# On two long-standing conjectures concerning trace nonnegativity

Sabine Burgdorf

Universität Konstanz,
Université de Rennes 1

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# Introduction – Real algebra

- $f \in \mathbb{R}[\underline{X}]$ in commuting variables $\underline{X} = (X_1, \ldots, X_n)$
- $f \geq 0$ if $f(\underline{x}) \geq 0$ for all $\underline{x} \in \mathbb{R}^n$
- $f \geq 0$ on $S$ if $f(\underline{x}) \geq 0$ for all $\underline{x} \in S$
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- Certificates of positivity or non-negativity

### Example

- $f = \sum g_i^2$ (sos) $\implies f \geq 0$.
- $f \geq 0 \implies f$ sos, if
  - $f \in \mathbb{R}[X]$
  - $\deg f = 2$ or
  - $f \in \mathbb{R}[X_1, X_2], \deg f \leq 4$

### Example (Motzkin polynomial)

$m = X_1^4 X_2^2 + X_2^4 X_1^2 - 3X_1^2 X_2^2 + 1 \geq 0$ on $\mathbb{R}^2$ but not sos

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- Quadratic module: $M \subset \mathbb{R}[\underline{X}], 1 \in M, M + M \subset M, \mathbb{R}[\underline{X}]^2 M \subset M$
  - $\Sigma^2 = \{f \in \mathbb{R}[\underline{X}] \mid f = \sum_i g_i^2\}$
  - $M(1 - X_i^2) := \{f \in \mathbb{R}[\underline{X}] \mid f \in \Sigma^2 + \sum_i (1 - X_i^2)\Sigma^2\}$

**Theorem (Putinar)**

Let $f \in \mathbb{R}[\underline{X}]$, $f \geq 0$ on $[-1, 1]^n$. Then $\forall \varepsilon > 0 : f + \varepsilon \in M(1 - X_i^2)$.

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& + (\frac{1}{n} + \frac{1}{n}(1 - X_1^2)^2 \sum_{k=0}^{n-2} (n - 1 - k) X_1^{2k})(1 - X_2^2)
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# Introduction – non commutative setting

**Idea:** Replace $\underline{x}$ with $x_i \in \mathbb{R}$ by $\underline{A}$ with $A_i \in \operatorname{Sym}\mathbb{R}^{t\times t}$

- $f \in \mathbb{R}[\underline{X}]$
- $f \geq 0$
- $f$ sos $\implies f \geq 0$
- Quadratic module

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- $f \in \mathbb{R}[\underline{X}]$
  - $f \in \mathbb{R}\langle \underline{X} \rangle$ in non commuting variables $\underline{X} = (X_1, \ldots, X_n)$
  - $\mathbb{R}$-algebra freely generated by $X_1, \ldots, X_n$
- $f \geq 0$
  - first guess: $f(\underline{A}) \succeq 0$ for all $\underline{A}$
  - trace nonnegativity: $\operatorname{tr}(f(\underline{A})) \geq 0$ for all $\underline{A}$

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- $\operatorname{tr}(f(\underline{A})) \geq 0$
- $f$ sos $\implies f \geq 0$
  - $A^2$ is not psd for all $A \in \operatorname{Sym} \mathbb{R}^{t \times t}$ but $A^*A$
  - $\sum g_i^2$ replaced by $\sum g_i^* g_i$ (sohs)
  - Involution $*$: $a^* = a$ for $a \in \mathbb{R}$, $X_i^* = X_i$,
    $(X_1 X_3 X_2^2)^* = X_2^2 X_3 X_1$
- Quadratic module
  - $M(1 - X_i^2) := \{g \in \mathbb{R}[\underline{X}] \mid g = \sum_j h_j^* h_j + \sum_{i,j} h_{ij}^* (1 - X_i^2) h_{ij}\}$

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**Fact:** $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ for all $A, B \in \operatorname{Sym} \mathbb{R}^{t \times t}$

$\rightarrow$ equivalence relation $\overset{\text{cyc}}{\sim}$

- $\operatorname{tr}([A, B]) = 0$
  - $v \overset{\text{cyc}}{\sim} w \Leftrightarrow v - w = [u_1, u_2] = u_1 u_2 - u_2 u_1$
  - $v \overset{\text{cyc}}{\sim} w \Leftrightarrow \exists u_1, u_2 : v = u_1 u_2, w = u_2 u_1$
  - $v \overset{\text{cyc}}{\sim} w \Leftrightarrow v = \sigma(w)$ for a cyclic permutation $\sigma$
- tr linear
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**Useful properties**

- $f \overset{\text{cyc}}{\sim} g \implies \operatorname{tr}(f(\underline{A})) = \operatorname{tr}(g(\underline{A}))$ for all $\underline{A}$.
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# BMV conjecture

**Conjecture (Bessis, Moussa, Villani, 1975)**

For all hermitian $A, B \in \mathbb{C}^{t\times t}$, $B \geq 0$, $t \in \mathbb{N}$, exists a measure $\mu \geq 0$ s.t.

$$\mathrm{tr}(e^{A-tB}) = \int e^{-tx} \mathrm{d}\mu(x).$$

- Gibbs density matrix $e^{-\beta H}$ of equilibrium at $k_B T = 1/\beta$
- $e^{-\beta H_0} = \int_0^\infty e^{-\beta E} dP_E$ spectral decomposition
- perturbation theory: $H = H_0 + tH_1$, $H_1$ psd
- partition function $Z(t) := \mathrm{tr}(e^{-\beta(H_0+tH_1)}) = \mathrm{tr}(e^{A-tB})$

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- $[A, B] = 0$: classical physics
- N-body system of bosons with local interaction:

  $H_0 = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + V(\underline{q})$, $H_1 = V'(\underline{q})$
- $A, B \in \operatorname{Sym} \mathbb{C}^{2\times 2}$
- in average: i.i.d. random matrices

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- Padé approximation
  - approximation of $f$ by rational function $R_{[m/n]}(t) = \frac{P_m(t)}{Q_n(t)}$
  - $P_m, Q_n \in \mathbb{R}[t]$, $\deg P_m = m$, $\deg Q_n = n$
  - $f(0) = R_{[m/n]}(0)$, $f'(0) = R'_{[m/n]}(0)$, $\ldots$, $f^{(m+n)}(0) = R^{(m+n)}_{[m/n]}(0)$
  - If $Z(t) = \int e^{-tx} \mathrm{d}\mu(x)$ for some $\mu \geq 0$, then:
    - $(R_{[m-1/m]}(t))_m$ monotone increasing lower bound of $Z(t)$
    - $(R_{[m/m]}(t))_m$ monotone decreasing upper bound of $Z(t)$

## Conjecture (Lieb, Seiringer, 2003)

Let $A, B \in \mathbb{C}^{t\times t}$ be hermitian. The following statements are equivalent:

1. For all $A, B$ with $B \geq 0$, exists a measure $\mu \geq 0$:

$$\operatorname{tr}(e^{A-tB}) = \int e^{-tx} \mathrm{d}\mu(x).$$

2. For all $A, B$ with $B \geq 0$, the function $f : t \mapsto \operatorname{tr}(e^{A-tB})$ is completely monotone.
3. For all psd $A, B$ and all $m \in \mathbb{N}$, the polynomial

$$p_{A,B,m}(t) := \operatorname{tr}((A + tB)^m) = \sum_k \operatorname{tr}(S_{m,k}(A, B))t^k \in \mathbb{R}[t]$$

has only nonnegative coefficients.

$p(t)$ is completely monotone if $(-1)^k \frac{\partial^k}{\partial t^k} p(t) \geq 0$ for all $t \geq 0$ ▸ result

# Proof 1/2

1 $\iff$ 2: Theorem of Bernstein

3 $\implies$ 2:

$$\begin{aligned}\operatorname{tr}(e^{A-tB}) &= e^{-\|A\|}\sum_m \frac{1}{m!}\operatorname{tr}((A+\|A\|\mathbf{1}-tB)^m)\\ &= e^{-\|A\|}\sum_m \frac{1}{m!}p_{A',B,m}(-t)\end{aligned}$$

Further

$$\begin{aligned}(-1)^k\frac{\partial^k}{\partial t^k}p(-t) &= (-1)^{2k}\frac{\partial^k}{\partial t^k}p(t)\\ &= \sum_{k=s}^{m}\frac{k!}{(k-s)!}\operatorname{tr}(S_{m,k}(A',B))t^{k-s} \geq 0 \text{ for } t \geq 0.\end{aligned}$$

# Proof 2/2

1 $\Longrightarrow$ 3:

$$(A+tB)^{-m} = \frac{1}{\Gamma(m)} \int_0^\infty e^{-\lambda(A+tB)} \lambda^{m-1} d\lambda$$

Thus

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Further if $A^{-1}$ exists

$$\begin{aligned}\mathrm{tr}(S_{m,k}(A,B)) &= \frac{\partial^k}{\partial t^k} \mathrm{tr}((A+tB)^{m+k})|_{t=0} \\ &= \frac{m+k}{m}(-1)^k \frac{\partial^k}{\partial t^k} \mathrm{tr}((A^{-1}+tA^{-\frac{1}{2}}BA^{-\frac{1}{2}})^{-m})|_{t=0} \geq 0\end{aligned}$$

Finish by continuity.

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Finish by continuity.

## Conjecture (BMV)

1. For all $A, B$ with $B \geq 0$, exists $\mu \geq 0$ : $\operatorname{tr}(e^{A-tB}) = \int e^{-tx} d\mu(x)$.
2. For all psd $A, B$ and all $m \in \mathbb{N}$:
$p_{A,B,m}(t) = \operatorname{tr}((A+tB)^m) = \sum_k \operatorname{tr}(S_{m,k}(A,B))t^k \in \mathbb{R}_+[t]$.

**Results**

- If $\operatorname{tr}(S_{M,K}(A,B)) \geq 0$, then $\operatorname{tr}(S_{m,k}(A,B)) \geq 0$ for all $m, k$ with $m \leq M, k \leq K, m-k \leq M-K$ (Hillar)
- using $f \overset{\mathrm{cyc}}{\sim} \sum g_i^* g_i$:
  - $m \leq 13, k \leq m$ (Klep, Schweighofer; Hägele)
  - $k \leq 4, m \in \mathbb{N}$ (Landweber, Speer; B.)
  - almost all other possibilities of $m, k$ not sohs (L., S.; Collins, Dykema)

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**Goal:** Find new certificates of trace-nonnegativity !

Let $\mathbb{R}_1^{t\times t}$ be the set of $\underline{B}$ of selfadjoint contractions in $\mathbb{R}^{t\times t}$, $t \in \mathbb{N}$.

**Real algebra:**

### Theorem (Putinar)

Let $f \in \mathbb{R}[\underline{X}]$, $f \geq 0$ on $[-1,1]^n$. Then $\forall \varepsilon > 0 : f + \varepsilon \in M(1 - X_i^2)$.

### Theorem (Helton, McCullough)

Let $f \in \mathbb{R}\langle\underline{X}\rangle$, $f \succeq 0$ on $\mathbb{R}_1^{t\times t}$, then $\forall \varepsilon > 0 :\ f + \varepsilon \in M(1 - X_i^2)$.

### Conjecture

Let $f \in \mathbb{R}\langle\underline{X}\rangle$, $\operatorname{tr}(f) \geq 0$ on $\mathbb{R}_1^{t\times t}$, then $\forall \varepsilon > 0 :\ f + \varepsilon \overset{\text{cyc}}{\sim} g$ for some $g \in M(1 - X_i^2)$.

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# Connes' embedding conjecture

## Theorem (Klep, Schweighofer, 2008)

Let $\mathcal{F}$ be a separable $\mathrm{II}_1$ factor with faithful trace $\tau$. The following statements are equivalent:

1. Let $\omega$ be a free ultrafilter on $\mathbb{N}$ and $\mathcal{R}$ be the hyperfinite $\mathrm{II}_1$ factor. Then $\mathcal{F}$ can be embedded into the ultrapower $\mathcal{R}^\omega$.
2. $\forall \varepsilon > 0, n, k \in \mathbb{N}, A_1, \dots, A_n \in \mathcal{F}_1 \; \exists B_1, \dots B_n \in \mathbb{C}_1^{t\times t}$:
$$\forall w \in \langle \underline{X} \rangle_k : \; \left|\tau(w(\underline{A})) - \frac{1}{t}\operatorname{tr}(w(\underline{B}))\right| < \varepsilon.$$
3. Let $f \in \mathbb{C}\langle \underline{X} \rangle, f = f^*, \operatorname{tr}(f) \geq 0$ on $\mathbb{C}_1^{t\times t}$, then $\forall \varepsilon > 0 : f + \varepsilon \overset{\mathrm{cyc}}{\sim} g$ for some $g \in M(1 - X_i^2)$.

proof

# Conclusion

- Relations between

| | | |
|---|---|---|
| problems in quantum physics<br>problems in operator theory | $\leftrightarrow$ | non commutative real algebra<br>with trace-nonnegativity |

## General question

Which questions/theorems can be transferred to solve problems by other methods ?

1. $\mathcal{F}$ can be embedded into $\mathcal{R}^\omega$.
2. $\forall \varepsilon > 0, \underline{A} \subset \mathcal{F}_1\ \exists \underline{B} \subset \mathbb{C}_1^{t\times t} : |\tau(w(\underline{A})) - \frac{1}{t}\operatorname{tr}(w(\underline{B}))| < \varepsilon.$
3. $f \in \mathbb{C}\langle \underline{X} \rangle, \operatorname{tr}(f) \geq 0$ on $\mathbb{C}_1^{t\times t}$, then $\forall \varepsilon > 0 :\ f + \varepsilon \overset{\text{cyc}}{\sim} g$ for some $g \in M(1 - X_i^2)$.

- (1) $\iff$ (2) by definition of ultrapower
- (3) $\implies$ (2) by Hahn-Banach separation theorem:
  - $k, \underline{A}$ fixed: $L \in \mathbb{C}\langle \underline{X} \rangle_k^\vee$ given by $L(p) := \tau(p(\underline{A}))$
  - $C = \operatorname{conv}\{\text{linear forms } p \mapsto \frac{1}{t}\operatorname{tr}(p(\underline{B})) \text{ for some } \underline{B} \subset \mathbb{C}^{t\times t}\}$
  - Hahn-Banach: $L \in C$
  - Conclude by rational approximation.
- (2) $\implies$ (3) by

## Theorem

Let $\mathcal{F}$ be a separable $\mathrm{II}_1$ factor with faithful trace $\tau$. Let $f \in \mathbb{C}\langle \underline{X} \rangle, f = f^*$, $\tau(f(\underline{A})) \geq 0$ on $\mathcal{F}_1$, then $\forall \varepsilon > 0 :\ f + \varepsilon \overset{\text{cyc}}{\sim} g$ for some $g \in M(1 - X_i^2)$.

Let $\mathcal{F}$ be a separable $\mathrm{II}_1$ factor with faithful trace $\tau$. Let $f \in \mathbb{C}\langle \underline{X} \rangle, f = f^*$, $\tau(f(\underline{A})) \geq 0$ on $\mathcal{F}_1$, then $\forall \varepsilon > 0: \ f + \varepsilon \overset{\text{cyc}}{\sim} g$ for some $g \in M(1 - X_i^2)$.

- $M := \{h \mid h \overset{\text{cyc}}{\sim} g \text{ for some } g \in M(1 - X_i^2)\}$ convex cone in $\mathbb{C}\langle \underline{X} \rangle$.
- If $f \notin M$ by separation $\exists L : \mathbb{C}\langle \underline{X} \rangle \to \mathbb{C}$ with $L(1) = 1$, $L(g^* g) \geq 0$, $L(fg) = L(gf), |L(w)| \leq 1$ for $w \in \langle \underline{X} \rangle$ and $L(f) \notin \mathbb{R}_+$.
- GNS construction:
  - $N := \{p \in \mathbb{C}\langle \underline{X} \rangle \mid L(p^* p) = 0\}$
  - bilinear form $\langle p, q \rangle := L(q^* p)$ on $\mathbb{C}\langle \underline{X} \rangle / N$
  - Completion to Hilbert space $E$
  - bounded s.a. operator $\hat{X}_i$ (left multiplication)
- $\mathcal{F}$ von Neumann algebra generated by $\hat{X}_1, \ldots \hat{X}_n$ $\tau(\sum_w a_w \hat{w}) := L(\sum_w a_w w)$.
- Then $\tau(\hat{f}) \geq 0$ by assumption, but $\tau(\hat{f}) = L(f) \notin \mathbb{R}_+$.

## Theorem

The following statements are equivalent:

1. $\mathcal{F}$ can be embedded into $\mathcal{R}^\omega$.
2. $\forall \varepsilon > 0, \underline{A} \subset \mathcal{F}_1 \ \exists \underline{B} \subset \mathbb{C}_1^{t\times t} : \ \forall w \in \langle \underline{X} \rangle_k \ |\tau(w(\underline{A})) - \frac{1}{t}\,\mathrm{tr}(w(\underline{B}))| < \varepsilon$
3. $f \in \mathbb{C}\langle \underline{X} \rangle, \mathrm{tr}(f) \geq 0$ on $\mathbb{C}_1^{t\times t}$, then $\forall \varepsilon > 0 : f + \varepsilon \overset{\text{cyc}}{\sim} g$ for some $g \in M(1 - X_i^2)$.

## Simplification

- it suffices to consider real polynomials and symmetric contractions
- Radulescu: Reduction to $\deg f \leq 4$, $n \in \mathbb{N}$
- Every $\mathrm{II}_1$ von Neumann algebra can be generated by 2 elements: Reduction to $n = 2$ but arbitrary degree

# Conclusion

- Relations between

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|---|---|---|

**General question**

Which questions/theorems can be transferred to solve problems by other methods ?