Large Sparse SVD in CUDA

1 Abstract

In this project report, we review the theory of the Singular Value Decomposition (SVD), applications of the SVD to Principal Component Analysis (PCA), different algorithms for computing the SVD, and state-of-the-art computational implementations for the SVD. We also present a CUDA implementation using cuBLAS and cuSPARSE for Golub-Kahan-Lanczos Bidiagonalization procedure, which is the most expensive step in computing the SVD of large sparse matrices.

2 The Singular Value Decomposition

The Singular Value Decomposition (SVD) of a rectangular matrix $A \in \mathbb{R}^{m \times n}$ is given by $A = U\Sigma V^T$, where $U \in \mathbb{R}^{m \times n}$ is orthogonal, $\Sigma \in \mathbb{R}^{n \times n}$ is diagonal, and $V \in \mathbb{R}^{n \times n}$ is orthogonal [4]. The columns of U, also known as the left singular vectors, form an orthogonal basis for the column space of A, while the columns of V, also known as the right singular vectors, form an orthogonal basis for the column space of A^T. The SVD of a matrix A is related to the eigenvalue decomposition of $A^T A$ because the eigenvectors of $A^T A$ are the columns of V and the eigenvalues of $A^T A$ are the square of the singular values of A. Another useful property of the SVD is due to the Eckhart-Young Theorem, which says that if $k < r$, where r is the rank of A, and $A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T$ where the singular values σ_i are of decreasing magnitude, the u_i are the columns of U, and the v_i are the columns of V, then A_k is the closest rank-k approximation to A in the 2-norm and the Frobenius norm. If the singular values of the matrix decay rapidly, then approximating A by A_k for a small k will significantly reduce storage requirements while maintaining a very good approximation of the original matrix.

3 Principal Component Analysis

Principal Component Analysis (PCA) was invented in 1901 by Karl Pearson in the context of statistical correlation theory. Let a dataset be represented by a matrix, where a data point is represented by column in that matrix. For instance, the Netflix matrix of users and ratings has each column represent a user's set of ratings for each movie. The first principal component of a dataset accounts for as much variability in the data as possible, and each next principle component has the highest possible variance in a direction orthogonal to all preceding components. It turns out that PCA can be computed using the SVD. Typically, only the first $k << n$ principal components are needed because it is know that a small number of orthogonal vectors can describe the variance in the data very well. For the Netflix matrix, it has been shown that peoples ratings can often

be described by a small low-rank subset of factors, like preference for historical drama, psychological thrillers, or comedy movies starring Vince Vaughn. Computing the top k principal components corresponds to computing the top k singular triplets: σ_i, u_i, v_i for $i = 1, \ldots, k$. As we will see, there are different ways of computing the SVD: some compute all n singular triplets, while some allow you to compute just a subset of $k << n$. For PCA, computing the full SVD is would be followed by discarding the non-principal components. Thus, it would be more efficient to only compute the principal components necessary in the first place. Related problems such as Noisy Matrix Completion and Noisy Robust PCA require computing the top k singular triplets at each step of an iterative method for convex constrained optimization such as Accelerated Proximal Gradient [8].

4 Algorithms for Computing the SVD

4.1 Dense SVD Frameworks

Many SVD algorithms start by Householder reduction to bidiagonal form. Then using the Golub-Kahan step, Demmel-Kahan step, Bisection step, or the Divide and Conquer method of Gu and Eisenstat (1995), it is possible to compute the singular values and singular vectors of the bidiagonal matrix [3]. Combining the singular vectors with the Householder reduction, we can form the SVD of the matrix as a whole. Other methods such as Biorthogonalization and Jacobi Rotation iterate directly on the input matrix [3]. All of these methods require the whole matrix to be in memory and can only compute the full SVD.

4.2 Sparse SVD Frameworks

Instead of assuming that the whole matrix is in memory, let's assume that we have an efficient way of applying our matrix A to a vector x. This can be a sparse matrix vector multiplication, or any other way of applying A to a vector which takes less than $O(mn)$ flops. The Lanczos procedure builds an orthogonal basis for the k dimensional Krylov subspace of A given by span$\{r, Ar, \ldots, A^{k-1}r\}$ for some vector r with just matrix vector products. The Golub-Kahan-Lanczos Bidiagonalization procedure uses this approach to reduce any rectangular matrix A to bidiagonal form without the hassle of requiring dense intermediate matrices, as is required by the Householder reduction to bidiagonal form. Even further, Golub-Kahan-Lanczos Bidiagonalization can compute top k singular triplets for any $k \leq n$, so it doesn't need to compute the full SVD. This bidiagonalization procedure would then be followed by an algorithm for computing the singular values and singular vectors of a bidiagonal matrix, such as the Divide and Conquer method of Gu and Eisenstat, which is considered state-of-the-art.

Algorithm 1 describes the Golub-Kahan-Lanczos Bidiagonalization procedure. The input consists of a matrix $A \in \mathbb{R}^{m \times n}$ where $A(1:n, 1:n)$ is nonsingular, a unit vector $u_c \in \mathbb{R}^n$ and the number of desired singular triplets $K \leq n$. Output is $\alpha \in \mathbb{R}^k, \beta \in \mathbb{R}^k, U \in \mathbb{R}^{m \times k}, V \in \mathbb{R}^{k \times k}, p \in \mathbb{R}^m$, such that $AV(:, 1{:}k) = U(:, 1{:}k)B(1{:}k, 1{:}k) + p_k e_k^T$ where $1 \leq k \leq K, B = \text{spdiags}([\alpha, \beta], [0, -1], k, k)$ and e_k is the k-th column of the k by k identity matrix. The first column of U is u_c. Notice that most of the work goes into matrix-vector multiplication at lines 5 and 8.

Algorithm 1 Golub-Kahan-Lanczos Bidiagonalization

 1: **procedure** GKL-BIDIAG(A, u_c, K)
 2:     $k := 1, p_0 = u_c, \beta_1 = 1, v_0 = 0$
 3:     **while** $\beta_k > 0, k < K$ **do**
 4:         $u_k := p_{k-1}/\beta_k$
 5:         $r_k := A^T u_k - \beta_k v_{k-1}$ ▷ Matrix-vector multiply
 6:         $\alpha_k := \|r_k\|_2$
 7:         $v_k := r_k/\alpha_k$
 8:         $p_k := Av_k - \alpha_k u_k$ ▷ Matrix-vector multiply
 9:         $\beta_{k+1} := \|p_k\|_2$
10:         $k := k + 1$
11:     **end while**
12:     **return** $\alpha, \beta, U = [u_1|\cdots|u_k], V = [v_1|\cdots|v_k], p_k$
13: **end procedure**

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5   Current SVD Implementations

Both of the dense categories described below require the entire matrix in memory and can only compute the full SVD. The sparse category only requires a function for matrix vector multiplication and the software mentioned is best suited for computing the largest $k << n$ singular triplets of large sparse matrices.

5.1   Dense Serial SVD Software

State-of-the-art routines for the SVD of a dense matrix include LAPACK [2] and Intel MKL [10] implementations of xGESVD (Householder reduction to bidiagonal form followed by Demmel-Kahan bidiagonal SVD) and xGESDD (Householder reduction to bidiagonal form followed by Divide and Conquer bidigaonal SVD). xGESVD uses less memory than xGESDD, but xGESDD is typically faster. MATLAB decides internally whether to use xGESVD or xGESDD in the svd function. LAPACK is free research software while Intel MKL is proprietary.

5.2   Dense Shared Memory Parallel SVD Software

In shared memory, MAGMA [1] and CULA [5] implement xGESVD and xGESDD. They both use cuBLAS [9] to speedup the corresponding dense serial algorithms. MAGMA is completely free and open source research software while CULA is commercial and closed source.

5.3   Sparse SVD Software

Both ARPACK [7] and PROPACK [6] can use an operator for matrix vector multiplication instead of storing the whole matrix in memory, and are both considered state-of-the-art software for computing the largest $k << n$ singular triplets of large sparse matrices. ARPACK, which called by MATLAB's eigs and svds functions, is designed to solve eigenvalue problems, but it can be adapted for SVD computation with some post-processing. ARPACK has a distributed memory Fortran implementation. PROPACK

is specifically for SVD computations and consistently outperforms ARPACK for large
sparse SVD problems in serial.

6   Sparse SVD Implementation in CUDA

Given the three categories in the previous section, one would expect that there should
also be a section for Sparse Shared Memory Parallel SVD computation. However, after
doing some research, I could not find a standard state-of-the-art software package for large
sparse SVD computations in shared memory. Hence, I present a CUDA implementation
the Golub-Kahan-Lanczos Bidiagonalization procedure to allow for computation of the
top k singular triplets of large sparse matrices. I make significant use of the cuBLAS
and cuSPARSE libraries from NVIDIA. I use cublasSscal for scaling a vector by a scalar,
cublasScopy to copy a vector into another vector, cusparseScsrmv for sparse matrix vec-
tor multiplication using Compressed Sparse Row storage of the matrix, cublasSaxpy for
adding a vector by a scaled vector, and cublasSnrm2 to get the 2-norm of a vector. The
core of the implementation, excluding malloc's and memcpy's, is below:

```
beta[0] = 1;
int k = 0;
// Begin iteration
while (k < K && beta[k] > 0)
{
  if (k > 0)
  {
    // U(:,k) = p/beta(k);
    work = 1/beta[k];
    cublasStatus = cublasSscal(cublasHandle, N, &work, d_p, 1);
    cublasStatus = cublasScopy(cublasHandle, M, d_p, 1, &d_U[k*M], 1);
    // r = A'*U(:,k) - beta(k)*V(:,k-1);
    cusparseScsrmv(cusparseHandle, CUSPARSE_OPERATION_TRANSPOSE, M, N, nz,
                   &one, descr, d_val, d_row, d_col, &d_U[k*M], &zero, d_r);
    work = -beta[k];
    cublasStatus = cublasSaxpy(cublasHandle, N, &work, &d_V[(k-1)*N], 1, d_r, 1);
  } else {
    // U(:,k) = p;
    cublasStatus = cublasScopy(cublasHandle, M, d_p, 1, &d_U[k*M], 1);
    // r = A'*U(:,k);
    cusparseScsrmv(cusparseHandle, CUSPARSE_OPERATION_TRANSPOSE, M, N, nz,
    &one, descr, d_val, d_row, d_col, &d_U[k*M], &zero, d_r);
  }
  // alpha(k) = norm(r);
  cublasSnrm2(cublasHandle, N, d_r, 1, &alpha[k]);
  // V(:,k) = r/alpha(k);
  work = 1/alpha[k];
  cublasStatus = cublasSscal(cublasHandle, N, &work, d_r, 1);
  cublasStatus = cublasScopy(cublasHandle, N, d_r, 1, &d_V[k*M], 1);
  // p = A*V(:,k) - alpha(k)*U(:,k);
  cusparseScsrmv(cusparseHandle, CUSPARSE_OPERATION_NON_TRANSPOSE, M, N, nz,
```

```
                &one, descr, d_val, d_row, d_col, &d_V[k*M], &zero, d_p);
  work = -alpha[k];
  cublasStatus = cublasSaxpy(cublasHandle, N, &work, &d_U[k*N], 1, d_p, 1);
  // if k < n
  if (k < N)
  {
    // beta(k+1) = norm(p);
    cublasSnrm2(cublasHandle, N, d_p, 1, &beta[k+1]);
  }
  // end
  cudaThreadSynchronize();
  printf("iteration = %d\n", k);
  // k = k + 1;
  k++;
}
```

References

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