

Bilinear Operations with Structured Tensors

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We consider approximate multiplication of d -dimensional matrices $\tilde{\mathbf{C}} \approx \mathbf{C} = \mathbf{A} \circ \mathbf{B}$, where \mathbf{A} and \mathbf{B} are given as Tucker or canonical decomposition with mode ranks r , “ \circ ” denotes any bilinear operation, and the result of this operation should be approximated also in the Tucker format with optimal values of ranks possible in the desired accuracy bound ε . Since mode sizes n can be very large, and mode ranks r also can reach values of about several hundreds, matrix \mathbf{C} should not appear as full array or as Tucker decomposition with mode ranks r^2 .

We address a number of algorithms to solve this problem. First, we propose by independent factor filtering and modified variable-rank Tucker-ALS procedure without a priori knowledge of ranks. We also propose cheap initialization of Tucker-ALS using an intrinsic tensor structure in $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}$. Then, we investigate the merits and drawbacks of the Tucker approximation via Krylov subspaces and the pre-filtering of individual mode factors. Finally, we show how one can apply recently developed Cross3D algorithm to the discussed recompression problem and obtain very fast and quite robust heuristic method.

Numerical examples include structured evaluation of typical operators from Hartree-Fock/Kohn-Sham model, by means of Canonical-to-Tucker and Tucker-to-Tucker multiplication.

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References

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