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Joint Usage / Research Center for Interdisciplinary Large-scale Information Infrastructures

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High-performance Randomized Matrix Computations for Big Data **Analytics and Applications**



Background

- Developing random sketching algorithms with high-performance implementations on supercomputers to compute singular value decomposition (SVD) and linear system (LS) solutions of very large-scale matrices.
- Few numerical solvers, especially randomized algorithms, are designed to tackle very large-scale matrix computations on the latest supercomputers..
- We intend to develop efficient sketching schemes to compute approximate SVD and LS solutions of large-scale matrices. The main idea is to sketch the matrices by randomized algorithms to reduce the computational dimensions and then suitably integrate the **sketches** to improve the accuracy and to lower the computational costs.
- We intend to implement the proposed algorithms on supercomputers. One essential component of this project is to develop effective automatic software auto-tuning (AT) technologies, so that the package can fully take advantage of the computational capabilities of the target supercomputers that include CPU homogeneous and CPU-GPU heterogeneous parallel computers.

Members

- Takahiro Katagiri (Nagoya U., Japan): AT (ppOpen-AT), parallel eigenvalue algorithms, and supercomputer implementations.
- Weichung Wang (National Taiwan U., Taiwan): Numerical linear algebra, parallel computing, and AT (surrogate-assisted turning). and big data
- Su-Yun Huang (Institute of Statistical Science, Academia Sinica, Taiwan): Mathematical statistics and machine learning (random sketching algorithm).
- Kengo Nakajima (U. Tokyo, Japan): Parallel algorithms in numerical iterative method (hybrid MPI/OpenMP execution).
- Osni Marques (LBNL, USA): Eigenproblem and its implementation (LAPACK, SVD algorithms).
- Feng-Nan Hwang (National Central U., Taiwan): Eigenproblem and its parallelization (SLEPc, SVD algorithms)
- Toshio Endo (TITECH, Japan): System software (optimizations for hierarchical memory and adaptation of its AT)
- (Collaborator) Akihiro Ida (U. Tokyo, Japan): Providing matrices by H-Matrix

iSVD Algorithm

Rank-k SVD

$oldsymbol{A}pproxoldsymbol{U}_{k}oldsymbol{\Sigma}_{k}oldsymbol{V}_{k}^{\perp}$

 U_k is an $m \times k$ orthonormal matrix that k < m, Σ_k is a $k \times k$ diagonal matrix, and V_k is an $n \times k$ orthonormal matrix. The columns of U_k and V_k are the leading left singular vectors and right singular vectors of A, respectively. The diagonal entries of Σ_k are the k largest singular values of A.

Research Plan

- Year 1 (FY2016): Algorithm development and testing environments deployment. (A prototyping)
- Year 2 (FY2017): Large-scale implementation and software integrations.
- Year 3: Auto-tuning of large-scale codes and tests of applications.

[By Ting-Li Chen, Su-Yun Huang, Hung Chen, David Chang, Chen-Yao Lin, and Weichung Wang]

Algorithm 2 Integrated SVD with multiple sketches (iSVD). **Require:** Input **A** (real $m \times n$ matrix), k (desired rank of approximate SVD), p (oversampling parameter), $\ell = k + p$ (dimension of the sketched column space), q(power of projection), N (number of random sketches) Ensure: Approximate rank-k SVD of $\boldsymbol{A} \approx \widehat{\boldsymbol{U}}_k \widehat{\boldsymbol{\Sigma}}_k \widehat{\boldsymbol{V}}_k^{\top}$ Generate $n \times \ell$ random matrices $\Omega_{[i]}$ for i = 1, ...

- 2: Assign $Y_{[i]} \leftarrow (AA^{\top})^q A\Omega_{[i]}$ for i = 1, ..., N with $\Omega_{[i]} = \Omega_{qp}$ or Ω_{cs} (in parallel) Compute $Q_{[i]}$ whose columns are orthonormal basis of $Y_{[i]}$ (in parallel)
- 4: Integrate $\overline{Q} \leftarrow \{Q_{[i]}\}_{i=1}^N$ (by Algorithm 3 or Algorithm 4)
- 5: Compute SVD of $\overline{Q}^{\top} A = \widehat{W}_{\ell} \widehat{\Sigma}_{\ell} \widehat{V}_{\ell}$
- Assign $\widehat{U}_{\ell} \leftarrow \overline{Q}\widehat{W}_{\ell}$
- 7: Extract the largest k singular-pairs from \widehat{U}_{ℓ} , $\widehat{\Sigma}_{\ell}$, \widehat{V}_{ℓ} to obtain \widehat{U}_{k} , $\widehat{\Sigma}_{k}$, \widehat{V}_{k}

Test Problem Test Problem for Low Rank Approximation ■Static electric field analysis size: N=300 × 300 Potential low-rank matrix := $\int_{\Gamma} \frac{1}{4\pi ||x - y||} u(y)dy$, Induced surface charge is calculated in half-infinite domain Permutation Mirror Image & partition by H-matrices (By Prof. Ida at U. Tokyo)

Errors

2.5E-15

2.0E-15

2.2E-15

1.0E+07 1.0E+06 1.0E+05 1.0E+03 1.0E+03 1.0E+02 1.0E+01 1.0E+01 1.0E+00 1.0E-01 • Frobenius Norm (FB) $||A - U\Lambda V^T||_F / ||A||_F$ $\sum_{i=1}^{T} (\|A - U\Lambda V^T\|_F / \|A\|_F)_i / T$ $\sqrt{(\sum_{i=1}^{T}(\|A - U\Lambda V^{T}\|_{F}/\|A\|_{F} - mean)_{i})^{2}}$

Distribution of Singular Values of A

(Full matrix: 300x300)

Value

Where T is the number of test trials of iSVD

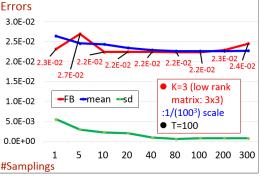
K=300 (low rank

·1/1 scale

● T=100

matrix: 300x300)

Results (Accuracy of Low Rank Approximation by iSVD)



Errors 1.4E-06 • K=30 (low rank 1.2E-06 matrix: 30x30) -FB -mean -sd 1.0E-06 :1/(103) scale T=100 8.0E-07 6.0E-07 4.0E-07 4.0E-07 3.7E-07 3.4E-07 3.2E-07 3.1E-07 3.1E-07 3.1E-07 2.0E-07 0.0E + 0010 20 40 80 100 200 300

1.5E-15 1.5E-15 1.4E-15 1.4E-15 1.0E-15 5.0F-16 0.0F+00 10 20 40 80 100 200 300

-FB -mean -sd

 $\bullet \Rightarrow$ If you accept accuracy of O(2E-02),

computation complexity is reduced to $O(1/100^3) = O(1/1,000,000)$

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