Communications in NLA

September 14, 2020

Mixed Precision Low Rank Compression of Data Sparse Matrices

Theo Mary

Sorbonne Université, CNRS, LIP6 https://www-pequan.lip6.fr/~tmary/ Slides available at https://bit.ly/CommNLA



Patrick Amestoy



Olivier Boiteau



Alfredo Buttari



Matthieu Gerest



Fabienne Jézéquel



Jean-Yves L'Excellent



	Bits			
	Signif. (†)	Exp.	Range	$u = 2^{-t}$
bfloat16	8	8	$10^{\pm 38}$	4×10^{-3}
fp16	11	5	$10^{\pm 5}$	5×10^{-4}
fp32	24	8	$10^{\pm 38}$	6×10^{-8}
fp64	53	11	$10^{\pm 308}$	1×10^{-16}
fp128	113	15	$10^{\pm 4932}$	1×10^{-34}

Half precision increasingly supported by hardware:

- Fp16 used by NVIDIA GPUs, AMD Radeon Instinct MI25 GPU, ARM NEON, Fujitsu A64FX ARM
- Bfloat16 used by Google TPU, NVIDIA GPUs, Arm, Intel

Benefits from low precisions

- Reduced storage and communications
- Increased speed, e.g., with GPU Tensor Cores



fp32 \rightarrow fp16 speedup evolution: P100: 2× V100: 8× A100: 16× (announced)

- Correspondingly low accuracy \Rightarrow mixed precision algorithms
- Mixed precision algs. highly successful in NLA: linear systems, matrix factorizations, matrix multiplication, iterative methods, least squares, EVD, SVD, matrix functions, FFT, and many others (see some references at the end of the slides)

Low rank compression

 $A \approx X Y^{T}$ $n \times n \qquad n \times r r \times n$ \longrightarrow

• ε -rank of A:

smallest r_{ε} such that $\exists T$, rank $(T) = r_{\varepsilon}$, $||A - T|| \le \varepsilon ||A||$

 Optimal ε-approximation given by truncated SVD (Eckart-Young)

$$A = U\Sigma V^{T} \quad \Rightarrow \quad T = U_{\varepsilon} \Sigma_{\varepsilon} V_{\varepsilon}^{T} = \sum_{i=1}^{r_{\varepsilon}} u_{i} \sigma_{i} v_{i}^{T}$$

- What precision should we store T in ?
- Naive answer: lowest possible precision with unit roundoff safely smaller than ε (e.g., fp64 if $\varepsilon < u_{\text{fp32}} \approx 6 \times 10^{-8}$)







• Assume $\varepsilon = 10^{-9} \Rightarrow \|A - U_{\varepsilon} \Sigma_{\varepsilon} V_{\varepsilon}^{T}\| \le \varepsilon \|A\|$



- Assume $\varepsilon = 10^{-9} \Rightarrow ||A U_{\varepsilon} \Sigma_{\varepsilon} V_{\varepsilon}^{T}|| \le \varepsilon ||A||$
- Naive approach: use **double precision** because $u_{\rm fp32} > \varepsilon$



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- Naive approach: use **double precision** because $u_{\rm fp32} > \varepsilon$
- Let $U_{\varepsilon} = [U_1 \ U_2]$, $\Sigma_{\varepsilon} = \text{diag}(\Sigma_1, \Sigma_2)$, and $V_{\varepsilon} = [V_1 \ V_2]$, such that $\|\Sigma_2\| \le \varepsilon/u_{\text{fp32}} \approx 2 \times 10^{-2}$



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- Let $U_{\varepsilon} = [U_1 \ U_2]$, $\Sigma_{\varepsilon} = \text{diag}(\Sigma_1, \Sigma_2)$, and $V_{\varepsilon} = [V_1 \ V_2]$, such that $\|\Sigma_2\| \le \varepsilon/u_{\text{fp32}} \approx 2 \times 10^{-2}$
- Our idea: converting U₂ and V₂ to single precision only introduces an error of order u_{fp32} ||Σ₂|| = ε

Error analysis

• Can use any number of precisions $u_1 \leq \varepsilon < u_2 < \ldots < u_p$

$$S_{k} = \left\{ i \leq r_{\varepsilon} : \frac{\varepsilon}{u_{k+1}} < \frac{\sigma_{i}}{\sigma_{1}} \leq \frac{\varepsilon}{u_{k}} \right\}, \quad k = 1: p$$
$$U_{k} \Sigma_{k} V_{k}^{T} = \sum_{i \in S_{k}} u_{i} \sigma_{i} v_{i}^{T} \quad \text{and} \quad \widehat{T} = \sum_{k=1}^{p} \widehat{U}_{k} \Sigma_{k} \widehat{V}_{k}^{T}$$

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where \widehat{U}_k and \widehat{V}_k are stored in precision u_k . Since for $k \geq 2$

$$\|U_k \Sigma_k V_k^{\mathsf{T}} - \widehat{U}_k \Sigma_k \widehat{V}_k^{\mathsf{T}}\| \le (2u_k + u_k^2) \|\Sigma_k\| \le (2 + u_k)\varepsilon \|\mathsf{A}\|$$

we obtain
$$\|A - \widehat{T}\| \le (2p - 1 + \sum_{k=2}^{p} u_k)\varepsilon\|A\| = O(\varepsilon)\|A\|$$

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$$\|\boldsymbol{A} - \widehat{\boldsymbol{T}}\| \leq (2p - 1 + \sum_{k=2}^{p} u_k)\varepsilon \|\boldsymbol{A}\| = O(\varepsilon)\|\boldsymbol{A}\|$$

Applicable to any low rank matrix XY^T = Σ^{rε}_{i=1} x_iy^T_i with decaying ||x_iy^T_i||. Example: AP ≈ QεRε = Q1R1 + ... + QpRp

Both matrices have ε -rank 30 (with $\varepsilon = 10^{-9}$) but present very different potential for mixed precision



Examples of spectrum



Data sparse matrices

• Data sparse matrices arise in several applications: BEM, PDEs, covariance matrices, ...



- They possess a block low rank structure: a block B represents the interaction between two subdomains
 ⇒ singular values decay rapidly for far away subdomains
- \Rightarrow High potential for mixed precision compression

BLR matrices (Amestoy et al.) use a flat 2D block partitioning



- Diagonal blocks are full rank
- Off-diagonal ones are stored in low rank form if their ε-rank is small enough

•
$$\varepsilon = 10^{-15} \rightarrow 50\%$$
 entries kept

Example of a BLR matrix (Schur complement of a 64^3 Poisson problem with block size 128)

BLR matrices (Amestoy et al.) use a flat 2D block partitioning



• Diagonal blocks are full rank

 Off-diagonal ones are stored in low rank form if their ε-rank is small enough

$$ho~arepsilon=10^{-15}
ightarrow$$
 50% entries kept

•
$$\varepsilon = 10^{-12} \rightarrow 36\%$$
 entries kept

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Example of a BLR matrix (Schur complement of a 64^3 Poisson problem with block size 128)

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- $\varepsilon = 10^{-15} \rightarrow 50\%$ entries kept
- $\varepsilon = 10^{-12} \rightarrow 36\%$ entries kept

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$$\varepsilon = 10^{-9} \
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 23% entries kept

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- $\varepsilon = 10^{-15} \rightarrow 50\%$ entries kept
- $\varepsilon = 10^{-12} \rightarrow 36\%$ entries kept
- $\varepsilon = 10^{-9} \
 ightarrow$ 23% entries kept

Example of a BLR matrix (Schur complement of a 64^3 Poisson problem with block size 128)

Hierarchical data sparse matrices (\mathcal{H} , HSS, ...) not covered in this talk, but could also benefit from mixed precision

Local vs global uniform precision compression

Should we approximate block $A_{ij} \approx T_{ij}$ such that

 $\|A_{ij} - T_{ij}\| \le \varepsilon \|A_{ij}\|$ (local compression)

or $\|A_{ij} - T_{ij}\| \le \varepsilon \|A\|$ (global compression)?

- Global compression increases approximation error by a factor at most the number of block-rows/columns
- Generally worth the extra compression coming from blocks of norm less than ||A|| (Higham & M., 2020)



Local compression (38% entries kept)



Global compression (23% entries kept)

• The set of singular vectors stored in precision u_k for block $A_{ij} = U^{(ij)} \Sigma^{(ij)} V^{(ij)T}$ is

$$S_{k}^{(ij)} = \left\{ \ell \leq r_{\varepsilon} : \frac{\varepsilon}{u_{k+1}} < \frac{\sigma_{\ell}^{(ij)}}{\sigma_{1}^{(ij)}} \leq \frac{\varepsilon}{u_{k}} \right\} \quad \text{(local compression)}$$
$$S_{k}^{(ij)} = \left\{ \ell \leq r_{\varepsilon} : \frac{\varepsilon}{u_{k+1}} < \frac{\sigma_{\ell}^{(ij)}}{\|A\|} \leq \frac{\varepsilon}{u_{k}} \right\} \quad \text{(global compression)}$$

⇒ With global compression, S_1 may be empty for some blocks Example: with double and single precisions, blocks such that $||A_{ij}|| \le \varepsilon/u_{\text{fp32}}||A||$ can be stored entirely in single precision





• Full rank blocks (near field) are in double precision



- Full rank blocks (near field) are in double precision
- Far field blocks are in single precision



- Full rank blocks (near field) are in double precision
- Far field blocks are in single precision
- Mid field blocks are in mixed precision

• Dense matrices obtained from the root separator (Schur complement) of sparse matrices

Matrix	Application	n
audikw_1	Structural	3768
Fault_639	Structural	7983
nd24k	2D/3D	7785
GaAsH6	Chemistry	6232
cage12	Graph	7323
thermal2	Thermal	1382

• Block size is set to 128





Up to 1.7 imes storage reduction with almost no error increase

14/18



14/18

Up to 2.2 imes storage reduction with almost no error increase



14/18

Up to 2.7 imes storage reduction with almost no error increase



Gain due to mixed precision increases with problem size: $1.6\times$ (smallest) $\rightarrow 1.9\times$ (largest) storage reduction

Mixed precision factorization of data sparse matrices

- Data sparse matrices can be factorized at a much lower cost than dense matrices
- Mixed precision can be used to further reduce this cost
- Example: a mixed precision low rank matrix \widehat{T} can be multiplied with a vector v

$$\widehat{T}\mathbf{v} = \left(\sum_{k=1}^{p} \widehat{U}_k \Sigma_k \widehat{V}_k^T\right) \mathbf{v} = \sum_{k=1}^{p} \widehat{U}_k \Sigma_k \widehat{V}_k^T \mathbf{v}$$

by computing $\widehat{U}_k \Sigma_k \widehat{V}_k v$ in precision u_k

• Other NLA operations can also be accelerated

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- Other NLA operations can also be accelerated
- Error analysis of BLR factorization in uniform precision *u* (Higham and M., 2020) shows that

 $A + \Delta A = LU, \quad \|\Delta A\| \le c_1 \varepsilon \|A\| + c_2 u \|L\| \|U\|$

• Analysis can be generalized to mixed precision (ongoing work) with only a modest increase of c_1



Flops compression ($\varepsilon = 10^{-9}$) fp64 fp64/fp32 fp64/fp32/bf16 30 Compression 20 10 0 audikw_1 Fault_639 nd24k GaAsH6 cage12 thermal2 Error ($\varepsilon = 10^{-9}$) 10⁻⁷ 10⁻⁸ 10-9 audikw 1 Fault_639 nd24k GaAsH6 cage12 thermal2

Up to 3.3 imes flops reduction with almost no error increase

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ightarrow 3.3 imes time reduction??

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ightarrow 3.3 imes time reduction?? 7.0 imes with GPU tensor cores

Conclusions

Mixed precision SVD

- Given a matrix A and a target accuracy ε , in what precision should we represent A?
- Naive answer: the lowest precision with unit roundoff less than arepsilon
- Our answer: it depends on its singular values!
- \Rightarrow If rapidly decaying, precisions lower than arepsilon can be used
 - Also applicable to QR and many other low rank decompositions

Mixed precision compression of data sparse matrices

- Data sparse matrices are an ideal application due to their block low-rank structure
- Achieved up to $2.7 \times$ storage reduction with fp64/fp32/bfloat16
- Can also accelerate factorization, up to $3.3 \times$ flops reduction
- \Rightarrow Much work still needed to transform flops into time reduction!

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