Singular value decomposition of complexes

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May 16, 2019

Abstract

Singular value decompositions of matrices are widely used in numerical linear algebra with many applications. In this paper, we extend the notion of singular value decompositions to finite complexes of vector spaces. We provide two methods to compute them and present several applications.

1 Introduction

For a matrix $A \in \mathbb{R}^{m \times k}$, a singular value decomposition (SVD) of A is

$$A = U \cdot \Sigma \cdot V^t$$

where $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{k \times k}$ are orthogonal and $\Sigma \in \mathbb{R}^{m \times k}$ is diagonal with nonnegative real numbers on the diagonal. The diagonal entries of Σ, say $\sigma_1 \geq \cdots \geq \sigma_{\min\{m,k\}} \geq 0$ are called the singular values of A and the number of nonzero singular values is equal to the rank of A. Extensions to matrices in $\mathbb{C}^{m \times k}$ simply involve replacing orthogonal with unitary and transpose with Hermitian transpose (conjugate transpose). Singular value decomposition is used to solve many problems in numerical linear algebra such as pseudoinversion, least squares solving, and low-rank matrix approximation. For example, the Eckart-Young theorem [EY36] shows that for $r = 0, \ldots, \min\{m, k\} - 1$, σ_{r+1} is the 2-norm distance between A and the set of matrices of rank at most r. In fact,

$$A_r = U \cdot \operatorname{diag}(\sigma_1, \ldots, \sigma_r, 0, \ldots, 0)_{m \times k} \cdot V^t$$

has rank at most r with $\sigma_{r+1} = \|A - A_r\|_2$ and solves

$$\min_{B\in\mathbb{R}^{m\times k}} \{\|A - B\|_2 \mid \operatorname{rank} B \le r\}. \tag{1}$$

A matrix $A \in \mathbb{R}^{m\times k}$ defines a linear map $A : \mathbb{R}^k \to \mathbb{R}^m$ via $x \mapsto Ax$ denoted

$$\mathbb{R}^m \xleftarrow{A} \mathbb{R}^k.$$

Geometrically, the singular values of A are the lengths of the semi-axes of the ellipsoid arising as the image of the unit sphere under this map defined by A.

Matrix multiplication simply corresponds to function composition. For example, if $B \in \mathbb{R}^{\ell\times m}$, then $B \circ A : \mathbb{R}^k \to \mathbb{R}^\ell$ is defined by $x \mapsto BAx$ denoted

$$\mathbb{R}^\ell \xleftarrow{B} \mathbb{R}^m \xleftarrow{A} \mathbb{R}^k.$$

If $B \circ A = 0$, then this composition forms a *complex* denoted

$$0 \longleftarrow \mathbb{R}^\ell \xleftarrow{B} \mathbb{R}^m \xleftarrow{A} \mathbb{R}^k \longleftarrow 0.$$

In general, a finite complex of finite-dimensional $\mathbb{R}$-vector spaces

$$0 \longleftarrow C_0 \xleftarrow{A_1} C_1 \xleftarrow{A_2} \dots \xleftarrow{A_{n-1}} C_{n-1} \xleftarrow{A_n} C_n \longleftarrow 0$$

consists of vector spaces $C_i \cong \mathbb{R}^{c_i}$ and differentials given by matrices A_i so that $A_i \circ A_{i+1} = 0$. We denote such a complex by $C_\bullet$ and its i^{th} homology group as

$$H_i = H_i(C_\bullet) = \frac{\ker A_i}{\operatorname{image} A_{i+1}}$$

with $h_i = \dim H_i$. Complexes are standard tools that occur in many areas of mathematics including differential equations, e.g. [AFW06, AFW10]. One of the reasons for developing a singular value decomposition of complexes is to compute the dimensions h_i efficiently and robustly via numerical methods when each A_i is only known approximately, say B_i. For example, if the rank of each A_i is known, say r_i, then each h_i can easily be computed via

$$h_i = c_i - (r_i + r_{i+1}).$$

One option would be to compute the singular value decomposition of each B_i in order to compute the rank of A_i since the singular value decomposition is an excellent rank-revealing numerical method. However, simply decomposing each B_i ignores the important information that the underlying matrices A_i form a complex.

The key point of this paper is that we can utilize information about the complex to provide more specific information that reflects the structure it imposes.

Theorem 1.1 (Singular value decomposition of complexes)**.** *Let $A_1, \ldots, A_n$ with $A_i \in \mathbb{R}^{c_{i-1} \times c_i}$, $r_i = \operatorname{rank} A_i$, and $h_i = c_i - (r_i + r_{i+1})$ be a sequence of matrices which define a complex $C_\bullet$, i.e., $A_i \circ A_{i+1} = 0$. Then, there exists sequences $U_0, \ldots, U_n$ and $\Sigma_1, \ldots, \Sigma_n$ of orthogonal and diagonal matrices, respectively, such that*

$$U_{i-1}^t \circ A_i \circ U_i = \begin{matrix} & r_i & r_{i+1} & h_i \\ r_{i-1} & 0 & 0 & 0 \\ r_i & \Sigma_i & 0 & 0 \\ h_{i-1} & 0 & 0 & 0 \end{matrix} \tag{2}$$

where all diagonal entries of Σ_i are strictly positive. Moreover, if every $r_i > 0$ and at least one $h_i > 0$, then the orthogonal matrices U_i can be chosen such that $\det U_i = 1$, i.e., each U_i is a special orthogonal matrix.

The diagonal entries of $\Sigma_1, \ldots, \Sigma_n$ are the *singular values of the complex* which are described in Remark 4.3. Just as with matrices, singular value decomposition of complexes naturally extends to complexes involving entries with complex numbers by simply replacing orthogonal with unitary and transpose with Hermitian transpose (conjugate transpose). However, such an extension is not needed for the applications in this article.

We develop two methods that utilize the structure of the complex $C_\bullet$ to compute a singular value decomposition of $C_\bullet$. The successive projection method described in Algorithm 3.1 uses the orthogonal projection

$$P_{i-1} \colon C_{i-1} \to \ker A_{i-1}$$

together with the singular value decomposition of the matrix $P_{i-1} \circ A_i$. The second method, described in Algorithm 3.3, is based on using each *Laplacian*

$$\Delta_i = A_i^t \circ A_i + A_{i+1} \circ A_{i+1}^t.$$

Both of these methods can be applied to numerical approximations B_i of A_i.

The organization of this paper is as follows. Section 2 proves Theorem 1.1 and collects a number of basic facts along with defining the pseudoinverse of a complex. Section 3 describes the algorithms mentioned above and illustrates them on an example. Section 4 considers projecting an arbitrary sequence of matrices onto a complex. Section 5 provides an application to computing Betti numbers of minimal free resolutions of graded modules over the polynomial ring $\mathbb{Q}[x_0, \ldots, x_n]$ which combines our method with ideas from [EMSS16].

Acknowledgement. DAB and JDH were supported in part by NSF grant ACI-1460032. JDH was also supported by in part by Sloan Research Fellowship BR2014-110 TR14 and NSF grant CCF-1812746. AJS was supported in part by NSF ACI-1440607. FOS is grateful to Notre Dame for its hospitality when developing this project. This work is a contribution to his Project 1.6 of the SFB-TRR 195 "Symbolic Tools in Mathematics and their Application" of the German Research Foundation (DFG). MES was supported in part by NSF grant DMS-1502294 and is grateful to Saarland University for its hospitality during a month of intense work on this project. The authors thank the anonymous referees for their comments which helped to improve this paper.

2 Basics

We first prove our main theorem on singular value decomposition of complexes.

Proof of Theorem 1.1. For convenience, let $A_0 = A_{n+1} = 0$ compliment the matrices $A_1, \ldots, A_n$ that describe the complex $C_\bullet$. By the homomorphism theorem,

$$(\ker A_i)^\perp \cong \operatorname{image} A_i.$$

The singular value decomposition for a complex follows by applying singular value decomposition to this isomorphism and extending an orthonormal basis of these spaces to an orthonormal basis of $\mathbb{R}^{c_{i-1}}$ and $\mathbb{R}^{c_i}$. Since $\operatorname{image} A_{i+1} \subset \ker A_i$, we have an orthogonal direct sum

$$(\ker A_i)^\perp \oplus \operatorname{image} A_{i+1} \subset \mathbb{R}^{c_i}$$

with

$$H_i := ((\ker A_i)^\perp \oplus \operatorname{image} A_{i+1})^\perp = \ker A_i \cap \operatorname{image} A_{i+1}^\perp \cong \frac{\ker A_i}{\operatorname{image} A_{i+1}}.$$

With respect to these subspaces, we can decompose A_i as

$$\begin{array}{l} \\ (\ker A_{i-1})^\perp \\ \operatorname{image} A_i \\ H_{i-1} \end{array} \begin{array}{c} \begin{array}{ccc} (\ker A_i)^\perp & \operatorname{image} A_{i+1} & H_i \end{array} \\ \begin{pmatrix} 0 & 0 & 0 \\ \Sigma_i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{array}.$$

Indeed, A_i has no component mapping to $(\operatorname{image} A_i)^\perp$, which explains six of the zero blocks, and $\ker A_i = (\ker A_i)^{\perp\perp} = \operatorname{image} A_{i+1} \oplus H_i$ explains the remaining two. Take U_i to be the orthogonal matrix whose column vectors form the orthonormal basis of the spaces $(\ker A_i)^\perp$ and $\operatorname{image} A_{i+1}$ induced from the singular value decomposition of $(\ker A_i)^\perp \to \operatorname{image} A_i$ and $(\ker A_{i+1})^\perp \to \operatorname{image} A_{i+1}$ extended by an orthogonal basis of H_i in the decomposition

$$(\ker A_i)^\perp \oplus \operatorname{image} A_{i+1} \oplus H_i = \mathbb{R}^{c_i}.$$

The linear map A_i has, in terms of these bases, the description $U_{i-1}^t \circ A_i \circ U_i$ which has the desired shape.

Finally, to achieve $\det U_i = 1$, we may, for $1 \le k \le r_i$, change signs of the k^{th} column in U_i and $(r_{i-1}+k)^{\text{th}}$ column of U_{i-1} without changing the result of the conjugation. If $h_i > 0$, then changing the sign of any of the last h_i columns of U_i does not affect the result either. Thus, this gives us enough freedom to reach $\det U_i = 1$ for all $i = 0, \dots, n$. □

The singular values of a matrix A are the square roots of the eigenvalues of $A^t \circ A$. The following generalizes this relationship to singular values of a complex and eigenvalues of the Laplacians.

Corollary 2.1 (Repetition of eigenvalues)**.** *Suppose that $A_1, \dots A_n$ define a complex with $A_0 = A_{n+1} = 0$. Let $\Delta_i = A_i^t \circ A_i + A_{i+1} \circ A_{i+1}^t$ be the corresponding Laplacians. Then, using the orthonormal bases described by the U_i's from Theorem 1.1, the Laplacians Δ_i have the shape*

$$\begin{array}{c} \\ r_i \\ r_{i+1} \\ h_i \end{array}\begin{array}{c} \begin{array}{ccc} r_i & r_{i+1} & h_i \end{array} \\ \begin{pmatrix} \Sigma_i^2 & 0 & 0 \\ 0 & \Sigma_{i+1}^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{array}.$$

In particular,

1. $\ker \Delta_i = H_i$*;*
2. *if* $r_i = \operatorname{rank} A_i$ *and* $\sigma_1^i \ge \sigma_2^i \ge \dots \ge \sigma_{r_i}^i > 0$ *are the singular values of* A_i*, then each* $(\sigma_k^i)^2$ *is an eigenvalue of both* Δ_i *and* Δ_{i-1}*.*

Proof. The structure of Δ_i follows immediately from the structure described in Theorem 1.1. The remaining assertions are immediate consequences. □

Let A_i^+ denote the Moore-Penrose pseudoinverse of the A_i. Thus, a singular value decomposition

$$A_i = U_{i-1} \circ \begin{pmatrix} 0 & 0 & 0 \\ \Sigma_i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \circ U_i^t \quad \text{yields} \quad A_i^+ = U_i \circ \begin{pmatrix} 0 & \Sigma_i^{-1} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \circ U_{i-1}^t.$$

Proposition 2.2. *Suppose that* $A_1, \ldots, A_n$ *define a complex with* $A_0 = A_{n+1} = 0$. *Then,* $A_{i+1}^+ \circ A_i^+ = 0$ *and*

$$id_{\mathbb{R}^{c_i}} - (A_i^+ \circ A_i + A_{i+1} \circ A_{i+1}^+)$$

defines the orthogonal projection of $\mathbb{R}^{c_i}$ *onto the homology* H_i.

Proof. We know that $A_i^+ \circ A_i$ defines the projection onto $(\ker A_i)^\perp$ and $A_{i+1} \circ A_{i+1}^+$ defines the projection onto $\operatorname{image} A_{i+1}$. The result follows immediately since these spaces are orthogonal and $H_i = ((\ker A_i)^\perp \oplus \operatorname{image} A_{i+1})^\perp$. □

For a complex $C_\bullet$ with

$$0 \longleftarrow \mathbb{R}^{c_0} \xleftarrow{A_1} \mathbb{R}^{c_1} \xleftarrow{A_2} \ldots \xleftarrow{A_n} \mathbb{R}^{c_n} \longleftarrow 0,$$

the *pseudoinverse complex*, denoted $C_\bullet^+$, is

$$0 \longrightarrow \mathbb{R}^{c_0} \xrightarrow{A_1^+} \mathbb{R}^{c_1} \xrightarrow{A_2^+} \ldots \xrightarrow{A_n^+} \mathbb{R}^{c_n} \longrightarrow 0.$$

Remark 2.3. If the matrices A_i have entries in a subfield $K \subset \mathbb{R}$, then the pseudoinverse complex is also defined over K. This follows since the pseudoinverse is uniquely determined by the Penrose relations [Pen55]:

$$\begin{aligned} A_i \circ A_i^+ \circ A_i &= A_i, & A_i \circ A_i^+ &= (A_i \circ A_i^+)^t, \\ A_i^+ \circ A_i \circ A_i^+ &= A_i^+, & A_i^+ \circ A_i &= (A_i^+ \circ A_i)^t, \end{aligned}$$

which form an algebraic system of equations for the entries of A_i^+ with a unique solution whose coefficients are in K. In particular, this holds for $K = \mathbb{Q}$.

If the entries of the matrices are in the finite field $\mathbb{F}_q$, the pseudoinverse of A_i is well defined over $\mathbb{F}_q$ with respect to the dot-product on $\mathbb{F}_q^{c_i}$ and $\mathbb{F}_q^{c_{i-1}}$ if

$$\ker A_i \cap (\ker A_i)^\perp = 0 \subset \mathbb{F}_q^{c_i} \quad \text{and} \quad \operatorname{image} A_i \cap (\operatorname{image} A_i)^\perp = 0 \subset \mathbb{F}_q^{c_{i-1}}.$$

We have implemented the computation of the pseudoinverse complex for double precision floating-point numbers $\mathbb{R}_{53}$, the rationals $\mathbb{Q}$, and finite fields $\mathbb{F}_q$ in our Macaulay2 package SVDComplexes.

3 Algorithms

We present two algorithms for computing a singular value decomposition of a complex followed by some examples.

Algorithm 3.1 (Successive projection method)**.**
INPUT: Sequence $A_1, \ldots, A_n$ of real matrices forming a complex $C_\bullet$.
OUTPUT: Integers $r_1, \ldots, r_n$, orthogonal matrices $U_0, \ldots, U_n$ and diagonal matrices $\Sigma_1, \ldots, \Sigma_n$ forming a singular value decomposition of $C_\bullet$.

1. Set $r_0 = 0$, $Q_0 = 0$, and $P_0 = \mathrm{id}_{C_0}$.
2. For $i = 1, \ldots, n$
   a. Compute the $(c_{i-1} - r_{i-1}) \times c_i$ matrix $\widetilde{A}_i = P_{i-1} \circ A_i$.
   b. Compute a singular value decomposition of $\widetilde{A}_i$, say $\widetilde{A}_i = \widetilde{U}_i \circ \widetilde{\Sigma}_i \circ \widetilde{V}_i^t$.
   c. Set $r_i = \operatorname{rank} \widetilde{\Sigma}_i$.
   d. Decompose
   $$\widetilde{V}_i^t = \begin{pmatrix} Q_i \\ P_i \end{pmatrix}$$
   into submatrices consisting of the first r_i and last $c_i - r_i$ rows of $\widetilde{V}_i^t$.
   e. Compute
   $$U_{i-1}^t = \begin{pmatrix} Q_{i-1} \\ \widetilde{U}_{i-1}^t \circ P_{i-1} \end{pmatrix}.$$
   f. If $i = n$, set $U_n = \widetilde{V}_n^t$ and then compute $\Sigma_1, \ldots, \Sigma_n$ satisfying (2).
3. Return $r_1, \ldots, r_n$, $U_0, \ldots, U_n$, and $\Sigma_1, \ldots, \Sigma_n$.

Proof of correctness. By induction on i, we will see that P_i defines the orthogonal projection $C_i \to \ker A_i$. Since V_i^t is orthogonal,

$$\begin{pmatrix} Q_i \\ P_i \end{pmatrix} \circ \begin{pmatrix} Q_i^t & P_i^t \end{pmatrix} = \begin{pmatrix} \mathrm{id}_{r_i} & 0 \\ 0 & \mathrm{id}_{c_i - r_i} \end{pmatrix}$$

where id_k denotes a $k \times k$ identity matrix, we additionally conclude that Q_i is the orthogonal projection $C_i \to (\ker A_i)^\perp$. This is trivially true for $A_0 = 0$.

For the induction step, $\operatorname{image} A_i \subset \ker A_{i-1}$ implies that $Q_{i-1} \circ A_i = 0$. Hence, A_i and $P_{i-1} \circ A_i = \widetilde{A}_i$ have the same nonzero singular values. From

$$\widetilde{A}_i = \widetilde{U}_i \circ \widetilde{\Sigma}_i \circ \widetilde{V}_i^t \qquad \text{and} \qquad \widetilde{V}_i^t = \begin{pmatrix} Q_i \\ P_i \end{pmatrix},$$

we see that P_i defines the orthogonal projection $C_i \to \ker A_i$. Moreover,

$$\begin{aligned}
U_{i-1}^t \circ A_i \circ U_i &= \begin{pmatrix} Q_{i-1} \\ \widetilde{U}_{i-1}^t \circ P_{i-1} \end{pmatrix} \circ A_i \circ \begin{pmatrix} Q_i^t & P_i^t \circ \widetilde{U}_i \end{pmatrix} \\
&= \begin{pmatrix} 0 \\ \widetilde{U}_{i-1}^t \circ \widetilde{A}_i \end{pmatrix} \circ \begin{pmatrix} Q_i^t & P_i^t \circ \widetilde{U}_i \end{pmatrix} \\
&= \begin{pmatrix} 0 \\ \widetilde{U}_{i-1}^t \circ \widetilde{U}_{i-1} \circ \widetilde{\Sigma}_i \circ \begin{pmatrix} Q_i \\ P_i \end{pmatrix} \end{pmatrix} \circ \begin{pmatrix} Q_i^t & P_i^t \circ \widetilde{U}_i \end{pmatrix} \\
&= \begin{pmatrix} 0 \\ \widetilde{\Sigma}_i \circ \begin{pmatrix} \mathrm{id}_{r_i} & 0 \\ 0 & \mathrm{id}_{c_i - r_i} \widetilde{U}_i \end{pmatrix} \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 \\ \Sigma_i & 0 \\ 0 & 0 \end{pmatrix}
\end{aligned}$$

since

$$\widetilde{\Sigma}_i \circ \begin{pmatrix} 0 \\ \mathrm{id}_{c_i - r_i} \end{pmatrix} = 0.$$

Hence, Algorithm 3.1 computes a singular value decomposition of $C_\bullet$. □

Remark 3.2. Algorithm 3.1 was presented using exact input data $A_1, \ldots, A_n$ for the complex $C_\bullet$ and exact computations. When using numerical approximations $B_1, \ldots, B_n$ for the matrices $A_1, \ldots, A_n$, this algorithm can be easily modified to use floating-point arithmetic to produce a good numerical approximation of a singular value decomposition for $C_\bullet$ provided that:

i) the approximations $B_1, \ldots, B_n$ of $A_1, \ldots, A_n$ are sufficiently accurate,

ii) the correct rank is identified in Step 2c, and

iii) floating-point arithmetic using sufficiently high precision is utilized.

We can alter Step 2c when using floating-point arithmetic to obtain more confidence in the correctness of the computation of $r_1, \ldots, r_n$. One natural approach is to start with two approximations $B_1, \ldots, B_n$ and $B_1', \ldots, B_n'$ in different precisions and determine $r_1, \ldots r_n$ as the number of stable singular values, i.e., the singular values which have approximately the same value in both computations. Moreover, since orthogonal matrices have unit condition number, they maintain lengths so that the rank r_i can be reliably computed in Step 2c for all $i = 1, \ldots, n$.

The second method for computing a singular value decomposition is based on using the Laplacians and Corollary 2.1 which generalizes the description of singular values of a matrix A as the square roots of the eigenvalues of $A^t \circ A$.

Algorithm 3.3 (Laplacian method)**.**
INPUT: Sequence $A_1, \ldots, A_n$ of real matrices forming a complex $C_\bullet$.
OUTPUT: Integers $r_1, \ldots, r_n$, orthogonal matrices $U_0, \ldots, U_n$ and diagonal matrices $\Sigma_1, \ldots, \Sigma_n$ forming a singular value decomposition of $C_\bullet$.

1. Compute an eigendecomposition of $\Delta_0 = A_1 \circ A_1^t$, i.e., compute an orthogonal matrix $U_0 \in \mathbb{R}^{c_0 \times c_0}$ and diagonal matrix $D_0 \in \mathbb{R}^{c_0 \times c_0}$ where the diagonal entries are listed in decreasing order such that

$$\Delta_0 = U_0 \circ D_0 \circ U_0^t.$$

2. Let r_1 be the number of nonzero diagonal entries of D_0, $\widetilde{V}_1$ be the first r_1 columns of U_0, $\Sigma_1 \in \mathbb{R}^{r_1 \times r_1}$ be the diagonal matrix with $(\Sigma_1)_{jj} = \sqrt{(D_0)_{jj}}$, and $\widetilde{U}_1 = A_1^t \circ \widetilde{V}_1 \circ \Sigma_1^{-1}$.

3. For $i = 1, \ldots, n-1$:

   a. Extend $\widetilde{U}_i$ to an orthogonal matrix $U_i \in \mathbb{R}^{c_i \times c_i}$ forming a eigenbasis for $\Delta_i = A_{i-1}^t \circ A_{i-1} + A_i \circ A_i^t$ such that

   $$\Delta_i = U_i \circ D_i \circ U_i^t$$

   where $D_i \in \mathbb{R}^{c_i \times c_i}$ is a diagonal matrix of the form

   $$D_i = \begin{pmatrix} \Sigma_i^2 & \\ & \Lambda_i \end{pmatrix}$$

   and the diagonal entries in Λ_i are listed in decreasing order.

b. Let r_{i+1} be the number of nonzero diagonal entries of Λ_i, $\widetilde{V}_{i+1}$ be the $r_i+1,\ldots,r_i+r_{i+1}$ columns of U_i, $\Sigma_{i+1} \in \mathbb{R}^{r_{i+1}\times r_{i+1}}$ be the diagonal matrix with $(\Sigma_{i+1})_{jj} = \sqrt{(\Lambda_i)_{jj}}$, and $\widetilde{U}_{i+1} = A_{i+1}^t \circ \widetilde{V}_{i+1} \circ \Sigma_{i+1}^{-1}$.

c. If $i = n-1$, extend $\widetilde{U}_n$ to an orthogonal matrix $U_n \in \mathbb{R}^{c_n\times c_n}$.

4. Return $r_1,\ldots,r_n$, $U_0,\ldots,U_n$, and $\Sigma_1,\ldots,\Sigma_n$.

Proof of correctness. Since each Δ_i is symmetric, it is diagonlizable, i.e., has an orthonormal basis consisting of eigenvectors. By construction, the first r_i columns of U_i form a basis for $(\ker A_i)^\perp$, the next r_{i+1} columns of U_i form a basis for $\operatorname{image} A_{i+1}$ and the last $h_i = c_i - (r_i + r_{i+1})$ columns of U_i form a basis for H_i. By the homomorphism theorem, $(\ker A_i)^\perp \cong \operatorname{image} A_i$ means that we can reuse r_i columns from U_{i-1} which form a basis for $\operatorname{image} A_i$ as the first r_i columns of U_i forming a basis for $(\ker A_i)^\perp$. This immediately yields that

$$U_{i-1}^t \circ A_i \circ U_i = \begin{pmatrix} 0 & 0 & 0 \\ \Sigma_i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

thereby computing a singular value decomposition for $C_\bullet$. □

Remark 3.4. If all of the eigenvalues of all of the Laplacians are distinct, then every eigenvector of length one is defined uniquely up to sign. Hence, one can compute eigendecompositions of the Δ_i's independently, e.g., using parallel computations. A singular value decomposition can then be computed by simply rearranging and changing signs on the eigenvectors as needed.

Remark 3.5. The comments in Remark 3.2 in reference to Algorithm 3.1 related to using numerical approximations hold for Algorithm 3.3 modulo identifying the correct rank in Steps 2 and 3b. The key aspect is to use sufficiently high precision to distinguish between small nonzero and zero eigenvalues due to the squaring of the singular values.

Example 3.6. We consider the complex

$$0 \longleftarrow \mathbb{R}^3 \xleftarrow{A_1} \mathbb{R}^5 \xleftarrow{A_2} \mathbb{R}^5 \xleftarrow{A_3} \mathbb{R}^3 \longleftarrow 0$$

where the matrices A_1, A_2, A_3, respectively, are

$$\begin{pmatrix} 14 & -4 & 16 & 3 & -9 \\ 14 & -5 & 20 & 9 & 1 \\ 4 & 1 & -4 & -12 & -24 \end{pmatrix}, \begin{pmatrix} -43 & -50 & -27 & -51 & 9 \\ 12 & -24 & 36 & 0 & -12 \\ 35 & 34 & 27 & 39 & -9 \\ -3 & -10 & 3 & -6 & -1 \\ -11 & -10 & -9 & -12 & 3 \end{pmatrix}, \begin{pmatrix} -8 & -16 & -12 \\ -5 & -1 & -15 \\ -1 & 13 & -14 \\ 12 & 12 & 28 \\ -1 & 25 & -24 \end{pmatrix}.$$

Printed with 4 digits only, the orthogonal matrices $U_0, \ldots, U_3$, respectively, are

$$\begin{pmatrix} -0.6553 & 0.2393 & -0.7165 \\ -0.7549 & -0.1745 & 0.6322 \\ 0.0262 & 0.9551 & 0.2950 \end{pmatrix}, \begin{pmatrix} -0.5694 & 0.1646 & -0.7702 & -0.1318 & 0.1950 \\ 0.1862 & 0.0303 & 0.0679 & -0.9710 & 0.1301 \\ -0.7448 & -0.1213 & 0.6010 & -0.0706 & 0.2537 \\ -0.2631 & -0.4289 & -0.0790 & -0.1821 & -0.8411 \\ 0.1309 & -0.8794 & -0.1862 & 0.0404 & 0.4162 \end{pmatrix},$$

$$\begin{pmatrix} 0.5019 & -0.1770 & 0.2288 & 0.5338 & 0.6160 \\ 0.5257 & 0.6126 & 0.3335 & 0.1127 & -0.4738 \\ 0.3586 & -0.7250 & 0.3461 & -0.3015 & -0.3677 \\ 0.5735 & 0.0970 & -0.5972 & -0.5061 & 0.2210 \\ -0.1195 & 0.2417 & 0.6000 & -0.5961 & 0.4604 \end{pmatrix}, \begin{pmatrix} -0.2525 & -0.2843 & -0.9249 \\ 0.1813 & -0.9528 & 0.2434 \\ -0.9505 & -0.1062 & 0.2921 \end{pmatrix}$$

Hence, for $i = 1, 2, 3$, the matrices $\overline{\Sigma}_i = U_{i-1}^t \circ A_i \circ U_i$ are

$$\begin{pmatrix} 34.489 & 0 & 0 & 0 & 0 \\ 0 & 28.714 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 114.08 & 0 & 0 & 0 & 0 \\ 0 & 47.193 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 45.993 & 0 & 0 \\ 0 & 35.209 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

showing that $r_i = \operatorname{rank} A_i = 2$ and $h_i = \dim H_i = 1$ for $i = 1, 2, 3$. In particular, the following diagram commutes:

$$\begin{array}{ccccccccccc} 0 & \longleftarrow & \mathbb{R}^3 & \xleftarrow{A_1} & \mathbb{R}^5 & \xleftarrow{A_2} & \mathbb{R}^5 & \xleftarrow{A_3} & \mathbb{R}^3 & \longleftarrow & 0 \\ & & \uparrow{\scriptstyle U_0} & & \uparrow{\scriptstyle U_1} & & \uparrow{\scriptstyle U_2} & & \uparrow{\scriptstyle U_3} & & \\ 0 & \longleftarrow & \mathbb{R}^3 & \xleftarrow[\overline{\Sigma}_1]{} & \mathbb{R}^5 & \xleftarrow[\overline{\Sigma}_2]{} & \mathbb{R}^5 & \xleftarrow[\overline{\Sigma}_3]{} & \mathbb{R}^3 & \longleftarrow & 0 \end{array}$$

One can use this singular value decomposition to compute the pseudoinverse complex. For example, A_1^+, printed with 6 decimal places is

$$\begin{pmatrix} 0.012191 & 0.011463 & 0.005043 \\ -0.003285 & -0.004260 & 0.001150 \\ 0.013141 & 0.017040 & -0.004601 \\ 0.001425 & 0.008366 & -0.014466 \\ -0.009815 & 0.002481 & -0.029152 \end{pmatrix}$$

which is a numerical approximation of the exact matrix

$$\begin{pmatrix} 5978/490373 & 5621/490373 & 2473/490373 \\ -1611/490373 & -2089/490373 & 564/490373 \\ 6444/490373 & 8356/490373 & -2256/490373 \\ 699/490373 & 8205/980746 & -14187/980746 \\ -4813/490373 & 2433/980746 & -28591/980746 \end{pmatrix}.$$

Moreover, this simple example is fairly stable against errors. For example, the algorithms predict the dimension of the homology groups correctly upon perturbing the entries of the matrices A_i on the order of $\leq 10^{-3}$ and using a threshold of 10^{-2} to compute the ranks, e.g., see SVDComplexes.

Example 3.7. We compared Algorithms 3.1 and 3.3 for verifying the dimension of homology groups for randomly generated complexes of various sizes with known homology group dimensions. Table 1 compares the timings of these algorithms.

c_0	c_1	c_2	c_3	h_0	h_1	h_2	h_3	Alg. 3.1 (sec)	Alg. 3.3 (sec)
7	21	28	14	2	3	2	1	0.00211	0.0110
8	27	35	17	3	6	4	2	0.00225	0.0182
9	33	42	20	4	9	6	3	0.00254	0.0294
10	39	49	23	5	12	8	4	0.00291	0.0647
11	45	56	26	6	15	10	5	0.00355	0.1090
12	51	63	29	7	18	12	6	0.00442	0.1150

Table 1: Comparison of timings using Algorithms 3.1 and 3.3.

Example 3.8. We constructed a series of examples from Stanley-Reisner simplicial complexes of N randomly chosen squarefree monomial ideals in a polynomial ring with k variables. The results are summarized in Table 2.

4 Projection

One application of using the singular value decomposition of a complex is to compute the pseudoinverse complex as described in Section 2. The following projects a sequence of matrices onto a complex.

Algorithm 4.1 (Projection to a complex)**.**
INPUT: A sequence $B_1, \ldots, B_n$ of $c_{i-1} \times c_i$ matrices and a sequence $h_0, \ldots, h_n$ of desired dimension of homology groups.
OUTPUT: If possible, a sequence $A_1, \ldots, A_n$ of matrices which define a complex with desired homology.

1. Set $r_0 = 0$ and compute $r_1, \ldots, r_{n+1}$ from $h_i = c_i - (r_i + r_{i+1})$ recursively. If $r_i < 0$ or $r_i > \operatorname{rank} B_i$ for some i or $r_{n+1} \neq 0$, then return the error message: "The desired dimension of homology groups cannot be satisfied."

k	N	c_0	c_1	c_2	$\ldots$							Alg 3.1
		h_0	h_1	h_2	$\ldots$							(sec)
8	20	8	27	44	30							
		1	0	0	1							0.0019
9	21	9	35	74	85	46						
		1	0	0	0	0						0.0036
10	23	10	45	118	190	173	69					
		1	0	0	0	3	0					0.0198
11	26	11	55	165	326	431	361	156	19			
		1	0	0	0	0	0	2	0			0.2410
12	30	12	66	218	474	694	664	375	101			
		1	0	0	0	0	0	2	0			1.29
13	35	13	78	286	712	1253	1553	1291	639	141		
		1	0	0	0	0	0	0	6	1		39.7
14	41	14	91	364	996	1948	2741	2687	677	559	75	
		1	0	0	0	0	0	0	7	0	0	355.

Table 2: Comparison of timings using Algorithm 3.1.

2. Set $Q_0 = 0$ and $P_0 = \mathrm{id}_{C_0}$.

3. For $i = 1, \ldots, n$

   a. Compute the $(c_{i-1} - r_{i-1}) \times c_i$ matrix $\widetilde{B}_i = P_{i-1} \circ B_i$.

   b. Compute the singular value decomposition

   $$\widetilde{B}_i = \widetilde{U}_{i-1} \circ \widetilde{\Sigma}_i \circ \widetilde{V}_i^t.$$

   c. Compute

   $$\overline{\Sigma}_i = \begin{matrix} \\ r_{i-1} \\ r_i \\ h_{i-1} \end{matrix} \begin{matrix} \begin{matrix} r_i & r_{i+1} & h_i \end{matrix} \\ \begin{pmatrix} 0 & 0 & 0 \\ \Sigma_i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{matrix}$$

   as a block matrix where Σ_i is a diagonal matrix whose entries are the largest r_i singular values of $\widetilde{B}_i$.

   d. Decompose

   $$\widetilde{V}_i^t = \begin{pmatrix} Q_i \\ P_i \end{pmatrix}$$

   into submatrices consisting of the first r_i and last $c_i - r_i$ rows of $\widetilde{V}_i^t$.

e. Compute

$$U_{i-1}^t = \begin{pmatrix} Q_{i-1} \\ \widetilde{U}_{i-1}^t \circ P_{i-1} \end{pmatrix}.$$

f. If $i = n$, then set $U_n = \widetilde{V}_n^t$.

4. Set $A_i = U_{i-1} \circ \overline{\Sigma}_i \circ U_i^t$ and return $A_1, \ldots, A_n$.

Proof of correctness. It is clear that the construction of the A_i's yields a complex presented in the form of (2). □

Example 4.2. In our package RandomComplexes, we have implemented several methods to produce complexes over the integers. The first function randomChainComplex takes as input sequences $h_1, \ldots, h_n$ and $r_1, \ldots, r_n$ of desired dimension of homology groups and ranks of the matrices, respectively. It uses the LLL algorithm [LLL82] to produce examples of desired moderate height. It runs fast for complexes with $c_i \leq 100$ but is slow for larger examples because of the use of the LLL-algorithm. Example 3.6 was produced this way.

For a given a complex, only allowing one homology group to change provides a description of its singular values. This is summarized in the following.

Remark 4.3. For a matrix $A \in \mathbb{R}^{m \times k}$, σ_{r+1} is the distance between A and set of matrices of rank at most r via (1). Singular values of a complex have a similar description. In particular, if $A_1, \ldots, A_n$ define a complex $C_\bullet$ with $A_i \in \mathbb{R}^{c_{i-1} \times c_i}$, $r_i = \operatorname{rank} A_i$, and $A_0 = A_{n+1} = 0$, then, for $r = 0, \ldots, r_i - 1$, the $(r+1)^{\text{st}}$ singular value of A_i, namely σ_{r+1}^i, is equal to

$$(3) \qquad \min_{B \in \mathbb{R}^{c_{i-1} \times c_i}} \{ \|A_i - B\|_2 \mid \operatorname{rank} B \leq r,\ A_{i-1} \circ B = 0,\ B \circ A_{i+1} = 0 \}$$

which one can view as the distance between the complex $C_\bullet$ and the set of complexes consisting of matrices $A_1, \ldots, A_{i-1}, B, A_{i+1}, \ldots, A_n$ where $\operatorname{rank} B \leq r$. Moreover, one can solve (3) using a singular value decomposition for $C_\bullet$ with, say, orthogonal matrices $U_0, \ldots, U_n$ and diagonal matrices $\Sigma_1, \ldots, \Sigma_n$. In particular, with $\Sigma_i = \operatorname{diag}(\sigma_1^i, \ldots, \sigma_{r_i}^i)_{r_i \times r_i}$, the matrix

$$B_r^i = U_{i-1} \circ \begin{pmatrix} 0 & 0 & 0 \\ \Lambda_r^i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \circ U_i^t$$

solves (3) where $\Lambda_r^i = \operatorname{diag}(\sigma_1^i, \ldots, \sigma_r^i, 0, \ldots, 0)_{r_i \times r_i}$ and $\sigma_{r+1}^i = \|A_i - B_r^i\|_2$.

Measuring distances between two sequences of matrices where only one matrix is different can be viewed as equivalent to simply measuring the distance between the only differing matrices. Remark 4.3 uses this to describe the singular values of complex. Algorithm 4.1 also uses this idea via a greedy approach at each step in its construction. In general, one can construct equivalent norms on sequences of matrices by building from the norms of the individual entries of the matrices. Given a sequence of matrices $B_1, \ldots, B_n$ and constants $\alpha_i, \beta_i > 0$, then

$$\sum_{i=1}^{n} \alpha_i \|B_i\|_2 \quad \text{and} \quad \max\{\beta_i \|B_i\|_2 \mid i = 1, \ldots, n\}$$

are easily seen to be equivalent norms. Therefore, given a norm on a sequence of matrices, we leave it as an open problem to compute the nearest complex with desired homology group dimensions to a given sequence of matrices.

5 Application to syzygies

We conclude with an application concerning the computation of Betti numbers in free resolutions. Let $S = K[x_0, \ldots, x_n]$ be the standard graded polynomial ring and M a finitely generated graded S-module. Then, by Hilbert's syzygy theorem, M has a finite free resolution:

$$0 \longleftarrow M \longleftarrow F_0 \xleftarrow{\varphi_1} F_1 \xleftarrow{\varphi_2} \ldots \xleftarrow{\varphi_c} F_c \longleftarrow 0$$

by free graded S-modules $F_i = \sum_j S(-i-j)^{b_{ij}}$ of length $c \leq n+1$. Here $S(-\ell)$ denotes the free S-module with generator in degree ℓ.

If we choose in each step a minimal number of homogenous generators, i.e., if $\varphi_i(F_i) \subset (x_0, \ldots x_n)F_{i-1}$, then the free resolution is unique up to an isomorphism. In particular, the Betti numbers b_{ij} of a minimal resolution are numerical invariants of M. On the other hand, for basic applications of free resolutions such as the computation of Ext and Tor-groups, any resolution can be used.

Starting with a reduced Gröbner basis of the submodule $\varphi_1(F_1) \subset F_0$ there is, after some standard choices on orderings, a free resolution such that at each step the columns of φ_{i+1} form a reduced Gröbner basis of $\ker \varphi_i$. This resolution is uniquely determined however, in most cases, highly nonminimal. An algorithm to compute this standard nonminimal resolution was developed in [EMSS16] which turned out to be much faster than the computation of a minimal resolution by previous methods.

The following forms the examples which we use as test cases.

Proposition 5.1 (Graded Artinian Gorenstein Algebras)**.** *Let $f \in \mathbb{Q}[x_0, \dots, x_n]$ be a homogeneous polynomial of degree d. In $S = \mathbb{Q}[\partial_0, \dots, \partial_n]$, consider the ideal $I = \langle D \in S \mid D(f) = 0 \rangle$ of constant differential operators which annihilate f. Then, $A_f^{\perp} := S/I$ is an artinian Gorenstein Algebra with socle in degree d.*

For more information on this topic see, e.g., [RS00].

Example 5.2. Let $f = \ell_1^4 + \ldots + \ell_{18}^4 \in \mathbb{Q}[x_0, \dots, x_7]$ be the sum of 4^{th} powers of 18 sufficiently general chosen linear forms ℓ_s. The Betti numbers b_{ij} of the minimal resolution $M = A_f^{\perp}$ as an S-module are zero outside the range $i = 0, \dots, 8, j = 0, \dots, 4$. In this range, they take the values:

$j \setminus i$	0	1	2	3	4	5	6	7	8
0	1	.	.	.	.	.	.	.	.
1	.	18	42	.	.	.	.	.	.
2	.	10	63	288	420	288	63	10	.
3	.	.	.	.	.	.	42	18	.
4	.	.	.	.	.	.	.	.	1

which, for example, says that $F_2 = S(-3)^{42} \oplus S(-4)^{63}$. We note that the symmetry of the table is a well-known consequence of the Gorenstein property.

On the other hand the Betti numbers of the uniquely determined nonminimal resolution are much larger:

$j \setminus i$	0	1	2	3	4	5	6	7	8
0	1	.	.	.	.	.	.	.	.
1	.	18	55	75	54	20	3	.	.
2	.	23	145	390	580	515	273	80	10
3	.	7	49	147	245	245	147	49	7
4	.	1	7	21	35	35	21	7	1

To deduce from this resolution the Betti numbers of the minimal resolution, we can use the formula

$$b_{ij} = \dim \operatorname{Tor}_i^S(M, \mathbb{Q})_{i+j}.$$

For example, to deduce $b_{3,2} = 288$, we have to show that the 5^{th} constant strand of the nonminimal resolution

$$0 \longleftarrow \mathbb{Q}^1 \longleftarrow \mathbb{Q}^{49} \longleftarrow \mathbb{Q}^{390} \longleftarrow \mathbb{Q}^{54} \longleftarrow 0$$

has homology only in one position.

The matrices defining the differential in the nonminimal resolution have polynomial entries whose coefficients in $\mathbb{Q}$ can have very large height such that the computation of the homology of the strands becomes infeasible. There are two options, how we can get information about the minimal Betti numbers:

- Pick a prime number p which does not divide any numerator of the normalized reduced Gröbner basis and then reduce modulo p yielding a module $M(p)$ with the same Hilbert function as M. Moreover, for all but finitely many primes p, the Betti numbers of M as an $\mathbb{Q}[x_0, \ldots, x_n]$-module and of $M(p)$ as $\mathbb{F}_p[x_0, \ldots, x_n]$-module coincide.

- Pass from a normalized reduced Gröbner basis of $\varphi_1(F_1) \subset F_0$ to a floating-point approximation of the Gröbner basis. Since in the algorithm for the computation of the uniquely determined nonminimal resolution [EMSS16], the majority of ground field operations are multiplications, we can hope that this computation is numerically stable and that the singular value decompositions of the linear strands will detect the minimal Betti numbers correctly.

Example 5.3. We experimented with artinian graded Gorenstein algebras constructed from randomly chosen forms $f \in \mathbb{Q}[x_0, \ldots, x_7]$ in 8 variables which were the sum of n 4^{th} powers of linear forms where $11 \leq n \leq 20$. This experiment showed that roughly 95% of the Betti table computed via floating-point arithmetic coincided with one computed over a finite field. The reason for this was that the current implementation uses only double precision floating-point computations which caused difficulty in detecting zero singular values correctly. This could be improved following Remark 3.2 using higher precision arithmetic.

We now consider a series of examples related to the famous Green's conjecture on canonical curves which was proved in a landmark paper [Voi05] for generic curves. In $S = \mathbb{Q}[x_0, \ldots, x_a, y_0, \ldots, y_b]$, consider the homogeneous ideal J_e generated by the 2×2 minors of

$$\begin{pmatrix} x_0 & x_1 & \ldots & x_{a-1} \\ x_1 & x_2 & \ldots & x_a \end{pmatrix} \text{ and } \begin{pmatrix} y_0 & y_1 & \ldots & y_{b-1} \\ y_1 & y_2 & \ldots & y_b \end{pmatrix}$$

together with the entries of the $(a-1) \times (b-1)$ matrix

$$\begin{pmatrix} x_0 & x_1 & x_2 \\ x_1 & x_2 & x_3 \\ \vdots & \vdots & \vdots \\ x_{a-2} & x_{a-1} & x_a \end{pmatrix} \begin{pmatrix} 0 & 0 & e_2 \\ 0 & -e_1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} y_0 & y_1 & \ldots & y_{b-2} \\ y_1 & y_2 & \ldots & y_{b-1} \\ y_2 & y_3 & \ldots & y_b \end{pmatrix}$$

for some parameters $e_1, e_2 \in \mathbb{Q}$. Then, by [ES18], J_e is the homogeneous ideal of an arithmetically Gorenstein surface $X_e(a,b) \subset \mathbb{P}^{a+b+1}$ with trivial canonical bundle. Moreover, the generators of J_e form a Gröbner basis. To verify the generic Green's conjecture for curves of odd genus $g = 2a+1$, it suffices to prove, for some values $e = (e_1, e_2) \in \mathbb{Q}^2$, that $X_e(a,a)$ has a "natural" Betti table, i.e., for each k there is at most one pair (i,j) with $i+j=k$ and $b_{ij}(X_e(a,a)) \neq 0$. For special values of $e = (e_1, e_2)$, e.g., $e = (0,-1)$, it is known that the resolution is not natural, see [ES18].

Example 5.4. For $a = b = 6$, our implementation computes the following Betti numbers for the nonminimal resolution: as

	0	1	2	3	4	5	6	7	8	9	10	11
	1	.	.	.	.	.	.	.	.	.	.	.
	.	55	320	930	1688	2060	1728	987	368	81	8	.
	.	.	39	280	906	1736	2170	1832	1042	384	83	8
	.	.	.	1	8	28	56	70	56	28	8	1

For $e = (2,-1)$ and $e = (0,-1)$, our implementation correctly computes the following Betti numbers, respectively, of the minimal resolutions:

	0	1	2	3	4	5	6	7	8	9	10	11
	1	.	.	.	.	.	.	.	.	.	.	.
	.	55	320	891	1408	1155	.	.	.	.	.	.
	.	.	.	.	.	.	1155	1408	891	320	55	.
	.	.	.	.	.	.	.	.	.	.	.	1

	1	.	.	.	.	.	.	.	.	.	.	.
	.	55	320	900	1488	1470	720	315	80	9	.	.
	.	.	9	80	315	720	1470	1488	900	320	55	.
	.	.	.	.	.	.	.	.	.	.	.	1

Each of these computations took several minutes and the results agree with those presented in [ES18] using exact methods which took several hours. To consider larger examples, more efficient algorithms and/or implementations for computing the singular value decomposition of a complex are needed.

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