

# HODGE LAPLACIANS ON GRAPHS\*

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**Abstract.** This is an elementary introduction to the Hodge Laplacian on a graph, a higher-order generalization of the graph Laplacian. We will discuss basic properties including cohomology and Hodge theory. The main feature of our approach is simplicity, requiring only knowledge of linear algebra and graph theory. We have also isolated the algebra from the topology to show that a large part of cohomology and Hodge theory is nothing more than the linear algebra of matrices satisfying  $AB = 0$ . For the remaining topological aspect, we cast our discussions entirely in terms of graphs as opposed to less-familiar topological objects like simplicial complexes.

**Key words.** Cohomology, Hodge decomposition, Hodge Laplacians, graphs

**AMS subject classifications.** 05C50, 58A14, 20G10

**1. Introduction.** The primary goal of this article is to introduce readers to the Hodge Laplacian on a graph and discuss some of its properties, notably the Hodge decomposition. To understand its significance, it is inevitable that we will also have to discuss the basic ideas behind cohomology, but we will do so in a way that is as elementary as possible and with a view towards applications in the information sciences.

If the classical Hodge theory on Riemannian manifolds [37, 60] is “differentiable Hodge theory,” the Hodge theory on metric spaces [6, 55] “continuous Hodge theory,” and the Hodge theory on simplicial complexes [26, 28] “discrete Hodge theory,” then the version here may be considered “graph-theoretic Hodge theory.”

Unlike physical problems arising from areas such as continuum mechanics or electromagnetics, where the differentiable Hodge–de Rham theory has been applied with great efficacy for both modeling and computations [1, 2, 27, 40, 47, 58, 59], those arising from data analytic applications are likely to be far less structured [3, 9, 11, 14, 15, 17, 22, 30, 36, 38, 41, 42, 48, 49, 51, 52, 61, 62, 63]. Often one could at best assume some weak notion of proximity of data points. The Hodge theory introduced in this article requires nothing more than the data set having the structure of an undirected graph and is conceivably more suitable for non-physical applications such as those arising from the biological or information sciences (see Section 6.3).

Our simple take on cohomology and Hodge theory requires only linear algebra and graph theory. In our approach, we have isolated the algebra from the topology to show that a large part of cohomology and Hodge theory is nothing more than the linear algebra of matrices satisfying  $AB = 0$ . For the remaining topological aspect, we cast our discussions entirely in terms of graphs as opposed to less-familiar topological objects like simplicial complexes. We believe that by putting these in a simple framework, we could facilitate the development of applications as well as communication with practitioners who may not otherwise see the utility of these notions.

We write with a view towards readers whose main interests may lie in machine

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learning, matrix computations, numerical PDEs, optimization, statistics, or theory of computing, but have a casual interest in the topic and may perhaps want to explore potential applications in their respective fields. To enhance the pedagogical value of this article, we have provided complete proofs and fully worked-out examples in Section 5.

The occasional whimsical section headings are inspired by [10, 44, 45, 53, 54].

**2. Cohomology and Hodge theory for pedestrians.** We will present in this section what we hope is the world's most elementary approach towards *cohomology* and *Hodge theory*, requiring only linear algebra.

**2.1. Cohomology on a bumper sticker.** Given two matrices  $A \in \mathbb{R}^{m \times n}$  and  $B \in \mathbb{R}^{n \times p}$  satisfying the property that

$$(2.1) \quad AB = 0,$$

a property equivalent to

$$\text{im}(B) \subseteq \ker(A),$$

the *cohomology group* with respect to  $A$  and  $B$  is the quotient vector space

$$\ker(A)/\text{im}(B),$$

and its elements are called *cohomology classes*. The word ‘group’ here refers to the structure of  $\ker(A)/\text{im}(B)$  as an abelian group under addition.

We have fudged a bit because we haven't yet defined the matrices  $A$  and  $B$ . Cohomology usually refers to a special case where  $A$  and  $B$  are certain matrices with topological meaning, as we will define in Section 3.

**2.2. Harmonic representative.** The definition in the previous section is plenty simple, provided the reader knows what a quotient vector space is, but can it be further simplified? For instance, can we do away with quotient spaces and equivalence classes<sup>1</sup> and define cohomology classes as actual vectors in  $\mathbb{R}^n$ ?

Note that an element in  $\ker(A)/\text{im}(B)$  is a set of vectors

$$x + \text{im}(B) := \{x + y \in \mathbb{R}^n : y \in \text{im}(B)\}$$

for some  $x \in \ker(A)$ . We may avoid such equivalence classes if we could choose an  $x_H \in x + \text{im}(B)$  in some unique way to represent the entire set. A standard way to do this is to pick  $x_H$  so that it is orthogonal to every other vector in  $\text{im}(B)$ . Since  $\text{im}(B)^\perp = \ker(B^*)$ , this is equivalent to requiring that  $x_H \in \ker(B^*)$ . Hence we should pick an  $x_H \in \ker(A) \cap \ker(B^*)$ . Such an  $x_H$  is called a *harmonic representative* of the cohomology class  $x + \text{im}(B)$ .

The map that takes the cohomology class  $x + \text{im}(B)$  to its unique harmonic representative  $x_H$  gives a natural isomorphism of vector spaces (see Theorem 5.3)

$$(2.2) \quad \ker(A)/\text{im}(B) \cong \ker(A) \cap \ker(B^*).$$

So we may redefine the cohomology group with respect to  $A$  and  $B$  to be the subspace  $\ker(A) \cap \ker(B^*)$  of  $\mathbb{R}^n$ , and a cohomology class may now be regarded as an actual vector  $x_H \in \ker(A) \cap \ker(B^*)$ .

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<sup>1</sup>Practitioners tend to dislike working with equivalence classes of objects. One reason is that these are often tricky to implement in a computer program.

A word about our notation:  $B^*$  denotes the adjoint of the matrix  $B$ . Usually we will work over  $\mathbb{R}$  with the standard  $l^2$ -inner product on our spaces and so  $B^* = B^\top$ . However we would like to allow for the possibility of working over  $\mathbb{C}$  or with other inner products.

*Linear algebra interlude.* For those familiar with numerical linear algebra, the way we choose a unique harmonic representative  $x_H$  to represent a cohomology class  $x + \text{im}(B)$  is similar to how we would impose uniqueness on a solution to a linear system of equations by requiring that it has minimum norm among all solutions [31, Section 5.5]. More specifically, the solutions to  $Ax = b$  are given by  $x_0 + \ker(A)$  where  $x_0$  is any particular solution; we impose uniqueness by requiring that  $x_0 \in \ker(A)^\perp = \text{im}(A^*)$ , which gives the minimum norm (or pseudoinverse) solution  $x_0 = A^\dagger b$ . The only difference above is that we deal with two matrices  $A$  and  $B$  instead of a single matrix  $A$ .

**2.3. Hodge theory on one foot.** We now explain why an element in  $\ker(A) \cap \ker(B^*)$  is called ‘harmonic.’ Again assume that  $AB = 0$ , the *Hodge Laplacian* is the matrix

$$(2.3) \quad A^*A + BB^* \in \mathbb{R}^{n \times n}.$$

We may show (see Theorem 5.2) that

$$(2.4) \quad \ker(A^*A + BB^*) = \ker(A) \cap \ker(B^*).$$

So the harmonic representative  $x_H$  that we constructed in Section 2.2 is a solution to the *Laplace equation*

$$(2.5) \quad (A^*A + BB^*)x = 0.$$

Since solutions to the Laplace equation are called *harmonic* functions, this explains the name ‘harmonic’ representative.

With this observation, we see that we could also have defined the cohomology group (with respect to  $A$  and  $B$ ) as the kernel of the Hodge Laplacian since

$$\ker(A)/\text{im}(B) \cong \ker(A^*A + BB^*).$$

We may also show (see Theorem 5.2) that there is a *Hodge decomposition*, an orthogonal direct sum decomposition

$$(2.6) \quad \mathbb{R}^n = \text{im}(A^*) \oplus \ker(A^*A + BB^*) \oplus \text{im}(B).$$

In other words, whenever  $AB = 0$ , every  $x \in \mathbb{R}^n$  can be decomposed uniquely as

$$x = A^*w + x_H + Bv, \quad \langle A^*w, x_H \rangle = \langle x_H, Bv \rangle = \langle A^*w, Bv \rangle = 0,$$

for some  $v \in \mathbb{R}^p$  and  $w \in \mathbb{R}^m$ .

Recall the well-known decompositions (sometimes called the Fredholm alternative, see Theorem 5.1) associated with the four fundamental subspaces [57] of a matrix  $A \in \mathbb{R}^{m \times n}$ ,

$$(2.7) \quad \mathbb{R}^n = \ker(A) \oplus \text{im}(A^*), \quad \mathbb{R}^m = \ker(A^*) \oplus \text{im}(A).$$

The Hodge decomposition (2.6) may be viewed as an analogue of (2.7) for a pair of matrices satisfying  $AB = 0$ . In fact, combining (2.6) and (2.7), we obtain

$$\mathbb{R}^n = \underbrace{\text{im}(A^*) \oplus \text{ker}(A^*A + BB^*)}_{\text{ker}(A)} \oplus \text{im}(B).$$

The intersection of  $\text{ker}(A)$  and  $\text{ker}(B^*)$  gives  $\text{ker}(A^*A + BB^*)$ , confirming (2.4). Since  $A^*A + BB^*$  is Hermitian, it also follows that

$$(2.8) \quad \text{im}(A^*A + BB^*) = \text{im}(A^*) \oplus \text{im}(B).$$

For the special case when  $A$  is an arbitrary matrix and  $B = 0$ , the Hodge decomposition (2.6) becomes

$$(2.9) \quad \mathbb{R}^n = \text{im}(A^*) \oplus \text{ker}(A^*A),$$

which may also be deduced directly from the Fredholm alternative (2.7) since

$$(2.10) \quad \text{ker}(A^*A) = \text{ker}(A).$$

*Linear algebra interlude.* To paint an analogy like that in the last paragraph of Section 2.2, our characterization of cohomology classes as solutions to the Laplace equation (2.5) is similar to the characterization of solutions to a least squares problem  $\min_{x \in \mathbb{R}^n} \|Ax - b\|$  as solutions to its normal equation  $A^*Ax = A^*b$  [31, Section 6.3]. Again the only difference is that here we deal with two matrices instead of just one.

**2.4. Terminologies.** One obstacle that the (impatient) beginner often faces when learning cohomology is the considerable number of scary-sounding terminologies that we have by-and-large avoided in the treatment above.

In Table 1, we summarize some commonly used terminologies for objects in Sections 2.1, 2.2, and 2.3. Their precise meanings will be given in Sections 3 and 4, with an updated version of this table appearing as Table 3. As the reader can see, there is some amount of redundancy in these terminologies; e.g., saying that a cochain is exact is the same as saying that it is a coboundary. This can sometimes add to the confusion for a beginner. It is easiest to just remember equations and disregard jargons. When people say things like ‘a cochain is harmonic if and only if it is closed and coclosed,’ they are just verbalizing (2.4).

In summary, we saw *three different ways of defining cohomology*: If  $A$  and  $B$  are matrices satisfying  $AB = 0$ , then the cohomology group with respect to  $A$  and  $B$  may be taken to be any one of the following,

$$(2.11) \quad \text{ker}(A)/\text{im}(B), \quad \text{ker}(A) \cap \text{ker}(B^*), \quad \text{ker}(A^*A + BB^*).$$

For readers who may have heard of the term *homology*, that can be defined just by taking adjoints. Note that if  $AB = 0$ , then  $B^*A^* = 0$  and we may let  $B^*$  and  $A^*$  play the role of  $A$  and  $B$  respectively. The homology group with respect to  $A$  and  $B$  may then be taken to be any one of the following,

$$(2.12) \quad \text{ker}(B^*)/\text{im}(A^*), \quad \text{ker}(B^*) \cap \text{ker}(A), \quad \text{ker}(BB^* + A^*A).$$

As we can see, the last two spaces in (2.11) and (2.12) are identical, i.e., there is no difference between cohomology and homology in our context (see Theorem 5.3 for a proof and Section 6.1 for caveats).

Table 1: Topological jargons (first pass)

NAME	MEANING
coboundary maps	$A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{n \times p}$
cochains	elements $x \in \mathbb{R}^n$
cochain complex	$\mathbb{R}^p \xrightarrow{B} \mathbb{R}^n \xrightarrow{A} \mathbb{R}^m$
cocycles	elements of $\ker(A)$
coboundaries	elements of $\text{im}(B)$
cohomology classes	elements of $\ker(A)/\text{im}(B)$
harmonic cochains	elements of $\ker(A^*A + BB^*)$
Betti numbers	$\dim \ker(A^*A + BB^*)$
Hodge Laplacians	$A^*A + BB^* \in \mathbb{R}^{n \times n}$
$x$ is closed	$Ax = 0$
$x$ is exact	$x = Bv$ for some $v \in \mathbb{R}^p$
$x$ is coclosed	$B^*x = 0$
$x$ is coexact	$x = A^*w$ for some $w \in \mathbb{R}^m$
$x$ is harmonic	$(A^*A + BB^*)x = 0$

**3. Coboundary operators and Hodge Laplacians on graphs.** The way we discussed cohomology and Hodge theory in Section 2 relies solely on the linear algebra of operators satisfying  $AB = 0$ ; this is the ‘algebraic side’ of the subject. There is also a ‘topological side’ that is just one step away, obtained by imposing the requirement that  $A$  and  $B$  be *coboundary operators*. Readers may remember from vector calculus identities like  $\text{curl grad} = 0$  or  $\text{div curl} = 0$  in  $\mathbb{R}^3$  — these are in fact pertinent examples of when  $AB = 0$  naturally arises; and as we will soon see,  $\text{div}, \text{grad}, \text{curl}$  are our most basic examples of coboundary operators. Restricting our choices of  $A$  and  $B$  to coboundary operators allows us to attach topological meanings to the objects in Section 2.

Just like the last section requires nothing more than elementary linear algebra, this section requires nothing more than elementary graph theory. We will discuss simplicial complexes (family of subsets of vertices), cochains (functions on a graph), and coboundary operators (operators on functions on a graph) — all in the context of the simplest type of graphs: undirected, unweighted, no loops, no multiple edges.

**3.1. Graphs.** Let  $G = (V, E)$  be an undirected graph where  $V := \{1, \dots, n\}$  is a finite set of vertices and  $E \subseteq \binom{V}{2}$  is the set<sup>2</sup> of edges. Note that once we have specified  $G$ , we automatically get *cliques* of higher order — for example, the set of triangles or 3-*cliques*  $T \subseteq \binom{V}{3}$  is defined by

$$\{i, j, k\} \in T \quad \text{iff} \quad \{i, j\}, \{i, k\}, \{j, k\} \in E.$$

More generally the set of  $k$ -*cliques*  $K_k(G) \subseteq \binom{V}{k}$  is defined by

$$\{i_1, \dots, i_k\} \in K_k(G) \quad \text{iff} \quad \{i_p, i_q\} \in E \text{ for all } 1 \leq p < q \leq k,$$

<sup>2</sup>Henceforth  $\binom{V}{k}$  denotes the set of all  $k$ -element subsets of  $V$ . In particular  $E$  is not a multiset since our graphs have no loops nor multiple edges.

i.e., all pairs of vertices in  $\{i_1, \dots, i_k\}$  are in  $E$ . Clearly, specifying  $V$  and  $E$  uniquely determines  $K_k(G)$  for all  $k \geq 3$ . In particular we have

$$K_1(G) = V, \quad K_2(G) = E, \quad K_3(G) = T.$$

In topological parlance, a nonempty family  $K$  of finite subsets of a set  $V$  is called a *simplicial complex* (more accurately, an abstract simplicial complex) if for any set  $S$  in  $K$ , every  $S' \subseteq S$  also belongs to  $K$ . Evidently the set comprising all cliques of a graph  $G$ ,

$$K(G) := \bigcup_{k=1}^{\omega(G)} K_k(G),$$

is a simplicial complex and is called the *clique complex* of the graph  $G$ . The *clique number*  $\omega(G)$  is the number of vertices in a largest clique of  $G$ .

There are abstract simplicial complexes that are not clique complexes of graphs. For example, we may just exclude cliques of larger sizes —  $\bigcup_{k=1}^m K_k(G)$  is still an abstract simplicial complex for any  $m = 3, \dots, \omega(G) - 1$ , but it would not in general be a clique complex of a graph.

**3.2. Functions on a graph.** Given a graph  $G = (V, E)$ , we will consider real-valued functions on its vertices  $f : V \rightarrow \mathbb{R}$ . We will also consider real-valued functions on  $E$  and  $T$  and  $K_k(G)$  in general but we shall require them to be *alternating*. By an alternating function on  $E$ , we mean one of the form  $X : V \times V \rightarrow \mathbb{R}$  where

$$X(i, j) = -X(j, i)$$

for all  $\{i, j\} \in E$ , and

$$X(i, j) = 0$$

for all  $\{i, j\} \notin E$ . An alternating function on  $T$  is one of the form  $\Phi : V \times V \times V \rightarrow \mathbb{R}$  where

$$\Phi(i, j, k) = \Phi(j, k, i) = \Phi(k, i, j) = -\Phi(j, i, k) = -\Phi(i, k, j) = -\Phi(k, j, i)$$

for all  $\{i, j, k\} \in T$ , and

$$\Phi(i, j, k) = 0$$

for all  $\{i, j, k\} \notin T$ . More generally, an alternating function is one where permutation of its arguments has the effect of changing its value by the sign of the permutation, as we will see in (4.1).

In topological parlance, the functions  $f, X, \Phi$  are called 0-, 1-, 2-*cochains*. These are discrete analogues of *differential forms* on manifolds [60]. Those who prefer to view them as such often refer to cochains as *discrete differential forms* [23, 24, 35] and in which case,  $f, X, \Phi$  are 0-, 1-, 2-*forms* on  $G$ .

Observe that a 1-cochain  $X$  is completely specified by the values it takes on the set  $\{(i, j) : i < j\}$  and a 2-cochain  $\Phi$  is completely specified by the values it takes on the set  $\{(i, j, k) : i < j < k\}$ . We may equip the spaces of cochains with inner products, for example, as weighted sums

$$(3.1) \quad \begin{aligned} \langle f, g \rangle_V &= \sum_{i=1}^n w_i f(i) g(i), & \langle X, Y \rangle_E &= \sum_{i < j} w_{ij} X(i, j) Y(i, j), \\ \langle \Phi, \Psi \rangle_T &= \sum_{i < j < k} w_{ijk} \Phi(i, j, k) \Psi(i, j, k), \end{aligned}$$

where the weights  $w_i, w_{ij}, w_{ijk}$  are given by any positive values invariant under arbitrary permutation of indices. When they take the constant value 1, we call it the

*standard  $L^2$ -inner product.* By summing only over the sets<sup>3</sup>  $\{(i, j) : i < j\}$  and  $\{(i, j, k) : i < j < k\}$ , we count each edge or triangle exactly once in the inner products.

We will denote the Hilbert spaces of 0-, 1-, and 2-cochains as  $L^2(V)$ ,  $L^2_\wedge(E)$ ,  $L^2_\wedge(T)$  respectively. The subscript  $\wedge$  is intended to indicate ‘alternating’. Note that  $L^2_\wedge(V) = L^2(V)$  since for a function of one argument, being alternating is a vacuous property. We set  $L^2_\wedge(\emptyset) := \{0\}$  by convention. The  $L^2$  prefix is merely to indicate the presence of an inner product.  $L^2$ -integrability is never an issue since the spaces  $V$ ,  $E$ ,  $T$  are finite sets; e.g., any function  $f : V \rightarrow \mathbb{R}$  will be an element of  $L^2(V)$  as  $\|f\|_V^2 = \langle f, f \rangle_V$  is just a finite sum and thus finite.

The elements of  $L^2_\wedge(E)$  (i.e., 1-cochains) are well-known in graph theory, often called *edge flows*. While the graphs in this article are always undirected and unweighted, a directed graph is simply one equipped with a choice of edge flow  $X \in L^2_\wedge(E)$  — an undirected edge  $\{i, j\} \in E$  becomes a directed edge  $(i, j)$  if  $X(i, j) > 0$  or  $(j, i)$  if  $X(i, j) < 0$ ; and the magnitude of  $X(i, j)$  may be taken as the weight of that directed edge. So  $L^2_\wedge(E)$  encodes all weighted directed graphs that have the same underlying undirected graph structure.

**3.3. Operators on functions on a graph.** We consider the graph-theoretic analogues of grad, curl, div in multivariate calculus. The *gradient* is the linear operator  $\text{grad} : L^2(V) \rightarrow L^2_\wedge(E)$  defined by

$$(\text{grad } f)(i, j) = f(j) - f(i)$$

for all  $\{i, j\} \in E$  and zero otherwise. The *curl* is the linear operator  $\text{curl} : L^2_\wedge(E) \rightarrow L^2_\wedge(T)$  defined by

$$(\text{curl } X)(i, j, k) = X(i, j) + X(j, k) + X(k, i)$$

for all  $\{i, j, k\} \in T$  and zero otherwise. The *divergence* is the linear operator  $\text{div} : L^2_\wedge(E) \rightarrow L^2(V)$  defined by

$$(\text{div } X)(i) = \sum_{j=1}^n \frac{w_{ij}}{w_i} X(i, j)$$

for all  $i \in V$ .

Using these, we may construct other linear operators, notably the well-known *graph Laplacian*, the operator  $\Delta_0 : L^2(V) \rightarrow L^2(V)$  defined by

$$\Delta_0 = -\text{div grad},$$

which is a graph-theoretic analogue of the Laplace operator (see Lemma 5.6). Less well-known is the *graph Helmholtzian* [38], the operator  $\Delta_1 : L^2_\wedge(E) \rightarrow L^2_\wedge(E)$  defined by

$$\Delta_1 = -\text{grad div} + \text{curl}^* \text{curl},$$

which is a graph-theoretic analogue of the vector Laplacian. We may derive (see Lemma 5.5) an expression for the adjoint of the curl operator,  $\text{curl}^* : L^2_\wedge(T) \rightarrow L^2_\wedge(E)$  is given by

$$(\text{curl}^* \Phi)(i, j) = \sum_{k=1}^n \frac{w_{ijk}}{w_{ij}} \Phi(i, j, k)$$

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<sup>3</sup>Our choice is arbitrary; any set that includes each edge or triangle exactly once would also serve the purpose. Each such choice corresponds to a choice of direction or orientation on the elements of  $E$  or  $T$ .

for all  $\{i, j\} \in E$  and zero otherwise.

The gradient and curl are special cases of *coboundary operators*, discrete analogues of *exterior derivatives*, while the graph Laplacian and Helmholtzian are special cases of *Hodge Laplacians*.

The matrices  $A$  and  $B$  that we left unspecified in Section 2 are coboundary operators. We may show (see Theorem 5.7) that the composition

$$(3.2) \quad \text{curl grad} = 0$$

and so setting  $A = \text{curl}$  and  $B = \text{grad}$  gives us (2.1).

Note that divergence and gradient are negative adjoints of each other:

$$(3.3) \quad \text{div} = -\text{grad}^*,$$

(see Lemma 5.4). With this we get  $\Delta_1 = A^*A + BB^*$  as in (2.3).

If the inner products on  $L^2(V)$  and  $L_\wedge^2(E)$  are taken to be the standard  $L^2$ -inner products, then (3.3) gives  $\Delta_0 = B^*B = B^\top B$ , a well-known expression of the graph Laplacian in terms of vertex-edge incidence matrix  $B$ . The operators

$$\text{grad}^* \text{grad} : L^2(V) \rightarrow L^2(V) \quad \text{and} \quad \text{curl}^* \text{curl} : L_\wedge^2(E) \rightarrow L_\wedge^2(E)$$

are sometimes called the *vertex Laplacian* and *edge Laplacian* respectively. The vertex Laplacian is of course just the usual graph Laplacian but note that the edge Laplacian is not the same as the graph Helmholtzian.

*Physics interlude.* Take the standard  $L^2$ -inner products on  $L^2(V)$  and  $L_\wedge^2(E)$ , the divergence of an edge flow at a vertex  $i \in V$  may be interpreted as the *netflow*,

$$(3.4) \quad (\text{div } X)(i) = (\text{inflow } X)(i) - (\text{outflow } X)(i),$$

where *inflow* and *outflow* are defined respectively for any  $X \in L_\wedge^2(E)$  and any  $i \in V$  as

$$(\text{inflow } X)(i) = \sum_{j: X(i,j) < 0} X(i,j), \quad (\text{outflow } X)(i) = \sum_{j: X(i,j) > 0} X(i,j).$$

Sometimes the terms *incoming flux*, *outgoing flux*, *total flux* are used instead of inflow, outflow, netflow. Figure 2 shows two *divergence-free* edge flows, i.e., inflow equals outflow at every vertex.

Let  $X \in L_\wedge^2(E)$ . A vertex  $i \in V$  is called a *sink* of  $X$  if  $X(i,j) < 0$  for every neighbor  $\{i,j\} \in E$  of  $i$ . Likewise a vertex  $i \in V$  is called a *source* of  $X$  if  $X(i,j) > 0$  for every neighbor  $\{i,j\} \in E$  of  $i$ . In general, an edge flow may not have any source or sink<sup>4</sup> but it can be written as

$$X = -\text{grad } f$$

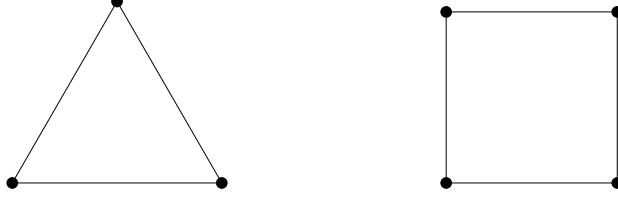
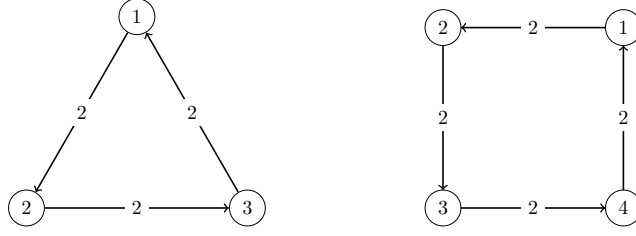
for some  $f \in L^2(V)$ , often called a *potential* function, then  $X$  will have the property of flowing from sources (local maxima of  $f$ ) to sinks (local minima of  $f$ ).

*Example 3.1.* We highlight a common pitfall regarding curl on a graph. Consider  $C_3$  and  $C_4$ , the *cycle graphs* on three and four vertices in Figure 1.

Number the vertices and consider the edge flows in Figure 2. What are the values of their curl? For the one on  $C_3$ , the answer is  $2 + 2 + 2 = 6$  as expected. But the answer for the one on  $C_4$  is not  $2 + 2 + 2 + 2 = 8$ , it is in fact 0.

<sup>4</sup>There is an alternative convention that defines  $i \in V$  to be a source (resp. sink) of  $X$  as long as  $\text{div } X(i) > 0$  (resp.  $\text{div } X(i) < 0$ ) but our definition is much more restrictive.



Fig. 1: Cycle graphs  $C_3$  (left) and  $C_4$  (right).Fig. 2: Edge flows on  $C_3$  (left) and  $C_4$  (right).

The second answer may not agree with a physicist's intuitive idea of curl and is a departure from what one would expect in the continuous case. However it is what follows from definition. Let  $X \in L^2_\wedge(E(C_3))$  denote the edge flow on  $C_3$  in Figure 2. It is given by

$$X(1,2) = X(2,3) = X(3,1) = 2 = -X(2,1) = -X(3,2) = -X(1,3),$$

and the curl evaluated at  $\{1,2,3\} \in T(C_3)$  is by definition indeed

$$(\text{curl } X)(1,2,3) = X(1,2) + X(2,3) + X(3,1) = 6.$$

On the other hand  $C_4$  has no 3-cliques and so  $T(C_4) = \emptyset$ . By convention  $L^2_\wedge(\emptyset) = \{0\}$ . Hence  $\text{curl} : L^2_\wedge(E(C_4)) \rightarrow L^2_\wedge(T(C_4))$  must have  $\text{curl } X = 0$  for all  $X \in L^2_\wedge(E(C_4))$  and in particular for the edge flow on the right of Figure 2.

Table 2: Electrodynamics/fluid dynamics jargons

NAME	MEANING	ALTERNATE NAME(S)
divergence-free	element of $\ker(\text{div})$	solenoidal
curl-free	element of $\ker(\text{curl})$	irrotational
vorticity	element of $\text{im}(\text{curl}^*)$	vector potential
conservative	element of $\text{im}(\text{grad})$	potential flow
harmonic	element of $\ker(\Delta_1)$	
anharmonic	element of $\text{im}(\Delta_1)$	
scalar field	element of $L^2(V)$	scalar potential
vector field	element of $L^2_\wedge(E)$	

**3.4. Helmholtz decomposition for graphs.** The usual graph Laplacian  $\Delta_0 : L^2(V) \rightarrow L^2(V)$ ,

$$\Delta_0 = -\operatorname{div} \operatorname{grad} = \operatorname{grad}^* \operatorname{grad},$$

has been an enormously useful construct in the context of spectral graph theory [20, 56], with great impact on many areas. We have nothing more to add except to remark that the Hodge decomposition associated with the graph Laplacian  $\Delta_0$  is given by (2.9),

$$L^2(V) = \ker(\Delta_0) \oplus \operatorname{im}(\operatorname{div}).$$

Recall from (2.10) that  $\ker(\Delta_0) = \ker(\operatorname{grad})$ . Since  $\operatorname{grad} f = 0$  iff  $f$  is piecewise constant, i.e., constant on each connected component of  $G$ , the number  $\beta_0(G) := \dim \ker(\Delta_0)$  counts the number of connected component of  $G$  — a well known fact in graph theory.

The Hodge decomposition associated with the graph Helmholtzian  $\Delta_1 : L_\wedge^2(E) \rightarrow L_\wedge^2(E)$ ,

$$\Delta_1 = -\operatorname{grad} \operatorname{div} + \operatorname{curl}^* \operatorname{curl} = \operatorname{grad} \operatorname{grad}^* + \operatorname{curl}^* \operatorname{curl}.$$

is called the *Helmholtz decomposition*. It says that the space of edge flows admits an orthogonal decomposition into subspaces

$$(3.5) \quad L_\wedge^2(E) = \underbrace{\operatorname{im}(\operatorname{curl}^*) \oplus \ker(\Delta_1)}_{\ker(\operatorname{curl})} \oplus \operatorname{im}(\operatorname{grad}),$$

and moreover the three subspaces are related via

$$(3.6) \quad \ker(\Delta_1) = \ker(\operatorname{curl}) \cap \ker(\operatorname{div}), \quad \operatorname{im}(\Delta_1) = \operatorname{im}(\operatorname{curl}^*) \oplus \operatorname{im}(\operatorname{grad}).$$

In particular, the first equation is a discrete analogue of the statement “a vector field is curl-free and divergence-free if and only if it is a harmonic vector field.”

There is nothing really special here — as we saw in Section 2.3, any matrices  $A$  and  $B$  satisfying  $AB = 0$  would give such a decomposition: (3.5) and (3.6) are indeed just (2.6), (2.4), and (2.8) where  $A = \operatorname{curl}$  and  $B = \operatorname{grad}$ . This is however a case that yields the most interesting applications (see Section 6.3 and [14, 38]).

*Example 3.2* (Beautiful Mind problem on graphs). This is a discrete analogue of a problem<sup>5</sup> that appeared in a blockbuster movie: Let  $G = (V, E)$  be a graph. If  $X \in L_\wedge^2(E)$  is curl-free, then is it true that  $X$  is a gradient? In other words, if  $X \in \ker(\operatorname{curl})$ , must it also be in  $\operatorname{im}(\operatorname{grad})$ ? Clearly the converse always holds by (3.2) but from (3.5), we know that

$$(3.7) \quad \ker(\operatorname{curl}) = \ker(\Delta_1) \oplus \operatorname{im}(\operatorname{grad})$$

and so it is not surprising that the answer is generally no. We would like to describe a family of graphs for which the answer is yes.

The edge flow  $X \in L_\wedge^2(E(C_4))$  on the right of Figure 2 is an example of one that is curl-free but not a gradient. It is trivially curl-free since  $T(C_4) = \emptyset$ . It is not a gradient since if  $X = \operatorname{grad} f$ , then

$$f(2) - f(1) = 2, \quad f(3) - f(2) = 2, \quad f(4) - f(3) = 2, \quad f(1) - f(4) = 2,$$

<sup>5</sup>Due to Dave Bayer [12]. See Figure 3.

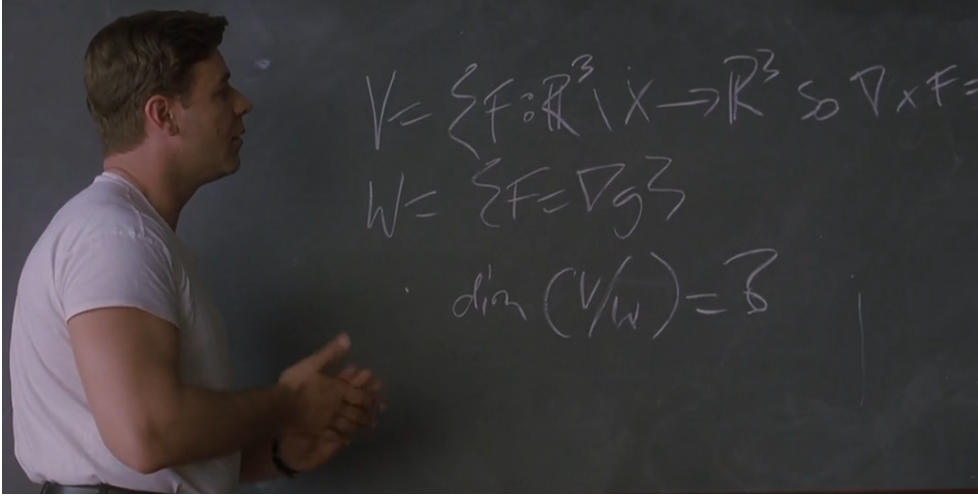


Fig. 3: Problem from *A Beautiful Mind*:  $V = \{F : \mathbb{R}^3 \setminus X \rightarrow \mathbb{R}^3 \text{ so } \nabla \times F = 0\}$ ,  $W = \{F = \nabla g\}$ ,  $\dim(V/W) = ?$

and summing them gives ‘ $0 = 8$ ’ — a contradiction. Note that  $X$  is also divergence-free by (3.4) since  $\text{inflow } X = \text{outflow } X$ . It is therefore harmonic by (3.6), i.e.,  $X \in \ker(\Delta_1)$  as expected.

Every divergence-free edge flow on  $C_4$  must be of the same form as  $X$ , taking constant value on all edges or otherwise we would not have  $\text{inflow } X = \text{outflow } X$ . Since all edge flows on  $C_4$  are automatically curl-free,  $\ker(\Delta_1) = \ker(\text{div})$  and is given by the set of all constant multiples of  $X$ . The number

$$\beta_1(G) = \dim \ker(\Delta_1)$$

counts the number of ‘1-dimensional holes’ of  $G$  and in this case we see that indeed  $\beta_1(C_4) = 1$ . To be a bit more precise, the ‘1-dimensional holes’ are the regions that remain uncovered after the cliques are filled in.

We now turn our attention to the contrasting case of  $C_3$ . Looking at Figure 1, it may seem that  $C_3$  also has a ‘1-dimensional hole’ as in  $C_4$  but this is a fallacy — holes bounded by triangles are not regarded as holes in our framework.

For  $C_3$  it is in fact true that every curl-free edge flow is a gradient. To see this, note that as in the case of  $C_4$ , any divergence-free  $X \in L_\Delta^2(E(C_3))$  must be constant on all edges and so

$$(\text{curl } X)(1, 2, 3) = X(1, 2) + X(2, 3) + X(3, 1) = c + c + c = 3c,$$

for some  $c \in \mathbb{R}$ . If a divergence-free  $X$  is also curl-free, then  $c = 0$  and so  $X = 0$ . Hence for  $C_3$ ,  $\ker(\Delta_1) = \{0\}$  by (3.7) and  $\ker(\text{curl}) = \text{im}(\text{grad})$  by (3.6). It also follows that  $\beta_1(C_3) = 0$  and so  $C_3$  has no ‘1-dimensional hole’.

What we have illustrated with  $C_3$  and  $C_4$  extends to any arbitrary graph. A moment’s thought would reveal that the property  $\beta_1(G) = 0$  is satisfied by any *chordal graph*, i.e., one for which every cycle subgraph of four or more vertices has a *chord*, an edge that connects two vertices of the cycle subgraph but that is not part of the cycle subgraph. Equivalently, a chordal graph is one where every chordless cycle subgraph is  $C_3$ .

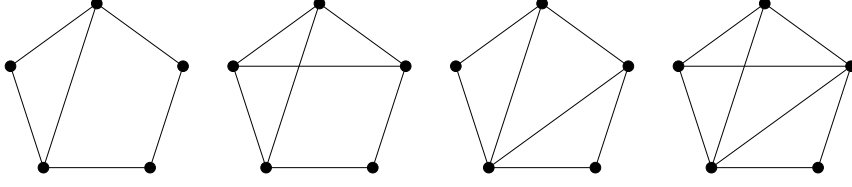


Fig. 4: Left two graphs: not chordal. Right two graphs: chordal.

**4. Higher order.** We expect the case of alternating functions on edges, i.e.,  $k = 1$ , discussed in Section 3 to be the most useful in applications. However for completeness and since it is no more difficult to generalize to  $k > 1$ , we provide the analogue of Section 3 for arbitrary  $k$  here.

**4.1. Higher-order cochains.** Let  $K(G)$  be the clique complex of a graph  $G = (V, E)$  as defined in Section 3.1. We will write  $K_k = K_k(G)$  for simplicity.

A  $k$ -cochain (or  $k$ -form) is an alternating function on  $K_{k+1}$ , or more specifically,  $f : V \times \cdots \times V \rightarrow \mathbb{R}$  where

$$(4.1) \quad f(i_{\sigma(0)}, \dots, i_{\sigma(k)}) = \text{sgn}(\sigma) f(i_0, \dots, i_k)$$

for all  $\{i_0, \dots, i_k\} \in K_{k+1}$  and all  $\sigma \in \mathfrak{S}_{k+1}$ , the symmetric group of permutations on  $\{0, \dots, k\}$ . We set  $f(i_0, \dots, i_k) = 0$  if  $\{i_0, \dots, i_k\} \notin K_{k+1}$ .

Again, we may put an inner product on  $k$ -cochains,

$$\langle f, g \rangle = \sum_{i_0 < \dots < i_k} w_{i_0 \dots i_k} f(i_0, \dots, i_k) g(i_0, \dots, i_k),$$

with any positive weights satisfying  $w_{i_{\sigma(0)} \dots i_{\sigma(k)}} = w_{i_0 \dots i_k}$  for all  $\sigma \in \mathfrak{S}_{k+1}$ .

We denote the resulting Hilbert space by  $L^2_{\wedge}(K_{k+1})$ . This is a subspace of  $L^2(\wedge^{k+1} V)$ , the space of alternating functions with  $k+1$  arguments in  $V$ . Clearly,

$$\dim L^2_{\wedge}(K_{k+1}) = \#K_{k+1}.$$

A word of caution regarding the terminology: a  $k$ -cochain is a function on a  $(k+1)$ -clique and has  $k+1$  arguments. The reason is due to the different naming conventions — a  $(k+1)$ -clique in graph theory is called a  $k$ -simplex in topology. In topological lingo, a vertex is a 0-simplex, an edge a 1-simplex, a triangle a 2-simplex, a tetrahedron a 3-simplex.

**4.2. Higher-order coboundary operators.** The  $k$ -coboundary operators  $\delta_k : L^2_{\wedge}(K_k) \rightarrow L^2_{\wedge}(K_{k+1})$  are defined by

$$(4.2) \quad (\delta_k f)(i_0, \dots, i_{k+1}) = \sum_{j=0}^{k+1} (-1)^j f(i_0, \dots, i_{j-1}, i_{j+1}, \dots, i_{k+1}),$$

for  $k = 0, 1, 2, \dots$ . Readers familiar with differential forms may find it illuminating to think of coboundary operators as discrete analogues of exterior derivatives. Note that  $f$  is a function with  $k+1$  arguments but  $\delta_k f$  is a function with  $k+2$  arguments. A convenient and often-used notation is to put a carat over the omitted argument

$$(4.3) \quad f(i_0, \dots, \widehat{i_j}, \dots, i_{k+1}) := f(i_0, \dots, i_{j-1}, i_{j+1}, \dots, i_{k+1}).$$

The crucial relation  $AB = 0$  in Section 2 is in fact

$$(4.4) \quad \delta_k \delta_{k-1} = 0,$$

which may be verified using (4.2) (see Theorem 5.7). The equation (4.4) is often verbalized as “the coboundary of a coboundary is zero.” It generalizes (3.2) and is sometimes called the *fundamental theorem of topology*.

As in Section 2.1, (4.4) is equivalent to saying that  $\text{im}(\delta_{k-1})$  is a subspace of  $\ker(\delta_k)$ . We define the  $k$ th *cohomology group* of  $G$  to be the quotient vector space

$$(4.5) \quad H^k(G) = \ker(\delta_k) / \text{im}(\delta_{k-1}),$$

for  $k = 1, 2, \dots, \omega(G) - 1$ .

To keep track of the coboundary operators, it is customary to assemble them into a sequence of maps written in the form

$$L_{\wedge}^2(K_0) \xrightarrow{\delta_0} L_{\wedge}^2(K_1) \xrightarrow{\delta_1} \dots \xrightarrow{\delta_{k-1}} L_{\wedge}^2(K_k) \xrightarrow{\delta_k} L_{\wedge}^2(K_{k+1}) \xrightarrow{\delta_{k+1}} \dots \xrightarrow{\delta_{\omega}} L_{\wedge}^2(K_{\omega}).$$

This sequence is called a *cochain complex*. It is said to be *exact* if  $\text{im}(\delta_{k-1}) = \ker(\delta_k)$  or, equivalently,  $H^k(G) = \{0\}$ , for all  $k = 1, 2, \dots, \omega(G) - 1$ .

For  $k = 1$ , we get  $\delta_0 = \text{grad}$ ,  $\delta_1 = \text{curl}$ , and the first two terms of the cochain complex are

$$L^2(V) \xrightarrow{\text{grad}} L_{\wedge}^2(E) \xrightarrow{\text{curl}} L_{\wedge}^2(T).$$

**4.3. Hodge theory.** The *Hodge  $k$ -Laplacian*  $\Delta_k : L_{\wedge}^2(K_k) \rightarrow L_{\wedge}^2(K_k)$  is defined as

$$\Delta_k = \delta_{k-1} \delta_k^* + \delta_k^* \delta_k.$$

We call  $f \in L_{\wedge}^2(K_k)$  a *harmonic  $k$ -cochain* if it satisfies the Laplace equation

$$\Delta_k f = 0.$$

Applying the results in Section 2.3 with  $A = \delta_k$  and  $B = \delta_{k-1}$ , we obtain the unique representation of cohomology classes as harmonic cochains

$$H^k(G) = \ker(\delta_k) / \text{im}(\delta_{k-1}) \cong \ker(\delta_k) \cap \ker(\delta_{k-1}^*) = \ker(\Delta_k),$$

as well as the Hodge decomposition

$$(4.6) \quad L_{\wedge}^2(K_k) = \overbrace{\text{im}(\delta_k^*) \oplus \ker(\Delta_k)}^{\ker(\delta_{k-1}^*)} \oplus \underbrace{\text{im}(\delta_{k-1})}_{\ker(\delta_k)},$$

and the relation

$$\text{im}(\Delta_k) = \text{im}(\delta_k^*) \oplus \text{im}(\delta_{k-1}).$$

*Example 4.1* (Hearing the shape of a graph). Two undirected graphs  $G$  and  $H$  on  $n$  vertices are said to be *isomorphic* if they are essentially the same graph up to relabeling of vertices. The *graph isomorphism problem*, an open problem in computer science, asks whether there is a polynomial-time algorithm<sup>6</sup> for deciding if two given graphs are isomorphic [4]. Clearly two isomorphic graphs must be *isospectral* in the

<sup>6</sup>An astounding recent result of Babai [5] is that there is a *quasipolynomial*-time algorithm.

sense that the eigenvalues (ordered and counted with multiplicities) of their graph Laplacians are equal,

$$\lambda_i(\Delta_0(G)) = \lambda_i(\Delta_0(H)), \quad i = 1, \dots, n,$$

a condition that can be checked in polynomial time. Not surprisingly, the converse — the graph theoretic analogue of Kac’s famous problem [39] — is not true, or we would have been able to determine graph isomorphism in polynomial time. We should mention that there are several definitions of isospectral graphs, in terms of the adjacency matrix, graph Laplacian, normalized Laplacian, signless Laplacian, etc; see [13, 32] for many interesting examples of nonisomorphic isospectral graphs.

The reader may perhaps wonder what happens if we impose the stronger requirement that the eigenvalues of all their higher-order Hodge  $k$ -Laplacians be equal as well?

$$\lambda_i(\Delta_k(G)) = \lambda_i(\Delta_k(H)), \quad i = 1, \dots, n, \quad k = 0, \dots, m.$$

For any  $m \geq 1$ , these indeed give a stronger set of sufficient conditions that can be checked in polynomial time. For example, the eigenvalues of  $\Delta_0$  for the two graphs in Figure 5 are 0, 0.76, 2, 3, 3, 5.24 (all numbers rounded to two decimal figures). On the other hand, the eigenvalues of  $\Delta_1$  are 0, 0.76, 2, 3, 3, 3, 5.24 for the graph on the left and 0, 0, 0.76, 2, 3, 3, 5.24 for the graph on the right, allowing us to conclude that they are not isomorphic. These calculations are included in Section 5.3.

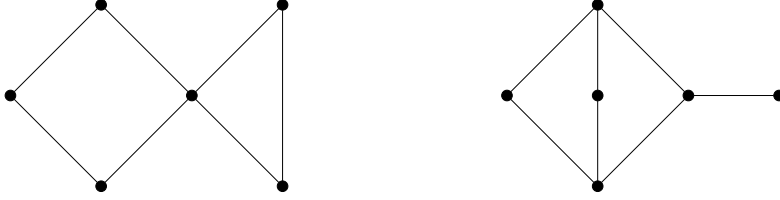


Fig. 5: These graphs have isospectral Laplacians (Hodge 0-Laplacians) but not Helmholtzians (Hodge 1-Laplacians).

Non-isomorphic graphs can nevertheless have isospectral Hodge Laplacians of all order. The two graphs in Figure 6 are clearly non-isomorphic. Neither contains cliques of order higher than two, so their Hodge  $k$ -Laplacians are zero for all  $k > 2$ . We may check (see Section 5.3) that the first three Hodge Laplacians  $\Delta_0$ ,  $\Delta_1$ ,  $\Delta_2$ , of both graphs are isospectral.

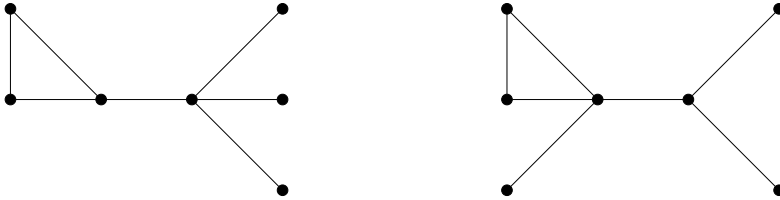


Fig. 6: Non-isomorphic graphs with isospectral Hodge  $k$ -Laplacians for all  $k = 0, 1, 2, \dots$

Table 3: Topological jargons (second pass)

NAME	MEANING
coboundary maps	$\delta_k : L_{\wedge}^2(K_k) \rightarrow L_{\wedge}^2(K_{k+1})$
cochains	elements $f \in L_{\wedge}^2(K_k)$
cochain complex	$\cdots \rightarrow L_{\wedge}^2(K_{k-1}) \xrightarrow{\delta_{k-1}} L_{\wedge}^2(K_k) \xrightarrow{\delta_k} L_{\wedge}^2(K_{k+1}) \rightarrow \cdots$
cocycles	elements of $\ker(\delta_k)$
coboundaries	elements of $\text{im}(\delta_{k-1})$
cohomology classes	elements of $\ker(\delta_k)/\text{im}(\delta_{k-1})$
harmonic cochains	elements of $\ker(\Delta_k)$
Betti numbers	$\dim \ker(\Delta_k)$
Hodge Laplacians	$\Delta_k = \delta_{k-1}\delta_{k-1}^* + \delta_k^*\delta_k$
$f$ is closed	$\delta_k f = 0$
$f$ is exact	$f = \delta_{k-1}g$ for some $g \in L_{\wedge}^2(K_{k-1})$
$f$ is coclosed	$\delta_{k-1}^* f = 0$
$f$ is coexact	$f = \delta_k^* h$ for some $h \in L_{\wedge}^2(K_{k+1})$
$f$ is harmonic	$\Delta_k f = 0$

**5. Detailed proofs and calculations.** In this section, we provide proofs of the linear algebraic facts in Section 2, verify various claims in Sections 3 and 4, and work out the details of Example 4.1.

**5.1. Linear Algebra over  $\mathbb{R}$ .** We provide routine proofs for some linear algebraic facts that we have used freely in Section 2. We will work over  $\mathbb{R}$  for convenience but every statement in Theorems 5.1, 5.2, 5.3 extends to any subfield of  $\mathbb{C}$ .

**THEOREM 5.1.** *Let  $A \in \mathbb{R}^{m \times n}$ . Then*

- ①  $\ker(A^*A) = \ker(A)$ ,
- ②  $\text{im}(A^*A) = \text{im}(A^*)$ ,
- ③  $\ker(A^*) = \text{im}(A)^\perp$ ,
- ④  $\text{im}(A^*) = \ker(A)^\perp$ ,
- ⑤  $\mathbb{R}^n = \ker(A) \oplus \text{im}(A^*)$ .

*Proof.*

- ① Clearly  $\ker(A) \subseteq \ker(A^*A)$ . If  $A^*Ax = 0$ , then  $\|Ax\|^2 = x^*A^*Ax = 0$ , so  $Ax = 0$ , and so  $\ker(A^*A) \subseteq \ker(A)$ .
- ② Applying rank-nullity theorem twice with ①, we get

$$\begin{aligned} \text{rank}(A^*A) &= n - \text{nullity}(A^*A) \\ &= n - \text{nullity}(A) = \text{rank}(A) = \text{rank}(A^*). \end{aligned}$$

Since  $\text{im}(A^*A) \subseteq \text{im}(A^*)$ , the result follows.

- ③ If  $x \in \text{im}(A)^\perp$ , then  $0 = \langle x, Ay \rangle = \langle A^*x, y \rangle$  for all  $y \in \mathbb{R}^n$ , so  $A^*x = 0$ . If  $x \in \ker(A^*)$ , then  $\langle x, Ay \rangle = \langle A^*x, y \rangle = 0$  for all  $y \in \mathbb{R}^n$ , so  $x \in \text{im}(A)^\perp$ .
- ④ By ③,  $\text{im}(A^*)^\perp = \ker(A^{**}) = \ker(A)$  and result follows.
- ⑤  $\mathbb{R}^n = \ker(A) \oplus \ker(A)^\perp = \ker(A) \oplus \text{im}(A^*)$  by ④.  $\square$

Our next proof ought to convince readers that the Hodge decomposition theorem ⑨ is indeed an extension of the Fredholm alternative theorem ⑤ to a pair of matrices.

**THEOREM 5.2.** *Let  $A \in \mathbb{R}^{m \times n}$  and  $B \in \mathbb{R}^{n \times p}$  with  $AB = 0$ . Then*

- ⑥  $\ker(A^*A + BB^*) = \ker(A) \cap \ker(B^*)$ ,
- ⑦  $\ker(A) = \operatorname{im}(B) \oplus \ker(A^*A + BB^*)$ ,
- ⑧  $\ker(B^*) = \operatorname{im}(A^*) \oplus \ker(A^*A + BB^*)$ ,
- ⑨  $\mathbb{R}^n = \operatorname{im}(A^*) \oplus \ker(A^*A + BB^*) \oplus \operatorname{im}(B)$ ,
- ⑩  $\operatorname{im}(A^*A + BB^*) = \operatorname{im}(A^*) \oplus \operatorname{im}(B)$ .

*Proof.* Note that  $\operatorname{im}(B) \subseteq \ker(A)$  as  $AB = 0$ ,  $\operatorname{im}(A^*) \subseteq \ker(B^*)$  as  $B^*A^* = 0$ .

⑥ Clearly  $\ker(A) \cap \ker(B^*) \subseteq \ker(A^*A + BB^*)$ . Let  $x \in \ker(A^*A + BB^*)$ . Then  $A^*Ax = -BB^*x$ .

- Multiplying by  $A$ , we get  $AA^*Ax = -ABB^*x = 0$  since  $AB = 0$ . So  $A^*Ax \in \ker(A)$ . But  $A^*Ax \in \operatorname{im}(A^*) = \ker(A)^\perp$  by ④. So  $A^*Ax = 0$  and  $x \in \ker(A^*A) = \ker(A)$  by ①.
- Multiplying by  $B^*$ , we get  $0 = B^*A^*Ax = -B^*BB^*x$  since  $B^*A^* = 0$ . So  $BB^*x \in \ker(B^*)$ . But  $BB^*x \in \operatorname{im}(B) = \ker(B^*)^\perp$  by ③. So  $BB^*x = 0$  and  $x \in \ker(BB^*) = \ker(B^*)$  by ①.

Hence  $x \in \ker(A) \cap \ker(B^*)$ .

⑦ Applying ⑤ to  $B^*$ ,

$$\begin{aligned} \ker(A) &= \mathbb{R}^n \cap \ker(A) = [\ker(B^*) \oplus \operatorname{im}(B)] \cap \ker(A) \\ &= [\ker(B^*) \cap \ker(A)] \oplus [\operatorname{im}(B) \cap \ker(A)] \\ &= \ker(A^*A + BB^*) \oplus \operatorname{im}(B), \end{aligned}$$

where the last equality follows from ⑥ and  $\operatorname{im}(B) \subseteq \ker(A)$ .

⑧ Applying ⑤,

$$\begin{aligned} \ker(B^*) &= \mathbb{R}^n \cap \ker(B^*) = [\ker(A) \oplus \operatorname{im}(A^*)] \cap \ker(B^*) \\ &= [\ker(A) \cap \ker(B^*)] \oplus [\operatorname{im}(A^*) \cap \ker(B^*)] \\ &= \ker(A^*A + BB^*) \oplus \operatorname{im}(A^*), \end{aligned}$$

where the last equality follows from ⑥ and  $\operatorname{im}(A^*) \subseteq \ker(B^*)$ . Alternatively, apply ⑦ with  $B^*, A^*$  in place of  $A, B$ .

⑨ Applying ⑤ to  $B^*$  followed by ⑧, we get

$$\mathbb{R}^n = \ker(B^*) \oplus \operatorname{im}(B) = \operatorname{im}(A^*) \oplus \ker(A^*A + BB^*) \oplus \operatorname{im}(B).$$

⑩ Applying ⑤ to  $A^*A + BB^*$ , which is self-adjoint, we see that

$$\operatorname{im}(A^*A + BB^*) = \ker(A^*A + BB^*)^\perp = \operatorname{im}(A^*) \oplus \operatorname{im}(B),$$

where the last equality follows from ⑨. □

Any two vector spaces of the same dimension are isomorphic. So saying that two vector spaces are isomorphic isn't saying very much — just that they have the same dimension. The two spaces in (2.11) are special because they are *naturally isomorphic*, i.e., if you construct an isomorphism, and the guy in the office next door constructs an isomorphism, both of you would end up with the same isomorphism, namely, the one below.

**THEOREM 5.3.** *Let  $A \in \mathbb{R}^{m \times n}$  and  $B \in \mathbb{R}^{n \times p}$  with  $AB = 0$ . Then the following spaces are naturally isomorphic*

$$\ker(A)/\operatorname{im}(B) \cong \ker(A) \cap \ker(B^*) \cong \ker(B^*)/\operatorname{im}(A^*).$$



*Proof.* Let  $\pi : \mathbb{R}^n \rightarrow \text{im}(B)^\perp$  be the orthogonal projection of  $\mathbb{R}^n$  onto the orthogonal complement of  $\text{im}(B)$ . So any  $x \in \mathbb{R}^n$  has a unique decomposition into two mutually orthogonal components

$$\begin{aligned}\mathbb{R}^n &= \text{im}(B)^\perp \oplus \text{im}(B), \\ x &= \pi(x) + (1 - \pi)(x).\end{aligned}$$

Let  $\pi_A$  be  $\pi$  restricted to the subspace  $\ker(A)$ . So any  $x \in \ker(A)$  has a unique decomposition into two mutually orthogonal components

$$\begin{aligned}\ker(A) &= (\ker(A) \cap \text{im}(B)^\perp) \oplus \text{im}(B), \\ x &= \pi_A(x) + (1 - \pi_A)(x),\end{aligned}$$

bearing in mind that  $\ker(A) \cap \text{im}(B) = \text{im}(B)$  since  $\text{im}(B) \subseteq \ker(A)$ .

As  $\pi$  is surjective, so is  $\pi_A$ . Hence  $\text{im}(\pi_A) = \ker(A) \cap \text{im}(B)^\perp$ . Also, for any  $x \in \ker(A)$ ,  $\pi_A(x) = 0$  iff the component of  $x$  in  $\text{im}(B)^\perp$  is zero, i.e.,  $x \in \text{im}(B)$ . Hence  $\ker(\pi_A) = \text{im}(B)$ . The first isomorphism theorem,

$$\ker(A)/\ker(\pi_A) \cong \text{im}(\pi_A) = \ker(A) \cap \text{im}(B)^\perp$$

yields the required result since  $\text{im}(B)^\perp = \ker(B^*)$  by ③. The other isomorphism may be obtained as usual by using  $B^*, A^*$  in place of  $A, B$ .  $\square$

In mathematics, *linear algebra* usually refers to a collection of facts that follow from the defining axioms of a field and of a vector space. In this regard, every single statement in Theorems 5.1, 5.2, 5.3 is false as a statement in linear algebra — they depend specifically on our working over a subfield of  $\mathbb{C}$  and are not true over arbitrary fields. For example, consider the finite field of two elements  $\mathbb{F}_2 = \{0, 1\}$  and take

$$A = B = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}.$$

Then  $A^* = A = B = B^*$ , and  $AB = B^*A^* = A^*A = BB^* = A^*A + BB^* = 0$ , which serves as a counterexample to ①, ②, ⑤, ⑦, ⑧, ⑨, ⑩, and Theorem 5.3.

**5.2. Div, Grad, Curl, and All That.** We provide routine verifications of statements claimed in Sections 3 and 4.

LEMMA 5.4. *Equip  $L^2(V)$  and  $L_\Delta^2(E)$  with the inner products in (3.1), we have*

$$\text{grad}^* X(i) = - \sum_{j=1}^n \frac{w_{ij}}{w_i} X(i, j) = -\text{div } X(i).$$

*Proof.* The required expression follows from

$$\begin{aligned}\langle \text{grad}^* X, f \rangle_V &= \langle X, \text{grad } f \rangle_E \\ &= \sum_{i < j} w_{ij} X(i, j) \text{grad } f(i, j) \\ &= \sum_{i < j} w_{ij} X(i, j) [f(j) - f(i)] \\ &= \sum_{i < j} w_{ij} X(i, j) f(j) + \sum_{i < j} w_{ij} X(j, i) f(i) \\ &\stackrel{\textcircled{1}}{=} \sum_{j < i} w_{ji} X(j, i) f(i) + \sum_{i < j} w_{ij} X(j, i) f(i)\end{aligned}$$

$$\begin{aligned}
&\stackrel{\textcircled{2}}{=} \sum_{j < i} w_{ij} X(j, i) f(i) + \sum_{i < j} w_{ij} X(j, i) f(i) \\
&= \sum_{i \neq j} w_{ij} X(j, i) f(i) \\
&= \sum_{i=1}^n w_i \left[ \sum_{j: j \neq i} \frac{w_{ij}}{w_i} X(j, i) \right] f(i) \\
&\stackrel{\textcircled{3}}{=} \sum_{i=1}^n w_i \underbrace{\left[ \sum_{j=1}^n \frac{w_{ij}}{w_i} X(j, i) \right]}_{\text{grad}^* X(i)} f(i).
\end{aligned}$$

① follows from swapping labels  $i$  and  $j$  in the first summand.

② follows from  $w_{ij} = w_{ji}$ .

③ follows from  $X(i, i) = 0$ .  $\square$

LEMMA 5.5. Equip  $L_\wedge^2(E)$  and  $L_\wedge^2(T)$  with the inner products in (3.1), we have

$$\text{curl}^* \Phi(i, j) = \sum_{k=1}^n \frac{w_{ijk}}{w_{ij}} \Phi(i, j, k).$$

*Proof.* The required expression follows from

$$\begin{aligned}
\langle \text{curl}^* \Phi, X \rangle_E &= \langle \Phi, \text{curl} X \rangle_T = \sum_{i < j < k} w_{ijk} \Phi(i, j, k) \text{curl} X(i, j, k) \\
&= \sum_{i < j < k} w_{ijk} \Phi(i, j, k) [X(i, j) + X(j, k) + X(k, i)] \\
&= \sum_{i < j < k} w_{ijk} \Phi(i, j, k) X(i, j) + \sum_{i < j < k} w_{ijk} \Phi(i, j, k) X(j, k) \\
&\quad + \sum_{i < j < k} w_{ijk} \Phi(i, j, k) X(k, i) \\
&\stackrel{\textcircled{1}}{=} \sum_{i < j < k} w_{ijk} \Phi(i, j, k) X(i, j) + \sum_{i < j < k} w_{ijk} \Phi(j, k, i) X(j, k) \\
&\quad + \sum_{i < j < k} w_{ijk} \Phi(k, i, j) X(k, i) \\
&\stackrel{\textcircled{2}}{=} \sum_{i < j < k} w_{ijk} \Phi(i, j, k) X(i, j) + \sum_{k < i < j} w_{kij} \Phi(i, j, k) X(i, j) \\
&\quad + \sum_{i < k < j} w_{ikj} \Phi(j, i, k) X(j, i) \\
&\stackrel{\textcircled{3}}{=} \sum_{i < j < k} w_{ijk} \Phi(i, j, k) X(i, j) + \sum_{k < i < j} w_{kij} \Phi(i, j, k) X(i, j) \\
&\quad + \sum_{i < k < j} w_{ikj} \Phi(i, j, k) X(i, j) \\
&= \sum_{i < j} \left[ \left( \sum_{k=j+1}^n + \sum_{k=1}^{i-1} + \sum_{k=i+1}^{j-1} \right) w_{ijk} \Phi(i, j, k) \right] X(i, j) \\
&= \sum_{i < j} w_{ij} \left[ \sum_{k: k \neq i, j} \frac{w_{ijk}}{w_{ij}} \Phi(i, j, k) \right] X(i, j) \\
&\stackrel{\textcircled{4}}{=} \sum_{i < j} w_{ij} \underbrace{\left[ \sum_{k=1}^n \frac{w_{ijk}}{w_{ij}} \Phi(i, j, k) \right]}_{\text{curl}^* \Phi(i, j)} X(i, j).
\end{aligned}$$

① follows from the alternating property of  $\Phi$ .

② follows from relabeling  $j, k, i$  as  $i, j, k$  in the second summand and swapping labels  $j$  and  $k$  in the third summand.

③ follows from  $\Phi(j, i, k) X(j, i) = \Phi(i, j, k) X(i, j)$  since both changed signs.

④ follows from  $\Phi(i, j, i) = \Phi(i, j, j) = 0$ .  $\square$

LEMMA 5.6. *The operator  $\Delta_0 = -\operatorname{div} \operatorname{grad}$  gives us the usual graph Laplacian.*

*Proof.* Let  $f \in L^2(V)$ . By definition,

$$\operatorname{grad} f(i, j) = \begin{cases} f(j) - f(i) & \text{if } \{i, j\} \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Define the adjacency matrix  $A \in \mathbb{R}^{n \times n}$  by

$$a_{ij} = \begin{cases} 1 & \text{if } \{i, j\} \in E, \\ 0 & \text{otherwise.} \end{cases}$$

The gradient may be written as  $\operatorname{grad} f(i, j) = a_{ij}(f(j) - f(i))$  and so

$$\begin{aligned} (\Delta_0 f)(i) &= -[\operatorname{div}(\operatorname{grad} f)](i) = -[\operatorname{div} a_{ij}(f(j) - f(i))](i) \\ (5.1) \quad &= -\sum_{j=1}^n a_{ij}[f(j) - f(i)] = d_i f(i) - \sum_{j=1}^n a_{ij} f(j), \end{aligned}$$

where for any vertex  $i = 1, \dots, n$ , we define its degree as

$$d_i = \deg(i) = \sum_{j=1}^n a_{ij}.$$

If we regard a function  $f \in L^2(V)$  as a vector  $(f_1, \dots, f_n) \in \mathbb{R}^n$  where  $f(i) = f_i$  and set  $D = \operatorname{diag}(d_1, \dots, d_n) \in \mathbb{R}^{n \times n}$ , then (5.1) becomes

$$\Delta_0 f = \begin{bmatrix} d_1 - a_{11} & -a_{12} & \cdots & -a_{1n} \\ -a_{21} & d_2 - a_{22} & \cdots & -a_{2n} \\ \vdots & & \ddots & \vdots \\ -a_{n1} & -a_{n2} & \cdots & d_n - a_{nn} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix} = (D - A)f.$$

So  $\Delta_0$  may be regarded as  $D - A$ , the usual definition of a graph Laplacian.  $\square$

THEOREM 5.7. *We have that*

$$\operatorname{curl} \operatorname{grad} = 0, \quad \operatorname{div} \operatorname{curl}^* = 0,$$

and more generally, for  $k = 1, 2, \dots$ ,

$$\delta_k \delta_{k-1} = 0, \quad \delta_{k-1}^* \delta_k^* = 0.$$

*Proof.* We only need to check  $\delta_k \delta_{k-1} = 0$ . The other relations follow from taking adjoint or specializing to  $k = 1$ . Let  $f \in L_\Lambda^2(K_{k-1})$ . By (4.2) and (4.3),

$$\begin{aligned} (\delta_k \delta_{k-1} f)(i_0, \dots, i_{k+1}) &= \sum_{j=0}^{k+1} (-1)^j \delta_{k-1} f(i_0, \dots, \widehat{i}_j, \dots, i_{k+1}) \\ &\stackrel{\textcircled{1}}{=} \sum_{j=0}^{k+1} (-1)^j \left[ \sum_{\ell=0}^{j-1} (-1)^\ell f(i_0, \dots, \widehat{i}_\ell, \dots, \widehat{i}_j, \dots, i_{k+1}) \right. \\ &\quad \left. + \sum_{\ell=j+1}^{k+1} (-1)^{\ell-1} f(i_0, \dots, \widehat{i}_j, \dots, \widehat{i}_\ell, \dots, i_{k+1}) \right] \\ &= \sum_{j < \ell} (-1)^j (-1)^\ell f(i_0, \dots, \widehat{i}_j, \dots, \widehat{i}_\ell, \dots, i_{k+1}) \end{aligned}$$

$$\begin{aligned}
& + \sum_{j > \ell} (-1)^j (-1)^{\ell-1} f(i_0, \dots, \widehat{i}_\ell, \dots, \widehat{i}_j, \dots, i_{k+1}) \\
& \stackrel{\textcircled{2}}{=} \sum_{j < \ell} (-1)^{j+\ell} f(i_0, \dots, \widehat{i}_j, \dots, \widehat{i}_\ell, \dots, i_{k+1}) \\
& \quad + \sum_{\ell > j} (-1)^{j+\ell-1} f(i_0, \dots, \widehat{i}_j, \dots, \widehat{i}_\ell, \dots, i_{k+1}) \\
& = \sum_{j < \ell} (-1)^{j+\ell} f(i_0, \dots, \widehat{i}_j, \dots, \widehat{i}_\ell, \dots, i_{k+1}) \\
& \quad - \sum_{j < \ell} (-1)^{j+\ell} f(i_0, \dots, \widehat{i}_j, \dots, \widehat{i}_\ell, \dots, i_{k+1}) = 0.
\end{aligned}$$

The power of  $-1$  in the third sum in  $\textcircled{1}$  is  $\ell - 1$  because an argument preceding  $\widehat{i}_\ell$  is omitted and so  $\widehat{i}_\ell$  is the  $(\ell - 1)$ th argument (which is also omitted).  $\textcircled{2}$  follows from swapping labels  $j$  and  $\ell$  in the second sum.  $\square$

**5.3. Calculations.** We will work out the details of Example 4.1. While we have defined coboundary operators and Hodge Laplacians as abstract, coordinate-free linear operators, any actual applications would invariably involve ‘writing them down’ as matrices to facilitate calculations. Readers might perhaps find our concrete approach here instructive.

A simple recipe for writing down a matrix representing a coboundary operator or a Hodge Laplacian is as follows: Given an undirected graph, label its vertices and edges arbitrarily but differently for easy distinction (e.g., we used numbers for vertices and letters for edges) and assign arbitrary directions to the edges. From the graphs in Figure 5, we get the labeled directed graphs  $G_1$  (left) and  $G_2$  (right) in Figure 7.

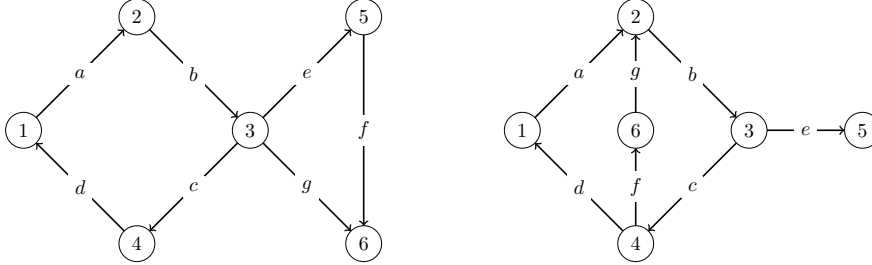


Fig. 7: The graphs in Figure 5, with vertices and edges arbitrarily labeled and directions on edges arbitrarily assigned.

The next step is to write down a matrix whose columns are indexed by the vertices and the rows are indexed by the edges and whose  $(i, j)$ th entry is  $+1$  if  $j$ th edge points into the  $i$ th vertex,  $-1$  if  $j$ th edge points out of the  $i$ th vertex, and  $0$  otherwise. This matrix represents the gradient operator  $\delta_0 = \text{grad}$ . We get

$$A_1 = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 \end{matrix} \\ \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \end{matrix} & \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & -1 & 0 & 0 & 1 \end{bmatrix} \end{matrix}, \quad A_2 = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 \end{matrix} \\ \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \end{matrix} & \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & -1 \end{bmatrix} \end{matrix}$$

for  $G_1$  and  $G_2$  respectively. Note that every row must contain exactly one  $+1$  and one  $-1$  since every edge is defined by a pair of vertices. This matrix is also known as a vertex-edge incidence matrix of the graph. Our choice of  $\pm 1$  for in/out-pointing edges is also arbitrary — the opposite choice works just as well as long as we are consistent throughout.

The graph Laplacians may either be computed from our definition as

$$L_1 = A_1^* A_1 = \begin{array}{c} \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \left[ \begin{array}{cccccc} 2 & -1 & 0 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 4 & -1 & -1 & -1 \\ -1 & 0 & -1 & 2 & 0 & 0 \\ 0 & 0 & -1 & 0 & 2 & -1 \\ 0 & 0 & -1 & 0 & -1 & 2 \end{array} \right] \end{array},$$

$$L_2 = A_2^* A_2 = \begin{array}{c} \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \left[ \begin{array}{cccccc} 2 & -1 & 0 & -1 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 \\ 0 & -1 & 3 & -1 & -1 & 0 \\ -1 & 0 & -1 & 3 & 0 & -1 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & -1 & 0 & 2 \end{array} \right] \end{array},$$

or written down directly using the usual definition [20, 56],

$$\ell_{ij} = \begin{cases} \deg(v_i) & \text{if } i = j, \\ -1 & \text{if } v_i \text{ is adjacent to } v_j, \\ 0 & \text{otherwise.} \end{cases}$$

We obtain the same Laplacian matrix irrespective of the choice of directions on edges and the choice of  $\pm 1$  for in/out-pointing edges. For us there is no avoiding the gradient operators since we need them for the graph Helmholtzian below.

We may now find the eigenvalues of  $L_1$  and  $L_2$  and see that they are indeed the values we claimed in Example 4.1:

$$\lambda(L_1) = (0, 3 - \sqrt{5}, 2, 3, 3, 3 + \sqrt{5}) = \lambda(L_2).$$

To write down the graph Helmholtzians, we first observe that  $G_1$  has exactly one triangle (i.e., 2-clique) whereas  $G_2$  has none<sup>7</sup>. We will need to label and pick an arbitrary orientation for the triangle in  $G_1$ : We denote it as  $T$  and orient it clockwise  $3 \rightarrow 5 \rightarrow 6 \rightarrow 3$ . A matrix representing the operator  $\delta_1 = \text{curl}$  may be similarly written down by indexing the columns with edges and the rows with triangles. Here we make the arbitrary choice that if the  $j$ th edge points in the same direction as the orientation of the  $i$ th triangle, then the  $(i, j)$ th entry is  $+1$  and if it points in the opposite direction, then the entry is  $-1$ . For  $G_1$  we get

$$B_1 = T \begin{array}{c} \begin{array}{cccccc} a & b & c & d & e & f \end{array} \\ \left[ \begin{array}{cccccc} 0 & 0 & 0 & 0 & 1 & 1 \\ -1 & 1 & 1 & 0 & 0 & 0 \end{array} \right].$$

<sup>7</sup>Those who see two triangles should note that these are really squares, or  $C_4$ 's to be accurate. See also Example 3.1.

Since  $G_2$  contains no triangles,  $B_2 = 0$  by definition.

We compute the graph Helmholtzians from definition,

$$H_1 = A_1 A_1^* + B_1^* B_1 = \begin{matrix} & \begin{matrix} a & b & c & d & d & e & f \end{matrix} \\ \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \end{matrix} & \begin{bmatrix} 2 & -1 & 0 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & -1 & 0 & -1 \\ 0 & -1 & 2 & -1 & 1 & 0 & 1 \\ -1 & 0 & -1 & 2 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 3 \end{bmatrix} \end{matrix}$$

$$H_2 = A_2 A_2^* + B_2^* B_2 = \begin{matrix} & \begin{matrix} a & b & c & d & d & e & f \end{matrix} \\ \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \end{matrix} & \begin{bmatrix} 2 & -1 & 0 & -1 & 0 & 0 & 1 \\ -1 & 2 & -1 & 0 & -1 & 0 & -1 \\ 0 & -1 & 2 & -1 & 1 & -1 & 0 \\ -1 & 0 & -1 & 2 & 0 & 1 & 0 \\ 0 & -1 & 1 & 0 & 2 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 2 & -1 \\ 1 & -1 & 0 & 0 & 0 & -1 & 2 \end{bmatrix} \end{matrix}$$

and verify that they have different spectra, as we had claimed in Example 4.1,

$$\lambda(H_1) = (0, 3 - \sqrt{5}, 2, 3, 3, 3, 3 + \sqrt{5}) \neq (0, 0, 3 - \sqrt{5}, 2, 3, 3, 3 + \sqrt{5}) = \lambda(H_2).$$

We now repeat the routine and convert the undirected graphs in Figure 6 into labeled directed graphs  $G_3$  (left) and  $G_4$  (right) in Figure 8. We label both triangles

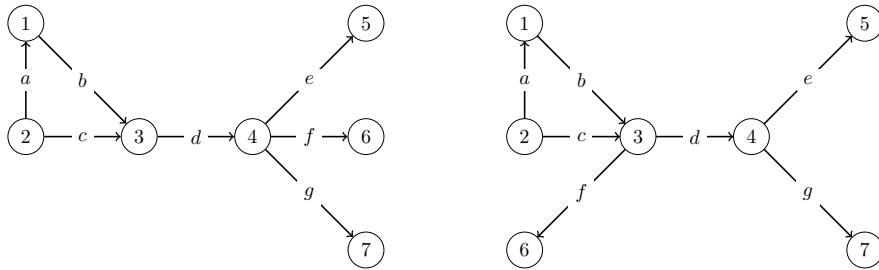


Fig. 8: Labeled directed versions of the graphs in Figure 6.

in  $G_3$  and  $G_4$  as  $T$  and orient it clockwise  $2 \rightarrow 1 \rightarrow 3 \rightarrow 2$ , giving us a matrix that represents both curl operators on  $G_3$  and  $G_4$ ,

$$B_3 = B_4 = T \begin{bmatrix} a & b & c & d & e & f & g \\ 1 & 1 & -1 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

With these choices, we obtain the following matrix representations of the gradi-

ents, Laplacians, and Helmholtzians on  $G_3$  and  $G_4$ ,

$$A_3 = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{matrix} \\ \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \end{matrix} & \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{bmatrix} \end{matrix},$$

$$A_4 = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{matrix} \\ \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \end{matrix} & \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{bmatrix} \end{matrix},$$

$$L_3 = A_3^* A_3 = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \end{matrix} & \begin{bmatrix} 2 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 4 & -1 & -1 & -1 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{bmatrix} \end{matrix},$$

$$L_4 = A_4^* A_4 = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \end{matrix} & \begin{bmatrix} 2 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 3 & -1 & 0 & -1 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{bmatrix} \end{matrix},$$

$$H_3 = A_3 A_3^* + B_3^* B_3 = \begin{matrix} & \begin{matrix} a & b & c & d & e & f & g \end{matrix} \\ \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \end{matrix} & \begin{bmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 3 & -1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 2 & -1 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & 1 & 1 \\ 0 & 0 & 0 & -1 & 1 & 2 & 1 \\ 0 & 0 & 0 & -1 & 1 & 1 & 2 \end{bmatrix} \end{matrix},$$

$$H_4 = A_4 A_4^* + B_4^* B_4 = \begin{matrix} & \begin{matrix} a & b & c & d & e & f & g \end{matrix} \\ \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \end{matrix} & \begin{bmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & -1 & 0 & -1 & 0 \\ 0 & 0 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & -1 & 2 & -1 & 1 & -1 \\ 0 & 0 & 0 & -1 & 2 & 0 & 1 \\ 0 & -1 & -1 & 1 & 0 & 2 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 2 \end{bmatrix} \end{matrix}.$$

As we intend to show that  $G_3$  and  $G_4$  have isospectral Hodge  $k$ -Laplacians for all  $k$ , we will also need to examine the Hodge 2-Laplacian  $\Delta_2$ . Since  $G_3$  and  $G_4$  have no cliques of order higher than two,  $\delta_k = 0$  for all  $k > 2$  and in particular  $\Delta_2 = \delta_1 \delta_1^*$ . So the  $1 \times 1$  matrix representing  $\Delta_2$  is just

$$P_3 := B_3 B_3^* = [3] = B_4 B_4^* =: P_4$$

for both  $G_3$  and  $G_4$ .

Finally, we verify that the spectra of the Hodge  $k$ -Laplacians of  $G_3$  and  $G_4$  are identical for  $k = 0, 1, 2$ , as we had claimed in Example 4.1:

$$\begin{aligned}\lambda(L_3) &= (0, 0.40, 1, 1, 3, 3.34, 5.26) = \lambda(L_4), \\ \lambda(H_3) &= (0.40, 1, 1, 3, 3, 3.34, 5.26) = \lambda(H_4), \\ \lambda(P_3) &= 3 = \lambda(P_4).\end{aligned}$$

Observe that three eigenvalues of  $L_3, L_4, H_3, H_4$  have been rounded to two decimal places — these eigenvalues have closed form expressions (zeros of a cubic polynomial) but they are unilluminating and a hassle to typeset. So to verify that they are indeed isospectral, we check their characteristic polynomials instead, as these have integer coefficients and can be expressed exactly:

$$\begin{aligned}\det(L_3 - xI) &= -21x + 112x^2 - 209x^3 + 178x^4 - 73x^5 + 14x^6 - x^7 \\ &= -x(x-3)(x-1)^2(x^3 - 9x^2 + 21x - 7) = \det(L_4 - xI), \\ \det(H_3 - xI) &= 63 - 357x + 739x^2 - 743x^3 + 397x^4 - 115x^5 + 17x^6 - x^7 \\ &= -(x-3)^2(x-1)^2(x^3 - 9x^2 + 21x - 7) = \det(H_4 - xI).\end{aligned}$$

**6. Topology, computations, and applications.** We conclude our article with this final section that (a) highlights certain deficiencies of our simplistic approach and provides pointers for further studies (Section 6.1); (b) discusses how one may compute the quantities in this article using standard numerical linear algebra (Section 6.2); and (c) proffers some high-level thoughts about applications to the information sciences (Section 6.3).

**6.1. Topological caveats.** The way we defined cohomology in Section 2.1 is more or less standard. The only simplification is that we had worked over a field. The notion of cohomology in topology works more generally over arbitrary rings where our simple linear algebraic approach falls short, but not by much — all we need is to be willing to work with modules over rings instead of modules over fields, i.e., vector spaces. Unlike a vector space, a module may not have a basis and we may not necessarily be able to represent linear maps by matrices, a relatively small price to pay.

However the further simplifications in Sections 2.2 and 2.3 to avoid quotient spaces only hold when we have a field of characteristic zero (we chose  $\mathbb{R}$ ). For example, if instead of  $\mathbb{R}$ , we had the field  $\mathbb{F}_2$  of two elements with binary arithmetic (or indeed any field of positive characteristic), then we can no longer define inner products and statements like  $\ker(B)^\perp = \text{im}(B^*)$  make no sense. While the adjoint of a matrix may still be defined without reference to an inner product, statements like  $\ker(A^*A) = \ker(A)$  are manifestly false in positive characteristic, as we saw at the end of Section 5.1.

We mentioned in Section 2.4 that in the way we presented things, there is no difference between cohomology and homology. This is an artifact of working over



a field. In general cohomology and homology are different and are related via the universal coefficient theorem [34].

From the perspective of topology, the need to restrict to fields of zero characteristic like  $\mathbb{R}$  and  $\mathbb{C}$  is a big shortcoming. For example, one would no longer be able to detect ‘torsion’ and thereby perform basic topological tasks like distinguishing between a circle and a Klein bottle, which is a standard utility of cohomology groups over rings or fields of positive characteristics. We may elaborate on this point if the reader is willing to accept on faith that the cohomology group  $H^k(G)$  in (4.5) may still be defined even (i) when  $G$  is a manifold, and (ii) when we replace our field of scalars  $\mathbb{R}$  by a ring of scalars  $\mathbb{Z}$ . We will denote these cohomology groups over  $\mathbb{R}$  and  $\mathbb{Z}$  by  $H^k(G; \mathbb{R})$  and  $H^k(G; \mathbb{Z})$  respectively. For the circle  $S^1$ , techniques standard in algebraic topology [34] but beyond the scope of this article allow us to compute these:

$$(6.1) \quad H^k(S^1; \mathbb{Z}) = \begin{cases} \mathbb{Z} & k = 0, \\ \mathbb{Z} & k = 1, \\ 0 & k \geq 2, \end{cases} \quad H^k(S^1; \mathbb{R}) = \begin{cases} \mathbb{R} & k = 0, \\ \mathbb{R} & k = 1, \\ 0 & k \geq 2. \end{cases}$$

Likewise, for the Klein bottle  $K$ , one gets

$$(6.2) \quad H^k(K; \mathbb{Z}) = \begin{cases} \mathbb{Z} & k = 0, \\ \mathbb{Z} & k = 1, \\ \mathbb{Z}_2 & k = 2, \\ 0 & k \geq 3, \end{cases} \quad H^k(K; \mathbb{R}) = \begin{cases} \mathbb{R} & k = 0, \\ \mathbb{R} & k = 1, \\ 0 & k \geq 2. \end{cases}$$

Here  $\mathbb{Z}_2 = \{0, 1\}$  with addition performed modulo 2; and whenever a cohomology group contains a nonzero element of finite order,<sup>8</sup> we say that it has *torsion*. There can never be torsion in  $H^k(G; \mathbb{R})$  since every nonzero real number has infinite order. As we can see from (6.1) and (6.2),  $S^1$  and  $K$  have identical cohomology groups over  $\mathbb{R}$ , i.e., we cannot tell apart a circle from a Klein bottle with cohomology over  $\mathbb{R}$ . On the other hand, since  $H^2(K; \mathbb{Z}) = \mathbb{Z}_2 \neq 0 = H^2(S^1; \mathbb{Z})$ , cohomology over  $\mathbb{Z}$  allows us to tell them apart.

Despite the aforementioned deficiencies, if one is primarily interested in engineering and scientific applications, then we believe that our approach in Sections 2, 3, and 4 is by-and-large adequate. Furthermore, even though we have restricted our discussions in Sections 3 and 4 to clique complexes of graphs, they apply verbatim to any simplicial complex.

We should add that although we did not discuss it, one classical use of cohomology and Hodge theory is to deduce topological information about an underlying topological space. Even over a field of characteristic zero, if we sample sufficiently many points  $V$  from a sufficiently nice metric space  $\Omega$ , and set  $G = (V, E)$  to be an appropriately chosen nearest neighbor graph, then

$$(6.3) \quad \beta_k(G) = \dim H^k(G) = \dim \ker(\Delta_k)$$

gives the number of ‘ $k$ -dimensional holes’ in  $\Omega$ , called the *Betti number*. While the kernel or 0-eigenspace captures qualitative topological information, the nonzero eigenspaces often capture quantitative geometric information. In the context of graphs

<sup>8</sup>Recall that the order of an element is the number of times it must be added to itself to get 0; but if this is never satisfied we say it has infinite order. In  $\mathbb{Z}_2$ ,  $1 + 1 = 0$  so 1 has order two.

[20, 56], this is best seen in  $\Delta_0$  — its 0-eigenpair tells us whether a graph is connected ( $\beta_0(G)$  gives the number of connected components of  $G$ , as we saw in Section 3.4) while its smallest nonzero eigenpair tells us how connected the graph is (eigenvalue by way of the Cheeger inequality [20, p. 26] and eigenvector by way of the Fiedler vector [50]).

**6.2. Computations.** A noteworthy point is that the quantities appearing in Sections 3 and 4 are all computationally tractable<sup>9</sup> and may in fact be computed using standard numerical linear algebra. In particular, the Hodge decomposition (4.6) can be efficiently computed by solving least squares problems, which among other things gives us Betti numbers via (6.3) [29]. For simplicity we will use the basic case in Section 3 for illustration but the discussions below apply almost verbatim to the higher order cases in Section 4 as well.

Since  $V$  is a finite set,  $L^2(V)$ ,  $L^2_\wedge(E)$ ,  $L^2_\wedge(T)$  are finite-dimensional vector spaces. We may choose bases on these spaces and get

$$L^2(V) \cong \mathbb{R}^p, \quad L^2_\wedge(E) \cong \mathbb{R}^n, \quad L^2_\wedge(T) \cong \mathbb{R}^m$$

where  $p, n, m$  are respectively the number of vertices, edges, and triangles in  $G$ . See also Section 5.3 for examples of how one may in practice write down matrices representing  $k$ -coboundary operators and Hodge  $k$ -Laplacians for  $k = 0, 1, 2$ .

Once we have represented cochains as vectors in Euclidean spaces, to compute the Helmholtz decomposition in (3.5) for any given  $X \in L^2_\wedge(E)$ , we may solve the two least squares problems

$$\min_{f \in L^2(V)} \|\text{grad } f - X\| \quad \text{and} \quad \min_{\Phi \in L^2_\wedge(T)} \|\text{curl}^* \Phi - X\|,$$

to get  $X_H$  as  $X - \text{grad } f - \text{curl}^* \Phi$ . Alternatively, we may solve

$$\min_{Y \in L^2_\wedge(E)} \|\Delta_1 Y - X\|$$

for the minimizer  $Y$  and get  $X_H$  as the residual  $X - \Delta_1 Y$  directly. Having obtained  $\Delta_1 Y$ , we may use the decomposition (2.8),

$$\begin{aligned} \text{im}(\Delta_1) &= \text{im}(\text{grad}) \oplus \text{im}(\text{curl}^*), \\ \Delta_1 Y &= \text{grad } f + \text{curl}^* \Phi, \end{aligned}$$

and solve either

$$\min_{f \in L^2(V)} \|\text{grad } f - \Delta_1 Y\| \quad \text{or} \quad \min_{\Phi \in L^2_\wedge(T)} \|\text{curl}^* \Phi - \Delta_1 Y\|$$

to get the remaining two components.

We have the choice of practical, efficient, and stable methods like Krylov subspace methods for singular symmetric least squares problems [18, 19] or specialized methods for the Hodge 1-Laplacian with proven complexity bounds [21].

**6.3. Applications.** Traditional applied mathematics largely involves using partial differential equations to model physical phenomena and traditional computational mathematics largely revolves around numerical solutions of PDEs.

<sup>9</sup>Although other related problems with additional conditions can be NP-hard [25].

However, one usually needs substantial and rather precise knowledge about a phenomenon in order to write it down as PDEs. For example, one may need to know the dynamical laws (e.g., laws of motions, principle of least action, laws of thermodynamics, quantum mechanical postulates, etc) or conservation laws (e.g., of energy, momentum, mass, charge, etc) underlying the phenomenon before being able to ‘write down’ the corresponding PDEs (as equations of motion, of continuity and transfer, constitutive equations, field equations, etc). In traditional applied mathematics, it is often taken for granted that there are known physical laws behind the phenomena being modeled.

In modern data applications, this is often a luxury. For example, if we want to build a spam filter, then it is conceivable that we would want to understand the ‘laws of emails.’ But we would quickly come to the realization that these ‘laws of emails’ would be too numerous to enumerate and too inexact to be formulated precisely, even if we restrict ourselves to those relevant for identifying spam. This is invariably the case for any human generated data: movie ratings, restaurant reviews, browsing behavior, clickthrough rates, newsfeeds, tweets, blogs, instagrams, status updates on various social media, etc, but it also applies to data from biology and medicine [43].

For such data sets, all one has is often a rough measure of how similar two data points are and how the data set is distributed. Topology can be a useful tool in such contexts [16] since it requires very little — essentially just a weak notion of separation, i.e., is there a non-trivial open set that contains those points?

If the data set is discrete and finite, which is almost always the case in applications, we can even limit ourselves to simplicial topology, where the topological spaces are simplicial complexes (see Section 3.1). Without too much loss of generality, these may be regarded as clique complexes of graphs (see Section 6.1): data points are vertices in  $V$  and proximity is characterized by cliques: a pair of data points are near each other iff they form an edge in  $E$ , a triplet of data points are near one another iff they form a triangle in  $T$ , and so on.

In this article we have implicitly regarded a graph as a discrete analogue of a Riemannian manifold and cohomology as a discrete analogue of PDEs: standard partial differential operators on Riemannian manifolds — gradient, divergence, curl, Jacobian, Hessian, scalar and vector Laplace operators, Hodge Laplacians — all have natural counterparts on graphs. An example of a line of work that carries this point of view to great fruition may be found in [7, 8, 46]. Also, in this article we have only scratched the surface of cohomological and Hodge theoretic techniques in graph theory; see [33] for results that go much further.

In traditional computational mathematics, discrete PDEs arise as discretizations of continuous PDEs, intermediate by-products of numerical schemes, and this accounts for the appearance of cohomology in numerical analysis [1, 2, 27]. But in data analytic applications, discrete PDEs tend to play a more central and direct role. The discrete partial differential operators on graphs introduced in this article may perhaps serve as a bridge on which insights from traditional applied and computational mathematics could cross over and be brought to bear on modern data analytic applications. Indeed we have already begun to see some applications of the Hodge Laplacian and Hodge decomposition on graphs to:

- (i) ranking [3, 36, 38, 48, 61],
- (ii) graphics and imaging [23, 47, 59],
- (iii) games and traffic flows [14, 15],
- (iv) brain networks [42],
- (v) data representations [17],

- (vi) deep learning [11],
- (vii) denoising [52],
- (viii) dimension reduction [49],
- (ix) link prediction [9],
- (x) object synchronization [30],
- (xi) sensor network coverage [63],
- (xii) cryo-electron microscopy [62],
- (xiii) generalizing effective resistance to simplicial complexes [41],
- (xiv) modeling biological interactions between a set of molecules or communication systems with group messages [51].

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