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Improved variants of the Hutch++ algorithm for trace estimation

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This work is concerned with two improved variants of the Hutch++ algorithm [2] for estimating the trace $\mathrm{tr}(\mathbf{A})$ of a square matrix $\mathbf{A}$, implicitly given through matrix-vector products. Hutch++ combines randomized low-rank approximation in a first phase with stochastic trace estimation in a second phase. In turn, Hutch++ only requires $O\left(\varepsilon^{-1}\right)$ matrix-vector products to approximate $\mathrm{tr}(\mathbf{A})$ within a relative error ε with high probability. This compares favorably with the $O\left(\varepsilon^{-2}\right)$ matrix-vector products needed when using stochastic trace estimation alone. In Hutch++, the number of matrix-vector products is fixed a priori and distributed in a prescribed fashion among the two phases. In this work, we derive an adaptive variant of Hutch++, which outputs an estimate of $\mathrm{tr}(\mathbf{A})$ that is within some prescribed error tolerance with a prescribed success probability, while splitting the matrix-vector products in a near-optimal way among the two phases. For the special case of symmetric positive semi-definite $\mathbf{A}$, we present another variant of Hutch++, called Nyström++, which utilizes the so called Nyström approximation [1] and requires only one pass over the matrix $\mathbf{A}$, as compared to two passes with Hutch++. We prove that the theoretical results on Hutch++ extend to Nyström++. Numerical experiments demonstrate the effectiveness of our two new algorithms.

References

[1] A. Gittens, M. W. Mahoney, *Revisiting the Nyström approximation for improved large-scale machine learning*, J. Mach. Learn., (2016), pp. 3977–4041.

[2] R. A. Meyer, C. Musco, C. Musco, D. P. Woodruff, *Hutch++: Optimal stochastic trace estimation*, In *Symposium on Simplicity in Algorithms (SOSA)*, SIAM, (2021), pp. 142–155.