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DS-GPS
A Deep Statistical Graph Poisson Solver

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Motivations

- Numerical simulations of fluid flow play an essential role in modelling many physical phenomena but solving the incompressible Navier-Stokes equations at scale remains daunting.
- The splitting scheme method requires the costly resolution of a Poisson problem to compute the pressure field that guarantees the incompressibility constraint.
- Leverage data-driven methods to enhance the Poisson pressure problem (PPE) resolution.

Objectives

- Develop a GNN-based algorithm to speed-up the resolution of the PPE on unstructured meshes.
- Design a model flexible to different domains, boundary conditions and initial solutions.
- The model should respect the boundary conditions by design and provide convergence guarantees.

Statistical Problem

Continuous Poisson Problem

\[ -\Delta u_p = f_p \in \Omega_p \]
\[ u_p = g_p \in \partial\Omega_p \]

Discretized Poisson Problem

\[ A_p U_p = B_p \]

Define a loss function

\[ \mathcal{L}_{\text{stat}}(U_p, A_p, B_p) = ||A_p U_p - B_p||^2 \]

Machine-Learning solver

\[ U_p = \text{solvers}(A_p, B_p) \]

\[ \theta^* = \arg\min_{\theta} \mathbb{E}_{U_p \sim \mathcal{P}}[\mathcal{L}_{\text{stat}}(\text{solvers}(U_p, A_p, B_p), A_p, B_p)] \]

Architecture

Deep Equilibrium GNNs

- Use a black-box solver to find the root of the GNN function:
  \[ H^* = \text{RootFind}(g_H, x) \quad \text{with} \quad g_H = f_0(H, g) - H \]
- The GNN function incorporates the different Message Passing:
  \[ \phi_{x,i} = \sum_{j \in \mathcal{N}(i)} \Phi_{x,j}(H_i, H_j, e_{ij}) \]
- The number of Message Passing is automatically determined by the “RootFind” black-box solver (a quasi-Newton method)!

Results

<table>
<thead>
<tr>
<th>Residual</th>
<th>MSE w.r.t LU solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.27e-3</td>
<td>1.06e-2</td>
</tr>
</tbody>
</table>

The Data

- Random 2D domains with coordinates in the unit square.
- \( \approx 500 \) nodes per geometry (Minimum : 221 - Maximum : 713).
- Force and boundary functions are defined as polynomials with randomly sampled coefficients.

Conclusion

This paper proposes a novel GNN-based approach to solve a Poisson problem with Dirichlet boundary conditions. Leveraging the implicit layer theory and a node-specific architecture, our method extends to any mesh size and shape, provides convergence guarantees and satisfies boundary conditions by design. By directly minimizing the residual of the problem, the model learns the physics of the equation and can output a solution ten times faster than traditional solvers.

References:

Top Left : Data-driven solution to be compared to Top Right : LU solution.
Bottom : Evolution of the residual and MSE loss across the RootFind solver iterations.