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▶ Trace estimator

Given a symmetric invertible matrix A, an important task, for example in computational chemistry and statistics, is to compute the trace of its inverse:

$$\mathrm{tr}(A^{-1}),$$

where $\mathrm{tr}(\cdot)$ denotes the trace of a matrix, that is, the sum of its diagonal elements. The main goal of this project is to implement Algorithm 2 from [1] for estimating $\mathrm{tr}(A^{-1})$.

a) Work out the details of the first part of Section 2.2 (everything before Algorithm 1) from [1] by establishing the precise connection between quadrature and the Lanczos algorithm.

b) Implement Algorithm 1 from [1] with Gauss-Radau quadrature.

c) Derive Proposition 4.1 from [1].

d) Implement Algorithm 2.

e) Reproduce all numerical experiments from [1], for which the matrices are available.

Compare the execution time of Algorithm 2 with

- Typing **trace(inv(A))**.
- Computing $\mathrm{tr}(A^{-1})$ by solving n linear systems.
- Computing $\mathrm{tr}(A^{-1})$ by estimating $e_i^T A^{-1} e_i$ for $i = 1, \ldots, n$ using Algorithm 1.

(This of course depends on the requested accuracy; so run this experiment with different accuracies.)

f) **Bonus:** There is a mistake in the paper [1] in Equation (12). Explain why (12) cannot always hold.

Hint: Consider the case in which $m = 1$ and the quadratic form is computed exactly, that is, $L_1 = U_1$.

▶ References

[1] Zhaojun Bai, Gark Fahey, and Gene Golub. Some large-scale matrix computation problems. *Journal of Computational and Applied Mathematics*, 74(1-2):71–89, 1996.