

Two-stage Stochastic Standard Quadratic Optimization

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Vienna Graduate School on
Computational Optimization



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- 2 Stochastic Standard Quadratic Problem
 - Problem Formulation
- 3 Lower Bounds Based on Dissecting Probability Measures
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 - A Chain of Lower Bounds
- 4 Solving the Scenario Problems
 - Lower Bounds Based on Copositive Optimization
 - Upper Bounds based on Awaystep Franke-Wolfe Algorithm
- 5 Numerical Experiments

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The Standard Quadratic Problem

Definition

The (deterministic) **Standard Quadratic Problem** (DStQP) is to optimize a quadratic form over the Standard Simplex (Probability Simplex)

$$\text{(DStQP)} \quad z_{\text{det}}^* := \min \left\{ q(z) := z^T Q z : z \in \Delta^n \right\}$$

where $\Delta^n = \{z \in \mathbb{R}_+^n : \bar{e}^T z = 1\}$ and \bar{e} is the vector of all ones.

The DStqP arises in many different contexts such as

- the Maximum-Clique- and the Maximum-Weight-Clique-Problem,
- Evolutionary Game Theory,
- Portfolio Selection and
- Dominant-Set Clustering

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where $\Delta^n = \{z \in \mathbb{R}_+^n : \bar{e}^T z = 1\}$ and \bar{e} is the vector of all ones.

- DStqP defines a class of NP-Hard optimization problems.
- Many polynomial time approximation schemes.
- Well performing local algorithms (e.g. based on immunization-infection dynamics).
- Many nice analytic bounds.

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Uncertain blocks in the objective matrix

- Henceforth, we assume that the quadratic form has uncertain entries:

$$\tilde{Q} := \begin{bmatrix} A & \tilde{B}^T \\ \tilde{B} & \tilde{C} \end{bmatrix}.$$

- Only the matrix $A \in \mathbb{R}^{n_1 \times n_1}$ is known exactly.
- The matrices $\tilde{B} \in \mathbb{R}^{n_2 \times n_1}$, $\tilde{C} \in \mathbb{R}^{n_2 \times n_2}$ are only known to follow a certain, known probability distribution $[\tilde{B}, \tilde{C}] =: \xi \sim \mathcal{P}$.

Two-Stage Decision Process

- We split the decision vector in two parts $z = (x, y(\xi))$.
- x is the here and now decision, to be made immediately
- $y(\xi)$ is the second stage decision, that may adapt to the uncertain outcome.

Definitions

Decomposing $z := (x, y(\xi))$, we arrive at

$$q(x, y(\xi)) = x^T A x + 2x^T \tilde{B}^T y(\xi) + y(\xi)^T \tilde{C} y(\xi)$$

The two stage Stochastic version of the StQP is then given by

$$\min_{x \in T^{n_1}} \left\{ x^T A x + \mathbb{E}_{\xi} \left[\min_{y(\xi) \geq 0} \left\{ 2x^T \tilde{B}^T y(\xi) + y(\xi)^T \tilde{C} y(\xi) : e^T x + e^T y(\xi) = 1 \right\} \right] \right\} \quad (1)$$

⇒ We want to find a first stage decision, that optimizes the expected performance of our second stage decision.

The Scenario Problem

- We can approximate the true probability distribution with an discretization.
- We get a discrete probability measure p_1, \dots, p_S ,
- associated realizations of the random data B_1, \dots, B_S and C_1, \dots, C_S

The problem then reduces to the so called *scenario problem*:

$$\begin{aligned} \min_{x, y_1, \dots, y_S} \quad & x^T A x + \sum_{i=1}^S p_s (2y_s^T B_s x + y_s^T C_s y_s) \\ \text{s.t. :} \quad & e^T x + e^T y_s = 1, \quad s = 1, \dots, S, \\ & x \geq 0, \\ & y_s \geq 0, \quad s = 1, \dots, S, \end{aligned}$$

Non-convex QP with linear constraints!

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Wait-and-See Approach

Suppose the following:

- ξ has a finite support $\Xi = \{\xi_1, \dots, \xi_S\}$,
- Finite number of possible scenarios $\xi_s = (B_s, C_s)$.
- Positive probabilities $p_s, s = 1, \dots, S$.

Deterministic optimization problem under scenario s :

$$z_s^* := \min \left\{ q_s(z) := z^T Q_s z : z \in \Delta^n \right\},$$

Wait and See Solution (WS)

$$z^{1*} := \sum_{s=1}^S p_s z_s^* \leq z_{\text{stoch}}^*$$

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Refinement of the Probability Measure

Consider the following **successively refining partition of the sample space**:

$$\begin{aligned} \Xi &= \{\xi_1, \dots, \xi_S\} \\ &\dots \\ &(\Xi_1^{(j)}, \Xi_2^{(j)}, \dots, \Xi_{m_j}^{(j)}) \\ &\dots \\ &(\Xi_1^{(2)}, \Xi_2^{(2)}, \dots, \Xi_{m_2}^{(2)}) \\ &(\{\xi_1\}, \{\xi_2\}, \dots, \{\xi_S\}), \end{aligned}$$

- Each row is a collection of subsets of the probability space Ξ .
- The whole space $\Xi = \cup_i \Xi_i^{(j)}$ for all j .
- $\Xi_i^{(j)}$ is the union of sets from the next more refined collection

A Chain of Lower Bounds

Denoting with

$$z^{j*} = \sum_{i=1}^{m_j} \pi_i^{(j)} z^*(\Xi_i^{(j)}),$$

where $\pi_i^{(j)} = \sum_{\xi_s \in \Xi_i^{(j)}} p_s$, we get to a chain of lower bounds expressed as follows

$$z^{1*} \leq z^{2*} \leq \dots \leq z^{j*} \leq \dots \leq z_{\text{stoch}}^*. \quad (2)$$

- The higher the index j , the fewer problems have to be solved,
- but with an increasing number of scenarios.

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Convex Reformulations of QCQPs in a Nutshell

$$\min_{x \in \mathbb{R}^2} q_{11}x_1^2 + 2q_{12}x_1x_2 + q_{22}x_2^2$$

$$\text{s.t. : } 2x_1^2 + x_2^2 \leq 12,$$

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$$4x_1^2 + x_2^2 \geq 4,$$

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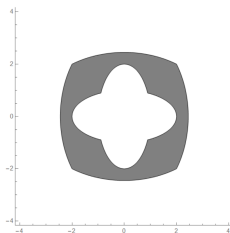
$$\min_{X \in \mathcal{S}_+^2} q_{11}X_{11} + 2q_{12}X_{21} + q_{22}X_{22}$$

$$\text{s.t. : } 2X_{11} + X_{22} \leq 12,$$

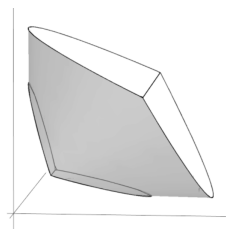
$$X_{11} + 2X_{22} \leq 12,$$

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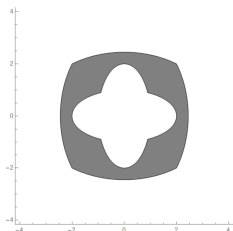


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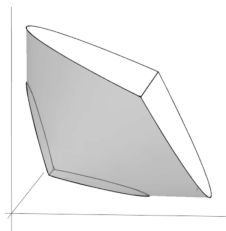


$\mathcal{G}(\mathcal{F})$

Convex Reformulations of QCQPs in a Nutshell



\mathcal{F}



$\mathcal{G}(\mathcal{F})$

- We can lift the space of variables by replacing $xx^T \rightarrow X$
- Then all quadratic expression become $x^T Ax = \text{tr}(Axx^T) \rightarrow \text{tr}(AX) = A \bullet X$, hence linear.
- Since not all psd-matrices are of the form xx^T the lifted problem is a relaxation.
- If the extreme points of the lifted feasible set matrices of the form xx^T , we get a feasible solution for the original problem.
- Thus, in these cases the relaxation is tight!

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Exact CPP-Reformulation

Burer (2009) proves the tightness of the CPP-relaxation

$$\min_{x, y_1, \dots, y_S} A \bullet X + \sum_{i=1}^S \rho_s (2B_s \bullet Z_s + {}^T C_s \bullet Y_s)$$

$$\text{s.t. : } e^T x + e^T y_s = 1, \quad s = 1, \dots, S,$$

$$E \bullet X + E \bullet Y_s + 2E \bullet Z_s = 1, \quad s = 1, \dots, S,$$

(CPP1)

$$\begin{pmatrix} 1 & x^T & y_1^T & \dots & y_S^T \\ x & X & Z_1^T & \dots & Z_S^T \\ y_1 & Z_1 & Y_1 & \dots & Y_{1,S}^T \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y_S & Z_S & Y_{1,S} & \dots & Y_S \end{pmatrix} \in \mathcal{CPP} \left(\mathbb{R}_+^{n_1 + S n_2 + 1} \right) := \{ B B^T : B \geq 0 \}$$

^aS. Burer. On the copositive representation of binary and continuous nonconvex quadratic programs. *Mathematical Programming*, 120(2) 2009

DNN Relaxation

We can further relax the problem in order to obtain a **tractable lower bound**

$$\min_{x, y_1, \dots, y_S} A \bullet X + \sum_{i=1}^S p_s \left(2B_s \bullet Z_s + {}^T C_s \bullet Y_s \right)$$

$$\text{s.t. : } e^T x + e^T y_s = 1, \quad s = 1, \dots, S,$$

$$E \bullet X + E \bullet Y_s + 2E \bullet Z_s = 1, \quad s = 1, \dots, S,$$

$$\begin{pmatrix} 1 & x^T & y_1^T & \dots & y_S^T \\ x & X & Z_1^T & \dots & Z_S^T \\ y_1 & Z_1 & Y_1 & \dots & Y_{1,S}^T \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y_S & Z_S & Y_{1,S} & \dots & Y_S \end{pmatrix} \in \mathcal{DNN}^{n_1+S n_2+1} := \mathcal{S}_+^{n_1+S n_2+1} \cap \mathcal{N}^{n_1+S n_2+1}$$

(DNN1)

Cheaper CPP-Relaxation

A **cheaper lower bound** is given by the problem

$$\begin{aligned} \min_{x, y_1, \dots, y_S} \quad & A \bullet X + \sum_{i=1}^S p_s (2B_s \bullet Z_s + C_s \bullet Y_s) \\ \text{s.t. :} \quad & e^T x + e^T y_s = 1, & s = 1, \dots, S, \\ & E \bullet X + E \bullet Y_s + 2E \bullet Z_s = 1, & s = 1, \dots, S, \quad (\text{CPP2}) \\ & \begin{pmatrix} 1 & x^T & y_s^T \\ x & X & Z_s^T \\ y & Z_s & Y_s \end{pmatrix} \in \text{CPP}(\mathbb{R}_+^{n_1+n_2+1}) & s = 1, \dots, S, \end{aligned}$$

Cheaper DNN Relaxation

We can relax the problem in the same way as before:

$$\begin{aligned} \min_{x, y_1, \dots, y_S} \quad & A \bullet X + \sum_{i=1}^S p_s \left(2B_s \bullet Z_s + {}^T C_s \bullet Y_s \right) \\ \text{s.t.} \quad & e^T x + e^T y_s = 1, \quad s = 1, \dots, S, \\ & E \bullet X + E \bullet Y_s + 2E \bullet Z_s = 1, \quad s = 1, \dots, S, \\ & \begin{pmatrix} 1 & x^T & y_s^T \\ x & X & Z_s^T \\ y & Z_s & Y_s \end{pmatrix} \in \mathcal{S}_+^{n_1+n_2+1} \cap \mathcal{N}^{n_1+n_2+1} \quad s = 1, \dots, S, \end{aligned}$$

(DNN2)

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The Franke-Wolfe Algorithm in a Nutshell

Algorithm 0: A fast way to solve $\min_{x \in P} f(x)$, for a polytope P .

Result: v^*

set $k = 1$

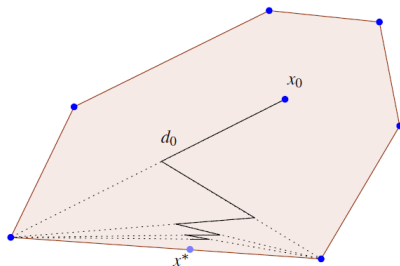
set $x_1 \in P$

repeat

 solve $\min_{y_+ \in P} \nabla f(x_k)^\top y_+$

 move to best vertex i.e. : $x_{k+1} = x_k + \alpha(y_+ - x_k)$

until *Some criterium is met*



The Pairwise Franke-Wolfe Algorithm in a Nutshell

Algorithm 1: An even faster way to solve $\min_{x \in P} f(x)$, for a polytope P .

Result: v^*

set $k = 1$

set $x_1 \in P$

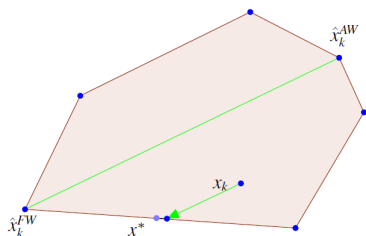
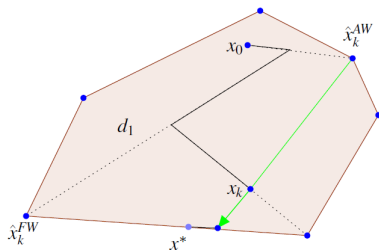
choose $S_k \subseteq P$

repeat

solve $\min_{y_+ \in P} \nabla f(x_k)^T y_+$ and $\max_{y_- \in S_k} \nabla f(x_k)^T y_-$; move towards best and away from worst vertex i.e. : $x_{k+1} = x_k + \alpha(y_+ - y_-)$

Update S_k

until *Some criterium is met*



Adapting AS-FW for the scenario problem

- The gradient is easily calculated from the problem data since $\nabla_{\mathbf{x}}^T Q\mathbf{x} = 2Q\mathbf{x}$.
- The vertices of the feasible set of $\left\{ (x, y_1, \dots, y_s) \in \mathbb{R}_+^{n_1 + Sn_2} : e^T x + e^T y_s = 1, s = 1, \dots, S \right\}$ are simply $V(P) = \{e_i : i \in [1:n_1]\} \cup \left\{ \sum_{s=1}^S e_{j_s + n_1 + (s-1)n_2} : j \in [1:n_2]^S \right\}$
- Thus, solving the linear optimization problem amounts to finding $S + 1$ largest/smallest values.
- S_k is easily updated by dropping coordinates that became zero.
- We can choose different starting points and pick the best solution.

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Comparing the copositive bounds

Results

- Test with different sizes of instances.
- 20 randomly generated instances per size category.
- Average %-gap between the upper bound and the two lower bounds.

(n_1, n_2, S)	Time		Gap		max Gap		Vs.	
	DNN1	DNN2	DNN1	DNN2	DNN1	DNN2	avgG	maxG
(5,5,10)	1.647	0.191	1.075%	1.373%	13.26%	14.167%	0.019%	0.016%
(5,10,10)	28.05	0.237	0.003%	0.039%	0.056%	0.379%	0.001%	0.001%
(5,20,10)	1132.45	0.754	0.428%	1.281%	5.136%	18.633%	0.001%	0.001%
(10,5,10)	2.942	0.438	1.365%	1.665%	17.201%	18.306%	0.014%	0.011%
(20,5,10)	5.515	0.977	9.432%	9.305%	35.772%	35.824%	0.002%	0.001%
(5,5,20)	37.588	0.546	0.807%	1.394%	13.756%	14.317%	0.029%	0.023%
(5,5,40)	1504.456	0.998	1.09%	1.579%	21.536%	21.625%	0.006%	0.004%

Comparing different Upperbounds

(n_1, n_2, S)	Time					Gap				
	DNN	Gurobi	fmincon	PFW	PFWM	DNN	Gurobi	fmincon	PFW	PFWM
(10,5,10)	0,274	291,987	0,701	0,031	5,419	16,33%	0,32%	3,01%	1,92%	0,25%
(20,5,10)	0,492	300,406	0,994	0,061	7,170	50,41%	2,13%	10,57%	2,10%	0,23%
(5,10,10)	0,362	300,483	2,622	0,039	8,463	15,24%	0,09%	2,31%	1,32%	0,08%
(5,20,10)	0,614	300,743	2,872	0,082	16,843	13,76%	0,15%	2,86%	1,88%	0,04%
(5,5,10)	0,362	296,317	0,764	0,024	4,207	19,06%	0,32%	0,94%	1,26%	0,32%
(5,5,20)	0,108	300,527	1,698	0,050	13,319	19,58%	0,15%	1,29%	2,54%	0,15%

Table: Results of cold-starting the upper-bound procedures

- Multistarting PFW yields small gaps in reasonable time.

Warmstarting primal procedures

(n_1, n_2, S)	Gap				Time			
	DNN+FW+Gurobi	DNN+fmincon	DNN+Gurobi	DNN+FW	DNN+FW+Gurobi	DNN+fmincon	DNN+Gurobi	DNN+FW
(10,5,10)	0,26%	0,63%	0,31%	0,27%	292,431	1,139	291,379	0,534
(20,5,10)	0,54%	1,43%	1,87%	0,82%	301,150	1,797	301,163	0,796
(5,10,10)	0,08%	0,72%	0,09%	0,10%	301,038	1,819	301,048	0,591
(5,20,10)	0,04%	0,47%	0,17%	0,04%	301,598	6,654	301,595	0,908
(5,5,10)	0,32%	0,33%	0,32%	0,34%	301,769	1,125	301,419	0,548
(5,5,20)	0,15%	0,25%	0,15%	0,21%	301,089	1,982	301,006	0,505

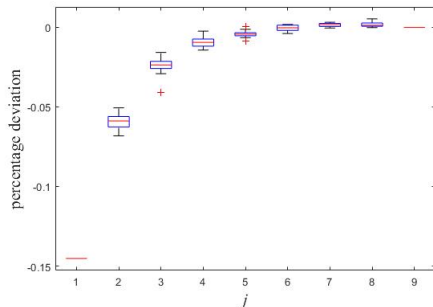
Table: Warmstarting the upper bound procedures: gaps and runtimes

- Using the upper bounds to warm start primal algorithms can be advantageous.

Experiments on dissecting the probability measure

Recall the **successively refining partition of the sample space**:

$$\begin{aligned} \Xi &= \{\xi_1, \dots, \xi_S\} \\ &\dots \\ (\Xi_1^{(j)}, \Xi_2^{(j)}, \dots, \Xi_{m_j}^{(j)}) \\ &\dots \\ (\Xi_1^{(2)}, \Xi_2^{(2)}, \dots, \Xi_{m_2}^{(2)}) \\ (\{\xi_1\}, \{\xi_2\}, \dots, \{\xi_S\}), \end{aligned}$$



Application to Mean-Variance Portfolio Optimization

- We consider the historical mean return and variance of returns of ten assets based on ten time series.
- For assets $i \in [1:5]$ a longer time series of 48 days is available while for assets $i \in [6:10]$ only a short time series of 12 days is available.
- Hence, we consider the portion of the covariance matrix that involve the latter assets to be uncertain and we consider the model:

$$\min_{x \in T^5} \left\{ \mu_x^T x + x^T \Sigma_{xx} x + \mathbb{E} \left[\min_{y \in P_x} \mu_y^T y + 2x^T \Sigma_{xy} y + y^T \Sigma_{yy} y \right] \right\} \quad (3)$$

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Despite the presence of a linear term, the above optimization problem can be rewritten as

$$\min_{x \in T^5} \left\{ x^T \bar{\Sigma}_{xx} x + \mathbb{E} \left[\min_{y \in P_x} 2x^T \bar{\Sigma}_{xy} y + y^T \bar{\Sigma}_{yy} y \right] \right\}$$

where

$$\begin{aligned} \bar{\Sigma}_{xx} &:= \Sigma_{xx} + \frac{1}{2} (\mu_x e^T + e \mu_x^T), \\ \bar{\Sigma}_{xy} &:= \Sigma_{xy} + \frac{1}{2} (\mu_x e^T + e \mu_y^T), \\ \bar{\Sigma}_{yy} &:= \Sigma_{yy} + \frac{1}{2} (\mu_y e^T + e \mu_y^T). \end{aligned}$$

- We approximated the problem via the scenario approach
- the covariance matrix were generated from a elementwise normal distribution, i.e. $(\Sigma)_{ij} \sim N((\hat{\Sigma})_{ij}, \sigma)$ with $\hat{\Sigma}$ the empirical covariance matrix and $\sigma = 1$
- Scenarios with $S \in \{100, 500, 1000, 5000, 10000\}$ were generated.

Numerical experiments on portfolio optimization

S	Obj	Gap	Time
100	163.59	0,00%	0.47
500	163.60	0,00%	1.07
1000	163.60	0,00%	2.27
5000	163.57	0,00%	10.84
10000	163.58	0,00%	22.49

Table: Results of the portfolio optimization experiment

- In our experiments, all instances were solved using merely the reduced conic relaxation
- Hence, there are real-world applications where gaps can be closed confidently using the basic strategies.

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Thank you