Adiabatic Quantum Graph Matching with Permutation Matrix Constraints

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Overview

- Matching problems on 3D shapes and images often lead to difficult combinatorial, quadratic assignment problems (QAPs)
- We address the question, how quantum annealers can help solving QAPs.
- For this we develop multiple methods to write following optimization over permutations $\mathbb{P}_n$

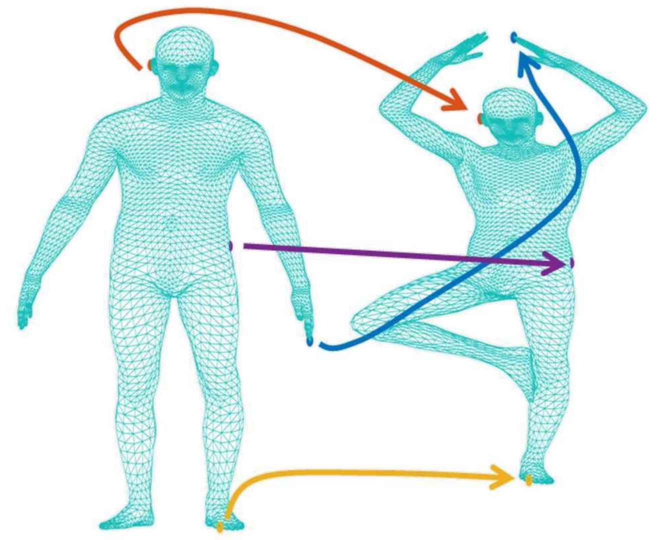
$$\arg\min_{X \in \mathbb{P}_n} \quad \mathbf{x}^{\mathrm{T}} W \mathbf{x}, \qquad (1)$$

where $X \in \mathbb{R}^{n \times n}$ and $\mathbf{x} := \mathrm{vec}(X) \in \mathbb{R}^{n^2}$, in an unconstrained form.

- We perform experiments on a quantum annealer as well as numerical simulations and compare the methods with each other.

Shape Matching

- Given two sets of points on a body. How can we find the correspondences?



- For isometric transformations $\phi : \mathbb{R}^3 \to \mathbb{R}^3 \quad \forall i \exists! j : v_i^1 \mapsto v_j^2$ the (geodesic) distances $d(\cdot,\cdot)$ do not change: $d_1(v_i^1, v_k^1) = d_1(\phi(v_i^1), \phi(v_k^1))$
- The non-negative term:

$$\sum_{i,j,k,l} X_{i,j} X_{k,l} |d_1(v_i^1, v_k^1) - d_2(v_j^2, v_l^2)|,$$

with $X \in \mathbb{P}_n$ is zero for the correct permutation matrix.

- This motivates equation (1).
- The optimization problem (1) is NP-hard

Quantum Computing

- The idea of quantum computing is to use quantum-mechanical systems to gain a computational advantage.
- Most prominent, general applications of quantum computing include:
  - Simulation of many-body physics[1,2]
  - Shor's algorithm for integer factorization[3]
  - Grover's algorithm for search in an unsorted database[4]
- *Quantum Annealing* can be used to solve:

$$\arg\min_{\mathbf{s} \in \{-1,1\}^m} \quad \mathbf{s}^T Q \mathbf{s} + \mathbf{q}^T \mathbf{s}, \qquad (2)$$

with an $m \times m$ matrix Q and an m dimensional vector $\mathbf{q}$.

Website (Code is available):

http://gvv.mpi-inf.mpg.de/projects/QGM/

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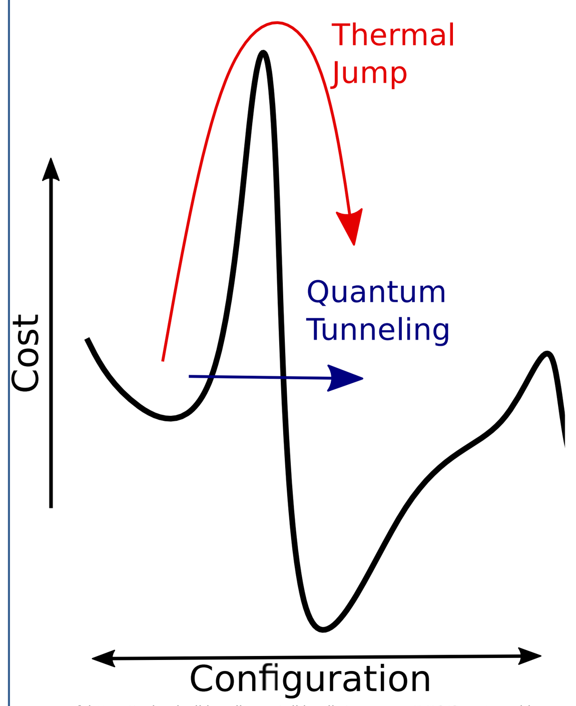
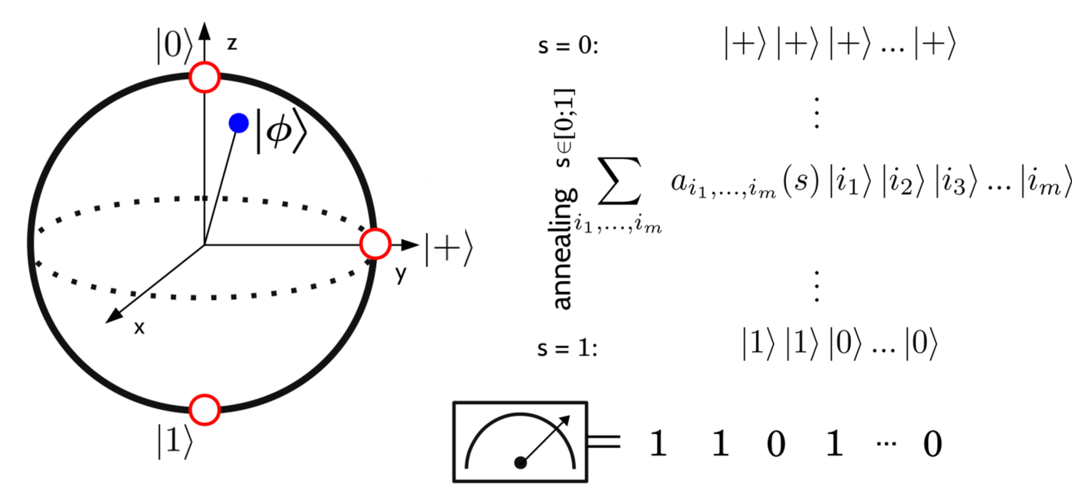
Quantum Annealing

- Stochastic algorithm comparable to simulated annealing, but with advantage for high, narrow peaks:[5]



cf. https://upload.wikimedia.org/wikipedia/commons/1/12/Quant-annl.jpg



- Major progress in recent experimental realization: D-Wave 2000Q has 2048 superconducting flux qubits
- Free access over cloud with D-Wave leap.[6]
- Computer Vision applications are researched.[7,8]

Conversion from (1) to (2)

- The equality constraints $\sum_i X_{i,j} = \sum_i X_{j,i} = 1$ are of the form $A\mathbf{x} = \mathbf{b}$, where A is a matrix and $\mathbf{b}$ is a vector.
- For sufficiently large λ, λ_j:

$$\begin{aligned} &\min_{\{\mathbf{x} \in \{0,1\}^{n^2} | \quad A\mathbf{x}=\mathbf{b}\}} \quad \mathbf{x}^{\mathrm{T}} W \mathbf{x} + \mathbf{c}^{\mathrm{T}} \mathbf{x} \\ = &\min_{\{\mathbf{x} \in \{0,1\}^{n^2}\}} \quad \mathbf{x}^{\mathrm{T}} W \mathbf{x} + \mathbf{c}^{\mathrm{T}} \mathbf{x} + \lambda ||A\mathbf{x} - \mathbf{b}||^2 \quad (Baseline) \\ = &\min_{\{\mathbf{x} \in \{0,1\}^{n^2}\}} \quad \mathbf{x}^{\mathrm{T}} W \mathbf{x} + \mathbf{c}^{\mathrm{T}} \mathbf{x} + \sum_j \lambda_j |(A\mathbf{x})_j - \mathbf{b}_j|^2 \quad (Row-wise) \end{aligned}$$

- Third method: Inserting the equalities to eliminate variables $(Inserted)$

Lower Bounds for the Penalty Parameters

- The minimizers of the constrained and the unconstrained problem coincide provided that:

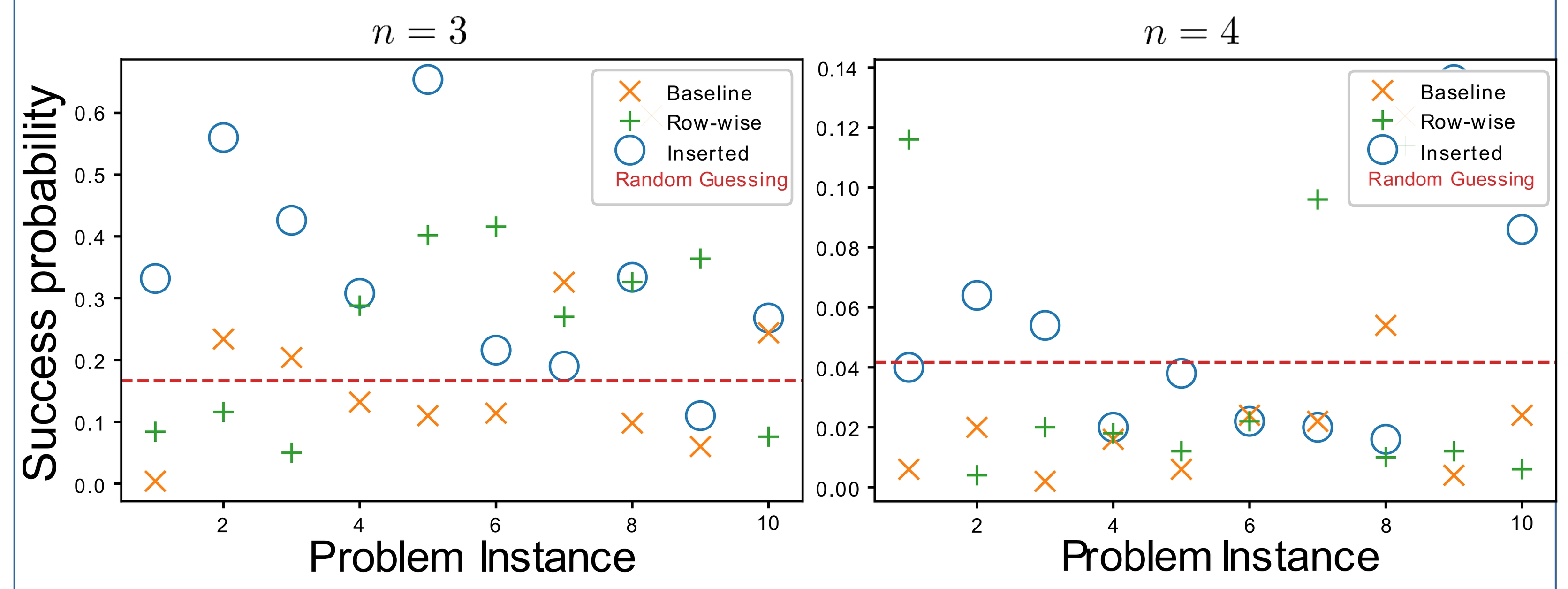
$$\lambda_i > \lambda_i^0 := D_{\mathcal{J}_i} + \frac{1}{2} D_{\{1,\dots,n^2\}},$$

where $\mathcal{J}_i$ denotes the indices that belong to a column or a row enumerated by the rows of A and

$$D_{\mathcal{J}} := \max_{k \in \mathcal{J}} \left(\sum_i |(W_{k,i} + W_{i,k})| + |W_{k,k}| + |c_k| \right).$$

- Similar propositions are proven for the other methods
- Lower bounds for the regularization parameter are important, since dominant regularization terms enhance errors

Experiments on D-Wave 2000Q



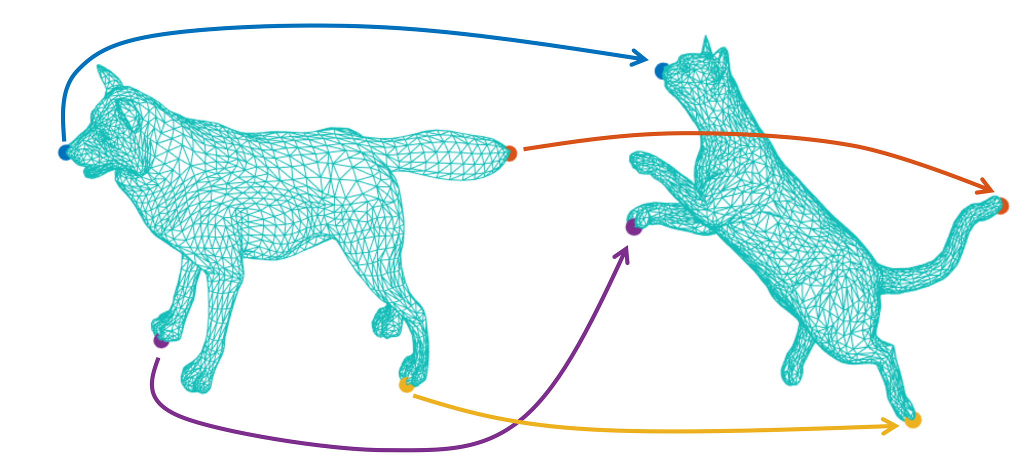
$$\text{Success Probability} = \frac{\#\ \text{Optimum was returned}}{\text{Number of runs}}$$

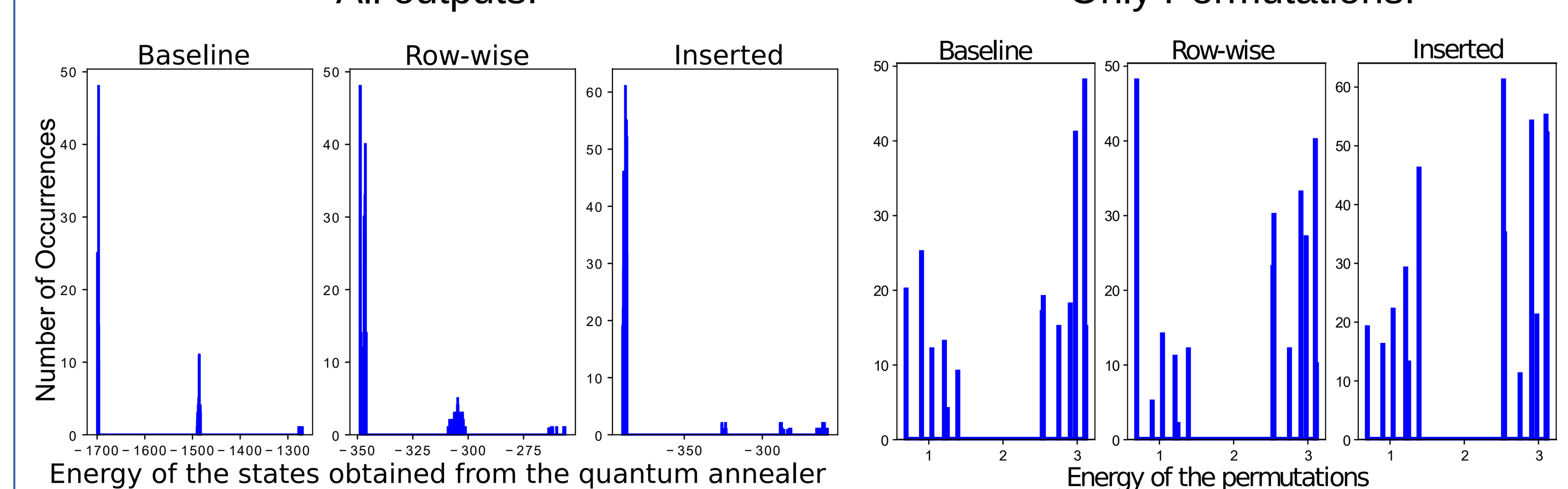
Ablative Study for n=4

- For $n = 4$ the results are worse than random guessing, despite numerical simulations confirming the validity of the algorithm.
- Hypothesis: Regularization term is too big compared to the rest

➡ Experimental errors in the couplings make the energy differences between the permutations insignificant.

Real Data (e.g. Near-Isometric Shape Matching):





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