A combinatorial approach to hypermatrix algebra

Edinah K. Gnang*

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Abstract

We present a formulation of the Cayley-Hamilton theorem for hypermatrices in conjunction with the corresponding combinatorial interpretation. Finally we discuss how the formulation of the Cayley-Hamilton theorem for hypermatrices leads to new graph invariants which in some cases results in symmetry breakings among cospectral graphs.

1 Introduction

The importance of a graph theoretical perspective of linear algebra is well established [BC, Z]. We show in this brief note that the insights provided by the combinatorial lens naturally extend to the algebra of hypermatrices. We denote by a hypermatrix, a finite set of complex numbers each of which is indexed by a unique member of an integer Cartesian product set of the form \( \{0, \ldots, (n_0 - 1)\} \times \cdots \times \{0, \ldots, (n_l - 1)\} \). Such a hypermatrix is said to be of order \( l \) and more conveniently called an \( l \)-hypermatrix. The algebra of hypermatrices arises as an attempt to generalize familiar concepts from linear algebra. A survey of important results concerning hypermatrices can be found in [L, LQ]. The algebra discussed here differs somewhat from the conventional hypermatrix algebras surveyed in [L]. The hypermatrix algebra discussed here will center around the Bhattacharya-Mesner hypermatrix product introduced in [BM1, BM2, B] and followed up in [GER]. Although the scope of the Bhattacharya-Mesner algebra extends to hypermatrices of all integral order, we restrict the discussion for notational convenience to 3-hypermatrices. We remark that all the results presented here generalize straightforwardly to other orders. Our main result is the formulation of a Cayley-Hamilton theorem for hypermatrices coupled with the corresponding combinatorial interpretation. Finally we discuss how the formulation of the Cayley-Hamilton theorem for hypermatrices leads to new graph invariants which in some cases results in symmetry breakings among cospectral graphs.

2 Generalization of the Cayley–Hamilton theorem.

2.1 The bare bones of a hypermatrix Cayley–Hamilton theorem.

The Cayley-Hamilton theorem for matrices is a statement about the maximum dimension of the span of the vector space of consecutive powers of a generic \( n \times n \) matrix. While it is clear that the dimension of the vector space spanned by Hadamard powers of a generic \( n \times n \) matrix is maximal over the vector space of all \( n \times n \) matrices, it is a rather surprising fact that the maximum dimension of the vector space spanned by consecutive matrix powers for a generic matrix is \( n \). Consequently we shall think of formulating the Cayley-Hamilton theorem for hypermatrices as

*School of Mathematics, Institute for Advanced Study. Email: gnang@ias.edu.
statement concerning the maximum dimension of the span of “powers” of a hypermatrix. In order to spell out what is meant here by powers we briefly review the Bhattacharya-Mesner hypermatrix product operation introduced in [BM1, BM2, B]. Given complex entred 3-hypermatrices $A$, $B$, and $C$ respectively of dimensions $m \times k \times p$, $m \times n \times k$, and $k \times n \times p$ their product yields a hypermatrix $D$ of size $m \times n \times p$ with entries specified by

$$d_{i_0i_1i_2} = \sum_{0 \leq j < k} a_{i_0ji_2} b_{i_0i_1j} c_{ji_1i_2}$$  \hspace{1cm} (1)$$ and noted \hfill (2) 

We now spell out what we mean by “powers”. In the context of 3-hypermatrices, powers refers to composition of Bhattacharya-Mesner hypermatrix product computation as depicted in the composition tree displayed in Fig1.

It follows from the ternary nature of the product that the composition always involves an odd number of operands. Incidentally the number of products which involve the same number of hypermatrices is determined by the sequence $C_n$ which in turn is determined by the recurrence relation

$$C_{2x1+1} = 1, \quad C_{2x_n+1} = \sum_{0<i,j,i+j<2x_n+1} C_i \times C_j \times C_{(2x_n+1)-(i+j)}.$$  \hspace{1cm} (3)$$

The recurrence $C_n$ defined above corresponds to a special case of the Fuss-Catalan numbers [E] and hence

$$C_{2n+1} = \frac{(3n)_n}{2n+1}$$  \hspace{1cm} (4)$$

Assuming (as suggested by $2 \times 2 \times 2$, $3 \times 3 \times 3$ and $4 \times 4 \times 4$ hypermatrices) that $n \times n \times n$ 3-hypermatrix composition products span a vector space of maximum dimension specified by some fixed polynomial in the $n$ say $f(n) \leq n^3$, it will suffice by the polynomial argument to exhibit explicitly such matrices for the values of $n \in \{1, 2, 3, 4\}$ to establish that the maximum dimension of the span of powers of a generic 3-hypermatrix is $n^3$. Therefore maximum number of operands to be considered when computing composition of products for a given $n \times n \times n$ 3-hypermatrix correspond to $l(n)$ defined by

$$l(n) = \min \{m\}, \text{ such that } n^3 \leq \sum_{0<2k+1 \leq m} C_{(2k+1)}$$  \hspace{1cm} (5)$$

hence

$$l(n) = \min \{m\}, \text{ such that } n^3 \leq \sum_{0<2k+1 \leq m} (2k+1)^{-1} \binom{3k}{k}$$  \hspace{1cm} (6)$$
incidentally for $n = 2$, it follows that
\[ l(2) = 4 \] (7)
and hence the number of distinct powers to be considered is given by
\[ 17 = \sum_{0 < 2k + 1 \leq 4} (2k + 1)^{-1} \binom{3k}{k} \] (8)

In particular we can verify that each one of the $\binom{17}{2}$ possible matrices which arise from possible choices of $2^3$ distinct composition of product of $2 \times 2 \times 2$ hypermatrices (stacked up individually as column vectors the square matrix), yield a matrix of full rank. We further conjecture that for every $n$ there exist some hypermatrix for which each one of the $\left( C_{2k+1}^{(n)} \right)_{n^3}$ possible matrices resulting from choices of $n^3$ composition products (individually stacked up as column vectors of a square matrix) yield a matrix of full rank. By the the combinatorial Nullstellensatz argument \[ \mathbf{A} \] it follows that in order to establish this fact, it is sufficient to show that the polynomial for some family of hypermatrices
\[ \det \left( \prod_{0 \leq k < C_{2k+1}^{(n)} \mathbb{C}_{2k+1}^{(n)}} M_k \right) \]
is not identically zero (the matrices $\{M_k\}_{k}$ correspond to distinct $n^3 \times n^3$ matrices which arise from distinct choices of collection $n^3$ of hypermatrix composition of products each of which are canonically vectorized and stacked up as column vectors of a square matrix).

Having thus asserted the maximality of the span, we use Cramer’s rule to express the linear dependence between any $n^3 + 1$ collection of the powers of a given hypermatrix of size $n \times n \times n$. Let $\mathbf{A}$ denote an $n \times n \times n$, we therefore formulate the Cayley–Hamilton theorem by asserting that
\[ \exists \left\{ p_k \left( a_{000}, \ldots, a_{(n-1)(n-1)(n-1)} \right) \right\}_{0 \leq k < n^3} \subset \mathbb{Q} \left( a_{000}, \ldots, a_{(n-1)(n-1)(n-1)} \right) \] (9)
such that
\[
\mathbf{0}_{n \times n \times n} = \mathbf{A} \ p_0 \left( a_{000}, \ldots, a_{(n-1)(n-1)(n-1)} \right) + \\
\circ (\mathbf{A}, \mathbf{A}, \mathbf{A}) \ p_2 \left( a_{000}, \ldots, a_{(n-1)(n-1)(n-1)} \right) + \\
\circ (\circ (\mathbf{A}, \mathbf{A}, \mathbf{A}), \mathbf{A}, \mathbf{A}) \ p_3 \left( a_{000}, \ldots, a_{(n-1)(n-1)(n-1)} \right) + \\
\circ (\mathbf{A}, \circ (\mathbf{A}, \mathbf{A}, \mathbf{A}), \mathbf{A}) \ p_4 \left( a_{000}, \ldots, a_{(n-1)(n-1)(n-1)} \right) + \\
\circ (\mathbf{A}, \mathbf{A}, \circ (\mathbf{A}, \mathbf{A}, \mathbf{A})) \ p_5 \left( a_{000}, \ldots, a_{(n-1)(n-1)(n-1)} \right) + \\
\ldots + \circ (\circ \ldots (\mathbf{A}, \ldots \mathbf{A}) \] (10)
and as mentioned before Cramer’s rule yields the formal expression for the rational functions
\[ \left\{ p_k \left( a_{000}, \ldots, a_{(n-1)(n-1)(n-1)} \right) \right\}_{0 \leq k < n^3} \]
thereby determining a formulation of the Cayley–Hamilton theorem for hypermatrices. We note that unlike the matrix case, the maximum dimension of the span associated with the vector space of powers of a generic hypermatrix matches the dimension of the span of the vector space of all hypermatrices.
2.2 A combinatorial interpretation of the hypermatrix Cayley-Hamilton theorem.

Let $A$ denote an $m \times n \times p$ 3-hypermatrix. Corresponding to $A$ we define a directed tripartite 3-uniform hypergraph $H(A)$ having $m + n + p$ vertices each of which is colored either red, green or blue. The vertices of $H(A)$ are colored such that $m$ of the vertices are colored red and also considered to be in one-to-one correspondence with the row slices of the adjacency hypermatrix $A$, which for convenience are labeled by integers from the set $\{0, 1, \cdots, m-1\}$. Furthermore the subsequent $n$ vertices of $H(A)$ are colored green and considered to be in one-to-one correspondence with the column slices of the hypermatrix $A$ which are also conveniently labeled with integers from the set $\{0, 1, \cdots, n-1\}$. Finally the remaining $p$ vertices of $H(A)$ are colored blue and considered to be in one-to-one correspondence with the depth slices of the hypermatrix $A$ conveniently labeled with integers from the set $\{0, 1, \cdots, p-1\}$. The tripartite hypergraph vertex coloring scheme is designed so as to establish a one to correspondence between entries of the adjacency hypermatrices and red, green, blue triplets of vertices of the tripartite 3-uniform hypergraph $H(A)$. More precisely the unique directed hyperedge whose initial red vertex is labeled $i$ (noted $R_i$), also having its middle green vertex label $j$ (noted $G_j$) and its terminal red vertex labeled $k$ (noted $R_k$), will be associated with the hypermatrix entry $a_{ijk}$. We will often refer to $a_{ijk}$ as the weight associated with the hyperedge $(R_i, G_j, B_k)$ of the 3-uniform hypergraph $H(A)$. The proposed directed tripartite hypergraph $H(A)$ described here is a natural extension of the the Konig directed bipartite graph associated with a matrix, further described in [BC]. We shall incidentally call the resulting hypergraph the Konig directed tripartite hypergraph associated with the 3-hypermatrix $A$.

2.3 Hypergraph composition

By analogy to the matrix case, the Konig directed tripartite hypergraph yields a combinatorial interpretation of the Bhattacharya-Mesner product operation. The hypergraph composition is defined by the following vertex and induced edge identification scheme. Consider tripartite hypergraphs such that $H(A)$ is of type $m$ by $t$ by $p$, $H(B)$ is of type $m$ by $n$ by $t$ and finally $H(C)$ of type denote a $t$ by $n$ by $p$. It is crucial for the construction that the number of red vertices of $H(A)$ matches the number of red vertices of $H(B)$, furthermore the number of green vertices of $H(B)$ must match the number of green vertices of $H(C)$ and the number of blue vertices of $H(A)$ must equal the number of blue vertices of $H(C)$. The preceding constraints will be understood as the pairwise constraints between the hypergraph pairs $(H(A), H(B))$, $(H(B), H(C))$ and $(H(A), H(C))$. We also point out the crucial triplet constraints which asserts that the number of green vertices of $H(A)$ must equal the number of blue vertices of $H(B)$ which in turn equals the number of red vertices of $H(C)$. If the three pairwise constraints in addition to the triplet constraints are satisfied one can perform the composition of the hypergraphs $H(A)$, $H(B)$, and $H(C)$ noted $\ast (H(A), H(B), H(C))$. The result of the composition as to be expected is again a directed tripartite hypergraph of type $m$ by $n$ by $p$, obtained by the following identification. In accordance with the pairwise constraint $(H(A), H(B))$ the red vertices of $H(A)$ are identified via their label correspondence with the red vertices of $H(B)$. Also in accordance with the pairwise constraints $(H(B), H(C))$ the green vertices of the hypergraphs $H(B)$ are identified via their label correspondence with the vertices of the graph $H(C)$. Finally in accordance with the pairwise constraint $(H(A), H(C))$ the blue vertices of the hypergraphs $H(A)$ are identified via label correspondence with the blue vertices of the graph $H(C)$. We conclude the identification scheme by considering all possible ways of identifying simultaneously together via label correspondence the remaining green vertex of $H(A)$ with the label corresponding blue vertex of $H(B)$ and finally with the label corresponding red vertex of $H(C)$. (The last identification step is only possible due to the triplet constraints relating the vertices hypergraphs $H(A)$, $H(B)$ and $H(C)$). We note that the last identification results into neither a red, nor a green nor a blue vertex lets say that the last vertex identification resulted in a white vertex. Therefore the weight associated with every ordered triplet $(R_r, G_g, B_b)$ of the resulting tripartite directed 3-uniform hypergraph is determined by the
summing out the unwanted white vertices as follows

\[
[\ast (H(A), H(B), H(C))]_{r,g,b} = \sum_{0 \leq w < t} a_{r,w,b} b_{r,g,w} c_{w,g,b},
\]

the weighting of the resulting vertices correspond precisely to the Bhattacharya-Mesner product. It therefore follows from the proposed construction that

\[
H(\circ (A, B, C)) = \ast (H(A), H(B), H(C)).
\]

It may be noted that each term of the form \(a_{r,w,b} b_{r,g,w} c_{w,g,b}\) in the sum can be thought off as describing a tetrahedron construction which connects the faces \((r, w, b)\), \((r, g, w)\) and \((w, g, b)\). It is therefore legitimate to deduce from the proposed identification scheme that the edges (or sides) of the triangular faces are also being appropriately identified. In particular, given an \(n \times n \times n\) hypermatrix \(A\) with binary entries the sum

\[
\sum_{0 \leq r < g < b < n} [\circ (A, A, A)]_{r,g,b}
\]

counts the number tetrahedron construction possible using the hyperedge from \(H(A)\). In particular for some particular choice of ordered triplet \((r, g, b)\) such that \(0 \leq r < g < b < n\) the entry \([\circ (A, A, A)]_{r,g,b}\) counts the number of tetrahedron in \(H(A)\) which admit the ordered hyperedge \((r, g, b)\) as one of the faces the tetrahedron. Furthermore the sum

\[
[\circ (\circ (A, A, A), A, A)]_{r,g,b} = \sum_{w_1} \left( \sum_{w_0} a_{r,w_0,b} a_{r,w_1,w_0} a_{w_0,w_1,b} \right) a_{r,g,w_1} a_{w_1,g,b}
\]

counts the number of tetrahedral simplices which can be constructed by gluing two tetrahedrons at a face of the form \((r, w_1, b)\) as depicted in the figure below where the face \((r, w_1, b)\) is colored blue.

Furthermore

\[
[\circ (A, \circ (A, A, A))_{r,g,b}] = \sum_{w_1} a_{r,w_1,b} \left( \sum_{w_0} a_{r,w_0, w_1} a_{r,g,w_0} a_{w_0,g, w_1} \right) a_{w_1,g,b}
\]
counts the number of tetrahedral simplices which can be constructed by gluing two tetrahedrons which are glue at a face of the form \((r, g, w_1)\) as depicted in the figure below where the face \((r, g, w_1)\) is colored red.

and finally the sum

\[
\left[ \circ (A, A, \circ (A, A)) \right]_{r,g,b} = \sum_{w_1} a_{r,w_1,b} a_{r,g,w_1} \left( \sum_{w_0} a_{w_1,w_0,b} a_{w_1,g,w_0} a_{w_0,g,b} \right)
\]

counts the number of tetrahedral simplices which can be constructed by gluing two tetrahedrons which are glue at a face of the form \((w_1, g, b)\) as depicted in the figure below where the face \((w_1, g, b)\) is colored green.

2.4 Graph invariants via inflation to hypergraphs.

We shall aim to show here that the natural inflation scheme from graph to hypergraphs introduced in [AFW] combined with the combinatorial invariants deduced from the generalization of the Cayley-Hamilton theorem leads
to symmetry breaking for some infinite families of cospectral graphs. It is well known that the cospectrality for a pair of graphs \( G_1 \) and \( G_2 \) is equivalent to the assertion that there exist coefficients \( \{ \alpha_k \}_{0 < k \leq n} \) such that

\[
0 = \sum_{0 < k \leq n+1} (\# \text{ Walks of length } k \text{ connecting vertex } i \text{ to } j \text{ in } G_1) \alpha_k = \sum_{0 < k \leq n+1} (\# \text{ Walks of length } k \text{ connecting vertex } i \text{ to } j \text{ in } G_2) \alpha_k
\]

where \( \alpha_{n+1} = 1 \), which algebraically expressed by the following equality in terms of the adjacency matrices

\[
\left( \sum_{0 < k \leq n+1} \alpha_k B^k \right) = 0 = \left( \sum_{0 < k \leq n+1} \alpha_k A^k \right)
\]  (15)

Incidentally the property can be equivalently stated for an arbitrary sequence of consecutive integer powers of \( A \), namely for some arbitrary integer \( \tau \geq 0 \)

\[
\left( \sum_{0 < k \leq n+1} \alpha_k B^{\tau+k} \right) = 0 = \left( \sum_{0 < k \leq n+1} \alpha_k A^{\tau+k} \right)
\]  (16)

This fact follows from the fact the vector space of powers of a matrix has a span of dimension at most \( n \) therefore we can more generally state the cospectral invariance property by stating that

\[
0 = \sum_{0 < k \leq n+1} (\# \text{ Walks of length } \tau + k \text{ connecting vertex } i \text{ to } j \text{ in } G_1) \alpha_k = \sum_{0 < k \leq n+1} (\# \text{ Walks of length } \tau + k \text{ connecting vertex } i \text{ to } j \text{ in } G_2) \alpha_k
\]  (17)

Similarly for hypermatrices we may consider the equivalence classes between 3-uniform hypergraphs induced by the

\[
0 = \sum_{0 < k \leq n^3+1} (\# k - \text{Tetrahedral Simplex spanning the directed triplet } (u, v, w) \text{ in } H_1) \alpha_k = \sum_{0 < k \leq n^3+1} (\# k - \text{Tetrahedral Simplex spanning the directed triplet } (u, v, w) \text{ in } H_2) \alpha_k
\]  (18)

(where a \( k \)-Tetrahedral Simplex denotes a simplex using \( k \) vertices in addition to the boundary triangle vertices). The coefficient set \( \{ \alpha_k \}_{0 < k \leq n^3+1} \) where \( \alpha_{n^3+1} = 1 \), constitutes an invariant for hypergraph under the action of the symmetric group on the vertices of the hypergraph. To show that such invariant are stronger then the spectral invariant it suffice to consider the pair of adjacency matrices with the smallest number of vertices which have the properties that their adjacency matrices are cospectral. A tripartite 3-uniform hypergraph is deduced from a graph as follows. We associate with to every directed path in the original graph of length two of the form \( v_r \rightarrow v_g \rightarrow v_b \), an ordered hyperedge \((R_r, G_g, B_b)\) of a hypergraph, thereby setting the \( a_{rgb} \) entry of the adjacency hypermatrix to 1. We refer to such a construction as an inflation. An easy rank argument on the compositions of products reveals that the inflation scheme in conjunction with the tetrahedral simplex counts indeed breaks the symmetry between the original two input graphs and incidentally establishes the existence of an infinite family of graphs for which the inflation scheme breaks the cospectrality symmetry.
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References

[A] N. Alon, Combinatorial Nullstellensatz, Comb. Prob. Comput. 8 , 7-29, (1999).

[AFW] N. Alon, U. Feige, A. Wigderson, D. Zuckerman, “Derandomized Graph Products”, Computational Complexity, pp. 60-75, 1995.

[B] P. Bhattacharya, “A new 3-D transform using a ternary product,” IEEE Trans. on Signal Processing 43(12):3081-3084, 1995.

[BC] R. A. Brualdi, D. Cvetkovic, “A Combinatorial Approach to Matrix Theory and Its Applications”, Discrete Mathematics and Its Applications, Chapman and Hall/CRC.

[BM1] D. M. Mesner and P. Bhattacharya, “Association schemes on triples and a ternary algebra,” J. Comb. Theory, ser. A, vol. 55, pp. 204-234, 1990.

[BM2] D. M. Mesner and P. Bhattacharya, “A ternary algebra arising from an association scheme on triples,” J. Algebra. vol. 164, no. 1 pp. 595-613, 1994.

[F] N. I. Fuss, “Solutio quaestionis, quot modis polygonum n laterum in polygona m laterum, per diagonales resolvi quaeat,” Nova Acta Academiae Scientiarum Imperialis Petropolitanae, vol. 9, pp. 243–251, 1791.

[GER] E. K. Gnang, A. Elgammal and V. Retakh, “A Spectral NA NA

[L] L.-H. Lim, "Tensors and hypermatrices," in: L. Hogben (Ed.), Handbook of Linear Algebra, 2nd Ed., CRC Press, Boca Raton, FL, 2013.

[LQ] L. Qi, “The Spectral Theory of Tensors”, preprint arXiv:1201.3424 [math.SP], 2012.

[S6] W. A. Stein et al., Sage Mathematics Software (Version 6.0), The Sage Development Team, ( 2013 ) , http://www.sagemath.org.

[Z] D. Zeilberger, “A combinatorial approach to matrix algebra”, Discrete Math. 56, 61-72 (1985).