The Laplacian

In the previous chapter we learned about smoothing operations by averaging or by using physical processes. Central to all of these operations was the second derivative of the function to be smoothed in the spatial dimension. In this chapter we will learn how to generalize this second derivative to two (and more) dimensions with an operator called the *Laplacian*.

For a completely rigorous mathematical explanation of all these topics (as well as for a definitive reference for all things Laplacian), I recommend the book by Evans [1], from which a lot of the theory in this chapter is taken.

Motivation

In the last chapter we looked at the diffusion and heat equations that model natural smoothing processes. Here we will go through, first, the Poisson equation, and then the heat equation from a theoretical view.

Poisson's equation

The Poisson equation has appears everywhere in physics. One such place is electrostatics.

Definition 1: Electric Field

> Given a charge distribution f in space $\mathbb{R}^3$, the electric field $\mathbf{E}$ of this charge distribution is given by Gauss's law,[1]
>
> $$\nabla \cdot \mathbf{E} = f\,, \tag{1}$$
>
> where $\nabla\,\cdot$ is the divergence operator.

Definition 2: Divergence

> The divergence operator is defined, in $\mathbb{R}^d$, as
>
> $$\nabla \cdot \mathbf{E} = \frac{\partial \mathbf{E}_1}{\partial x_1} + \ldots + \frac{\partial \mathbf{E}_d}{\partial x_d} \tag{2}$$

The *electric field* $\mathbf{E}$ is the force experienced by a unit charged particle from the charge distribution f. The *electric energy* u measures the work required to move that unit charge particle through the field $\mathbf{E}$. In electrostatics (where the electric and magnetic fields do not change over time), the amount of work requried is independent of the precise path, and only depends on the start (x_0) and end (x_1) points: $u(x_1) - u(x_0)$.

Definition 3: Electric Energy

> The electric energy is defined as
>
> $$\nabla u = -\mathbf{E}\,. \tag{3}$$

Combining Definition 1 and Definition 3, we get the equation for the electrostatic equation, the *Poisson equation*,

[1] Well, up to a constant, but we say that the constant is folded into the charge distribution f.

Definition 4: Electrostatic Poisson equation

The electrostatic Poisson equation is defined as

$$-\nabla \cdot \nabla u = f \,. \tag{4}$$

This object, $-\nabla \cdot \nabla$ is the Laplacian Δ, and we will rigorously define it in this class. The poisson equation is one way to generalize the second derivative from the smoothing applications to higher dimensions. The electric potential is another function that is smooth in nature, and that we can exploit to find smooth solutions to a variety of problems.

Heat equation

In the last chapter we introduced the one-dimensional heat equation, $\frac{\partial u}{\partial t} = \rho \frac{\partial^2 u}{\partial x^2}$. Heat distribution in $\mathbb{R}^d$ is modeled by the d-dimensional heat equation.

Definition 5: Heat equation

The heat equation in $\mathbb{R}^d$ is defined as

$$\frac{\partial u}{\partial t} = \rho \nabla \cdot \nabla u \,. \tag{5}$$

The heat equation in Definition 5 is not the same thing as the Poisson equation – it contains a time component as well as a space component. While the Poisson equation (4) finds the smoothest function for some scenario, the heat equation Definition 5 takes a function and smoothes it, bit by bit, over time. See Figure 1 for an overview of the difference.

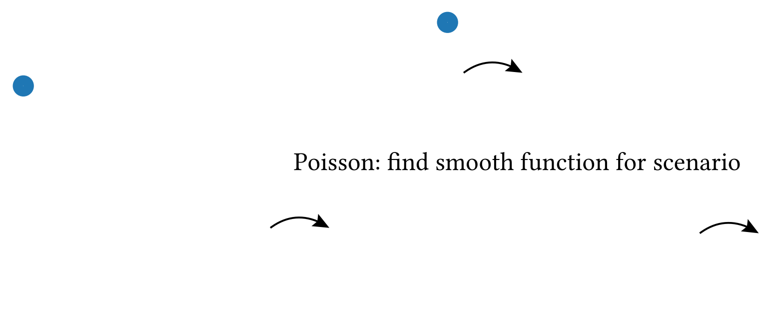

Figure 1: Solving a poisson equation to find the smoothest function in some scenario vs. solving a heat equation to smooth a function bit by bit.

Calculus background

The gradient, divergence, and Laplacian operators used in the previous section are easy enough to define in Euclidean space $\mathbb{R}^d$. But what do we do on a two-dimensional surface $\Omega \subseteq \mathbb{R}^3$?

Gradient

In Euclidean space $\mathbb{R}^d$, the gradient of a function $u : \mathbb{R}^d \to \mathbb{R}$ is defined as

$$\nabla u = \begin{pmatrix} \frac{\partial u}{\partial x_1} \\ \cdots \\ \frac{\partial u}{\partial x_d} \end{pmatrix} . \tag{6}$$

This does not work on surfaces, where we can't take partial derivatives as easily. If the surface is given by embedding, i.e., $\Omega = \varphi\left([0,1]^d\right)$, $\eta = \varphi^{-1}$, then we can define the gradients via chain rule.

Definition 6: Gradient via embedding

Let $u : \Omega \to \mathbb{R}$. Let there be a bijective function $\varphi : \mathbb{R}^d \to \Omega \subseteq \mathbb{R}^k$ such that $\Omega = \varphi\left([0,1]^d\right)$, $\eta = \varphi^{-1}$.

We define the Jacobian J_φ of φ as the matrix $J_\varphi = \begin{pmatrix} \frac{\partial \varphi_1}{\partial x_1} & \dots & \frac{\partial \varphi_1}{\partial x_d} \\ \dots & & \dots \\ \frac{\partial \varphi_k}{\partial x_1} & \dots & \frac{\partial \varphi_k}{\partial x_d} \end{pmatrix}$

We define $v = u \circ \varphi : \mathbb{R}^d \to \mathbb{R}$, i.e., $u = v \circ \eta$.

Then the gradient of u is

$$\nabla u(x) = J_{\varphi(x)} \nabla v(x). \tag{7}$$

We can make the computation from Definition 6 a little bit more concrete with the following example. Consider the spherical coordinates. There,

$$\varphi(\theta, \alpha) = \begin{pmatrix} \sin\theta\cos\alpha \\ \sin\theta\sin\alpha \\ \cos\theta \end{pmatrix}. \tag{8}$$

Thus, the Jacobian is

$$J_\varphi = \begin{pmatrix} \cos\theta\cos\alpha & -\sin\theta\sin\alpha \\ \cos\theta\sin\alpha & \sin\theta\cos\alpha \\ -\sin\theta & 0 \end{pmatrix}. \tag{9}$$

This means that the function $\theta(\theta - \pi)$ has the gradient

$$J_\varphi \nabla(\theta(\theta-\pi)) = \begin{pmatrix} \cos\theta\cos\alpha & -\sin\theta\sin\alpha \\ \cos\theta\sin\alpha & \sin\theta\cos\alpha \\ -\sin\theta & 0 \end{pmatrix} \begin{pmatrix} 2\theta - \pi \\ 0 \end{pmatrix} = (2\theta - \pi) \begin{pmatrix} \cos\theta\cos\alpha \\ \cos\theta\sin\alpha \\ -\sin\theta \end{pmatrix} \tag{10}$$

In practice, if the transformations φ, η are isometries, this will be much simpler. Our goal when computing gradients in practice will thus be to reduce everything to situations where φ and η are as simple as possible.

Another way to think of the gradient is to define it via extension:

Definition 7: Gradient via extension

Let $u : \Omega \to \mathbb{R}$. Let $\tilde{u} : \mathbb{R}^k \to \mathbb{R}$ such that the restriction to Ω is equal to u, i.e., $\tilde{u}|_\Omega = u$. We call $\tilde{u}$ an *extension* of u into Euclidean space.

Then we can define the gradient of u via orthogonal projection to Ω,

$$\nabla u(x) = \mathrm{P}_{\Omega,x} \nabla \tilde{u}(x), \tag{11}$$

where $\mathrm{P}_{\Omega,x}$ is the orthogonal projection of vectors onto the tangent plane of Ω at the point x.

Divergence

Again, as with the gradient, the divergence is easy to define in Euclidean space (Definition 2). But what about our curved surface Ω? Like with the gradient, we can define divergence via embedding or via extension.

Definition 8: Divergence via embedding

> Let $\boldsymbol{u} : \Omega \to \mathbb{R}^k$ be a tangent vector field to Ω. Let there be a bijective function $\varphi : \mathbb{R}^d \to \Omega \subseteq \mathbb{R}^k$ such that $\Omega = \varphi\left([0,1]^d\right)$, $\eta = \varphi^{-1}$.
>
> We define $\boldsymbol{v} = \boldsymbol{u} \circ \varphi : \mathbb{R}^d \to \mathbb{R}^k$, i.e., $\boldsymbol{u} = \boldsymbol{v} \circ \eta$.
>
> Then the divergence of u is
>
> $$\operatorname{trace}\left(J_\varphi J_{\boldsymbol{v}}^T\right) \tag{12}$$

Let's try this with our spherical coordinate example again. What is the divergence of $\begin{pmatrix} -\sin\alpha \\ \cos\alpha \\ 0 \end{pmatrix}$?

$$J_{\boldsymbol{v}} = \begin{pmatrix} 0 & -\cos\alpha \\ 0 & -\sin\alpha \\ 0 & 0 \end{pmatrix}. \tag{13}$$

So,

$$\begin{aligned} J_\varphi J_{\boldsymbol{v}}^T &= \begin{pmatrix} \cos\theta\cos\alpha & -\sin\theta\sin\alpha \\ \cos\theta\sin\alpha & \sin\theta\cos\alpha \\ -\sin\theta & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ -\cos\alpha & -\sin\alpha & 0 \end{pmatrix} \\ &= \begin{pmatrix} \sin\theta\sin\alpha\cos\alpha & \sin\theta\sin^2\alpha & 0 \\ -\sin\theta\cos^2\alpha & -\sin\theta\cos\alpha\sin\alpha & 0 \\ 0 & 0 & 0 \end{pmatrix}. \end{aligned} \tag{14}$$

The trace of this matrix is zero, so

$$\nabla \cdot \begin{pmatrix} -\sin\alpha \\ \cos\alpha \\ 0 \end{pmatrix} = 0\,. \tag{15}$$

Laplacian

You might have seen the Laplacian defined in Euclidean space $\mathbb{R}^d$ as the sum of second partial derivatives, like this:

$$\Delta u = -\frac{\partial^2 u}{\partial x_1^2} - \ldots - \frac{\partial^2 u}{\partial x_d^2}\,. \tag{16}$$

This does not work on surfaces for the same reason the gradient and the divergence did not work like this – there is no easy way to take these partial derivatives. Luckily, all the work we did for the gradient and the divergence pays off now, and there is a very simple way to define the Laplacian using these two operators.

Definition 9: Laplacian

> Let $u : \Omega \to \mathbb{R}$. The Laplacian of u is defined as[2]
>
> $$\Delta u = -\nabla \cdot \nabla u\,. \tag{17}$$

This was a lot of work, but we now have a firm grasp on the operator that is responsible for all the smoothing and denoising.

[2]Laplacian conventions vary. Some places (including the assignments) might define the Laplacian as minus what we are using here.

Boundary conditions

Is there a unique solution to the Poisson equation $\Delta u = f$? Even in only one dimension we know this is for sure not the case. Consider the simple example $f = 0$ and $u : [0,1] \to \mathbb{R}$. Then by simple antidifferentiation we know that u has the form

$$ax + b\,, \tag{18}$$

where a and b are two arbitrary scalars, and no matter what we set them to, $\Delta u = 0$.

What do we need to do in order to ensure that the Poisson equation is solvable? We will add boundary conditions to it.[3] Instead of merely asking ourselves the question "Which u solves $\Delta u = f$?", we will ask "Which u fulfilling this set of boundary conditions solves $\Delta u = f$?"

Dirichlet conditions

Dirichlet conditions are the boundary conditions where the value of the solution is given at the boundary.

Definition 10: Dirichlet conditions

Let $u : \Omega \to \mathbb{R}$.

Let $\partial\Omega$ be the boundary of Ω, and let $g : \partial\Omega \to \mathbb{R}$.

Dirichlet boundary conditions are when the solution to a PDE prescribes the value at the boundary:

$$u|_{\partial\Omega} = g\,, \qquad \text{i.e.,} \qquad u(x) = g(x) \quad \forall x \in \partial\Omega\,. \tag{19}$$

Solving a Poisson equation with Dirichlet boundary conditions means finding a solution to $\Delta u = f$ such that $u|_{\partial\Omega} = g$.

For our one-dimensional toy example $\Delta u = 0$ on the interval $[0,1]$ we can see that supplying two values at $x = 0$ and $x = 1$ will exactly eliminate a and b:

$$u(x) = (u(1) - u(0))x + u(0)\,. \tag{20}$$

Neumann conditions

Instead of supplying values, we can also supply the normal derivative at the boundary.

[3]There is more to the solvability of the Poisson equation than merely the boundary conditions. For example, the geometry of the boundary must also fulfill certain conditions. We will not go into this here, and just assume that the boundary geometry is always appropriate.

Definition 11: Neumann conditions

Let $u : \Omega \to \mathbb{R}$.

Let $\partial\Omega$ be the boundary of Ω, and let $g : \partial\Omega \to \mathbb{R}$.

Let $\boldsymbol{\nu}$ be the outward-pointing normal at the boundary. This is *not* the surface normal, it is the normal that points across the boundary curve of a surface (and is tangent to the surface).

Neumann boundary conditions are when the solution to a PDE prescribes the normal derivative at the boundary:

$$(\nabla u \cdot \boldsymbol{\nu})|_{\partial\Omega} = g\,, \qquad \text{i.e.,} \qquad \nabla u(x) \cdot \boldsymbol{\nu}(x) = g(x) \quad \forall x \in \partial\Omega\,. \tag{21}$$

Solving a Poisson equation with Neumann boundary conditions means finding a solution to $\Delta u = f$ such that $u|_{\partial\Omega} = g$ and such that $\int_\Omega u\,dx = 0$. This is not always possible: Neumann boundary conditions are only valid if the following compatibility condition holds:

$$\int_\Omega f\,dx = \int_{\partial\Omega} g\,dx\,. \tag{22}$$

Our 1D toy example also has a solution with Neumann boundary conditions. Let the normal derivative at 0 be -1, and the normal derivative at 1 be 1. Then every solution of the form $x + b$ fulfills the Neumann conditions as well as the Poisson equation. But only $x - \frac{1}{2}$ fulfills $\int_\Omega u\,dx = 0$, so that is the unique solution.

Mixed conditions

Dirichlet and Neumann conditions can be freely mixed with each other. It is not uncommon to see one part of the boundary subject to Dirichlet and another subject to Neumann conditions. If there is even a small part of the boundary that is subject to Dirichlet conditions, the compatibility conditions and the average integral condition for the Neumann boundary conditions become obsolete.

Weak formulation

You are probably used to look at PDEs and other equations in mathematics in the form $\Delta u(x) = f(x) \quad \forall x \in \Omega$. This is called the *strong form*: It is one equation for each point in the domain Ω. An alternate way to look at equations that is very popular in the theory of partial differential equations is the *weak form*. Instead of formulating the problem as

For every point in the domain, some equation should hold.

we demand that

For every test function, some equation should hold.

What is a test function? A test function is a function which we will multiply our equation by and then integrate. Let $v : \Omega \to \mathbb{R}$ be an arbitrary smooth (infinitely differentiable) function. Then, if u solves the Poisson equation, it must hold that

$$\int_\Omega \Delta u\, v\,dx = \int_\Omega f\, v\,dx\,, \tag{23}$$

where we multiplied both sides of the Poisson equation with v and integrated over the domain Ω. We no longer have an equation that holds for all points $x \in \Omega$ (we removed the dependence on x by integrating), but we now have an equation that must hold for all smooth *test functions* $v : \Omega \to \mathbb{R}$. It turns out that this is an almost equivalent way to phrase the Poisson equation, just instead of asking that something hold for all points, we ask that something hold for all functions.

One neat thing that you can not do with the strong form, but you can with the weak form, is transform the equation using integration by parts. Let's assume we have zero Neumann boundary conditions.[4] Then, by integration by parts.[5]

$$\int_\Omega \Delta u\, v\, dx = \int_\Omega -\nabla \cdot \nabla u\, v\, dx = -\int_{\partial\Omega} \boldsymbol{\nu} \cdot \nabla u\, v\, dx + \int_\Omega \nabla u \cdot \nabla v\, dx\,. \tag{24}$$

Applying the Neumann boundary condition, $\int_{\partial\Omega} \boldsymbol{\nu} \cdot \nabla u\, v\, dx = 0$.

This gives us the weak formulation for the Poisson problem:

Definition 12: Poisson equation (weak formulation)

> The weak formulation for the Poisson equation is as follows: Find a smooth function $u : \Omega \to \mathbb{R}$ such that
>
> $$\int_\Omega \nabla u \cdot \nabla v\, dx = \int_\Omega f\, v\, dx \qquad \forall \text{ smooth } v : \Omega \to \mathbb{R}\,. \tag{25}$$
>
> Boundary conditions / integral conditions / compatibility conditions apply, just like with the strong equation.

"Something to think about" 1: Strong vs. weak

> Is the weak formulation always equivalent to the strong formulation? Are strong solutions always weak solutions? Are weak solutions always strong solutions?

Why would people want to look at the weak formulation instead of the strong one? One reason is that while the strong formulation involves the Laplacian (a second-order operator with two derivatives), the weak formulation involves only the gradient (a first-order operator with one derivative). This makes many calculations easier, and even makes some calculations that are not possible at all with second-order operations possible (as we will see in the next chapter).

Energy formulation

We have seen the Poisson equation formulated as "for every point an equation must hold" as well as "for every test function an equation must hold". The third way the Poisson equation is often formulated is as an energy problem:

> Find a function that minimizes an energy.

For the Poisson equation, the energy that is minimized is called the *Dirichlet energy*.

[4] The same thing works for zero Dirichlet conditions, but then we must test with functions that also fulfill zero Dirichlet. If you want to use non-zero Dirichlet or non-zero Neumann, things become complicated.

[5] This is a well-known calculus trick that I have sneakily applied to gradient and divergence on the surface without proving you that this works. It works.

Definition 13: Dirichlet energy

The Dirichlet energy of a function $u : \Omega \to \mathbb{R}$ is

$$E(u) = \frac{1}{2} \int_\Omega \|\nabla u\|^2 \, dx \,. \tag{26}$$

Minimizing the Dirichlet energy E yields functions that solve the weak Poisson equation (25). We will show this with a quick variational calculation. Let $w : \Omega \to \mathbb{R}$ be an arbitrary smooth function. We now investigate $u + hw$, where $h > 0$ is some small scalar that we will take the limit of towards zero. This is the same thing as taking the partial derivative in the direction of w, just in the infinite dimensional space of smooth functions – for the partial derivative we consider the infinitesimal variation $\boldsymbol{x} + h(0 \ \ldots \ 0 \ 1 \ 0 \ \ldots \ 0)^T$.

$$E(u + hw) = \frac{1}{2} \int_\Omega \|\nabla u + h \nabla w\|^2 \, dx \,. \tag{27}$$

We now differentiate this expression with respect to h and evaluate it at $h = 0$ to get the derivative at u:

$$\frac{\partial}{\partial h} E(u + hw)|_{h=0} = \int_\Omega (\nabla u + h \nabla w) \cdot \nabla w \, dx|_{h=0} = \int_\Omega \nabla u \cdot \nabla w \, dx \,. \tag{28}$$

The functions that minimize the Dirichlet energy E will be its critical points, so they will have zero partial derivative in all directions w. This means that for every smooth $w : \Omega \to \mathbb{R}$, (28) must be 0:

$$\int_\Omega \nabla u \cdot \nabla w \, dx = 0 \,. \tag{29}$$

But this is exactly the weak formulation from Definition 12. Thus we can minimize the Dirichlet energy to find solutions to the Poisson equation.

Bibliography

[1] Lawrence C. Evans. 2010. *Partial Differential Equations* (2nd ed.). American Mathematical Society.