A Supplementary Figures and Tables

Lemma 1. *If A and B are the adjacency matrices of simple graphs that are isomorphic to one another, then the minimum of rQAP is equal to the minimum of QAP.*

Proof. Because any feasible solution to GM is also a feasible solution to rQAP, we must only show that the optimal objective function value to rQAP can be no better than the optimal objective function value of QAP. Let $A = PBP^\mathsf{T}$, so that $\langle A, PBP^\mathsf{T}\rangle = 2m$, where m is the number of edges in A. If rQAP could achieve a lower objective value, then it must be that there exists a $D \in \mathcal{D}$ such that $\langle A, DBD^\mathsf{T}\rangle > \langle A, PBP^\mathsf{T}\rangle = 2m$ (remember that we are minimizing the negative Euclidean inner product). For that to be the case, it must be that $(DBD^\mathsf{T})_{uv} \geq 1$ for some (u, v). That this is not so may be seen by the submultiplicativity of the norm induced by the ℓ_∞ norm: $\|Dx\|_\infty \leq \|D\|_{\infty,\infty} \|x\|_\infty$. Applying this twice (once for each doubly stochastic matrix multiplication) yields our result. $\square$

Linear Assignment Problems The standard way of writing a Linear Assignment Problem (LAP) is

$$\begin{array}{ll} \text{minimize} & \sum_{u,v\in[n]} a_{u\pi(v)} b_{uv} \\ \text{subject to} & P \in \mathcal{P}. \end{array}$$

The LAP objective function, like the QAP objective function, enjoys a number of equivalent formulations, including

$$\text{(LAP)} \qquad \begin{array}{ll} \text{minimize} & \langle P, AB^\mathsf{T}\rangle \\ \text{subject to} & P \in \mathcal{P}. \end{array} \tag{11}$$

The binary constraints of LAP—like those of QAP—make solving even this problem computationally tricky. Nonetheless, in the last several decades, there has been much progress in accelerating algorithms for solving LAPs, starting with exponential time, all the way down to $\mathcal{O}(n^3)$ for general LAPs, and even faster for certain special cases (e.g., sparse matrices) [24, 12].

To see that Eq. (7) is identical to Eq. (12), simply let $A = \nabla_P^{(i)}$ and $B = I$ (the $n \times n$ identity matrix).

To solve a LAP, consider a continuous relaxation of LAP, specifically, relaxing the permutation matrix constraint to a doubly stochastic matrix constraint:

$$\text{(rLAP)} \qquad \begin{array}{ll} \text{minimize} & \langle P, AB^\mathsf{T}\rangle \\ \text{subject to} & P \in \mathcal{D}. \end{array} \tag{12}$$

As it turns out, the minima of LAP and rLAP are equal to one anther [12]. This relaxation motivates our approach to approximating QAP.

Pseudocode 1 `FAQ` for finding a local optimum of rQAP

Input: graphs A and B as well as stopping criteria
Output: $\widehat{P}$, an estimated permutation matrix

1: Choose an initialization, $P^{(0)} = \mathbf{1}\mathbf{1}^\mathsf{T}/n$
2: **while** stopping criteria not met **do**
3:    Compute the gradient of f at the current point via Eq. (6)
4:    Compute the direction $Q^{(i)}$ by solving Eq. (7) via the Hungarian algorithm
5:    Compute the step size $\alpha^{(i)}$ by solving Eq. (8)
6:    Update $P^{(i)}$ according to Eq. (9)
7: **end while**
8: Obtain $\widehat{P}$ by solving Eq. (10) via the Hungarian algorithm.

Table 1: Comparison of FAQ with optimal objective function value and previous state-of-the-art for directed graphs. The best (lowest) value is in **bold**. Asterisks indicate achievement of the global minimum. The number of vertices for each problem is the number in its name (second column).

#	Problem	Optimal	FAQ	EPATH	GRAD
1	lipa20a	3683	**3791**	3885	3909
2	lipa20b	27076	**27076***	32081	**27076***
3	lipa30a	13178	**13571**	13577	13668
4	lipa30b	151426	**151426***	**151426***	**151426***
5	lipa40a	31538	**32109**	32247	32590
6	lipa40b	476581	**476581***	**476581***	**476581***
7	lipa50a	62093	**62962**	63339	63730
8	lipa50b	1210244	**1210244***	**1210244***	**1210244***
9	lipa60a	107218	**108488**	109168	109809
10	lipa60b	2520135	**2520135***	**2520135***	**2520135***
11	lipa70a	169755	**171820**	172200	173172
12	lipa70b	4603200	**4603200***	**4603200***	**4603200***
13	lipa80a	253195	**256073**	256601	258218
14	lipa80b	7763962	**7763962***	**7763962***	**7763962***
15	lipa90a	360630	**363937**	365233	366743
16	lipa90b	12490441	**12490441***	**12490441***	**12490441***

Table 2: Comparison of FAQ with optimal objective function value and the best result on the undirected benchmarks. Note that FAQ restarted 100 times finds the optimal objective function value in 3 of 16 benchmarks, and that FAQ restarted 3 times finds a minimum better than the previous state-of-the-art on all 16 particularly difficult benchmarks.

#	Problem	Optimal	FAQ_{100}	FAQ_{3}	previous min
1	chr12c	11156	**12176**	13072	13072
2	chr15a	9896	**9896***	17272	19086
3	chr15c	9504	**10960**	14274	16206
4	chr20b	2298	**2786**	3068	3068
5	chr22b	6194	**7218**	7876	8482
6	esc16b	292	**292***	294	296
7	rou12	235528	**235528***	238134	253684
8	rou15	354210	**356654**	371458	371458
9	rou20	725522	**730614**	743884	743884
10	tai10a	135028	**135828**	148970	152534
11	tai15a	388214	**391522**	397376	397376
12	tai17a	491812	**496598**	511574	529134
13	tai20a	703482	**711840**	721540	734276
14	tai30a	1818146	**1844636**	1890738	1894640
15	tai35a	2422002	**2454292**	2460940	2460940
16	tai40a	3139370	**3187738**	3194826	3227612