Solving the Heat Equation with Neural Networks

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Abstract

Standard methods for solving Partial Differential Equations (PDEs) include Euler steps, Runge-Kutta, Galerkin methods, and others. These methods mesh the domain in which we want to solve the PDE and then take small steps to solve the PDE. However, the combination of an exponentially increasing number of both grid points and steps and decreasing numerical stability makes this process infeasible for high-dimensional problems. In this paper we attempt to solve the Heat Equation, a well-studied PDE, using the Deep Galerkin Method, which uses deep neural networks to approximate a solution to the PDE via the Universal Approximation Theorem.

1 Background

The Deep Galerkin Method was first proposed in 2018 by Justin Sirignano and Konstantinos Spiliopoulos, who used the method to numerically solve the Black-Scholes equation for options pricing. This main advantage of the DGM is that it is mesh-free, and as a result does not suffer from the curse of dimensionality, allowing us to compute values in feasible time for higher-dimensional setups. Sirignano and Spiliopoulos proved rigorously that using a deep neural network, as the number of layers goes to infinity, the network approximation converges point wise to the true solution. This is done by choosing a loss function which consists of distance from some initial condition, distance from some boundary condition, and distance from the size of the differential operator applied to the function. By minimizing the sum of these three terms, the method aims to generate a function which closely approximates the initial condition, boundary condition, and a solution on the interior of the domain, thereby giving a numerical solution to the PDE.
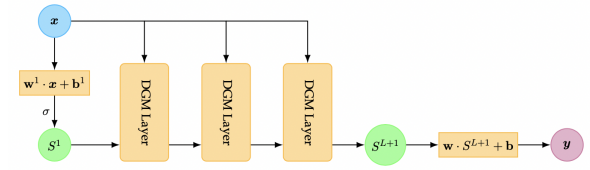
2 Methods

2.1 DGM Architecture

Figure 5.2: *Bird's-eye perspective of overall DGM architecture.*

The overall DGM architecture consists of stacked DGM layers that take as input the original x and the output of the previous DGM layer, as well as two linear layers, one at the start and one at the end.
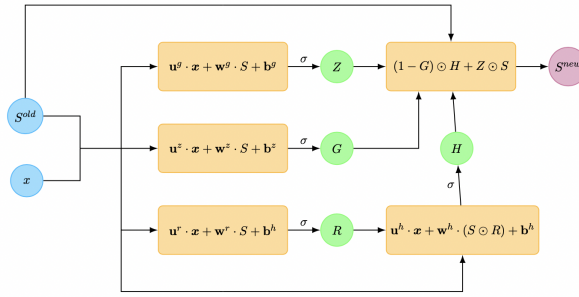
2.2 Individual DGM layer

Figure 5.3: *Operations within a single DGM layer.*

Each individual DGM layer consists of four sums of linear maps and an output function. In total, each layer contains eight weight matrices, four bias vectors, and four activation functions, which are eventually combined in the layer's output function.

3 Results

4 Conclusion

References

References follow the acknowledgments. Use unnumbered first-level heading for the references. Any choice of citation style is acceptable as long as you are consistent. It is permissible to reduce the font size to `small` (9 point) when listing the references. **Remember that you can use a ninth page as long as it contains *only* cited references.**

2

[1] Al-Aradi A. Correia A. Naiff D. Jardim G. Solving Nonlinear High-Dimensional Partial Differential Equations via Deep Learning.

[2] Han. J. Solving High-dimensional PDEs Using Deep Learning. https://www.pnas.org/content/pnas/115/34/8505.fu

[3] Penko V. https://github.com/vitkarpenko/FEM-with-backward-Euler-for-the-heat-equation

[4] Sirignano. J, spiliopoulos K. DGM: A deep learning algorithm for solving partial differential equations. https://arxiv.org/abs/1708.07469

There is a new style file for papers submitted in 2016!
NIPS requires electronic submissions. The electronic submission site is

<div align="center">https://cmt.research.microsoft.com/NIPS2016/</div>

Please read carefully the instructions below and follow them faithfully.

4.1   Style

Papers to be submitted to NIPS 2016 must be prepared according to the instructions presented here. Papers may only be up to eight pages long, including figures. Since 2009 an additional ninth page *containing only acknowledgments and/or cited references* is allowed. Papers that exceed nine pages will not be reviewed, or in any other way considered for presentation at the conference.

The margins in 2016 are the same as since 2007, which allow for ∼15% more words in the paper compared to earlier years.

Authors are required to use the NIPS LaTeX style files obtainable at the NIPS website as indicated below. Please make sure you use the current files and not previous versions. Tweaking the style files may be grounds for rejection.

4.2   Retrieval of style files

The style files for NIPS and other conference information are available on the World Wide Web at

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The file `nips_2016.pdf` contains these instructions and illustrates the various formatting requirements your NIPS paper must satisfy.

The only supported style file for NIPS 2016 is `nips_2016.sty`, rewritten for LaTeX 2_ε. **Previous style files for LaTeX 2.09, Microsoft Word, and RTF are no longer supported!**

The new LaTeX style file contains two optional arguments: `final`, which creates a camera-ready copy, and `nonatbib`, which will not load the `natbib` package for you in case of package clash.

At submission time, please omit the `final` option. This will anonymize your submission and add line numbers to aid review. Please do *not* refer to these line numbers in your paper as they will be removed during generation of camera-ready copies.

The file `nips_2016.tex` may be used as a "shell" for writing your paper. All you have to do is replace the author, title, abstract, and text of the paper with your own.

The formatting instructions contained in these style files are summarized in Sections 5, 6, and 7 below.

5   General formatting instructions

The text must be confined within a rectangle 5.5 inches (33 picas) wide and 9 inches (54 picas) long. The left margin is 1.5 inch (9 picas). Use 10 point type with a vertical spacing (leading) of 11 points. Times New Roman is the preferred typeface throughout, and will be selected for you by default. Paragraphs are separated by $^1/_2$ line space (5.5 points), with no indentation.

The paper title should be 17 point, initial caps/lower case, bold, centered between two horizontal rules. The top rule should be 4 points thick and the bottom rule should be 1 point thick. Allow ¼ inch space above and below the title to rules. All pages should start at 1 inch (6 picas) from the top of the page.

For the final version, authors' names are set in boldface, and each name is centered above the corresponding address. The lead author's name is to be listed first (left-most), and the co-authors' names (if different address) are set to follow. If there is only one co-author, list both author and co-author side by side.

Please pay special attention to the instructions in Section 7 regarding figures, tables, acknowledgments, and references.

6   Headings: first level

All headings should be lower case (except for first word and proper nouns), flush left, and bold.

First-level headings should be in 12-point type.

6.1   Headings: second level

Second-level headings should be in 10-point type.

6.1.1   Headings: third level

Third-level headings should be in 10-point type.

Paragraphs   There is also a \paragraph command available, which sets the heading in bold, flush left, and inline with the text, with the heading followed by 1 em of space.

7   Citations, figures, tables, references

These instructions apply to everyone.

7.1   Citations within the text

The natbib package will be loaded for you by default. Citations may be author/year or numeric, as long as you maintain internal consistency. As to the format of the references themselves, any style is acceptable as long as it is used consistently.

The documentation for natbib may be found at

    http://mirrors.ctan.org/macros/latex/contrib/natbib/natnotes.pdf

Of note is the command \citet, which produces citations appropriate for use in inline text. For example,

    \citet{hasselmo} investigated\dots

produces

    Hasselmo, et al. (1995) investigated...

If you wish to load the natbib package with options, you may add the following before loading the nips_2016 package:

```
\PassOptionsToPackage{options}{natbib}
```

If `natbib` clashes with another package you load, you can add the optional argument `nonatbib` when loading the style file:

```
\usepackage[nonatbib]{nips_2016}
```

As submission is double blind, refer to your own published work in the third person. That is, use "In the previous work of Jones et al. [4]," not "In our previous work [4]." If you cite your other papers that are not widely available (e.g., a journal paper under review), use anonymous author names in the citation, e.g., an author of the form "A. Anonymous."

7.2   Footnotes

Footnotes should be used sparingly. If you do require a footnote, indicate footnotes with a number[1] in the text. Place the footnotes at the bottom of the page on which they appear. Precede the footnote with a horizontal rule of 2 inches (12 picas).

Note that footnotes are properly typeset *after* punctuation marks.[2]

7.3   Figures

All artwork must be neat, clean, and legible. Lines should be dark enough for purposes of reproduction. The figure number and caption always appear after the figure. Place one line space before the figure caption and one line space after the figure. The figure caption should be lower case (except for first word and proper nouns); figures are numbered consecutively.

You may use color figures. However, it is best for the figure captions and the paper body to be legible if the paper is printed in either black/white or in color.
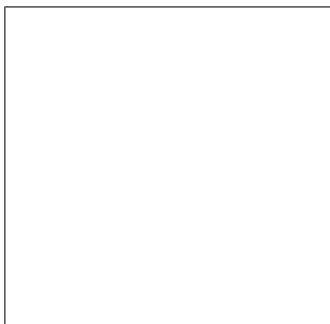
Figure 1: Sample figure caption.

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[1] Sample of the first footnote.
[2] As in this example.

Table 1: Sample table title

	Part		Size (μm)
Name	Description		
Dendrite	Input terminal		$\sim$100
Axon	Output terminal		$\sim$10
Soma	Cell body		up to 10^6

7.4   Tables

All tables must be centered, neat, clean and legible. The table number and title always appear before the table. See Table 1.

Place one line space before the table title, one line space after the table title, and one line space after the table. The table title must be lower case (except for first word and proper nouns); tables are numbered consecutively.

Note that publication-quality tables *do not contain vertical rules.* We strongly suggest the use of the `booktabs` package, which allows for typesetting high-quality, professional tables:

https://www.ctan.org/pkg/booktabs

This package was used to typeset Table 1.

8   Final instructions

Do not change any aspects of the formatting parameters in the style files. In particular, do not modify the width or length of the rectangle the text should fit into, and do not change font sizes (except perhaps in the **References** section; see below). Please note that pages should be numbered.

9   Preparing PDF files

Please prepare submission files with paper size "US Letter," and not, for example, "A4."

Fonts were the main cause of problems in the past years. Your PDF file must only contain Type 1 or Embedded TrueType fonts. Here are a few instructions to achieve this.

- You should directly generate PDF files using `pdflatex`.

- You can check which fonts a PDF files uses. In Acrobat Reader, select the menu Files>Document Properties>Fonts and select Show All Fonts. You can also use the program `pdffonts` which comes with `xpdf` and is available out-of-the-box on most Linux machines.

- The IEEE has recommendations for generating PDF files whose fonts are also acceptable for NIPS. Please see http://www.emfield.org/icuwb2010/downloads/IEEE-PDF-SpecV32.pdf

- `xfig` "patterned" shapes are implemented with bitmap fonts. Use "solid" shapes instead.

- The `\bbold` package almost always uses bitmap fonts. You should use the equivalent AMS Fonts:

  ```
  \usepackage{amsfonts}
  ```

  followed by, e.g., `\mathbb{R}`, `\mathbb{N}`, or `\mathbb{C}` for $\mathbb{R}$, $\mathbb{N}$ or $\mathbb{C}$. You can also use the following workaround for reals, natural and complex:

  ```
  \newcommand{\RR}{I\!\!R} %real numbers
  \newcommand{\Nat}{I\!\!N} %natural numbers
  \newcommand{\CC}{I\!\!\!\!C} %complex numbers
  ```

  Note that `amsfonts` is automatically loaded by the `amssymb` package.

If your file contains type 3 fonts or non embedded TrueType fonts, we will ask you to fix it.

9.1   Margins in LaTeX

Most of the margin problems come from figures positioned by hand using `\special` or other commands. We suggest using the command `\includegraphics` from the `graphicx` package. Always specify the figure width as a multiple of the line width as in the example below:

```
\usepackage[pdftex]{graphicx} ...
\includegraphics[width=0.8\linewidth]{myfile.pdf}
```

See Section 4.4 in the graphics bundle documentation (`http://mirrors.ctan.org/macros/latex/required/graphics/grfguide.pdf`)

A number of width problems arise when LaTeX cannot properly hyphenate a line. Please give LaTeX hyphenation hints using the `\-` command when necessary.

Acknowledgments

Use unnumbered third level headings for the acknowledgments. All acknowledgments go at the end of the paper. Do not include acknowledgments in the anonymized submission, only in the final paper.

References

References follow the acknowledgments. Use unnumbered first-level heading for the references. Any choice of citation style is acceptable as long as you are consistent. It is permissible to reduce the font size to `small` (9 point) when listing the references. **Remember that you can use a ninth page as long as it contains *only* cited references.**

[1] Alexander, J.A. & Mozer, M.C. (1995) Template-based algorithms for connectionist rule extraction. In G. Tesauro, D.S. Touretzky and T.K. Leen (eds.), *Advances in Neural Information Processing Systems 7*, pp. 609–616. Cambridge, MA: MIT Press.

[2] Bower, J.M. & Beeman, D. (1995) *The Book of GENESIS: Exploring Realistic Neural Models with the GEneral NEural SImulation System.* New York: TELOS/Springer–Verlag.

[3] Hasselmo, M.E., Schnell, E. & Barkai, E. (1995) Dynamics of learning and recall at excitatory recurrent synapses and cholinergic modulation in rat hippocampal region CA3. *Journal of Neuroscience* **15**(7):5249-5262.