A Quantum Algorithm for the Sub-Graph Isomorphism Problem

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Sub-graph isomorphism (SGI)

We consider an *(finite) undirected graph* $\mathcal{A} = (V_\mathcal{A}, E_\mathcal{A})$, where

- $V_\mathcal{A}$ is the finite set of vertices,
- $E_\mathcal{A}$ is the set of elements of the form $\{i, j\}$, representing the edge connecting vertex $i \in V_\mathcal{A}$ to $j \in V_\mathcal{A}$.

To each graph $\mathcal{A}$, with $n = |V_\mathcal{A}|$, we associate the corresponding $n \times n$ *adjacency matrix* A whose entries are

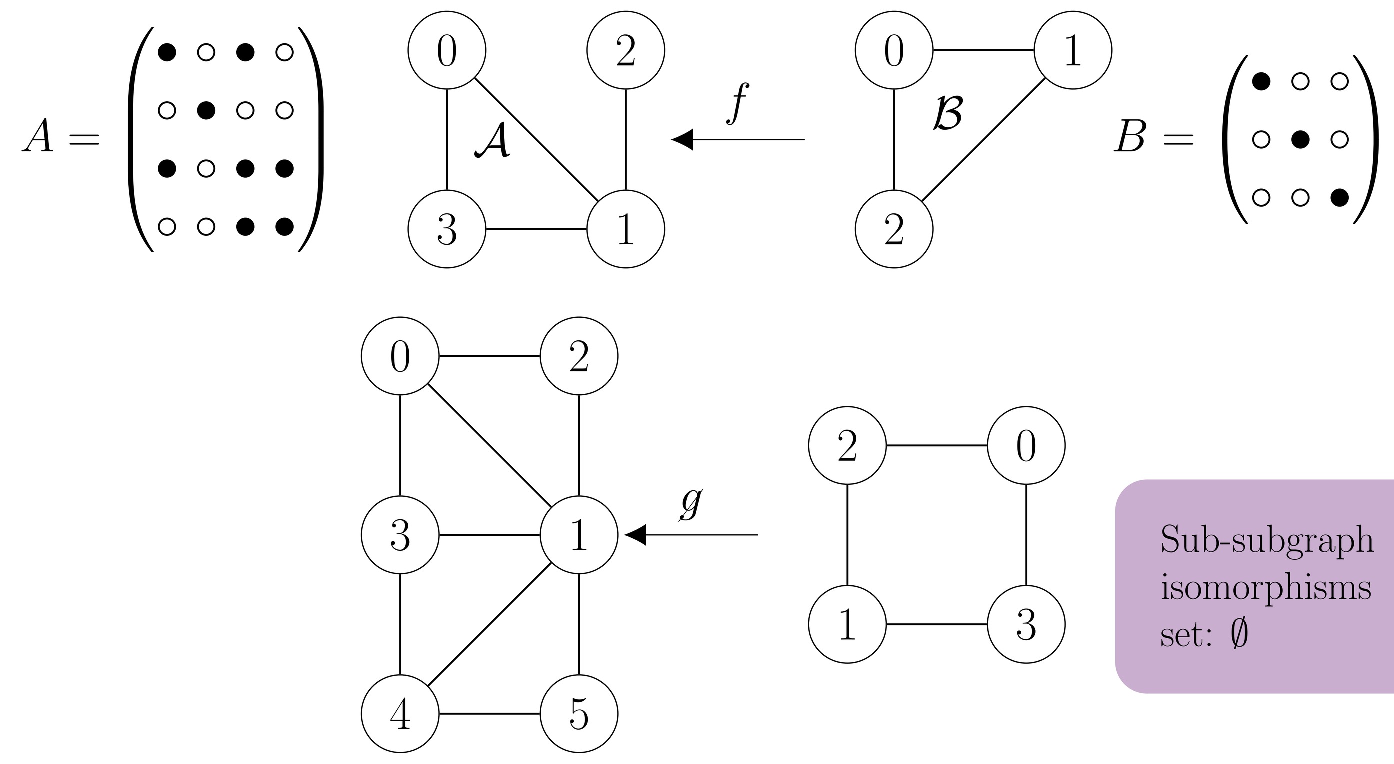
$$A_{i,j} = \begin{cases} 1, & \{i,j\} \in E_\mathcal{A} \\ 0, & \text{otherwise,} \end{cases}$$

A graph $\mathcal{B}$ is said to be an *induced subgraph* of a graph $\mathcal{A}$ if $V_\mathcal{B} \subset V_\mathcal{A}$ and for all $i, j \in V_\mathcal{B}$, $\{i, j\} \in E_\mathcal{A} \iff \{i, j\} \in E_\mathcal{B}$.

Let $n = |V_\mathcal{A}|$, $m = |V_\mathcal{B}|$, then the sub-graph isomorphisms are the $(n \times n)$ permutations P that make the following cost function vanish

$$\ell_{A,B}(P) = \left\| SPAP^\top S^\top - B \right\|_F^2,$$

where $S = (\mathbb{I}_m \mid \mathbb{O}_{m,n-m})$. The space of m-permutation of n has size $\frac{n!}{(n-m)!}$, which becomes $n!$ when $n = m$.



Sub-subgraph isomorphisms set: $\emptyset$

Applications

Graph databases, biochemistry, computer vision, social network analysis, knowledge graph query and anti-money laundry.

The hat representation $\widehat{(\cdot)}$

Given graph $\mathcal{A}$ and the corresponding adjacency matrix $A \in \mathcal{S}_N(\mathbb{Z}_2)$, with $N = 2^k = |V_\mathcal{A}|$ for some $k > 1$, we define the *unitary operator representation* denoted $\widehat{A} \in \mathsf{U}(2N^2)$, as

$$\widehat{A} := H^{\otimes(2k+1)} \left(\mathbb{I}_{N^2} \oplus \sum_{i,j} (-1)^{A_{i,j}} |i,j\rangle \langle i,j| \right) H^{\otimes(2k+1)}, \tag{1}$$

where H is the 2×2 matrix corresponding to the Hadamard operator on a single qubit.

Given the $N \times N$ permutation P we define the representation

$$\check{P} := \mathbb{I}_2 \otimes \left(H^{\otimes 2k} \cdot P^{\otimes 2} \cdot H^{\otimes 2k} \right). \tag{2}$$

Properties of $\widehat{(\cdot)}$ and $\check{(\cdot)}$

For all $A, B \in \mathcal{S}_N(\mathbb{Z}_2)$,

(i) $\widehat{(A +_2 B)} = \widehat{A} \cdot \widehat{B} = \widehat{B} \cdot \widehat{A}$, $\quad \widehat{\mathbb{O}_N} = \mathbb{I}_{2N^2}$ (group-homomorphism)

(ii) $A \neq B \implies \widehat{A} \neq e^{\imath\phi}\widehat{B}$, $\quad \forall \phi \in \mathbb{R}$ ('physical injectivity')

(iii) $\widehat{PAP^\top} = \check{P} \cdot \widehat{A} \cdot \check{P}^\top$

Also $\widehat{(\cdot)}$ requires $\log_2(2N^2) = 2k + 1$ qubits w.r.t. the number of vertices N.

The cost function

For simplicity consider the *graph isomorphism* (GI) case. We define the *classical disparity function* $\Psi_\mathrm{C} : \mathcal{S}_N(\mathbb{Z}_2) \times \mathcal{S}_N(\mathbb{Z}_2) \to \mathbb{R}$ as

$$\Psi_\mathrm{C}(A, B) := \frac{1}{N^2} \|A - B\|_\mathrm{F}^2 = \frac{1}{N^2} \sum_{i,j} (A_{i,j} - B_{i,j})^2. \tag{4}$$

We define the corresponding *quantum disparity function* as

$$\Psi_\mathrm{Q}^\mathrm{GI}(A, B) := 1 - \left| \langle 0|^{\otimes(2k+1)} \widehat{B} \cdot \widehat{A} \, |0\rangle^{\otimes(2k+1)} \right|, \tag{5}$$

also we prove that $\Psi_\mathrm{C}(A, B) = \Psi_\mathrm{Q}^\mathrm{GI}(A, B)$.

For the SGI case we obtain the corresponding disparity function $\Psi_\mathrm{Q}^\mathrm{SGI}(A, B)$, not requiring $|V_\mathcal{A}| = |V_\mathcal{B}|$ also we prove again that $\Psi_\mathrm{C}(SAS^\top, B) = \Psi_\mathrm{Q}^\mathrm{SGI}(A, B)$.

Now we introduce a permutation P to obtain

$$\Psi_\mathrm{Q}^\mathrm{GI}(PAP^\top, B) := 1 - \left| \langle 0|^{\otimes(2k+1)} \widehat{B} \cdot \check{P} \cdot \widehat{A} \, |0\rangle^{\otimes(2k+1)} \right|. \tag{6}$$

Next step

We substitute the fixed permutation P with an Ansatz $\widetilde{P}_\mathfrak{G}(\theta)$ producing a tunable superposition of permutations.

The Ansatz

Given a vector of parameters $\theta \in \mathbb{R}^c$, we propose an Ansatz of the form

$$\widetilde{P}_\mathfrak{G}(\theta) = e^{\imath\phi} \prod_{i=1}^{c} \exp\left(-\imath \frac{\theta_i}{2} P_i \right), \tag{3}$$

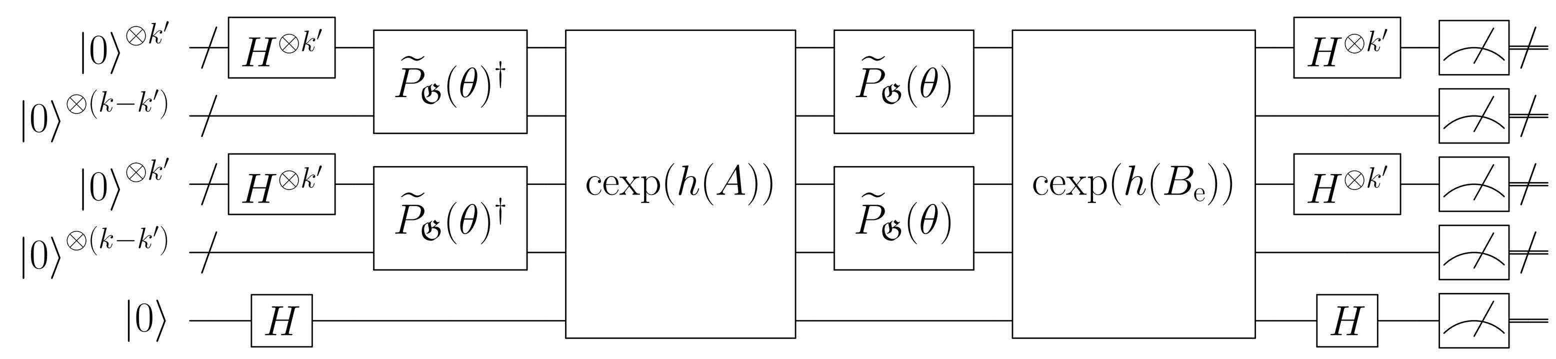
where P_i are permutation matrices acting on k qubits, such that $P_i^2 = \mathbb{I}_{2^k}$. Also, the structure of the P_i is determined by the hyperparameters $\mathfrak{G}$. Equation (3) can be expanded to reveal the tunable superposition of permutations structure

$$\widetilde{P}_\mathfrak{G}(\theta) = \sum_{j=1}^{2^c} \alpha_j(\theta) Q_j,$$

where Q_i are permutation matrices (not necessarily unique) and the functions $\alpha_j : \mathbb{R}^c \to \mathbb{C}$ map the parameters to the complex coefficients of the Q_j. Moreover, we show that the subset of parameters $\{\theta \in \mathbb{R}^c | \theta_i \in \{0, \pi\}\}$ determines $\widetilde{P}_\mathfrak{G}(\theta)$ to produce each Q_i individually.

The quantum circuit

Consider graphs $\mathcal{A}$ and $\mathcal{B}$ having $|V_\mathcal{A}| = 2^k$ and $|V_\mathcal{B}| = 2^{k'}$ vertices, respectively $(k > k')$. Given the Ansatz $\widetilde{P}_\mathfrak{G}(\theta)$, we obtain the QC for the SGI utility function $\mathcal{L}_\mathrm{Q}^\mathrm{SGI}(\theta)$.



Where

$$\mathrm{cexp}(h(A)) = \mathbb{I}_{N^2} \oplus \sum_{i,j} (-1)^{A_{i,j}} |i,j\rangle \langle i,j|$$

is a *diagonal operator* depending on the adjacency matrix A.

Algorithm 1: The sub-graph isomorphism algorithm (simplified)

Data: Adjacency matrices A and B for graphs $\mathcal{A}$ and $\mathcal{B}$, respectively. Permutation Ansatz hyper-parameters $\mathfrak{G}$.

`// The matrices` A `and` B `have sizes` $N \times N$ `and` $N_B \times N_B, N = 2^k$, $N_B = 2^{k'}$, $k' < k$

Result: R; `// Set of partial permutation matrices`

$R \leftarrow \emptyset$;

$\mathcal{L}_\mathrm{Q}^\mathrm{SGI}(\theta) \longleftarrow \mathrm{CircuitFactory}(A, B, \mathfrak{G})$;

$\theta \leftarrow \mathrm{SampleUniform}([0,\pi]^c)$; `// Sample initial` $\theta \in \mathbb{R}^c$ `from` $[0,\pi]^c$

for $t_1 \leftarrow 1$ **to maxsteps do**

  $\theta \leftarrow \theta - \eta \widetilde{\nabla}^{(t_1)} \left(-\mathcal{L}_\mathrm{Q}^\mathrm{SGI}(\theta) \right)$; `// Update` θ `with SGD step`

  $\mathbf{p} \leftarrow (\Lambda(\theta_i/\pi))_i$; `// Obtain vector of distances of` θ_i/π `from closest even integer`

  for $t_2 \leftarrow 1$ **to samples do**

    $\mathbf{u} \leftarrow \mathrm{SampleUniform}([0,1]^c)$;

    $\mathbf{g} \leftarrow \left(\chi_{[0,\infty)}(p_i - u_i) \right)_i$; `// Sample vector in` $\{0,1\}^c$ `according to probabilities` $\mathbf{p}$

    $P \leftarrow \widetilde{P}_\mathbf{h}(\pi \cdot \mathbf{g})$; `// Obtain a classical permutation, note` $\pi \cdot \mathbf{g} \in \{0,\pi\}^c$

    $d \leftarrow \left\| SPAP^\top S^\top - B \right\|_F^2$; `// Check discrepancy classically`

    if $d = 0$ **then** $R \leftarrow R \cup \{SP\}$;

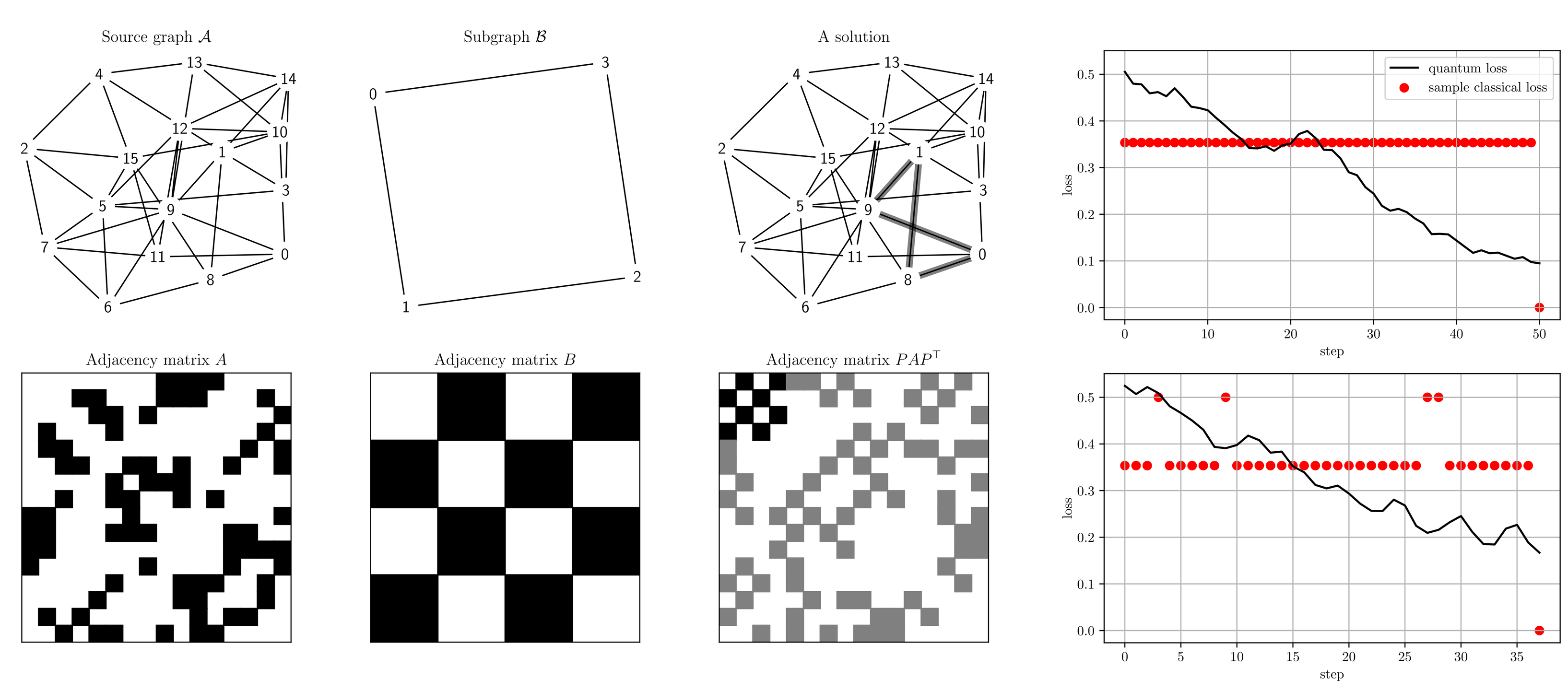
  end

  if $|R| \neq 0$ **then break**;

end

Results

Below a practical example of SGI (columns 1-3) and two samples of the SGD evolution (fourth column).



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