

From Manifolds to Graphs

The Laplacian Operator



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Background Introduction



Shape Analysis Course Chapter 9

- ▶ The textbook Chapter 9, and the course slides (mostly 8-10) (Could be found from Geometric Data Processing Group)
- ▶ Shape Analysis (Lectures 12-13): The Laplacian operator on intervals, regions, graphs, and manifolds — On YouTube
- ▶ Shape Analysis (Lectures 13, extra content): Divergence of tangent vector fields — On YouTube
- ▶ Shape Analysis (Lectures 14): Laplacian operators via first-order Galerkin finite elements (FEM) — On YouTube
- ▶ Shape Analysis (Lectures 14, extra content): A simple Laplacian on point clouds — On YouTube
- ▶ Shape Analysis (Lecture 15): Applications of the Laplacian in graphics, vision, and learning — On YouTube

Basic Approach of Shape Analysis: Operator Base.

- ▶ Understanding the structure of operators on functions.

The main operator we focus on: Laplacian

- ▶ Input: function on a manifold
- ▶ Output: the function which is the second derivative of the input at every point
- ▶ Eigenvalues and Eigenvectors of Laplacian infer a lot of information about the shape / manifold
- ▶ Discrete Laplacian Operators enables a lot of applications, following the outline: find some matrix approximating Laplacian, do linear algebra calculation, find something...
- ▶ Same calculation from low to high dimensional space, a “sledgehammer”

No clear convention on the sign of Laplacian among mathematicians, physics, computer scientists.

Here we try to stick to the convention:

- ▶ Non-negative Eigenvalues
- ▶ It is minus the sum of the second derivatives
- ▶ Discretize it to be a positive semidefinite matrix

Not gonna have time to build up the theory of Laplacian Operator from the ground up (i.e. function, spaces, differentiable manifolds, etc.).

Instead: feel of how it behaves, how it is constructed, etc.

Can One Hear the Shape of a Drum?

CAN ONE HEAR THE SHAPE OF A DRUM?

MARK KAC, The Rockefeller University, New York

To George Eugene Uhlenbeck on the occasion of his sixty-fifth birthday

"La Physique ne nous donne pas seulement l'occasion de résoudre des problèmes . . . , elle nous fait présenter la solution." H. POINCARÉ.

Before I explain the title and introduce the theme of the lecture I should like to state that my presentation will be more in the nature of a leisurely excursion than of an organized tour. It will not be my purpose to reach a specified destination at a scheduled time. Rather I should like to allow myself on many occasions the luxury of stopping and looking around. So much effort is being spent on streamlining mathematics and in rendering it more efficient, that a solitary transgression against the trend could perhaps be forgiven.

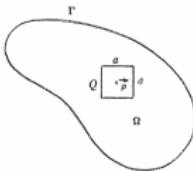


FIG. 1

Around 1960s, not the first one on the topic, but the most memorable one.

What is it asking?

- ▶ From the sound you hear from a drum, can you reconstruct the shape of that drum?
- ▶ Can I reconstruct a piece of geometry from an audio signal?
- ▶ From the 1-D frequency signal, can we reconstruct the high dimensional shape?

Sounds impossible at first but...

What is it asking?

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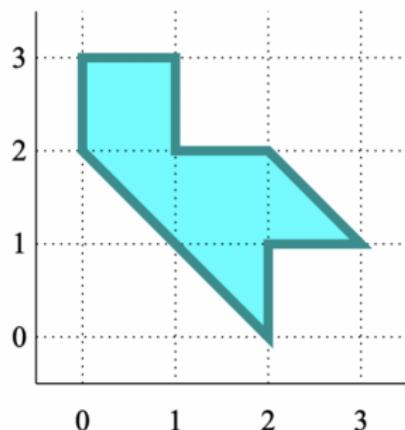
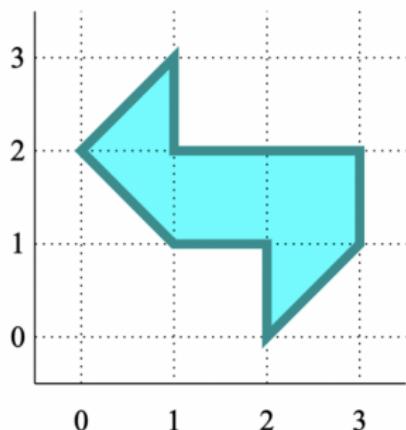
A 1-D version of the question:

- ▶ Can we reconstruct the length of string (of a guitar) from the sound it makes?

There is a relationship between the length of the string (the shape) and the frequency of vibration you hear.

The answer in the 1-D space is YES, but for the drum is NO.

Reason: There are drums that are either spectral (but very rare). There are two drums in the universe that makes exactly the same vibrations but have different shape.



Decompose the vibration modes into a list of frequencies and eigenfunctions. Revealing quite a bit of the shape.

http://pngimg.com/upload/hammer_PNG3886.png



You can learn a lot
about a shape by
hitting it (lightly)
with a hammer!

What can you learn about a shape based on its: (1) vibration frequencies and (2) oscillation patterns?

- ▶ We can compute it via Laplacian.
- ▶ Ends up in (1) eigenvalues and (2) eigenvectors.

$$\Delta f = \lambda f$$

Linear Operator L is something that satisfies:

$$L[\mathbf{x} + \mathbf{y}] = L[\mathbf{x}] + L[\mathbf{y}]$$

$$L[c\mathbf{x}] = cL[\mathbf{x}]$$

The finite dimensional case (but it will be dangerous to infer it this way when infinite dimensional space would be involved):

$$L[\mathbf{x}] = \mathbf{A}\mathbf{x},$$

where \mathbf{A} is a matrix and \mathbf{x} is a vector.

Theorem.

*Suppose a complex square matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ is **Hermitean**.¹ Then, \mathbf{A} has an **orthogonal basis** of n eigenvectors. If \mathbf{A} is **positive definite**, the corresponding eigenvalues are **nonnegative**.*

Orthogonal basis: any two eigenvector correspond to different eigenvalues are necessarily orthogonal.

¹Equal to its own conjugate transpose.

In the real-value case Hermitian means symmetric.

And these eigenvectors **span** \mathbb{R}^n .

Row Theorem of $A \in \mathbb{R}^{n \times n}$:

$\text{Span}(\text{columns of } A) = \mathbb{R}^n \iff$ There is a pivot in every row
 $Ax = b$ is consistent for every b

How to examine “there is a pivot in every row”: apply row addition / subtraction and guarantee that in the end no row becomes 0.

Suppose a real square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is **Hermitian** i.e. Symmetric.

$$\mathbf{Ax} = \lambda \mathbf{x} \quad \mathbf{Ay} = \mu \mathbf{y} \quad \mathbf{x} \neq \mathbf{0}, \mathbf{y} \neq \mathbf{0}, \lambda \neq \mu$$

If \mathbf{x} and \mathbf{y} are orthogonal, then $\mathbf{x}^T \mathbf{y} = 0$.

Proof:

$$\begin{aligned}\lambda \mathbf{x}^T \mathbf{y} &= (\mathbf{Ax})^T \mathbf{y} = \mathbf{x}^T \mathbf{A}^T \mathbf{y} = \mathbf{x}^T (\mathbf{Ay}) \\ &= \mathbf{x}^T \mu \mathbf{y} = \mu \mathbf{x}^T \mathbf{y} \\ \therefore 0 &= (\lambda - \mu) \mathbf{x}^T \mathbf{y}\end{aligned}$$

Given $\lambda \neq \mu$, we have $\mathbf{x}^T \mathbf{y} = 0$.

Will be able to extend to Hermitian operators that satisfies $\langle \mathbf{x}, \mathbf{Ay} \rangle = \langle \mathbf{Ax}, \mathbf{y} \rangle$.

Suppose a real square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is **Hermitian** i.e.
Symmetric. and positive definite.

$$\lambda = \lambda \mathbf{x}^T \mathbf{x} = \mathbf{x}^T (\lambda \mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x} > 0,$$

because of that \mathbf{A} is positive definite. (If positive-semidefinite
then ≥ 0)

This is something we'll use frequently in computation.

$$\int_a^b u(x)v'(x)dx = [u(x)v(x)]_a^b - \int_a^b u'(x)v(x)dx$$

Or, let $u = u(x)$ and $du = u'(x)dx$, while $v = v(x)$ and $dv = v'(x)dx$

$$\int udv = uv - \int vdu$$

Wave Equation



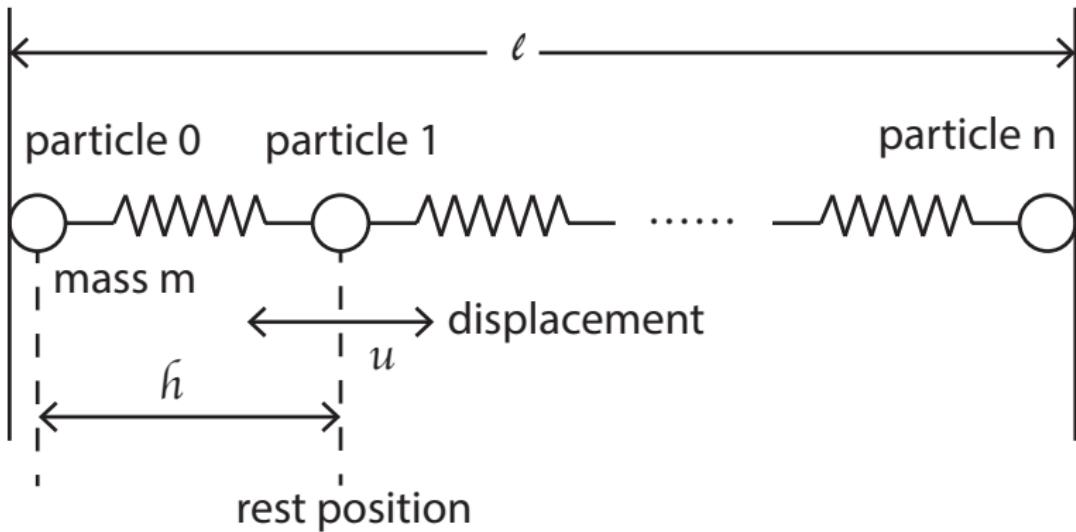
“Can You Hear the Shape of a Line Segment?” /
“Can You Hear the Length of an Interval?”

A many-particle physical system with $n + 1$ particles, each with mass m , along the interval of length ℓ , attached by strings with constant k , and rest length 0.

The particles are spaced distance $h = \ell/n$ apart, and particles 0 and n are fixed in place.

Suppose at time $t = 0$, each particle i is displaced horizontally (i.e. 1-D vibration) by **signed** distance u_i from its rest position $\ell i/n$.

Our goal is to track their motion over time.



Positive u_i : displaced to the right; Negative u_i : displaced to the left. Fix the end particles (0 and n). $\ell = 0$ when we are not stretching it (rest length).

From Newton's second law: $ma = F$ and we consider only the neighbors,

$$m \frac{d^2 u_i}{dt^2} = k(u_{i+1} - u_i) + k(u_{i-1} - u_i) = k(u_{i+1} + u_{i-1} - 2u_i),$$

suppose $i \in \{1, 2, \dots, n\}$ and $n \rightarrow \infty$.

The right hand side approximates a second derivative.

$u(x, t)$: the displacement of particle at position x when t . Then as $n \rightarrow \infty$, it resembles the solution of the partial differential equation known as *wave equation*:

$$\frac{\partial^2 u(x, t)}{\partial t^2} = c^2 \frac{\partial^2 u(x, t)}{\partial x^2},$$

where c^2 absorbs all physical constants.

Since:

$$F = m \frac{d^2 u_i}{dt^2} = k(u_{i+1} + u_{i-1} - 2u_i),$$

Therefore, if we stack the unknown u values into a vector-valued function $\mathbf{u}(t) \in \mathbf{R}^{n-1}$, then the second derivative $\mathbf{u}''(t) = -c^2 L \mathbf{u}(t)$, where

$$L = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & \ddots & \ddots & \ddots \\ & & & -1 & 2 \end{bmatrix}$$

$$\mathbf{u}''(t) = -c^2 L \mathbf{u}(t),$$

If we assume that x is the direction of the string, then:

$$\frac{d^2 u_i}{dx^2} \approx \frac{\frac{u_{i+1}-u_i}{h} - \frac{u_i-u_{i-1}}{h}}{h} = \frac{u_{i+1} + u_{i-1} - 2u_i}{h}$$

$$L = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & \ddots & \ddots & \ddots \\ & & & -1 & 2 \end{bmatrix} \approx \frac{d^2}{dx^2}$$

If we take $n \rightarrow \infty$:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0$$

We will think of our operators as acting on functions spatially.

The “string” abstraction:

$$\{f(\cdot) \in C^\infty([0, \ell]) : f(0) = f(\ell) = 0\}$$

$f(0) = f(\ell) = 0$: “Dirichlet boundary conditions”.

$$\mathcal{L}[\cdot] : u \mapsto -\frac{\partial^2 u}{\partial x^2}$$

Can be interpreted as positive (semi-)definite matrix.

$$\begin{aligned} u^T L u &= \sum_{i=1}^{n-1} u_i (Lu)_i \quad // u_0 = u_n = 0 \\ &= \sum_{i=1}^{n-1} u_i (2u_i - u_{i-1} - u_{i+1}) \\ &= 2 \sum_{i=1}^{n-1} u_i^2 - \sum_{i=1}^{n-1} u_i u_{i-1} - \sum_{i=1}^{n-1} u_i u_{i+1} \\ &= \sum_{i=0}^n u_i^2 + \sum_{i=0}^n u_{i-1}^2 - 2 \sum_{i=0}^n u_i u_{i-1} \\ &= \sum_{i=0}^n (u_i - u_{i-1})^2 \geq 0 \end{aligned}$$

The discrete version is simple. The continuous version:

$$\mathcal{L}[\cdot] : u \mapsto -\frac{\partial^2 u}{\partial x^2}$$

$$\begin{aligned}\langle u, \mathcal{L}[u] \rangle &= \int_a^b u(x) \cdot -\frac{\partial^2 u(x)}{\partial x^2} dx \\ &= \left[-\frac{\partial^2 u(x)}{\partial x^2} u(x) \right]_a^b + \int_a^b \frac{\partial u(x)}{\partial x} \cdot \frac{\partial u(x)}{\partial x} dx \\ &= \int_a^b \left(\frac{\partial u(x)}{\partial x} \right)^2 dx \quad // \text{ boundary term is equal to zero} \\ &\geq 0 \quad // \text{ where } a = 0, b = \ell\end{aligned}$$

$\int_a^b \left(\frac{\partial u(x)}{\partial x} \right)^2 dx$: “Dirichlet Energy of function u ”

Again we consider:

$$\mathcal{L}[\cdot] : u \mapsto -\frac{\partial^2 u}{\partial x^2}$$

Then we have eigenfunctions as:

$$\phi_k(x) = \sqrt{\frac{2}{\ell}} \sin\left(\frac{\pi kx}{\ell}\right), \quad \lambda_k = \left(\frac{\pi k}{\ell}\right)^2$$

Applying the \mathcal{L} operator:

$$\mathcal{L}[\phi_k(x)] = -\sqrt{\frac{2}{\ell}} \left(\frac{\pi k}{\ell}\right)^2 \sin\left(\frac{\pi kx}{\ell}\right) = \lambda_k \phi_k(x)$$

$$\langle \phi_k, \phi_m \rangle = \delta_{km} \quad \delta_{km} \text{ is 1 iff } k = m \text{ otherwise } \delta_{km} = 0$$

Fourier series with the help of eigenvalue & eigenvector
(discrete) / eigenfunction (smooth), solve the wave equation in
some sort of closed form.

$$\mathbf{u}''(t) = -c^2 L \mathbf{u}(t)$$

$$\frac{\partial^2 u}{\partial t^2} = -c^2 \mathcal{L}[u]$$

$$\mathbf{u}''(t) = -c^2 L \mathbf{u}(t),$$

with L already proved to be positive semi-definite. According to the spectrum theory: \exists eigenvectors ϕ_k , eigenvalues λ_k , where the ϕ_k are orthonormal and span \mathbb{R}^n .

$$\mathbf{u}(t) = \sum_k u^k(t) \phi_k$$

Then we have:

$$\begin{aligned}\sum_k (u^k)''(t) \phi_k &= \mathbf{u}''(t) = -c^2 L \mathbf{u}(t) \\ &= -c^2 L \sum_k u^k(t) \phi_k = -c^2 \sum_k u^k(t) \lambda_k \phi_k \\ (u^k)''(t) &= -c^2 u^k(t) \lambda_k\end{aligned}$$

We now have the ordinary differential equation in just one variable:

$$(u^k)''(t) = -c^2 u^k(t) \lambda_k$$

A standard solution of this ODE shows as a consequence that

$$u^k(t) = a^k \sin(c\sqrt{\lambda_k}t) + b^k \cos(c\sqrt{\lambda_k}t)$$

After knowing λ_k and parameter c , we can compute the actual value of a^k and b^k from some known data points e.g. when $t = 0$ and then we can construct the closed form solution of the wave equation.

The continuous case $\frac{\partial^2 u}{\partial t^2} = -c^2 \mathcal{L}[u]$ have similar form of solution.

$$u^k(t) = a^k \sin(c\sqrt{\lambda_k}t) + b^k \cos(c\sqrt{\lambda_k}t),$$

with continuous ϕ ,

$$\phi_k(x) = \sqrt{\frac{2}{\ell}} \sin\left(\frac{\pi k x}{\ell}\right), \quad \lambda_k = \left(\frac{\pi k}{\ell}\right)^2$$

So the answer to the question:

“Can You Hear the Length of an Interval?”
is: YES. We hear it from λ_k .

The n -dimensional version is not much more complicated than the 1-dimensional version.

$$\frac{\partial^2 u}{\partial t^2} = -\Delta u$$

$$\Delta := - \sum_i \frac{\partial^2}{\partial (x^i)^2} = -\nabla \cdot \nabla ,$$

where ∇ is the gradient operator.

We first consider wave equation on a compact domain $\Omega \subseteq \mathbb{R}^n$, the flat region on an n -dimensional space. Its boundary $\partial\Omega \subset \mathbb{R}^n$ is a smooth $(n - 1)$ -dimensional submanifold.

When $n = 2$, it encapsulates the case of a vibrating drum head.

We consider the wave modeled by $u(\mathbf{x}, t)$, $t \geq 0$. This time $\mathbf{x} \in \Omega$ is location/particle in an N-D domain, instead of on a 1-D string.

$$\frac{\partial^2 u(\mathbf{x}, t)}{\partial t^2} = \sum_i \frac{\partial^2 u(\mathbf{x}, t)}{\partial (x^i)^2}$$

$$\mathbf{u}|_{\partial\Omega} \equiv 0 \quad (\text{the Dirichlet boundary conditions})$$

Following similar steps we've had in 1-D space, we are motivated to find the eigenvalues of the operator:

$$\Delta[\cdot] : u(\mathbf{x}, t) \mapsto - \sum_i \frac{\partial^2 u(\mathbf{x}, t)}{\partial(x^i)^2}$$

which takes the place of \mathcal{L} , and is also called a Laplacian (in the \mathbb{R}^n space), often denoted as

$$\Delta := - \underbrace{\nabla}_{\text{divergence}} \cdot \underbrace{\nabla}_{\text{gradient}}$$

$$\Delta := - \sum_i \frac{\partial^2}{\partial(x^i)^2} = - \underbrace{\left(\frac{\partial}{\partial x^1} \quad \cdots \quad \frac{\partial}{\partial x^n} \right)}_{\nabla^T} \underbrace{\begin{pmatrix} \frac{\partial}{\partial x^1} \\ \vdots \\ \frac{\partial}{\partial x^n} \end{pmatrix}}_{\nabla}$$

It is not yet clear from the following expression:

$$\frac{\partial^2 u(\mathbf{x}, t)}{\partial t^2} = \sum_i \frac{\partial^2 u(\mathbf{x}, t)}{\partial (x^i)^2}$$
$$\mathbf{u}|_{\partial\Omega} \equiv 0$$

that $\Delta = -\nabla \cdot \nabla$ is invariant to rigid motion (because of i).

This property can be verified by this Proposition:

Suppose $g(\mathbf{x}) := f(R\mathbf{x} + \mathbf{t})$, where $R^T R = RR^T = I_{n \times n}$.
Then, $\Delta g(\mathbf{x}) = [\Delta f](R\mathbf{x} + \mathbf{t})$.

Checking invariance to translation by verifying that \mathbf{y} and \mathbf{x} have the same Laplacian, starting with chain rule:

$$\mathbf{y} := R\mathbf{x} + \mathbf{t}$$

$$\frac{\partial}{\partial x^i} = \sum_j \frac{\partial y^j}{\partial x^i} \frac{\partial}{\partial y^j} = \sum_j R_i^j \frac{\partial}{\partial y^j}$$

$$\begin{aligned}\Delta_{\mathbf{x}} &= - \sum_i \frac{\partial^2}{\partial(x^i)^2} = - \left(\sum_j R_i^j \frac{\partial}{\partial y^j} \right) \cdot \left(\sum_j R_i^j \frac{\partial}{\partial y^j} \right) \\ &= - \sum_j \frac{\partial^2}{\partial(y^j)^2} = \Delta_{\mathbf{y}}\end{aligned}$$

Or from an abstract level what we did:

$$\nabla_{\mathbf{x}} = R^T \nabla_{\mathbf{y}}$$
$$\Delta_{\mathbf{x}} = -\nabla_{\mathbf{x}}^T \nabla_{\mathbf{x}} = -\nabla_{\mathbf{y}}^T R R^T \nabla_{\mathbf{y}} = -\nabla_{\mathbf{y}}^T \nabla_{\mathbf{y}} = \Delta_{\mathbf{y}}$$

Conclusion: our Laplacian operator is coordinate i independent.
It is okay to rotate it / move it and it still have the same
Laplacian.

Now we move out of the scope of the drum scenario. There are a lot more that Laplacian can handle.

One most obvious thing is that Laplacian could be used to measure how **smooth** a function is.

Here we have the example of *Dirichlet Energy* and *Harmonic Functions*. This example has little to do with Physics.

Suppose $u : \partial\Omega \mapsto \mathbb{R}$, we wish to interpolate u o the interior of Ω . We have the Dirichlet energy of function u , which measures the total norm of its gradient.

$$E[u] := \frac{1}{2} \int_{\Omega} \|\nabla u(\mathbf{x})\|_2^2 d\mathbf{x}$$

Here we would like to seek a smooth function (small norm gradient) that satisfies our boundary constraints.

$$\min_{u(\mathbf{x}) : \Omega \mapsto \mathbb{R}} E[u]$$

subject to $u|_{\partial\Omega}$ prescribed

The solution would be $\Delta u(\mathbf{x}) \equiv 0$, which is called a “*Harmonic function*” or “*Laplace equation*”.

The way we solve it (\oint for contour integral): ²

$$\min_{u(\mathbf{x}): \Omega \rightarrow \mathbb{R}} E[u]$$

subject to $u|_{\partial\Omega}$ prescribed

$$\begin{aligned} E[u] &= \frac{1}{2} \int_{\Omega} \|\nabla u(\mathbf{x})\|_2^2 d\mathbf{x} \\ &= \frac{1}{2} \int_{\Omega} \nabla u(\mathbf{x}) \cdot \nabla u(\mathbf{x}) d\mathbf{x} \\ &= \frac{1}{2} \oint_{\partial\Omega} u(\mathbf{x}) \nabla u(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) d\mathbf{x} + \frac{1}{2} \int_{\Omega} u(\mathbf{x}) \Delta u(\mathbf{x}) d\mathbf{x} \end{aligned}$$

The fancy way of write $\int_{\Omega} u(\mathbf{x}) \Delta u(\mathbf{x}) d\mathbf{x}$ could be $\langle u(\mathbf{x}), \Delta u(\mathbf{x}) \rangle$,
the inner product form.

²see: multi-variable integration by parts.

$\frac{1}{2} \oint_{\partial\Omega} u(\mathbf{x}) \nabla u(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) d\mathbf{x}$ is the prescribed boundary term. We will use variational derivative to prove that $\Delta u(\mathbf{x}) \equiv 0$.

First, assume we have a perturbation $w : \Omega \mapsto \mathbb{R}$, $w|_{\partial\Omega} \equiv 0$; and we assume that u is optimal.

Then we know: $u + hw$ will satisfy the boundary constraints.

$$\frac{d}{dh} E[u + hw]|_{h=0} = 0$$

Why does:

$$\frac{d}{dh} E[u + hw]|_{h=0} = 0$$

the equation holds?

Why does:

$$\frac{d}{dh} E[u + hw]|_{h=0} = 0$$

the equation holds?

Because: u is optimal, minimizing $E[\cdot]$ to the local minimum.
When $h = 0$ we are at the local minimum point. Otherwise
 $E[u + hw]$ goes higher in both direction.

We can ignore the boundary term because that part has nothing to do with h .

$$\frac{d}{dh} E[u + hw]|_{h=0} = 0$$

$$\frac{d}{dh} \left[\frac{1}{2} \int_{\Omega} (u + hw)(\mathbf{x}) \Delta((u + hw)(\mathbf{x})) d(\mathbf{x}) \right]_{h=0} = 0$$

Applying the product rule (to pass the $\frac{d}{dh}$ inside the integral):

$$\begin{aligned} & \frac{1}{2} \int_{\Omega} w(\mathbf{x}) \Delta u(\mathbf{x}) + u(\mathbf{x}) \Delta w(\mathbf{x}) d\mathbf{x} \\ &= \int_{\Omega} w(\mathbf{x}) \Delta u(\mathbf{x}) d\mathbf{x} = 0 \end{aligned}$$

It is true for $\forall w : \Omega \mapsto \mathbb{R}$, $w|_{\partial\Omega} \equiv 0$ that,

$$\int_{\Omega} w(\mathbf{x}) \Delta u(\mathbf{x}) d\mathbf{x} = 0$$

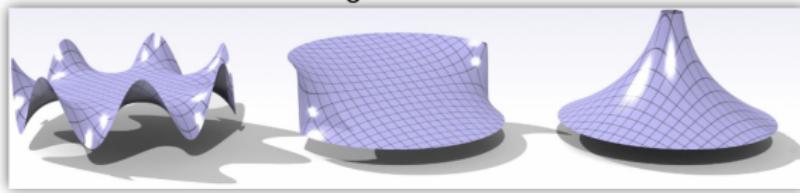
Therefore, $\Delta u(\mathbf{x}) \equiv 0$ in the interior of Ω .

That is the Harmonic functions, whose:

- ▶ Boundaries are prescribed;
- ▶ Interior is smooth.

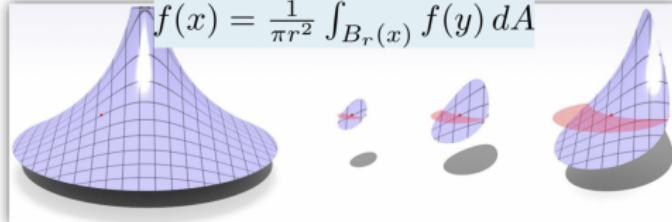
Harmonic functions satisfies a lot of nice properties, such as the **mean value property**: *If you pick an area in the domain, the center value is equal to the average of the area.*

$$\Delta f \equiv 0$$



Mean value property:

$$f(x) = \frac{1}{\pi r^2} \int_{B_r(x)} f(y) dA$$



Images made by E. Vouga

Cage-Based Deformation: compute the inner points as a linear combination of the boundary points.

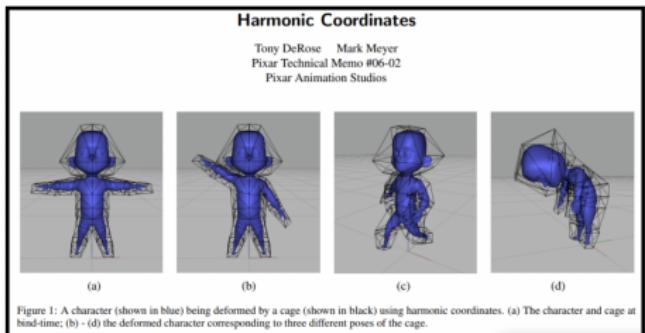


Figure 1: A character (shown in blue) being deformed by a cage (shown in black) using harmonic coordinates. (a) The character and cage at bind-time; (b) - (d) the deformed character corresponding to three different poses of the cage.

Abstract

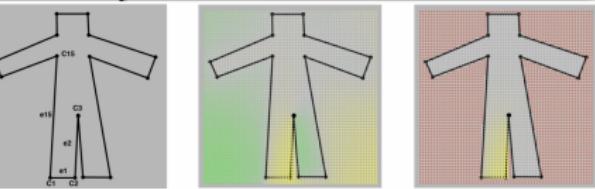
Generalizations of barycentric coordinates in two and higher dimensions have been shown to be useful in many areas, including finite element surfaces, the definition of S-patches (n-sided generalizations of Bézier surfaces), free-form deformations, mesh parametrization, and interpolation. In this paper we present a new form of dimensional generalization barycentric coordinates. The new coordinates are defined as solutions to Laplace's equation subject to carefully chosen boundary conditions. Since solutions to Laplace's equation are called harmonic functions, we call the new construction harmonic coordinates. We show that harmonic coordinates possess several properties that make them more attractive than mean value coordinates when used to define two and three dimensional deformations.

ways, one of the simplest being to isying the interpolation conditions:

$$\beta_i(T_j) = \delta_{i,j}$$

Similarly, barycentric coordinates defined relative to a non-degenerate $T_1, T_2, T_3, T_4 \in \mathbb{R}^3$ as the unique line 2 where the indices i and j run from 1 to 3.

As described in Ju et al., Ju et al. barycentric coordinates stem from the interpolating functions. Gouraud shading colors c_1, c_2, c_3 assigned to the vertices of a triangle are interpolated across the triangle according to the formula



Also based on the fact that in 3-D case we have closed-form solution for harmonic functions etc. (*)

Given $\{f(\cdot) \in C^\infty : f|_{\partial\Omega} \equiv 0\}$. Define the Laplacian as:

$$\mathcal{L} := \Delta f$$

and the inner product as:

$$\langle f, g \rangle := \int_{\Omega} f(\mathbf{x})g(\mathbf{x})d\mathbf{x}$$

The Laplacian is:

- ▶ Positive: $\langle f, \mathcal{L}[f] \rangle \geq 0$ (“positive semi-definite”)
- ▶ Self-adjoint: $\langle f, \mathcal{L}[g] \rangle = \langle \mathcal{L}[f], g \rangle$ (“symmetric”)

Note that $f(\mathbf{x}) \equiv 0$ on the boundary $\partial\Omega$. The integral on the boundary results in zero (using the trick of integration by parts).

$$\begin{aligned}\langle f, \mathcal{L}[f] \rangle &= - \int_{\Omega} f(\mathbf{x}) \nabla \cdot \nabla f(\mathbf{x}) d\mathbf{x} \\ &= - \oint_{\partial\Omega} f(\mathbf{x}) \nabla f(\mathbf{x}) d\mathbf{x} + \int_{\Omega} \nabla f(\mathbf{x}) \nabla f(\mathbf{x}) d\mathbf{x} \\ &= \int_{\Omega} \|\nabla f(\mathbf{x})\|_2^2 d\mathbf{x} \geq 0\end{aligned}$$

Similarly we have (f and g are both $\equiv 0$ on the boundary):

$$\begin{aligned}\langle f, \mathcal{L}[g] \rangle &= - \int_{\Omega} f(\mathbf{x}) \nabla \cdot \nabla g(\mathbf{x}) d\mathbf{x} \\ &= - \oint_{\partial\Omega} f(\mathbf{x}) \nabla g(\mathbf{x}) d\mathbf{x} + \int_{\Omega} \nabla f(\mathbf{x}) \nabla g(\mathbf{x}) d\mathbf{x} \\ &= \int_{\Omega} \nabla f(\mathbf{x}) \nabla g(\mathbf{x}) d\mathbf{x} \\ &= \langle g, \mathcal{L}[f] \rangle\end{aligned}$$

$$\begin{aligned} \min_{u(\mathbf{x}): \Omega \mapsto \mathbb{R}} \quad & \frac{1}{2} \int_{\Omega} \|\nabla u(\mathbf{x})\|_2^2 d(\mathbf{x}) \\ \text{subject to} \quad & \int_{\Omega} u(\mathbf{x})^2 d\mathbf{x} = 1 \end{aligned}$$

Why we set $u(\mathbf{x})^2 d\mathbf{x} = 1$ instead of $= 0$? Because:

- ▶ scaling a function by a constant does not affect its qualitative structure;
- ▶ 0 is super smooth but a not interesting case.

We seek to solve $\Delta u = \lambda u$, where the eigenvalue λ is the Lagrange multiplier, and it actually is equal to the Dirichlet energy of u .

The eigenvalue λ is equal to the Dirichlet energy of u . The larger λ is, the higher Dirichlet Energy, and the more “wiggly” the corresponding eigenfunction would be.

$$\Delta u_k = \lambda_k u_k$$

we are going to see infinite sequence of it — finding a new eigenfunction u_k by changing λ_k .

Weyl’s Law: you can sense the dimensionality of domain Ω by looking at the sequence of Laplacian eigenvalues.

The formal version of the “Can you hear the shape of a drum?” problem:

Do there exist two domains Ω with the same sequence of eigenvalues?

Discretization



We define the graphs as $G = \{V, E\}$ where there is a value assigned to each vertex $v_i \in V$.

Question: what is the Dirichlet Energy of a function on a graph?

We define the graphs as $G = \{V, E\}$ where there is a value assigned to each vertex $v_i \in V$.

Question: what is the Dirichlet Energy of a function on a graph?

Answer: Dirichlet Energy measures smoothness. We can estimate “smoothness” in this way:

$$DE[f] = \sum_{(i,j) \in E} (f(v_i) - f(v_j))^2$$

The differencing operator $D \in \{-1, 0, 1\}^{|E| \times |V|}$ is defined as:

$$D_{ev} := \begin{cases} -1 & \text{if } j \in V, (v, j) \in E \\ 1 & \text{if } i \in V, (i, v) \in E \\ 0 & \text{otherwise} \end{cases}$$

The computation is cumulative. e.g. If there are 2 “in-edge” at a node then we do $+2$ on it, for 3 “out-edge” we do -3 , etc.

Given $\mathbf{f} \in \mathbb{R}^n$ on $G = (V, E)$ where there are $|V| = n$ vertices.
The Dirichlet Energy can be formally re-defined as:

$$E[\mathbf{f}] := \sum_{(i,j) \in E} (f^i - f^j)^2 = \|D\mathbf{f}\|_2^2 = \mathbf{f}^T D^T D \mathbf{f} := \mathbf{f}^T L \mathbf{f}$$

where L is the **unweighted** Graph Laplacian.

The unweighted graph Laplacian $L \in \mathbb{R}^{|V| \times |V|}$ on an undirected graph is defined as:

$$L_{ij} := D^T D = A - \overline{D} = \begin{cases} -1 & \text{if } (i, j) \in E \text{ or } (j, i) \in E \\ \text{degree}(i) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

where A is the adjacency matrix, \overline{D} is the diagonal Degree matrix, D is the Differencing Operator.

It is easy to see that L_{ij} is:

- ▶ Symmetric when the graph is undirected;
- ▶ Positive Semi-Definite because the Dirichlet Energy is non-negative.

Labeled graph	Degree matrix	Adjacency matrix	Laplacian matrix
	$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$

More interesting correlations would be found if we consider a line-graph special case, and compare it to where we started to dive in — the line segment with many particles. (*)

The second smallest graph eigenvector: (*)

- ▶ The smallest graph eigenvalue: 0, not exciting;
- ▶ The second smallest graph eigenvalue: the corresponding eigenvector becomes very interesting, called the Fiedler vector, or the “algebraic connectivity” of the graph.
- ▶ Intuitive understanding: not being trapped in a local optimal point, being the smoothiest possible, thus providing suggestion for graph partitioning.

Mean value property satisfied:

$$(Lx)^v = 0 \iff \text{value at } v \text{ is average of neighboring values}$$

This property is useful for e.g. surface parameterization.

Kirchoff's Theorem

Number of spanning trees equals

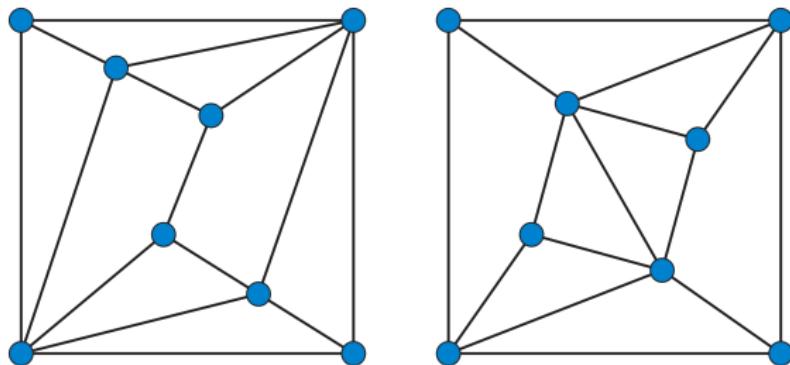
$$t(G) = \frac{1}{|V|} \prod_{k=2}^{|V|} \lambda_k$$

For more: Spectral Graph Theory

Can You Hear the Shape of a Graph?

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That is: can you re-construct the graph structure from the eigenvalues?

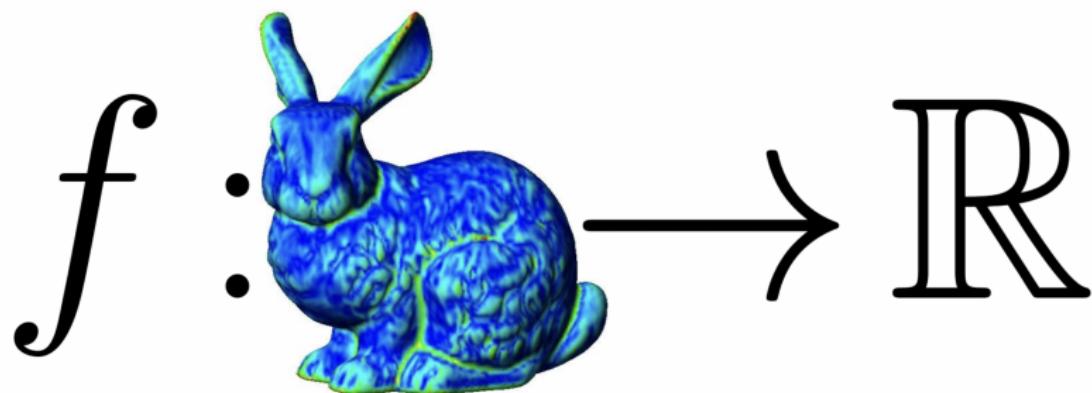


Many reasons to say “**NO**” include but not limited to this case of a pair of **cospectral Enneahedron**.

Surfaces & Manifolds



Function f on a manifold maps the points to real numbers.



e.g. Color function as a scalar associated with every point.

Linear map of tangent spaces:

$$d\varphi_{\mathbf{p}}(\gamma'(0)) := (\varphi \circ \gamma)'(0)$$

Formally, $\varphi : \mathcal{M} \rightarrow \mathcal{N}$ is a map from a submanifold $\mathcal{M} \subseteq \mathbb{R}^k$ into a submanifold $\mathcal{N} \subseteq \mathbb{R}^\ell$, and the differential of φ at point $\mathbf{p} \in \mathcal{M}$, $d\varphi_{\mathbf{p}} : T_{\mathbf{p}}\mathcal{M} \rightarrow T_{\varphi(\mathbf{p})}\mathcal{N}$ is given by

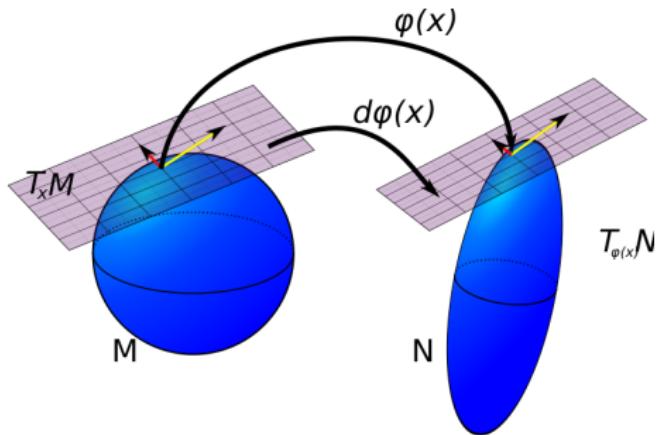
$$d\varphi_{\mathbf{p}}(\gamma'(\mathbf{v})) := (\varphi \circ \gamma)'(0),$$

$\gamma : (-\epsilon, \epsilon) \rightarrow \mathcal{M}$ is any curve with $\gamma(0) = \mathbf{p}$ and $\gamma'(0) = \mathbf{v} \in T_{\mathbf{p}}\mathcal{M}$.

$T_{\mathbf{p}}\mathcal{M}$ denotes the tangent space of \mathcal{M} at \mathbf{p} .

The image is from Wikipedia Pushforward.

$$d\varphi_p(\gamma'(0)) := (\varphi \circ \gamma)'(0)$$



If φ is a map from one space to another, then the differential of a map φ at a particular point on my source domain \mathcal{M} is a function that is linear on the tangent plane to my manifold.

What it does: For every tangent vector, it maps it to the directional derivative of the map φ in that tangent vector direction.

That is the definition of the differential of a map.

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In our case, we are mapping the manifold to \mathbb{R} so it is not complicated at this part.

Beyond that, we will need to define the gradient so that we will be able to define the Dirichlet Energy and the Laplacian.

Given manifold $\mathcal{M} \subseteq \mathbb{R}^m$ and $f : \mathcal{M} \rightarrow \mathbb{R}$. For each $\mathbf{p} \in \mathcal{M}$, there exists a unique vector $\nabla f(\mathbf{p}) \in T_{\mathbf{p}}\mathcal{M}$ so that $\forall \mathbf{v} \in T_{\mathbf{p}}\mathcal{M}$:

$$df_{\mathbf{p}}(\mathbf{v}) = \mathbf{v} \cdot \nabla f(\mathbf{p})$$

In the flat case, this fancy feature is saying that there exists a gradient vector. Now we are extending it to the curved surface.

Take basis $\mathbf{b}_i, \dots, \mathbf{b}_m \in T_{\mathbf{p}}\mathcal{M}$ (where m is the dimension of our manifold) for the tangent space at \mathbf{p} of our manifold $T_{\mathbf{p}}\mathcal{M}$.

Define $a_i := df_{\mathbf{p}}(\mathbf{b}_i)$.

- We are taking the directional derivative of f at each of the basis directions and getting the scalar a_i .

Define the inner product matrix with elements:

$$g_{ij} = \mathbf{b}_i \cdot \mathbf{b}_j,$$

with inverse matrix g^{-1} being g^{ij} .

We are going to define a matrix and check that it is the gradient we want. Claim,

$$\nabla f(\mathbf{p}) = \mathbf{x} := \sum_{ij} a_i g^{ij} \mathbf{b}_j$$

$\forall \mathbf{v} \in T_{\mathbf{p}}\mathcal{M}$, decompose it into the linear combination of basis $\mathbf{v} = \sum_i v^i \mathbf{b}_i$. Then, by definition of \mathbf{v} and \mathbf{x} ,

$$\mathbf{v} \cdot \mathbf{x} = \sum_i v^i \mathbf{b}_i \cdot \sum_{k\ell} a_k g^{k\ell} \mathbf{b}_\ell$$

Next, by definition of $g_{ij} = \mathbf{b}_i \cdot \mathbf{b}_j$,

$$\begin{aligned}\sum_i v^i \mathbf{b}_i \cdot \sum_{k\ell} a_k g^{k\ell} \mathbf{b}_\ell &= \sum_{ik\ell} v^i a_k g^{k\ell} \mathbf{b}_i \mathbf{b}_\ell \\ &= \sum_{ik\ell} v^i a_k g^{k\ell} g_{i\ell}\end{aligned}$$

The term $g^{k\ell} g_{i\ell}$ could be regarded as $(g^{-1}g)_i^k$, which is essentially $\delta_{k=i}$. We are cancelling the matrix and its inverse. Therefore,

$$\sum_{ik\ell} v^i a_k g^{k\ell} g_{i\ell} = \sum_i v^i a_i$$

By definition of a_k we have,

$$\sum_i v^i a_i = \sum_i v^i df_{\mathbf{P}}(\mathbf{b}_i)$$

By linearity,

$$\sum_i v^i df_{\mathbf{P}}(\mathbf{b}_i) = df_{\mathbf{P}}\left(\sum_i v^i \mathbf{b}_i\right) = df_{\mathbf{P}}(\mathbf{v})$$

All in all,

$$\mathbf{v} \cdot \mathbf{x} = df_{\mathbf{P}}(\mathbf{v})$$

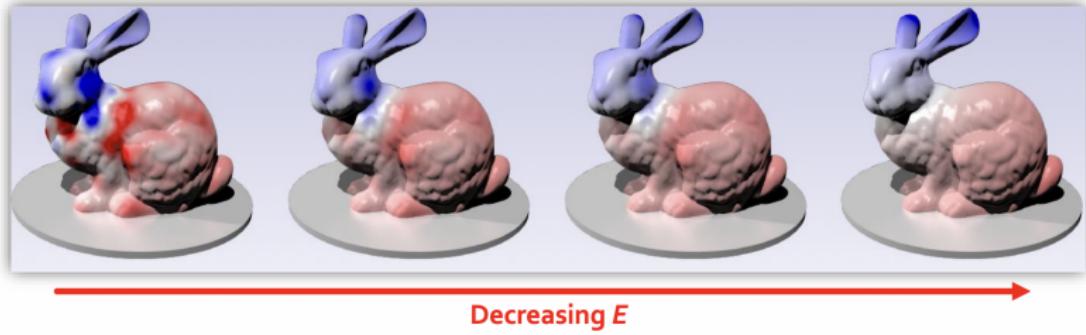
for any \mathbf{v} , thus \mathbf{x} is the gradient vector.

\mathbf{x} is unique. There is no other \mathbf{x} satisfying this condition. (*)

The Dirichlet Energy of a function $f : \mathcal{M} \rightarrow \mathbb{R}$:

$$E[f] := \int_S \|\nabla f\|_2^2 dA$$

where $A = \text{vol}(\mathbf{p})$. ³



³https://en.wikipedia.org/wiki/Volume_form

“Motivated” by finite-domain linear algebra, inner product of the gradients of f and g :

$$\begin{aligned}\langle f, g \rangle_{\Delta} &:= \int_S \nabla f(x) \nabla g(x) dA \\ &= \langle f, \Delta g \rangle = \langle \Delta f, g \rangle\end{aligned}$$

It implies that $\langle f, f \rangle \geq 0$

Relating it back to the graph ($G = (V, E)$) case, where D is the Differencing Operator:

$$\begin{aligned}(Df)^T(Dg) &= f^T D^T D g = f^T (D^T D) g = f^T L g \\ &= f^T (D^T D g) = f^T \Delta g\end{aligned}$$

Laplace-Beltrami Operator: Laplace Operator, associated to smooth manifolds.

Suppose \mathcal{M} has no boundary. Then, for each smooth function $f : \mathcal{M} \rightarrow \mathbb{R}$, there is a smooth function Δf so that for all smooth $g : \mathcal{M} \rightarrow \mathbb{R}$,

$$\begin{aligned}\langle f, g \rangle_{\Delta} &:= \int_{\mathcal{M}} \nabla f(\mathbf{p}) \nabla g(\mathbf{p}) d\text{vol}(\mathbf{p}) \\ &= \int_{\mathcal{M}} [\Delta f](\mathbf{p}) g(\mathbf{p}) d\text{vol}(\mathbf{p})\end{aligned}$$

Formal proof will need Riesz representation theorem. (*)
In the manifold case, $\Delta = -\nabla \cdot \nabla$ still holds.

Laplacian is the divergence of gradient.

$$\Delta = -\nabla \cdot \nabla$$

Now what we can do is to define the divergence (previously we had the gradient defined).

The divergence of a tangent vector field \mathbf{v} to a submanifold $\mathcal{M} \subseteq \mathbb{R}^n$ at point $\mathbf{p} \in \mathcal{M}$ is given by

$$\nabla \cdot \mathbf{v}(\mathbf{p}) := \sum_{k=1}^m \mathbf{e}_k \cdot d\mathbf{v}(\mathbf{e}_k)$$

where $\mathbf{e}_1, \dots, \mathbf{e}_m \in T_{\mathbf{p}}\mathcal{M}$ form an orthonormal basis.⁴

⁴Sometimes we write $\nabla \cdot \mathbf{v}(\mathbf{p})$ as $(\nabla \cdot \mathbf{v})_{\mathbf{p}}$.

Suppose that $n = 3$ and $m = 2$, we have:

$$\nabla \cdot \mathbf{v}(\mathbf{p}) := \sum_{i=1}^2 \mathbf{e}_i \cdot d\mathbf{v}(\mathbf{e}_i) = \sum_{i=1}^2 \langle \mathbf{e}_i, d\mathbf{v}(\mathbf{e}_i) \rangle_{\mathbf{p}}$$

Regarded as an extension of the **plane** case, which says:

$$\nabla \cdot \mathbf{v}(\mathbf{x}) := \sum_i \frac{\partial v^i(\mathbf{x})}{\partial x^i}$$

(*) Some other way of obtaining divergence: Flux Density backward definition. A more physical point of view — look at a ball on the manifold and look at a flux of a vector field out of it, relative to its volume.⁵

⁵<https://en.wikipedia.org/wiki/Flux>

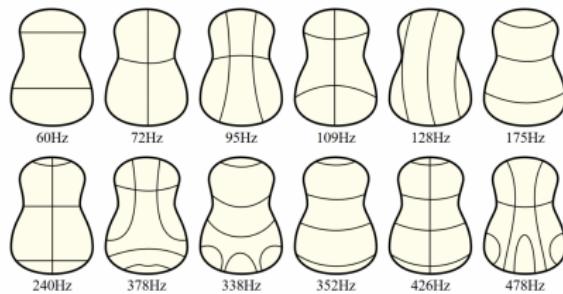
Eigenfunctions are still available.

$$\Delta\psi_i = \lambda_i\psi_i$$

But be careful: it represents the vibration mode of the **surface**, instead of the volume.

Theorem (Courant).

The n -th eigenfunction of the Dirichlet boundary value problem has at most n nodal domains.



The surface is wiggling up & down in response to the vibration frequencies (coming from the sound).



- ▶ In place where the eigenfunction is equal to 0, called “*nodal domains*”, the surface isn’t vibrating. The nodal domains happen to be the stationary points.

⁶<https://www.youtube.com/watch?v=CGiiS1MFF1I>

Example 2: Violin Back Plate Tuning ⁷

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A strategy used by violin makers for a long time.



- ▶ We need a sound post in the body of a violin. The body of the violin is expected to vibrate according to the sound made by the strings. The sound post brings vibration from one piece of wood to another.
- ▶ To avoid adding extra stress to the instrument, we find the nodal domains to place the sound post.

⁷<https://www.youtube.com/watch?v=3uMZZVvnSiU>

The Heat Equation:

$$\frac{\partial u}{\partial t} = -\Delta u$$

- ▶ Can be written in the form almost identical to the wave equation, but instead of the second derivative it uses the first derivative.

The Spherical Harmonics:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0$$

The Mean Curvature Flow compute Laplacian of xyz function:

$$\Delta x = Hx$$

- ▶ Intuition: Laplacian measures difference with neighbors.