Solving partial differential equations with neural networks

FYS-STK4155: Project 3

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github.com/mortele/FYS-STK4155

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Abstract

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I. INTRODUCTION

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II. THEORY

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A. The heat equation

The heat equation is a partial differential equation (in space x and time t) which describes the evolution of temperature differences in a region of space over a time interval. It is based on *Fourier's law*; the rate of heat flow through a surface is proportional to the temperature gradient across the surface, i.e.

$$\mathbf{q} = -k\nabla T = -k\frac{\partial T}{\partial x}, \tag{1}$$

where $\mathbf{q}$ denotes the heat flux density, k is the thermal conductivity of the surface material, and T represents the temperature. Changes in temperature are proportional to changes in internal energy, with the proportionality constant being the specific heat capacity c_p. With the arbitrary energy zero point placed at absolute zero, this can be written as

$$Q = c_p\rho T, \tag{2}$$

with Q being the internal energy and ρ denoting the mass density. This is essentially just a restatement of (a shifted) *first law of thermodynamics*, in the absence of applied work. The total heat energy contained in a region $[a, b]$ is given by the integral

$$\int_a^b \mathrm{d}x\, c_p\rho T(x,t). \tag{3}$$

Integrating over a small region of space and considering the change in internal energy over a short time interval (assuming c_p and ρ are both time-independent and spatially homogenous) gives

$$\begin{aligned}\Delta Q =& c_p\rho \int_x^{x+\Delta x} \mathrm{d}\chi \left[T(\chi, t+\Delta t) - T(\chi, t)\right] \\ =& c_p\rho \int_x^{x+\Delta x} \mathrm{d}\chi \int_t^{t+\Delta t} \mathrm{d}\tau\, \frac{\partial T}{\partial \tau}.\end{aligned} \tag{4}$$

Over a short time period Δt, the change in internal energy of a short segment of length Δx must be entirely due to the heat flux in/out of the boundaries,

$$\begin{aligned}\Delta Q &= k\int_t^{t+\Delta t} \mathrm{d}\tau \left[\frac{\partial T(x+\Delta x, \tau)}{\partial x} - \frac{\partial T(x,\tau)}{\partial x}\right] \\ &= k\int_t^{t+\Delta t} \mathrm{d}\tau \int_x^{x+\Delta x} \mathrm{d}\chi\, \frac{\partial^2 T}{\partial \chi^2}.\end{aligned} \tag{5}$$

By conservation of energy, the difference between Eq. (4) and Eq. (5) must obviously vanish. Since we are integrating over the same spatial and temporal regions in both equations, this means that the integrand must vanish identically:

$$\frac{k}{c_p\rho}\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t}. \tag{6}$$

This is known as the *heat equation* and is a special case of the more general diffusion equation.

B. Closed form solution

The 1D heat equation may be solved by applying a separation of variables ansatz, i.e. we assume the solution $u(x,t)$ takes the form

$$u(x,t) = X(x)T(t), \tag{7}$$

with $X(x)$ carrying all the x-dependence, and $T(t)$ carrying the corresponding time dependence. Introducing the compact notation

$$u_x \equiv \partial_x u = \frac{\partial u}{\partial x}, \quad \text{and} \quad u_t \equiv \partial_t u = \frac{\partial u}{\partial t}, \tag{8}$$

we find by insertion of the ansatz into Eq. (6):

$$\begin{aligned}
\alpha^2\, u_{xx} &= u_t \\
\alpha^2\, \partial_x \Big[\partial_x X(x) T(t)\Big] &= \partial_t X(x) T(t) \\
\alpha^2\, \partial_x \Big[X_x T + X T_x\Big] &= X_t T + X T_t \\
\alpha^2 \Big[X_{xx} T + 2 X_x T_x + X T_{xx}\Big] &= X T_t \\
\frac{1}{X(x)} \frac{\partial^2 X(x)}{\partial x^2} &= \frac{1}{\alpha^2\, T(t)} \frac{\partial T(t)}{\partial t},
\end{aligned} \tag{9}$$

where we defined $\alpha^2 \equiv k/c_p\rho$ and used the fact that $X_t = T_x = 0$. As the left hand side is independent of t and the right hand side is independent of x, the equality can only be achieved if both sides are constant. This reduces the original partial differential equation into a set of two ordinary differential equations

$$\frac{1}{X(x)} \frac{\partial^2 X(x)}{\partial x^2} = k \tag{10}$$

$$\frac{1}{\alpha^2\, T(t)} \frac{\partial T(t)}{\partial t} = k, \tag{11}$$

with k an undetermined constant.

Depending on the value of k, the spatial part has solutions $X(x) = Ax + B$ (if $k = 0$), $X(x) = A\mathrm{e}^{\mu x} + B\mathrm{e}^{-\mu x}$ (if $k = \mu^2 > 0$), or $X(x) = A\mathrm{e}^{\mathrm{i}\mu x} + B\mathrm{e}^{-\mathrm{i}\mu x}$ (if $k = -\mu^2 < 0$). The temporal equation has solutions $T(t) = C$ (if $k = 0$), or $T(t) = C\mathrm{e}^{\alpha^2\mu^2 x}$ (otherwise).

Applying the boundary conditons

In order to make progress, we need to apply the specific boundary and initial conditions. In our case, the boundaries at $x = 0$ and $x = L = 1$ vanish, and the initial spatial solution takes the form $u(x, t = 0) = \sin \pi x$. If the k constant of Eq. (10) vanishes, then both constants A and B vanish due to the boundary conditions. The same is true if $k = \mu^2 > 0$. It follows that the only non-trivial solutions arise when $k = -\mu^2 < 0$, in which case we find (left boundary)

$$X(0) = A \cos \mu x + B \sin \mu x = 0 \Rightarrow A = 0$$

and (right boundary)

$$X(1) = B \sin \mu x = 0 \Rightarrow \mu = \pi n.$$

This gives rise to an infinite set of equations—one for each n—which determine the Fourier coefficients of the initial condition $u(x, t = 0)$:

$$u(x, t = 0) = \sum_{n=1}^{\infty} B_n \sin(n\pi x), \tag{12}$$

with

$$B_n = 2 \int_0^1 \mathrm{d}x\, u(x, t = 0)\, \sin(n\pi x). \tag{13}$$

The temporal equation, Eq. (11), can now be solved only applying the boundary conditions. With the value of μ fixed at $\mu = n\pi$, we obtain

$$T(t) = \mathrm{e}^{-n^2\pi^2\alpha^2 t}. \tag{14}$$

Applying the initial condition

Combining the $X(x)$ and $T(t)$ solutions we obtain a series representation of the solution in terms of the Fourier coefficients of the initial condition $u(x, t = 0)$, in which the higher frequency modes of the initial solution decays more rapidly than the corresponding lower frequency modes,

$$u(x, t) = \sum_{n=1}^{\infty} B_n \sin(n\pi x)\, \mathrm{e}^{-n^2\pi^2\alpha^2 t}. \tag{15}$$

It is easy to see that the steady-state solution is achieved when $u(x, t) = 0$, since both boundaries (left and right) act as sinks for the initial heat energy contained in the system, and no heat is ever *added.* In our case, the initial condition makes the general solution Eq. (15) take on a very simple form. Applying $u(x, t = 0) = \sin \pi x$, it is trivial to evaluate

$$B_n = 2 \int_0^1 \mathrm{d}x\, \sin(\pi x)\, \sin(n\pi x) = \delta_{1n}, \tag{16}$$

due to the orthogonality of $\sin(n\pi x)$ and $\sin(m\pi x)$. This means $B_1 = 1$ and $B_2, B_3, \cdots = 0$, and the full solution to Eq. (6) is given by

$$u(x, t) = \sin(\pi x)\, \mathrm{e}^{-\pi^2\alpha^2 t}. \tag{17}$$

III. FINITE DIFFERENCE METHOD

The most straightforward way to solve Eq. (6) numerically is through *finite difference methods*, i.e. discretizing time and space on a grid and Taylor expanding the solution to obtain algebraic equation sets. A multitude of different strategies and schemes exists, but we will consider the *explicit forward Euler* scheme.

The spatial region $[0, L]$ is discretized by splitting it into N segments, and considering only the functional values on the points $x_i = i\Delta x$ with $i \in [0, N-1]$. We denote a function $f(x,t)$ evaluated at x_i (and at time t) by $f_i^t = f(x_i, t)$. Considering N spatial points gives a step size Δx between each point of

$$\Delta x = \frac{L}{N-1}. \tag{18}$$

In addition, we introduce a discretization in the temporal dimension with step size Δt.

Let us consider the Taylor expansion of a function $f(x,t)$ considered at fixed t, $f(x;t)$, around a spatial point x. We use the shorthand $h \equiv (x-a)$, and consider the expansion at a point $a \neq x$. The expansions of $f(x+h;t)$ and $f(x-h;t)$ are given by,

$$f(x+h) \approx f(x) + hf'(x) + h^2 f''(x), \tag{19}$$

$$f(x-h) \approx f(x) - hf'(x) + h^2 f''(x), \tag{20}$$

respectively. As t is considered a fixed parameter for the moment, we supressed the second functional argument for notational brevity. The shorthand $f'(x)$ is here used to denote differentiation w.r.t. x. Note that both equations hold with equality if an overall error term proportional to h^3 is added on the right hand side, i.e. $\mathcal{O}(h^3)$. Adding Eqs. (19) and (20) and dividing through by h^2 yields

$$\begin{aligned} f(x+h) + f(x-h) &= 2f(x) + h^2 f''(x) + \mathcal{O}(h^4) \\ f''(x) &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2), \end{aligned} \tag{21}$$

which is the three-point central difference approximation to the second derivative. Note that the resulting error is proportional to h^2 because the third order contributions from Eqs. (19) and (20)—$h^3 f'''(x+h)$ and $-h^3 f'''(x+h)$—cancel exactly. A corresponding temporal first order derivative approximation may be found by simply considering Eq. (19), and considering h to be a small temporal step, x to be a fixed parameter, and varying t. This gives

$$f'(t) = \frac{f(t+h) - f(t)}{h} + \mathcal{O}(h), \tag{22}$$

where the error term is proportional to h^2 when disregarding the last term on the right hand side of Eq. (19), which gives $\mathcal{O}(h)$ after dividing through by h.

Let us now consider Eq. (21) on the previously defined grid, and take $h = \Delta x$. In the Eq. (22) case, we define $h = \Delta t$, and equate $\alpha^2 f''(x)$ with $f'(t)$ as in the heat equation Eq. (6). The result can be solved for $f(x, t+\Delta t)$, i.e. the *next* time step given that the previous step is known:

$$\begin{aligned} \frac{f_i^{j+1} - f_i^j}{\Delta t} &= \alpha^2 \frac{f_{i+1}^j - 2f_i^j + f_{i-1}^j}{\Delta x^2} \\ f_i^{j+1} &= f_i^j + \beta\Big[f_{i+1}^j - 2f_i^j + f_{i-1}^j\Big], \end{aligned} \tag{23}$$

where f_i^j denotes the discretized $f(x_i, t_j)$ and

$$\beta \equiv \alpha^2 \left(\frac{\Delta t}{\Delta x^2}\right). \tag{24}$$

Equation (23) is known as the *explicit Euler* scheme, and can be solved directly for $f(x, t+\Delta t)$ since the right hand side is all known at time step t.

C. Solving differential equations with neural networks

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IV. RESULTS AND DISCUSSION

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V. CONCLUSION

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