

Partial differential equations

Sol'n's are functions of more than one variable

Example: $\frac{\partial}{\partial t} f(x,t) = D \frac{\partial^2}{\partial x^2} f(x,t)$ "Heat" / "Diffusion" equation

[Shorthand notation: $\dot{f} = Df''$]

Always try "separation of variables":

guess: $f(x,t) = X(x)T(t)$

Substitute:

$$\frac{X \dot{T}}{D X T} = \frac{D T X''}{D T X}$$

$$\frac{\dot{T}}{D T} = \frac{X''}{X} = -k^2$$

constant,
units
distance⁻²

only depends
on t

only depends
on x

2nd order ODE:

$$X'' = -k^2 X$$

$$X(x) = B(k)e^{ikx} \quad (-\infty < k < \infty)$$

1st order ODE

$$\dot{T} = -Dk^2 T$$

$$T(t) = C(k)e^{-Dk^2 t}$$

general sol'n:

$$f(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{-Dk^2 t} e^{ikx} dk$$

Initial conditions:

$$f(x, t=0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk$$

But how to determine $A(k)$ from $f(x,t=0)$??

Application of Initial Conditions: "Fourier Transform"

Change of basis in an orthonormal function space

Analogy with Euclidean vector space:

Vectors: $\vec{F} = \sum_i A_i \vec{V}_i$ (\vec{V}_i 's are "orthonormal basis vectors")

(2D) example: $\vec{F} = 2\hat{x} + 3\hat{y}$

The diagram shows a 2D coordinate system with a horizontal x-axis and a vertical y-axis. The x-axis is labeled \vec{V}_1 and the y-axis is labeled \vec{V}_2 . A vector \vec{F} is drawn in the first quadrant. It is decomposed into two components: $2\hat{x}$ along the x-axis and $3\hat{y}$ along the y-axis. Arrows point from the coefficient '2' to the unit vector \hat{x} and from the coefficient '3' to the unit vector \hat{y} .

Functions: $F(x) = \int_{-\infty}^{\infty} A(k) u_k(x) dk$

($u_k(x)$'s are "orthonormal basis functions")

($u_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}}$ for Fourier Transform)

Determine Coefficients

Vectors $\vec{F} = \sum_i A_i \vec{v}_i$

"inner product": $\vec{v}_j \cdot \vec{F} = \vec{v}_j \cdot \sum_i A_i \vec{v}_i = \sum_i A_i (\vec{v}_j \cdot \vec{v}_i)$

$$= \sum_i A_i \delta_{ij} \leftarrow \text{"Kronecker delta"} = 0 \quad i \neq j$$
$$= 1 \quad i = j$$
$$= A_j$$
$$\Rightarrow A_i = \vec{v}_i \cdot \vec{F}$$

Example: $A_1 = \vec{v}_1 \cdot \vec{F} = \hat{x} \cdot (2\hat{x} + 3\hat{y}) = 2(\hat{x} \cdot \hat{x}) + 3(\hat{x} \cdot \hat{y}) = 2$

We can also find coefficients in a different basis! for example, if $\vec{v}_1 = \frac{\hat{x} + \hat{y}}{\sqrt{2}}$, $\vec{v}_2 = \frac{\hat{x} - \hat{y}}{\sqrt{2}}$, then in this basis,

$$A_1 = \vec{v}_1 \cdot \vec{F} = \left(\frac{\hat{x} + \hat{y}}{\sqrt{2}} \right) \cdot (2\hat{x} + 3\hat{y}) = \frac{5}{\sqrt{2}}, \quad A_2 = \vec{v}_2 \cdot \vec{F} = \left(\frac{\hat{x} - \hat{y}}{\sqrt{2}} \right) \cdot (2\hat{x} + 3\hat{y}) = -\frac{1}{\sqrt{2}}$$

Determine Coefficients

functions $F(x) = \int_{-\infty}^{\infty} A(k) u_k(x) dk$

take inner product w/ another basis function:

$$\int_{-\infty}^{+\infty} u_{k'}^*(x) F(x) dx = \int_{-\infty}^{+\infty} u_{k'}^*(x) \left[\int_{-\infty}^{\infty} A(k) u_k(x) dk \right] dx$$

$$= \int_{-\infty}^{\infty} A(k) \left[\int_{-\infty}^{\infty} u_{k'}^*(x) u_k(x) dx \right] dk$$

$$= \int_{-\infty}^{\infty} A(k) \delta(k-k') dk$$

$$= A(k')$$

"Dirac delta f_n ":
 $\delta(k-k') = 0 \quad k \neq k'$
But $\int_{-\infty}^{\infty} \delta(k-k') dk = 1$

$$\Rightarrow A(k) = \int_{-\infty}^{\infty} u_k^*(x) F(x) dx$$

"Fourier transform" of $F(x)$

This formula now allows us to solve our P.D.E., given initial conditions!

Diffusion Equation, revisited

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}$$

solution: use F.T.

$$f(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k, t) e^{ikx} dk$$

$$\int_{-\infty}^{\infty} \frac{e^{-ik'x}}{\sqrt{2\pi}} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k, t) e^{ikx} dk \right] dx = \int_{-\infty}^{\infty} \frac{e^{-ik'x}}{\sqrt{2\pi}} \left[-D \int_{-\infty}^{\infty} k^2 \tilde{f}(k, t) e^{ikx} dk \right] dx$$

$$\int_{-\infty}^{\infty} \tilde{f}(k, t) \left[\int_{-\infty}^{\infty} \frac{e^{-ik'x}}{\sqrt{2\pi}} \frac{e^{ikx}}{\sqrt{2\pi}} dx \right] dk = -D \int_{-\infty}^{\infty} k^2 \tilde{f}(k, t) \left[\int_{-\infty}^{\infty} \frac{e^{-ik'x}}{\sqrt{2\pi}} \frac{e^{ikx}}{\sqrt{2\pi}} dx \right] dk$$

$$\int_{-\infty}^{\infty} \tilde{f}(k, t) \delta(k-k') dk = -D \int_{-\infty}^{\infty} k^2 \tilde{f}(k, t) \delta(k-k') dk$$

$$\tilde{f}(k', t) = -D k'^2 \tilde{f}(k', t)$$

an O.D.E we know how to solve!

$$\tilde{f}(k, t) = A(k) e^{-Dk^2 t}$$

Then,

$$f(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{-Dk^2 t} e^{ikx} dk$$

same as solution by separation of variables!

Closed-form solution of Diffusion Eqn

$$f(x, t=0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk \quad \begin{array}{c} \text{Fourier} \\ \longleftrightarrow \\ \text{Transform} \end{array} \quad A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x, t=0) e^{-ikx} dx$$

Example: $f(x, t=0) = \delta(x)$ "impulse" initial conditions

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}}$$

So,

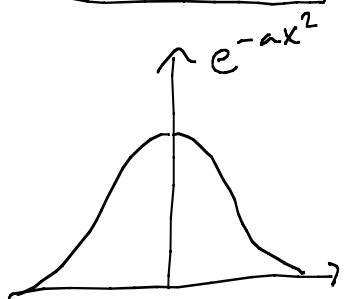
$$f(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{-Dk^2 t} e^{ikx} dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-Dk^2 t} e^{ikx} dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-D+(k^2 - \frac{ikx}{Dt})} dk$$

"Complete the square": $= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-D+(k - \frac{ix}{2Dt})^2} e^{-\frac{x^2}{4Dt}} dk$

$$= \frac{1}{2\pi} e^{-\frac{x^2}{4Dt}} \int_{-\infty}^{\infty} e^{-D+(k - \frac{ix}{2Dt})^2} dk$$

transform variables $y = \sqrt{Dt} \left(k - \frac{ix}{2Dt} \right)$, $dk = \frac{dy}{\sqrt{Dt}}$: $= \frac{1}{2\pi} e^{-\frac{x^2}{4Dt}} \left[\int_{-\infty}^{\infty} e^{-y^2} dy \right] \frac{1}{\sqrt{Dt}}$ $\sqrt{\pi}$ (see next page)

Integrating the Gaussian



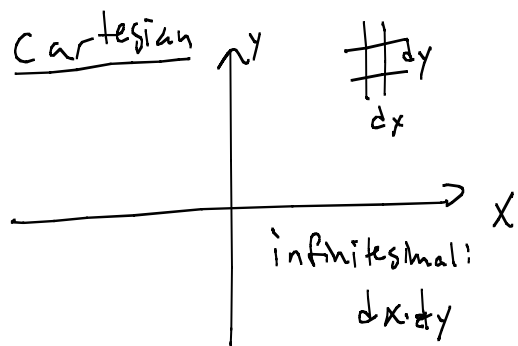
$$I_1 = \int_{-\infty}^{\infty} e^{-ax^2} dx$$

How to do this integral?

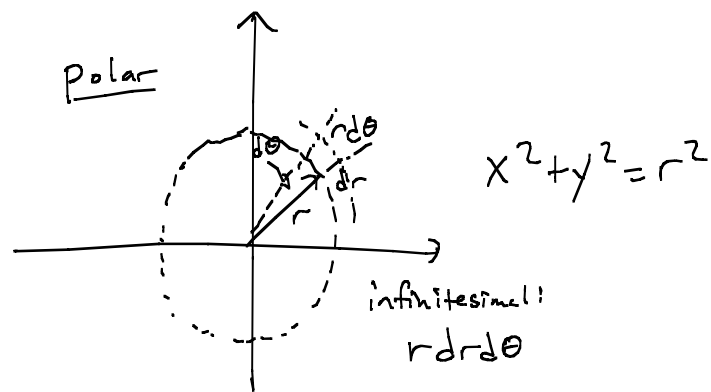
$$I_2 = \int_{-\infty}^{\infty} e^{-ay^2} dy$$

Note this is the same, so $I_1 = \sqrt{I_1 \cdot I_2}$

$$I_1 \cdot I_2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-ax^2} e^{-ay^2} dx dy = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-a(x^2+y^2)} dx dy$$



Coordinate transformation



$$I_1 \cdot I_2 = \int_0^{2\pi} \int_0^{\infty} e^{-ar^2} r dr d\theta = 2\pi \int_0^{\infty} r e^{-ar^2} dr = 2\pi \left. \frac{e^{-ar^2}}{-2a} \right|_0^{\infty} = \frac{\pi}{a}$$

So $I_1 = \sqrt{\frac{\pi}{a}}$. Note this can be used to normalize: $\int_{-\infty}^{\infty} \sqrt{\frac{a}{\pi}} e^{-ax^2} dx = 1$

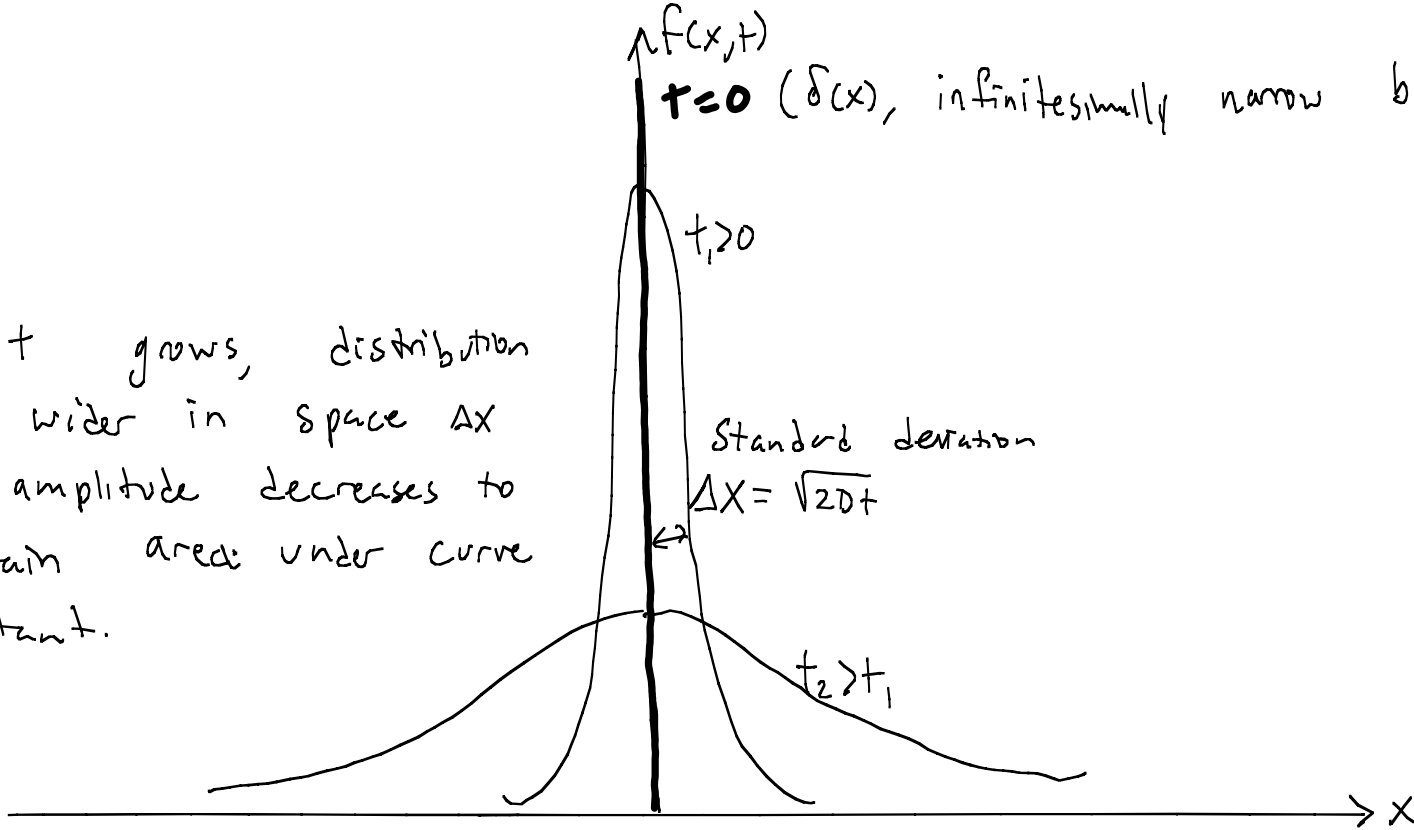
Solution to Diffusion Eqn w/ impulse initial conditions

$$f(x,t) = \frac{1}{\sqrt{2\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

Normalized "Gaussian" in x

$t=0$ ($\delta(x)$, infinitesimally narrow but $\int_{-\infty}^{\infty} f(x) dx = 1$)

As t grows, distribution gets wider in space Δx and amplitude decreases to maintain area under curve constant.



In general, normalized gaussian has form $f(x) = \frac{1}{\Delta x \sqrt{2\pi}} e^{-\frac{x^2}{2\Delta x^2}}$ such that $\Delta x = \sqrt{\Delta x^2} = \sqrt{\int_{-\infty}^{\infty} (x - \langle x \rangle)^2 f(x) dx}$ (note that $\langle x \rangle = 0$)