Applications of the Hodge Decomposition to Biological Structure and Function Modeling

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joint work with

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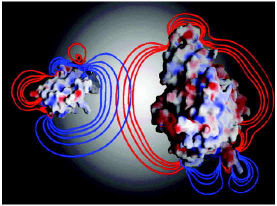
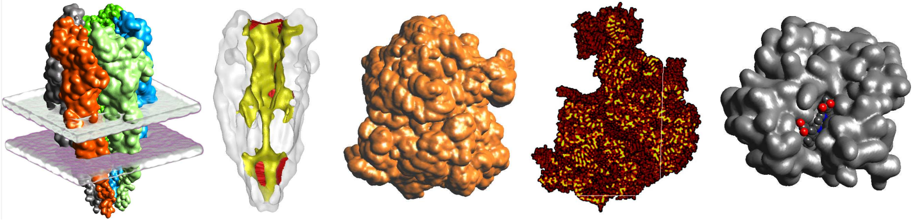
Introduction



- Molecular dynamics are governed by electrostatic forces of attraction and repulsion.
- These forces are described as the solutions of a PDE over the molecular surfaces.
- Molecular surfaces may have complicated topological features affecting the solution.



The Hodge Decomposition relates topological properties of the surface to solution spaces of PDEs over the surface.

(space of forms) $\cong$ (solutions to $\Delta u = f \neq 0$) $\oplus$ (non-trivial deRham classes)

Outline

Outline

1. The Hodge Decomposition for smooth differential forms

2. The Hodge Decomposition for discrete differential forms

3. Applications of the Hodge Decomposition to biological modeling

Differential Forms

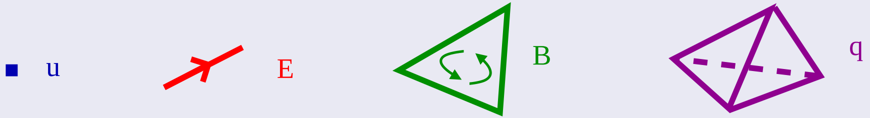
Let Ω denote a smooth n-manifold and $T_x(\Omega)$ the tangent space of Ω at x. A k**-form** ω is a mapping from Ω to the space of alternating k-tensors on the tangent space of Ω at the input point:

$$\omega : \Omega \to \Lambda^k[T_x(\Omega)^*], \qquad \omega(x) : \bigoplus_{i=1}^{k} T_x(\Omega) \to \mathbb{R},$$

where $\omega(x)$ is an alternating k-tensor. The space of k-forms is denoted $\Lambda^k(\Omega)$.

Alternate Characterization of k-forms

A k-form represents an intrinsically k-dimensional phenomena and can be integrated over a k-dimensional region.



electric potential is point−valued

electric fields are valued based on a linear current flow

magnetic fields are are dual to electric fields and valued on planes

charge density is valued over a volume

The Exterior Derivative Operator

The **exterior derivative** operator denoted by d is

$$d : \Lambda^k(\Omega) \to \Lambda^{k+1}(\Omega),$$

defined as follows. Let $I := \{i_1, \ldots, i_k\}$ denote an increasing sequence of k indices ($i_j < i_{j+1}$) and let $dx_I = dx_1 \wedge \cdots \wedge dx_k$. Given $\omega = \sum_I a_I dx_I$ define

$$d\omega := \sum_I da_I \wedge dx_I \quad \text{where} \quad da_I := \sum_{i \in I} \frac{\partial a_I}{\partial x_i} dx_i$$

The exterior derivative generalizes the familiar operators grad, curl, and div for $\Omega = \mathbb{R}^3$:

$$0 \longrightarrow \Lambda^0(\Omega) \xrightarrow[\text{grad}]{d} \Lambda^1(\Omega) \xrightarrow[\text{curl}]{d} \Lambda^2(\Omega) \xrightarrow[\text{div}]{d} \Lambda^3(\Omega) \longrightarrow 0$$

Example: Given $f \in \Lambda^0(\mathbb{R}^3)$, we have $f : \mathbb{R}^3 \to \mathbb{R}$. Accordingly:

$$\text{grad } f := \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right) = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz =: df$$

Stokes' Theorem

Stokes' Theorem

Given a compact, oriented n-dimensional manifold Ω with boundary $\partial\Omega$ and a smooth $(n-1)$ form ω on Ω, the following equality holds:

$$\int_{\partial\Omega} \omega = \int_{\Omega} d\omega$$

Alternate Characterization of d

Let ω be a k-form on a compact oriented n-manifold Ω $(0 \leq k < n)$. Then $d\omega$ is the unique $(k+1)$-form such that on any $(k+1)$-dimensional submanifold $\Pi \subset \Omega$ the following holds

$$\int_{\Pi} d\omega = \int_{\partial\Pi} \omega$$

Inner Products

We would like to construct an operator going the other way in the sequence:

$$0 \longleftarrow \Lambda^0(\Omega) \xleftarrow{\delta} \Lambda^1(\Omega) \xleftarrow{\delta} \Lambda^2(\Omega) \xleftarrow{\delta} \Lambda^3(\Omega) \xleftarrow{\delta} 0$$

To do so, we must first fix an inner product on our space.

An **inner product** $(\cdot,\cdot)_V$ on a vector space V is linear in each variable, symmetric, and non-degenerate, i.e. given $\alpha \in V$: $\quad (\alpha, \beta) = 0 \quad \forall \beta \iff \alpha = 0$.

An inner product $(\cdot,\cdot)_V$ on V extends to an inner product $(\cdot,\cdot)$ on $\Lambda(V)$

Let $\{e_1, \ldots, e_n\}$ be an orthonormal basis of V. We say that elements of the form $e_{i_1} \wedge \ldots \wedge e_{i_k}$ have **grading** k. Define the inner product of elements with different gradings to be zero. Define

$$(e_{i_1} \wedge \ldots \wedge e_{i_k}, e_{j_1} \wedge \ldots \wedge e_{j_k}) := det \begin{pmatrix} (e_{i_1}, e_{j_1})_V & \cdots & (e_{i_1}, e_{j_k})_V \\ \vdots & \ddots & \vdots \\ (e_{i_k}, e_{j_1})_V & \cdots & (e_{i_k}, e_{j_k})_V \end{pmatrix} \in \{-1, 0, 1\}$$

Extend the above definitions bilinearly for arbitrary elements of $\Lambda(V)$.

The Hodge Star Operator

The **Hodge Star** operator denoted by $\star$ is

$$\star : \Lambda^k(\Omega) \to \Lambda^{n-k}(\Omega).$$

Let $\{e_1, \ldots, e_n\}$ be an orthonormal basis for V with positive orientation. For $0 < k < n$, let $\sigma \in S_n$ satisfy $\sigma(1) < \cdots < \sigma(k)$ and $\sigma(k+1) < \cdots < \sigma(n)$. Define

$$\star \left(e_{\sigma(1)} \wedge \ldots \wedge e_{\sigma(k)}\right) := sign(\sigma) \left(e_{\sigma(k+1)} \wedge \ldots \wedge e_{\sigma(n)}\right).$$

For $k = 0$ and $k = n$, $\star$ is defined by $\star(1) = \pm e_1 \wedge \cdots \wedge e_n$ and $\star(e_1 \wedge \cdots \wedge e_n) = \pm 1$.

Example: $\star dxdz = \star dx_1 \wedge dx_3 = sign\ (1\ 3\ 2) dx_2 = -dx_2 = -dy$

Alternate Characterization of $\star$

The Hodge Star is the unique operator satisfying the relationship

$$\alpha \wedge \star\beta = (\alpha, \beta)\mu \quad \forall \alpha, \beta \in \Lambda^k(V),$$

where $\mu := e_1 \wedge \cdots \wedge e_n$ is the volume element of $\Lambda(V)$.

The Codifferential Operator

The (exterior) **codifferential** operator denoted by δ is

$$\delta : \Lambda^k(\Omega) \to \Lambda^{k-1}(\Omega)$$

defined as the formal adjoint to d with respect to the inner product $(\cdot,\cdot)$ on $\Lambda(\Omega)$. That is, given $\eta \in \Lambda^k(\Omega)$, $\delta\eta$ is the unique element of $\Lambda^{k-1}(\Omega)$ satisfying

$$(d\omega, \eta) = (\omega, \delta\eta)$$

for all $\omega \in \Lambda^{k-1}(\Omega)$.

Alternate Characterization of δ

Given an inner product on $\Lambda(V)$, where V has dimension n, the action of δ on a k-form is given by

$$\delta = (-1)^{nk+1} \star d \star$$

Example: $\delta(xyz\,dxdz) = (-1)^{3(2)+1} \star d(-xyz\,dy) = \star d(xyz\,dy)$

$$= \star(yz\,dxdy - xy\,dydz) = yz\,dz - xy\,dx$$

The Laplacian Operator

The **Laplacian operator** denoted by Δ is

$$\Delta : \Lambda^k(\Omega) \to \Lambda^k(\Omega)$$

given by

$$\Delta := d\delta + \delta d$$

Note that Δ reduces to the typical Laplacian operator when $k = 0$. By the definitions, $d_0 = \nabla$ and $\delta_1 = \text{div}$. Hence

$$\Delta_0 = d_{-1}\delta_0 + \delta_1 d_0 = \delta_1 d_0 = \text{div}\nabla = \nabla \cdot \nabla = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}.$$

Therefore, understanding solutions to the differential form problem $\Delta\omega = \alpha$ for a given form α will shed light on the Laplace and Poisson PDE problems.

The Hodge Decomposition

The space of **harmonic k-forms** is

$$\mathfrak{H}^k := \{\omega \in \Lambda^k(\Omega) : \Delta\omega = 0\}$$

The Hodge Decomposition Theorem

For each integer k with $0 \leq k \leq n$, $\mathfrak{H}^k$ is finite dimensional and we have the following orthogonal direct sum decompositions of $\Lambda^k(\Omega)$ of smooth k-forms on Ω:

$$\begin{aligned} \Lambda^k(\Omega) &= \Delta(\Lambda^k) \oplus \mathfrak{H}^k \\ &= d\delta(\Lambda^k) \oplus \delta d(\Lambda^k) \oplus \mathfrak{H}^k \\ &= d(\Lambda^{k-1}) \oplus \delta(\Lambda^{k+1}) \oplus \mathfrak{H}^k. \end{aligned}$$

Consequently, the equation $\Delta\omega = \alpha$ has a solution $\omega \in \Lambda^k(\Omega)$ if and only if the k-form α is orthogonal to the space of harmonic k-forms.

Relation to Cohomology

Recall that the **deRham complex** on Ω is

$$0 \longrightarrow \Lambda^0(\Omega) \xrightarrow{d_0} \Lambda^1(\Omega) \xrightarrow{d_1} \cdots \xrightarrow{d_{n-1}} \Lambda^n(\Omega) \longrightarrow 0.$$

The k**th deRham cohomology group** is denoted $H^k_{dR}(\Omega)$ and is given by

$$H^k_{dR} := \ker d_k / \mathrm{im} d_{k-1}$$

Lemma

Let Ω be a compact oriented Riemannian n-manifold Ω without boundary and $0 \leq k \leq n$. Then

$$H^k_{dR}(\Omega) \cong \mathfrak{H}^k.$$

Abbreviated Proof:

$$H^k_{dR} = \left[d(\Lambda^{k-1}) \oplus \mathfrak{H}^k \right] / d(\Lambda^{k-1}) \cong \mathfrak{H}^k$$

Summary of Smooth Hodge Decomposition Facts

Summary of results in the smooth setting:

- k-forms are meant to be integrated over k dimensional regions
- $d : \Lambda^k \to \Lambda^{k+1}$ is characterized by Stokes' theorem
- $\star : \Lambda^k \to \Lambda^{n-k}$ is characterized by $\alpha \wedge \star\beta = (\alpha, \beta)\mu$
- $\delta : \Lambda^k \to \Lambda^{k-1}$ is characterized by $\delta = (-1)^{nk+1} \star d \star$
- The Hodge Decomposition is $\Lambda^k = d\Lambda^{k-1} \oplus \delta\Lambda^{k+1} \oplus \mathfrak{H}^k$
- Solutions to the Poisson equation $\Delta\omega = \alpha$ lie in $d\Lambda^{k-1} \oplus \delta\Lambda^{k+1}$
- Solutions to the Laplace equation $\Delta\omega = 0$ are exactly the harmonic forms $\mathfrak{H}^k$
- Each k-cohomology class of Ω has a unique harmonic k-form representative.

How can we recreate these results on a discrete level for computational modeling?

$$
\begin{tikzcd}
\text{smooth:} & 0 & \Lambda^0 \arrow[l, "\delta_0"'] \arrow[r, shift left, "d_0"] \arrow[d, shift left] & \Lambda^1 \arrow[l, shift left, "\delta_1"] \arrow[r, shift left, "d_1"] \arrow[d, shift left] & \Lambda^2 \arrow[l, shift left, "\delta_2"] \arrow[r, shift left, "d_2"] \arrow[d, shift left] & \Lambda^3 \arrow[l, shift left, "\delta_3"] \arrow[r, "d_3"] \arrow[d, shift left] & 0 \\
\text{discrete:} & 0 \arrow[r] & \mathcal{C}^0 \arrow[r] \arrow[u, shift left] & \mathcal{C}^1 \arrow[r] \arrow[u, shift left] & \mathcal{C}^2 \arrow[r] \arrow[u, shift left] & \mathcal{C}^3 \arrow[r] \arrow[u, shift left] & 0
\end{tikzcd}
$$

Outline

Discrete Differential Forms

- *k-forms are meant to be integrated over k dimensional regions*

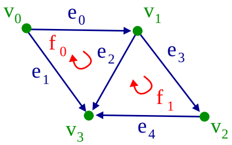
Let $\mathfrak{T}$ be a triangulation of a smooth compact n-manifold Ω. Let $\mathfrak{T}_k$ denote the k-simplicies of $\mathfrak{T}$. A k**-chain** c is a linear combination of the elements of $\mathfrak{T}_k$:

$$c = \sum_{\tau \in \mathfrak{T}_k} c_\tau \tau, \quad c_\tau \in \mathbb{R}$$

The set of all such chains form the **vector space of k-chains** is denoted $\mathcal{C}_k$.
A k**-cochain** ω is a linear map

$$\omega : \mathcal{C}_k \longrightarrow \mathbb{R}$$

The vector space of k-cochains is denoted $\mathcal{C}^k$.



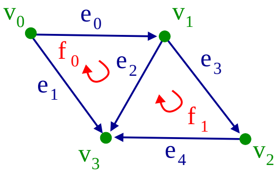
Cochains are the discrete analogues of differential forms.

The Boundary Operator

The k**th boundary operator** denoted by ∂_k takes a k-chain to its $(k-1)$-chain boundary. Its action on a k-simplex is

$$\partial_k[v_0, v_1, \cdots, v_k] := \sum_{i=0}^{k} (-1)^i [v_0, \cdots, \widehat{v_i}, \cdots, v_k]$$

where $\widehat{v_i}$ indicates that v_i is omitted.



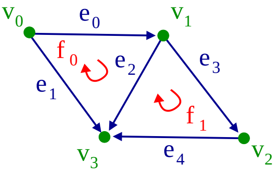
Let $c = f_1 + f_2$. Then $\partial_k c = \begin{bmatrix} 1 & 0 \\ -1 & 0 \\ 1 & -1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 0 \\ 1 \\ 1 \end{bmatrix} = e_0 - e_1 + e_3 + e_4$

Discrete Exterior Derivative

- $d : \Lambda^k \to \Lambda^{k+1}$ *is characterized by Stokes' theorem*

The k**th discrete exterior derivative** is the transpose of the $(k+1)$st boundary operator: $\mathbb{D}_k = \partial_{k+1}^T$

Example: Let ω be the 1-cochain $\omega(e_i) := i$.



$$\mathbb{D}_1\omega = \begin{bmatrix} 1 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 1 \\ 5 \end{bmatrix}$$

$$\int_{e_0 - e_1 + e_3 + e_4} \omega = \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}^T \begin{bmatrix} 1 \\ -1 \\ 0 \\ 1 \\ 1 \end{bmatrix} = -1+3+4 = 6 = 1+5 = \begin{bmatrix} 1 \\ 5 \end{bmatrix}^T \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \int_{f_0+f_1} \mathbb{D}_1\omega$$

Maps Between Smooth and Discrete Forms

To pass our theory between smooth and discrete settings, we will need maps:

$$\begin{tikzcd} \Lambda^k \arrow[d, shift left, "\mathcal{R}_k"] \\ \mathcal{C}^k \arrow[u, shift left, "\mathcal{I}_k"] \end{tikzcd} \qquad \begin{tikzcd} \Omega \arrow[d, shift left, "h^{-1}"] \\ \mathfrak{T}^k \arrow[u, shift left, "h"] \end{tikzcd}$$

The k**th deRham map** $\mathcal{R}_k : \Lambda^k \to \mathcal{C}^k$ is defined as follows. Let $\mathfrak{T}$ be a triangulation of Ω with $h : \mathfrak{T} \to \Omega$ a homeomorphism. Given $\omega \in \Lambda^k$ and $c \in \mathcal{C}_k$ a chain, define

$$(\mathcal{R}_k \omega)(c) := \int_{h(c)} \omega$$

The map $\mathcal{R}$ satisfies $\mathcal{R}d = \mathbb{D}\mathcal{R}$, i.e. the following is a commutative diagram:

$$\begin{tikzcd} \Lambda^k \arrow[r, "d_k"] \arrow[d, "\mathcal{R}_k"] & \Lambda^{k+1} \arrow[d, "\mathcal{R}_{k+1}"] \\ \mathcal{C}^k \arrow[r, "\mathbb{D}_k"] & \mathcal{C}^{k+1} \end{tikzcd}$$

Maps Between Smooth and Discrete Forms

The map $\mathcal{I}_k : \mathcal{C}^k \to \Lambda^k$ is called an interpolation map and has no canonical choice since $\mathcal{R}$ is not invertible. We can require, however, that $\mathcal{I}_k$ be chosen such that:

- $\mathcal{R}\mathcal{I} = \mathrm{id}$ (consistency)
- $\mathcal{I}\mathcal{R} = \mathrm{id} + O(h^s)$ (approximation)

where $h \in \mathbb{R}_{>0}$ is the partition size of the mesh and $s \in \mathbb{R}_{>0}$ is the approximation order.

Whitney Maps

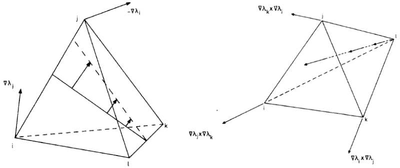
The Whitney map is a commonly used interpolation operator. The idea is to construct a basis of k-forms whose support is defined relative to a particular k-simplex.

Let $\tau := [v_0, \ldots, v_k]$ denote a k-simplex and $[\mu_0, \ldots, \mu_k]$ the barycentric coordinate functions of τ. The **Whitney form** $\eta_\tau \in \Lambda^k$ associated to this simplex is defined by

$$\eta_\tau := k! \sum_{i=0}^{k} (-1)^i \mu_i d\mu_0 \wedge \ldots \wedge \widehat{d\mu_i} \wedge \ldots \wedge d\mu_k$$

where $\widehat{d\mu_i}$ indicates that $d\mu_i$ is omitted. Given $\omega \in \mathcal{C}^k$ a k-cochain, its **Whitney interpolant** $\mathcal{I}(\omega)$ is

$$\mathcal{I}(\omega) := \sum_{\tau \in \mathcal{C}_k} \omega(\tau)\eta_\tau$$



Discrete Hodge Star

- $\star : \Lambda^k \longrightarrow \Lambda^{n-k}$ is characterized by $\alpha \wedge \star\beta = (\alpha, \beta)\mu$

To capture this relationship, we have two choices:

1. Define an inner product of two cochains and induce a discrete Hodge Star.
2. Define a discrete Hodge Star and induce an inner product.

We will examine each in turn.

Discrete Hodge Star via Inner Product

- $\star : \Lambda^k \rightarrow \Lambda^{n-k}$ is characterized by $\alpha \wedge \star\beta = (\alpha, \beta)\mu$

1. Define an inner product of two cochains and induce a discrete Hodge Star.

Let $a, b \in \mathcal{C}^k$. The **inner product of k-cochains** is defined by $(a, b)_{\mathcal{C}^k} := (\mathcal{I}a, \mathcal{I}b)_{\Lambda^k}$

This definition allows for two possible discrete Hodge stars.

- The **natural** discrete $\star$, given by $\overset{\mathrm{N}}{\star} := \mathcal{R} \star \mathcal{I}$ so that

$$(a, \overset{\mathrm{N}}{\star} b)_{\mathcal{C}^k} = (\mathcal{I}a, \mathcal{I}\mathcal{R} \star \mathcal{I}b)_{\Lambda^k}$$

  which implies $\overset{\mathrm{N}}{\star}\mathcal{R} = \mathcal{R}\star$

- The **derived** discrete $\star$, induced by $\int a \wedge \overset{\mathrm{D}}{\star} b := \int \mathcal{I}a \wedge \star\mathcal{I}b$ so that

$$(a, \overset{\mathrm{D}}{\star} b)_{\mathcal{C}^k} = (\mathcal{I}a, \star\mathcal{I}b)_{\Lambda^k}$$

  which implies $\int a \wedge \overset{\mathrm{D}}{\star} a = (a, a)$ for $a \in \mathcal{C}^k$

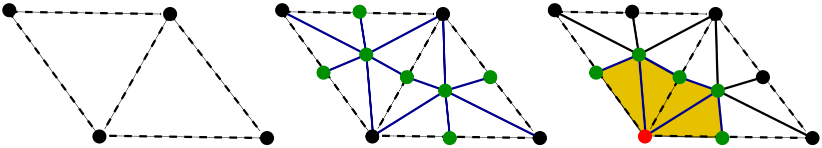
Remark: the property implied by one definition is *not* implied by the other!

Discrete Hodge Star directly

- $\star : \Lambda^k \to \Lambda^{n-k}$ is characterized by $\alpha \wedge \star\beta = (\alpha, \beta)\mu$

2. Define a discrete Hodge Star and induce an inner product.

Observe that an $(n-k)$-cochain is defined by its action on $(n-k)$-chains, however there is no canonical way to map a k-simplex to an $(n-k)$-simplex in the same mesh.



Since we would like the discrete $\star$ to be a square matrix, we ask that it associate a k-cochain on the ***primal*** mesh to an $(n-k)$-cochain on the ***dual*** mesh. The i, j entry of the discrete $\star$ should be a weight w_{ij} of the ith primal k-chain to the jth dual $(n-k)$-chain.

Discrete Hodge Star directly

- $\star : \Lambda^k \longrightarrow \Lambda^{n-k}$ is characterized by $\alpha \wedge \star\beta = (\alpha, \beta)\mu$

One simple but concrete approach is the following (from Desbrun, Kanso, Tong 2006):

Let $\{\tau_i\}$ be the k-simplicies of a triangulation $\mathfrak{T}$ of a smooth n-manifold. Let $*\tau$ denote the dual of τ and $|\tau|$ the measure of τ. Then the **discrete Hodge Star** $\star_k$ is a matrix of size $|\mathcal{C}_k| \times |\mathcal{C}_k|$ with diagonal entries

$$(\star_k)_{ii} := |*\tau_i|/|\tau_i|$$

and all other entries zero.

To achieve the desired characterization, we define the inner product accordingly.

Let α, β be k-cochains. Then their **inner product** is

$$(\alpha, \beta) := \alpha^T \star_k \beta = \sum_{i=1}^{|\mathcal{C}_k|} \alpha_i \left(\frac{|*\tau_i|}{|\tau_i|} \right) \beta_i$$

where $\alpha = [\alpha_1 \cdots \alpha_{|\mathcal{C}_k|}]^T$, $\beta = [\beta_1 \cdots \beta_{|\mathcal{C}_k|}]^T$

Discrete Codifferential and Hodge Decomposition

- $\delta : \Lambda^k \to \Lambda^{k-1}$ is characterized by $\delta = (-1)^{nk+1} \star d \star$

A discrete codifferential is defined based on the choice of discrete Hodge star.

Let ω be a k-cochain and $\star$ a discrete Hodge star. The **discrete codifferential** of ω is given by the matrix multiplications

$$\delta\omega := (-1)^{nk+1} \star \mathbb{D} \star \omega$$

Remark: Alternatively, we could define δ based on the relationship $(\alpha, \delta\beta) = (\mathbb{D}\alpha, \beta)$ however this may differ from the above definition by $O(h^s)$.

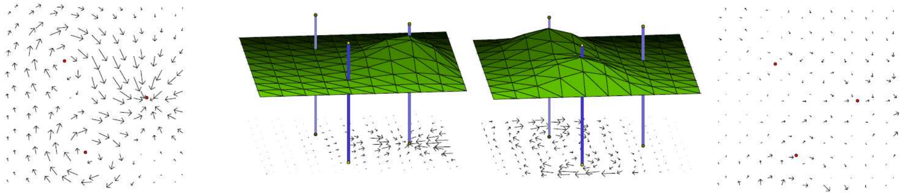
We now consider how this is implemented and its implications for biological modeling.

Outline

Prior Work

POLTHIER AND PREUSS *Identifying vector fields singularities using a discrete hodge decomposition* Proc. of Vis. Math. III, 2003
TONG, LOMBEYDA, HIRANI AND M. DESBRUN *Discrete multiscale vector field decomposition* ACM Trans. Graph., 22(3), 2003.

- Detect and classify singularities of 2D (former) and 3D (latter) vector fields by minimizing certain functionals to capture the divergence-free and curl-free components.



- Arguably more robust than Jacobian-based methods of singularity detection since there is no need to approximate partial derivatives.
- Requires solving a global linear system which may be unfeasible for the large data sets encountered in the biological domain.

Prior Work

ARNOLD, FALK AND WINTHER *Finite element exterior calculus, homological techniques, and applications* Acta Numerica, 2006.

- Give spaces of polynomials defined over a mesh and operators $\mathcal{R}$ and $\mathcal{I}$ such that a discrete Hodge decomposition is obtained.
- Establish bounds on the size of each component in the discrete Hodge decomposition. These bounds are shown to be independent of h (the mesh size) using approximation properties of the projections and elliptic regularity.
- Prove that the spaces described ensure stability of the method in the sense characterized by the Babuska inf-sup condition. (Loosely, this means the computed solution depends continuously on the input data).

Prior Work

TARHASAARI, KETTUNEN, BOSSAVIT *Some realizations of a discrete Hodge operator: a reinterpretation of finite element techniques* IEEE Trans. Magnetics 35:3, 1999
HIRANI *Discrete Exterior Calculus* Dissertation, Cal Tech, 2003.
BOCHEV AND HYMAN *Principles of Mimetic Discretizations of Differential Operators* in "Compatible Spatial Discretizations," 2006.
BELL *Algebraic Multigrid for Discrete Differential Forms* Dissertation, UIUC, 2008.

- Using Whitney interpolation for $\mathcal{I}_k$, define a "mass matrix" $\mathbb{M}$:

$$\mathbb{M}_k(i,j) := (\mathcal{I}_k e_i, \mathcal{I}_k e_j)$$

- The discrete Hodge Decomposition of a k-cochain ω^k is then

$$\omega^k = \mathbb{D}_{k-1}\alpha^{k-1} + \mathbb{M}_k^{-1}\mathbb{D}_k^T\mathbb{M}_{k+1}\beta^{k+1} + h^k$$

- The components can be computed by finding a basis for the space of harmonic k-cochains and projecting ω^k onto the basis elements.

Research Questions

- Is Bell's method appropriate for use in biological domains? Can we instead develop a domain-sensitive selection of bases for molecular force field vector components?

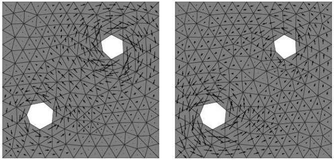


Figure 7.2: Initial harmonic basis.

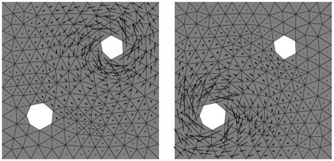


Figure 7.3: Localized harmonic basis.

- What is the relative strength of the components of the force field given by the Hodge decomposition in biological settings? How much does this depend upon the choice of discrete Hodge star ($\overset{N}{\star}, \overset{D}{\star}, \star_k, \ldots$)?
- Can Hodge-based analysis aid in the construction of a stable solution of molecular force fields using low degree algebraic spline vector finite elements (e.g. A-patches)?

Acknowledgements

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- A copy of these slides is available at

  http://www.math.utexas.edu/users/agillette/