

► **Trace estimator**

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

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

where  $\text{tr}(\cdot)$  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  $\text{tr}(A^{-1})$ .

- 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  $\text{tr}(A^{-1})$  by solving  $n$  linear systems.
- Computing  $\text{tr}(A^{-1})$  by estimating  $e_i^T A^{-1} e_i$  for  $i = 1, \dots, n$  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.