Boundary Conditions, Differential Equations & Neural Forms

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Abstract

In the framework of Neural Networks (NNs), Differential Equations (DEs) with Dirichlet boundary conditions (BCs), are easier to treat in comparison to those with prescribed Neumann BCs. In this text we show how to transform the problem of a second order linear DE with one Dirichlet and one Neumann BC, to a problem with two Dirichlet BCs.

1 Problem description in the Neural Form setting

Let $\mathcal{L}$ be a linear second order differential operator, and $f(x)$ a known function. We want to transform the problem:

$$\mathcal{L}\psi(x) = f(x), \text{ with } x \in [a, b], \text{ s.t.: } \psi(a) = \psi_a, \frac{d\psi(b)}{dx} = \psi'_b \tag{1}$$

to a problem with two Dirichlet type of conditions, namely:

$$\mathcal{L}\psi(x) = f(x), \text{ with } x \in [a, b], \text{ s.t.: } \psi(a) = \psi_a, \psi(b) = \psi_b \tag{2}$$

A trial solution for the problem in eq. (2) may be written as:

$$\Psi_T(x, w) = \psi_a \frac{b - x}{b - a} + \psi_b \frac{x - a}{b - a} + (x - a)(x - b)N(x, w) \tag{3}$$

where $N(x, w)$ is a NN with weights w. The derivative of the trial solution is given as:

$$\frac{d\Psi_T(x, w)}{dx} = \frac{\psi_b - \psi_a}{b - a} + (2x - a - b)N(x, w) + (x - a)(x - b)\frac{dN(x, w)}{dx} \tag{4}$$

and at $x = b$, $\psi'_b = \dfrac{d\Psi_T(b, w)}{dx} = \dfrac{\psi_b - \psi_a}{b - a} + (b - a)N(b, w)$ and from this:

$$\psi_b = \psi_a + (b - a)\psi'_b - (b - a)^2 N(b, w) \tag{5}$$

leading to the following trial solution:

$$\Psi_T(x, w) = \psi_a + \psi'_b(x - a) - (b - a)(x - a)N(b, w) + (x - a)(x - b)N(x, w) \tag{6}$$

2 A simple illustrative example

We considered the ODE:

$$\frac{d^2\psi(x)}{dx^2} + x^2\psi(x) = (1+x^2)e^x, \;\; x \in [0,1] \tag{7}$$
$$\psi(0) = 1, \quad \text{and} \quad \frac{d\psi(x)}{dx}\Big|_{x=1} = e$$

The analytic (exact) solution is $\psi(x) = e^x$. Using eq. (6) one obtains:

$$\Psi_T(x, w) = 1 + ex - xN(1, w) + x(x-1)N(x, w) \tag{8}$$

Using a single hidden layer sigmoid perceptron with six nodes, i.e.:

$$N(x, w) = \sum_{i=1}^{6} w_{3i-2}\sigma(w_{3i-1}x + w_{3i}) \tag{9}$$

we have obtained a MSE for the equation residuals of $E(w^*) \approx 7.14 \times 10^{-20}$ and a maximum deviation from the exact solution: $\max_x |\Psi_T(x, w^*) - e^x| \approx 10^{-11}$. The grid consisted of 50 equidistant points in $[0, 1]$. The numerical values found for the optimal weights $\{w^*\}$, are listed below.

$w^*_{1\to3}$	0.146015806075384	2.012287065216300	-4.23664769775313
$w^*_{4\to6}$	0.912548971565254	1.102611308747920	-2.61861750144132
$w^*_{7\to9}$	0.241302113163382	3.147846842902310	-7.75931239686514
$w^*_{10\to12}$	0.933256798350501	0.615693699319356	-1.05493916158718
$w^*_{13\to15}$	0.911365237108423	0.177242748720129	-0.187659063306668
$w^*_{16\to18}$	0.331005021852551	-0.766858074110213	-94.8027539978478

The MSE of the residuals is given by (with $M = 50$ in our example):

$$E(w) = \tfrac{1}{M}\sum_{i=1}^{M}\left(\Psi''_T(x_i, w) + x_i^2\Psi_T(x_i, w) - (1 + x_i^2)e^{x_i}\right)^2 \tag{10}$$

3 Neumann BCs at both ends

In this case let the trial solution be written as:

$$\Psi_T(x, w) = \psi_a\frac{(x-b)^2}{(b-a)^2} + \psi_b\frac{(x-a)^2}{(b-a)^2} + (x-a)(x-b)N(x, w) \tag{11}$$

$$\begin{aligned}\frac{d\Psi_T(x, w)}{dx} &= \psi_a\frac{2(x-b)}{(b-a)^2} + \psi_b\frac{2(x-a)}{(b-a)^2} + \\ &+ (2x - a - b)N(x, w) + (x-a)(x-b)\frac{dN(x, w)}{dx}\end{aligned} \tag{12}$$

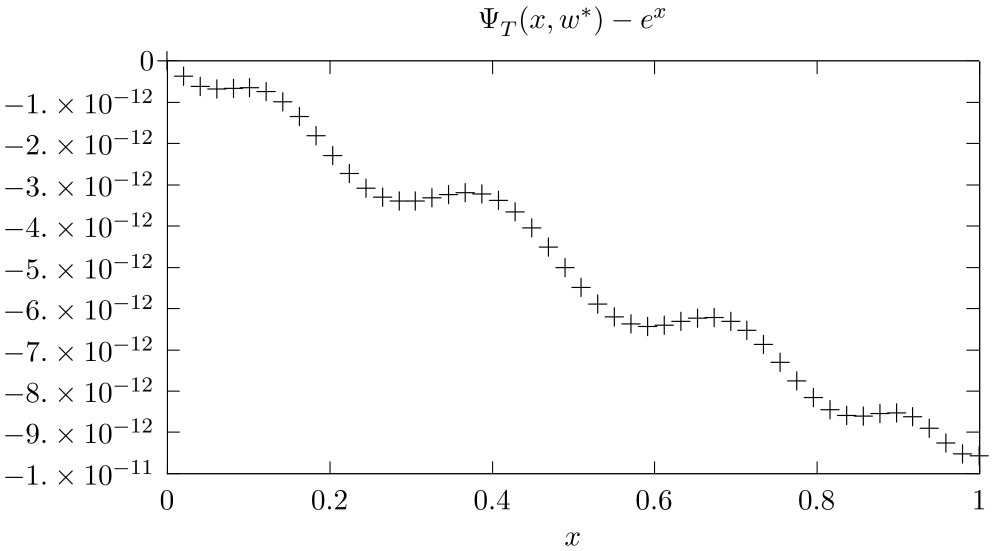

Figure 1: Plot of the difference $\Psi_T(x, w^*) - e^x$

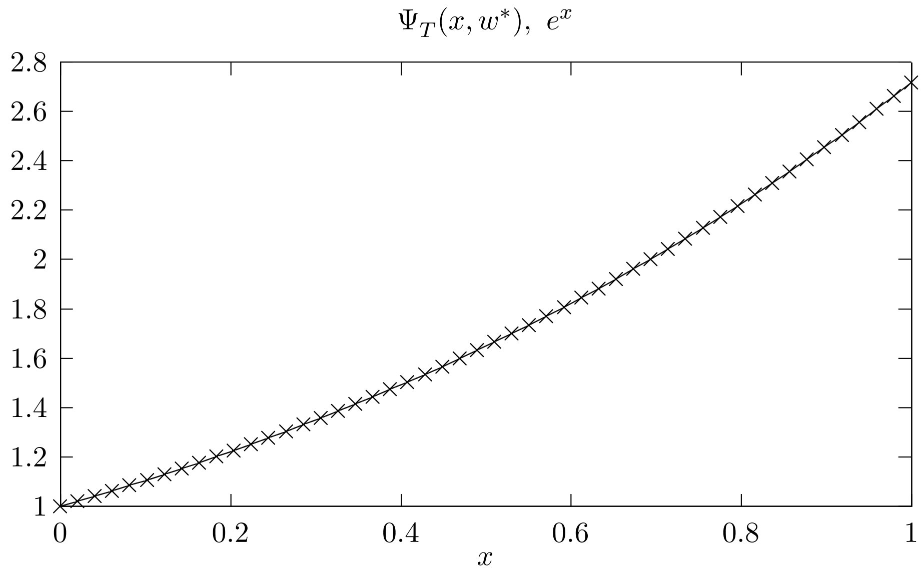

Figure 2: Plots of $\Psi_T(x, w^*)$ and of the exact solution e^x

leading to the following values for $\psi_a,\ \psi_b$:

$$\psi_a = -\frac{b-a}{2}\left[\psi'_a + (b-a)N(a,w)\right],\ \psi_b = \frac{b-a}{2}\left[\psi'_b - (b-a)N(b,w)\right] \qquad (13)$$

with the trial solution becoming:

$$\begin{aligned}\Psi_T(x,w) = & -\frac{1}{2}\left[\psi'_a + (b-a)N(a,w)\right]\frac{(x-b)^2}{(b-a)} + \\ & + \frac{1}{2}\left[\psi'_b - (b-a)N(b,w)\right]\frac{(x-a)^2}{(b-a)} + (x-a)(x-b)N(x,w)\end{aligned} \tag{14}$$

We solved again the same example equation with the BCs: $\psi'(0) = 1, \psi'(1) = e$ (again the exact solution is $\psi(x) = e^x$), and obtained similarly highly accurate results.