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The critical exponent conjecture for powers of doubly nonnegative matrices ☆

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ABSTRACT

Doubly nonnegative matrices arise naturally in many setting including Markov random fields (positively banded graphical models) and in the convergence analysis of Markov chains. In this short note, we settle a recent conjecture by C.R. Johnson et al. [Charles R. Johnson, Brian Lins, Olivia Walch, The critical exponent for continuous conventional powers of doubly nonnegative matrices, Linear Algebra Appl. 435 (9) (2011) 2175–2182] by proving that the critical exponent beyond which all continuous conventional powers of n-by-n doubly nonnegative matrices are doubly nonnegative is exactly $n-2$. We show that the conjecture follows immediately by applying a general characterization from the literature. We prove a stronger form of the conjecture by classifying all powers preserving doubly nonnegative matrices, and proceed to generalize the conjecture for broad classes of functions. We also provide different approaches for settling the original conjecture.

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1. Introduction and main result

The study of operations preserving different notions of positivity is an important topic in matrix analysis (see e.g. Bhatia [2], Horn and Johnson [5]). The purpose of this short note is to prove the *critical exponent conjecture* for doubly nonnegative matrices formulated recently by Johnson et al. [6]. A real symmetric matrix A is said to be *doubly nonnegative* if it is both positive semidefinite, and entrywise nonnegative. Given a real function $f:[0,\infty)\to[0,\infty)$ and a doubly nonnegative matrix A, we define the matrix $f(A)$ using the spectral decomposition of A. Namely, if $A=UDU^T$,

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where U is orthogonal and $D = \operatorname{diag}(d_{11}, \ldots, d_{nn})$ is diagonal, define $f(A) := Uf(D)U^T$, where $f(D) := \operatorname{diag}(f(d_{11}), \ldots, f(d_{nn}))$. Assuming A is doubly nonnegative, it is very natural to seek conditions under which $f(A)$ is also doubly nonnegative.

A similar question can be asked when the function f is applied entrywise to the elements of A. Denote by $f[A] := (f(a_{ij}))$. In the particular case where $f(x) = x^\alpha$ for $0 \leqslant \alpha \in \mathbb{R}$, it has been shown by FitzGerald and Horn [4] (see also Horn and Johnson [5, Chapter 6.3]) that $f[A]$ is doubly nonnegative for every doubly nonnegative matrix A if and only if $\alpha \in \mathbb{N} \cup [n-2, \infty)$. Note that in each of the two questions above, one of the two nonnegativity conditions is merely used to ensure that $f(A)$ or $f[A]$ is well defined, and the real question is whether the other notion of nonnegativity is preserved.

Johnson et al. are interested in the first question above for the power functions $f(x) = x^\alpha$ for real α. Namely, which conventional powers preserve the set of doubly nonnegative matrices of a given order? This problem was also considered by Audenaert [1]. In [6], the following phase transition was shown to occur for every integer $n > 0$.

Theorem 1.1. *(See [6, Theorem 2.1].) There is a function $\mu : \mathbb{N} \to [0, \infty)$ such that for any n-by-n doubly nonnegative matrix A, the matrix $f(A) = A^\alpha$ is doubly nonnegative for $\alpha \geqslant \mu(n)$.*

The smallest such $\mu(n)$ always exists by continuity and is denoted by $m(n)$. The quantity $m(n)$ is called the (conventional) *critical exponent* (see [6]), and it is of great interest to identify it. Johnson et al. [6] provide a lower bound for $m(n)$ for all n, and a sharp upper bound for small values of n.

Theorem 1.2. *(See [6, Theorems 3.1, 3.2, 4.1].) The critical exponent $m(n) \geqslant n-2$. If $n < 6$, then the critical exponent $m(n) = n-2$.*

The authors then proceed to conjecture if the above result is true in general:

Conjecture 1.3. *(See Johnson, Lins, and Walch (2011) [6].) For all integers $n \geqslant 2$, the critical exponent $m(n) = n-2$.*

The goal of this note is to settle this conjecture and prove that indeed $m(n) = n-2$ for all $1 < n \in \mathbb{N}$. More generally, we prove this conjecture (in fact, a stronger statement of it) for a larger class of functions. In order to state our main result, we first need some notation.

Definition 1.4. Let $n \geqslant 2$ be an integer. Denote the set of doubly nonnegative $n \times n$ matrices by DN_n. Now given a function $f : [0, \infty) \to [0, \infty)$, define the *critical exponent* for f to be

$$m(f, n) := \inf\{0 \leqslant t \in \mathbb{R} : \ A^\alpha f(A) \in DN_n, \ \forall A \in DN_n, \ \forall \alpha \geqslant t\}. \tag{1.5}$$

We now state the main result of this paper.

Theorem 1.6 *(Critical exponent conjecture, stronger form). Given $u > 0$ and $\beta \in \mathbb{R}$, the critical exponent for $f(x) := (x+u)^{-\beta}$ is $m(f, n) = n-2+\max(\beta, 0)$. Moreover, below the critical exponent there are only finitely many values $0 \leqslant \alpha < m(f, n)$ such that the map $g(x) = x^\alpha (x+u)^{-\beta}$ preserves DN_n, and these are contained in the set*

$$\{m + \max(\beta, 0) : \ m = 0, 1, \ldots, n-3\}. \tag{1.7}$$

Remark 1.8. Note that the critical exponent Conjecture 1.3 for powers by Johnson et al. [6] is the special case where $\beta = 0$. Additionally, Theorem 1.6 strengthens the statement of the critical exponent conjecture significantly in two ways: (1) it discusses the behavior of $A^\alpha f(A)$ for values of α lower than the critical exponent, and (2) it considers more general functions than conventional matrix powers.

We will also see in Section 2.1 that showing that $g(x) = x^{n-1}(x+u)^{-1}$ preserves DN_n for all $u > 0$ actually implies the critical exponent conjecture. This reason also motivates our trying to prove Theorem 1.6 which is a more general result than the standard form of the critical exponent conjecture.

2. Proof of the strong critical exponent conjecture

We now settle Conjecture 1.3 by proving the more general result given by Theorem 1.6. To do so, we shall employ the following result from the literature.

Theorem 2.1. *(See Micchelli and Willoughby [7, Corollary 3.1].) Suppose $g(x) \geqslant 0$ is continuous for $x \geqslant 0$. Then g preserves DN_n if and only if all the divided differences of g in $[0, \infty)$ of order $1, 2, \ldots, n-1$ are nonnegative.*

Theorem 2.1 is shown by replacing g by the Newton interpolation polynomial taking values $g(\lambda_i)$ at the eigenvalues $0 \leqslant \lambda_1 \leqslant \cdots \leqslant \lambda_n$ of A, and proving that each summand is doubly nonnegative, i.e.,

$$(A - \lambda_1 I) \cdots (A - \lambda_k I) \in DN_n, \quad \forall A \in DN_n,\ 1 \leqslant k \leqslant n-1. \tag{2.2}$$

Note that if g is C^{n-1}, then g preserves DN_n if and only if $g^{(i)}(x) \geqslant 0$ for all $0 \leqslant i < n$ and $x > 0$ (by the mean value theorem for divided differences). As a consequence, we have the following corollary.

Corollary 2.3. *Conjecture 1.3 holds for all integers $n \geqslant 2$. Moreover, $g(x) = x^\alpha$ preserves DN_n if and only if $\alpha \in \mathbb{N} \cup [n-2, \infty)$.*

Proof. Immediate by considering $g(x) = x^\alpha$. □

Note that the set of powers which preserves DN_n for conventional powers (Corollary 2.3) is exactly the same as for Hadamard powers [4]: $\alpha \in \mathbb{N} \cup [n-2, \infty)$.

Remark 2.4. Besides settling the critical exponent conjecture for powers, Theorem 2.1 can also be used to establish the existence of a critical exponent in very general settings. For instance, a family of smooth functions $(f_\alpha)_{\alpha \geqslant 0}$ will have a "critical index" $m(n)$ for DN_n, if and only if

$$f_\alpha^{(i)}(x) \geqslant 0, \quad \forall x > 0,\ i = 0, 1, \ldots, n-1, \tag{2.5}$$

for all α large enough. A stronger statement would be that (2.5) holds if and only if $\alpha \in S(n) \cup [m(n), \infty)$ for some finite set $S(n)$. We show in Theorems 1.6 and 3.1 that this is indeed the case for large families of functions.

To prove Theorem 1.6 using Theorem 2.1, we need the following preliminary result.

Lemma 2.6. *For all $\alpha, \beta \in \mathbb{R}$, $u, x > 0$, and $0 \leqslant r \in \mathbb{Z}$,*

$$\begin{aligned} \frac{d^r}{dx^r}\frac{x^\alpha}{(x+u)^\beta} &= \frac{x^{\alpha-r}}{(x+u)^{\beta+r}} \sum_{i=0}^{r} \binom{r}{i} u^i x^{r-i} \prod_{j=0}^{i-1}(\alpha - j) \prod_{j=i}^{r-1}(\alpha - \beta - j) \\ &= \frac{x^{\alpha-r}}{(x+u)^{\beta+r}} \sum_{i=0}^{r} \binom{r}{i} u^i x^{r-i} \frac{\Gamma(\alpha+1)\Gamma(\alpha-\beta-i+1)}{\Gamma(\alpha-i+1)\Gamma(\alpha-\beta-r+1)}. \end{aligned}$$

The proof follows by induction on r. It is straightforward but long and tedious, and is hence omitted.

Finally, we now prove the main result of this note.

Proof of Theorem 1.6. Suppose first that $\alpha \geqslant n-2+\max(\beta,0)$. Then for all $0 \leqslant i < n$ and $x > 0$, the ith derivative

$$\frac{d^i}{dx^i}\frac{x^\alpha}{(x+u)^\beta}$$

is indeed defined and can be computed using Lemma 2.6. It is easy to check that all of these derivatives are nonnegative, since $x, u > 0$, and $\alpha - (n-2)$ and $\alpha - \beta - (n-2)$ are nonnegative. By Theorem 2.1 (see the remarks preceding Corollary 2.3), we infer that $x^\alpha (x+u)^{-\beta}$ preserves DN_n for all $\alpha \geqslant n-2+\max(\beta,0)$.

To complete the proof, suppose now that $0 \leqslant \alpha < n-2+\max(\beta,0)$ and α is not in the set (1.7). Define $g(x) = x^\alpha (x+u)^{-\beta} : [0,\infty) \to [0,\infty)$. By Theorem 2.1, it suffices to show that there is at least one $0 \leqslant i < n$ and $x > 0$ such that $g^{(i)}(x) < 0$. There are two cases:

(1) Suppose $\beta < 0$. Now compute by Lemma 2.6,

$$g^{(m+2)}(x) = \frac{x^{\alpha-m-2}}{(x+u)^{\beta+m+2}}\left[u^{m+2}\prod_{j=0}^{m+1}(\alpha-j) + x\sum_{i<m+2}\binom{m+2}{i}u^i x^{m+1-i}\prod_{j=0}^{i-1}(\alpha-j)\prod_{j=i}^{m+1}(\alpha-\beta-j)\right].$$

Now if $\alpha \in (m, m+1)$ for some integer $m \in [0, n-3]$, then $u^{m+2}\prod_{j=0}^{m+1}(\alpha-j)$ is the smallest degree term in x and is negative. Therefore $g^{(m+2)}(x) < 0$ for small $x > 0$.

(2) Suppose $\beta \geqslant 0$. Once again using Lemma 2.6,

$$g^{(m+2)}(x) = \frac{x^{\alpha-m-2}}{(x+u)^{\beta+m+2}}\left[x^{m+2}\prod_{j=0}^{m+1}(\alpha-\beta-j) + x\sum_{i>0}\binom{m+2}{i}u^i x^{m+1-i}\prod_{j=0}^{i-1}(\alpha-j)\prod_{j=i}^{m+1}(\alpha-\beta-j)\right].$$

Now if $\alpha - \beta \in (m, m+1)$ for some integer $m \in [0, n-3]$, then a similar analysis as in the previous case, but this time with $x \to \infty$, implies that $g^{(m+2)}(x) < 0$ for some $x > 0$. □

2.1. Alternate proof

We now provide an alternate proof of the original critical exponent conjecture in [6]. Similar to Johnson et al. result in [6] (see Theorem 1.2), we only show the conjecture (i.e., that $m(f,n) = n-2$ for $f(x) \equiv 1$) for small values of n, although we also indicate an approach for all n.

The first simplification is in showing that to verify whether or not a given function f preserves DN_n, it is enough to focus on a particular off-diagonal entry:

Lemma 2.7. *Given $f : [0,\infty) \to [0,\infty)$ and a fixed pair of integers $1 \leqslant i \neq j \leqslant n$, the matrix $f(A)$ is doubly nonnegative for all $A \in DN_n$ if and only if $(f(A))_{ij} \geqslant 0$ for each $A \in DN_n$.*

Proof. One implication is immediate from the definition. Conversely, given any $A = UDU^T$ with U orthogonal and D diagonal, note that $f(A) = Uf(D)U^T$ is positive semidefinite. Hence its diagonal entries are nonnegative. We now consider the off-diagonal entries of $f(A)$. Note that for every n-by-n permutation matrix P,

$$f\left(PAP^T\right) = f\left((PU)D(PU)^T\right) = (PU)f(D)(PU)^T = Pf(A)P^T.$$

Since conjugating by P preserves DN_n, hence $(Pf(A)P^T)_{ij} \geqslant 0$ for all P, A. This is equivalent to saying that $f(A)_{i'j'} \geqslant 0$ for all $i' \neq j'$. □

Next, note by Theorem 2.1 and Lemma 2.6, that for every $n \in \mathbb{N}$,

$$A^{n-1}(A+uI)^{-1} \in DN_n, \quad \forall A \in DN_n,\ u > 0. \tag{2.8}$$

We now show that this fact alone implies the critical exponent Conjecture 1.3.

Proposition 2.9. *Fix an integer $n = n_0 \geqslant 2$. Then Eq. (2.8) for $n = n_0$ implies the critical exponent Conjecture 1.3 for $n = n_0$.*

Proof. By [6, Theorem 3.2], we know that $m(n_0) \geqslant n_0 - 2$. To show that $m(n_0) = n_0 - 2$, assume first that $A \in DN_{n_0}$ is nonsingular. Clearly, A^k is doubly nonnegative if $A \in DN_{n_0}$ and $k \in \mathbb{N}$. Therefore, it suffices to prove that A^q is doubly nonnegative for every $k < q < k+1$ and every integer $k \geqslant n_0 - 2$. To show this, note that for $k < q < k+1$ and $x > 0$, the following formula holds:

$$x^q = \frac{\sin((q-k)\pi)}{\pi} \int_0^\infty t^{q-k-1} x^{k+1} (x+t)^{-1}\, dt. \tag{2.10}$$

Eq. (2.10) is shown by a standard contour integration followed by an application of the residues theorem (see e.g. [3, Chapter V, Example 2.12]). But now the matrix $A^q = U D^q U^T$ can be written as:

$$A^q = \frac{\sin((q-k)\pi)}{\pi} \int_0^\infty t^{q-k-1} A^{k+1} (A+tI)^{-1}\, dt = \frac{\sin((q-k)\pi)}{\pi} \int_0^\infty t^{q-k-1} f_{k,t}(A)\, dt, \tag{2.11}$$

where $f_{k,t}(x) := x^{k+1}(x+t)^{-1}$ for $t \geqslant 0$ and $x > 0$. Note that $\sin((q-k)\pi) > 0$ since $0 < q-k < 1$. Moreover, since for every $A \in DN_{n_0}$ and $k \geqslant n_0 - 2$, the matrix $f_{k,t}(A)$ is doubly nonnegative by Eq. (2.8), it follows immediately that A^q is doubly nonnegative.

Finally, if A is singular, then $A^q = \lim_{u \to 0^+} (A+uI)^q$ and the result follows. □

Remark 2.12. Eq. (2.11) is frequently used in the study of positive definite matrices. See e.g. Bhatia [2, Theorem 1.5.8].

Given Proposition 2.9, it is thus of interest to prove Eq. (2.8) from first principles in order to provide an elementary proof of the critical exponent conjecture in [6]. We conclude this section with a case-by-case verification of Eq. (2.8) for $n \leqslant 3$. Such an approach (but using different arguments) was adopted by Johnson et al. in [6] when they showed the conjecture for $n < 6$.

Proposition 2.13. *The critical exponent Conjecture 1.3 holds for $n \leqslant 3$.*

Proof. In light of Proposition 2.9, it suffices to show that Eq. (2.8) holds (for $n \leqslant 3$). First note that $A^{n-1}(A+uI)^{-1}$ is clearly positive semidefinite. By using Lemma 2.7, it now suffices to show that the $(1,2)$-entry of $A^{n-1}(A+uI)^{-1}$ is nonnegative. Denote this entry by $a_{12,n}$. It is then easily shown that for $A \in DN_2$,

$$a_{12,2} = \frac{a_{12}u}{\det(A+uI_2)} \geqslant 0.$$

Similarly, for $n = 3$,

$$a_{12,3} = \det(A+uI_3)^{-1}\big(a_{12}\det A + a_{12}u(C_{11}+C_{22}+C_{33}) + u^2(a_{12}a_{11} + a_{12}a_{22} + a_{13}a_{23})\big),$$

where C_{ii} are the principal cofactors/minors of A, hence are nonnegative. This concludes the proof since all entries of A are nonnegative. □

3. Generalization of the strong critical exponent conjecture

Note that Theorem 2.1 can be used to systematically study and resolve the (strong) critical exponent conjecture for broad classes of functions. We conclude this note by showing such a result.

Theorem 3.1. *Let $f : [0,\infty) \to [0,\infty)$ be a C^{n-1} function satisfying*

$$f(x) > 0, \qquad \lim_{x\to 0^+} f(x) > 0, \qquad f^{(i)}(x) \geqslant 0, \qquad \lim_{x\to 0^+} f^{(i)}(x) = M_i < \infty,$$
$$\forall x > 0,\ 0 < i < n. \tag{3.2}$$

Then the values $0 \leqslant \alpha \in \mathbb{R}$ such that $x^\alpha f(x)$ preserves DN_n are $\mathbb{N} \cup [n-2,\infty)$. In particular, the critical exponent for all such functions f is $m(f,n) = n-2$.

Proof. Set $g(x) := x^\alpha f(x)$. In order to use Theorem 2.1, we evaluate $g^{(i)}(x)$ using the product rule:

$$g^{(i)}(x) = \sum_{l=0}^{i} \binom{i}{l} \prod_{j=0}^{l-1} (\alpha - j) x^{\alpha-l} f^{(i-l)}(x).$$

If $\alpha \in \mathbb{N}$ then every product $\prod_{j=0}^{l-1}(\alpha - j)$ that includes a negative term also includes 0, whence all derivatives of g are nonnegative at $x > 0$. Similarly, if $\alpha \geqslant n-2$, then $g^{(i)}(x) \geqslant 0$ for $x > 0$. Finally if $\alpha \notin \mathbb{N}$ and $\alpha < n-2$, assume $\alpha \in (m, m+1)$ for some integer $m \in [0, n-3]$. Then the $l = m+2$ term for $g^{(m+2)}(x)$ is negative, and hence $g^{(m+2)}(x) < 0$ for small values of $x > 0$ by (3.2). □

Remark 3.3. Note that the critical exponent conjecture in [6] is again a special case of Theorem 3.1 – with $f(x) \equiv 1$. Moreover, the cone $\mathscr{F}$ of functions f satisfying (3.2) is a very large family that contains all absolutely monotonic functions with nonzero constant term as well as exponential-type functions such as e^x and $\cosh(x)$. Additionally, $\mathscr{F}$ is closed under multiplication, exponentiation, composition, and taking nontrivial nonnegative linear combinations.

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