# Generalised Eikonal Equations on graphs with applications to semi-supervised learning

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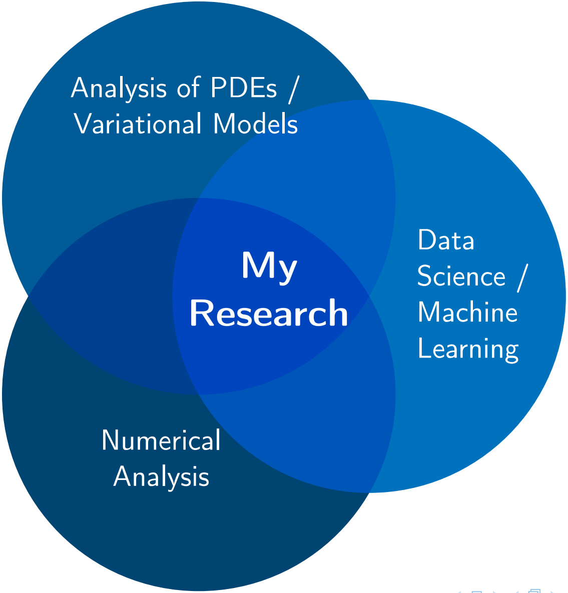
**Mathematics for Deep Learning Opening Workshop**
April 21, 2022

# My Research


Analysis of PDEs / Variational Models
Data Science / Machine Learning
Numerical Analysis
My Research

# Goal: Numerical modelling across scales

**MICROSCOPIC FORMULATION**
agent-based models (high-dimensional equations)
for properties (e.g. positions) of large number of agents

rigorous bridge

**MACROSCOPIC FORMULATION**
mean-field equations (low-dimensional equations)
for macroscopic structures (e.g. density functionals)

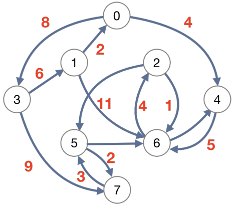
separate approaches

## Originality:

- **New perspective:** bridge micro- and macroscopic description
- **Importance:**
  - probe microscopic system via macroscopic observables
  - two different approaches for the development of computational methods
  - rigorous bridge implying reliability of approaches

# Motivation

- Computational methods for semi-supervised and unsupervised classification based on variational models and PDEs (e.g. algorithms based on phase fields, MBO scheme, p-Laplacians)
- Success of Eikonal equations in the continuum setting (e.g. continuum shortest path problem, electromagnetism, ray optics)
- Shortest path graph distances are widely used in data science and machine learning

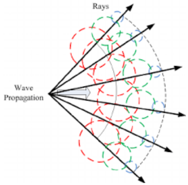



$\Rightarrow$ **Development of discrete generalised eikonal equations on graphs for semi-supervised learning**

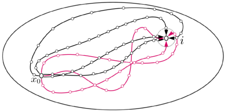
# Models for information propagation on graphs

We propose three models for the propagation of information on graphs [1]:

- **Front propagation models:** information propagation as an evolving front, i.e. evolving front separates region for which the wave has arrived from the remainder




- **First arrival times:** finding the smallest travel time over a set of possible paths, i.e. consider subsets of set of admissible paths and optimise travel times over these sets




[1] Dunbar, Elliott, LMK, arXiv:2201.07577

# Models for information propagation on graphs

- **Discrete generalised eikonal models:**
  - Continuum eikonal equation

$$\|\nabla u\|_2 = s \quad \text{in } \Omega\backslash\{x_0\}$$

with boundary conditions

$$\begin{aligned} u(x_0) &= 0, \\ \nabla u(x) \cdot \nu(x) &\geqslant 0 \quad \text{for } x \in \Gamma \end{aligned}$$

  - Discrete one-sided derivatives:

$$\nabla_w^+ u_i = (w_{j,i}(u_i - u_j)^+)_{j \in N(i)}$$

$\Rightarrow$ Define discrete generalised eikonal equations for any $1 \leqslant p \leqslant \infty$ as

$$\begin{aligned} \|\nabla_w^+ u_i\|_p &= s_i, \quad i \in \mathring{V}, \\ u_i &= 0, \quad i \in \partial V \end{aligned}$$

# Theoretical results

We show

- Equivalence of models (front propagation, first arrival times and discrete generalised eikonal models) depending on parameter $p$
  $\Rightarrow$ **Sufficient to focus on discrete generalised eikonal models**

- Formal limit for specific regular grids for any $p$ where $w_{ij} = \eta(\|X_i - X_j\|_2)$:
  - **Square grid:** $\eta(1)\|\nabla U\|_p = S$
  - **Triangular grid:** $\eta(1)\|(\nabla U \cdot \xi_k)_{k=1,2,3}\|_p = S$ with $\xi_1 = (1,0), \xi_2 = (\cos(\pi/3), \sin(\pi/3))$ and $\xi_3 = (\cos(2\pi/3), \sin(2\pi/3))$

  $\Rightarrow$ **Limiting PDE** of the form $\|A\nabla U(x)\|_p = S(x)$ for $A \in \mathbb{R}^{2\times 2}$

- Formal limit for regular $\kappa$-neighbor grid for $\kappa$ even and $p = 2$

and we perform **numerical experiments**...

# Close-up views of underlying graphs

Square ($S$) Triangular ($T$) Hexagonal ($H$) Rhombus ($R$) Uniform ($U$)

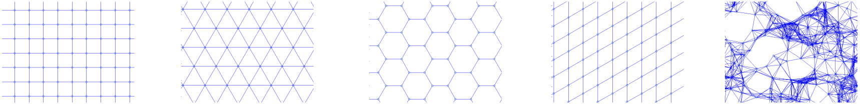
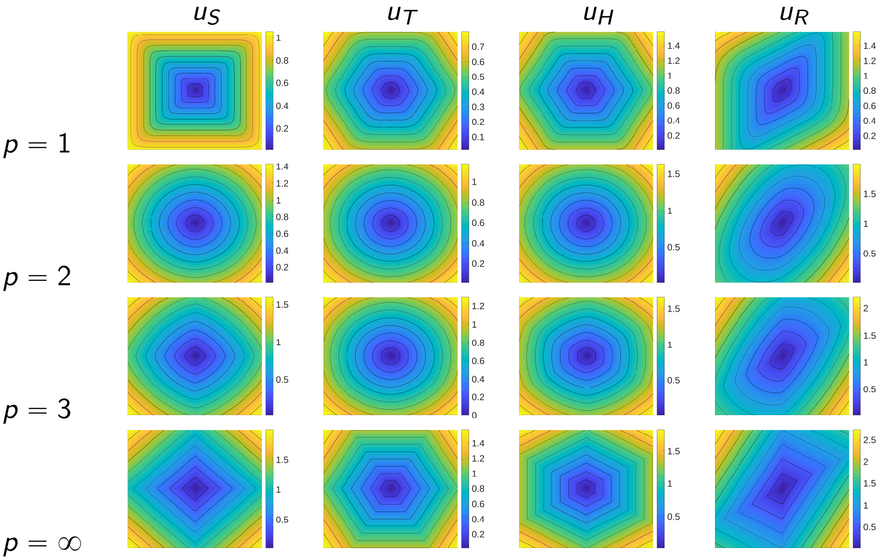


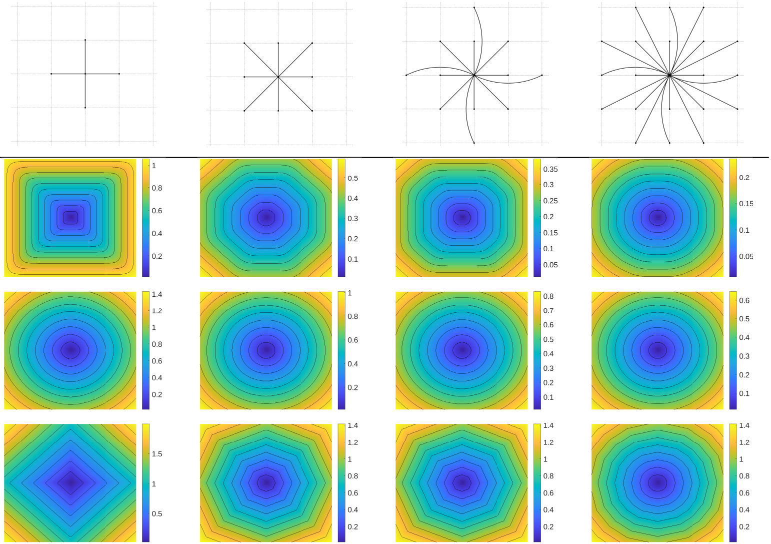
Figure: The $S$, $T$, $H$, and $R$ grids are regular, and we take a small interior angle of $\pi/3$, for the rhombus grid $R$. The $U$ graph is created from connecting uniformly random points to nearest neighbours upto a cut-off radius 0.04 (leading to 12 average neighbours).

# Discrete solution on different structured grids



# Discrete solutions for the generalised Eikonal equation

Stencil: 4 8 12 20




$p = 1$

$p = 2$

$p = \infty$

# Traveltime fields and classification for two moons problem

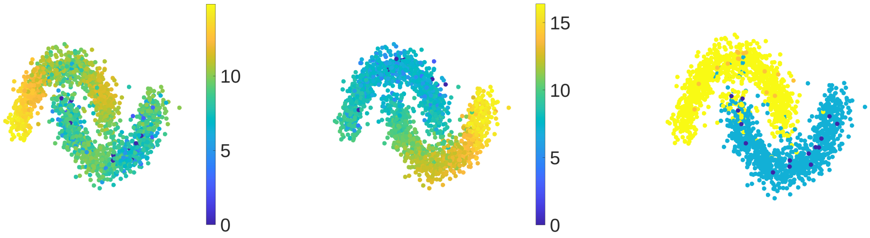



Figure: Left and centre panels: traveltime field for label 1 and 2 respectively. Right panel: classification with predicted label 1 (blue) and predicted label 2 (yellow) solved with initially known labels 1 (orange), and 2 (dark blue). The accuracy was 94.7%.

# Mean (standard deviation) of classification for the two moons example

| $w_{i,j}$ | Eikonal model | Two moons accuracy % |
|---|---|---|
| | $p = 1$ | 92.7 (3.81) |
| $\exp\left(-\frac{\|x_i - x_j\|^2}{\sqrt{d_{10}(x_i) d_{10}(x_j)}}\right)$ | $p = 2$ | 92.0 (2.80) |
| | $p = \infty$ | 89.5 (2.96) |

# Performance of on data sets Cora and CiteSeer

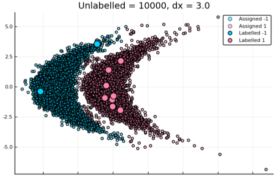
| $w_{i,j}$ | Eikonal model | Cora accuracy | CiteSeer accuracy |
|---|---|---|---|
| $1/\|x_i - x_j\|_{\ell^2}$ | $p = 1$ | 69.0 (7.49) | 64.3 (1.64) |
| | $p = 2$ | 68.9 (6.86) | 62.6 (1.87) |
| | $p = \infty$ | 68.1 (3.86) | 61.0 (2.26) |
| $\exp(-\frac{\|x_i - x_j\|_{\ell^2}^2}{500})$ | $p = 1$ | 72.4 (1.58) | 64.3 (1.91) |
| | $p = 2$ | 71.8 (1.88) | 62.5 (2.12) |
| | $p = \infty$ | 69.2 (2.50) | 60.8 (2.25) |
| $\exp(-\frac{\|x_i - x_j\|_{\ell^2}^2}{100\sqrt{d_{\max}(x_i)d_{\max}(x_j)}})$ | $p = 1$ | 72.4 (1.56) | 64.3 (2.06) |
| | $p = 2$ | 71.7 (1.91) | 62.5 (2.08) |
| | $p = \infty$ | 69.0 (2.42) | 60.7 (2.22) |

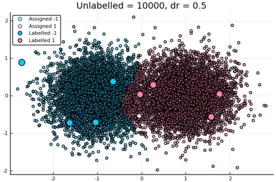
Table: Mean (standard deviation) of classification accuracy given as percentages, for the examples using different choices of weights. The function $d_{\max}(x)$ is the Euclidean distance from $x_i$ to its furthest neighbour.

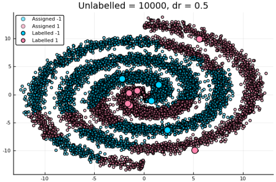
$\Rightarrow$ Comparably performance to flaship methods Planetoid-T and Planetoid-I

# Conclusion: PDEs on graphs for semi-supervised learning

- **Model development:** Discrete models on graphs (front propagation, first arrival time and discrete eikonal models)
- **Derivation of continuum models**
  - Generalised eikonal equations Dunbar, Elliott, LMK, arXiv:2201.07577
  - Second-order PDEs LMK, Wolfram, arXiv:2007.12516
- **Quantitative behaviour:** Analytic results on equivalence of models
- **Computational experiments** for semi-supervised learning



Thank you very much for your attention!

Happy to answer any questions!

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