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An Approximate Singular Value Decomposition of Large Matrices in Julia

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Motivation behind an Approximate SVD

- The singular value decomposition (SVD) is a widely used algorithm:
 - Data compression: allows for compact representation of matrices
 - Data assimilation: determine fastest growing perturbations
- Does not scale well: $O(n^3)$ for a square matrix

$$\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$$

- Approximate algorithm based on Friedland et al., (2009)
 $\mathbf{B} pprox \mathbf{A}_k = \mathbf{U}_k \mathbf{\Sigma}_k \mathbf{V}_k^T$
- Two attractive features:
 - Better scaling: $O(kn^2)$ for a square matrix
 - Small memory footprint



Description of the Algorithm

Psuedocode

1	C =	rand_cols(A,k)
2	x =	run_orth(C)
3	(Bx,By) =	compute_B(X,A,k)
4	N =	compute_norm(Bx,By,k)
5	while iter	== true
6	С	= rand_cols(A, ℓ)
7	Х	<pre>= run_orth(hcat(X,C))</pre>
8	G	= compute_G(X, A, $k+l$)
9	(\bigcirc, λ)	= eig_G(G, k, <i>l</i>)
10	(U,S)	= $svd_G(X, O, \lambda)$
11	(Bx,By)	= compute_B(U,A,k)
12	N	<pre>= compute_norm(Bx,By,k)</pre>
13	end	

Algorithm

Explanation

- 1 Randomly draw "k" columns from "A"
- 2 Obtain an orthonormal set from the columns
- 3 Construct the "B" matrix using the \perp set
- 4 Compute the norm of "B"
- 5 Begin iterating
- 6 Randomly draw "*l*" more columns
- 7 Obtain a new \perp set
- 8 Construct the "G" matrix using the \perp set
- 9 Compute the eigenvectors/values of "G"
- 10 Compute the SVD of "G"
- 11 Compute the "B" using the SVD of "G"
- 12 Compute the norm of "B"
- 13 Iterate
- Iteratively sample A and obtain orthonormal sets
 - Uses QR factorization to obtain orthonormal set

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- Apply orthonormal sets to the A matrix
 - Main bottleneck: O(kmn) complexity

Algorithm

- Takes either AbstractMatrices or DArrays
 - Algorithm proceeds differently depending on the array type
- Compactly store matrices as, $\mathbf{B} = \mathbf{x}_1 \mathbf{y}_1^T + \mathbf{x}_2 \mathbf{y}_2^T + \ldots + \mathbf{x}_k \mathbf{y}_k^T$
- k pairs of $[m \times 1]$, $[n \times 1]$ vectors instead of an $[m \times n]$ matrix
 - k(m+n) elements instead of mn elements
- Never actually construct the full B



▶ Two validation cases: "rand (N_x, N_y)" & "randn (N_x, N_y)"

• True error:
$$\epsilon_T = \frac{||\mathbf{A} - \mathbf{A}_k||_F}{||\mathbf{A}||_F}$$

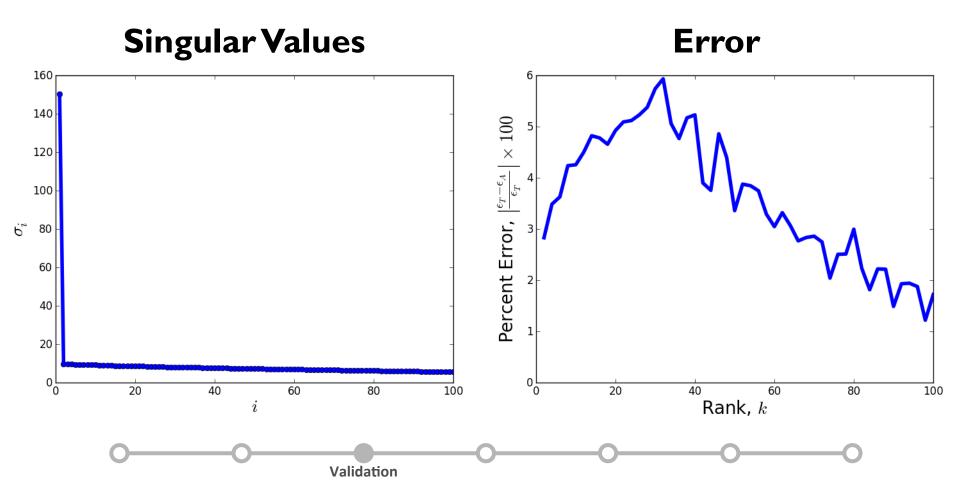
• Approximation error:
$$\epsilon_A = rac{||\mathbf{A} - \mathbf{B}||_F}{||\mathbf{A}||_F}$$

Validation

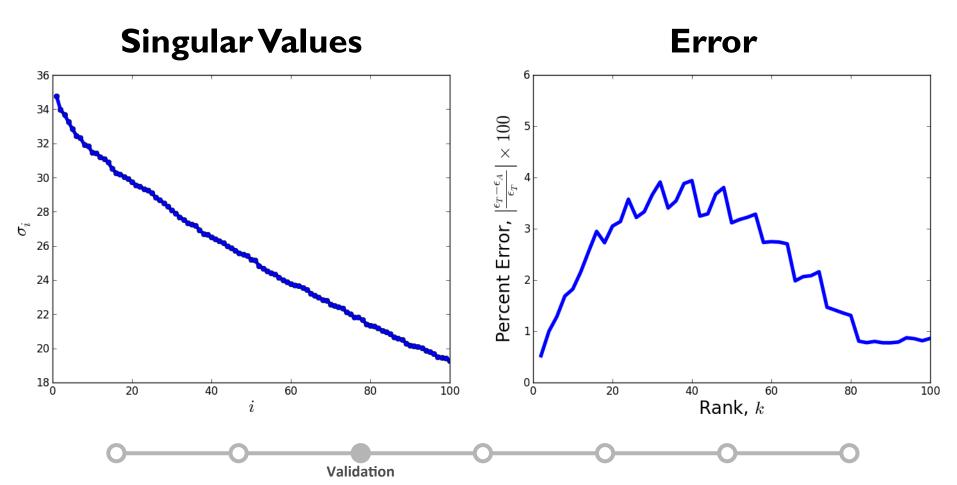
• Error added from approximation: $\epsilon =$

$$= \left| \frac{\epsilon_T - \epsilon_A}{\epsilon_T} \right| \times 100$$

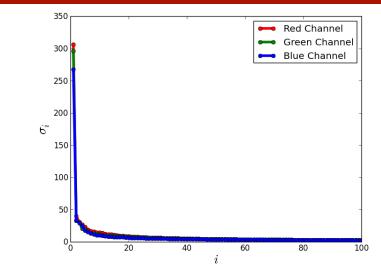
- ▶ "rand (N_x, N_y)" case
 - Sharp dropoff in the eigenvalue spectrum
 - ▶ N_x, N_y = 300



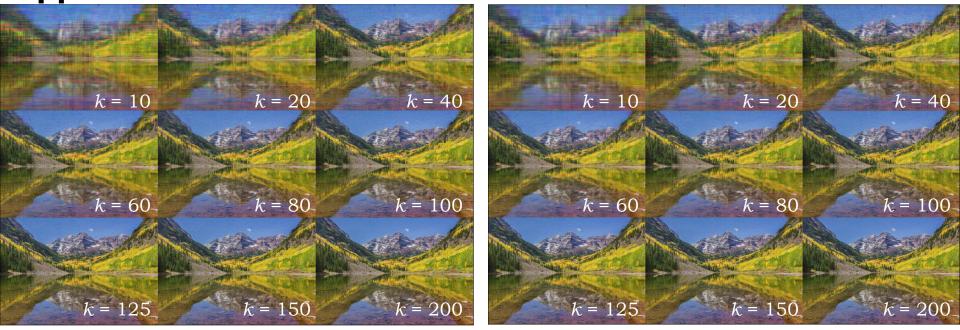
- "randn (N_x, N_y)" case
 - Smooth dropoff in the eigenvalue spectrum
 - ▶ N_x, N_y = 300



- Testing with a real image
- Fairly sharp eigenvalue dropoff
 - Original image is [800×542]



Approximated



Validation

True

Profiling the Code

Profiling

- Developed a code profiler
- Allowed me to quickly determine bottlenecks
 - Helped me choose the norm
- Helped me choose default parameters

julia> svd approx(rand(10000,10000)) ITER 0: rand cols - 43.20% ITER 0: run_orth - 2.44% ITER 0: compute B - 48.75% ITER 0: compute norm - 5.61% ITER 0: 1.65529299 seconds ITER 1: rand cols - 3.82% 1: run_orth - 2.32% ITER ITER 1: compute G - 44.73% ITER 1: eig_G - 2.10% ITER 1: svd G - 0.33% ITER 1: compute B - 43.40% ITER 1: compute norm - 3.29% TTER 1: 3.21842003 seconds Exited at iter 8 in 64.67 seconds

Optimizations

- Direct calls to the BLAS/LAPACK
 - QR factorization (DGEQRF + DORGQR)
 - Matrix-Vector multiplication (DGEMV)
- Parallel matrix multiplication
 - ▶ Need to perform k matrix-vector multiplications at every iteration:

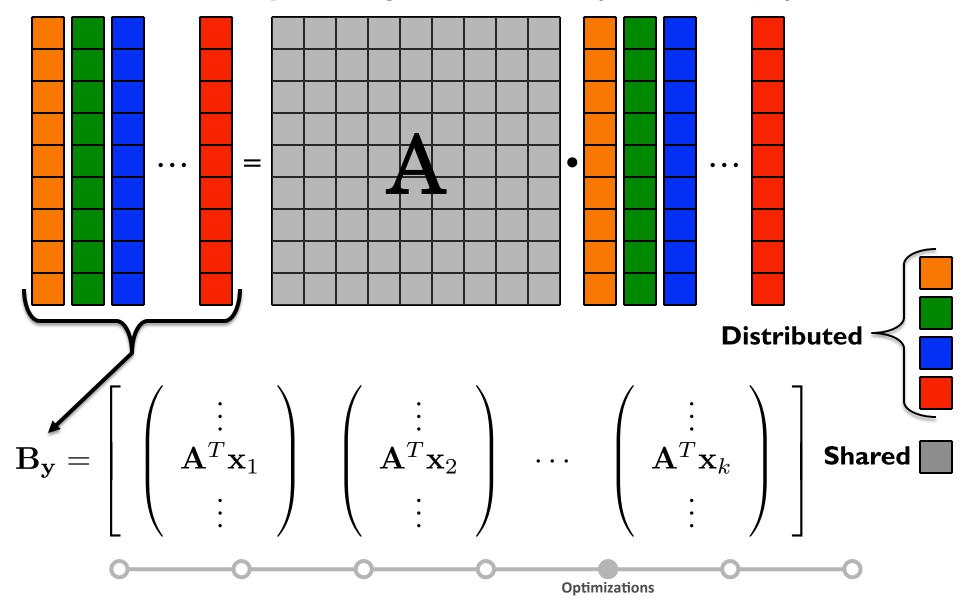
$$\mathbf{B} = \sum_{i=1}^{k} \mathbf{x}_{i} \left(\mathbf{A}^{T} \mathbf{x}_{i} \right)^{T}$$

 Can do them in simultaneously in parallel or can break them into smaller matrix-vector multiplications

Optimizations

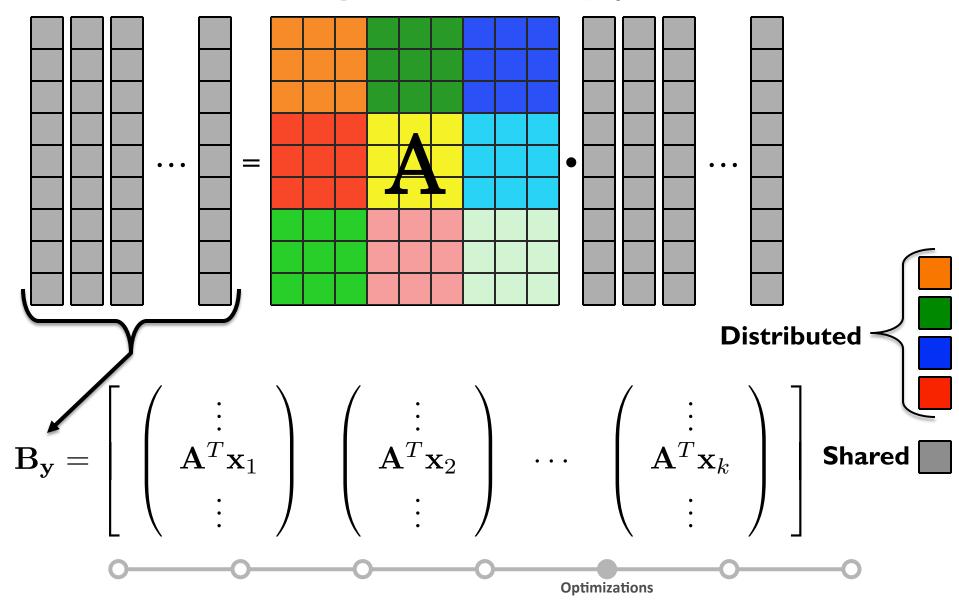
Optimizations: A Tale of Two DGEMVs

Shared Memory: k large DGEMVs in parallel on p processors



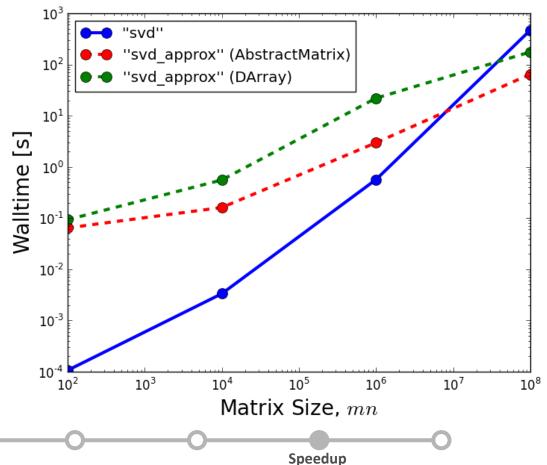
Optimizations: A Tale of Two DGEMVs

Distributed Memory: A broken into *p* parts, *k* serial DGEMVs



Speedup: Matrix Size

- For the approximate SVD against the built in serial SVD ("(U, S, V) = svd(A)")
 - "svd (A)" should scale as O(mn²)
 - "svd_approx(A)" should scale as O(kmn)
- Approximate SVD does exhibit better scaling
 - ▶ svd_approx @ 10⁸:64s
 - ▶ svd @ 10⁸: 468s
- Only use approximate
 SVD for large matrices



Summary

- Implemented an approximate SVD in Julia

 - Scales as O(kmn) instead of $O(mn^2)$ for standard SVD
- Currently works with both AbstractMatrices and DArrays
 - Different algorithm based on the user input
- Excellent speedup for large matrices (>10⁸ elements)