particular using Gaussian processes, has proven very effective under these conditions. Much less research is available in the combinatorial case. In this paper, we propose and analyze an estimation-of-distribution (EDA) algorithm based on a Mallows probabilistic model and compare it with CEGO, a Bayesian optimization algorithm for combinatorial optimization. Experimental results show that the Bayesian algorithm is able to obtain very good solutions with very few evaluations, however, at a significant computational cost, whereas the proposed EDA outperforms CEGO when the number of solutions evaluated approaches 400, and it is significantly faster. These results suggest that the combination of Bayesian optimization and a Mallows-based EDA may be an interesting direction for future research.

Keywords: Combinatorial optimization · Bayesian optimization · Expensive black-box optimization · Estimation of distribution algorithms

1 Introduction

Motivation: Manuel

In many practical optimization problems, the objective function contexts
Related work: Ekhine
Our contribution: Ekhine

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Zaefferer et al. [5, 6] Pérez Cáceres et al. [4]
[3]

2 Background

Permutations are defined as bijections of the set $[n]$ integer onto itself. The set of all permutations of n items is denoted as S_n and has cardinality $n!$. We denote permutations with Greek letters with exception of the inverse permutation denoted as $e = 1, 2, 3, \ldots, n$. We denote the composition of σ and π as $\sigma\pi$ and the inverse of σ as σ^{-1}, for which the relation $\sigma\sigma_{-1} = e$ always holds.

Distributions over permutations are functions that assign a probability value to each of the permutations in S_n, $p(\sigma) \in [0, 1]$ [**?**]. One of the most popular distributions is the Mallows Model (MM), which is considered as an analogous to the Gaussian distribution for permutations. The MM defines the probability of each permutation σ as follows:

$$p(\sigma) = \frac{\exp(-\theta d(\sigma, \sigma_0))}{\psi} \tag{1}$$

with two parameters, θ and σ_0, where permutation σ_0 a reference permutation that has the largest probability value, i.e., the mode of the distribution. The probability of every permutation $\sigma \in S_n$ decays exponentially as its distance $d(\sigma, \sigma_0)$ increases, and θ, the dispersion parameter controls this decay. The distance $d(\sigma, \sigma_0)$ is the Kendall's-τ distance. The normalization constant ψ can be easily computed for the Kendall's-τ distance as well as for the Hamming, Cayley and Ulam distance [**?**].

One of the most common problems related ti probability distributions is that of learning the maximum likelihood parameters given a sample of data S. For the MM, this problem tranlates to learning θ and σ_0 that best describe a sample of permutations.

The learning process is divide in two stages: first, we estimate the central permutation of the distribution, $\hat{\sigma}0$ and, second, compute the dispersion parameter, $\hat{\theta}$.

The exact maximum likelihood estimation is computationally hard [**?**]. However, the approximate learning requires polynomilal computational time and is guarantied to obtain high quality parameters [**? ?**].

This process of sample S is as follows: first, compute $\hat{\sigma}0$ with the Borda count algorithm. Borda orders the items $[n]$ by their *Borda score* increasingly, where the Borda score $B(i)$ is the average of each position i, $B(i) \propto \sum_{t \in S} \sigma_t(i)$. Second, the computation of θ is casted as a numerical optimization problem [**?**].

Recently, it has been proposed an extension of Borda by the name of uBorda. uBorda considers a sample of permutations S along with a weight $w(\sigma)$ for each permutation σ []. Intuitively it is equivalent to replicating the permutations in the sample proportionally to their weight. It has been used to learn a MM in an evolving preference context. In this paper, we propose to use uBorda where each permutation in the sample $\sigma \in S$ is weighted by its fitness function $w(\sigma) = f(\sigma)$.

LOP: Ekhine

Quizás luego: PFSP y QAP

3 Methods

~~CEGO: Manuel.~~

Combinatorial Efficient Global Optimization (CEGO) [6] is an extension of the well-known EGO method [2] to unconstrained black-box combinatorial optimization problems. In EGO, Gaussian process models are used as a surrogate of the landscape of the expensive original problem. An optimization method searches for solutions in the surrogate model by optimizing the expected improvement criterion, which balances the expected mean and variance of the chosen solution. Once a solution is chosen, it is evaluated on the actual objective function and the result is used to update the surrogate-model, hopefully increasing its predictive power.

CEGO replaces the Euclidean distance measure, used by the surrogate model in EGO, with a distance measure appropriate to combinatorial landscapes [5], such as the Kendall distance for permutations [**?**]. In CEGO, the surrogate model is explored by a GA with crossover and mutation operators appropriate for the particular combinatorial problem. The original paper notes that coupling the GA with local search does not improve the results significantly since the model is anyway an inexact estimation of the original objective function [6, p. 875].

What else do we need to say?
Description of UMM: Ekhine
new approach: add sample, learn distri, sample distri
learn distri: uMM with param ρ and binary search rho
sample: peakig distri
Quality guarantees

4 Experimental setup

We use the implementation of GECO provided by the authors[3]. Following the authors of CEGO [5, 6], we use and the GA that optimizes the surrogate models uses a population size of 20, crossover rate of 0.5, mutation rate of 1, tournament selection of size 2 and probability of 0.9, interchange mutation (i.e., exchanging two randomly selected elements of the permutation) and cycle crossover for permutations. The budget of each run of the GA is 10^4 evaluations using the surrogate-model. Although it is never stated in the original paper, the implementation of CEGO generates a set of initial solutions of size m_{ini} by means of a max-min-distance sequential design: new solutions are added to the set sequentially by maximizing the minimum distance to solutions already in the set. These initial solutions are then evaluated on the actual objective function and the result is used to build the initial surrogate model. Here we use $m_{\text{ini}} = 20$.[4]

The CPU time required for a single run of CEGO using these settings is larger than a week. For simplicity, we use Kendall Tau distance [**?**] in all experiments[5].

[3] https://cran.r-project.org/package=CEGO
[4] **[MANUEL: Zaefferer et al. [5] uses 10 so we may want to change this]**
[5] **[MANUEL: Zaefferer et al. [5] claims this is called Swap distance, could you double-check?]**

Nevertheless, Zaefferer et al. [6] points out that CEGO performs best on the QAP when using Hamming distance. We plan to extend our analysis of uMM to other distance measures and to the dynamic selection of distance measures [5].

In all experiments, we consider a maximum budget of $FE_{\max} = 400$ evaluations of the actual objective function. In a white-box context, state-of-the-art algorithms for the problems considered here typically evaluate hundreds? thousands? of solutions, thus, the budget considered here for the black-box context is extremely limited.

We implemented UMM in Python 3. The parameter settings that we use are...

Complete this with details of uMM: MANUEL

~~Computing system details: MANUEL~~All experiments were run on Intel Xeon E5-2640 CPUs at 2.50 GHz, 64 GB RAM running CentOS Linux release 7.4.1708 (Core).

Describir como se generan las intancias de LOP: Ekhine

Describir las instancias: Ekhine

For the LOP, we generated synthetic instances of size $n = 20$, $m = 200$, $\phi \in \{0.5, 0.7, 0.9\}$[6]

In the case of the QAP and PFSP, we consider the same instances as Zaefferer et al. [5, 6], i.e., `nug12`,`nug30`,`tho30` and `kra32` for the QAP, with n equal to the number in the instance name, and `reC05`, `reC13`, `reC19`, `reC31` for the PFSP, with $n \in \{20, 20, 30, 50\}$, respectively.

5 Experimental analysis

Bayesian optimization methods using a global GP model, such as CEGO, are known to have trouble optimizing locally [1]. Our intuition is that this problem becomes worse in rugged combinatorial landscapes, where small steps may produce drastic changes.

6 Conclusions

Open questions:

- How difficult is to extend uMM to other distance metrics?
- Can we plot the posterior probability of the optimal solution?

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[6] **[MANUEL: what is m?]**

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