Minimum energy configurations on a toric lattice as a quadratic assignment problem.

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General form of quadratic assigment problems (QAPs)

QAP in Koopmans-Beckmann form

$$QAP(A, B) = \min_{\varphi \in S_n} \sum_{i,j=1}^{n} a_{ij} b_{\varphi(i)\varphi(j)}$$

where

- $A = (a_{ij}), B = (b_{ij}) \in \mathbb{R}^{n \times n}$
- S_n is the set of all permutations of n elements

We will study a specific example from **energy minimization**.

QAP example: Particles on a grid

Problem:

- Minimize the total energy of repulsive particles
- Periodic tiling of size $n_1 \times n_2$
- Density $m/(n_1 n_2)$

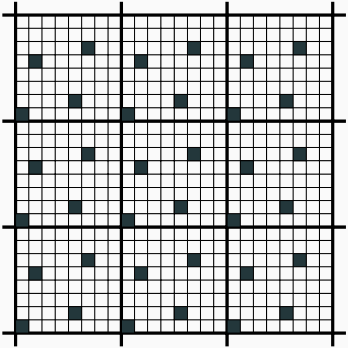


Figure 1: A $n_1 \times n_2 = 8 \times 8$ grid tiling with $m = 4$

Tiling to torus

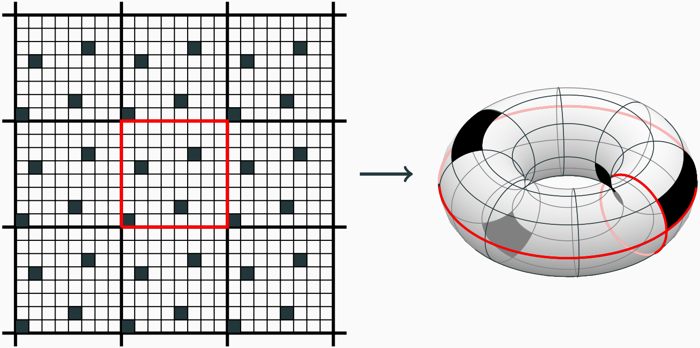


Figure 2: Example of a $n_1 \times n_2 = 8 \times 8$ grid tiling with $m = 4$, and the corresponding toroidal interpretation of the 8×8 grid.

Potential function and formal definition

Choice of potential function and metric, here:

$$f_{(x_1,y_1),(x_2,y_2)} = \frac{1}{d_{\mathrm{Lee}}((x_1,y_1),(x_2,y_2))},$$

and $f_{i,i} = 0$, where d_{Lee} is the **Lee distance** given by the shortest path metric on the toroidal grid.

Thus for fixed n_1,n_2,m the problem is

$$\min_{\substack{T \subseteq [n_1] \times [n_2] \\ |T| = m}} \sum_{a,b \in T} f_{a,b}.$$

Reformulation as QAP

For the the reformulation as QAP we assume an ordering on the grid points. We set $n = n_1 n_2$.

Let $A, B \in \mathbb{R}^{n\times n}$ be the matrices

$$A_{ij} = \begin{cases} 1, & \text{if } i, j \leq m \\ 0, & \text{otherwise.} \end{cases}, \qquad B_{i,j} = f_{i,j} = f_{(x_i,y_i),(x_j,y_j)}.$$

Then their corresponding QAP is the energy minimization problem:

$$\min_{\substack{T\subseteq[n_1]\times[n_2] \\ |T|=m}} \sum_{a,b\in T} f_{a,b} = \min_{\pi\in S_n} \sum_{i,j=1}^{n} a_{ij} b_{\pi(i)\pi(j)}$$

Complexity of QAPs

QAPs are NP-complete.

$\Rightarrow$ Instead look for approximations, heuristics and *bounds*.

We consider three known bounds:

- A projected eigenvalue bound
- A convex quadratic programming bound
- A semidefinite programming bound

Projection-based bounds

- $V \in \mathbb{R}^{n\times(n-1)}$ s.t. $\mathcal{R}(V) = e^{\perp}$ and $V^T V = I_{n-1}$,
- $\tilde{A} = V^T A V$, $\tilde{B} = V^T B V$,
- $\lambda_{\tilde{A}}$ and $\mu_{\tilde{B}}$ are the vectors of eigenvalues of $\tilde{A}$ and $\tilde{B}$

Projected eigenvalue bound

Proposition (Hadley, Rendl, Wolkowicz (1990))

Set $D = \frac{2}{n} A e e^T B$*. The* projection lower bound *for the symmetric* $\mathrm{QAP}(A, B)$ *is given by*

$$\mathrm{PB}(A, B) := \langle \lambda_{\tilde{A}}, \mu_{\tilde{B}} \rangle^- + \min_{\varphi \in S_n} \sum_{i=1}^{n} d_{i\varphi(i)} - \frac{(e^T A e)(e^T B e)}{n^2},$$

where $\langle x, y \rangle^- = \min_{\varphi \in S_n} \sum_{i=1}^{n} x_{\varphi(i)} y_i$.

Convex quadratic programming bound

Let A and B be symmetric matrices, and set

$$(S^*, T^*) = \arg\max \left\{ \mathrm{tr}(S+T) \colon \tilde{B} \otimes \tilde{A} - I \otimes S - T \otimes I \succcurlyeq 0 \right\},$$

so the matrix

$$\hat{Q} := \tilde{B} \otimes \tilde{A} - I \otimes S^* - T^* \otimes I \succcurlyeq 0$$

is positive semidefinite, and $\mathrm{tr}(S^* + T^*) = \langle \lambda_{\tilde{A}}, \mu_{\tilde{B}} \rangle^-$.

Convex quadratic programming bound (ctd.)

Proposition (Anstreicher, Brixius (2001))

A bound at least as good as $PB(A,B)$ is

$$QPB(A,B) := \min_{\substack{X \geq 0 \text{ doubly stochastic} \\ X = \frac{1}{n} ee^T + VYV^T \\ y = \mathrm{vec}(Y)}} y^T \hat{Q} y + \langle \lambda_{\tilde{A}}, \mu_{\tilde{B}} \rangle^- + \frac{2}{n} \mathrm{tr}\,(BJAX) - \frac{(e^T A e)(e^T B e)}{n^2}.$$

Semidefinite bound

Proposition (Povh, Rendl (2009), equivalent to earlier bound by Zhao, Karisch, Rendl, Wolkowicz (1998))

The following is a semidefinite relaxation of $\mathrm{QAP}(A, B)$ *for symmetric* A, B*:*

$$\begin{aligned} SDPQAP(A,B) := \min\ & \langle B \otimes A, Y\rangle \\ \text{s.t. } & \langle I \otimes E_{jj}, Y\rangle = 1 \text{ for } j = 1, \ldots, n, \\ & \langle E_{jj} \otimes I, Y\rangle = 1 \text{ for } j = 1, \ldots, n, \\ & \langle I \otimes (J - I) + (J - I) \otimes I, Y\rangle = 0, \\ & \langle J \otimes J, Y\rangle = n^2, \\ & Y \in S_+^{n^2} \cap \mathbb{R}_{\geq 0}^{n^2 \times n^2}. \end{aligned}$$

Bound comparison

Theorem

For symmetric matrices A and B we have

$$PB(A,B) \le QPB(A,B) \le SDPQAP(A,B) \le QAP(A,B).$$

Proof idea.

- We only need to show that $QPB(A,B) \le SDPQAP(A,B)$
- We prove the inequality for a weaker SDP bound, which uses the projection of the other bounds.

□

We now compare these bounds to an eigenvalue bound for the energy minimization problem.

Eigenvalue bound for energy minimization

The relaxation

$$\begin{aligned} EVB(n, m, B) := \min \;& x^T B x \\ \text{s.t.} \;& x^T x = x^T e = m, \end{aligned}$$

gives a closed-form lower bound for the energy minimization problem in terms of eigenvalues of B.

Proposition (Bouman, Draisma, Van Leeuwaarden (2013))

Let $\lambda_{\min}$ be the smallest eigenvalue of B, and $\lambda_1 = e_1^T B e$. Then

$$EVB(n, m, B) = \lambda_1 \frac{m^2}{n} + \lambda_{\min} \left(m - \frac{m^2}{n} \right)$$

is a lower bound for the potential energy of m particles.

Bound comparison

Theorem

For all n_1,n_2,m, with A,B as before, we have

$$PB(A, B) = QPB(A, B) = EVB(n, m, B) \leq SDPQAP(A, B).$$

Only the SDP bound has a chance of improving existing bounds.

Problem: The matrices appearing in the SDP bound are of size $(n_1 n_2)^2 \times (n_1 n_2)^2$.

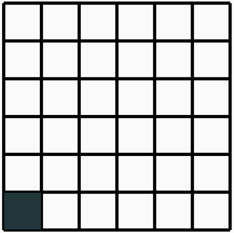
Solution: Symmetry reduction (in form of a Jordan reduction) to size $\mathcal{O}(\sqrt{n_1 n_2}) \times \mathcal{O}(\sqrt{n_1 n_2})$.

Results

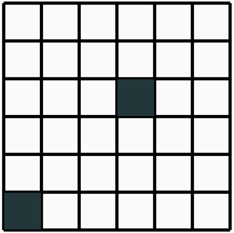
Bounds

$n_1 = n_2$	m	$PB(A, B)$	$SDPQAP(A, B)$	Upper bounds from simulated annealing
6	1	−1.51	0.00	0.00
	2	−2.13	0.33	0.33
	4	−0.64	3.00	3.00
	12	41.47	44.00	44.00
	18	111.00	111.00	111.00
7	1	−1.54	0.00	0.00
	2	−2.29	0.33	0.33
8	1	−1.67	0.00	0.00
	2	−2.65	0.25	0.25
	4	−2.57	2.27	2.27
	32	286.67	286.67	286.67
10	1	−1.72	0.00	0.00
	2	−2.88	0.20	0.20
	4	−3.57	1.81	1.81
	20	70.23	81.43	81.43
	50	588.33	588.33	588.33

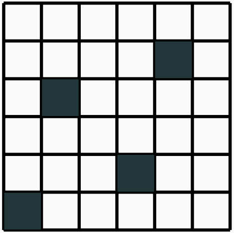
Optimal arrangements on a 6×6 grid



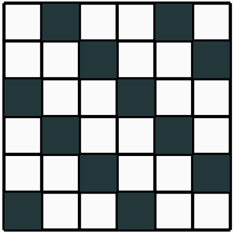
$m = 1$



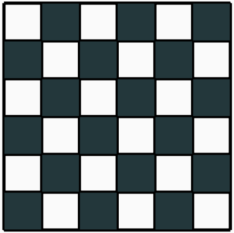
$m = 2$



$m = 4$

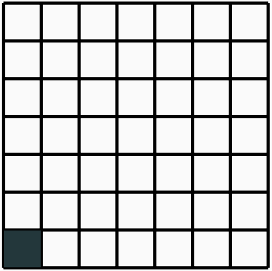


$m = 12$

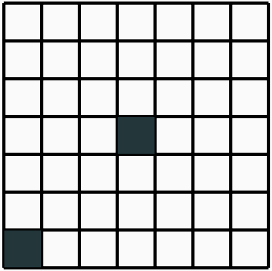


$m = 18$

Optimal arrangements on a 7×7 grid

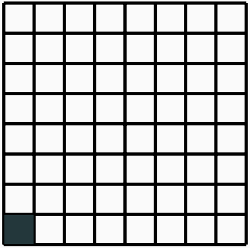


$m = 1$

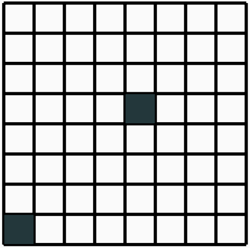


$m = 2$

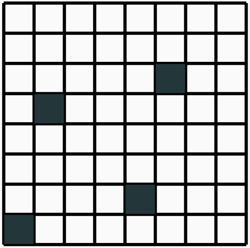
Optimal arrangements on a 8×8 grid



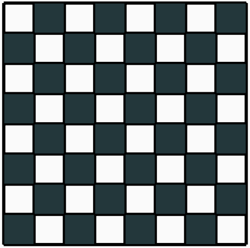
$m = 1$



$m = 2$

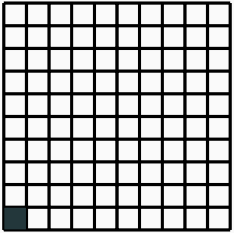


$m = 4$

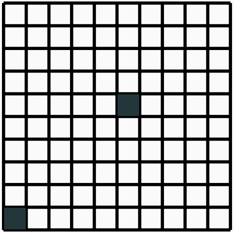


$m = 32$

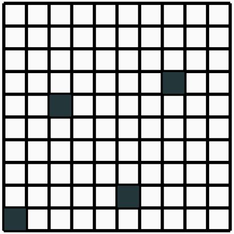
Optimal arrangements on a 10×10 grid



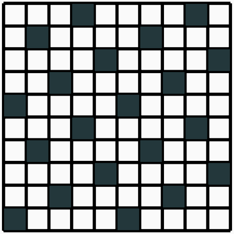
$m = 1$



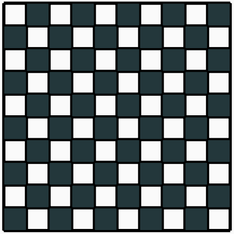
$m = 2$



$m = 4$



$m = 20$



$m = 50$

Any questions?

Weaker SDP bound

$$
\begin{aligned}
SDPPB(A,B) := \min \ & \langle \tilde{B} \otimes \tilde{A}, U \rangle + \frac{2}{n}\mathrm{vec}(V^T BJAV)^T u \\
& + \frac{1}{n^2}(e^T A e)(e^T B e) \\
\text{s.t.} \ & \begin{pmatrix} 1 & u^T \\ u & U \end{pmatrix} \succcurlyeq 0, \\
& \langle E_{ij} \otimes I_{n-1}, U \rangle = \delta_{ij} \quad \forall i,j = 1,\dots,n-1, \\
& \langle I_{n-1} \otimes E_{ij}, U \rangle = \delta_{ij} \quad \forall i,j = 1,\dots,n-1, \\
& (V \otimes V) u \geq -\frac{1}{n} e \otimes e.
\end{aligned}
$$

Symmetry Reduction

Conic form

We assume the problem is given in the form

$$\begin{aligned} \mathsf{P} = \min\ & \langle C, X\rangle \\ \text{s.t. } & X \in X_0 + \mathcal{L} \\ & X \in \mathcal{K} \end{aligned} \qquad\qquad \begin{aligned} \mathsf{D} = \min\ & \langle X_0, Y\rangle \\ \text{s.t. } & Y \in C + \mathcal{L}^\perp \\ & Y \in \mathcal{K}^*. \end{aligned}$$

where

- $\mathcal{K} \subseteq \mathcal{V}$ is a convex cone in a real vectorspace,
- X_0 and C are elements of $\mathcal{V}$,
- $\mathcal{L} \subseteq \mathcal{V}$ a linear subspace.

Constraint set invariance conditions (CSICs)

Definition

A projection $P\colon \mathcal{V} \to \mathcal{V}$ fulfills the CSICs for $(\mathcal{K}, X_0 + \mathcal{L}, C)$ if

(i) $P(\mathcal{K}) \subseteq \mathcal{K}$ (the projection is positive),

(ii) $P(X_0 + \mathcal{L}) \subseteq X_0 + \mathcal{L}$,

(iii) $P^*(C + \mathcal{L}^\perp) \subseteq C + \mathcal{L}^\perp$,

where P^* is the adjoint of P.

If P is an orthogonal projection P_S to a linear subspace S, we call S **admissible**.

Symmetry reduction

For admissible S, the following programs have the same objective values as **P** and **D**:

$$\begin{aligned} \min \quad & \langle P_S(C), X \rangle \\ \text{s.t.} \quad & X \in P_S(X_0) + \mathcal{L} \cap S \\ & X \in \mathcal{K} \cap S \end{aligned} \qquad \begin{aligned} \min \quad & \langle P_S(X_0), Y \rangle \\ \text{s.t.} \quad & Y \in P_S(C) + \mathcal{L}^\perp \cap S \\ & Y \in \mathcal{K}^* \cap S \end{aligned}$$

Jordan reduction

Proposition (Permenter (2017))

If $\mathcal{V}$ is an euclidian Jordan-algebra and $\mathcal{K}$ its cone of squares, then an unital subspace $S \subseteq \mathcal{V}$ is admissible if

$$\begin{aligned} &S \ni P_{\mathcal{L}}(C), P_{\mathcal{L}^\perp}(X_0), \\ &S \supseteq P_{\mathcal{L}}(S), \\ &S \supseteq \{X^2 \mid X \in S\} \quad [S \textit{ is a subalgebra.}]. \end{aligned}$$

The converse holds if J is special.

Its enough to know here that S^n is a special euclidian Jordan-algebra and its cone of squares is S^n_+.

Extension to the doubly nonnegative cone

Proposition

An orthogonal projection P_S onto an unital subspace $S \subseteq \mathcal{V}$ fulfills

$$P_S(D^n) \subseteq D^n$$

if and only if

$$P_S(S^n_+) \subseteq S^n_+$$

and S has a basis of nonnegative matrices with disjoint supports.

A simple algorithm

We further restrict ourselves to a Partition $P = S$. Then the following algorithm gives us the optimal admissible partition subspace:

$P \leftarrow \mathrm{part}(P_{\mathcal{L}}(C)) \wedge \mathrm{part}(P_{\mathcal{L}^\perp}(X_0))$
repeat
  $P \leftarrow P \wedge \mathrm{part}(P_{\mathcal{L}}(P))$
  $P \leftarrow P \wedge \mathrm{part}(\mathrm{span}\{X^2 \mid X \in P\})$
until *converged*;

Here part returns the partition given by unique entries, and $\wedge$ the smallest refinement of two partitions.