Binary Quadratic Optimization

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Preface

The work on this thesis began in April 2010 when I started my Master's Thesis. I officially began my PhD research in November 2010 at the Center of Excellence in Optimization and Systems Engineering at Åbo Akademi University. I am very grateful for all help I have gotten from my adviser, professor Tapio Westerlund. A big thank you goes to Ray Pörn, without your mathematical understanding and formulations that you have tried to explain to me this thesis would not exist. Thank you Axel Nyberg for your comments on my thesis, they have been of much help. I also want to thank everyone at the Process Design and Systems Engineering Laboratory for a great working/coffee environment. I also want to thank all the followers of the "Matdiktator", for our wonderful and often long lunches, I do not know how I would have finished this thesis without you. Finally, I want to thank Jonna for always being there for me.

Åbo, June 2016
Otto Nissfolk

Contribution of the author

Paper I: The Coulomb Glass - Modeling and Computational Experience with a Large Scale 0-1 QP Problem
Paper I is written by Ray Pörn and I am responsible for the optimization and result presentation. Other co-authors are Fredrik Jansson and Tapio Westerlund. In this paper the 0-1 formulation for the Coulomb glass problem is introduced.

Paper II: A Mixed Integer Quadratic Reformulation of the Quadratic Assignment Problem with Rank-1 Matrix
Paper II is written by me and I am responsible for implementing the models and solving of the optimization problem. The co-authors are Ray Pörn, Tapio Westerlund and Fredrik Jansson. In this paper we introduce a formulation for Rank-1 QAP problems.

Paper III: A Metaheuristic Optimization Algorithm for Binary Quadratic Problems
Paper III is written by me with guidance from my supervisor Tapio Westerlund. In this paper we tried a new metaheuristic method in order to acquire good solutions to binary quadratic problems.

Paper IV: Reformulation of 0-1 Quadratic Programs using Non-diagonal Perturbations
Paper IV is mainly written by Ray Pörn and I am responsible for the implementation of the mathematical models, the optimization and the presentation of the results. Other co-authors are Anders Skjäl and Tapio Westerlund.

Paper V: Testing the non-diagonal quadratic convex reformulation technique
Paper V is written by me and I am responsible for the implementations as well as the computations. The mathematical background and formulations are from Papers II and IV. The co-authors are Ray Pörn and Tapio Westerlund. In this paper we test how different numbers of non-diagonal elements included in the NDQCR affect the solution times.

Svensk sammanfattning

Optimering är ett viktigt verktyg vid beslutsfattande och speciellt då man undersöker och förbättrar produktionen i en fabrik. Matematiskt inbegriper lösningen av ett optimeringsproblem att hitta den bästa lösningen av alla tillåtna lösningar till problemställningen. Ett optimeringsproblem består av en objektsfunktion, variabler och bivillkor. Objektsfunktionen är ett matematiskt uttryck vilket man vanligen vill minimera eller maximera. Till exempel inom en fabrik vill man maximera vinsten eller minimera produktionskostnader. Variablerna beskriver till exempel hur mycket av en viss sorts resurs som behövs eller hur mycket tid som går åt i olika produktionssteg. Binära variabler kan vara beslutsvariabler som till exempel bestämmer ifall en fabrik skall placeras på en ort eller inte. Bivillkorena är funktioner som begränsar de tillåtna värdena för variablerna, till exempel att mängden använda resurser inte kan överstiga mängden tillgängliga resurser.

Denna doktorsavhandling är baserad på de fem artiklar som finns bifogade i slutet av avhandlingen. Avhandlingens huvudtema är binärkvadratisk optimering. Det vill säga att objektfunktionen innehåller kvadratiska och bilinjära delar samt linjära delar. Huvudproblemet som granskats är Coulombglas-problemet. Coulombglas är en modell för en lätt dopad halvledare vid mycket låga temperaturer (några K) där elektronerna är belägna på vissa orenheter och elektronerna växelverkar kraftigt med varandra. Optimeringsproblemet är att placera ut elektronerna för att minimera totalenergin för systemet och då hitta grundtillståndet för materialet. En uppsättning testproblem med koppling till digital färganalys som jag även undersökt är de så kallade tai*xxx*c problemen. Dessa så kallade gråskalaproblem är problemställningar där man har ett rutmönster och skall fylla en del av rutorna med svart färg och en del med vit färg, målet är att den gråa färg som ögat uppfattar skall vara så jämn som möjligt.

Contents

Introduction

Optimization is an important activity in decision making, in analyzing and in improving production in a factory. In mathematical terms, an optimization problem is the problem of finding the best solution out of all feasible solutions. An optimization problem consists of an objective function, variables and constraints. The objective function is a mathematical function expressing what we want to maximize or minimize. For example, in manufacturing we may want to maximize the profits or minimize the cost of production. The variables can express how much resources are needed or the time spent in various production steps. Binary variables can be decision variables expressing whether a factory should be built at a location or not. The constraints are functions that define the boundaries for the variables, e.g. the amount of resources used cannot exceed the available resources.

1.1 Optimization

In order to solve a problem to optimality, the problem often needs to be convex, that means that a local minimum is also the global one. If the problem is not convex it can be convexified. In this thesis, we work with quadratic problems and in order to obtain a convex problem the quadratic matrix needs to be positive-semidefinite, that is that all eigenvalues of the matrix are in the positive half-space of the complex plane.

If the optimal solution cannot be obtained we can still obtain indications on how good the solution is with a upper bound (UB) and a lower bound (LB). A upper bound is a solution that fulfills all constraints and is therefore a feasible solution. The lower bound is a relaxed solution where some of the constraints may not be active. When the upper and the lower bound are alike, the problem is solved to optimality. The gap is a measure of the quality of the solution, it is calculated as:

$$\text{gap} = \frac{UB - LB}{UB} * 100\%.$$

A linear program (LP) is a problem formulation including only continuous variables and linear constraints. When introducing integer variables, the problem goes from LP to mixed integer linear programming (MILP). If there are quadratic terms in the objective function, the problem is called quadratic program (QP) and if there are as well quadratic constraints, it is a quadratically constrained quadratic program (QCQP).

One can use heuristic methods in order to obtain good solutions in a short amount of time. However, the solution is neither guaranteed to be the optimal solution, nor can any bounds for the solution be obtained.

1.2   Scope of work

This thesis is about new convexification and solution methods for binary quadratic problems. This thesis is organized as follows: In chapter 2, binary quadratic programming is introduced. In chapter 3, the relaxation and convexification using Quadratic Convex Reformulation and Non-Diagonal Quadratic Convex Reformulation is described. In chapter 4, the main problem looked at, the Coulomb glass problem, is presented. In chapter 5, the connection to a special case of Quadratic Assignment Problem is presented. In chapter 6, the contents of my papers and the main ideas are summarized. Chapter 7 concludes this thesis.

1.3   List of publications

This thesis is based on the following papers:

- Paper I: Ray Pörn, Otto Nissfolk, Fredrik Jansson and Tapio Westerlund. The coulomb glass - modeling and computational experience with a large scale 0-1 QP problem. 21st European Symposium on Computer Aided Process Engineering, volume 29 of Computer Aided Chemical Engineering, pages 658-662. Elsevier, 2011. doi: http://dx.doi.org/10.1016/B978-0-444-53711-9.50132-2

- Paper II: Otto Nissfolk, Ray Pörn, Tapio Westerlund and Fredrik Jansson. A mixed integer quadratic reformulation of the quadratic assignment problem with rank-1 matrix. 11th International Symposium on Process Systems Engineering, volume 31 of Computer Aided Chemical Engineering, pages 360-364. Elsevier, 2012. doi: http://dx.doi.org/10.1016/B978-0-444-59507-2.50064-0

- Paper III: Otto Nissfolk and Tapio Westerlund. A metaheuristic optimization algorithm for binary quadratic problems. 23rd European Symposium on Computer Aided Process Engineering, volume 32 of Computer Aided Chemical Engineering, pages 469-474. Elsevier, 2013. doi: http://dx.doi.org/10.1016/B978-0-444-63234-0.50079-8

- Paper IV: Ray Pörn, Otto Nissfolk, Anders Skjäl and Tapio Westerlund. Reformulation of 0-1 quadratic programs using non-diagonal perturbations. Submitted to Journal of Optimization Theory and Applications, February 2016.

- Paper V: Otto Nissfolk, Ray Pörn and Tapio Westerlund. Testing the Non-Diagonal Quadratic Convex Reformulation Technique. Accepted to 26th European Symposium on Computer Aided Process Engineering.

Binary Quadratic Programming

Quadratic Programming (QP) is the optimization of a quadratic objective function (e.g. $6x_1^2 + 3x_2^2 - 5x_1x_2 + 7x_3$) subject to linear constraints. The quadratic objective function means that it can include squared, bi-linear and linear terms. The quadratic program can be represented as:

$$
\begin{aligned}
\text{minimize} \quad & \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x} + \mathbf{c}^T\mathbf{x}, \\
\text{subject to} \quad & \mathbf{A}\mathbf{x} = \mathbf{a}, \\
& \mathbf{B}\mathbf{x} \leq \mathbf{b}, \qquad \mathbf{x} \in R^n,
\end{aligned}
\tag{2.1}
$$

where $\mathbf{Q}$ is a symmetric $n \times n$ matrix, $\mathbf{A}$ an $m \times n$ matrix, $\mathbf{c}$ an n-dimensional vector, $\mathbf{a}$ an m-dimensional vector and $\mathbf{x}$ is an n-dimensional vector with variables. The example problem would be:

$$
\min \frac{1}{2}\left[\begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} 12 & -5 & 0 \\ -5 & 6 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \right] + \begin{pmatrix} 0 & 0 & 7 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}.
$$

Binary Quadratic Programming (BQP) is a QP with binary variables. A general binary quadratic programming problem can be written as follows:

$$
\begin{aligned}
\text{minimize} \quad & \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x} + \mathbf{c}^T\mathbf{x}, \\
\text{subject to} \quad & \mathbf{A}\mathbf{x} = \mathbf{a}, \\
& \mathbf{B}\mathbf{x} \leq \mathbf{b}, \\
& \mathbf{x} \in \{0,1\}^n,
\end{aligned}
\tag{2.2}
$$

the dimensions are the same as the corresponding matrices and vectors in formulation 2.1.

Quadratic Convex Reformulation and Non-Diagonal Quadratic Convex Reformulation

Ji et al. [2013] introduced a variant of the QCR that included non-diagonal elements. Ji et al. did not name the method, so we named it Non-Diagonal Quadratic Convex Reformulation (NDQCR). NDQCR can be used to convexify 0-1 QP problems. A general BQP is given by:

$$
\begin{aligned}
\text{minimize} \quad & \mathbf{x}^T \mathbf{Q} \mathbf{x} + \mathbf{c}^T \mathbf{x}, \\
\text{subject to} \quad & \mathbf{A}\mathbf{x} = \mathbf{a}, \\
& \mathbf{B}\mathbf{x} \leq \mathbf{b}, \\
& \mathbf{x} \in \{0,1\}.
\end{aligned} \tag{3.1}
$$

The standard semidefinite relaxation of the problem 3.1 is:

$$
\begin{aligned}
\text{minimize} \quad & \mathbf{Q} \bullet \mathbf{X} + \mathbf{c}^T \mathbf{x}, \\
\text{subject to} \quad & \mathbf{A}\mathbf{x} = \mathbf{a}, \\
& \mathbf{B}\mathbf{x} \leq \mathbf{b}, \\
& \text{diag}(\mathbf{X}) = \mathbf{x}, \\
& \begin{bmatrix} 1 & \mathbf{x}^T \\ \mathbf{x} & \mathbf{X} \end{bmatrix} \geq 0, \\
& \mathbf{x} \in R^n, \mathbf{X} \in S^n,
\end{aligned} \tag{3.2}
$$

where $\mathbf{Q} \bullet \mathbf{X}$ denotes the scalar product of the matrices i.e. the sum of the products of the corresponding elements in the matrices $\mathbf{Q}$ and $\mathbf{X}$ respectively. ≥ 0 indicate that the matrix on the left hand side should be positive semidefinite. The 3.2 formulation can

be strengthened by adding squared norm constraints [Faye and Roupin, 2007] and RLT
inequalities [Roupin, 2004] to the formulation. These constraints are given by:

$$\|\mathbf{Ax} - \mathbf{a}\|^2 = \mathbf{x}^T \mathbf{A}^T \mathbf{Ax} - 2\mathbf{a}^T \underbrace{\mathbf{Ax}}_{\mathbf{a}} + \mathbf{a}^T \mathbf{a} = \mathbf{x}^T \mathbf{A}^T \mathbf{Ax} - \mathbf{a}^T \mathbf{a} = 0,$$

and

$$
\begin{aligned}
x_i x_j &\leq x_i & &\forall\, i \neq j, \\
x_i x_j &\leq x_j & &\forall\, i \neq j, \\
x_i x_j &\geq x_i + x_j - 1 & &\forall\, i \neq j, \\
x_i x_j &\geq 0 & &\forall\, i \neq j.
\end{aligned}
\tag{RLT}
$$

The formulation has the following form:

$$
\begin{aligned}
\min \quad & \mathbf{x}^T \mathbf{Q} \mathbf{x} + \mathbf{c}^T \mathbf{x}, \\
s.t. \quad & \mathbf{Ax} = \mathbf{a}, \\
& \mathbf{Bx} \leq \mathbf{b}, \\
& \mathbf{x}^T \mathbf{A}^T \mathbf{Ax} = \mathbf{a}^T \mathbf{a}, \\
& x_i x_j \geq x_i + x_j - 1 & &\forall\, i \neq j, \\
& x_i x_j \geq 0 & &\forall\, i \neq j, \\
& x_i x_j \leq x_i & &\forall\, i \neq j, \\
& x_i x_j \leq x_j & &\forall\, i \neq j, \\
& \mathbf{x} \in \{0, 1\}.
\end{aligned}
\tag{3.3}
$$

The NDQCR strengthened semidefinite relaxation of the problem is

$$
\begin{aligned}
\min \quad & \mathbf{Q} \bullet \mathbf{X} + \mathbf{c}^T \mathbf{x}, \\
s.t. \quad & \mathbf{Ax} = \mathbf{a}, & &: \lambda \\
& \mathbf{Bx} \leq \mathbf{b}, & &: \mu \\
& x_i^2 = x_i & \forall\, i, & : \delta \\
& \mathrm{diag}(\mathbf{X}) = \mathbf{x}, \\
& \mathbf{A}^T \mathbf{A} \bullet \mathbf{X} = \mathbf{a}^T \mathbf{a}, & &: \alpha \\
& X_{ij} \geq 0 & \forall\, i \neq j, & : \mathbf{S} \\
& X_{ij} \geq x_i + x_j - 1 & \forall\, i \neq j, & : \mathbf{T} \\
& X_{ij} \leq x_i & \forall\, i \neq j, & : \mathbf{U} \\
& X_{ij} \leq x_j & \forall\, i \neq j, & : \mathbf{V} \\
& \begin{bmatrix} 1 & \mathbf{x}^T \\ \mathbf{x} & \mathbf{X} \end{bmatrix} \geq 0, \\
& \mathbf{x} \in R^n, \mathbf{X} \in S^n.
\end{aligned}
\tag{3.4}
$$

The optimal set of Lagrangian multipliers are extracted from the solution of formulation 3.4. Continuous variables y_{ij} and z_{ij} $(i < j)$ coupled with the RLT constraints

$$y_{ij} \geq 0, \quad y_{ij} \geq x_i + x_j - 1, \quad z_{ij} \leq x_i, \quad z_{ij} \leq x_j$$

are included in the problem. This linearization procedure gives rise to the following convex mixed integer reformulated problem:

$$\min \quad \mathbf{x}^T \overline{\mathbf{Q}}^* \mathbf{x} + \overline{\mathbf{c}}^{*T} \mathbf{x} + \overline{\mathbf{q}}^* + 2 \sum_{i=1}^{n} \sum_{j=i+1}^{n} (S_{ij}^* + T_{ij}^*) y_{ij} - 2 \sum_{i=1}^{n} \sum_{j=i+1}^{n} (U_{ij}^* + V_{ij}^*) z_{ij},$$

$$
\begin{aligned}
s.t. \quad & \mathbf{Ax} = \mathbf{a}, \\
& \mathbf{Bx} \leq \mathbf{b}, \\
& y_{ij} \geq 0, \quad y_{ij} \geq x_i + x_j - 1, \\
& z_{ij} \leq x_i, \quad z_{ij} \leq x_j, \\
& \mathbf{x} \in \{0,1\}, \\
& y_{ij}, \quad z_{ij} \in R_+ \ (i < j),
\end{aligned}
\qquad \text{(NDQCR)}
$$

where

$$
\begin{aligned}
\bar{\mathbf{Q}}^* &= \mathbf{Q} + \mathrm{Diag}(\boldsymbol{\delta}^*) + \alpha^* \mathbf{A}^T \mathbf{A} - \mathbf{S}^* - \mathbf{T}^* + \mathbf{U}^* + \mathbf{V}^*, \\
\bar{\mathbf{c}}^* &= \mathbf{q} + \mathbf{A}^T \boldsymbol{\lambda}^* + \mathbf{B}^T \boldsymbol{\mu}^* - \boldsymbol{\delta}^*, \\
\bar{\mathbf{q}}^* &= -\boldsymbol{\lambda}^{*T} \mathbf{a} - \boldsymbol{\mu}^{*T} - \alpha^* \mathbf{a}^T \mathbf{a}.
\end{aligned}
$$

The convexification using the QCR method is done by adding the δ^*-vector to the diagonal of $\mathbf{Q}$ and the subtracting it with the $\mathbf{c}$-vector as follows:

$$
\begin{aligned}
\min \quad & \frac{1}{2}(\mathbf{x}^T (\mathbf{Q} - Diag(\boldsymbol{\delta}^*)) \mathbf{x}) + (\mathbf{c} - \boldsymbol{\delta}^*) \mathbf{x}, \\
s.t. \quad & \mathbf{Ax} = \mathbf{a}, \\
& \mathbf{Bx} \leq \mathbf{b}, \\
& \mathbf{x} \in \{0,1\}.
\end{aligned}
\qquad \text{(QCR)}
$$

The NDQCR method can be described as a four-step procedure:

- strengthen the 0-1 QP SDP-relaxation by including a set of redundant RLT inequalities

- solve the semidefinite relaxation

- MIQP problem is formed by using multipliers from the SDP solution

- the reformulated MIQP problem is solved with any suitable solver.

Examples for the usage of the QCR and NDQCR reformulation can be found in chapter 4.3.

The Coulomb glass Problem

4.1 Theory

Coulomb glass is a model for disordered materials in physics; the electrons are situated on impurities in the material and interact strongly with each other [Ortuño et al., 2008, Shklovskii and Efros, 1984, Tsigankov et al., 2003]. This can be observed in lightly doped semiconductors; this means that impurities are added into an extremely pure semiconductor, at very low temperatures, near 0 K. Typical for glass-like materials is that the dynamics for the material is very slow meaning that if cooled rapidly it takes a long time until the electrons reach equilibrium. It is presumed [Shklovskii and Efros, 1984] that the impurities are fixed to certain positions and that the electrons can move freely from one impurity to another and thus reach equilibrium.

Coulomb's law explains the electrostatic force between two electrons as follows [Benson, 1995]:

$$F = \frac{kqQ}{r^2},$$ (4.1)

where q and Q are two distinct electrons, r the distance between the electrons and k is Coulomb's constant. This constant is defined as:

$$k = \frac{1}{4\pi\varepsilon_0\varepsilon},$$ (4.2)

where ε_0 is the permittivity constant for vacuum and ε the material specific permittivity constant. If we calculate the force between two impurities in a disordered material, the charges q and Q are equal to the elementary charge e. By integrating the force in equation 4.1, the energy between two impurities is obtained according to:

$$\mathrm{d}W = -F(r)\mathrm{d}r$$

$$W = \int_{\infty}^{r_{ij}} -F(r)\mathrm{d}r = \int_{\infty}^{r_{ij}} -\frac{kqQ}{r^2}\mathrm{d}r \qquad (4.3)$$

$$= -kqQ \int_{\infty}^{r_{ij}} \frac{1}{r^2}\mathrm{d}r = kqQ\frac{1}{r_{ij}}$$

A Coulomb-gap can be seen when plotting the density of states versus the energy. The density of states gives how many impurities have an energy within a certain energy interval [Shklovskii and Efros, 1984]. When a Coulomb-gap appears, certain conditions must be met, these conditions are:

1.

$$x_i = 1 \text{ if } e_i < \epsilon_F$$

$$x_j = 0 \text{ if } e_j > \epsilon_F$$

where ϵ_F is the so called Fermi-energy.

2.

$$\Delta E = \underbrace{e_j - e_i}_{>0} - \frac{1}{r_{ij}} > 0$$

$$e_i = \sum_j \frac{x_j}{r_{ij}} + \epsilon_i$$

assume that $e_j = \epsilon_F + a$ and $e_i = \epsilon_F - a$

which leads to: $r_{ij} > \dfrac{1}{2a}$

4.2   Optimization of the Coulomb glass

The objective is to minimize the total energy of the Coulomb glass in order to find the ground state. The ground state for the system is defined as the electron configuration that has the lowest total energy. If one can find the ground state for a Coulomb glass, it is possible to model the properties for the semiconductor, for example how they conduct electricity and which excitations to higher energies are possible.

There will only be a force between two impurities if both are occupied. This is modeled using binary variables. These binary variables x_i and x_j tell whether or not the impurities i and j are occupied. By combining equation 4.2 with equation 4.3 and taking into account that both charges are electrons, the following equation is obtained:

$$E_{ij} = \frac{e^2}{4\pi\varepsilon_0\varepsilon} \frac{x_i x_j}{r_{ij}}$$

Assume that the system contains N impurities and that n of these are filled with electrons. Also, assuming that the empty impurities are neutral the total energy for the system can be defined as [Tsigankov et al., 2003]:
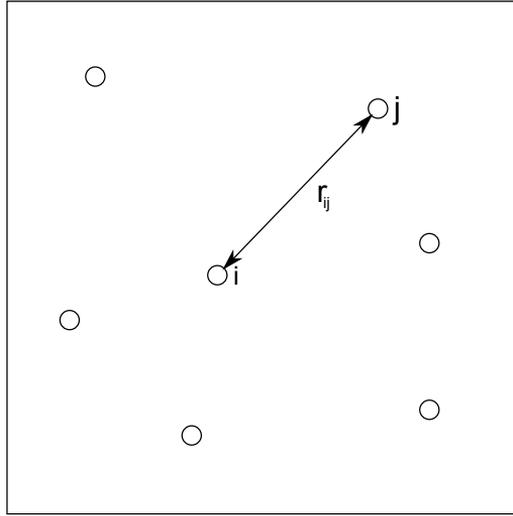
Figure 4.1: Figure that describes the distance between impurities i and j.

$$E = \frac{e^2}{4\pi\varepsilon_0\varepsilon} \frac{1}{2} \sum_{i}^{N} \sum_{j\neq i}^{N} \frac{x_i x_j}{r_{ij}} + \sum_{i}^{N} \epsilon_i x_i \qquad (4.4)$$

where r_{ij} is the distance between impurities i and j (illustrated in figure 4.1), ϵ_i is the energy for impurity i and x_i is a binary variable stating if impurity i is occupied or not. If n impurities are occupied then $\sum_{i}^{N} x_i = n$. Equation 4.4 can be reformulated using matrices and vectors to the following form:

$$E = \frac{1}{2}\mathbf{x}^{\mathbf{T}}\mathbf{Q}\mathbf{x} + \mathbf{c}^{\mathbf{T}}\mathbf{x} \qquad (4.5)$$

where element $Q_{ij} = \frac{1}{r_{ij}}$ and $c_i = \epsilon_i$.

Minimizing equation 4.5 with the constraint that all x_i are binary variables and that exactly n of those have to be equal to 1, gives us a binary quadratic optimization problem, BQP. One can search for the ground state using heuristic methods, i.e. simulated annealing [Díaz-Sánchez et al., 2000]. This method gives good solutions with low energy configurations fast but the solution found cannot be guaranteed to be the optimal solution and no lower bounds are obtained. By solving the problem as a BQP the problem can be solved to global optimality or at least an upper bound and a lower bound can be obtained. A drawback with the BQP formulation is that the systems being solved are vast which leads to a huge combinatorial problem. In order to obtain physically significant results the number of impurities should be very large, at least many thousand impurities. However, systems of that size are difficult to optimize. When generating the problems it is good to use periodic boundary conditions that is that every impurity sees the nearest copy of the impurities which is illustrated in figure 4.2. When using periodic boundary conditions there is no border in the system. If one is interested in how material behaves

far from the edge, but only small-scale simulations are possible, then periodic boundary conditions can help.
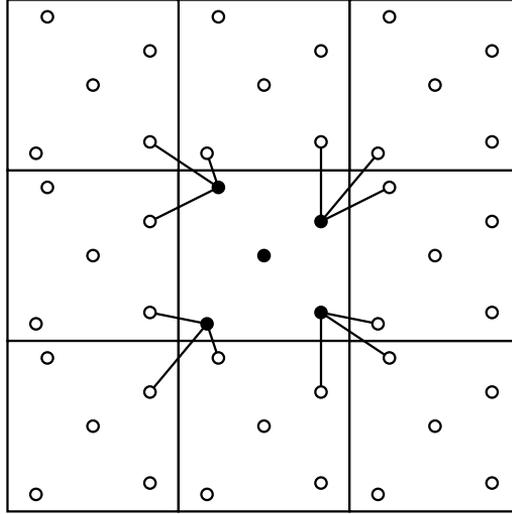
Figure 4.2: Figure describing the periodic boundary conditions.

The problem formulation that describes the system mathematically is defined as:

$$\begin{aligned}
\text{minimize} \quad & \frac{1}{2}\mathbf{x}^T \mathbf{Q}\mathbf{x} + \mathbf{c}^T \mathbf{x}, \\
\text{subject to} \quad & \sum_{i=1}^{N} x_i = n, \\
& x_i \in \{0,1\}.
\end{aligned} \tag{4.6}$$

If $\mathbf{Q}$ is not positive semidefinite one can, because the variables in $\mathbf{x}$ are binary, rewrite and convexify the problem into quadratic form by substituting $\mathbf{Q}$ with $\bar{\mathbf{Q}}$ so that $\bar{\mathbf{Q}} = \mathbf{Q} + \text{diag}(\alpha)$ where $\alpha \geq -\lambda_{\min}$ and $\lambda_{\min}$ is the smallest eigenvalue for $\mathbf{Q}$. $\mathbf{c}$ is substituted with $\bar{\mathbf{c}} = \mathbf{c} - \frac{\alpha}{2}\mathbf{e}$ where $\mathbf{e}$ is a column vector with all element equal to 1. The convexification can also be made according to the formulations presented in chapter 3.

$$\begin{aligned}
\text{minimize} \quad & \frac{1}{2}(\mathbf{x}^T \bar{\mathbf{Q}}\mathbf{x}) + \bar{\mathbf{c}}^T \mathbf{x}, \\
\text{subject to} \quad & \sum_{i=1}^{N} x_i = n, \\
& x_i \in \{0,1\}.
\end{aligned} \tag{4.7}$$

Formulation 4.7 gives the optimal solution to the problem formulated in 4.6 as long as $\alpha \geq -\lambda_{\min}$.

4.3 CGP Examples

In figure 4.3 an example of a CGP with 4 electron sites is shown.
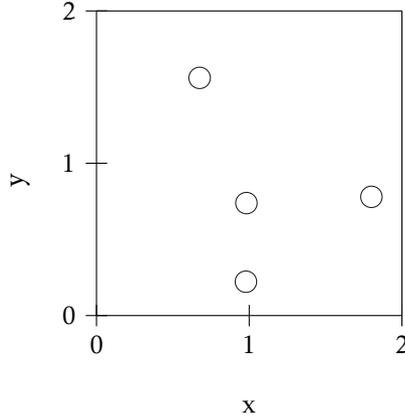
Figure 4.3: A CGP example.

The **Q**-matrix and **c**-vector from figure 4.3 is:

$$\mathbf{Q} = \begin{pmatrix} 0 & 0.9688 & 0.6065 & 0.6493 \\ 0.9688 & 0 & 1.2741 & 0.5280 \\ 0.6065 & 1.2741 & 0 & 0.5508 \\ 0.6493 & 0.5280 & 0.5508 & 0 \end{pmatrix}, \tag{4.8}$$

$$\mathbf{c} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{4.9}$$

The matrix 4.8 is not positive semidefinite because of the zeros in the diagonal. By checking the eigenvalues of the matrix 4.8 it is found that the smallest eigenvalue, λ_{min}, is: -1.36. This is added with changed signs to the diagonal of the matrix 4.8:

$$\bar{\mathbf{Q}} = \begin{pmatrix} 1.36 & 0.9688 & 0.6065 & 0.6493 \\ 0.9688 & 1.36 & 1.2741 & 0.5280 \\ 0.6065 & 1.2741 & 1.36 & 0.5508 \\ 0.6493 & 0.5280 & 0.5508 & 1.36 \end{pmatrix}. \tag{4.10}$$

The terms added to the diagonal are then subtracted from the $\bar{\mathbf{c}}$-vector:

$$\bar{\mathbf{c}} = \begin{pmatrix} -0.68 \\ -0.68 \\ -0.68 \\ -0.68 \end{pmatrix}. \tag{4.11}$$

The problem formulation $\frac{1}{2}\mathbf{x}^T\bar{\mathbf{Q}}\mathbf{x} + \bar{\mathbf{c}}^T\mathbf{x}$ with matrix 4.10 as $\bar{\mathbf{Q}}$ and vector 4.11 as $\bar{\mathbf{c}}$ is written as:

$$\min \frac{1}{2}\left[\begin{pmatrix} x_1 & x_2 & x_3 & x_4 \end{pmatrix} \begin{pmatrix} 1.36 & 0.9688 & 0.6065 & 0.6493 \\ 0.9688 & 1.36 & 1.2741 & 0.5280 \\ 0.6065 & 1.2741 & 1.36 & 0.5508 \\ 0.6493 & 0.5280 & 0.5508 & 1.36 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}\right],$$

$$+\begin{pmatrix} -0.68 & -0.68 & -0.68 & -0.68 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix},$$

s.t.

$$x_1 + x_2 + x_3 + x_4 = 2,$$

$$x_1, x_2, x_3, x_4 \in \{0, 1\}.$$

The optimal solution for this problem is 0.528. The solution is illustrated in figure 4.4. The root node solution for this formulation is 0.3481 that means that the root node solution gap to the optimum is 34.1%.
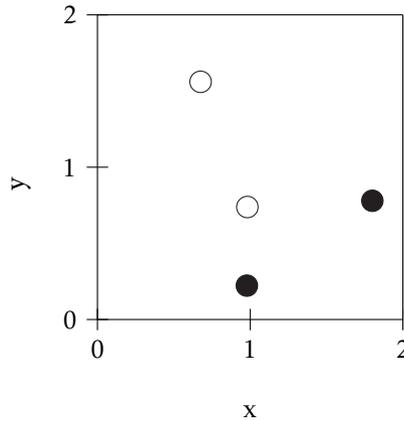
Figure 4.4: The solution to the CGP example.

When the same example is convexified using QCR we obtain the following optimal u-vector to be added to the diagonal:

$$\mathbf{u} = \begin{pmatrix} 0.7803 \\ 1.8902 \\ 1.0248 \\ 1.0700 \end{pmatrix}.$$

That gives us the following formulation:

$$\min \frac{1}{2}\left[(x_1 \quad x_2 \quad x_3 \quad x_4)\begin{pmatrix} 0.7803 & 0.9688 & 0.6065 & 0.6493 \\ 0.9688 & 1.8902 & 1.2741 & 0.5280 \\ 0.6065 & 1.2741 & 1.0248 & 0.5508 \\ 0.6493 & 0.5280 & 0.5508 & 1.0700 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}\right],$$

$$+(0.39015 \quad 0.9451 \quad 0.5124 \quad 0.535)\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix},$$

s.t.

$$x_1 + x_2 + x_3 + x_4 = 2,$$
$$x_1, x_2, x_3, x_4 \in \{0, 1\}.$$

The solution is of course the same as above and the root node value is 0.476 and the root node gap is 9.8%.

When solving the CG problem with NDQCR only the lower bounding triangle inequalities are included because all elements in the **Q** matrix are positive. The lower bounding inequalities are

$$x_i x_j \geq 0,$$
$$x_i x_j \geq x_i + x_j - 1.$$

The example with NDQCR gives the following matrices and vectors:

$$\lambda = \begin{pmatrix} 0.51 \\ 1.00 \\ 0.72 \\ 0.11 \end{pmatrix}, \mathbf{S} = \begin{pmatrix} 0.00 & 0.24 & 0.03 & 0.04 \\ 0.24 & 0.00 & 0.38 & 0.00 \\ 0.03 & 0.38 & 0.00 & 0.01 \\ 0.04 & 0.00 & 0.01 & 0.00 \end{pmatrix}, \mathbf{T} = \begin{pmatrix} 0.00 & 0.01 & 0.00 & 0.32 \\ 0.01 & 0.00 & 0.05 & 0.03 \\ 0.00 & 0.05 & 0.00 & 0.18 \\ 0.32 & 0.03 & 0.18 & 0.00 \end{pmatrix}, \alpha = 14.92.$$

Using the λ-vector, S-matrix, T-matrix and α-value we are able to create a convex problem as follows:

$$\bar{\mathbf{Q}}^* = \mathbf{Q} + \mathbf{Diag}(\lambda^*) + \alpha * \mathbf{A}^T\mathbf{A} - \mathbf{S}^* - \mathbf{T}^* = \begin{pmatrix} 15.43 & 15.64 & 15.50 & 15.20 \\ 15.64 & 15.90 & 15.77 & 15.42 \\ 15.50 & 15.77 & 15.64 & 15.28 \\ 15.20 & 15.40 & 15.28 & 15.03 \end{pmatrix},$$

$$\bar{\mathbf{c}}^* = \mathbf{c} - \lambda^* = \begin{pmatrix} -0.26 \\ -0.50 \\ -0.36 \\ -0.05 \end{pmatrix},$$

$$\bar{\mathbf{q}}^* = -\alpha^* a^T a = -29.84.$$

The reformulated problem is:

$$\text{minimize} \quad \frac{1}{2}(\mathbf{x}^T \bar{\mathbf{Q}}^* \mathbf{x}) + \bar{\mathbf{c}}^{*T} x + \bar{\mathbf{q}}^* + \sum_{i>j}^{N} S_{ij}^* y_{ij} + \sum_{i>j}^{N} T_{ij}^* y_{ij},$$

$$\text{subject to} \quad x_1 + x_2 + x_3 + x_4 = 2,$$

$$y_{ij} \geq 0 \quad \forall\, i > j,$$

$$y_{ij} \geq x_i + x_j - 1 \quad \forall\, i > j,$$

$$x_1, x_2, x_3, x_4 \in \{0, 1\}. \tag{4.12}$$

The solution is, of course, the same as for the other two examples, however, the optimal solution is already acquired in solution of the SDP problem (root node solution).

Connections to special cases of the Quadratic Assignment Problem

5.1 Introduction

The quadratic assignment problem (QAP) is a well-known combinatorial optimization problem introduced by Koopmans and Beckmann [1957]. The QAP is a problem where n facilities and n locations are given with specified flows and distances between the facilities and locations. The objective is to minimize the total cost of placing a facility at every location. The total cost derives from the distances and flows between the facilities and also additional costs for placing a facility at a certain location may be used. In its basic form the QAP is a non-convex 0-1 quadratic problem. The problem formulation looks as follows:

$$
\begin{aligned}
\text{minimize} \quad & \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n} f_{ik} d_{jl} x_{ij} x_{kl} + \sum_{i=1}^{n}\sum_{j=1}^{n} c_{ij} x_{ij}, \\
\text{subject to} \quad & \sum_{j=1}^{n} x_{ij} = 1 \quad \forall\, i \in N, \\
& \sum_{i=1}^{n} x_{ij} = 1 \quad \forall\, j \in N, \\
& x_{ij} \in \{0,1\} \quad \forall\, i,j \in N.
\end{aligned}
\tag{5.1}
$$

where f_{ik} is the flow between facilities i and k, d_{jl} is the distance between locations j and l, and c_{ij} is the cost of placing facility i at location j. The variable $x_{ij} = 1$ if facility i

is assigned to location j, otherwise, $x_{ij} = 0$ and $N = \{1, 2, \ldots, n\}$. With no loss of generality we can assume that $c_{ij} = 0$ and omit the linear term in (5.1).

5.2 Solving specially structured QAP using CGP-formulations

The taixxxc problems formulated by Taillard [1995] that can be found in the QAPLIB [2013] are gray-scale pattern problems with rank-1. Gray-scale problems are similar to CGP, the objective is to place black squares on a white grid in order to make the resulting color as gray as possible. The taixxxc problems can be formulated as QP problems. The taixxxc distance and flow matrices are defined as:

$$
\begin{aligned}
T_{rstu} &= \max_{v,w \in \{-1,0,1\}} \frac{1}{(r-t+nv)^2 + (s-u+nw)^2} \\
f_{ij} &= \begin{cases} 1 & \text{if } i \le m \text{ and } j \le m \\ 0 & \text{otherwise} \end{cases}, d_{ij} = d_{n(r-1)+s\,n(t-1)+u} = T_{rstu}
\end{aligned}
\tag{5.2}
$$

where (r, s) are the coordinates for i, (t, u) are the coordinates for j, n is the dimension of the problem and m is the amount of black squares.

The QAP can also be expressed using the trace-operator Edwards [1980], Nyberg [2014].

$$
\sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \sum_{l=1}^{n} f_{ik} d_{jl} x_{ij} x_{kl} = \operatorname{tr}(\mathbf{DXFX^T}),
$$

where, in the special case of Rank-1 $\mathbf{F}$-matrix,

$$
\mathbf{F} = \mathbf{qq}^T,
$$

that leads to

$$
\begin{aligned}
&= \operatorname{tr}(\mathbf{DXqq}^T\mathbf{X}^T), \\
&= \operatorname{tr}(\mathbf{q}^T\mathbf{X}^T\mathbf{DXq}), \\
&= \operatorname{tr}((\mathbf{Xq})^T\mathbf{DXq}),
\end{aligned}
$$

then

$$
\mathbf{Xq} = \mathbf{y},
$$

$$
= \operatorname{tr}(\mathbf{y}^T\mathbf{Dy}),
$$

$$
= \mathbf{y}^T\mathbf{Dy}.
$$

The QP formulation [Nissfolk et al., 2012], for the special case of Rank-1 QAP, is very similar to CGP:
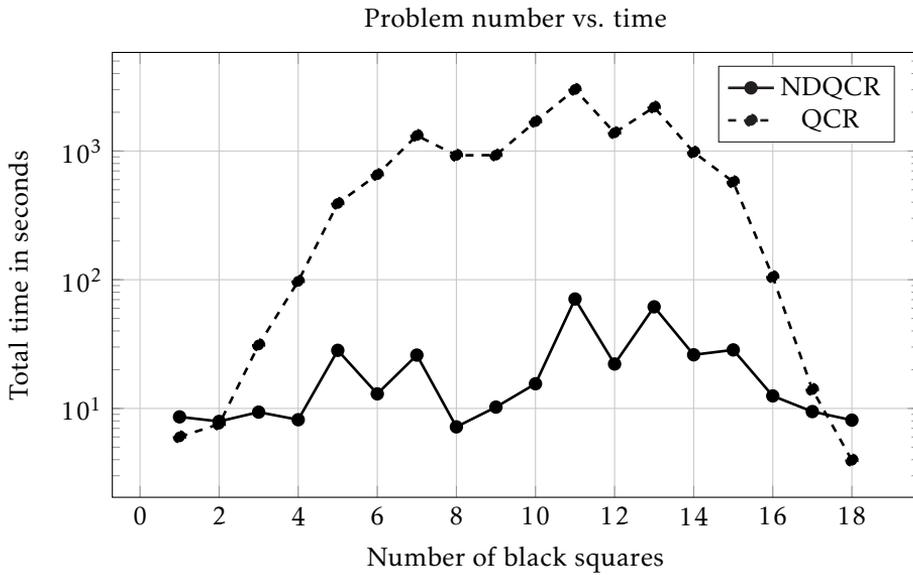
Figure 5.1: Solution times for tai36c

$$
\begin{aligned}
\text{minimize} \quad & \mathbf{y}^T \mathbf{D} \mathbf{y}, \\
\text{subject to} \quad & \sum_{j=1}^{n} x_{ij} = 1 && \forall\, i \in N, \\
& \sum_{i=1}^{n} x_{ij} = 1 && \forall\, j \in N, \\
& y_i = \sum_{j=1}^{n} x_{ij} q_j && \forall i \in N, \\
& \sum_{i=1}^{n} y_i = \sum_{j=1}^{n} q_j, \\
& x_{ij} \in \{0,1\} && \forall\, i,j \in N.
\end{aligned}
\tag{5.3}
$$

From the figure 5.1 one can clearly see that the NDQCR is better than the QCR, only in the case where we only have one black square or half the board is black is the problem convexified with QCR faster overall this is because the time spent in the NDQCR SDP part is longer.

From the QAP Library (2013), we found that nobody has yet been able to solve the problem tai256c to optimality and the previous tightest lower bound reported in QAPLIB is 43849646, obtained by Peng et al. [2010]. Further, the previous best known solution of tai256c reported in QAPLIB is 44759294, obtained by Ant colony technique.

When testing our NDQCR method on tai64c and tai256c we solved tai64c to optimal-

ity in 529 seconds and obtained a new best lower bound to tai256c. Our lower bound of 43849789 is also the root node for the MIQP and after solving for 8 months we have a lower bound of 44095200.

CHAPTER 6

Results and notes on the papers

6.1 Paper I

In this paper, the BQP formulation for the Coulomb glass problem is introduced. We looked at different ways to solve the problems, one was to obtain a lower bound using semidefinite programming and an upper bound from a heuristic algorithm based on randomized solutions using the covariance matrix from the SDP. Another was to extract Lagrangian multipliers from the SDP and use them in the MIQP solver in order to obtain tight lower bounds and solve the problems using a MIQP solver. Problem formulation 4.7 is the one that is called CG-QP in this paper.

6.2 Paper II

In this paper, we introduced a formulation for rank-1 QAPs. The only QAP that truly are Rank-1 are the tai*xxx*c problems by Taillard [1995]. The generated test problems were rank-1 and convexified using the QCR method and then solved using a MIQP solver.

6.3 Paper III

In this paper, we tried a new metaheuristic method in order to find good solutions to binary quadratic problems. However, the method used did not perform as good as we had hoped. When testing on the tai64c problem we found the optimal solution in only 30 s.

6.4 Paper IV

In this paper, we use a method by Ji et al. [2013] to convexify and solve binary quadratic problems. The method is an improvement of the QCR method and also makes use of

non-diagonal elements in order to obtain tighter lower bounding. It can be seen that, for larger test problems, the overall solution time is shorter with the NDQCR method than the QCR. However, for small test problems the overall solution time is longer due to the fact that much time is spent in the SDP solver. The lower bounds acquired using the NDQCR method are tighter than with the QCR.

Table 6.1: Average results for CG with QCR

| Size (n) | MIQP | | SDP | | Total |
	Gap	Time	Gap	Time	time
50	0.00 %	3.4	3.75 %	1.0	4.4
100	0.07 %	1456.2	1.55 %	3.6	1459.8
150	0.69 %	3600.1	1.51 %	6.9	3607.0
200	1.01 %	3600.5	1.05 %	6.9	3607.4

Table 6.2: Average results for CG with NDQCR

| Size (n) | MIQP | | SDP | | Total |
	Gap	Time	Gap	Time	time
50	0.00 %	1.6	0.01 %	12.6	14.2
100	0.00 %	17.8	0.03 %	18.7	36.6
150	0.00 %	122.4	0.03 %	19.4	141.7
200	0.00 %	687.0	0.02 %	25.0	712.0

Table 6.1 (Table 5 in the paper) and table 6.2 (Table 7 in the paper) show the benefit of the NDQCR method for the larger problems, however, for the smallest problem of size 50 the time spent in the SDP solver is so long that the total solution time is longer for the NDQCR method. It can clearly be seen that the lower bounds from NDQCR are much tighter than the ones obtained from the QCR method.

In this paper, we present a new lower bound for the largest problem in the QAPLIB, tai256c. Our new best lower bound from the solution of the SDP relaxation (which is also the solution of the root node of the reformulated quadratic programming problem using diagonal and non-diagonal elements obtained from the solution of the SDP) is 43849789 and the best lower bound in the QAPLIB is 43849646.

6.5   Paper V

In this continued work from Paper IV, we test how different numbers of non-diagonal elements affect the total solution time. It seems that when including more non-diagonal elements the lower bounding becomes tighter and also the solution time in the MIQP solver improves. However, the time spent in the SDP solver is longer.

Conclusions

The main goal of this thesis is to find new and improved solution strategies to the Coulomb glass problem. In particular, the non-diagonal quadratic convex reformulation technique presented in paper IV yields very good results in both lower bounds and solution times. The NDQCR method was also tested on binary least squares problems and on gray-scale problems because their problem formulation is very similar to the CGP. In this thesis, the choice of elements to include in the NDQCR is based on choosing the largest absolute values first. How to choose which elements to include in the NDQCR should be investigated further, one idea would be to first solve an SDP in order to determine which elements impact the MIQP model the most.

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