A Differential-Operator Approach to the Permanental Polynomial

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A recently published computational approach to the permanental polynomial scales very badly ($\sim 2^n$) with problem size, relying as it does on examining the entire augmented adjacency matrix for nonzero products. The present study presents an entirely different algorithm that relies on symbolic computation of second partial derivatives. This approach has previously been applied to the matching polynomial but not the permanental polynomial. The differential-operator algorithm scales much better with problem size. For fullerene-type structures without perimeters, the two algorithms take about the same time to compute $n = 32$. On one $n = 40$ structure, the new algorithm was >45 times faster. Relative performance is even better for polycyclic aromatic hydrocarbon structures, which have perimeters.

INTRODUCTION

Let **A** be the adjacency matrix of a graph, G(*V*,*E*,*F*) on |*V*| vertices with |*E*| edges forming a set of |*F*| faces, and let **I** be the identity matrix of order |*V*|. Then the much-studied characteristic polynomial[1] is just the determinant det(*x***I** − **A**). The *permanental polynomial*, per(*x***I** − **A**), on the other hand, has received only brief mention in the chemical[1−5] and mathematical[6−9] literature, probably because of the relative difficulty in computing it. Recently, a practical computational route to this polynomial appeared,[10] along with some results on chemical structures.[11,12] The practical limit of this method on generally available machines, however, remains ≤40 vertices, and the potential of this polynomial remains largely uninvestigated.

A number of years ago, Godsil and Gutman[13] and Rosenfeld and Gutman[14] laid the foundation for a method of computing graph-theoretic polynomials by symbolic manipulation of second partial derivatives. The notation used in those papers is adopted here, namely, the characteristic polynomial is denoted by $\phi^-(G,x)$, and the permanental polynomial by $\phi^+(G,x)$. The ordinary (and also much-studied) *acyclic* or *matching polynomial* (ref 1, pp 134ff) is $\alpha^-(G,x)$. Finally, ref 14 introduced a new polynomial, $\alpha^+(G,x)$, which has the same absolute coefficients as $\alpha^-(G,x)$, but with all signs positive. This polynomial does not have a specific name and has apparently never been studied, but *acyclic permanental polynomial* seems a good choice.

The following definitions from ref 14 are relevant here, the differential operator

$$\mathscr{D} = \sum_{rs\in E} \frac{\partial^2}{\partial x_r \partial x_s}$$

where the sum is over all edges in *G*, and the product

$$\mathscr{X} = \prod_{i=1}^{|V|} x_i$$

Then,

$$\mathscr{D}\mathscr{X} = \sum_{rs\in E} \frac{\mathscr{X}}{x_r x_s}$$

Finally, ref 14 demonstrated (Theorem 1, Corollary 1.2) that, for $x_1 = x_2 = x_3 = \ldots = x$

$$\alpha^{\pm}(G, x) = \exp(\pm\mathscr{D})\mathscr{X} = \prod_{rs\in E}\left(1 \pm \frac{\partial^2}{\partial x_r \partial x_s}\right)\mathscr{X}$$

Salvador et al.[15] published an implementation of this expression for $\alpha^-(G,x)$ that relied on the symbolic-algebra abilities of Mathematica. They mention its applicability to $\alpha^+(G,x)$ in passing.

Reference 14 defines three more operators for the purpose of expressing $\phi^{\pm}(G,x)$, namely,

$$\mathscr{Z}_t = \partial^z / \prod_{i=1}^{z} \partial x_i,\ \mathscr{C} = \sum_t 2^{c(t)}\,\mathscr{Z}_t \text{ and } \mathscr{H} = \mathscr{C} + \mathscr{D}$$

where, as before, *t* is a 2-regular subgraph of *G*, *z* is the number of vertices in *t*, *c*(*t*) is the number of vertex-disjoint cycles in *t*, and the summation is over cycles in *G*. (The notation has been changed somewhat from ref 14.) Just as D over edges produces all independent sets of edges, so too C over cycles produces all 2-regular subgraphs of *G*. Then, finally (ref 14, Theorem 5), again for $x_1 = x_2 = x_3 = \ldots = x$

$$\phi^{\pm}(G, x) = \exp(\pm\mathscr{H})\mathscr{X}$$

The key to this equation is the fact that, in the infinite-series

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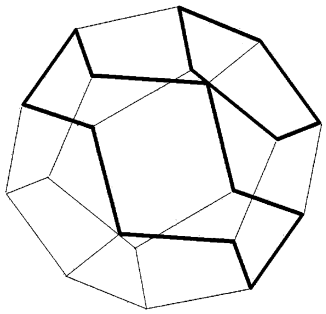

Figure 1. A 2-regular subgraph of the dodecahedron graph consisting of a 5-cycle and a 10-cycle.

expansion of the exponential function, only the first two terms are not equal to zero.

RESULTS AND DISCUSSION

In terms of a practical computation of the permanental polynomial, $\phi^+(G,x)$, the equation to be derived from all this is

$$\phi^+(G, x) = \alpha^+(G, x) + \sum_t 2^{c(t)}\alpha^+(G\backslash t, x)$$

where here the summation is explicitly over all 2-regular subgraphs of G, and $G\backslash t$ is G with all vertices and adjacent edges of each t deleted. (The determinantal version of this equation can be found in Gutman and Polansky.)[16] The Mathematica code of Salvador et al.[15] can easily be modified to compute α^+. The outstanding tasks are to enumerate and identify the subgraphs t and to ascertain the number of vertex-disjoint cycles in each t. As shown below, these problems have already been addressed.

The mathematical basis of $\alpha^+(G,x)$ is easily explained. A *2-regular subgraph* of G is a (not necessarily connected) subgraph, all vertices of which are of degree 2. A 2-regular subgraph therefore consists of one cycle or of ≥ 2 vertex-disjoint cycles. Using slightly different notation, Hosoya[17] represented the acyclic and characteristic polynomials as

$$\alpha^- = \sum_{k=0}^{\lfloor |V|/2 \rfloor} (-1)^2 p(G, k)x^{|V|-2k}$$

and

$$\phi^- = \sum_{k=0}^{\lfloor |V|/2 \rfloor} (-1)^2 p(G, k)x^{|V|-2k} + \sum_t^{\text{cycles}} (-2)^{c(t)} \sum_{k=0}^{\lfloor (|V|-|t|)/2 \rfloor} p(G\backslash t, k)x^{|V|-|t|-2k}$$

where $p(G, k)$ is the number of ways of choosing k disjoint edges, the summation over cycles, t, is over all 2-regular subgraphs of G, $c(t)$ is the number of vertex-disjoint cycles in each t, and $G\backslash t$ is G with all vertices of t and their adjacent edges deleted. Figure 1 illustrates a 2-regular subgraph of the dodecahedron graph with $c(t) = 2$. By an exact analogy, $\alpha^+(G,x)$ and $\phi^+(G,x)$ may be expressed as

$$\alpha^- = \sum_{k=0}^{\lfloor |V|/2 \rfloor} p(G, k)x^{|V|-2k}$$

$$\phi^+ = \sum_{k=0}^{\lfloor |V|/2 \rfloor} p(G, k)x^{|V|-2k} + \sum_t^{\text{cycles}} (-2)^{c(t)} \sum_{k=0}^{\lfloor (|V|-|t|)/2 \rfloor} p(G\backslash t, k)x^{|V|-|t|-2k}$$

Thus, $\alpha^+(G,x)$ is simply the permanental polynomial without the cyclic contributions in the same sense that the acyclic polynomial is the characteristic polynomial without the cyclic contributions. It is obvious from these expressions that for structures without any cycles, i.e., trees, the matching polynomial and acyclic permanental polynomial are identical to the characteristic and permanental polynomials, respectively.

Randić and Trinajstić[18] published an exceptionally useful discussion of the t-recognition problem: How can one identify all the 2-regular subgraphs in a multiring system? Specifically, they summarize a method that is very easy and fast on modern computers which can be recapitulated as follows. Number the vertices in G from 1 to $|V|$, the edges from 1 to $|E|$, and the faces from 1 to $|F|$. Generate an $|F| \times |E|$ $\{0,1\}$ matrix $\mathbf{Q}$ such that $\mathbf{Q}_{i,j} = 1$ if edge j forms part of the boundary of face i, and $\mathbf{Q}_{i,j} = 0$ otherwise. Each row, $\mathbf{Q}_i$, will be a $\{1,0\}$ vector. Consider each $\mathbf{Q}_i$ to be a binary integer B_i. Each B_i thus defined encodes the edge list of some face. Analogous encodings of all other 2-regular subgraphs t are generated by combining some set of B_i via the bitwise exclusive-OR (XOR) operation. In Mathematica code,[19] the sum and product of a vector of numbers are available from **Plus**@@*list* and **Times**@@*list*, respectively, where *list* is either an actual vector or a variable name referring to one. In an exactly analogous fashion, **BitXor**@@*list* produces the integer result of XORing a vector of integers all together. An example of this operation as it pertains to the problem at hand is shown in Figure 2.

The correspondence between selection of edges and XORing of integer representations relies on those two operations having the same selection rules. An edge is selected if it belongs to exactly one member of the subset of faces. Strictly speaking, XOR selects a bit that is set in any odd number of its binary integer arguments, but, since any given edge belongs to exactly 0, 1, or 2 of a set of faces, 1 is the only odd number possible.

For a polycyclic aromatic hydrocarbon graph that has a perimeter, there is a one-to-one correspondence between the set of 2-regular subgraphs and the possible combinations of faces $\binom{|F|}{i}$, $i = 1$ to $|F|$. For fullerene-type graphs that do not have a perimeter, the complete set of $\binom{|F|}{i}$ generates each 2-regular subgraph twice. This complication is easily handled, however, because the two sets of faces that generate a given 2-regular subgraph are always complementary. That is, each set of the pair contains just those faces that are not in the other set. An example for the dodecahedron graph is shown in Figure 3. For fullerene-type structures with $|F|$ odd, the problem is easily solved by considering only combinations of $i \leq [|F|/2]$ faces. With $|F|$ even, however, there is still duplication among the face sets with exactly $|F|/2$ members.

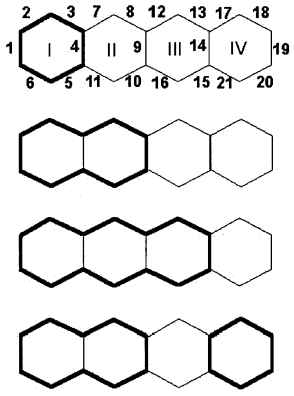

Figure 2. Several 2-regular subgraphs of tetracene, namely, those represented by **BitXor**@@{B_1}, **BitXor**@@{B_1,B_2}, **BitXor**@@{B_1,B_2 B_3}, and **BitXor**@@{B_1,B_2 B_4}. Bits are normally numbered from right to left, so B_1 = 111111, B_2 = 11111001000, B_3 = 1111100100000000, and B_4 = 111110010000000000000. **BitXor**@@{B_1,B_2 B_4} produces the binary integer representation of a subgraph consisting of a 10-cycle and a 6-cycle. $G\backslash t$ for this subgraph is two isolated vertices. The acyclic permanental polynomial of two isolated vertices is x^2, and $c(t) = 2$, so this subgraph contributes $2^2 \times x^2 = 4x^2$ to the permanental polynomial.

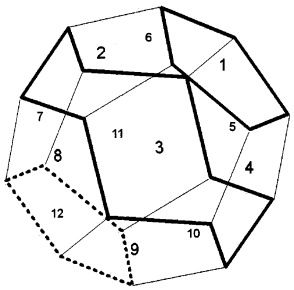

Figure 3. The same 2-regular subgraph of the dodecahedron graph shown in Figure 1. Here, the faces are numbered 1−12, with larger-type numbers for those that could be seen on a solid figure and smaller-type numbers for those that would be hidden. Note how the binary integer representation of this 2-regular subgraph results from both **BitXor**@@{B_2,B_3,B_4,B_5,B_6} and its complement **BitXor**@@{B_1,B_7,B_8,B_9,B_{10},B_{11},B_{12}}. $G \setminus t$ for this subgraph consists of the five vertices and five edges belonging to face 12, indicated by the dashed line.

This problem can be solved by choosing an arbitrary face and considering among face sets with $|F|/2$ members only those that contain (or, equivalently, do not contain) that face. Since all cyclic structures will have a face numbered 1, it is convenient to implement this solution by excluding integer lists that contain B_1.

Having found a reliable way to enumerate and identify all the 2-regular subgraphs of a given structure, the only barrier remaining to applying the equation

$$\phi^+(G, x) = \alpha^+(G, x) + \sum_t 2^{c(t)}\alpha^+(G\backslash t, x)$$

to an actual calculation is to find the values of $c(t)$ for the various t. This is simply a matter of generating the adjacency matrix of t (by eliminating from **A** the rows and columns not corresponding to vertices in t) and tracing the connections through it. Indeed, Mathematica code to perform exactly that task had already been written for another purpose[20] and could be adapted directly. The final result was a working Mathematica program that duplicated the results of the older algorithm for every problem on which it was tested. The program (but not Mathematica itself) is available from the author on request.

These algebraic manipulations would be of only academic interest if they did not result in an algorithm that clearly outperforms the one set forth in ref 10. Fortunately, the CPU time requirement of the present approach is at least a factor of 10 smaller for structures of any appreciable size, and the factor gets larger as the structures get larger. There are several barriers to generalizing timing comparisons. Prominent among these is that, for quite similar structures with the same $|V|$ and $|E|$, CPU times with the older algorithm can differ by a factor of 10.[10] Another is that, for larger structures where the difference is greater, it is simply not practical to run the older algorithm on an ordinary desktop machine. For example, using the old algorithm to find the permanental polynomial of the C_{40} 4−6 fullerene with C_1 symmetry took 1033 h on a single, 64-bit processor of a Cray T3E running at 600 MHz. The new algorithm solved the same problem on a 32-bit Pentium III running at 500 MHz in 38 h. Running the same $|V| = 36$ problem with the old algorithm on both machines gave the result that the Cray was 1.68× faster, but even that number may change with problem size.

Further complications arise from overflow of the 32-bit integer registers with the older algorithm. When there are more than 32 edges in a structure, some of the B_i representations will contain more than 32 bits. While this problem can be circumvented by breaking longer words into two parts (see, for example, Delic and Cash[21]), it cannot be ignored. Similarly, for fullerene-type structures larger than C_{36}, the largest coefficients will overflow the integer registers of a 32-bit machine if the older algorithm is used. These problems do not arise with the new algorithm because Mathematica performs integer calculations, including bitwise logical operations, to arbitrary precision, keeping all the digits, on both 32-bit and 64-bit machines.

For similar graphs on $|V|$ vertices, CPU time with the old algorithm scales as $2^{|V|}$. The new one scales much better, but there is too much variation in CPU time for structures with the same $|V|$ to quantify the improvement. The value of $|V|$ for which CPU times are about the same is 32 for fullerene-type structures and somewhat less for polycyclic aromatic hydrocarbons. A disadvantage of the new algorithm is that, because of its reliance on the code from ref 15, it requires Mathematica or some other commercial software capable of doing symbolic manipulations. Specifically, the second partial derivatives, $\partial^2/\partial x_r \partial x_s$, are evaluated without ever assigning numeric values to the symbols. The old algorithm, by contrast, exists as compiled, executable code that requires no other software to run except an operating system. Additional improvements in speed, not to mention portability, might result if some straightforward way could be found to substitute numeric manipulations in Fortran or C or Pascal, for the symbolic evaluations of the derivatives, and this is a likely target for future work.

These caveats notwithstanding, the algorithm described here for finding the permanental polynomial of a chemical graph offers a substantial increase in computation speed, especially for larger structures. This advantage will become more important as faster hardware brings more structures within the reach of generally available desktop computers.

CONCLUSIONS

The characteristic polynomial of molecular graphs has a long history in the literature of mathematical chemistry. Little has been done, however, with the superficially similar permanental polynomial because of the difficulty in calculating its coefficients with readily available hardware. Some progress was made in this direction a few years ago, but permanental polynomials still remained a computational challenge. The present study describes a working, tested algorithm which reduces the time required for these calculations by a factor of approximately 50 for structures with ~40 vertices and which scales much more favorably with problem size, where the previously published algorithm scales exponentially. Thus exploration of the permanental polynomial for molecules large enough to exhibit great structural variability is now possible.

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