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HEURISTIC APPROACHES TO STOCHASTIC QUADRATIC ASSIGNMENT PROBLEM: VAR AND CVAR CASES

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Abstract: *The goal of this paper is to continue our investigation of the heuristic approaches of solving the stochastic quadratic assignment problem (StoQAP) and provide additional insight into the behavior of different formulations that arise through the stochastic nature of the problem. The deterministic Quadratic Assignment Problem (QAP) belongs to a class of well-known hard combinatorial optimization problems. Working with several real-world applications we have found that their QAP parameters can (and should) be considered as stochastic ones. Thus, we review the StoQAP as a stochastic program and discuss its suitable deterministic reformulations. The two formulations we are going to investigate include two of the most used risk measures - Value at Risk (VaR) and Conditional Value at Risk (CVaR). The focus is on VaR and CVaR formulations and results of test computations for various instances of StoQAP solved by a genetic algorithm, which are presented and discussed.*

Keywords: *quadratic assignment problem, stochastic quadratic assignment problem, VaR and CVaR deterministic reformulations, genetic algorithm*

1 Introduction

The main aim of the paper is to deal with the Stochastic Quadratic Assignment Problem (StoQAP) as the (stochastic) generalization of the Quadratic Assignment Problem (QAP) by the of stochastic programming techniques. A short review of the well-known quadratic assignment problem with appropriate references is provided in Section 2 for completeness as it follows and quotes ideas from our previous papers from 2014 [16] and 2016 [26] dealing with this topic. Various original motivating applications from the Brno University of Technology research areas are mentioned as they serve as a motivation for the urge to consider some of parameters in the QAP to be random. The next section is devoted to the short review of selected basic concepts of stochastic programming. These concepts are applied to StoQAP in Section 4, and specifically to two original reformulations containing risk measures - Value at Risk (VaR) and Conditional Value at Risk (CVaR) that are introduced and solved by a metaheurestic implemented in MATLAB.

2 Quadratic assignment problem

The QAP was first formulated by T. C. Koopmans and M. Beckman in 1957, see [8]. Formally the problem is stated in the following way. Let us have a set of n facilities and a set of n locations. For each pair of locations, a distance is specified and for each pair of facilities a weight or a flow is specified. The task is to assign all facilities to different locations with the goal of minimizing the sum of the distances multiplied by the corresponding flows. The development of the QAP related approaches can be found, e.g., in [6], [21] and [16] for further references.

To build a QAP mathematical program, we denote $N = \{1, 2, \ldots, n\}$ and $n \times n$ matrix $\mathbf{X}$ having variable components satisfying the following assignment constraints that form the feasible set

$$\mathcal{C} = \left\{ \sum_{i=1}^{n} x_{ij} = 1, \sum_{j=1}^{n} x_{ij} = 1, x_{ij} \in \{0, 1\}, i, j = 1, 2, \ldots, n \right\}.$$

If the above conditions are met, then the QAP can be formulated as a quadratic binary program

$$\min_{x_{ij}} \left\{ \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n} d_{ij} f_{kl} x_{ik} x_{jl} \mid \mathbf{X} \in \mathcal{C} \right\}, \tag{1}$$

where $d_{ij}, \forall i, j \in N$ are distances and $f_{kl}, \forall k, l \in N$ are flows. The QAP (1) is proven to be an NP-complete problem by [30]. During our applied research collaboration, we have found inspiring engineering applications of QAP similar formulations at the Brno University of Technology (BUT). Among them, we can enlist a design of fiber concrete pieces [36] and placement of cooling equipment in the continuous casting process [34]. Both problems lead to a specific mixed integer nonlinear programming (MINLP) formulation, so the QAP experience can be useful. In addition, the next problem involves even random parameters. Together with process engineering department we also work on energy production related problems. Waste is often discussed as one of modern resources of energy. Its production places and produced amounts can randomly vary, so the distances and flows can be modeled as random, see [22]. Hence, we need to model QAPs where at least one of the aforementioned distance and flow matrices will be considered random.

3 Stochastic programming framework

We review a mathematical program (MP) as $\min_{\mathbf{x}}\{f(\mathbf{x}) \mid \mathbf{x} \in C\}$, where $C \subseteq \mathbb{R}^n$ is a feasible set, $n \in \mathbb{N}$, $f : C \longrightarrow \mathbb{R}$ is an objective function, and $\mathbf{x} \in C$ is a decision (vector) variable. MPs often involve important constant (deterministic) parameters. So, we can emphasize this fact by writing parameters explicitly in MP and we introduce a parametric MP (PMP) as $\min_{\mathbf{x}}\{f(\mathbf{x}, \mathbf{a}) \mid \mathbf{x} \in C\}$ where $\mathbf{a} \in \mathbb{R}^K$ is a constant parameter, $K \in \mathbb{N}$. Notice please that the introduced programs are constrained by deterministic constraints in the paper (cf. C and $\mathcal{C}$). We specify an underlying (stochastic) program (UP) as $\min_{\mathbf{x}}\{f(\mathbf{x}, \boldsymbol{\xi}) \mid \mathbf{x} \in C\}$, where $\boldsymbol{\xi} : \Omega \longrightarrow \mathbb{R}^K$ is a random vector, for $(\Omega, \mathcal{F}, P)$ given probability space. So, UP is obtained from PMP by replacing $\mathbf{a}$ with $\boldsymbol{\xi}$. As $\boldsymbol{\xi}$ is an $\mathcal{F}$-measurable mapping, it induces a probability distribution on $\mathbb{R}^K$. We denote a probability space as $(\mathbb{R}^K, \mathcal{B}, \mathcal{P})$ or $(\Xi, \mathcal{B}, \mathcal{P})$, where Ξ is a support of $\mathcal{P}$. $\mathcal{B}$ is a σ-field of Borel sets on $\mathbb{R}^K$ or projections of those sets on Ξ. Derived probabilities are computed by the rule $\forall B \in \mathcal{B} : \mathcal{P}(B) = P(\{\omega \mid \boldsymbol{\xi}(\omega) \in B\})$. $\forall \omega^s \in \Omega : \boldsymbol{\xi}(\omega^s) \in \mathbb{R}^K$ is a realization (observation) of $\boldsymbol{\xi}$. In short, we write $\boldsymbol{\xi}^s$. Finally, we denote the presence of random parameters in the model in the following way: We write $(\boldsymbol{\xi})$ after letters denoting random parameters. So, the UP is defined in a correct syntactical way, however its semantics remains unclear. Thus, the first question that should be answered is when the decision will be made — before the random parameters $\boldsymbol{\xi}$ are observed or after the observations $\boldsymbol{\xi}^s$ are known.

According to Madansky [7] when the decision $\mathbf{x}$ is made after observing the randomness $\boldsymbol{\xi}$, this case is called the wait-and-see (WS) approach. However, many decision makers must often make decisions before the observations of $\boldsymbol{\xi}$ are known as in our case. So, they are using the so-called here-and-now (HN) approach. The decision $\mathbf{x}$ must be the same for any future realization of $\boldsymbol{\xi}$. Stochastic programming deals primarily with HN decisions because the typical decision situation is described by the lack of observations. Let the UP be given. For further computational comparisons we review its HN expected value (EV) deterministic reformulation as $\min_{\mathbf{x}}\{f(\mathbf{x}, E\boldsymbol{\xi}) \mid \mathbf{x} \in C\}$, where $E\boldsymbol{\xi}$ is an expected value of $\boldsymbol{\xi}$. We further specify a HN expected objective (EO) deterministic reformulation as $\min_{\mathbf{x}}\{E[f(\mathbf{x}, \boldsymbol{\xi})] \mid \mathbf{x} \in C\}$. Both EV and EO reformulations were applied to StoQAP in our previous paper [16]. The choice of expected value of $f(\mathbf{x}, \boldsymbol{\xi})$ was motivated by the basic idea to minimize "average costs". The idea is realistic when we have the chance to apply such a policy many times in the future. However, the average costs do not guarantee that there are no outlying costs. Therefore, we may need to introduce a different criterion that is more risk averse.

4 StopQAP, VaR_α and CVaR_α

In this section we introduce the QAP with stochastic parameters (StoQAP) within the context of the QAP and stochastic programming. There is still a considerable lack of research focused on StoQAP; a few exceptions to this apparent disinterest are several authors who have analyzed statistical properties of the flow and/or distance matrices, see, e. g. [28]. The first interesting insights into the HN StoQAP came from queueing related applications, see [10] and [32]. In comparison with previous research papers that included randomness only in the flow matrix, we deal with the StoQAP in a general way, as the uncertainty is included in both flow and distance matrices. So, an underlying program following the previously introduced notation is the following

$$\min_{x_{ij}} \left\{ \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n} d_{ij}(\boldsymbol{\xi}) f_{kl}(\boldsymbol{\xi}) x_{ik} x_{jl} \mid \mathbf{X} \in \mathcal{C} \right\}. \tag{2}$$

where $d_{ij}(\boldsymbol{\xi})$ and $f_{kl}(\boldsymbol{\xi})$ are random parameters. Thus, we can specify deterministic reformulations. We will write them in general, however, we will focus on a finite discrete probability distribution case with scenarios $s \in \mathcal{S}$. We will skip EV and EO reformulations here, as they are studied in paper [16] as well as the VO and MM reformulations that were investigated in paper [26].

So, given a confidence level $\alpha \in (0,1)$ a HN (here-and-now) VaR_α (Value at Risk at confidence level α) StoQAP reformulation is introduced:

$$\min_{x_{ij}} \left\{ \mathrm{VaR}_\alpha \left[\sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \sum_{l=1}^{n} d_{ij}(\boldsymbol{\xi}) f_{kl}(\boldsymbol{\xi}) x_{ik} x_{jl} \right] \mid \mathbf{X} \in \mathcal{C} \right\}, \tag{3}$$

where the VaR_α is the $\alpha-$quantile of the distribution of costs (given our initial decision $\mathbf{x}$). By choosing $\alpha = 1$ we would get the MM formulation studied in our previous paper.

Given a confidence level $\alpha \in (0,1)$ a HN CVaR_α (Conditional Value at Risk at confidence level α) StoQAP reformulation is the following:

$$\min_{x_{ij}} \left\{ \mathrm{CVaR}_\alpha \left[\sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \sum_{l=1}^{n} d_{ij}(\boldsymbol{\xi}) f_{kl}(\boldsymbol{\xi}) x_{ik} x_{jl} \right] \mid \mathbf{X} \in \mathcal{C} \right\}, \tag{4}$$

where the CVaR_α is defined as

$$\mathrm{CVaR}_\alpha = \frac{1}{1-\alpha} \int_\alpha^1 \mathrm{VaR}_\gamma \mathrm{d}\gamma, \tag{5}$$

i.e. it is the expected value of the tail (from α-quantile onward) of the distribution of costs (sometimes referred to as the Expected shortfall). For an in-depth information about the properties of the introduced risk measures, see [23].

Looking back to (3) and (4), we specify that all random variables have a finite discrete probability distributions with a finite number of scenarios and probabilities p_s or we use a scenario-based (SB) approach for the approximation of random elements of the flow and distance matrices with probabilities $p_s = 1/|\mathcal{S}|$. As we further use HN SB VaR and HN SB CVaR StoQAP, we utilize notation $d_{ij}^s = d_{ij}(\boldsymbol{\xi}^s)$ and $f_{kl}^s = f_{kl}(\boldsymbol{\xi}^s)$ where s denotes a scenario.

5 Computations and results

There are numerous possibilities of approaching the problems formulated in the previous sections. One of these approaches would be the traditional/optimization one, i.e. the model having $2n$ binary variables x_{ij} and $2n$ linear constraints and the way to solve this model would be the standard optimization technique for MINLPs - branch and bound, and cutting plane methods described in the rich integer programming literature. The drawback of this approach is that computational time (time to reach certified global optimum) explodes with increasing n as shown in our previous paper [16].

The approach used in our computations is a different one. The set of feasible solutions to the above mentioned problems is the set of n-by-n permutation matrices and as such can be described by a permutation vector p of length n. This formulation is not exactly useful for traditional optimization techniques; however, it is very convenient one for the use of specialized genetic algorithms. There are custom tailored mutation and crossover procedures that deal with permutation vectors (i.e. the result of these procedures is again a permutation vector), that are often used in the travelling salesman problem, and can be found, e.g., in [17]. The use of genetic algorithms cannot guarantee, that the solution found at the end of the procedure is truly the global optimum, nevertheless, its ability to find a "very good" solution in a fraction of time compared to the traditional approach makes it the "weapon of choice" for our computations.

The success of this approach hinges upon our ability to evaluate the fitness/objective function repeatedly for quite a large number of iterations. In this regard an efficient procedure for computing the quadruple (quintuple) sum is essential. In some software (MATLAB in our experience) an efficient way of computing the sum is in rewriting it into a matrix multiplication form that is detailed in our previous paper [26]. The computation of VaR_α in (3) is obtained by ordering the cost vector and finding the α-quantile. Similarly, CVaR_α in (4) is computed as the average of the values that are greater or equal to the VaR_α.

We investigated 3 cases with different correlation structure between $\mathbf{D}$ and $\mathbf{F}$. In the first case $d_{ij}(\boldsymbol{\xi}) \sim U(1,9)$ and $f_{ij}(\boldsymbol{\xi}) \sim U(1,9)$ are independent, with correlation $\rho = 0$. In the second case $f_{ij}(\boldsymbol{\xi}) \sim U(1,9)$ and $d_{ij}(\boldsymbol{\xi}) = f_{ij}(\boldsymbol{\xi}) + \epsilon_{i,j}$, where $\epsilon_{i,j} \sim U(-2,2)$; the resulting correlation $\rho = \frac{\sigma(F)}{\sigma(D)} = \sqrt{\frac{4}{5}}$. The last case is again $f_{ij}(\boldsymbol{\xi}) \sim U(1,9)$ and $d_{ij}(\boldsymbol{\xi}) = 10 - f_{ij}(\boldsymbol{\xi}) + \epsilon_{i,j}$; the resulting correlation $\rho = -\sqrt{\frac{4}{5}}$. Furthermore, we review the

HN SB EO (expected objective) reformulation to compare the more risk averse objectives of VaR_α and CaR_α to this quite commonly used one:

$$\min_{x_{ij}}\{\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n}\sum_{s=1}^{|\mathcal{S}|} p_s\left(d_{ij}^s f_{kl}^s\right) x_{ik}x_{jl} \mid \mathbf{X}\in\mathcal{C}\}. \tag{6}$$

The stopping criterion for the genetic algorithm was 150 stall generations (identical for all problem sizes). The computations were carried out on an ordinary machine (3.2 GHz i5-4460 CPU, 16 GB RAM). Then, the following results have been obtained for varying number of facilities/locations n, fixed number of scenarios $|\mathcal{S}| = 100$ and confidence level $\alpha = 0.9$, see Table 1 and Table 2.

Table 1: Results for $\rho = 0$ and $\rho = \sqrt{\frac{4}{5}}$.

	$\rho = 0$					$\rho = \sqrt{\frac{4}{5}}$				
n	objective	EO	VaR	CVaR	time [s]	objective	EO	VaR	CVaR	time [s]
10	EO	2484	2692	2768	73	EO	2469	2742	2857	77
	VaR	2497	2651	2772	84	VaR	2489	2699	2871	94
	CVaR	2491	2680	2738	76	CVaR	2490	2755	2821	76
20	EO	9948	10355	10524	167	EO	9934	10521	10772	205
	VaR	9992	10273	10536	150	VaR	10003	10442	10813	156
	CVaR	9977	10326	10437	186	CVaR	9999	10539	10682	160
30	EO	22402	22972	23210	315	EO	22349	23239	23496	328
	VaR	22470	22873	23286	257	VaR	22490	23018	23620	237
	CVaR	22453	22932	23083	377	CVaR	22470	23156	23348	380
40	EO	39837	40656	40908	715	EO	39802	40958	41285	921
	VaR	39936	40488	40934	606	VaR	39983	40769	41496	611
	CVaR	39935	40565	40676	767	CVaR	39949	40881	41044	889
50	EO	62271	63313	63751	1002	EO	62346	63988	64698	1113
	VaR	62425	63142	63850	732	VaR	62544	63582	64684	911
	CVaR	62405	63253	63448	1201	CVaR	62524	63836	64168	1156

Table 1 shows the results for the first two cases for specific sizes of problems identified by number of variables. Computational times are presented as well to underline how the problem quickly grows. The minimized objective is specified by rows. The validity of solution can be derived column related values, where the optimal solution obtained by the choice of reformulation (see rows) is substituted in the objective function specified by the reformulation (see columns). One interesting aspect of the results is the relative closeness of EO and CVaR solutions (in terms of the corresponding objectives), or, on the other hand that minimizing VaR produces solutions quite dissimilar to the other two (it has the worst EO and CVaR value in almost all cases).

Table 2: Results for $\rho = -\sqrt{\frac{4}{5}}$.

n	EO	VaR	CVaR	time [s]
10	1957	2060	2091	68
20	7865	8065	8110	202
30	17698	18010	18119	530
40	31872	32234	32346	1690
50	50970	51488	51677	2670

In Table 2, the results for the negative correlation case show a different behavior - namely that the minimal objective (be it EO, VaR or CVaR) was attained by the same solution. Furthermore the computational times

(in the table we report the average time for the three objectives) were much higher in comparison with the first two cases.

6 Conclusion

In this paper we continue our investigation of the StoQAP problem, started in [16] and [26], by introducing more risk averse formulations as the objective, namely CVaR and VaR, and comparing the solutions to these formulation with a standard EO formulation. The focus is on scenario-based reformulation and the subsequent mathematical program is solved by a genetic algorithm and the actual computations were implemented in MATLAB. All computations have followed the idea of test set for StoQAP introduced in [16].

The next line of research will take the direction of improving the algorithm as in [13], [14], [24], and [33]. We expect to utilize the results in the aforementioned areas of applications.

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