Fast Approximate Quadratic Programming for Large (Brain) Graph Matching

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Abstract

Quadratic assignment problems (QAPs) arise in a wide variety of domains, ranging from operations research to graph theory to computer vision to neuroscience. In the age of big data, graph valued data is becoming more prominent, and with it, a desire to run algorithms on ever larger graphs. Because QAP is **NP**-hard, exact algorithms are intractable. Approximate algorithms necessarily employ an accuracy/efficiency trade-off. We developed a fast approximate quadratic assignment algorithm (FAQ). FAQ finds a local optima in (worst case) time cubic in the number of vertices, similar to other approximate QAP algorithms. We demonstrate empirically that our algorithm is faster and achieves a lower objective value on over 80% of the suite of QAP benchmarks, compared with the previous state-of-the-art. Applying the algorithms to our motivating example, matching C. elegans connectomes (brain-graphs), we find that FAQ achieves the optimal performance in record time, whereas none of the others even find the optimum.

Keywords:
graph theory, neuroscience, nonlinear optimization

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

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Input: graphs $A$ and $B$ as well as stopping criteria
Output: $\widehat{P}$, an estimated permutation matrix
Choose an initialization, $P^{(0)} = \mathbf{1}\mathbf{1}^{\mathsf{T}}/n$
while stopping criteria not met do
    Compute the gradient of $f(P) = -tr(B^{\mathsf{T}}P^{\mathsf{T}}AP)$ at the current point:
    $\nabla f(P^{(i)}) = -AP^{(i)}B^{\mathsf{T}} - A^{\mathsf{T}}P^{(i)}B$.
    Compute the direction $Q^{(i)}$ by solving
    $\min_{P \in \mathcal{D}} f(P^{(i)}) + \nabla f(P^{(i)})^{\mathsf{T}}(P - P^{(i)})$ via the Hungarian algorithm.
    Compute the step size $\alpha^{(i)}$ by solving $\min_{\alpha \in [0,1]} f(P^{(i)} + \alpha^{(i)}Q^{(i)})$
    Update $P^{(i)}$ according to $P^{(i+1)} = P^{(i)} + \alpha^{(i)}Q^{(i)}$.
end while
Obtain $\widehat{P}$ by solving $\min_{P \in \mathcal{P}} -\langle P^{(i_{max})}, P\rangle$ via the Hungarian algorithm.
```