

# ESTIMATING THE VON NEUMANN ENTROPY OF LARGE MATRICES

MICHELE BENZI

ABSTRACT. The problem of approximating the von Neumann entropy of a symmetric positive semidefinite matrix  $A$ , defined as  $\text{tr}(f(A))$  where  $f(x) = -x \log x$ , is considered. After discussing some useful properties of this matrix function, approximation methods based on randomized trace estimation and probing techniques used in conjunction with polynomial and rational Krylov methods will be described. Bounds and heuristics used in the implementation of the algorithms will be discussed. The performance of the methods will be assessed using test problems arising in Network Science.

This is joint work with my students Michele Rinelli and Igor Simunec.

## REFERENCES

- [1] M. Benzi, M. Rinelli and I. Simunec, *Computation of the von Neumann entropy of large matrices via trace estimators and rational Krylov methods*, Numerische Mathematik, **155** (November 2023), 1–38.

CLASSE DI SCIENZE, SCUOLA NORMALE SUPERIORE, PIAZZA DEI CAVALIERI, 7, 56126 PISA, ITALY  
E-mail address: `michele.benzi@sns.it`