Immanants and Immanantal Polynomials of Chemical Graphs

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The much-studied determinant and characteristic polynomial and the less well-known permanent and permanental polynomial are special cases of a large class of objects, the immanants and immanantal polynomials. These have received some attention in the mathematical literature, but very little has appeared on their applications to chemical graphs. The present study focuses on these and also generalizes the acyclic or matching polynomial to an equally large class of acyclic immanantal polynomials, generalizes the Sachs theorem to immanantal polynomials, and sets forth relationships between the immanants and other graph properties, namely, Kekulé structure count, number of Hamiltonian cycles, Clar covering polynomial, and Hosoya sextet polynomial.

1. INTRODUCTION

A chemical graph is usually considered to be an undirected graph without loops or multiple edges that represents some chemical structure, and that definition is used here. A chemical graph is composed of a vertex set V representing atoms and an edge set E representing bonds between atoms. In some studies, weights are assigned to vertices and/or edges, often to account for the presence of heteroatoms, but here we consider only unweighted graphs. The adjacency matrix of such a graph $\mathbf{A}$ is a $|V| \times |V|$ matrix of elements $a_{i,j} = 1$ if an edge connects vertices i and j and $a_{i,j} = 0$ otherwise.

The characteristic polynomial is defined as the determinant of the difference between a diagonal matrix of the symbolic variable x and the adjacency matrix, $\mathscr{P}(G,x) = \det(x\mathbf{I} - \mathbf{A})$. The last term of this polynomial, $a_n x^0$, is just the determinant of $\mathbf{A}$. An extensive literature exists on the characteristic polynomials of adjacency matrices.[1] Some papers have also appeared on the permanental polynomial of $\mathbf{A}$ $\mathscr{P}^{\text{per}}(G,x) = \text{per}(x\mathbf{I} - \mathbf{A})$[2−6] and the corresponding last term, the permanent.[7−9] Just as $\mathscr{P}^{\text{per}}(G,x)$ is the permanental polynomial because it is the permanent of $(x\mathbf{I} - \mathbf{A})$, the characteristic polynomial might be thought of as the determinantal polynomial, although that term is never actually used. These two polynomials are representatives, extremes in one sense (described below), of a large class of polynomials that are the subject of this study.

The class of matrix functions to which these belong is the *immanantal polynomials*, $\mathscr{I}_\lambda(G,x)$, which are the corresponding *immanants*, $\text{imm}_\lambda(x\mathbf{I} - \mathbf{A})$. Various spellings of this term have appeared in the literature, but the one used here is the mathematical term coined by Littlewood[10] and is unrelated to the English words *immanent* and *imminent*. In usage corresponding to the determinant and permanent, the last (x^0) term of an immanantal polynomial $\mathscr{I}_\lambda(G,x)$ of a matrix is the immanant imm_λ of the matrix. For a graph G, the subscript λ refers to a nonincreasing partition of the integer $|V|$. The nonincreasing partitions of the integer 6, for example, are {1,1,1,1,1,1}, {2,1,1,1,1}, {2,2,1,1,1,1}, {2,2,2}, {3,1,1,1}, {3,2,1}, {3,3}, {4,1,1}, {4,2}, {5,1}, and {6}. In the mathematics literature, standard notation represents multiple occurrences by a superscript, e.g., {2,2,1,1,1,1} by $\{2^2,1^4\}$. For any n, the characteristic polynomial is the one associated with $\{1^n\}$, and the permanental polynomial is the one associated with $\{n\}$. This is the sense in which these two polynomials are "extreme" immanantals.

For an integer n, the number of distinct nonincreasing partitions is given by the partition function $P(n)$, a function long-studied by mathematicians.[11] From the example above, $P(6) = 11$. However, $P(n)$ increases very rapidly with n. A few more examples are $P(10) = 42$, $P(15) = 176$, $P(20) = 627$, $P(30) = 5604$, $P(40) = 37\,338$. An approximate general result is $P(n) \approx [\exp(\pi\sqrt{2n/3})]/4n\sqrt{3}$.[11] $P(n)$ is the number of distinct immanants and immanantal polynomials for a graph on n vertices. Detailed discussions of this matter have been published. See, for example, Merris and Watkins[12] and Botti and Merris[13] and references therein. A few results needed for the present study are summarized below.

There is a one-to-one correspondence between the partitions of n and the irreducible representations of the symmetric group S_n (see, for example, ref 14) of $n!$ permutations of n elements. The same one-to-one correspondence occurs between the individual characters of an irreducible representation and the partitions of n. Therefore, a complete table of irreducible characters of S_n will be a $P(n) \times P(n)$ matrix with elements $\chi(\lambda,\xi)$ indexed by a partition λ and a conjugacy class ξ. For a symmetric group S_n, a conjugacy class ξ is a set of all permutations σ of n elements that have the same cycle structure, i.e., the same numbers and lengths of cycles in the permutation. Computer programs for generating these matrices have been described;[15,16] however, the difficulties of executing these calculations in practice are discussed below.

Table 1 shows the matrix for $n = 6$. The same set of symbols, i.e., the nonincreasing partitions of n, is used to

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Table 1. Irreducible Character Matrix $\chi(\lambda,\xi)$ for $n = 6^a$

$\lambda\backslash\xi$	6	5,1	4,2	$4,1^2$	3^2	3,2,1	$3,1^3$	2^3	$2^2,1^2$	$2,1^4$	1^6
6	1	1	1	1	1	1	1	1	1	1	1
5,1	−1	0	−1	1	−1	0	2	−1	1	3	5
4,2	0	−1	1	−1	0	0	0	3	1	3	9
$4,1^2$	1	0	0	0	1	−1	1	−2	−2	2	10
3^2	0	0	−1	−1	2	1	−1	−3	1	1	5
3,2,1	0	1	0	0	−2	0	−2	0	0	0	16
$3,1^3$	−1	0	0	0	1	1	1	2	−2	−2	10
2^3	0	0	−1	1	2	−1	−1	3	1	−1	5
$2^2,1^2$	0	−1	1	1	0	0	0	−3	1	−3	9
$2,1^4$	1	0	−1	−1	−1	0	2	1	1	−3	5
1^6	−1	1	1	−1	1	−1	1	−1	1	−1	1

[a] Note that the characters for $\lambda = \{1^n\}$ (the determinantal partition) are all 1 for an even number of elements permuted and -1 for an odd number of elements permuted, while the characters for $\lambda = \{n\}$ (the permanental partition) are all 1. The character tables for all values of n have these properties.

designate both λ and ξ, but λ and ξ are mathematically different entities, namely, λ is an irreducible representation of S_n and ξ is a permutation cycle structure. An important property of character matrices is that they have full rank, i.e., the rows are linearly independent.[17] Most of the foregoing material, except that regarding characteristic and permanental polynomials, has appeared in the mathematics literature. Only Balasubramanian[18] and Chan et al.[19] seem to have applied these concepts explicitly to chemical graphs.

2. CALCULATION OF IMMANANTS AND IMMANANTAL POLYNOMIALS

The characteristic polynomial of a graph, $\mathscr{P}(G,x)$, is often given as

$$\mathscr{P}(G,x) = \sum_{i=0}^{n} \sum_{s \in G} (-1)^{p(s)} 2^{c(s)} x^{n-i}$$

(see, for example, refs 1 and 20), where the second summation is over all subgraphs s on i vertices consisting only of cycles and isolated edges, $p(s)$ is the total number of components in each s, and $c(s)$ is the number of cycles in each s. Subgraphs of this type are often called *Sachs graphs* in recognition of Sachs' original formulation,[21] now usually called the *Sachs theorem*. The factor $2^{c(s)}$ is present because each Sachs graph represents $2^{c(s)}$ permutations of the vertices, each cycle being permutable in either of two directions. In terms of the adjacency matrix **A**, this equation may be written as

$$\mathscr{P}(G,x) = \sum_{\sigma} \prod_{j=1}^{n} (x\boldsymbol{I} - \boldsymbol{A})_{j,\sigma(j)} = \sum_{i=0}^{n} \sum_{\sigma(i)} (-1)^{p(\sigma)} x^{n-i} \prod_{j=1}^{n} (\boldsymbol{I} - \boldsymbol{A})_{j,\sigma}(j)$$

where $p(\sigma)$ is the number of elements in the permutation corresponding to cycles or edges, and the matrix elements $(\mathbf{M})_{j,\sigma(j)}$ are taken such that $\sigma(j)$ is the jth position in the permutation σ. The summation over σ is over all permutations of n elements, while that over $\sigma(i)$ is over only those permutations that actually change i elements, i.e., leave $n - i$ elements unchanged. This operation is analogous to finding Sachs graphs on i vertices. The determinant of the adjacency matrix, det(**A**), is just the single part of the outer summation (of either equation) with $i = n$.

The following notation conventions for immanants and their relationship to irreducible characters of S_n are adopted here. A permutation is denoted by σ and a conjugacy class, a set of all σ for a given n that have the same cycle structure, by ξ. A $P(n) \times P(n)$ irreducible character matrix of S_n, is denoted by χ. The matrix element indexed by the row corresponding to the partition λ and the column corresponding to conjugacy class ξ is $\chi(\lambda,\xi)$. The irreducible character associated with a specific permutation σ is denoted as $\chi_\lambda(\sigma) = \chi(\lambda,\xi)$, where ξ is the conjugacy class to which σ belongs.

Observe that in the two equations above, the $(-1)^{p(\sigma)}$ terms are nothing more than the irreducible characters $\chi_\lambda(\sigma)$ corresponding to the determinantal partition $\{1^n\}$. It has been observed[22] that the permanent and permenantal polynomial may be obtained by substituting $(+1)^{p(\sigma)}$, the irreducible characters corresponding to the permanental partition $\{n\}$, for $(-1)^{p(\sigma)}$. What has apparently not been explicitly observed before, however, is that *all* immanants and immanantal polynomials may be obtained from the above equations if the irreducible characters $\chi(\lambda,\xi)$ are available. Thus,

$$\mathscr{I}_\lambda(G,x) = \sum_{i=0}^{n} \sum_{\sigma(i)} \chi_\lambda(\sigma) x^{n-i} \prod_{j=1}^{n} (\boldsymbol{I} - \boldsymbol{A})_{j,\sigma}(j)$$

and the corresponding immanant of the adjacency matrix, $\mathrm{imm}_\lambda(\mathbf{A})$, is the term with $i = n$. When $\lambda = \{1^n\}$, the above equation reduces to the Sachs theorem, as it must if the equation is valid.

The importance of this generalization from a computational perspective can hardly be overstated, since it means that immanants and immanantal polynomials can be obtained by adapting methods for computing permanents[7,23] and permanental polynomials.[3,6] The present study utilized a Mathematica implementation of published formulas for the irreducible representations[12,18] and for the permanent[8] and permanental polynomial.[3] Calculation of the irreducible characters requires the latest version of the add-on package Combinatorica.[24] An advantage of Mathematica for this task is its automatic handling of integers with any number of digits. All of the irreducible characters are integers, but some of them are very large, exceeding the capacity of a 32-bit CPU register even for modest n. Unfortunately, the fastest algorithm currently available for calculating the permanent of a (0,1) matrix[9] seems unusable for other immanants because the cycle structures of the individual permutations are lost.

Because of the rapid increase of $P(n)$ with n, the challenge of actually calculating either the complete set of irreducible characters for S_n or a complete set of immanantal polynomials for a graph on n vertices is considerable. The character table for S_{30} contains 31 404 816 integers, some of them quite large. A desktop computer operating at 1.4 Ghz required approximately 3 weeks to generate this table. Once generated, however, these tables can be saved to disk and used as needed, since they depend only on n and are not specific to any particular graph on n vertices.

3. ALGEBRAIC PROPERTIES OF IMMANANTS AND IMMANANTAL POLYNOMIALS

Since P(n) greatly exceeds n in magnitude, for any particular graph G, not all of the P(n) immanants or polynomials are linearly independent. However, as a general matter for any particular value of n, choosing a set of linearly independent immanantal polynomials depends on knowing the structure of G. Any two polynomials can be linearly independent in principle because the irreducible representations of S_n are all linearly independent.[17]

The situation for immanants is better defined. The only permutations σ that contribute to the immanant are the ones with no fixed points, i.e., those that permute no vertex into itself. In terms of a graph, this restriction corresponds to choosing Sachs graphs only on all n vertices. It has long been known[25] that the number of conjugacy classes comprising such permutations on n elements is P(n) − P(n −1), the difference between successive values of the partition function P.[11] For convenience, let us define Y(n) = P(n) − P(n −1), since this expression is often needed in the discussion that follows. Therefore, of the P(n) immanants of any graph G, only Y(n) are linearly independent. That is, their values are given by a system of Y(n) linearly independent equations in Y(n) unknowns. (This seemingly elementary observation has apparently not been published before.)

As an empirical matter, in every case tested in the present study, a linearly independent set of immanants could be found by choosing only those associated with partitions λ that have the first two elements (at least) of identical length. In other words, the partitions when represented as $\{a^x, b^y, c^z...\}$ must have $x \geq 2$. (Note that the determinantal partition $\{1^n\}$ meets this criterion, but the permanental partition $\{n\}$ does not.) These partitions of any n are exactly Y(n) in number because each one is the conjugate of a member of the set of Y(n) conjugacy classes with no fixed points. Partitions are often visualized as left-justified rows of dots called Ferrers diagrams. Thus, $\{5, 4^2, 3, 1^3\}$ is a row of 5 dots, two rows of 4 dots below it, a row of 3 dots below that, and finally 3 single dots. The conjugate of a partition may be visualized by reading down the columns of its Ferrers diagram instead of across the rows. The conjugate of $\{5, 4^2, 3, 1^3\}$ is $\{7, 4^2, 3, 1\}$. The mathematical basis for this linear independence appears not to have been investigated.

4. APPLICATIONS OF IMMANANTS AND IMMANANTAL POLYNOMIALS TO CHEMICAL GRAPHS

Excluding the determinant and permanent and their associated polynomials, very little concerning immanants and immanantal polynomials of adjacency matrices of chemical graphs has appeared in the literature,[18] although a relationship between the $\lambda = \{2, 1^{n-2}\}$ immanant of the Laplacian matrix of trees and their Wiener numbers was published.[19] A chemical graph is ordinarily one that directly represents a hydrocarbon structure, that is, a connected, undirected graph without loops or multiple edges, and with all vertices having degree ≤4. The various schemes that have been investigated for incorporating heteroatoms will not be considered here. Suppose that a set of Y(n) linearly independent immanants has been calculated, and the corresponding Y(n) irreducible representations of S_n have been calculated also. Of the P(n) characters $\chi(\lambda,\xi)$ in each irreducible representation, only those Y(n) ξ with no fixed points contribute to the immanant. Let us call this subset ξ^*. Then, each immanant is

$$\mathbf{imm}_\lambda(\mathbf{A}) = \sum_{\sigma\in\xi^*}\chi_\lambda(\sigma)\prod_{j=1}^{n}(\boldsymbol{A}+\boldsymbol{I})_{j,\sigma}(j)$$

Thinking about the graph instead of its adjacency matrix, it is more straightforward to write

$$\mathbf{imm}_\lambda(\mathbf{A}) = \sum_{\xi\in\xi^*}\mathbf{m}(\xi)\chi(\lambda,\xi)\,2^{c(\xi)}$$

where the m(ξ) are the number of ways of selecting a spanning subgraph corresponding to a permutation in ξ, and $c(\xi)$ is the number of cycles (elements > 2) in ξ. This operation can be illustrated with the simple example of the trigonal prism graph on 6 vertices. For $n = 6$, ξ^* is $\{2^3\}$, $\{3^2\}$, {4,2}, {6}. On a trigonal prism graph, there are 4 ways of selecting 3 isolated edges, one way of selecting two 3-cycles, 3 ways of selecting a 4-cycle plus an edge, and 3 ways of selecting a 6-cycle. Therefore, m($\{2^3\}$) = 4, m($\{3^2\}$) = 1, m({4,2}) = 3, and m({6}) = 3. The permanent, which has $\chi(\{6\},\xi) = 1$ for all ξ, should then be $\mathrm{imm}_{\{6\}}(\mathbf{A}) = (4 \times 1 \times 2^0) + (1 \times 1 \times 2^2) + (3 \times 1 \times 2^1) + (3 \times 1 \times 2^1) = 4 + 4 + 6 + 6 = 20$; independent calculation confirms this result. Substituting the appropriate values from Table 1 for the Y(n) linearly independent λ, we have

$$\mathrm{imm}_{\{1,1,1,1,1,1\}}(\mathbf{A}) = (4 \times -1 \times 2^0) + (1 \times 1 \times 2^2) + (3 \times -1 \times 2^1) + (3 \times 1 \times 2^1) = -4 + 4 - 6 + 6 = 0$$

$$\mathrm{imm}_{\{2,2,1,1\}}(\mathbf{A}) = (4 \times -3 \times 2^0) + (1 \times 0 \times 2^2) + (3 \times 1 \times 2^1) + (3 \times 0 \times 2^1) = -12 + 0 + 6 + 0 = -6$$

$$\mathrm{imm}_{\{2,2,2\}}(\mathbf{A}) = (4 \times 3 \times 2^0) + (1 \times 2 \times 2^2) + (3 \times -1 \times 2^1) + (3 \times 0 \times 2^1) = 12 + 8 - 6 + 0 = 14,$$

and

$$\mathrm{imm}_{\{3,3\}}(\mathbf{A}) = (4 \times -3 \times 2^0) + (1 \times 2 \times 2^2) + (3 \times -1 \times 2^1) + (3 \times 0 \times 2^1) = -12 + 8 - 6 + 0 = -10$$

The interest in applying this exercise to chemical graphs is that if, as we supposed, we have numerical values for the Y(n) immanants and the relevant Y(n)^2 $\chi(\lambda,\xi)$, then the set of Y(n) equations involving m(ξ) comprises a set of Y(n) equations in Y(n) unknowns which can be solved for the various m(ξ). Several of these m(ξ) are of long-standing interest. For example, the Kekulé structure count, the number of ways of selecting n/2 independent edges, is m($\{2^{n/2}\}$). The number of Hamiltonian cycles in the graph, i.e., the number of distinct n-cycles, is m({n}). The Clar covering polynomial of hexagonal (benzenoid) systems, as defined and investigated by Zhang,[26−29] has as coefficients the values of m($\{6^k, 2^{(n-6k)/2}\}$), $0 \leq k \leq n/6$. Zhang has also established some

Table 2. Complete Set of Immanantal Polynomials for the Trigonal Prism Graph (Prismane)

λ	$I_\lambda(G,x)$
6	$x^6 + 9x^4 - 4x^3 + 24x^2 - 24x + 20$
5,1	$5x^6 + 27x^4 - 4x^3 + 24x^2 + 20$
4,2	$9x^6 + 27x^4 + 12x^2 + 12x + 18$
$4,1^2$	$10x^6 + 18x^4 - 4x^3 - 36x^2 + 12x + 2$
3^2	$5x^6 + 9x^4 + 4x^3 - 12x^2 - 12x - 10$
3,2,1	$16x^6 + 8x^3 - 12x - 8$
$3,1^3$	$10x^6 - 18x^4 - 4x^3 - 36x^2 - 12x + 6$
2^3	$5x^6 - 9x^4 + 4x^3 + 24x^2 + 12x + 14$
$2^2,1^2$	$9x^6 - 27x^4 + 24x^2 + 12x - 6$
$2,1^4$	$5x^6 - 27x^4 - 8x^3 + 12x^2$
1^6	$x^6 - 9x^4 - 4x^3 + 12x^2$

connections between the Clar covering polynomial and the chromatic and sextet polynomials.[30−32] More direct connections between these polynomials and the m(ξ) values may exist but have not yet been established.

Table 2 lists the complete set of immanantal polynomials for the trigonal prism graph (prismane, $n = 6$), and comparison of these with the characters in Table 1 reveals how structural information is captured in the polynomials. In this graph, only a triangle contributes to $\xi = \{3,1^3\}$, and only $\xi = \{3,1^3\}$ contributes to the x^3 terms. Since there are two triangles in prismane, the coefficient of x^3 is $(-1)(2^1)\chi(\lambda,\{3,1^3\})$. Both $\xi = \{5,1\}$ and $\xi = \{3,2,1\}$ contribute to the x^1 term. There are six ways of selecting a 5-cycle and six ways of selecting a triangle plus a disjoint edge from prismane, so the coefficient of x^1 is $6(-1)(2^1)\chi(\lambda,\{5,1\}) + 6(-1)(2^1)\chi(\lambda,\{3,2,1\})$. The factor of -1 occurs because $\prod_{j=1}^{n} (\mathbf{I} - \mathbf{A})_{\sigma,j(\sigma)}$ is -1 for odd permutations, $+1$ for even permutations. The factor of $2^{c(\xi)}$ occurs because the $\chi(\lambda,\xi)$ count *conjugacy classes*, while the $\mathscr{I}_\lambda(G,x)$ count *permutations*, and each cycle can be permuted in two ways. Thus, with the character table for S_n and a complete set of $\mathscr{I}_\lambda(G,x)$ for some graph G, it is possible to obtain the count of permutations contributing to *each* conjugacy class ξ. One might, for example, obtain the counts of k disjoint hexagons in G, m($\{6^k,1^{n-6k}\}$).

Another thoroughly studied polynomial in chemical graph theory is the acyclic, or matching, polynomial (see, for example, ref 1, Chapter 7). The acyclic polynomial is variously described as the characteristic polynomial with the cyclic contributions subtracted out or the characteristic polynomial of an acyclic (and not physically realizable) "reference" structure. Within the context of the description of immanantal polynomials given above, however, the meaning of the acyclic polynomial is both completely straightforward and completely generalizable to all the other partitions besides $\{1^n\}$. Specifically, the matching polynomial is the sum of those contributions to the characteristic polynomial made by $\xi = \{2^k, 1^{n-2k}\}$, $0 \le k \le n/2$. In the ordinary matching polynomial, the signs alternate because the $\chi(\{1^n\},\{2^k, 1^{n-2k}\})$ are -1 for k odd and $+1$ for k even (see Table 1 for an example). An acyclic immanantal polynomial associated with any other partition $\lambda \neq \{1^n\}$ can be defined in exactly the same way as that part of the immanantal polynomial contributed by $\xi = \{2^k, 1^{n-2k}\}$. Computationally, since only one conjugacy class contributes to each coefficient of the matching polynomial, the coefficients of any other acyclic immanantal polynomial are related to the coefficients of the ordinary matching polynomial by the ratios of the corresponding irreducible characters, $\chi(\lambda,\{2^k, 1^{n-2k}\})/\chi(\{1^n\},\{2^k, 1^{n-2k}\})$. Thus, advantage could be taken of efficient algorithms available for calculating the matching polynomial.[33−35]

Merris has argued (personal communication) that an acyclic immanantal polynomial should be expressible as a linear combination of the P(n) ordinary immanantal polynomials. This is indeed the case. It is possible to write and solve P(n) simultaneous equations in P(n) unknowns (the coefficients by which the P(n) immanantal polynomials must be multiplied) to give the acyclic immanantal polynomial for any specified λ, and this exercise was done for the trigonal prism graph as a demonstration of concept. The solutions depend only on λ and are valid for any graph on n vertices. As a practical matter, however, this approach is very computationally intensive compared to other available methods. With the irreducible character matrices in hand, an entirely different set of P(n) polynomials is available for study, perhaps as different in their properties from the ordinary immanantals as the characteristic and matching polynomials are known to be from each other.

5. CONCLUSIONS

This study provided a description of a very large set of graph invariants (immanants) and their associated polynomials that have appeared with some frequency in the mathematics literature but are almost unknown in chemical graph theory. In addition, an equally large set, the acyclic immanantal polynomials, was described that has apparently not been previously considered at all. These were shown to be related to the characteristic and permanental polynomials, the study of which has historically proven very fruitful in chemistry. In addition, algebraic relationships that do not apply to any individual polynomial were demonstrated between chemically interesting graph invariants and the immanants and associated polynomials taken as a set.

The amount of territory in chemical graph theory waiting to be explored here is so vast, it is difficult to formulate initial directions for further study. Nevertheless, a few areas suggest themselves. (1) It seems reasonable that some relationships exist between the structure of a partition λ and the kind of chemical information its immanant, immanantal polynomial, and acyclic immanantal polynomial encode, but nothing at all about these relationships has been published. (2) The behavior of these mathematical objects within a set of related structures, say the fullerenes, or the catacondensed benzenoids, or the [N]phenylene isomers, has not been investigated. (3) The opportunities to investigate quantitative structure−property relationships (QSPRs) are practically unlimited. (4) As with most graph-theoretical approaches to QSPR, methods for incorporating heteroatoms are notably lacking. (5) Available computational algorithms are probably far from optimal.

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