Deep Variational Methods

Dominic Bair, Dominique Zosso

Department of Mathematical Sciences, Montana State University

MONTANA STATE UNIVERSITY

Motivation

- Partial Differential Equations (PDEs) are used to model systems in a wide variety of fields.
- PDEs are often impossible to solve analytically and difficult to solve numerically, especially in high dimensions.
- Machine learning has recently been applied in the area of PDEs with promising results.
- Calculus of variations can be used to solve some PDEs by restating them as a minimization problem.
- This minimization problem can potentially be used in conjunction with machine learning for increased computational performance in certain problems.

Deep Learning

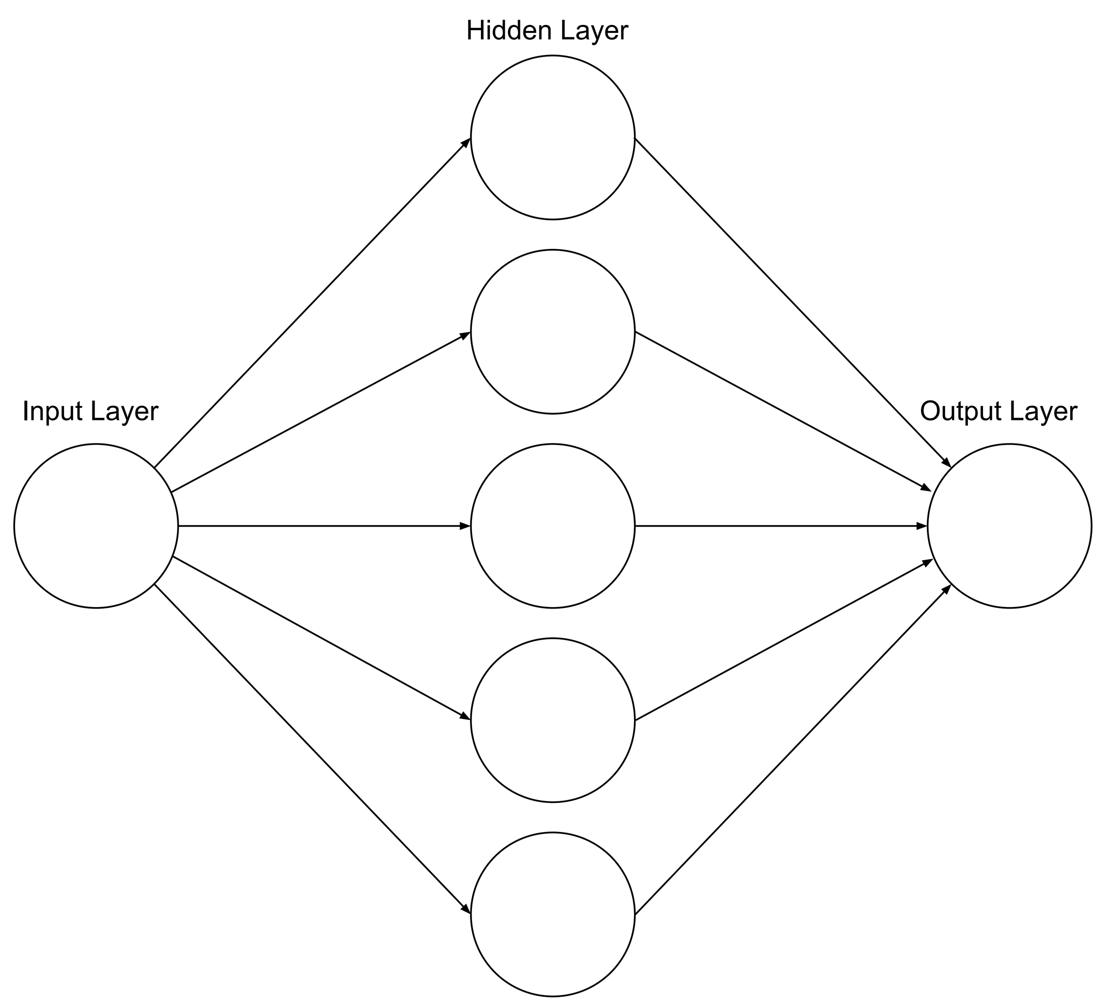

Figure: A visualization of a simple 1–layer Neural Network (NN).

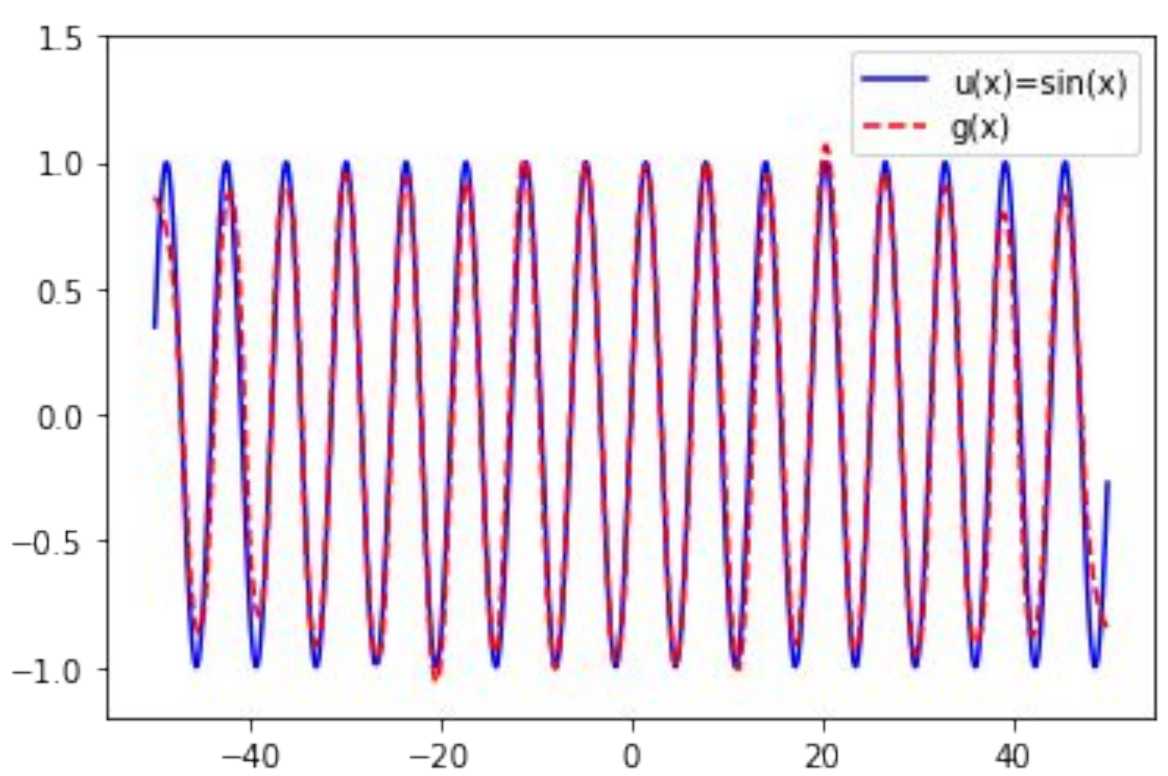

Figure: An output of a NN that has learned the sine function.

Deep Galerkin Methods (DGM)

Consider a general PDE with differential operator D, and initial and boundary conditions:

$$\begin{cases} Du = f, & (x,t) \in \Omega \times (0,T) \\ u = g, & (x,t) \in \partial\Omega \times (0,T) \\ u = h, & (x,0) \in \Omega \times \{0\} \\ \vdots & \end{cases} \tag{1}$$

We train a NN to solve (1) by minimizing a loss function: [1]

$$\begin{aligned} \text{Loss} = & \frac{1}{I}\sum_{i=1}^{I} |D\hat{u}(x_i,t_i) - f(x_i,t_i)|^2 \\ & + \frac{1}{J}\sum_{j=1}^{J} |\hat{u}(x_j,t_j) - g(x_j,t_j)|^2 \\ & + \frac{1}{K}\sum_{k=1}^{K} |\hat{u}(x_k,0) - h(x_k)|^2 + \cdots \end{aligned} \tag{2}$$

Calculus of Variations

Idea of Calculus of Variations

Find u that minimizes (or maximizes) the following functional: [2]

$$J = \int_\Omega L(x, u(x), \nabla u(x))\, dx \tag{3}$$

Euler–Lagrange Equation

We can find this u by solving the following equation:

$$\frac{\partial L}{\partial u} - \nabla \cdot \frac{\partial L}{\partial \nabla u} = 0 \tag{4}$$

Deep Variational Methods (DVM)

If a PDE has a variational formulation, we can solve it by training a NN to minimize the following loss function:

$$\begin{aligned} \text{Loss} = & \frac{\lambda}{I}\sum_{i=1}^{I} L(x_i) \\ & + \frac{1}{J}\sum_{j=1}^{J} |\hat{u}(x_j) - g(x_j)|^2 + \cdots \end{aligned} \tag{5}$$

Laplace Problem

Consider the following functional:

$$J = \frac{1}{2}\int_\Omega ||\nabla u||^2\, dx \quad \text{s.t. } u = f \text{ for } x \in \partial\Omega \tag{6}$$

We can minimize J by applying (4) to get the following PDE:

$$\begin{cases} \Delta u = 0, & x \in \Omega \\ u = f, & x \in \partial\Omega \end{cases} \tag{7}$$

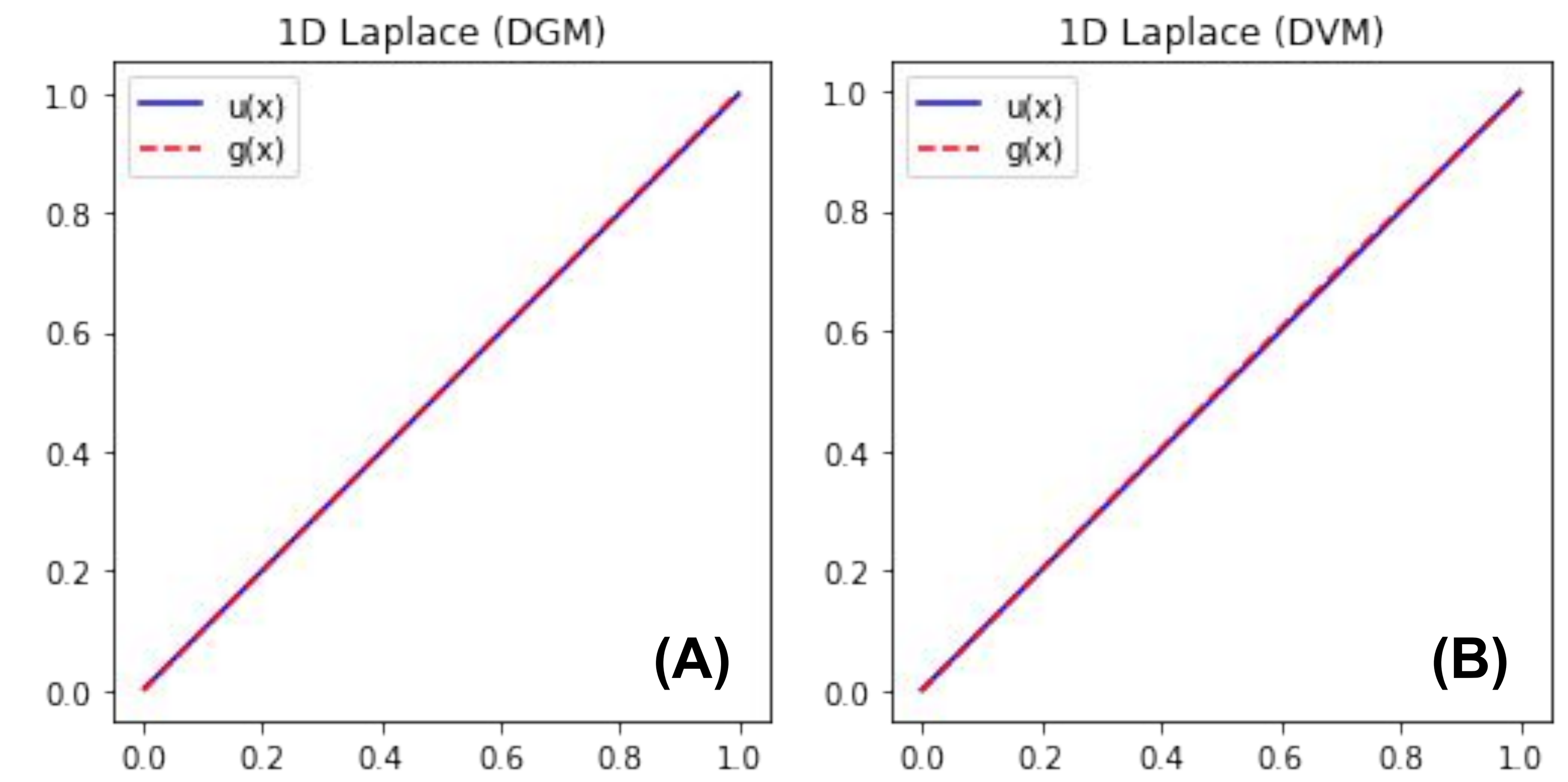

Figure: Examples of DGM and DVM in 1–D; note the slightly increased error in **(B)**.

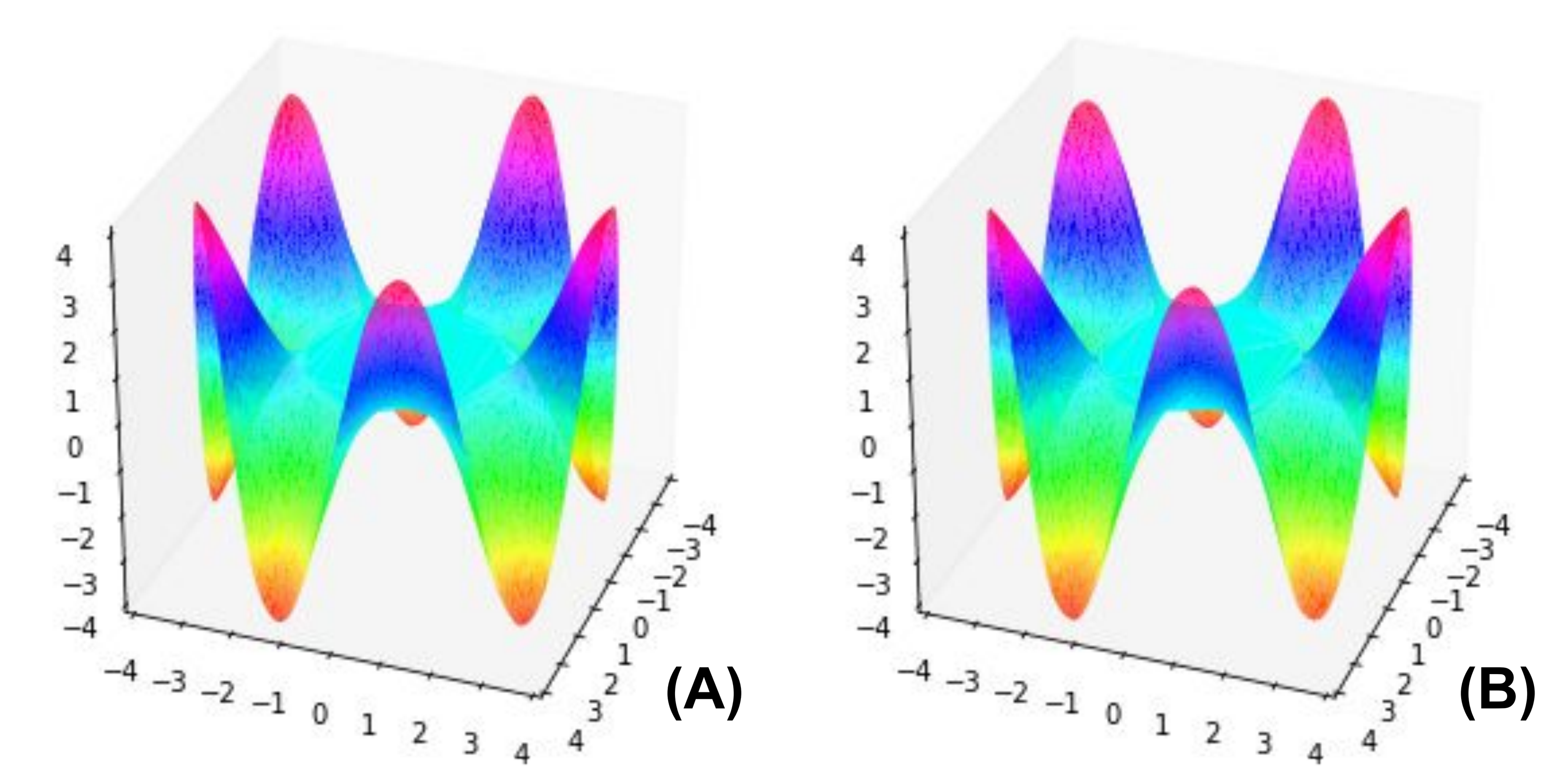

Figure: **(A)** a 2-D DGM solution to (7); **(B)** a 2-D DVM solution to (6); note the slightly decreased amplitude.

References & Acknowledgments

[1] Justin Sirignano and Konstantinos Spiliopoulos. Dgm: A deep learning algorithmfor solving partial differential equations.*Journal of Computational Physics Vol.375*, 2018.

[2] John R. Taylor. *Classical Mechanics*. University Science Books, 2005.

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