Global Optimization Strategies for Standard Quadratic Problems

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INTRODUCTION TO StQPs

Standard Quadratic Optimization Problems (StQPs):

$$\min_{x\in\mathbb{R}^n} \quad \frac{1}{2}x^TQx + c^Tx$$

$$\text{s.t.} \quad \boxed{\begin{array}{l} e^Tx = 1 \\ x \geq 0 \end{array}}$$

n-dimensional standard simplex

StQPs:
- **Not convex**
- **NP-hard problems**

StQPs are very important and these are some **applications**:
- **Portfolio Optimization**
- **Finding Maximum clique in graphs**

OBSERVATIONS ON StQP PROBLEMS

Given the structure of **StQP** problems, the following **observations** are valid:

- **First Observation**: *Matrix Q and vector c can always be re-defined in such a way that $Q_{ii} = 0$ for all $i = 1, \dots, n$, i.e. all diagonal elements of the Hessian matrix Q can be taken equal to 0.*

- **Second Observation**: *If the diagonal condition above holds, then all $Q_{ij} > 0$ can be set equal to 0, since at any optimal solution of the StQP problem, $Q_{ij} > 0$ implies that al least one among x_i and x_j is certainly equal to 0.*

SMO ALGORITHM

To solve the **StQP** problems, **a fast decomposition algorithm** has been applied.

↓

Sequential Minimal Optimization (SMO)

Main features:

- **Updates two variables** in closed form
- **Guarantees convergence** to a local minimum
- Efficient ***local solver*** within a global optimization strategy

A fundamental point of **SMO**:

- **Choice of the starting point**

Using a simple **Multi-Start strategy** with **SMO** as a **local solver**:

- **Global optimum** is often found and with relatively short computation times

THESIS AIM

Use a strategy that **allows to find the global minimum in a consistent way** with less computation times.

↓

Using the **Convexity Graph** associated to the **Hessian matrix** Q of the problem.

CONVEXITY GRAPH 1/3

A **graph** $G = (V, E)$ can be associated with a problem **StQP**, where:

- $V = \{1, \dots, n\}$ are vertices (or nodes) of the graph.
- $E = \{(i, j) : i, j \in \{1, \dots, n\}, Q_{ij} < 0\}$ are edges (or arcs).

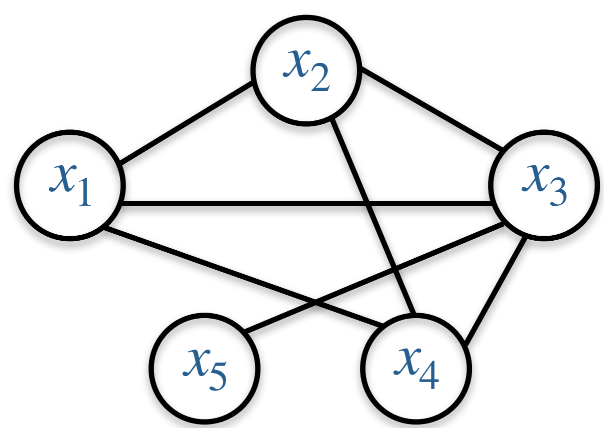
Def. Convexity Graph

> **Convexity Graph** *is graph in which every variable of the problem is associated with a node and an edge* (i, j) *is placed if and only if the objective function is strictly convex on the whole edge in the feasible set joining the nodes* x_i *and* x_j*.*

Example:

$$\begin{array}{cc} & \begin{array}{ccccc} x_1 & x_2 & x_3 & x_4 & x_5 \end{array} \\ \begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{array} & \begin{bmatrix} 0.0 & -2.1 & -2.9 & -3.8 & 0.0 \\ -2.1 & 0.0 & -2.7 & -2.0 & 0.0 \\ -2.9 & -2.7 & 0.0 & -0.3 & -2.3 \\ -3.8 & -2.0 & -0.3 & 0.0 & 0.0 \\ 0.0 & 0.0 & -2.3 & 0.0 & 0.0 \end{bmatrix} \end{array}$$

$\xrightarrow{\text{Convexity Graph}}$



CONVEXITY GRAPH 2/3

The **optimal solution** of the problem StQP must be attained in the relative interior of some face:

$F_C = \{x \in \Delta_n : x_i = 0,\ i \notin C\}$, where $C \subseteq V$ is a ***clique*** over the convexity graph G.

This implies that

In an **optimal solution** if there are **multiple non-zero components**, they must be in a ***clique***.

Def. Clique

A ***Clique*** *C in an undirected graph G is a subset of the vertices, such that every two distinct vertices are adjacent.*

CONVEXITY GRAPH 3/3

- Use the **convexity graph** for the **choice of the starting points** of the SMO algorithm
  - that is more efficient than a basic *Multistart* strategy (starts from the vertices of the standard simplex)

- Calculating the ***cliques*** is as difficult a problem as solving the starting problem
  - **good strategy**: look for initial solutions in which **only two components are different from zero**.

In an **optimal solution** these **two components** can be **simultaneously different from zero** only if they are **connected** in the **convexity graph**.

BUILD THE BINARY MATRIX

To choose the **starting point**, first you have to build the **binary matrix** H relating to the matrix Q of the problem, where:

- **Extra-diagonal elements:** $\dfrac{2Q_{ij} - Q_{ii} - Q_{jj}}{2}$

  if > 0 then $H_{ij} = 0$

  if < 0 then $H_{ij} = 1$

  with:
  $i = 1, \ldots, n$
  $j = 1, \ldots, n$

- **Diagonal elements:** $H_{ii} = 0$

This **binary matrix** H is necessary to efficiently choose the **starting point** from which to start the **SMO algorithm**.

CHOICE OF THE STARTING POINT

Pseudo-code:

Let $\boldsymbol{H} \in \mathbb{R}^{n \times n}$ be a **binary matrix** and let $\boldsymbol{x} \in \mathbb{R}^{n}$ be a **zeros-vector**.

1. Randomly choose $i \sim \mathcal{U}(1,\dots,n)$
2. $J = \{j \mid H_{ij} = 1\}$
3. $s = length(J)$
4. Randomly choose $k \sim ([0,\dots,s-1])$
5. $\hat{j} = J[k]$
6. $x = \left[0,0,0,\dots,\frac{1}{2},0,0,\dots,\frac{1}{2},0,\dots,0\right]$ where $x[i] = \frac{1}{2}$ and $x[\hat{j}] = \frac{1}{2}$
7. Return $\boldsymbol{x}$

DESCRIPTION OF DATASETS

For this thesis, the experiments were performed on **three different datasets**:

- **Generic Dataset**: **56 instances of StQP** problems with size $n \in \{10,30,50,100,200,500,1000\}$.
- **BSU Dataset**: **20 instances of StQP** problems with size $n \in \{5,\ldots,24\}$. These problems are *hard* because they have an exponential number of local minimums.
- **BHOSLIB Dataset**: **5 instances of StQP problems for each of the 8 different dimensions** in $\{450,595,760,945,1150,1272,1400,1534\}$. These are **maximum clique** problems and they are *hard*. For each problem, the real size of the maximum clique is known.

EXPERIMENTS ON GENERIC DATASET 1/2

Three algorithms were compared:

1. **Branch-and-bound** (exact algorithm that guarantees optimality)
2. **Multistart SMO** (starting points are the vertices of standard simplex)
3. **Multistart SMO based on convexity graph** (**SMO-CG**) (2000 iterations)

Some **results** are shown in the following tables:

Problem	Branch-and-bound		Multistart SMO		SMO-CG	
	Time to optimum (sec.)	Objective value	Time to optimum (sec.)	Objective value	Time to optimum (sec.)	Objective value
100x100(0.5)_5	20.65	**-6.18**	0.67	-6.14	**0.71**	**-6.18**
100x100(0.75)_1	55.58	**-6.57**	1.10	-6.51	**0.08**	**-6.57**
100x100(0.75)_2	101.57	**-6.53**	0.94	**-6.53**	**0.42**	**-6.53**
100x100(0.75)_3	1.82	**-6.63**	1.01	**-6.63**	**0.65**	**-6.63**
100x100(0.75)_4	47.32	**-6.56**	0.92	**-6.56**	**0.36**	**-6.56**
100x100(0.75)_5	42.48	**-6.81**	0.94	**-6.81**	**0.85**	**-6.81**

⋮

EXPERIMENTS ON GENERIC DATASET 2/2

⋮

Problem	Branch-and-bound		Multistart SMO		SMO-CG	
	Time to optimum (sec.)	Objective value	Time to optimum (sec.)	Objective value	Time to optimum (sec.)	Objective value
200x200(0.75)_1	Error	Error	3.58	**-6.70**	**0.30**	**-6.70**
200x200(0.75)_5	Error	Error	2.98	**-6.86**	**0.36**	**-6.86**
500x500(0.25)_1	Error	Error	9.72	**-6.81**	**4.24**	**-6.81**
500x500(0.25)_5	Error	Error	13.17	-6.58	**5.58**	**-6.66**
500x500(0.5)_2	Error	Error	12.63	-7.07	**6.81**	**-7.08**
500x500(0.5)_3	Error	Error	12.67	**-6.86**	**1.04**	**-6.86**
1000x1000(0.25)	Error	Error	39.58	**-6.76**	**20.88**	**-6.76**

Number of problems in which the optimum was found for each algorithm:

- **Branch-and-bound**: 40 of 56
- **Multistart SMO**: 47 of 56
- **SMO-CG**: **56 of 56**

EXPERIMENTS ON BSU DATASET

Three algorithms were compared:

1. **Branch-and-bound** (exact algorithm that guarantees optimality)
2. **Multistart SMO** (starting points are the vertices of standard simplex)
3. **Multistart SMO based on convexity graph** (**SMO-CG**) (2000 iterations)

Some **results** are shown in the following table:

Problem	Branch-and-bound	Multistart SMO	SMO-CG
	Time to optimum (sec.)	Time to optimum (sec.)	Time to optimum (sec.)
BSU5	0.51	0.0096	**0.0054**
BSU8	0.73	G.O Not Found	**0.01**
BSU9	0.70	G.O Not Found	**0.01**
BSU15	3.14	22.53	**1.32**
BSU20	1.46	1.764	**0.07**
BSU23	116.47	191.87	**52.46**
BSU24	679.74	6.19	**0.24**

EXPERIMENTS ON BHOSLIB DATASET 1/2

Two algorithms were compared:

1. **Multistart SMO** (starting points are the vertices of standard simplex)
2. **Multistart SMO based on convexity graph** (**SMO-CG**) (4000 iterations)

The **Branch-and-bound** was not used because it was unable to give a solution due to the greatness and complexity of the problems of this dataset.

The **size of the clique**, obtained after applying one of the two algorithms, is computed with the following formula:

$clique\_size = \dfrac{1}{1+f^\star}$ where $f^\star$ is the optimal solution of the problem

EXPERIMENTS ON BHOSLIB DATASET 2/2

Results with **Multistart SMO**:

Vertices	Max. Clique Size	P1 sol.	P2 sol.	P3 sol.	P4 sol.	P5 sol.	Avg. Time to Optimum (sec.)
450	30	**26**	26	25	25	**26**	35.70
595	35	30	**30**	29	31	30	**76.80**
760	40	33	33	**34**	**34**	33	**130.88**
945	45	37	35	35	37	37	**157.09**
1150	50	40	39	**43**	40	41	337.28
1272	53	**43**	45	43	44	**45**	526.01
1400	56	46	45	45	45	44	744.58
1534	59	48	47	46	48	48	1042.06

Multistart SMO gets **8 wins** compared to **SMO-CG**

Results with **SMO-CG**:

Vertices	Max. Clique Size	P1 sol.	P2 sol.	P3 sol.	P4 sol.	P5 sol.	Avg. Time to Optimum (sec.)
450	30	25	26	**26**	**26**	25	**19.01**
595	35	30	29	**30**	31	**31**	133.82
760	40	33	**35**	33	33	**34**	164.53
945	45	37	**37**	**36**	37	**38**	170.26
1150	50	40	**41**	42	40	41	**322.63**
1272	53	42	45	**44**	44	42	**307.07**
1400	56	46	45	45	**46**	**46**	**404.92**
1534	59	48	47	**48**	48	48	**936.40**

SMO-CG gets **14 wins** compared to **Multistart SMO**

CONCLUSIONS & FUTURE DEVELOPMENTS

- Implemented a technique that efficiently use **SMO** as a **local solver** within a **global optimization strategy**.

- The main challenge was to **choose an adequate starting point** for the algorithm
  - **Best results** using the **convexity graph** associated with the starting problem (**SMO-CG**).
  - **SMO-CG** was better, in terms of **performance**, compared to **SMO equipped with a simple Multistart strategy**
    - especially as the **size** of **StQP** problems **increases**.

A possible **Future Development** is:

1. Use strategies that **better use information relating to convexity graph**.

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