Performance of Random Sampling for Computing Low-rank Approximations of a Dense matrix on GPUs

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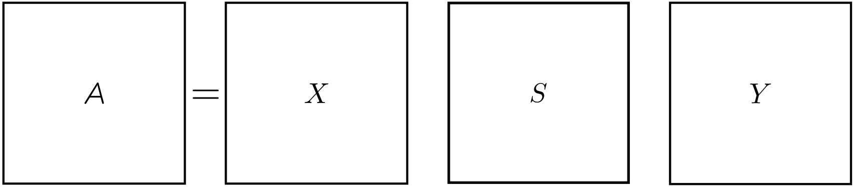
Take a dense matrix A of size $m \times n$ and compute its SVD $A = XSY$:



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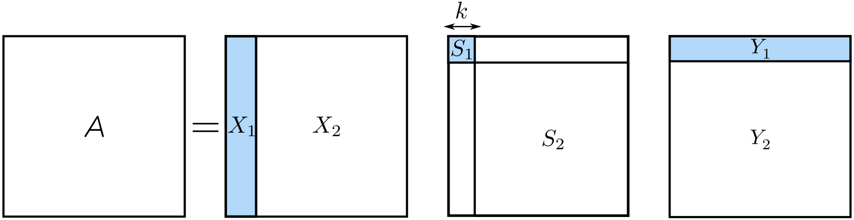

$$A = X_1 S_1 Y_1 + X_2 S_2 Y_2 \quad \text{with} \quad S_1(k,k) = \sigma_k > \varepsilon,\ S_2(1,1) = \sigma_{k+1} \leq \varepsilon$$

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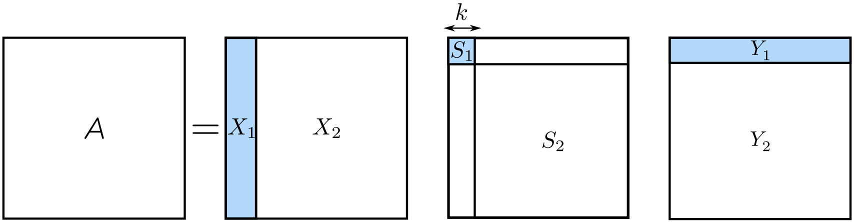

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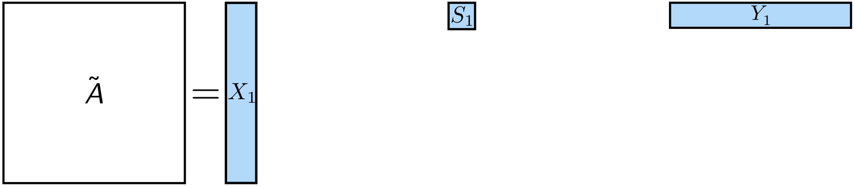

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If the singular values of A decay very fast (e.g. exponentially) then $k \ll \min(m,n)$ even for very small ε (e.g. 10^{-14})
$\Rightarrow$ memory and CPU consumption can be reduced considerably with a controlled loss of accuracy ($\leq \varepsilon$) if $\tilde{A}$ is used instead of A

QRCP Decomposition

- QR decomposition with Column Pivoting

$$AP = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_{11} & R_{12} \\ & R_{22} \end{pmatrix}$$

  with
  - $Q = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix}$ a $m \times n$ matrix with orthogonal colums;
  - $R = \begin{pmatrix} R_{11} & R_{12} \\ & R_{22} \end{pmatrix}$ a $n \times n$ upper triangular matrix;
  - P a $n \times n$ pivot matrix.
- Truncated QRCP

$$\underset{m \times n}{AP} \approx \underset{m \times k}{Q_1} \underset{k \times n}{\begin{pmatrix} R_{11} & R_{12} \end{pmatrix}}$$

LAPACK's QP3

- QP3 computes a QR with column pivoting factorization using BLAS-3 kernels.
- We modified the code to get the truncated version.
- Limitations:
  - Not only BLAS-3: also BLAS-2;
  - Synchronization at every step to pick pivot;
  - Limited parallelism and data locality;
  - Communications.
  - Column norms may diverge $\rightarrow$ need to recompute and update.

Random Sampling: Overview

- **Stage A**: generate Q, orthogonal subspace spanning the range of A, i.e.:
$$A \approx AQ^T Q$$
- **Stage B**: use Q to compute low-rank approximations of A (QR, SVD, ...) with standard deterministic methods.

Stage A: Sampling

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- To avoid round-off errors, we need to reorthogonalize B between each application of A and A^T.

Communications

- Two memory levels hierarchy: fast/slow (M = size of fast memory).

	#flops	#words
Random sampling		
Sampling (Gaussian)	$\mathcal{O}(mn\ell)$	$\mathcal{O}(mn\ell/M^{1/2})$
Sampling (FFT)	$\mathcal{O}(mn\log(m))$	$\mathcal{O}(mn\log(m)/\log(M))$
Iter. (mult.)	$\mathcal{O}(mn\ell q)$	$\mathcal{O}(mn\ell q/M^{1/2})$
Iter. (orth.)	$\mathcal{O}((m+n)\ell^2 q)$	$\mathcal{O}((m+n)\ell^2 q/M^{1/2})$
QRCP	$\mathcal{O}(n\ell^2)$	$\mathcal{O}(n\ell^2)$
QR	$\mathcal{O}(m\ell^2)$	$\mathcal{O}(m\ell^2/M^{1/2})$
Total	$\mathcal{O}(mn\ell(1+2q))$	$\mathcal{O}(mn\ell(1+2q)/M^{1/2})$
QP3	$\mathcal{O}(mnk)$	$\mathcal{O}(mnk)$
CAQP3	$\mathcal{O}(mn(m+n))$	$\mathcal{O}(mn^2/M^{1/2})$

Figure : Computation and communication costs on one GPU.

- Random sampling has a flop overhead (oversampling + power iterations), but...
- ...much better communications efficiency

Experimental Setups

- Compiled with `gcc` 4.4.7 and `nvcc` (CUDA 6.0.1), with `-O3` flag, linked to threaded MKL (version 10.3).
- Machine: two eight-core Genuine Intel(R) 2.60GHz CPUs and three NVIDIA Tesla K40c GPUs.

	Matrix Name		
	POWER	EXPONENT	HAPMAP
σ_i	$(i+1)^{-3}$	$10^{-i/10}$	--
σ_0	1	1	9.9e+03
σ_{k+1}	8e-06	1.3e-05	5e+02
$\kappa(A)$	1.3e+05	7.9e+04	2e+01
m	500,000	500,000	503,783
n	500	500	506
k	50	50	50
p	10	10	10
ℓ	60	60	60

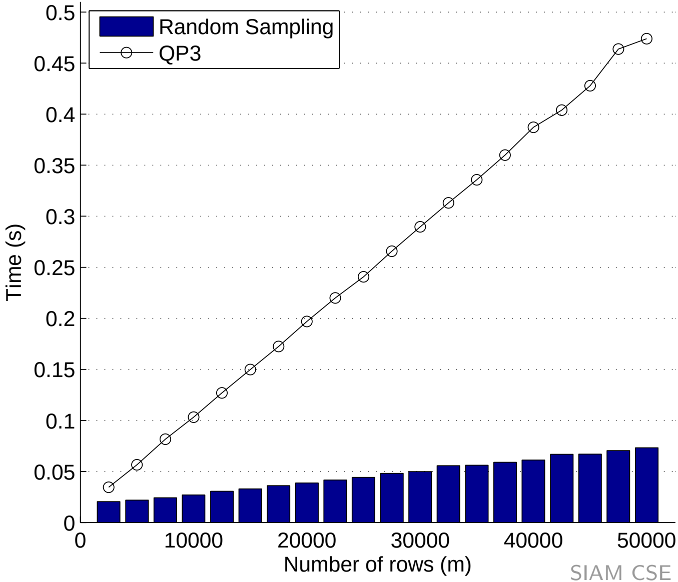
Table : Test matrices.

	QP3	Random Sampling		
		$q = 0$	$q = 1$	$q = 2$
POWER	4.47e-05	9.08e-05	4.59e-05	4.45e-05
EXPONENT	2.69e-05	5.18e-05	2.69e-05	2.69e-05
HAPMAP	5.99e-01	9.86e-01	8.74e-01	8.18e-01

Figure : Approximation error norm $\|AP - QR\| / \|A\|$.

The same order of accuracy is already reached with $q = 0$.

Time with different numbers of rows (m)



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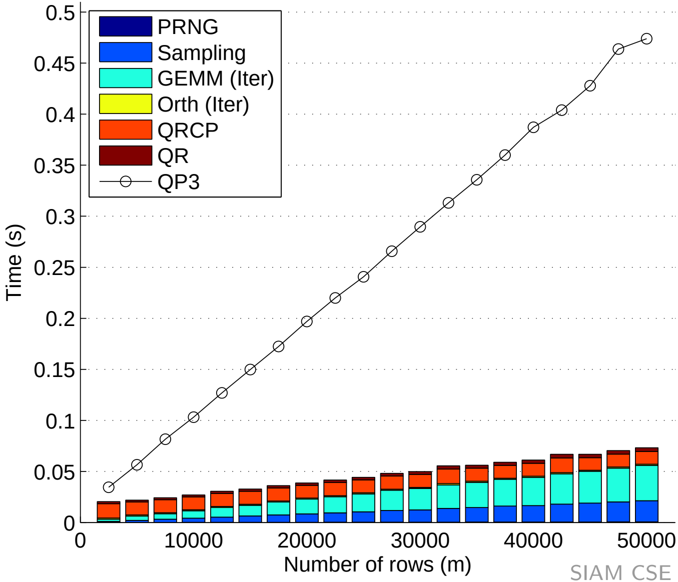
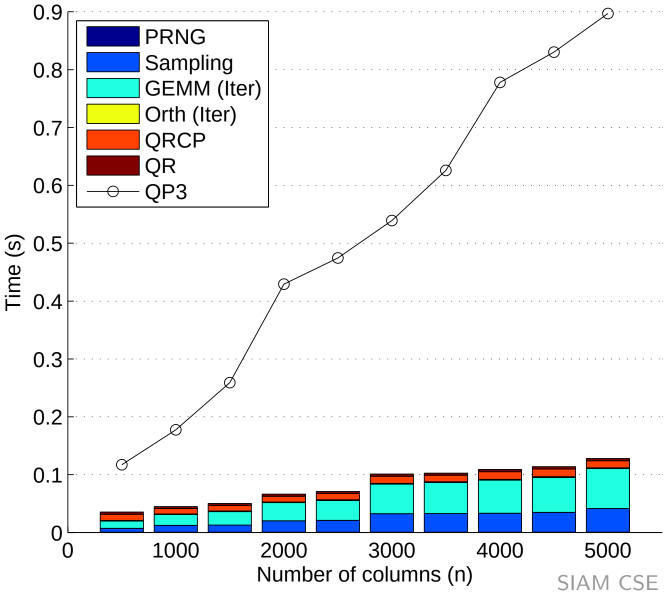
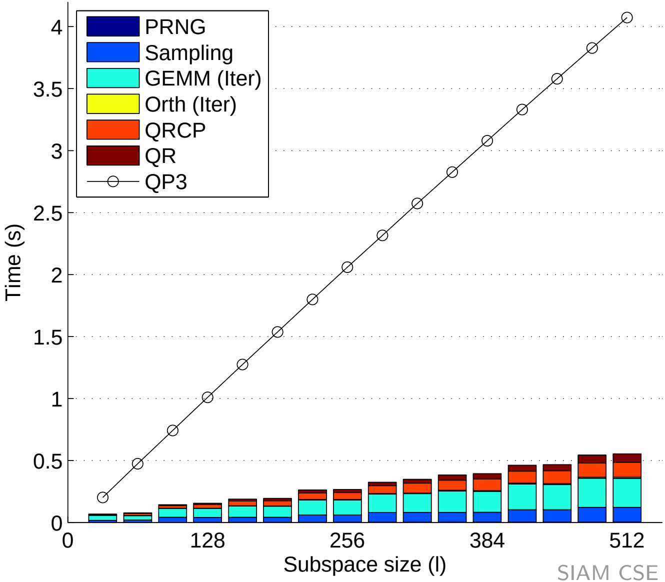


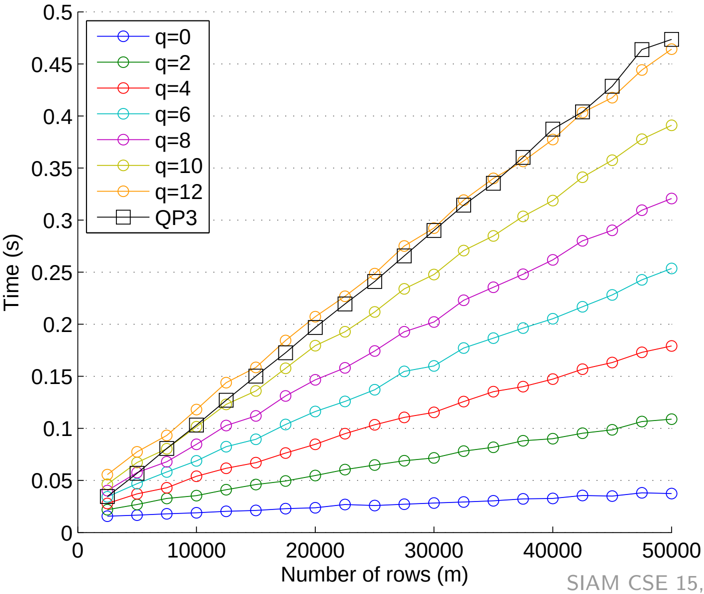
Time with different numbers of columns (n)



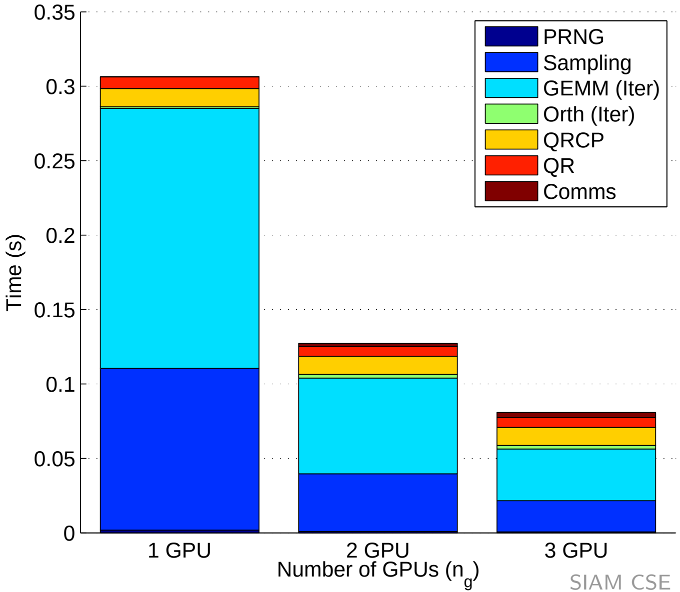
Time with different subspace sizes (ℓ)



Time with different numbers of iterations (q)



Time on 1, 2 and 3 GPUs



Conclusion

Summary: Random Sampling vs. QP3

- Comparable accuracy on the test matrices used.
- Small flop overhead but substantial communication improvement $\Rightarrow$ performance speedups above 13.
- Scaling on multiple GPUs.

Reference

- MS 266 & 291: Randomized Algorithms in Numerical Linear Algebra
  - Performance of Computing Low-Rank Approximation on Hybrid CPU/GPU Architectures

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Thanks!

Questions?