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The Random Quadratic Assignment Problem

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Abstract The quadratic assignment problem, QAP, is one of the most difficult of all combinatorial optimization problems. Here, we use an abbreviated application of the statistical mechanics replica method to study the asymptotic behavior of instances in which the entries of at least one of the two matrices that specify the problem are chosen from a random distribution P. Surprisingly, the QAP has not been studied before using the replica method despite the fact that the QAP was first proposed over 50 years ago and the replica method was developed over 30 years ago. We find simple forms for $C_{\min}$ and $C_{\max}$, the costs of the minimal and maximum solutions respectively. Notable features of our results are the symmetry of the results for $C_{\min}$ and $C_{\max}$ and their dependence on P only through its mean and standard deviation, independent of the details of P.

Keywords Quadratic assignment problem · Replica method

1 Introduction

Optimal assignment of classes to classrooms [11], design of DNA microarrays [9], cross species gene analysis [19], creation of hospital layouts [13], and assignment of components to locations on circuit boards [26] are a few of the many problems which have been formulated as a quadratic assignment problem (QAP). The QAP is a combinatorial optimization problem first introduced by Koopmans and Beckmann [20]. It is NP-hard and is considered to be one of the most difficult problems to be solved optimally. The problem was defined in the following context: A set of N facilities are to be located at N locations. The quantity of materials which flow between facilities i and j is A_{ij} and the distance between locations i and j is B_{ij}. The problem is to assign to each location a single facility so as to minimize

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(or maximize) the cost

$$C = \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} B_{p(i)p(j)}, \tag{1}$$

where $p(i)$ represents the location to which i is assigned.

In addition to being important in its own right, the QAP includes such other combinatorial optimization problems as the traveling salesman problem and graph partitioning as special cases. There is an extensive literature which addresses the QAP and is reviewed in [3, 6, 10, 17, 22, 24]. The QAP is exceedingly hard. With the exception of specially constructed cases, optimal algorithms have solved only relatively small instances with $N \leq 36$. Various heuristic approaches have been developed and applied to problems typically of size $N \approx 100$ or less. By contrast, a traveling salesman problem consisting of almost 25,000 towns in Sweden has been solved exactly [4].

Our approach makes use of the replica method of statistical mechanics. The replica method is notorious for the tremendously complicated calculations usually involved. However, we take advantage of the fact that if only the form of the solution is desired, the calculation is relatively straightforward. While we formulate the problem using the replica method, we proceed only through the first step which consists of averaging over the disorder represented by the random matrix. At this point, using elementary arguments, we can infer the form of the minimum and maximum costs.

We find that in the asymptotic limit in which the size of the problem $N \to \infty$, the costs of the minimum and maximum solutions, $C_{\min}$ and $C_{\max}$ respectively, are

$$C_{\min} = \mu_A \mu_B N^2 - \sigma_A f(B) N^{3/2} \tag{2}$$

$$C_{\max} = \mu_A \mu_B N^2 + \sigma_A f(B) N^{3/2}, \tag{3}$$

where A is a matrix the elements of which are chosen from the random distribution $P(A_{ij})$ and the elements of B are arbitrary. Here μ_A and σ_A are the mean and standard deviations of the distribution $P(A)$; μ_B is the mean of the entries of B, and f is a function of B and N. Equations (2) and (3) hold under the condition that both matrices are dense (have $O(N^2)$ non-zero entries). Our goal below is to argue for the *form* of (2) and (3). We do not attempt to determine the value of the functions $f(B)$.

2 Relation to Previous Work

Previous work on asymptotic properties of random QAP instances has been generally limited to the case in which the elements of *both* matrices are drawn from random (usually uniform) distributions [1, 2, 5, 7, 8, 14, 21, 25]. Here we consider the properties of solutions to the QAP under the requirement that the elements of only *one* of the matrices need be drawn from *any* random distribution P. Burkard and Fincke [8] implicitly studied the case in which only one matrix is random. They proved rigorously that, under certain conditions, asymptotically as $N \to \infty$, the ratio between $C_{\min}$ and $C_{\max}$ approaches 1, a result with which our (2) and (3) are consistent. Our work extends [8] by finding the closed form (2) and (3). Rhee [25] finds a closed form solution similar to (2) when *both* matrices are random and does *not* find the explicit dependence on σ_A. Finally, statistical mechanics methods have been previously used to study the random QAP [2, 5] although to the best of our knowledge the replica method had not been used heretofore.

3 Random Solution Cost

It is useful to first consider the solution for which $p = p^*$ is a random permutation. Because the elements of A are assigned randomly and since $p^*(i)$ and $p^*(j)$ are random, each B_{ij} in the sum is multiplied by a random value of A_{ij} the average of which is μ_A. Hence, the cost of a random permutation is

$$C_{\text{rand}} = \mu_A \sum_{i,j=1}^{N} B_{p^*(i)p^*(j)} = \mu_A \mu_B N^2. \tag{4}$$

4 Replica Analysis

We now use the replica method to derive the form for $C_{\min}$ and then derive the relationship of $C_{\max}$ to $C_{\min}$. Employing a Hamiltonian, $\mathcal{H}$, defined as the QAP cost function our goal is to compute the partition function

$$Z = \sum_{\{p\}} \exp\left[-\frac{H}{kT}\right] = \sum_{\{p\}} \exp\left[-\frac{1}{kT} \sum_{i,j=1}^{N} A_{ij} B_{p(i)p(j)}\right] \tag{5}$$

and the free energy

$$-\frac{F}{kT} = \lim_{N\to\infty} \ln Z \tag{6}$$

where k and T are the Boltzmann constant and temperature respectively. Then,

$$C_{\min} = F(T = 0). \tag{7}$$

Since the Hamiltonian includes a random matrix, A, we want to calculate the value of the free energy F averaged over the disorder specified by the probability distribution $P(A)$. However, averaging the log of the partition function is difficult. The replica method of statistical mechanics [12] was introduced to make calculation of this average possible. The replica method has been used not just on models of physical systems (such as spin glasses [12, 18, 23]) but also on such combinatorial optimization problems as graph partitioning and the traveling salesman problem [15, 16, 23]. The calculation of the average of the partition function is simplified using a mathematical identity known as the *replica trick*, $\ln(x) = \lim_{n\to 0}(x^n - 1)/n$. Then (6) becomes

$$-\frac{F}{kT} = \lim_{N\to\infty} \lim_{n\to 0} \frac{1}{n}\left(\overline{Z^n} - 1\right), \tag{8}$$

where

$$Z^n = \left(\sum_{\{p^1\}} \exp\left[-\frac{H(\{p^1\})}{kT}\right]\right) \cdots \left(\sum_{\{p^n\}} \exp\left[-\frac{H(\{p^n\})}{kT}\right]\right) \tag{9}$$

and $\overline{Z^n} \equiv \int P(A) Z^n \, dA$ denotes Z^n averaged over the disorder. Here each Hamiltonian represents a replica of the original system and the sum over $\{p^\alpha\}$ now denotes the sum over all permutations in all replicas.

In order to achieve physically sensible results with $f \equiv F/N$ intensive, we require the mean and standard deviation of $P(A)$ to scale as (see [15, 18, 23])

$$\begin{aligned} \mu_A &= \tilde{\mu}_A/N \\ \sigma_A &= \tilde{\sigma}_A/\sqrt{N} \end{aligned} \tag{10}$$

with $\tilde{\mu}_A$ and $\tilde{\sigma}_A$ independent of N. In Appendix A we then find that

$$\begin{aligned} \overline{Z^n} = \exp\left[-\frac{n\mu_A\mu_B N^2}{kT}\right] \\ \times \sum_{\{p^\alpha\}} \exp\left[\frac{\sigma_A^2}{2(kT)^2}\sum_{i,j}\left(\sum_\alpha B_{p^\alpha(i)p^\alpha(j)}\right)^2\right]. \end{aligned} \tag{11}$$

As explained in Appendix B, (11) holds under the condition that neither A nor B is sparse.

We can make the following observations based on (11) and (8):

- Consistent with (2), the dependence of F on A is only through μ_A and σ_A.
- If $\sigma_A = 0$ and/or $T \to \infty$, substituting (11) in (8) yields $F = \mu_A\mu_B N^2$ which is the cost of the random solution, (4). This is reasonable because (i) physically for high temperatures we expect randomness and (ii) if $\sigma_A = 0$, all entries in A are identical and all permutations yield the same costs.

We infer the form of $F(T = 0)$ as follows:

- In (11) σ_A appears in the combination σ_A/T. Thus, from (8) we see that in the $T \to 0$ limit, only a term linear in σ_A can survive in F.

  This linear dependence on σ_A as well as on μ_A is consistent with the simple case in which all of the elements in A are scaled by a constant, z, in which case $\sigma_A \to z\sigma_A$ and $\mu_A \to z\mu_A$. Clearly the optimal permutation is unchanged but the cost is also scaled by z. Thus, in this simple case, for any permutation (including the optimal one) the linear dependence on μ_A and σ_A must hold.
- Given that we obtained (11) by expanding in $1/\sqrt{N}$, we expect the second term in the expressions for $C_{\min}$ to be proportional $N^{3/2}$ since the leading term is proportional to N^2.

Given the considerations, above the only possible expression for the second term in F is $\sigma_A f(B) N^{3/2}$ where f is a function of B only.

The form of $C_{\max}$ follows directly as follows. Let $C_{\min}(A, B)$ and $C_{\max}(A, B)$ denote the optimal minimum and maximum costs respectively of the QAP problem with matrices A and B and let $-A$ denote a matrix with elements $-A_{ij}$. Since $C_{\max}(A, B) = -C_{\min}(-A, B)$ and since $\mu_{-A} = -\mu_A$ and $\sigma_{-A} = \sigma_A$, the form for $C_{\max}$ in equation (3) follows directly from the form for $C_{\min}$.

If the entries of B are also drawn from a random distribution as in previous work, it is straightforward to show that

$$\begin{aligned} C_{\min} &= \mu_A\mu_B N^2 - c\sigma_A\sigma_B N^{3/2} \\ C_{\max} &= \mu_A\mu_B N^2 + c\sigma_A\sigma_B N^{3/2} \end{aligned} \tag{12}$$

where c is a constant independent of A and B and σ_B is the standard deviation of the entries in B. The dependence of the $N^{3/2}$ term on A and B only through their standard deviations has not been shown before.

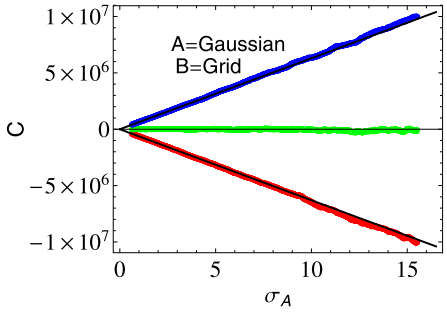

Fig. 1 For an $N = 100$ QAP instance consisting of an A matrix with elements from a Gaussian distribution and a B matrix representing a two-dimensional grid, (from top to bottom), $C_{\max}$, C_{rand}, and $C_{\min}$ versus standard deviation σ_A. For a given σ_A, $C_{\max}$ and $C_{\min}$ values are equidistant from C_{rand} value

5 Numerical Results

To confirm our findings, we use the tabu search (TS) [27] heuristic to obtain approximate numerical solutions for a number of QAP instances. We employ matrices of the types described in detail in Appendix D. We use the notation "*A matrix type*"-"*B matrix type*" to specify a QAP instance.

In Fig. 1, we plot $C_{\min}$ and $C_{\max}$ versus σ_A for an instance of type Gaussian-Grid. As expected, the plots are linear in σ_A and the absolute values of $C_{\min}$ and $C_{\max}$ are equal for a given σ. This is consistent with (2) and (3).

A stronger test is achieved by studying instances specified by a matrix that represents a random graph of average degree k. In this case,

$$\sigma_A(k) = \sqrt{k(N-1-k)} = \sqrt{\left(\frac{N-1}{2}\right)^2 - \left(k - \frac{N-1}{2}\right)^2} \tag{13}$$

which represents a circle with origin at $((N-1)/2, 0)$. In Fig. 2(a) we plot $C_{\min}$, C_{rand}, and $C_{\max}$ versus k, $0 \le k \le N-1$, for an instance of type Random-Grid. In order to illustrate the behavior of $C_{\min}$ and $C_{\max}$ in more detail, in Fig. 2(b), we plot $\Delta C_{\min/\max} \equiv C_{\min/\max} - C_{\text{rand}}$. The solid line is an ellipse of the form

$$C^{\text{theory}}_{\max/\min} = \pm\sigma_A(k) f(B) N^{3/2} \tag{14}$$

where $f(B)$ is chosen to best fit of (14) to the data. The fit is consistent with the theory, exhibiting both the expected linear dependence of the optimal costs on $\sigma_A(k)$ and the symmetry represented by (2) and (3). In Fig. 3 we show similar plots for other varied QAP instances.

We now study the dependence of ΔC on N. We treat instances in which the A matrix is random or random regular and consider different types of B matrix. To compare results for instances of different sizes, we define the normalized quantities ΔC_{norm} and k_{norm}

$$\Delta C_{\text{norm}} \equiv \frac{\Delta C}{\mu_B N^2}; \qquad k_{\text{norm}} \equiv \frac{k}{N-1}. \tag{15}$$

With this normalization we expect

$$\Delta C_{\text{norm}} \sim \sigma_A N^{-1/2}. \tag{16}$$

In Fig. 4(a), (c), and (e) we plot ΔC_{norm} for various values of N for various instance types. We confirm the $N^{-1/2}$ dependence by plotting

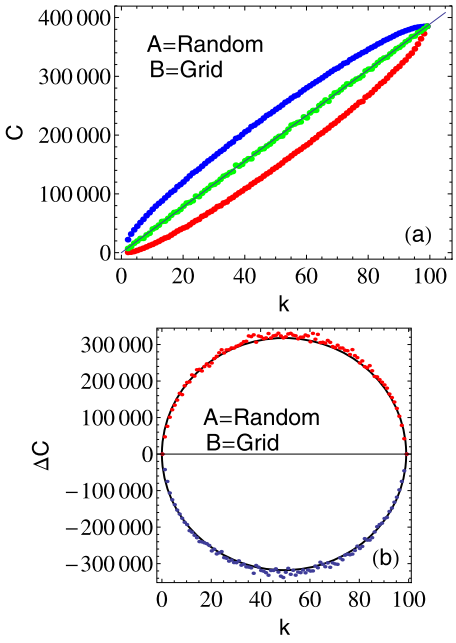

Fig. 2 For an $N = 100$ QAP instance consisting of an A matrix representing a random graph and B matrix representing a two-dimensional grid, (from top to bottom), (**a**) $C_{\max}$, C_{rand}, and $C_{\min}$ versus average degree k and (**b**) $\Delta C_{\max}$ and $\Delta C_{\min}$ versus k. In this and all following figures, the *upper* and *lower semi-circles* are the $\Delta C_{\max}$ and $\Delta C_{\min}$ plots, respectively. The *solid circular line* represents the theoretical prediction

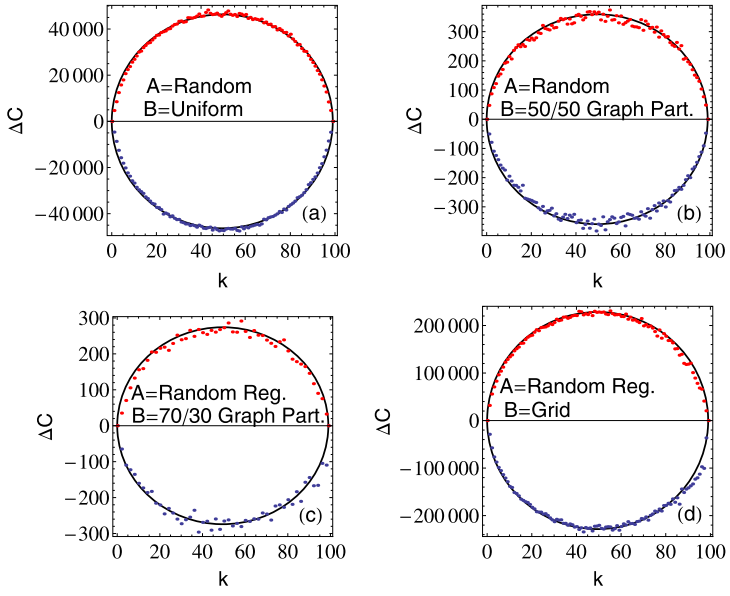

Fig. 3 For various $N = 100$ QAP instance, $\Delta C_{\max}$ and $\Delta C_{\min}$ versus k. The *solid circular line* represents the theoretical prediction

$$\Delta C_{\text{collapsed}} \equiv \Delta C_{\text{norm}} N^{1/2} \tag{17}$$

in Fig. 4(b), (d) and (f). The collapse is consistent with (16). Additional plots for other instance types are shown in Fig. 2 in the Supplement.

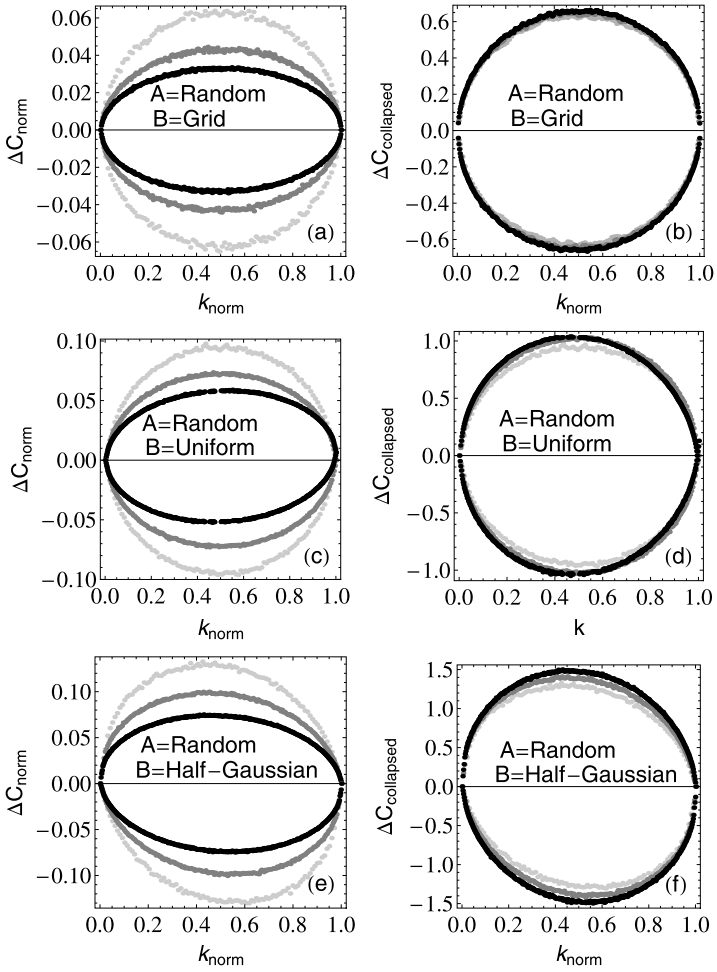

Fig. 4 (**a**), (**c**), (**e**) Normalized ΔC versus normalized k for instance sizes $N = 100$ (*light gray*); $N = 225$ for (**a**) and 200 for (**c**) and (**e**) (*medium gray*); and $N = 400$ (*black*). The *right hand column* contains the corresponding collapsed plots

6 Discussion and Summary

With an innovative use of the statistical mechanics replica method involving only elementary arguments and minimal mathematics, we determine the form of the values of the minimal and maximal costs for the random QAP. This is a significant advancement on a problem for which progress has been exceedingly slow. We find remarkably simple forms for $C_{\min}$ and $C_{\max}$ providing insight into what have heretofore been isolated numerical results. This work not only (i) presents concrete results for the QAP but also (ii) illustrates the power of the replica method to unify and extend results on a very difficult problem.

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Appendix A: Integration over Disorder

In the following we retain only terms which do not vanish in the $N \to \infty$ limit. This is equivalent to retaining terms only to second order in A_{ij}. Because we want to maintain the exponential form, we write

$$\begin{aligned}
\overline{Z^n} &= \int P(A) \sum_{\{p^\alpha\}} \exp\left[-\frac{1}{kT} \sum_{\alpha=1}^{n} \sum_{i,j=1}^{N} A_{ij} B_{p^\alpha(i) p^\alpha(j)} \right] \mathrm{d}A \\
&= \sum_{\{p^\alpha\}} \exp\left[\ln \int P(A) e^{-\frac{1}{kT} \sum_{i,j} \sum_{\alpha}^{n} A_{ij} B_{p^\alpha(i) p^\alpha(j)}} \, \mathrm{d}A \right] \\
&= \sum_{\{p^\alpha\}} \exp\left[\ln \prod_{i,j} \int P(A_{ij}) e^{-\frac{1}{kT} \sum_{\alpha}^{n} A_{ij} B_{p^\alpha(i) p^\alpha(j)}} \, \mathrm{d}A_{ij} \right] \\
&= \sum_{\{p^\alpha\}} \exp\left[\sum_{i,j} \ln \int P(A_{ij}) e^{-\frac{1}{kT} \sum_{\alpha}^{n} A_{ij} B_{p^\alpha(i) p^\alpha(j)}} \, \mathrm{d}A_{ij} \right] \\
&= \sum_{\{p^\alpha\}} \exp\left[\sum_{i,j} \ln(1 + y_{ij}) \right] \qquad (18)
\end{aligned}$$

where $y_{ij} \equiv \int P(A_{ij}) \exp[-\frac{1}{kT} \sum_{\alpha}^{n} A_{ij} B_{p^\alpha(i) p^\alpha(j)}] dA_{ij} - 1$. Expanding y_{ij} to second order in A_{ij} we have:

$$\begin{aligned}
y_{ij} &\sim \int P(A_{ij}) \left[1 - \frac{1}{kT} \sum_{\alpha}^{n} A_{ij} B_{p^\alpha(i) p^\alpha(j)} + \frac{(\sum_{\alpha}^{n} A_{ij} B_{p^\alpha(i) p^\alpha(j)})^2}{2(kT)^2} \right] \mathrm{d}A_{ij} - 1 \\
&= -\frac{\mu_A}{kT} \sum_{\alpha}^{n} B_{p^\alpha(i) p^\alpha(j)} + \frac{\mu_{2A}}{2(kT)^2} \left(\sum_{\alpha}^{n} B_{p^\alpha(i) p^\alpha(j)} \right)^2 \qquad (19)
\end{aligned}$$

where μ_{A2} is the second moment (around zero) of P. Expanding $\ln(1 + y_{ij})$ to the second order in y_{ij} and substituting (19), we have

$$\begin{aligned}
\ln(1 + y_{ij}) &\sim -\frac{\mu_A}{kT} \sum_{\alpha}^{n} B_{p^\alpha(i) p^\alpha(j)} + \frac{\mu_{2A}}{2(kT)^2} \left(\sum_{\alpha}^{n} B_{p^\alpha(i) p^\alpha(j)} \right)^2 - \frac{1}{2} \left(\frac{\mu_A}{kT} \sum_{\alpha}^{n} B_{p^\alpha(i) p^\alpha(j)} \right)^2 \\
&= -\frac{\mu_A}{kT} \sum_{\alpha}^{n} B_{p^\alpha(i) p^\alpha(j)} + \frac{\sigma_A^2}{2(kT)^2} \left(\sum_{\alpha}^{n} B_{p^\alpha(i) p^\alpha(j)} \right)^2 \qquad (20)
\end{aligned}$$

where we have only retained terms to $O(A_{ij}^2)$. Finally we have

$$\begin{aligned}
\overline{Z^n} &= \sum_{\{p^\alpha\}} \exp\left[\sum_{i,j} \left[-\frac{\mu_A}{kT} \sum_{\alpha}^{n} B_{p^\alpha(i) p^\alpha(j)} + \frac{\sigma_A^2}{2(kT)^2} \left(\sum_{\alpha}^{n} B_{p^\alpha(i) p^\alpha(j)} \right)^2 \right] \right] \\
&= \sum_{\{p^\alpha\}} \exp\left[-\frac{\mu_A \mu_B n N^2}{kT} + \frac{\sigma_A^2}{2(kT)^2} \sum_{i,j} \left(\sum_{\alpha}^{n} B_{p^\alpha(i) p^\alpha(j)} \right)^2 \right] \qquad (21)
\end{aligned}$$

where we use the fact that $\sum_{i,j} B_{p^\alpha(i) p^\alpha(j)}$ is independent of permutation.

Appendix B: Requirements on A and B Matrices

That μ_A and σ_A scale as in (10) in order to achieve physically sensible results with $f = F/N$ intensive (i.e. independent of N) is required so that the quantities in the exponents of (2) do not scale as N^2 which would ultimately result in f scaling as N as $N \to \infty$. The exponents will scale as N^2 if A and B are dense (have $O(N^2)$ non-zero elements). If, however, either matrix is sparse the exponents will scale as N and the requirements on u_A and σ_A do not hold. We cannot then expand equation (18) in A_{ij} as done in Appendix A. Thus our results do not apply to QAP instances in which both matrices are not dense, such as the traveling salesman problem. Our results do apply to graph partitioning of dense graphs including random graphs in which the average degree k of the graph scales such that k/N is a constant—the case we have treated here (see also Refs. [15, 28]).

The requirement that A and B must be dense appears to be equivalent to a requirement, specified by Burkhard and Fincke [8] in which they studied asymptotic properties of problems with sum (e.g. QAP) and bottleneck objective functions. They proved rigorously that, under certain conditions, asymptotically as $N \to \infty$, the ratio between $C_{\min}$ and $C_{\max}$ approaches 1, a result with which our (2) and (3) are consistent. A key condition is that $|S|$, the number of non-zero elements which contribute to the sum in the objective function, increases to infinity faster than the log of the number of feasible solutions $|T|$:

$$\lambda_0 |S| - \log |T| \to \infty \quad \text{as } N \to \infty \tag{22}$$

for a certain fixed constant $\lambda_0 > 0$.

For the QAP, $|T| \sim N!$ and $|S| \sim N^2$ if A and B are dense but $|S| \sim N$ if either is sparse. Equation (22) holds in the former case but not in the latter.

Using statistical mechanical methods in Ref. [2], Albrecher et al. also make use of the requirement of (22) to prove the results of Ref. [8] generalizing and repairing an earlier statistical mechanical approach [5].

Appendix C: Relationship to Graph Partitioning

The problem of partitioning a graph into two subgraphs of size rN and $(1-r)N$ with the minimum number of edges between the two subgraphs can be represented as a QAP as follows: One matrix, A, is the adjacency matrix of the graph to be partitioned. The other matrix, B, the *graph partitioning matrix*, is the adjacency matrix for a bipartite graph in which edges are present between two sets of vertices; one set contains rN vertices and the second set contains $(1-r)N$ vertices. The QAP cost function is the cost of partitioning the graph represented by A.

Appendix D: Matrix Types

We employ matrices of the following types:

- Uniform—the matrix elements are chosen from a uniform distribution on the interval $[0, 100]$.
- Gaussian—matrix elements are chosen from a Gaussian distribution with zero mean and standard deviation σ.

– Half-Gaussian—matrix elements are chosen from a Gaussian distribution as above but only elements with value greater or equal to zero are used.
– Random (graph)—the matrix is the adjacency matrix of a random graph with edges present with probability p. The average degree of the graph is $k = pN$.
– Random Regular (graph)—the matrix is the adjacency matrix of a random regular graph for which all vertices are degree k.
– Grid—the matrix elements are the Euclidean distances between points in a two-dimensional square grid. The distances between adjacent points along the x and y axes are 100.
– Graph Partitioning—the matrix is the graph partitioning matrix described in Appendix C.

All matrices are symmetrical with zero diagonal. For the Random and Random Regular matrices that represent graphs, we study cases of the graph degree k ranging from 0 to $N - 1$.

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