Conjecture. Let A, B be density matrices. Then,

$$\operatorname{tr}\sqrt{A^{1/2}\mathrm{B}A^{1/2}} \leq \int_0^1 \operatorname{tr} A^t B^{1-t}\,\mathrm{dt} \tag{1}$$

This is known to be true when A and B commute.

Finding a counterexample.

Fix $B = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$. Note, for any $H = [h_{ij}]$ the structure of B ensures that the spectrum $\sigma(H) = \{h_{11}, 0\}$. Let the following be a parametrized family of density matrices.

$$A(\theta, \lambda) = U_\theta D_\lambda U_\theta^T$$

$$\text{where} \quad U_\theta = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}, \quad D_\lambda = \begin{bmatrix} \lambda & 0 \\ 0 & 1-\lambda \end{bmatrix}, \quad \text{for} \quad 0 \leq \lambda \leq 1 \tag{2}$$

If $A = A(\theta, \lambda)$, then $\sigma(AB) = \sigma(UDU^T B) = \{\lambda\cos^2\theta + (1-\lambda)\sin^2\theta, 0\}$. But

$$\operatorname{tr}\sqrt{A^{1/2}\mathrm{B}A^{1/2}} = \sum_{\lambda \in \sigma(\mathrm{AB})} \sqrt{\lambda}$$

So,

$$\mathrm{LHS} = \sqrt{\lambda\cos^2\theta + (1-\lambda)\sin^2\theta} \tag{3}$$

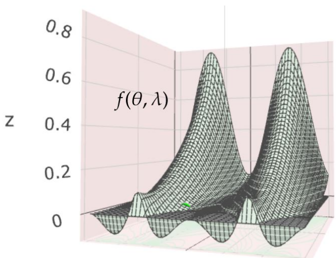
And $\operatorname{tr} A^t B^{1-t} = \operatorname{tr} U D^t U^T B = \lambda^t \cos^2\theta + (1-\lambda)^t \sin^2\theta$. So

$$\begin{aligned} \mathrm{RHS} &= \int_0^1 \lambda^t \cos^2\theta + (1-\lambda)^t \sin^2\theta \quad \mathrm{dt} \\ &= \cos^2\theta \frac{\lambda - 1}{\log\lambda} + \sin^2\theta \frac{-\lambda}{\log(1-\lambda)} \end{aligned} \tag{4}$$

Use (4) and (3) to define

$$f(\theta, \lambda) = \cos^2\theta \frac{\lambda - 1}{\log\lambda} + \sin^2\theta \frac{-\lambda}{\log(1-\lambda)} - \sqrt{\lambda\cos^2\theta + (1-\lambda)\sin^2\theta} \tag{5}$$

We can plot f for $0 \leq \lambda \leq 1$, and we see that the graph of f goes below the plane $z = 0$.



This implies there exists θ, λ such that $f(\theta, \lambda) < 0$. In particular

$$f\left(\frac{\pi}{4}, \frac{3}{4}\right) \quad = \quad \frac{1}{8}\left[\frac{3}{\log 4} + \frac{1}{\log 4 - \log 3} - 4\sqrt{2}\right] = -0.0021 < 0 \tag{6}$$

This shows that $A\left(\frac{\pi}{4}, \frac{3}{4}\right)$ and B are counterexamples to (1).

$\square$