$p(t) = \mathrm{Tr}[(A+tB)^m] \in \mathbf{R}_+[t]$

Progress on the BMV trace conjecture

Christopher Hillar
(Texas A&M University)

Introduction

In 1975, Bessis, Moussa, and Villani (BMV) introduced a positivity conjecture while studying partition functions of quantum mechanical systems. Let A and B be Hermitian n-by-n matrices with B positive semidefinite (PSD, for short) and consider the real valued function:

$$f(t) = \mathrm{Tr}[\exp(A - tB)]$$

Conjecture [BMV1]: The function f is completely monotone:

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

Despite being open for quite some time, general progress on the problem has been slow. We will focus on a local version, recently formulated by Lieb and Seiringer. Here, ***A* is also assumed PSD**.

Conjecture [BMV2]: The real polynomial $p(t) = \mathrm{Tr}[(A+tB)^m]$ has all nonnegative coefficients for any positive integer m.

Example: If $m = 2$, then conjecture BMV2 asserts that

$$\mathrm{Tr}[(A+tB)^2] = \mathrm{Tr}[B^2]\,t^2 + \mathrm{Tr}[AB+BA]\,t + \mathrm{Tr}[A^2]$$

has nonnegative coefficients. Since A and B are positive semidefinite, only the second one, $2\mathrm{Tr}[AB]$, poses any difficulty:

Lemma: If A, B are PSD, then AB has nonnegative eigenvalues.

In fact, this simple calculation proves BMV2 in the case $m = 2$, and similar tricks verify it up to $m = 5$. However, no simple approach can work for larger m as we will argue after introducing some notation.

Focusing on individual coefficients, we define matrices

$$S_{m,k}(A,B) = [t^k]\ (A+tB)^m,$$

the sum of all length m words in A and B with k Bs. For instance,

$$S_{2,1}(A,B) = AB + BA$$

$$S_{3,2}(A,B) = ABB + BAB + BBA$$

By a symmetry argument, it is easy to see that each $S_{m,k}(A,B)$ is Hermitian. Thus, each coefficient of $p(t)$ is real. But the matrix need not be PSD (even if $m = 2$, $k = 1$). We refine BMV2 by fixing m and k :

Conjecture [BMV3]: For all positive semidefinite A and B, the matrix $S_{m,k}(A,B)$ has nonnegative trace.

We focus on the case $m = 6$, $k = 3$ to illustrate the general difficulty of conjecture BMV3. A simple computation demonstrates

$$\mathrm{Tr}[S_{6,3}(A,B)] = 2\mathrm{Tr}[(AB)^3] + 6\mathrm{Tr}[A^3B^3] + 12\mathrm{Tr}[ABABBA]$$

Although the first two terms in the sum above are always nonnegative, it turns out the the third summand can be made negative (a fact only known recently [H,Johnson]) although not easily so. More remarkably, naively picking random A and B will fail to find such examples.

Conclusion: If the conjecture is true, almost certainly a proof must navigate a complicated cancellation of signs.

Known Results

- When the size of the matrices is $n = 2$, the conjecture is well-known; (in fact, it is known that any word $W(A,B)$ has nonnegative eigenvalues).

- If $AB = BA$ or $m < 6$, the conjectures are true.

- BMV1 is true in an "average" sense, the precise statement involving notions of free probability (matrix version of random variables) [Fannes,Petz]

- BMV2 is true when $n = 3$ and A and B are of a special (nontrivial) form [Drmota, et al]

- BMV3 is true for $n = 3$, $m = 6$, $k = 3$. [H,Johnson]

- BMV3 is true if either A or B have exactly 2 distinct e-values

Other than these facts, very little is known about this problem.

We now discuss some of our recent progress.

The first result should be surprising since it is not at all straightforward to get information about $S_{m+1,k}$ from $S_{m,k}$

Theorem 1 (Asymptotic Formulation): If there are PSD A,B and a power $m > 0$ showing BMV3 false, then there are PSD A,B making BMV3 false with power $m+1$.

Corollary: If conjecture BMV3 is false, then it is really false.

Corollary: If conjecture BMV2 is true for infinitely many m, then it is true for all m.

Theorem 2 (Transfer Principal): $\mathrm{Tr}[S_{m,k}(A,B)] \geq 0$ for all PSD A, B if and only if whenever $S_{m,k}(A,B) \neq 0$, it has at least one positive eigenvalue.

This last result essentially transfers the problem of showing that a sum of eigenvalues is nonnegative to that of showing one of them is.

In this regard, one is reminded of Perron's Theorem for nonnegative matrices. Fix PSD matrices A and B.

Conjecture: The matrix $S_{m,k}(A,B)$ either has a positive eigenvalue or it is the zero matrix.

Finally, the following reduces the number of parameters in a computational approach by 2.

Theorem 3 (Singular Reduction): It is enough to prove conjecture BMV3 in the case of singular matrices.

SOS Approaches

Real positive semidefinite matrices may be parameterized as

$$A = XX^{T},\ B = YY^{T}$$

For matrices X, Y of indeterminates. Thus, BMV3 naturally becomes a statement about sums of squares (there are also other ways to do this).

Problem: Can one find "nice" SOS representations for the polynomials $\mathrm{Tr}[S_{m,k}(A,B)]$ in the indeterminates X,Y?

Problem: Use SOS tools to find certificates of nonnegativity in the nontrivial (but known) case $m = 6$, $k = 3$, $n = 3$ and the (unknown) case $m = 7$, $k = 3$, $n = 3$.

Problem: Use real root counting to show that the characteristic polynomial of $S_{m,k}(A,B)$ has at least 1 nonnegative root (in at least the above cases).

Example (parameterization): A concrete setup for approaching these problems is to compute with the following parameterization of A and B in the case $n = 3$ ($0 < r < 1$; $u,b,x,y > 0$; $z < 0$)

(One may reduce the general 3-by-3 case to this one)

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & r & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$B = \begin{bmatrix} \left(x^2+u^2\right)/b & x & -z \\ x & b & y \\ -z & y & \left(x^2y^2+u^2y^2+2xbzy+z^2b^2\right)/u^2b \end{bmatrix}$$

References

D. Bessis, P. Moussa and M. Villani, *Monotonic converging variational approximations to the functional integrals in quantum statistical mechanics*, J. Math. Phys. **16** (1975), 2318 - 2325.

C. Hillar, Advances on the BMV conjecture, submitted.