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THE BMV CONJECTURE

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1. The BMV trace conjecture

In 1975, while studying partition functions of quantum mechanical systems, Bessis, Moussa, and Villania formulated a conjecture regarding a positivity property of traces of matrices [5]. If this property holds, explicit error bounds in a sequence of Padé approximants follow. Let A and B be $n \times n$ Hermitian matrices with B positive semidefinite, and let

$$\phi^{A,B}(t) = \mathrm{Tr}[\exp{(A - tB)}].$$

The original formulation of the conjecture asserts that $\phi^{A,B}$ is completely monotone; in other words, it is the Laplace transform of a positive measure:

$$\mathrm{Tr}[\exp{(A - tB)}] = \int_0^\infty \exp(-tx) d\mu^{A,B}(x).$$

Equivalently, the derivatives of the function $f(t) = \phi^{A,B}(t)$ alternate signs:

$$(-1)^m f^{(m)}(t) \geq 0, \quad t > 0,\ m = 0, 1, 2, \ldots.$$

Since the conjecture was introduced in [5], many partial results and extensive computational experimentation have been given all in favor of the conjecture's validity. For instance, there have been variational approaches [7, 8, 13, 14], hypergeometric approaches [9], free probability approaches [10], techniques using matrix analysis [12, 17, 24], and most recently noncommutative sum of squares approaches [6, 11, 20, 21] that have been combined with the technology of semidefinite programming [19]. However, despite much work, very little is known about the problem, and it has remained unresolved except in very special cases. Recently, Lieb and Seiringer in [23], and as previously communicated to us [17], have reformulated the conjecture of [5] as a question about the traces of certain sums of words in two positive definite matrices. (See also [18] for a generalization from traces to sums of principal minors).

Conjecture 1.1 (BMV). *The polynomial $p(t) = \mathrm{Tr}\left[(A + tB)^m\right]$ has all nonnegative coefficients whenever A and B are $n \times n$ positive semidefinite matrices.*

The coefficient of t^k in $p(t)$ is the trace of the sum, $S_{m,k}(A, B)$, of all words of length m in A and B, in which k B's appear. In [17], among other things, it was noted that, for $m < 6$, each constituent word in $S_{m,k}(A, B)$ has nonnegative trace. Thus, the above conjecture is valid for $m < 6$ and arbitrary positive integers n. It was also noted in [17] (see also [5]) that the conjecture is valid for arbitrary m and $n < 3$. Thus, the first case in which prior methods did not apply and the conjecture was in doubt, is $m = 6$ and $n = 3$. Even in this case, all coefficients, except $\mathrm{Tr}[S_{6,3}(A, B)]$, were known to be nonnegative (also as shown in [17]). It was only recently [14], using heavy computation, that Johnson and I showed this remaining coefficient to be nonnegative.

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Much of the subtlety of Conjecture 1.1 lies in the fact that the Hermitian matrix $S_{m,k}(A,B)$ need not have all nonnegative eigenvalues, and in addition that some terms within the sum defining $S_{m,k}(A,B)$ can have negative trace. This later fact was only proved recently in work with Johnson [17] (with the help of Shaun Fallat), in which we disproved the conjecture [17] that all positive definite words in two letters have positive trace (see the next section for an example).

In [13], I made progress on the conjecture with the following theorem.

Theorem 1.2. *Suppose that there exist integers m', k' and $n \times n$ positive definite matrices A and B such that $\mathrm{Tr}[S_{m',k'}(A,B)] < 0$. Then, for any $m \geq m'$ and $k \geq k'$ such that $m - k \geq m' - k'$, there exist $n \times n$ positive definite A and B making $\mathrm{Tr}[S_{m,k}(A,B)]$ negative.*

Corollary 1.3. *If the Bessis-Moussa-Villani conjecture is true for some exponent m_0, then it is also true for all $m < m_0$.*

Corollary 1.3 motivates a general program to solve the BMV conjecture, and there is evidence that this approach is more than a theoretical possibility. For instance, Hägele [11] has used this approach and Corollary 1.3 to prove the conjecture for all $m \leq 7$ (and all n). Inspired by Hägele's ideas, Klep and Schweighofer [19] used semidefinite programming and noncommutative sums of squares techniques to prove the conjecture for all $m \leq 13$. One of their motivations was the Connes' embedding conjecture on von Neumann algebras [20]. It should be noted that these techniques provably fail [11] for the difficult $m = 6$ case, making the appeal to Corollary 1.3 fundamental. Other work along these lines appears in the papers of Burgdorf [6] and Landweber-Speer [21].

Another approach is to use the following theorem found in [13]. It characterizes the BMV conjecture in terms of the eigenvalues of the matrix $S_{m,k}(A,B)$ and resembles the Perron-Frobenius theorem for nonnegative matrices.

Theorem 1.4. *Fix positive integers $m \geq k$ and n. Then, $\mathrm{Tr}[S_{m,k}(A,B)] \geq 0$ for all positive semidefinite A,B if and only if for all positive semidefinite A,B, the matrix $S_{m,k}(A,B)$ either has a positive eigenvalue or is the zero matrix.*

It follows that to prove the BMV conjecture, it is enough to show the positivity of only one of the eigenvalues of $S_{m,k}(A,B)$, rather than the sum of all of them.

2. An Abel Theorem for Word Equations

The Lieb and Seiringer formulation of the BMV trace conjecture says that the trace of $S_{m,k}(A,B)$, the sum of all words of length m in A and B with k Bs, is nonnegative for all positive semidefinite matrices A and B. In the case of 2×2 matrices, every word in two positive semidefinite letters has nonnegative trace (in fact, it has all nonnegative eigenvalues), thereby verifying the BMV conjecture for this case. It was unknown whether this fact held in general until Johnson and I [17] (with the assistance of Shaun Fallat) found that the word $W = BABAAB$ has negative trace with the matrices:

$$A_1 = \begin{bmatrix} 1 & 20 & 210 \\ 20 & 402 & 4240 \\ 210 & 4240 & 44903 \end{bmatrix} \quad \text{and} \quad B_1 = \begin{bmatrix} 36501 & -3820 & 190 \\ -3820 & 401 & -20 \\ 190 & -20 & 1 \end{bmatrix}.$$

Finding such examples is surprisingly difficult as the methods in [17] show, and randomly generating millions of matrices will fail to produce them [17]. Nonetheless, we believe that most words can have negative trace, and we made the following conjecture in [17].

Conjecture 2.1. *A word in two letters A and B has positive trace for every pair of real positive definite A and B if and only if the word is a palindrome or a product (juxtaposition) of 2 palindromes.*

Evidence for the conjecture can be found in [16], where we essentially proved it in the complex Hermitian case. Positive definite matrices which give a word a negative trace are potential counterexamples to the BMV conjecture, and it is useful to be able to generate many of these matrices. As remarked above, this is a difficult task since random sampling methods do not work.

We were led to constructing these matrices by solving positive definite word equations. Let W be a palindrome in the letters A and B. If the equation $W(A_1, X) = B_1$ may be solved for a positive definite X given A_1 and B_1, then the word $WAWAAW$ can have negative trace. This would allow us to construct many potential counterexamples to the BMV conjecture. In this regard, we were able to show the surprising result that every palindromic word equation $W(A, X) = B$ has a positive definite solution X for any pair of positive definite A and B [15]. The proof of this result uses fixed point methods, although for special cases, one may express X explicitly in terms of A, B, and their fractional powers. For instance, the Riccati equation $XAX = B$ has solution

$$X = A^{-1/2}\left(A^{1/2}BA^{1/2}\right)^{1/2}A^{-1/2}. \tag{2.1}$$

Even though solutions always exist (in fact, there are generically an odd number of them [3]), it is usually very difficult to solve word equations [3]. Solutions of the form (2.1), however, can be computed efficiently, and it is natural to try and determine those equations which can be solved similarly. The correct setting for this question is the category of *uniquely divisible groups* [4] (also called *universal*). These are groups G for which every $g \in G$ has a unique nth root for each positive integer n. Such groups have appeared recently in Aguiar's work on combinatorial Hopf algebras [1, 2]. Equation (2.1) is the unique solution to $XAX = B$ in any uniquely divisible group.

I have investigated this problem and formulated a conjecture that gives a complete description of those word equations that have solutions in terms of radicals.

Definition 2.2. *A word is called totally decomposable if it can be expressed as a composition of maps of the following forms applied to the letter X.*

- $\pi_{m,k}(W) = (WA^k)^m W$, *$m$ a positive integer, k a nonnegative integer*
- $r(W) = WA$
- $l(W) = AW$

It is not hard to prove that a decomposable word equation has solutions in terms of radicals. The following converse can be viewed as an Abel theorem for word equations.

Conjecture 2.3. *A word equation $W(X, A) = B$ is solvable in terms of radicals only if W is a totally decomposable word.*

I have developed a program to prove this conjecture. The idea involves gluing together an infinite sequence of specially constructed finite groups. It uses a pleasing blend of number theory (Dirichlet's theorem on arithmetic progressions and the Weil conjectures for curves) and combinatorics (a new word polynomial which characterizes total decomposability in terms of its factorability). With Levine, we can show that this program settles Conjecture 2.3 for words of length less than 20. I will continue to collaborate with Levine on this problem and carry out the remaining details of the program.

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