The hafnian of Toeplitz matrices of a special type, perfect matchings and Bessel polynomials

Dmitry Efimov^{*} Institute of Physics and Mathematics, Komi Science Centre UrD RAS, Syktyvkar, Russia

Abstract

We present a simple and convenient analytical formula for efficient exact computation of the hafnian of Toeplitz matrices of a special type. An interpretation of the obtained results is given in the language of perfect matchings and Bessel polynomials.

Introduction

Let $A = (a_{ij})$ be a symmetric matrix of order n = 2m over a commutative associative ring. Its hafnian is defined as

$$\mathrm{Hf}(A) = \sum_{(i_1 i_2 | \dots | i_{n-1} i_n)} a_{i_1 i_2} \dots a_{i_{n-1} i_n},$$

where the sum runs over all partitions of the set $\{1, 2, ..., n\}$ into disjoint pairs $(i_1i_2), ..., (i_{n-1}i_n)$ up to the order of pairs, and the order of elements in each pair. So, for example, if n = 4 then $Hf(A) = a_{12}a_{34} + a_{13}a_{24} + a_{14}a_{23}$. Equivalently, one can define the hafnian as

$$\operatorname{Hf}(A) = \frac{1}{m! 2^m} \sum_{\sigma \in S_n} a_{\sigma(1), \sigma(2)} \dots a_{\sigma(n-1), \sigma(n)},$$

where the sum runs over all permutations of the set $\{1, 2, ..., n\}$. Note that diagonal elements of the matrix are not present in the definition of the hafnian. We will take them equal to zero for convenience. The hafnian was introduced by E.R. Caianiello in one of his works on quantum field theory [1]. He gave the name to the new matrix function in honor of Copenhagen (Lat. Hafnia), the place where the idea of this mathematical concept first occurred to him. By this name he also emphasized connection with Pfaffian introduced by A. Cayley in 19th

^{*}e-mail: dmefim@mail.ru

century, from which the hafnian differs only by the signs of some components. Later it became clear that the hafnian also has a useful combinatorial property related to solving an important problem in graph theory: if M is the adjacency matrix of an unordered graph with even number of vertices, then Hf(M) equals the total number of perfect matchings of the graph.

Unfortunately the widespread use of the hafnian is limited by the fact that there are no effective algorithms for its calculation in the general case. Thus, in the recent work [2], the currently fastest exact algorithm to compute the hafnian of an arbitrary complex $n \times n$ matrix is described. It runs in $O(n^3 2^{n/2})$ time. And numerical benchmarks on the Titan supercomputer (the 7th place in the Top500 ranking as June 2018) indicated that it would require about a month and a half to compute the hafnian of a randomly generated 100×100 complex matrix using this algorithm.

Since in the general case calculation of the hafnian has a high computational complexity, the problem is actual of finding efficient analytical formulas expressing the hafnian for special classes of matrices. Thus, in many important cases (e.g., when considering adjacency matrices of planar graphs) one can reduce calculation of the hafnian of a given matrix to a much more efficient calculation of the Pfaffian for another matrix, associated with the former one by certain simple transformations [3]. Recall that a matrix is called Toeplitz if all elements of every of its diagonal parallel to the main one are the same. The paper [4] presents an algorithm for calculating the hafnian of banded Toeplitz matrices of order n and bandwidth m which runs in $O(2^{3m} \log n)$ time.

In this work we obtain an efficient analytical formula for calculating the hafnian of Toeplitz matrices of a special type, different from the one mention above. In a special case this formula reduces to computation of the value of the Bessel polynomial of the corresponding degree at a certain point. Using this formula, one can calculate the hafnian in linear time.

The main part

To begin with, consider two properties of the hafnian. The first property is quite obvious.

Proposition 1. Let A be a symmetric matrix of order 2m over a commutative associative ring R, and $c \in R$. Then

$$Hf(cA) = c^m Hf(A).$$
(1)

Let $Q_{k,n}$ denote the set of all (unordered) k-element subsets of the set $\{1, 2, \ldots, n\}$. Let A be a matrix of order n and $\alpha \in Q_{k,n}$. We denote by $A[\alpha]$ the submatrix of A formed by the rows and columns of A with numbers in α , and by $A(\alpha)$ the submatrix of A formed from A by removing the rows and columns with numbers in α . The following property proved in [5]:

Proposition 2. Let A, B be symmetric matrices of order 2m. Then

$$\operatorname{Hf}(A+B) = \sum_{k=0}^{m} \sum_{\alpha \in Q_{2k,2m}} \operatorname{Hf}(A[\alpha]) \operatorname{Hf}(B(\alpha)),$$
(2)

where $\operatorname{Hf}(A[\alpha]) = 1$ if $\alpha \in Q_{0,2m}$, and $\operatorname{Hf}(B(\alpha)) = 1$ if $\alpha \in Q_{2m,2m}$.

To prove our main result, we need also one combinatorial property of path graphs. Recall that a path graph is a graph that can be drawn so that all of its vertices and edges lie on a single straight line and all neighboring vertices are adjacent. We denote the path graph with n vertices by P_n (Fig. 1). Let k



Figure 1: The path graph P_n

be a non-negative integer less than n/2, and let E_n^k denote the number of ways to select k edges in P_n so that there are no two selected edges with a common vertex.

Proposition 3. The value of E_n^k equals the binomial coefficient C_{n-k}^k .

Proof. It is obvious that one can select k different edges in P_n in C_{n-1}^k ways. Now we replace the given path graph by a new one according to the following rule: we insert an additional edge after each of the first k-1 selected edges, counting left to right. As a result, we obtain a path graph with n + k - 1vertices and k selected edges, any two of which have no common vertices (Fig. 2). It is not hard to see that such a procedure and its inverse establishes a



Figure 2: Transition between the path graphs P_5 and P_7 with 3 selected (in red) edges

one-to-one correspondence between samples of k edges in a path graph with n vertices and samples of k edges, any two of which have no common vertices, in a path graph with n + k - 1 vertices. Therefore, $C_{n-1}^k = E_{n+k-1}^k$. \Box that $E_n^k = C_{n-k}^k$.

Now we can formulate and prove the main result.

Theorem 1. Let R be a commutative associative ring with unit element, and $a, b \in R$. Consider a symmetric matrix $T_{a,b}$ of order 2m whose elements on the main diagonal are zero, the elements on the subdiagonal and on the superdiagonal are equal to a, and all others elements are equal to b:

$$T_{a,b} = \begin{pmatrix} 0 & a & b \\ a & \ddots & \ddots & \\ & \ddots & \ddots & a \\ b & & a & 0 \end{pmatrix}.$$
 (3)

Assuming $0^0 = 1$, the following equality holds:

$$Hf(T_{a,b}) = \sum_{k=0}^{m} (a-b)^{m-k} b^k \frac{(m+k)!}{k!(m-k)!2^k} .$$
(4)

Proof. Let J_q denote a symmetric matrix of order 2m whose elements on the main diagonal are zero, and all others elements equal q. Directly from the definition of the hafnian it follows that

$$\operatorname{Hf}(J_q) = q^m \frac{(2m)!}{m! 2^m}.$$
(5)

Let U_q denote the matrix of order 2m whose elements on the subdiagonal and on the superdiagonal are equal to q, and all others elements are zeros. Since $T_{a,b} = J_b + U_{a-b}$, we can write the following chain of equalities using the formulas (1), (2), and (5):

$$Hf(T_{a,b}) = Hf(J_b + U_{a-b}) = \sum_{k=0}^{m} \sum_{\alpha \in Q_{2k,2m}} Hf(J_b[\alpha]) Hf(U_{a-b}(\alpha)) = \sum_{k=0}^{m} (a-b)^{m-k} b^k \frac{(2k)!}{k! 2^k} \sum_{\alpha \in Q_{2k,2m}} Hf(U_1(\alpha)).$$
(6)

Here we use the fact that $J_b[\alpha]$ has the same form as the initial matrix J_b , i.e., $J_b[\alpha]$ is a symmetric matrix of order 2k whose elements on the main diagonal are zeros, and all others elements are equal to b.

Let u_{ij} denote the elements of (0, 1)-matrix U_1 . If $\alpha \in Q_{2k,2m}$, then the matrix $U_1(\alpha)$ has the order 2m - 2k, and, by the definition,

$$\sum_{\alpha \in Q_{2k,2m}} \operatorname{Hf}(U_1(\alpha)) = \sum_{\alpha \in Q_{2k,2m}} \sum_P u_{i_1 i_2} \dots u_{i_{2m-2k-1} i_{2m-2k}},$$
(7)

where the inner sum runs over all partitions P of the set $\{1, 2, \ldots, 2m\}\setminus \alpha$ into disjoint pairs $(i_1i_2), \ldots, (i_{2m-2k-1}i_{2m-2k})$ up to an order of pairs and an order of elements in each pair. Since only the elements $u_{i,i+1}$ and $u_{i+1,i}$ of U_1 are equal to 1, the term $u_{i_1i_2} \ldots u_{i_{2m-2k-1}i_{2m-2k}}$ in the sum (7) equals 1 if and only if each

pair in the partition $(i_1i_2), \ldots, (i_{2m-2k-1}i_{2m-2k})$ consists of two neighboring indexes, otherwise this term equals zero. It follows that the sum (7) equals the number of different ways to select in the set $\{1, 2, \ldots, 2m\}$ a collection of m-kdisjoint pairs $(i_1, i_1 + 1), \ldots, (i_{m-k}, i_{m-k} + 1)$, up to an order of pairs. And this is nothing else than the number of ways to select m-k edges in the path graph P_{2m} so that any two edges do not have common vertices. By Proposition 3 this number equals $C_{2m-m+k}^{m-k} = C_{m+k}^{m-k}$. Thus substituting this value in (6), we get the desired expression:

$$\operatorname{Hf}(T_{a,b}) = \sum_{k=0}^{m} (a-b)^{m-k} b^k \frac{(2k)!}{k! 2^k} C_{m+k}^{m-k} = \sum_{k=0}^{m} (a-b)^{m-k} b^k \frac{(m+k)!}{k! (m-k)! 2^k}.$$

Now we make a few comments about the result. Let a, b be non-negative integers, and let $G_{a,b}$ denote the graph with the adjacency matrix $T_{a,b}$. If one draws $G_{a,b}$ in the form of an arc diagram, then the neighboring vertices will be connected by a arcs while all the other pairs of vertices by b arcs. In this case the formula (4) expresses the number of perfect matchings of the graph $G_{a,b}$.

Let a = 0, b = 1. The graph $G_{0,1}$ with *n* vertices is the complement of the path graph P_n (Fig. 3). And it is not hard to see that perfect matchings of the graph $G_{0,1}$ with 2m vertices are loopless linear chord diagrams with *m* chords considered in [6]. From (4) we get

$$Hf(T_{0,1}) = \sum_{k=0}^{m} (-1)^{m-k} \frac{(m+k)!}{k!(m-k)!2^k}.$$
(8)

Thus, the formula (8) expresses the number of loopless linear chord diagrams with m chords (the sequence A278990 in [7]).



Figure 3: The graph $G_{0,1}$ with six vertices and all its perfect matchings

Consider now the graph $G_{2,1}$. If one calculates by (4) the hafnian of its adjacency matrix for consecutive m, starting with m = 1, we get the sequence:

$$2, 7, 37, 266, 2431, 27007, \ldots$$

Its k-th member equals the number of perfect matchings of the graph $G_{2,1}$ with 2k vertices (Fig. 4). Note that this sequence has the notation A001515 in [7],



Figure 4: The graph $G_{2,1}$ with four vertices and all its perfect matchings

however its description does not contain the interpretation given here.

Recall (see [8], [9]) that the Bessel polynomial of degree m is a polynomial of the form:

$$y_m(x) = \sum_{k=0}^{m} \frac{(m+k)!}{k!(m-k)!} \left(\frac{x}{2}\right)^k$$

It follows from (4) that the hafnian of the matrix $T_{b+1,b}$ of order 2m equals the value of the Bessel polynomial of degree m at x = b:

$$\operatorname{Hf}(T_{b+1,b}) = y_m(b).$$

This is a rather curious and unexpected fact, the explanation of which is not clear so far.

Conclusion

We obtained a simple analytical formula for efficient exact calculation of the hafnian of Toeplitz matrices of the special type (3). Based on this formula, it is not hard to write an algorithm which calculates the hafnian of a matrix of order n in O(n) time. The resulting formula can be used to find the number of perfect matchings of special graphs, for example, complements of the path graphs. Along the way, we established an intresting connection between the hafnian of Toeplitz matrices and the Bessel polynomials. This connection requires more detailed study. Also, one could try, using the above methods, to find effective analitical formulas for calculating hafnians of other types of Toeplitz matrices.

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