

9. THE GAUSSIAN AND THE HEAT EQUATION ON THE LINE

9.1. The Gaussian

A “Gaussian” function is any function of the form e^{-ax^2} – or any constant multiple of that. Such functions have a rich history within mathematics and appear in a wide variety of settings. Perhaps the most famous setting is as “the curve” – *i.e.*, the classic bell-shaped curve of probability theory, more properly known as the *normal distribution*. To be exact, the density of the standard normal distribution – that is, of a normal distribution of mean 0 and standard deviation 1 – is $\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$ and the density of a more general normal distribution of mean μ and standard deviation σ is $\frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$.*

We have several computational tasks before us. The first is to compute the integral of a Gaussian. Right away we have a problem. If we take as the “elementary” or “familiar” functions those functions we worked with in Calculus I and II – powers and roots, the six trigonometric functions and their respective inverses, exponentials and logarithms, and anything we can assemble out of these pieces in a finite number of additions, multiplications, divisions, and compositions – then there is nothing in this class of functions whose derivative is e^{-x^2} . Put more concisely, e^{-x^2} has no elementary antiderivative. All of the devices in a calculus book’s chapter on “Techniques of Integration” get us exactly nowhere with this function. Some might consider this a failure; I prefer to think of it as an opportunity to escape from the same old boring list of functions. We can define a function to be the antiderivative of a Gaussian. (This has been done, as the error function – look up “erf x ” some time.) We can print tables of values of such functions. (This has also been done, most often as the “cumulative probability distribution function” of the normal distribution, but also as erf x .) It would be a simple Calculus II exercise† to find a power series for the antiderivative of a Gaussian. Finally, although we can’t find a closed-form antiderivative for a Gaussian, we can compute its improper integral over the whole real line in closed form. You should have seen the following argument in Calculus III, but I can never pass up the opportunity to repeat it.

FACT:

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} \quad (9.1)$$

Derivation: we start by defining I to be the quantity we want to compute: $I = \int_{-\infty}^{\infty} e^{-x^2} dx$.

Compute the integral over the whole of \mathbb{R}^2 (the x - y plane) of the function $e^{-(x^2+y^2)}$:

$$\begin{aligned} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2+y^2)} dx dy &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-x^2} e^{-y^2} dx dy \\ &= \int_{-\infty}^{\infty} e^{-y^2} \left[\int_{-\infty}^{\infty} e^{-x^2} dx \right] dy = \left[\int_{-\infty}^{\infty} e^{-x^2} dx \right] \left[\int_{-\infty}^{\infty} e^{-y^2} dy \right] = I^2 \end{aligned}$$

Next, repeat the same calculation, only use polar coordinates this time:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2+y^2)} dx dy = \int_0^{\infty} \int_0^{2\pi} e^{-r^2} r d\theta dr$$

*We use the expression “exp(x)” as a synonym for “ e^x ” when writing everything in the exponent would look awkward on paper.

†“A simple Calculus II exercise” – someone will pay for that remark, and it won’t be the author! See the first exercise at the end of this section.

$$= \int_0^\infty 2\pi r e^{-r^2} dr = -\pi e^{-r^2} \Big|_0^\infty = \pi$$

Hence, $I^2 = \pi$, and so $I = \sqrt{\pi}$.

By making the change of variables $u = (\sqrt{a})x$, we can extend this computation as follows:

$$e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \quad (9.2)$$

Our next task is to compute the Fourier transform of a Gaussian. Our goal is the following:

THE FOURIER TRANSFORM OF THE GAUSSIAN			
If	$f(x) = e^{-\pi x^2}$	then	$\hat{f}(s) = e^{-\pi s^2}$ (9.3)
If	$f(x) = e^{-ax^2}$	then	$\hat{f}(s) = \sqrt{\frac{\pi}{a}} \exp\left(-\frac{\pi^2 s^2}{a}\right)$ (9.4)
If	$f(x) = \sqrt{\frac{\pi}{a}} \exp\left(-\frac{\pi^2 x^2}{a}\right)$	then	$\hat{f}(s) = e^{-as^2}$ (9.5)

There are at least three ways of making this calculation, each of which is revealing in its own way. The first involves what appears to be a simple change of variables, but is actually an appeal to Cauchy's theorem on complex line integrals. The second uses a differential equation and the properties of the Fourier transform from chapter 7. The third - perhaps my favorite - uses a one-dimension-two-dimension trick very like the way we calculated formula (9.2), but since we have not yet introduced the two-dimensional Fourier transform, we will concentrate on the first two methods.

FIRST METHOD – COMPLETING THE SQUARE:

$$\begin{aligned} \text{If } f(x) = e^{-ax^2}, \text{ then } \hat{f}(s) &= \int_{-\infty}^{\infty} f(x) e^{-2\pi i s x} dx = \int_{-\infty}^{\infty} e^{-ax^2} e^{-2\pi i s x} dx \\ &= \int_{-\infty}^{\infty} e^{-a(x^2 - \frac{2\pi i s}{a} x)} dx = \int_{-\infty}^{\infty} \exp\left[-a\left(x^2 - \frac{2\pi i s}{a} x - \frac{\pi^2 s^2}{a^2}\right) - a\left(\frac{\pi^2 s^2}{a^2}\right)\right] dx \\ &= \exp\left(-\frac{\pi^2 s^2}{a}\right) \int_{-\infty}^{\infty} \exp\left[-a\left(x^2 - \frac{2\pi i s}{a} x - \frac{\pi^2 s^2}{a^2}\right)\right] dx \\ &= \exp\left(-\frac{\pi^2 s^2}{a}\right) \int_{-\infty}^{\infty} \exp\left[-a\left(x - \frac{\pi i s}{a}\right)^2\right] dx \end{aligned}$$

It now seems that all we have to do is to make the “harmless” substitution $u = x - \frac{\pi i s}{a}$ in this integral to get (by the use of equation (9.1)) that:

$$\hat{f}(s) = \exp\left(-\frac{\pi^2 s^2}{a}\right) \int_{-\infty}^{\infty} e^{-au^2} du = \exp\left(-\frac{\pi^2 s^2}{a}\right) \sqrt{\frac{\pi}{a}} = \sqrt{\frac{\pi}{a}} \exp\left(-\frac{\pi^2 s^2}{a}\right)$$

But is this substitution really harmless? Does a calculus book's section on making changes of variable in integrals justify such a substitution that involves complex numbers? A calculus book has no such justification - but a complex variables book does! In fact, what this change does is to shift a complex line integral from the real axis (the line $z = x$) to a parallel horizontal line (the line

$z = x + \frac{\pi is}{a}$). The function we are integrating, $f(z) = \exp \left[-a \left(z - \frac{\pi is}{a} \right)^2 \right]$, is an entire function (that is, analytic on the entire complex plane), so Cauchy's Theorem tells us that its integral over any simple closed curve is zero. We apply this to the rectangle that goes from $-R$ to R to $R + \frac{\pi is}{a}$ to $-R + \frac{\pi is}{a}$ back to $-R$, then take the limit as $R \rightarrow \infty$. The contributions of the two small vertical ends of this rectangle to the overall integral tend rapidly to zero, since the function becomes very small for $|\operatorname{Re} z|$ large. Hence, in the limit, we have that the integrals on the two parallel horizontal lines are equal to each other – and that's all we need to justify this calculation.

SECOND METHOD - A DIFFERENTIAL EQUATION:

Let $y = e^{-ax^2}$. We can readily verify that y satisfies the differential equation

$$\frac{dy}{dx} + 2axy = 0$$

Take the Fourier transform of this differential equation. From equation (7.15)

$$\widehat{\frac{dy}{dx}} = 2\pi is \widehat{y}$$

From the formula (7.27), we also see that

$$(2axy)^\wedge = 2a \widehat{xy} = \frac{1}{\pi} ai \frac{d}{ds} \widehat{y}$$

Substituting these into the differential equation, we get

$$2\pi is \widehat{y} + \frac{1}{\pi} ai \frac{d}{ds} \widehat{y} = 0$$

Divide by $\frac{ai}{\pi}$ to get $\frac{d}{ds} \widehat{y} + \frac{2\pi^2 s}{a} \widehat{y} = 0$.

So \widehat{y} satisfies another differential equation – a first order linear ordinary differential equation, which can be solved by the usual technique of finding a multiplying factor. The general solution turns out to be:

$$\widehat{y} = C \exp \left(-\frac{\pi^2 s^2}{a} \right).$$

where C is an unknown constant. To discover a value for C , we would need an initial condition – but we do have just that. After all,

$$\widehat{y}(0) = \int_{-\infty}^{\infty} f(x) e^{-2\pi i 0 x} dx = \int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

Thus, $C = \sqrt{\frac{\pi}{a}}$ and $\widehat{y} = \sqrt{\frac{\pi}{a}} \exp \left(-\frac{\pi^2 s^2}{a} \right)$ *q.e.d.*

Equation (9.5) follows from (9.4) by making a simple substitution and then multiplying both sides of the equation by the appropriate expression. Equation (9.3) – the easiest one of the three to remember – is just the special case $a = \pi$.

Those of you with sufficiently suspicious minds might well be justified in asking, “If the Fourier transform – like the Laplace transform – is supposed to turn differential equations into algebraic

equations, then why, in this last example, did it turn a differential equation into a differential equation?" The truth is that any of these transforms – Fourier transform, Fourier series, or Laplace transform – perform their differential-equation-to-algebraic-equation magic only on *constant coefficient linear differential equations*. The equation we used, although linear, did not have constant coefficients.

So, if we stick to constant coefficient linear equations, the Fourier transform will turn a differential equation into an algebraic equation. What happens if we try it on a partial differential equation? Let's say we have a (constant coefficient linear) P.D.E. in two variables. That makes it a differential equation in each of two directions. If we take the Fourier transform in just one of those directions – and that had better be a direction in which we have the whole of $(-\infty, \infty)$ to stretch out in – then what we will get will be an equation which is an algebraic equation (in fact, a linear equation) in one of the variables and an ordinary differential equation in the other variable. Let's see how this works in practice.

9.2. The heat equation on the line

Suppose we have an infinitely long straight rod of some uniform material that has perfectly insulated sides, and let $u(x, t)$ be the temperature in the bar at position x and time t ; alternatively, suppose we have an infinitely long straight pipe containing a non-moving fluid into which a contaminant has been introduced, and let $u(x, t)$ be the concentration of that contaminant at position x and time t . In either case, heat will flow from hotter regions to colder regions and the contaminant will diffuse from regions of higher concentration to regions of lower concentration, so the dependence on t is genuine. We know the initial state – that is, we know that $u(x, 0) = f(x)$, the initial temperature or initial concentration – and we would like to be able to predict from this what the temperature or concentration will be from now on. To answer this, we must solve the *heat equation* (also known as the *diffusion equation*) for the infinite line:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \text{ for } -\infty < x < \infty, 0 < t < \infty; u(x, 0) = f(x) \quad (9.6)$$

To solve it, we act as if $u(x, t)$ were a function of x alone and take its Fourier transform as a function of x . The result is a function $\widehat{u}(s, t)$ which depends on the wavenumber s and the time t . We need to know what this Fourier transform will do to the sides of the differential equation. Formula (7.15) tells us that

$$\widehat{\frac{\partial^2 u}{\partial x^2}} = -4\pi^2 s^2 \widehat{u}$$

whereas a simple argument involving differentiating under the integral sign is enough to show that

$$\widehat{\frac{\partial u}{\partial t}} = \frac{\partial}{\partial t} \widehat{u}$$

and doing this when $t = 0$ leaves us with

$$\widehat{u}(s, 0) = \widehat{f}(s).$$

$$\text{Thus we have } \frac{\partial}{\partial t} \widehat{u} = -4\pi^2 s^2 \widehat{u}; \widehat{u}(s, 0) = \widehat{f}(s) \quad (9.7)$$

But this is an ordinary differential equation – in fact, that first and most important of all differential equations: the equation of exponential growth or decay. Its solution is

$$\widehat{u}(s, t) = \widehat{f}(s)e^{-4\pi^2 s^2 t} = \widehat{f}(s)e^{-4\pi^2 t s^2}. \quad (9.8)$$

We have found that the Fourier transform of the solution is the product of two functions. Equation (8.16) now tells us that the solution may be written as the convolution of two other functions. In fact, if $W_t(x)$ is the function such that $\widehat{W}_t(s) = e^{-4\pi^2 ts^2}$, then

$$u(x, t) = (f * W_t)(x) \quad (9.9)$$

Equation (9.5) identifies $W_t(x)$ for us:

$$W_t(x) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right) \quad (9.10)$$

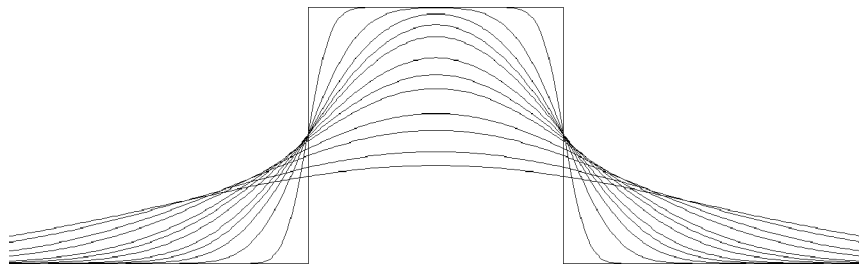
Using this, we can explicitly write out the convolution in (9.9) to get the Gauss-Weierstrass integral form of the solution to this differential equation:

$$\begin{aligned} u(x, t) &= \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} f(x - y) \exp\left(-\frac{y^2}{4t}\right) dy \\ &= \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} f(y) \exp\left(-\frac{(x - y)^2}{4t}\right) dy \end{aligned} \quad (9.11)$$

Of course, with the Gaussian being the way it is – a function without an elementary antiderivative – we know that we’re usually not going to be computing this integral in closed form. However, the existence of this explicit integral form gives us a wide range of numerical possibilities: we can use some direct means of numerical integration (e.g., Simpson’s rule) or we can use a power series, or we can look up values in a table of the normal distribution or of $\operatorname{erf} x$, or we can even use equation (9.8) together with an efficient algorithm for approximating Fourier transforms and inverse Fourier transforms. As an example, try numerically solving this problem for the following initial conditions:

$$u(x, 0) = f(x) = \begin{cases} 1 & \text{for } -1 \leq x \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

Plot (on the same set of axes) $f(x)$ and $u(x, t)$ as a function of x for the following (not necessarily evenly spaced) values of t : .01, .05, .1, .15, .2, .3, .4, .5, .75, 1.0, 1.5, and 2.0. We see the following graph:



(9.12)

An instructive contrast to this heat equation case is the case of Laplace’s equation for a half-plane. (The physical interpretations involve steady-state temperature or electrostatic potential or some such thing.) We would like to solve the following for $u(x, y)$:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \text{ for } -\infty < x < \infty, 0 < y < \infty; u(x, 0) = f(x) \quad (9.13)$$

subject to the condition that $u(x, y)$ remain bounded as $y \rightarrow \infty$, and assuming that $f(x)$ is an integrable function on $(-\infty, \infty)$ so that it has a Fourier transform.

As before, we take the Fourier transform with respect to x alone, getting the transformed function $\hat{u}(s, y)$. The differential equation transforms to:

$$-4\pi^2 s^2 \hat{u} + \frac{\partial^2 \hat{u}}{\partial y^2} = 0; \quad \hat{u}(s, 0) = \hat{f}(s).$$

This second order ordinary differential equation has for its solutions the following:

$$\hat{u}(s, y) = C_1 e^{2\pi s y} + C_2 e^{-2\pi s y}.$$

Now apply the condition that u – and hence also \hat{u} – remains bounded as $y \rightarrow \infty$. If $s > 0$, this means that $C_1 = 0$ and $C_2 = \hat{f}(s)$. If $s < 0$, this means that $C_1 = \hat{f}(s)$ and $C_2 = 0$. If $s = 0$, the details are different but the result is essentially the same. If we assemble these pieces, we get that

$$\hat{u}(s, y) = \hat{f}(s) e^{-2\pi |s| y} = \hat{f}(s) e^{-2\pi y |s|} \quad (9.14)$$

To finish the analogy to the heat equation example, we need a function $P_y(x)$ such that $\widehat{P_y}(s) = e^{-2\pi y |s|}$. From exercise 5.1, you know the answer: $P_y(x) = \frac{1}{\pi} \cdot \frac{y}{y^2 + x^2}$. The solution will be the convolution of the boundary conditions $f(x)$ with $P_y(x)$. That is, the solution is

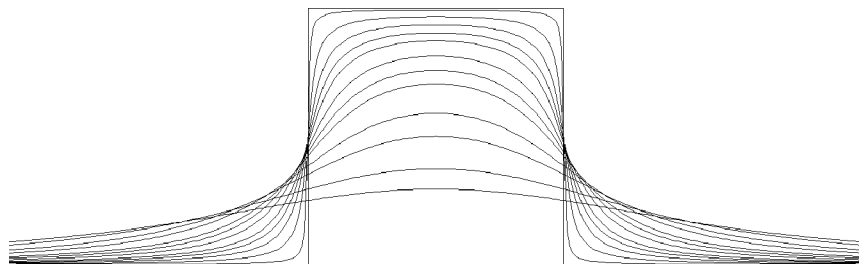
$$\begin{aligned} u(x, y) &= \frac{1}{\pi} \int_{-\infty}^{\infty} f(x-w) \frac{y}{y^2 + w^2} dw \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} f(w) \frac{y}{y^2 + (x-w)^2} dw \end{aligned} \quad (9.15)$$

Let's apply this to the same $f(x)$ that we used in the heat equation example, namely

$$u(x, 0) = f(x) = \begin{cases} 1 & \text{for } -1 \leq x \leq 1 \\ 0 & \text{otherwise} \end{cases}.$$

$$\text{Then } u(x, y) = \frac{1}{\pi} \int_{x-1}^{x+1} \frac{y}{y^2 + w^2} dw = \frac{1}{\pi} \left[\tan^{-1} \left(\frac{x+1}{y} \right) - \tan^{-1} \left(\frac{x-1}{y} \right) \right].$$

Figure 9.16 contains plots (on the same axes) of $f(x)$ and of $u(x, y)$ for the following values of y : .01, .05, .1, .15, .2, .3, .4, .5, .75, 1.0, 1.5, and 2.0. You should take careful note of the differences between this graph and figure 9.12. These differences reflect the different behaviors of the underlying differential equations.



(9.16)

9.3. Exercises

9.1. “A simple Calculus II exercise”:

- (a) Find a power series centered at 0 for $F(x) = \int e^{-x^2} dx$, subject to the initial condition $F(0) = 0$.
- (b) Use this power series to compute, accurate to 4 decimal places, $\int_0^1 e^{-x^2} dx$.

9.2. In this section of notes, we solved the heat equation on the infinite line:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \text{ for } -\infty < x < \infty, 0 < t < \infty; u(x, 0) = f(x)$$

To write the equation in exactly this form is to exercise the mathematician’s prerogative: “All physical constants are equal to 1.” If we admit that there are physical constants that stand for things like the heat conduction property of a particular material, then the equation should really be (for some such constant c):

$$\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2} \text{ for } -\infty < x < \infty, 0 < t < \infty; u(x, 0) = f(x)$$

Solve this version of the equation by the same techniques as in these notes.

9.3. Let $W(x, t)$ be the *Gauss-Weierstrass heat kernel* – that is, let $W(x, t)$ be the function we wrote as $W_t(x)$ in equation (9.10):

$$W(x, t) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right)$$

- (a) Verify directly that $W(x, t)$ satisfies the heat equation itself.
- (b) Show that for all $t > 0$, $\int_{-\infty}^{\infty} W(x, t) dx = 1$.
- (c) For any fixed $x \neq 0$, compute $\lim_{t \rightarrow 0^+} W(x, t)$.
- (d) Compute $\lim_{t \rightarrow 0^+} W(0, t)$.
- (e) Is the following a fair thing to say? “ $W(x, t)$ is the solution to the heat equation when the initial conditions are the Dirac delta (unit impulse) located at the origin.” (There’s no right answer to this now; we’ll know more later in the course.)