Accessing geometry via function spaces

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ROADMAP

- Limits of graphs
- Geometric objects of interest:
  - Intrinsic distances
  - Symmetries
- Why function spaces?
  - Visualization
  - Finding symmetries
  - Algebras on function space
LIMITS OF GRAPHS
DISCRETE FUNCTION SPACES

- Sequence of graphs \((V_n, E_n)\) approximating \(\Omega \supset V_n\)

- Define function spaces \(\ell(V_n) = \{f : V_n \to \mathbb{R}\}\)

  - \(\ell(V_n) \cong \mathbb{R}^N\) (where \(N\) is size of \(V_n\)) by \(\vec{f}_i = f(x_i)\)

  - Inner product \(f \cdot h = \sum_{x \in V_n} f(x)h(x)\)

  - Restriction of \(f : \Omega \to \mathbb{R}\) by \(\Pi_n f = f|_{V_n}\)
WHY FUNCTION SPACES?

- Sequence of graphs \((V_n, E_n)\) approximating \(\Omega \supset V_n\)
- Hard to define limit \((V_n, E_n) \rightarrow \Omega\)
- Assume \(V_n \subset V_{n+1}\) and \(V^* = \bigcup_n V_n\) dense in \(\Omega\)
- Easy to define limit \(f_n \rightarrow f\) by \(\|f_n - \Pi_n f\| \rightarrow 0\)
- Requires some assumptions on \(f\), e.g. smoothness
- Convergence of functions doesn’t tell us about geometry
- We need operators! Haven’t used the edges yet....
GRAPH LAPLACIANS

- Build a random walk
  - Assign weights to edges $K_{ij} \geq 0$ for $i \sim j$
  - Compute row sums $D_{ii} = \sum_j K_{ij}$
  - Divide rows by row sums $P = D^{-1}K$
  - $P$ is a Markov matrix (transition probabilities)

- Assume symmetric $K_{ij} = K_{ji}$ non-negative def. $\vec{v}^\top K \vec{v} \geq 0$

- Define the associated graph Laplacian $L = P - I$

- $L$ is called the generator of the random walk
# Discrete analogs of continuous objects

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<th>Continuous</th>
<th>Discrete</th>
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<td>( L^2(\Omega) )</td>
<td>( \mathbb{R}^N )</td>
</tr>
<tr>
<td>Functions, ( f : \mathcal{M} \rightarrow \mathbb{R} )</td>
<td>Vectors, ( \vec{f}_i = f(x_i) )</td>
</tr>
<tr>
<td>‘Basis’, ( \delta_x )</td>
<td>Basis, ( \vec{e}<em>i = \delta</em>{x_i} )</td>
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<tr>
<td>Operators, ( \mathcal{F} )</td>
<td>Matrices, ( \mathbf{F} )</td>
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<td>Laplacian, ( \Delta )</td>
<td>graph Laplacian, ( \mathbf{L} )</td>
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<tr>
<td>Eigenfunctions, ( \Delta \varphi_j = \lambda_j \varphi_j )</td>
<td>Eigenvectors, ( \mathbf{L} \vec{\varphi}_j = \lambda_j \vec{\varphi}_j )</td>
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<tr>
<td>Inner product, ( \langle f, h \rangle_{L^2} )</td>
<td>Dot Product, ( \vec{f} \cdot \vec{h} )</td>
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<td>Measure, ( \langle f, h \rangle_{L^2, d\mu} )</td>
<td>Diagonal matrix, ( \vec{f} \cdot_D \vec{h} = \vec{f}^\top D \vec{h} )</td>
</tr>
</tbody>
</table>
SEQUENCE OF GRAPHS \((V_n, E_n)\) approximating \(\Omega \supset V_n\)

Define a sequence graph Laplacians \(L_n = P_n - I\)

Find scaling factors \(c_n\) such that \(c_n L_n\) converges pointwise

Meaning that for nice functions \(f : \Omega \to \mathbb{R}\)

\[
\lim_{n \to \infty} \| c_n L_n \Pi_n f - \Pi_n \mathcal{L} f \| = 0
\]
**Example 1: Laplacians on Fractals**

- Sequence of graphs \((V_n, E_n)\) approximating \(\Omega \supset V_n\)
- Uniform random walk \(K_{ij} = 1\) if \(i \sim j\)
- For the Sierpinski gasket (SG, shown above) \(c_n = 5^n\)

\[
c_n \mathbf{L}_n \vec{f}_i = 5^n \sum_{j \sim i \text{ in } V_n} (f(x_j) - f(x_i)) \to \Delta f
\]

- \(\Delta\) is the foundation of analysis on SG
EXAMPLE 2: LAPLACIANS ON MANIFOLDS

- Sequence of graphs \((V_n, E_n)\) approximating \(\Omega \supset V_n\)
- Local random walk \(K_{ij} = \exp\left(-\frac{||x_i - x_j||^2}{4\delta^2}\right)\)
- For \(d\)-dimensional manifold \(c_n = \delta^{-2}\) where \(\delta = N^{-\frac{1}{6+d}}\)
  \[c_n L_n \vec{f}_i \rightarrow \Delta f\]
- \(\Delta\) is the Laplace-Beltrami operator
LAPLACIAN ON $S^1$, 10 POINTS

Parameterize $S^1 = \{\theta \in [0, 2\pi)\}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

Kernel $K$, Density $D = K1$, Normalized $\hat{K} = D^{-1}KD^{-1}$, Bias $\hat{D} = \hat{K}1$, Laplacian $L$

Index, $i$: $-5, 0, 5, 10$
Eigenvalue, $\lambda_i$: $0.5, 2.5, 4.5, 6.5, 8.5, 10.5$
Eigenfunction: $\sin(\theta)$

Graphs showing the kernel, density, normalized, and bias, along with their corresponding eigenvalues and eigenfunctions.
LAPLACIAN ON $S^1$, 100 POINTS

Parameterize $S^1 = \{\theta \in [0, 2\pi)\}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

Kernel $K$, Density $D = K1$, Normalized Kernel $\hat{K} = D^{-1}KD^{-1}$, Bias $\hat{D} = \hat{K}1$, Laplacian $L$
**Nonuniform \( S^1 \), 100 Points**

Parameterize \( S^1 = \{ \theta \in [0, 2\pi) \} \), Laplacian is \( \Delta = -\frac{d^2}{d\theta^2} \)

Kernel  \quad Density  \quad Normalized  \quad Bias  \quad Laplacian

\[
K_1 \quad D = K_1 \quad \hat{K} = D^{-1}KD^{-1} \quad \hat{D} = \hat{K}_1 \quad L
\]

<table>
<thead>
<tr>
<th>Eigenvalue, ( \lambda_i )</th>
<th>Index, ( i )</th>
<th>Eigenfunction</th>
<th>( \theta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-5, 5, 10, 15, 20, 25, 20, 15, 10, 5, 0</td>
<td>2, 4, 6, 8, 10</td>
<td>0, ( \pi ), 2( \pi )</td>
<td>0, ( \pi ), 2( \pi )</td>
</tr>
</tbody>
</table>

\( K \quad D = K_1 \quad \hat{K} = D^{-1}KD^{-1} \quad \hat{D} = \hat{K}_1 \quad L \)
REAL DATA $S^1$, 100 POINTS

Parameterize $S^1 = \{\theta \in [0, 2\pi)\}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

$K$  $D = K1$  $\hat{K} = D^{-1}KD^{-1}$  $\hat{D} = \hat{K}1$  $L$

Eigenvalue, $\lambda_i$

Index, $i$

Eigenfunction

$\theta$
REAL DATA $S^1$, 1000 POINTS

Parameterize $S^1 = \{\theta \in [0, 2\pi)\}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

$$K$$  $$D = K1$$  $$\hat{K} = D^{-1}KD^{-1}$$  $$\hat{D} = \hat{K}1$$  $$L$$

Eigenvalue, $\lambda_i$

$\theta$

Eigenfunction

Index, $i$
LESSON LEARNED SO FAR...

- We can approximate manifolds/fractals by graphs
- Nice convergence notions on functions/operators
- Graph Laplacians converge to continuous Laplacians
- Sampling is important!
A bit of Riemannian geometry

- Consider a smooth $d$-dimensional manifold $\mathcal{M}$
- There is no canonical inner product on tangent spaces
- A Riemannian metric $g$ is a choice of inner product
  \[ g_x : T_x \mathcal{M} \times T_x \mathcal{M} \to \mathbb{R} \]
  - $g_x$ is bilinear, symmetric, positive definite, and smooth in $x$
- **Example:** Let $\iota : \mathcal{M} \to \mathbb{R}^m$ be a smooth embedding
  \[ g_x(v, w) = \langle D\iota(x)v, D\iota(x)w \rangle_{\mathbb{R}^m} \]
- $g$ is called the induced metric
RIEMANNIAN VOLUME

- Choose coordinates $x^1, \ldots, x^d : U_x \rightarrow \mathbb{R}$

- Basis vectors $e_1, \ldots, e_d \in T_x \mathcal{M}$ where $e_i = \frac{\partial}{\partial x^i}$

- Represent $g_x$ as a matrix $g_{ij}(x) = g_x(e_i, e_j)$

- Define the volume form $dV(x) = \sqrt{\det(g(x))} \, dx^1 \cdots dx^d$

- $\text{vol}(\mathcal{M}) = \int_{x \in \mathcal{M}} 1 \, dV(x)$

- Now we can define a nice function space $L^2(\mathcal{M}, g)$
WHY IS THE RIEMANNIAN METRIC A GEOMETRY?

- Allows us to measure tangent vectors $\|v\|^2_g = g_x(v, v)$

- Given a differentiable curve $\gamma : [0, 1] \to M$ we can define the length, $L(\gamma) \equiv \int_0^1 \|\gamma'(t)\|dt$

- We define the intrinsic distance $d_I(x, y) \equiv \inf_\gamma L(\gamma)$

- If some $\gamma$ attain $d_I(x, y)$ it is a geodesic

- $(M, d_I)$ is called a path metric space
WHAT ARE ISOMETRIES?

- Let $\mathcal{T} : \mathcal{M} \rightarrow \mathcal{N}$ be a diffeomorphism

- We call $\mathcal{T}$ an isometry if $g_\mathcal{M} = \mathcal{T}^* g_\mathcal{N}$

  - Pick orthonormal bases $v_1, ..., v_d \in T_x \mathcal{M}$ and $w_1, ..., w_d \in T_{\mathcal{T}(x)} \mathcal{N}$
  
  - Represent $D\mathcal{T}(x) : T_x \mathcal{M} \rightarrow T_{\mathcal{T}(x)} \mathcal{N}$ in these bases
  
  - $\mathcal{T}$ is an isometry if $D\mathcal{T}(x)$ is an orthogonal matrix

- $\mathcal{T}$ is an isometry $\iff d_{I,\mathcal{M}}(x, y) = d_{I,\mathcal{N}}(\mathcal{T}(x), \mathcal{T}(y))$

- $\iff$ is Myers-Steenrod theorem (proves $\mathcal{T}$ is diffeo)
Isometries $\mathcal{T} : \mathcal{M} \to \mathcal{N}$ preserve the metric, $g$

Laplacian is defined by $g$

$$\Delta f = \text{div} \circ \nabla = \frac{1}{\sqrt{|g|}} \partial_i g^{ij} \sqrt{|g|} \partial_j f$$

Laplacian is preserved by isometries

$$\Delta_{\mathcal{N}}(f \circ \mathcal{T}) = \Delta_{\mathcal{M}}(f) \circ \mathcal{T}$$
Visualization: Diffusion Maps

- Eigenfunctions $\Delta \varphi_j = \lambda_j \varphi_j$ define isometric embedding

$$\Phi : x \mapsto c(e^{-\lambda_1 t} \varphi_1(x), e^{-\lambda_2 t} \varphi_2(x), ...)$$

- Embed $S^1 \subset \mathbb{R}^6$ by

$$t \mapsto (\cos(t), \sin(t), \cos(2t), \sin(2t), \cos(5t), \sin(5t))/\sqrt{30}$$

- Want to project back to $\mathbb{R}^3$
LEARNING NONLINEAR MAPS

- Assume we have two data sets \( \{ x_i \}_{i=1}^{N} \) and \( \{ y_i \}_{i=1}^{N} \)
- Related by a diffeomorphism \( y_i = \mathcal{H}(x_i) \)

\[
\begin{align*}
M & \xrightarrow{\mathcal{H}} \mathcal{H}(M) \\
\downarrow \phi & \quad \downarrow \Phi \\
\ell^2 \cong L^2(M, \tilde{g}) & \xrightarrow{U} \ell^2 \cong L^2(\mathcal{H}(M), g)
\end{align*}
\]

- \( \tilde{\phi} \) and \( \Phi \) are built with Local Kernels
- \( U \) is orthogonal linear map \( \Rightarrow \) Easy to fit
LEARNING NONLINEAR MAPS
WHAT ARE SYMMETRIES?

- Isometries preserve the Riemannian metric, $g$, and the intrinsic distance, $d_I$

- Consider isometries $\mathcal{T} : \mathcal{M} \rightarrow \mathcal{M}$

- Group structure: Composition of isometries is an isometry

- Laplacian is preserved $\Delta(f \circ \mathcal{T}) = \Delta(f) \circ \mathcal{T}$

- Hard Theorem: Isometries form a Lie group
**Symmetries and Eigenfunctions**

- Consider an non-trivial isometry \( T : M \rightarrow M \)
- Consider an eigenfunction \( \Delta \varphi_j = \lambda_j \varphi_j \)
  \[ \Delta (\varphi_j \circ T) = \lambda_j \varphi_j \circ T \]
- So \( \varphi_j \circ T \) is an eigenfunction with eigenvalue \( \lambda_j \)
- This implies that \( \lambda_j \) has multiplicity at least two and
  \[ \varphi_j \circ T = \sum_{\lambda_k = \lambda_j} a_{jk} \varphi_k \]
**Symmetries and Eigenfunctions**

- Isometries of $S^1 = [0, 2\pi) \Rightarrow T_s(t) = s + t \mod 2\pi$

- Eigenfunctions $\varphi_2(t) = \sin(t)$ and $\varphi_3(t) = \cos(t)$

- $(\varphi_2 \circ T_s)(t) = \sin(s + t) = \sin(s) \cos(t) + \cos(s) \sin(t)$

- $(\varphi_3 \circ T_s)(t) = \cos(s + t) = \cos(s) \cos(t) - \sin(s) \sin(t)$

$$
\begin{bmatrix}
\varphi_2 \circ T_s \\
\varphi_3 \circ T_s
\end{bmatrix} =
\begin{bmatrix}
\cos(s) & \sin(s) \\
-\sin(s) & \cos(s)
\end{bmatrix}
\begin{bmatrix}
\varphi_2 \\
\varphi_3
\end{bmatrix}
$$
**Symmetry Group Representation**

- For the $n$ eigenfunctions with eigenvalue $\lambda_j$

  \[ \varphi_j \circ T = \sum_{\lambda_k = \lambda_j} a_{jk} \varphi_k \]

- The matrix $A$ with entries $a_{jk}$ is orthogonal

- Composing isometries $T_1 \circ T_2$

  \[ \varphi_j \circ T_1 \circ T_2 = \sum_{\lambda_k = \lambda_j} a^1_{jk} \varphi_k \circ T_2 = \sum_{\lambda_\ell = \lambda_k = \lambda_j} a^1_{jk} a^2_{k\ell} \varphi_\ell \]

- Results in matrix multiplication

- We have a **representation** of the isometry group in $O(n)$!
Symmetry Group Representation

- Isometry group has representation in orthogonal transformations of the eigenfunctions of the Laplacian
- Isometry group determines multiplicity of eigenvalues
- We can use this to search for symmetries!
- Look for repeated eigenvalues then...
- Find orthogonal transformations that preserve eigenfunctions
**LAPLACIAN ON $S^1$, 100 POINTS**

Parameterize $S^1 = \{ \theta \in [0, 2\pi) \}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

Kernel $K$ \quad Density $D = K1$ \quad Normalized $\hat{K} = D^{-1}KD^{-1}$ \quad Bias $\hat{D} = \hat{K}1$ \quad Laplacian $L$
**Torus** $T^2$, 1200 Points

Parameterize $T^2 = \{(\theta, \phi) \in [0, 2\pi)^2\}$

- **Kernel**
- **Density**
- **Normalized**
- **Bias**
- **Laplacian**

**Formulas:**

\[
K = D = K1 = D^{-1}KD^{-1} = \hat{K}1 = \hat{D} = L
\]
**Flat Torus** $T^2$, 1200 Points

Parameterize $T^2 = \{ (\theta, \phi) \in [0, 2\pi)^2 \}$

**Kernel** $K$

**Density** $D = K1$

**Normalized** $\hat{K} = D^{-1}KD^{-1}$

**Bias** $\hat{D} = \hat{K}1$

**Laplacian** $L$

$K$ $D = K1$ $\hat{K} = D^{-1}KD^{-1}$ $\hat{D} = \hat{K}1$ $L$
**Sphere** $S^2$, 42 points

Parameterize $S^2 = \{(\theta, \phi) \in [0, 2\pi)^2\}$

Kernel $K$, Density $D = K1$, Normalized $\hat{K} = D^{-1}KD^{-1}$, Bias $\hat{D} = \hat{K}1$, Laplacian $L$
**Sphere $S^2$, 642 Points**

Parameterize $S^2 = \{(\theta, \phi) \in [0, 2\pi)^2\}$

<table>
<thead>
<tr>
<th>Kernel</th>
<th>Density</th>
<th>Normalized</th>
<th>Bias</th>
<th>Laplacian</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Kernel" /></td>
<td><img src="image2" alt="Density" /></td>
<td><img src="image3" alt="Normalized" /></td>
<td><img src="image4" alt="Bias" /></td>
<td><img src="image5" alt="Laplacian" /></td>
</tr>
</tbody>
</table>

$$K, \quad D = K1, \quad \hat{K} = D^{-1}KD^{-1}, \quad \hat{D} = \hat{K}1, \quad L$$
Z₃ SYMMETRY, 90 POINTS

Parameterize \( \{\theta \in [0, 2\pi)\} \)

\[
K \quad D = K1 \quad \hat{K} = D^{-1}KD^{-1} \quad \hat{D} = \hat{K}1 \quad L
\]
$Z_3$ SYMMETRY, 90 POINTS

Parameterize $\{\theta \in [0, 2\pi)\}$

\[ K, \quad D = K1, \quad \hat{K} = D^{-1}KD^{-1}, \quad \hat{D} = \hat{K}1, \quad L \]

Eigenfunction shifts

Nonsymmetric Shift
SAMPLING THEORY ON MANIFOLDS

- Want to generalize Shannon’s sampling theorem
- \( f \) has finite Fourier series \( \Leftrightarrow \) determined by values on grid
- Assume \( f(t) = a_0 + a_1 \sin(t) + a_2 \cos(t) \)
- We can determine \( f \) from values on 3 points
- Best points are \( \{0, 2\pi/3, 4\pi/3\} \)
- Orbit of finite subgroup \( Z_3 \subset O(2) \)
- Finite subgroups of \( O(2) \) \( \Rightarrow \) Best samples on \( S^1 \)
Sampling Theory on Manifolds

- Want to generalize sampling theorem to manifolds

- $\mathcal{H}_m = \text{span}\{\varphi_1, \ldots, \varphi_m\}$ and $K_m(x, y) = \sum_{j=1}^{m} \varphi_j(x)\varphi_j(y)$

- $f \in \mathcal{H}_m$ implies $\langle f, K_m(x, \cdot) \rangle = f(x)$ so $\mathcal{H}$ is RKHS

- Find points $x_i \in \Omega$ s.t. span$\{K_m(\cdot, x_i)\} = \mathcal{H}_m$

- **Sampling Theorem:** $f \in \mathcal{H}_m$ determined by $\bar{f}_i = f(x_i)$

- **Idea:** Sampling sets $\Leftrightarrow$ Orbits of finite subgroups of $T$
Good sampling sets $\Rightarrow$ Fast convergence $\Rightarrow$ Less data!
Think of eigenfunctions $\varphi_j$ as generalized Fourier basis

In the case of $S^1$ recover standard Fourier basis

On $S^1$ we also have multiplicative structure:

$$f \ast h(s) = \int_0^{2\pi} f(s - t)h(t) \, dt = \int_0^{2\pi} f(T_s(t))h(t) \, dt$$

Convolution defined in terms of translation symmetry

Fourier transform maps convolution to multiplication

Pontryagin duality: $\mathcal{F}(f \ast h) = \mathcal{F}(f)\mathcal{F}(h)$
Think of eigenfunctions $\varphi_j$ as generalized Fourier basis

Let $\mathcal{T}_{\vec{\theta}}$ be the isometry group parameterized by $\vec{\theta}$

For a ‘super-symmetric’ manifold: The isometry group parameterization gives natural coordinates on the manifold

Generalize convolution to ‘super-symmetric’ manifolds

$$f * h(x) = \int_{\mathcal{M}} f(\mathcal{T}_x(y)) h(y) \, dy$$

What does Pontryagin duality say?
Eigenfunctions of $\Delta$ are basis for $L^2(\mathcal{M}, g)$

$$\varphi_i \cdot \varphi_j = \sum_k c_{ijk} \varphi_k$$

$c_{ijk}$ are called the structure constants of the algebra

Ex: $\varphi_2(t)\varphi_3(t) = \sin(t) \cos(t) = \sin(2t)/2 = \varphi_4(t)/2$

Want to compute the Riemannian metric $g(v, w)$

Fact: Any vector field can be written as $v = \sum_{ij} a_{ij} \varphi_i \nabla \varphi_j$

So if I can compute $g(\nabla \varphi_j, \nabla \varphi_k)$ I know $g$
MULTIPLICATION FUNCTION ALGEBRA

- I need to compute $g(\nabla \varphi_j, \nabla \varphi_k)$, handy formula:

\[
g(\nabla \varphi_j, \nabla \varphi_k) = -\frac{1}{2} \left( \varphi_i \Delta \varphi_j + \varphi_j \Delta \varphi_i - \Delta(\varphi_i \varphi_j) \right)
\]

- Good thing we used eigenfunctions

\[
g(\nabla \varphi_j, \nabla \varphi_k) = -\frac{1}{2} \left( \varphi_i \lambda_j \varphi_j + \varphi_j \lambda_i \varphi_i - \Delta \left( \sum_k c_{ijk} \varphi_k \right) \right)
\]

- We need the structure constants!

\[
g(\nabla \varphi_j, \nabla \varphi_k) = -\frac{1}{2} \sum_k c_{ijk} (\lambda_j + \lambda_i - \lambda_k) \varphi_k
\]
Start with the smooth eigenfunctions $\Delta \varphi_i = \lambda_i \varphi_i$

Define a frame for 1-forms: $b^{ij} = \varphi_i d\varphi_j - \varphi_j d\varphi_i$

Define Laplace-de Rham operator on $b^{ij}$

$$\langle b^{kl}, \Delta^1 (b^{ij}) \rangle = \sum_r (c_{kir} c_{ljr} - c_{kjr} c_{lir})(\lambda_r^2 - \lambda_r (\lambda_k + \lambda_i + \lambda_l + \lambda_j))$$

$$+ c_{ijr} c_{klr}(\lambda_j - \lambda_i)(\lambda_l - \lambda_k)$$

Exterior calculus is determined by function algebra
SUMMARY

- Function spaces give useful notions of convergence
- Use graph Laplacians to define discrete calculus
- Manifold symmetries represented in Laplacian eigenspace
- Graph symmetries rep. in graph Laplacian eigenspace
- Connections to convolution algebra and sampling theory
- Eigenvalues + Structure constants ⇒ Exterior Calculus