Real Homology Cohomology and Harmonic Cochains, Least Squares, and Diagonal Dominance

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Abstract

We give new algorithms for computing basis cochains for real-valued homology, cohomology, and harmonic cochains on manifold simplicial complexes. We discuss only planar, surface, and solid meshes. Our algorithms are based on a least squares formulation. Previous methods for computing homology and cohomology have relied on persistence algorithm or Smith normal form, both of which have cubic complexity in worst case. Our algorithm is a Hodge decomposition using only the connectivity information of the mesh. This is a pair of least squares problems and thus can be solved using very reliable, efficient, classical iterative linear solvers which work in spite of nontrivial kernels, have guarantees on iteration counts, and work without forming the full linear system. Moreover, as we showed recently elsewhere, the corresponding normal equation matrices are diagonally dominant, allowing the use of recent developments in very fast solvers for such.

For harmonic cochains, one previous approach has been to find eigenvectors corresponding to zero eigenvalue of the Laplace-deRham operator. In another approach, earlier methods have required the solution of all lower dimensional problems. We find harmonic cochains by solving a single weighted least squares problem. Our method does not use any inverse Hodge star matrices, since these can be dense if Whitney forms are used. We also show diagonal dominance in certain cases depending on geometric properties of the mesh. Finally, we prove a discrete version of the Hodge-deRham theorem relating cohomology and harmonic cochains.

1 Introduction

The importance of harmonic functions is well-established in mathematics and its applications. Harmonic functions are the solutions of the most fundamental of all elliptic partial differential equations (PDEs), namely, Laplace’s equation. That is, these are the functions whose Laplacian is zero. Harmonic functions and their discrete incarnations are very useful objects in various fields like computer graphics [24, 25], machine learning [6, 55], complex analysis [14], analysis [4], and so on.

When the domain is generalized to surfaces, Laplacian becomes the Laplace-Beltrami operator. One can also generalize the objects that the operator acts on. If it acts on differential forms instead of functions, it is called the Laplace-deRham operator [1]. For example, in $\mathbb{R}^3$, the operator $\text{grad} \cdot \text{div} - \text{curl} \cdot \text{curl}$ is the vector Laplacian. For the standard inner product, it is equivalent to the Laplace-deRham on 1-forms. These and other Laplace-deRham operators are important in PDEs and differential geometry [37], numerical methods for such PDEs [3], computer graphics [49], and in many other fields. The kernel of these operators are called harmonic forms and these too find applications in the above fields. Perhaps the most striking manifestation of harmonic forms is in the link they yield between topology and analysis. This is the content of the Hodge-deRham theorem which relates cohomology space with the space of harmonic forms. As in discretizations of exterior calculus [2, 19, 20, 33], these operators have discrete counterparts that act on cochains instead of forms. These and related preliminaries are reviewed in Section 2.

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In this paper we give new algorithms for computing elements of real homology and cohomology and real valued harmonic cochains. We only discuss the case of planar, surface, and solid meshes. For the first two, the interesting cohomology is $H^1$ and for the solid case $H^1$ and $H^2$ are the interesting ones. Starting with a random cochain, we use least squares to find a representative for an element in $H^1$. This step is a Hodge decomposition, using only the connectivity information and taking the identity matrix as the inner product matrix on cochains.

The least squares problems can be solved by an iterative method like LSQR [43] which does not require the formation of the normal equation and works in spite of the existence of a nontrivial kernel. But in fact solvers approaching time optimality are available for this step as a consequence of our recent results in [35]. In [35] we showed that the matrix in the normal equations for cohomology calculation is diagonally dominant (it is of course symmetric). Thus the recent work of Spielman and Teng [45–48] and others and of Koutis et al. [39] can be used to approach time optimality. In the past, for real homology and cohomology calculations, researchers have relied on persistence algorithm [29, 56] followed by the use of Poincaré or Lefschetz duality [41]. This, for example, is the procedure followed by [20].

For computing the harmonic cochains we take the nontrivial cocycle from the previous step and solve a weighted least squares problem to obtain a unique harmonic cochain. This also gives us a discrete Hodge-deRham theorem. This method appears at first sight to be same as that in [20]. But in fact their algorithm and numerical properties of their matrices are very different. These differences and advantages of our method are highlighted in Section 6.

2 Review of Preliminaries

We need some basic terminology from exterior calculus and algebraic topology. Several recent papers in computational topology cover the relevant algebraic topology concepts. See for instance [21]. The classic textbooks are [31, 41]. Since we use discretization of exterior calculus, and there is no room for a detailed review, we point to several accessible treatments. We use two types of such discretizations. One involves simplicial oriented manifold complexes (primal mesh) and their circumcentric duals (dual mesh). (By manifold complex we mean a complex which is a manifold. Typically this is a simplicial approximation of a smooth manifold.) This discretization is called Discrete Exterior Calculus (DEC). The usual references for this are [19, 20, 33]. See also [36]. Another useful source is [23] which is one of the earliest references for discretization of Hodge theory.

The other discretization of exterior calculus is finite element exterior calculus. In particular, we use Whitney forms, which are piecewise smooth differential forms with tangential continuity across shared edges in 2D triangle meshes and normal continuity across shared triangles in 3D tetrahedral meshes. Some standard references for this material are [2, 3, 20, 23]. Our longtime favorite reference for smooth exterior calculus is the book [1]. The original definition of Whitney forms is from [54]. The most important object for this paper is a real-valued cochain. The space of $p$-dimensional cochains on a simplicial complex is the set of homomorphisms from the group of $p$-chains to reals. The space is denoted as $C^p(K; \mathbb{R})$ but we will shorten it to $C^p$. For the purpose of this paper it is enough to think of $C^p$ as a space of real-valued functions on the $p$-simplices which changes sign on a simplex when the simplex orientation is reversed. This is not a precise depiction. In reality cochains are functions on chains which are functions on the simplices. But the simplification above make the presentation easier. The space $C^p$ is a real vector space of dimension equal to the number of $p$-simplices.

Whitney forms can be thought of as an interpolation scheme from cochains to piecewise smooth forms. They are built from barycentric coordinate functions, with $\mu_i$ denoting the barycentric coordinate function corresponding to vertex $i$. For example, in a triangle, the Whitney form corresponding to edge $[i, j]$ is $\mu_i \, d\mu_j - \mu_j \, d\mu_i$. The Whitney 2-form corresponding to a triangle $[i, j, k]$ in a tetrahe-
Laplace-deRham operators in 2 and 3 dimensions. These are, in 2D, the discrete Hodge Laplacians given by the operator being 0 if we fall off either end of the diagrams above. These are sometimes referred to as the Hodge Laplacian of order equal to the number of faces minus the dimension of the manifold simplicial complex, which may be smaller than the embedding dimension. We will use either well-centered triangulations [52] in which the circumcenter lies in the interior of simplices, or Delaunay triangulations. Some recent work has shown that DEC works in Delaunay meshes [34]. See also [35]. For the Whitney forms version of exterior calculus we will not have the interior of simplices, or Delaunay triangulations. Some recent work has shown that DEC works in Delaunay meshes [34]. See also [36]. For the Whitney forms version of exterior calculus we will not have the interior of simplices, or Delaunay triangulations. Some recent work has shown that DEC works in Delaunay meshes [34]. See also [35].

In DEC one uses circumcentric dual cells of the primal simplices. This is the usual p vs n - p geometric duality common in algebraic topology [41] except that circumcenters are used instead of barycenters. Here n is the dimension of the manifold simplicial complex, which may be smaller than the embedding dimension. We will use either well-centered triangulations [52] in which the circumcenter lies in the interior of simplices, or Delaunay triangulations. Some recent work has shown that DEC works in Delaunay meshes [34]. See also [35]. For the Whitney forms version of exterior calculus we will not have the interior of simplices, or Delaunay triangulations. Some recent work has shown that DEC works in Delaunay meshes [34]. See also [35].

For simplicity we only describe the boundaryless case here. The boundary case works by taking into account the appropriate boundary conditions. The main operators are the discrete exterior derivative denoted \( d_p : C^p \to C^{p+1} \) which is just the coboundary operator. As a matrix it is the transpose of \( \partial_{p+1} : C_{p+1} \to C_p \), the boundary operator of algebraic topology acting on chains. Thus \( d_{p+1} \circ d_p = 0 \).

The other operator is the discrete Hodge star \( \ast_p : C^p \to D^{n-p} \). To mimic the properties of smooth Hodge star, we attach a \((-1)^p W^p\) whenever we write \( \ast^{-1} \). As a matrix \( \ast_p \) in DEC is a diagonal matrix of order equal to the number of p-simplices. The entry corresponding to a simplex \( \sigma^p \) is \(|\sigma^p|/|\ast \sigma^p|\), where \(|\sigma^p|\) in the numerator stands for p-dimensional volume, \( \ast \sigma^p \) stands for dual cell corresponding to \( \sigma^p \) and \(|\ast \sigma^p|\) stands for the \((n-p)\)-dimensional volume of the dual cell. It was shown recently [34] that if signed lengths are used (negative if circumcenter outside a simplex) then for Delaunay triangulation all diagonal entries of the diagonal matrix \( \ast_p \) are positive. The basic idea of the proof is that the circumcenters preserve the ordering of simplices in a Delaunay mesh. We will call the Hodge star matrix described above the DEC Hodge star.

If Whitney forms are used, then the matrix \( \ast_p \) is sparse but not diagonal in general. The entry \((i,j)\) is \( \int W_i W_j \) where \( W_i \) is the Whitney form corresponding to p-simplex number \( i \). The integral is over the n-simplices that contain both the p-simplices. The inner product is the one on differential forms [40]. For our cases of interest this is just the dot product of the proxy vector fields. We will refer to this \( \ast_p \) as the Whitney Hodge star matrix. Now we have the following chain complexes in 2 and 3 dimensions:

\[
\begin{array}{cccc}
C^0 & \xrightarrow{d_0} & C^1 & \xrightarrow{d_1} & C^2 \\
\downarrow \ast_0 & & \downarrow \ast_1 & & \downarrow \ast_2 \\
D^2 & \xrightarrow{d_0^T = d_0^T} & D^1 & \xrightarrow{d_1^T = d_1^T} & D^0 \\
C^0 & \xrightarrow{d_0} & C^1 & \xrightarrow{d_1} & C^2 & \xrightarrow{d_2} & C^3 \\
\downarrow \ast_0 & & \downarrow \ast_1 & & \downarrow \ast_2 & & \downarrow \ast_3 \\
D^3 & \xrightarrow{d_2^T = d_2^T} & D^2 & \xrightarrow{d_1^T = d_1^T} & D^1 & \xrightarrow{d_0^T = d_0^T} & D^0
\end{array}
\]

The discrete codifferential is defined as \( \delta_{p+1} : C^{p+1} \to C^p \), and \( \delta_{p+1} = (-1)^p \ast_p^{-1} d_p^T \ast_p \). With this we define the discrete Laplace-deRham operators as \( \Delta_p = d_{p-1} \delta_p + \delta_{p+1} d_p \) where we assume the operator is 0 if we fall off either end of the diagrams above. These are sometimes referred to as the discrete Hodge Laplacians. For convenience we list the explicit formulas for all the codifferentials and Laplace-deRham operators in 2 and 3 dimensions. These are, in 2D:

\[
\delta_0 = 0, \quad \delta_1 = \ast_0^{-1} d_0^T \ast_1, \quad \delta_2 = -\ast_1^{-1} d_1^T \ast_2, \quad \Delta_2 = d_{2-1} \delta_2 + \delta_2 d_{2+1}
\]
and

\[
\begin{align*}
\Delta_0 &= \delta_1 d_0 = *_{0}^{-1} d_{0}^{T} *_{1} d_{0}, \\
\Delta_1 &= d_0 \delta_1 + \delta_2 d_1 = d_0 *_{0}^{-1} d_{0}^{T} *_{1} + *_{1} d_{1}^{T} *_{2} d_{1}, \\
\Delta_2 &= d_1 \delta_2 = -d_{1} *_{1}^{-1} d_{1}^{T} *_{2} .
\end{align*}
\]

In 3D these are

\[
\begin{align*}
\delta_0 &= 0 , \\
\delta_1 &= *_{0}^{-1} d_{0}^{T} *_{1}, \\
\delta_2 &= *_{1}^{-1} d_{1}^{T} *_{2}, \\
\delta_3 &= *_{2}^{-1} d_{2}^{T} *_{3} ,
\end{align*}
\]

and

\[
\begin{align*}
\Delta_0 &= \delta_1 d_0 = *_{0}^{-1} d_{0}^{T} *_{1} d_{0}, \\
\Delta_1 &= d_0 \delta_1 + \delta_2 d_1 = d_0 *_{0}^{-1} d_{0}^{T} *_{1} + *_{1}^{-1} d_{1}^{T} *_{2} d_{1}, \\
\Delta_2 &= d_1 \delta_2 + \delta_3 d_2 = d_1 *_{1}^{-1} d_{1}^{T} *_{2} + *_{2}^{-1} d_{2}^{T} *_{3} d_{2}, \\
\Delta_3 &= d_2 \delta_3 = d_{2} *_{2}^{-1} d_{2}^{T} *_{3} .
\end{align*}
\]

### 3 Real Homology and Cohomology by Least Squares

We now describe a least-squares based method for finding a basis for real homology and cohomology. This allows us to use iterative linear solvers. We can use either classical solvers like conjugate gradient (CG) [32], MINRES [42] or LSQR [43], or modern ones like multigrid or KMP [39]. The latter can allow us to approach time optimality in some cases as described later and in [35].

For the simplicial complex $K$, we are interested in computing a basis for the vector spaces $H_p(K;\mathbb{R})$ and $H^p(K;\mathbb{R})$, the real-valued homology and cohomology vector spaces. For this section, the simplicial complex can be an arbitrary one; it need not be a manifold simplicial complex. But from the next section onwards we will assume $K$ is an oriented manifold simplicial complex. A basis for these vector spaces can be computed in many ways. One standard approach is to find the Smith normal form (SNF) for the boundary matrices [41]. By keeping track of the row and column operations a basis can be computed in terms of the original simplices. For SNF computation, one can work in several finite fields and infer the result for $\mathbb{Z}$, or work directly in $\mathbb{Z}$ and interpret the result as real numbers. The use of $\mathbb{Z}$ can make the algorithm expensive because the intermediate entries can become very large although there are algorithms to make the SNF computation polynomial time [38]. But the time complexity is cubic since row and column operations are involved. There can also be fill-in, i.e., zero entries becoming nonzero which can make the method impractical for very large complexes. If $K$ is a compact, orientable, $n$-dimensional manifold simplicial complex embedded in $\mathbb{R}^N$, then Poincaré or Lefschetz duality [41] can be used to construct a cohomology element starting from a homology element [49].

A second standard method is the persistence [27, 29] algorithm. This is usually implemented for the finite field $\mathbb{F}_2$ or other finite fields because of the same difficulty with $\mathbb{Z}$ that the naive SNF algorithm [41] has. The persistence algorithm however also has cubic complexity [28].

Our method for computing a basis element for $H^p(K;\mathbb{R})$ or $H_p(K;\mathbb{R})$ is an extension of our recent work [35]. We are only interested in $p = 1$ or $p = n - 1$. In this paper we are only concerned with the case of embedding dimension 2 or 3 and with $K$ being dimension 2 or 3. That is, we are only interested in the 1-dimensional cohomology of planar or surface meshes and 1- or 2-dimensional cohomology of solid meshes. We will only describe how to find a single element in the basis of $H^p(K;\mathbb{R})$, and then standard numerical linear algebra can be used to find the other basis elements. The $\dim(H^2(K;\mathbb{R}))$ will typically be small compared to the sizes of the matrices involved, since it is the second Betti number and corresponds to the cavities in the mesh. Similar comment applies to $\dim(H^1(K;\mathbb{R}))$. 

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The basic idea of our algorithm is to start with a random cochain and find its Hodge decomposition without using the metric information in the Hodge star. See [35] for an accessible introduction to Hodge decomposition in this context and for references on classical Hodge decomposition. We’ll call this procedure a topological Hodge decomposition. For concreteness we describe here the topological Hodge decomposition for finding a nontrivial 2-cocycle in a tetrahedral mesh.

Suppose there are \( N_2 \) triangles in \( K \). We first pick a random 2-cochain \( \rho \) by picking a random \( N_2 \)-vector. First we scale the entries of \( \rho \). In the present case, each entry is multiplied by the area of its corresponding triangle. This is not strictly required, but it removes the bias coming from the size of the simplex. Since a cochain is a discrete form and 2-cochain is a flux through a triangle, the same vector field would give a larger flux for a triangle with larger area. We then normalize \( \rho \) to have 2-norm 1. For simplicity of notation we’ll also call this final random 2-cochain \( \rho \).

To find a representative 2-cochain of an element of \( H^2(K; \mathbb{R}) \) we are interested in something which is in the kernel \( \ker d_2 \) but not in the image \( \text{im} d_1 \). Although this can be explained as Hodge decomposition, an equivalent explanation is in terms of least squares as pointed out in [35]. Refer to Figure 1 when reading the least squares-based algorithm that we now describe.

![Figure 1](image-url): Illustration of Hodge decomposition with identity inner product on cochains. The dark arrows are the initial, intermediate and final cochain and the dashed arrows show projections. We start with a 2-cochain \( \rho \) from which the component along \( \text{im} d_1 \) is first removed by a least squares computation. This yields \( \rho - d_1 \alpha \) which is in the space orthogonal to \( \text{im} d_1 \). A second projection via a least squares computation removes the component along \( \text{im} d_2^T \), resulting in the final nontrivial 2-cocycle \( \omega \).

We want a 2-cochain which is not in \( \text{im} d_1 \). The least squares projection of \( \rho \) into \( \text{im} d_1 \) will result in a residual which is not in \( \text{im} d_1 \). That is, we first solve the least squares problem

\[
d_1 \alpha \cong \rho. \tag{1}
\]

This can be done by LSQR, a classical, extremely reliable, and rapidly convergent method for solving least squares problems [43]. Since \( d_1 = d_2^T \) as a matrix, and hence contains only zeros or \( \pm 1 \), the presence of a nontrivial kernel for \( d_1 \) poses no challenge for any Krylov iterative method [8, 10, 30], including LSQR. Alternatively one can form the corresponding normal equations [9]

\[
d_1^T d_1 \alpha = d_1^T \rho. \tag{2}
\]
This equation can then be solved by a Krylov method like CG or MINRES. For all the iterative methods, conservative estimates on number of iterations can be made and for CG such estimates are given in [35]. Even with several hundred thousand rows in $d_1$, the actual number of iterations required to achieve a relative error of $10^{-8}$ or less is usually a few hundred or less [35].

Let $\alpha$ be the solution to the least squares problem. Then from standard linear algebra, the residual $\rho - d_1 \alpha$ is in im $d_1^T$, the orthogonal complement of im $d_1$. Thus we have achieved the first objective of producing a 2-cocochain which is not in im $d_1$.

Now we have to find a 2-cocochain in ker $d_2$, while staying out of im $d_1$. Since im $d_2 = ker d_2$, we do a least squares projection of $\rho - d_1 \alpha$ to im $d_2^T$ and then the residual will be in ker $d_2$. This is done by solving the least squares problem

$$d_2^T b \approx \rho - d_1 \alpha,$$

or because of orthogonality of im $d_2^T$ and im $d_1$ by solving the equivalent least squares problem

$$d_2^T b \approx \rho.$$

The normal equation corresponding to this system is

$$d_2 d_2^T b = d_2 \rho.$$

Instead of solving the two least squares problems (1) and (4), we can solve the equivalent least squares problem

$$[d_1 \quad d_2^T] \begin{bmatrix} a \\ b \end{bmatrix} \approx \rho.$$

Even though this looks incorrect because it appears that the matrix should be a $2 \times 2$ block matrix, this is correct because of orthogonality. If $\beta$ is the solution of (4), then

$$\omega = \rho - d_1 \alpha - d_2^T \beta$$

is the nontrivial 2-cocycle which is in ker $d_2$ and not in im $d_1$. Note that this $\omega$ is obtained from a Hodge decomposition of $\rho$ using an identity inner product matrix and so it is “harmonic” according to this inner product matrix. But for applications in graphics and numerical PDEs we are really interested in harmonic according to the inner product of the mesh, discretized as a DEC or Whitney Hodge star. In the next section we describe how, starting from $\omega$, we obtain such a harmonic cochain.

### 4 Harmonic Cochains using Optimization

In the previous section we showed how a nontrivial cocycle $\omega$ can be obtained by starting with a random cochain $\rho$ and solving two least squares problems. As mentioned earlier, this amounts to doing a topological Hodge decomposition of a random cochain. Now we describe how to obtain a harmonic cochain cohomologous to $\omega$, i.e., one that is in the same cohomology class as $\omega$. We will again use least squares, but now it will be weighted least squares. For simplicity, we again develop the theory for the case of boundaryless manifold simplicial complexes. The case with boundary follows by taking into account the appropriate boundary conditions as in the smooth theory [1].

In cohomology theory of smooth manifolds there is a remarkable theorem called Hodge-deRham theorem [37, Theorem 2.2.1]. It states that in each cohomology class there is exactly one harmonic form and it is the one with the smallest $L^2$ norm. Inspired by this, we formulate a discrete version of this theorem. First we derive the necessary stationarity conditions in the discrete case. For $\omega \in C^p$ s.t. $d_p \omega = 0$, we consider the optimization problem

$$\min_{\alpha \in C^{p-1}} (\omega + d_{p-1} \alpha, \omega + d_{p-1} \alpha),$$
where the $(\cdot, \cdot)$ is the $L^2$ inner product on $p$-cochains [7]. This is just the inner product using the discrete Hodge star as the inner product matrix. That is, we want to find

$$\min_{\alpha \in C^{p-1}} (\omega + d_{p-1} \alpha)^T *_p (\omega + d_{p-1} \alpha).$$

(8)

Writing this in terms of $\alpha$, we have $\min_{\alpha \in C^{p-1}} f(\alpha)$, where

$$f(\alpha) = \omega^T *_p \omega + \omega^T *_p d_{p-1} \alpha + \alpha^T d_{p-1}^T *_p d_{p-1} \alpha + \alpha^T d_{p-1}^T *_p \omega.$$

Stationary points are solutions of $Df(\alpha) = 0$ (here $D$ is the derivative with respect to the variable $\alpha$) and

$$Df(\alpha) = \omega^T *_p d_{p-1} + \omega^T *_p d_{p-1} + \alpha^T d_{p-1}^T *_p d_{p-1} + \alpha^T d_{p-1}^T *_p \omega.$$

By symmetry of the inner product matrix $*_p$ we have $Df(\alpha) = 2\omega^T *_p d_{p-1} + 2\alpha^T d_{p-1}^T *_p d_{p-1}$. Thus, if $Df(\alpha) = 0$ then $\alpha^T d_{p-1}^T *_p d_{p-1} = -\alpha^T *_p d_{p-1}$, that is,

$$d_{p-1}^T *_p d_{p-1} \alpha = -d_{p-1}^T *_p \omega.$$

(9)

Although this is a necessary condition for solving the optimization problem (8), the matrix $d_{p-1}^T *_p d_{p-1}$ may have a nontrivial kernel. In fact in the interesting cases it generally will. For example, for $p = 1$, the $\ker d_0$ will have dimension equal to the number of connected components in the complex. For $\alpha$ to be a minimizer we need that the Hessian, which is $d_{p-1}^T *_p d_{p-1}$, be at least positive semidefinite, which it is, because of the positive definiteness of $*_p$. In this case, $\alpha$ may not be unique, but as we will show in Theorem 4.2, $d_{p-1} \alpha$ will be unique. Theorem 4.2 is the discrete version of the Hodge-deRham theorem. Note that equation (9) is equivalent to $\delta_p d_{p-1} \alpha = -\delta_p \omega$ which is $\delta_p (\omega + d_{p-1} \alpha) = 0$. This should make the connection to $\omega + d_{p-1} \alpha$ being harmonic more transparent. This connection is proved in Theorem 4.2. But first we need a lemma.

**Lemma 4.1.** $\delta_{p+1}$ and $d_p$ are adjoints of each other.

**Proof.** We need to show that $(d_p \alpha, \beta) = (\alpha, \delta_{p+1} \beta)$ for any $\alpha \in C^p$ and $\beta \in C^{p+1}$. In matrix notation, we need to show that $\alpha^T d_p^T *_{p+1} \beta = \alpha^T *_p \delta_{p+1} \beta$. Since $\alpha$ and $\beta$ are arbitrary, this is equivalent to showing that $d_p^T *_{p+1} = *_p \delta_{p+1}$. But this is true by the definition of $\delta_{p+1}$. \hfill $\square$

**Theorem 4.2** (Discrete Hodge-deRham). Let $[\omega] \in H^p(K; \mathbb{R})$. Then

(i) there exists an $\alpha \in C^{p-1}(K; \mathbb{R})$, not necessarily unique, such that $\delta_p (\omega + d_{p-1} \alpha) = 0$;

(ii) $d_{p-1} \alpha$ such that $\delta_p (\omega + d_{p-1} \alpha) = 0$ is unique; and

(iii) $\delta_p (\omega + d_{p-1} \alpha) = 0$ if and only if $\Delta_p (\omega + d_{p-1} \alpha) = 0$.

**Proof.** (i) Consider the least squares problem $d_{p-1} \alpha \equiv \omega$. Let $-\alpha$ be a solution. Some such $\alpha$ always exists because least squares problems always have a solution. Note that the 2-norm used in formulating this problem as a residual minimization is the one induced from the Hodge star inner products on cochains. Specifically, the inner product matrix is $*_p$ and the least squares problem minimizes $(\omega + d_{p-1} \alpha)^T *_p (\omega + d_{p-1} \alpha)$ since $\omega - d_{p-1} (-\alpha) = (\omega + d_{p-1} \alpha)$. But from properties of least squares [9] the residual $(\omega + d_{p-1} \alpha)$ is orthogonal to $\im d_{p-1}$. Thus we have that $(\omega + d_{p-1} \alpha) \in \im d_{p-1}^\perp = \ker \delta_p$ since $\delta_p$ is the adjoint of $d_{p-1}$ in the Hodge star inner product on cochains by Lemma 4.1.

(ii) Uniqueness of $d_{p-1} \alpha$ follows from properties of least squares.

(iii) For the forward direction, we note that $\Delta_p (\omega + d_{p-1} \alpha) = (d_{p-1} \delta_p + \delta_{p+1} d_p) (\omega + d_{p-1} \alpha)$ which is $d_{p-1} \delta_p \omega - d_{p-1} \delta_p d_{p-1} \alpha$ since $\omega$ is in $\ker d_p$. Thus, $\Delta_p (\omega + d_{p-1} \alpha) = d_{p-1} (\delta_p \omega + \delta_p d_{p-1} \alpha) = 0$. The reverse direction is true since $\omega + d_{p-1} \alpha \in \ker \Delta_p = \ker \delta_p \cap \ker d_p$. \hfill $\square$
Remark 4.3. While the nontrivial cocycle computation required two least square solves, the harmonic cochain calculation requires only one. The equation (9) is the normal equation corresponding to the weighted least squares version of equation (2). One does not need to solve a weighted version of (5).

5 Approaching Time Optimality

In recent work, Koutis et al. [39] introduced a new algorithm for solving symmetric diagonally dominant (SDD) matrices. An SDD matrix is a symmetric square matrix $A$ with entries $a_{ij}$ such that $|a_{ii}| \geq \sum_{j \neq i} |a_{ij}|$. For a matrix of order $n$ with $m$ nonzeros, their algorithm has expected time complexity $\tilde{O}(m(\log n)^2 \log(\frac{1}{\epsilon}))$ for computing a solution with relative error bounded by $\epsilon$. The $\tilde{O}(\cdot)$ notation hides a factor of at most $(\log \log n)^4$.

Their work builds on that of Spielman and Teng [45–48] and others. See the references in these papers and in [39]. These algorithms start by associating a weighted graph and weighted graph Laplacian with the SDD matrix. The algorithms are multilevel and the matrices are made sparser and smaller. The sparsification is done by building low stretch trees.

As we point out in [35], our application is well-suited for KMP solver because the equations involved are derived from Laplacians to start with. In particular, the normal equation corresponding to equation (2) for the 1-cochain case has the normal equation $d_T^0 d_0 = \partial_T^{-1} \partial_T^{-1}$ which is the graph Laplacian. The second normal equation (5) for the 1-cochain case on the surface involves $d_1 d_T^1 = \partial_T^{-1} \partial_2$. This matrix is also SDD as shown in [35]. By an easy extension of the proof in [35] the matrix in the 2-cochain case for solids is also SDD. In these cases the representatives of real cohomology classes can be computed in the complexity of KMP solver, which is much better than cubic complexity of SNF followed by Poincaré-Lefschetz duality, or that of persistence. Thus one can approach time optimality in the sense of [39] in cohomology basis computation.

As mentioned in Remark 4.3, for the harmonic cochain computation, there is only one weighted least squares problem to be solved, namely (9). For the 1-cochain computation the matrix on the left in equation (9) is $d_T^0 \ast_1 d_0$. The SDDness of this matrix depends on the properties of the mesh. To see this we first need the following lemma.

Lemma 5.1. If $\ast_1$ is diagonal and with positive diagonal entries, then $d_T^0 \ast_1 d_0$ is SDD.

Proof. This follows from the fact that $d_T^0 \ast_1 d_0$ is the weighted graph Laplacian. \qed

If a well-centered mesh (e.g. acute-angled triangles in a triangle mesh) is used then the DEC Hodge star $\ast_1$ is diagonal with positive entries. For more on well-centered triangulations see [50–53]. It was shown recently [34, 36] that even for a Delaunay mesh this is true if signed lengths are used for the dual mesh, where the dual edge length is negative if the circumcenter is outside the triangle. Thus if the DEC Hodge star is used, then for Delaunay meshes, $d_T^0 \ast_1 d_0$ is SDD.

The matrix $d_T^0 \ast_1 d_0$ is the usual stiffness matrix that arises in the weak form of Poisson’s equation in finite element method [111]. The fact that its properties depend on the geometric properties of the mesh fits with the long tradition of the study of such effects in finite elements [5, 44]. When Whitney Hodge star is used, we have numerical evidence that the matrix is SDD when the mesh is acute angled. A simple manifestation of this, in the case of a single triangle is in Figure 2.

6 Comparisons with Other Methods

There are two methods for harmonic cochain computation that compete with our method. One is the method in [3] which involves a mixed finite element formulation [12] of Laplace’s equation. This is a first
order formulation, i.e., only first order derivatives appear. The harmonic cochain formulation in [3] continues the tradition of [2] in that it avoids the explicit discretization of Hodge star, and relies instead on the adjointness of $d$ and $\delta$. Since the harmonic cochains are the eigenvectors of the 0 eigenvalue of the Laplace-deRham operator, one can use, say a shifted version of power method on the finite element system matrix. However, eigenvalue and eigenvector methods are usually numerically not as well behaved as linear system solving for symmetric semidefinite systems.

The second method is in [20] and the second stage of it appears at first sight to be close to our method. However, there are several important numerical and algorithmic differences. They solve the equation $\Delta p \left( \omega + d_{p-1} \alpha \right) = 0$ for $\alpha$ directly, for which they solve all the lower dimensional versions first. Moreover, they appear to use the discrete Laplace-deRham operator directly. For large problems this can be problematic because $\Delta p = \pm d_{p-1} \ast^{p-1} \ast p \pm \ast p \ast^{p+1} d_p$ and the presence of $\ast^{-1}$ is troublesome if Whitney Hodge star is used. This is because in the Whitney case the $\ast^{p-1}$ is sparse but $\ast^{-1}$ will typically not be. (Note that while the $\ast p$ can be cancelled out, $\ast^{-1}$ is stuck between two operators and can’t be cancelled.) Another major difference is that they find the nontrivial cocycles by a persistence like method, which is a method in the same class as direct numerical linear algebra methods, thereby ruling out the use of faster iterative methods for approximation.

7 Experimental Results

Figures 3-6 show some example computations using our method. Computation of a harmonic cochain is shown for planar, surface and solid meshes. Figure 3 shows both stages of the calculation starting from a random cochain. The first stage least squares was solved using LSQR and the second using CG, although either solver could have been used for either stage.

In all of the figures the cochains are visualized as proxy vector fields obtained from a Whitney interpolation of the cochain. As mentioned earlier Whitney interpolation, i.e., the use of Whitney forms is a method for obtaining piecewise smooth differential forms, starting from cochains. The cochain values are Whitney interpolated inside the top dimensional simplices, converted to the corresponding proxy vector field and then sampled at the barycenter. These are the vector fields that are shown in the figures. For details on this procedure for visualizing cochains see [36].
For 1-cochains, we would expect to see the proxy vector fields of harmonic cochains circulating around holes and in the nontrivial directions of surface handles. For example a harmonic 1-cochain on a torus should go along the meridian, the longitude, or both. For the circulation around holes see Figure 4 and the sphere with a hole in Figure 5. The torus and a genus 3 surface is in Figure 5. A 2-cochain can be interpreted as the flux through the triangles. Thus we would expect to see a hedgehog like figure around cavities and this is visible in the solid annulus and solid torus with cavity in Figure 6.

8 Conclusions and Future Work

Since real numbers cannot be represented exactly, what we have described is really a rational approximation to real homology. However, an element in say, ker $d_2$ computed using least squares will not yield exactly 0 when $d_2$ is applied to it. While harmonic cochains generated in this way are sufficient for numerical PDEs and graphics applications, it would be interesting to study if there are techniques to “clean up” the computed cochain so that $d_2$ applied to it is exactly zero. One approach might be to use continued fractions approximations to represent finite precision numbers known to lie in certain intervals, as rational numbers. Another approach might be to find a cohomologous cochain with minimal 1-norm or for which the higher dimensional cochain has the minimal 1-norm [13, 17, 18, 22].

The relationship between the shapes of simplices and properties of the stiffness matrix is an important one and it would be interesting to explore these relationships for Whitney Hodge star following the techniques of [5, 16, 44]. As is well known, such relationships can be important for physical properties like the discrete maximum principle [15, 16, 26].

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References


Appendix

Figure 3: Different steps of our algorithm. First step is creation of a random cochain. One such random cochain normalized by edge lengths is shown on top left. (It is denser near the holes because the mesh is denser there.) Next step is the creation of a nontrivial cocycle, i.e., a cohomology class representative. This is obtained from a Hodge decomposition computed by least squares, without using any metric information. Top right figure shows the result. The bottom row is the final step in finding a harmonic cochain cohomologous to the one in top right. This is done by another Hodge decomposition computed using a weighted least squares, using the Hodge star matrix as the inner product matrix. We used the Whitney Hodge star for the bottom left and DEC Hodge star for the bottom right. The results look similar but are slightly different. All cochains are visualized by sampling the proxy vector field corresponding to the Whitney interpolation of the cochain values from the edges. Sampling is performed at the triangle barycenters.
Figure 4: Some harmonic 1-cochains on planar meshes computed using our method, using the Whitney Hodge star. The bottom figure is a zoomed-in view of the upper right figure.
**Figure 5:** Some harmonic 1-cochains on surface meshes embedded in $\mathbb{R}^3$ computed using our method, using the Whitney Hodge star. The upper figures are the torus and a genus three surface. The bottom figure is a sphere with holes near the north and south poles. (The inside of the sphere is visible in the hole.)
Figure 6: Some harmonic 2-cochains on solid (tetrahedral) meshes computed using our method, using the Whitney Hodge star. The upper left figure is a solid annulus, that is, a solid ball with a cavity. The upper right figure is a solid torus with an enclosed cavity. The lower figure is a zoomed-in and rotated view of the solid torus showing the proxy vector field around the cavity.