Deep Statistical Solvers

Course Project — DS303: Machine Learning

Team AlphaSolvers

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Overview

Problem Statement

- **Optimization Problem:** The elementary question is to solve the following optimization problem for a given Interaction Graph G

$$U^*(G) = \arg\min_{U \in \mathcal{U}} L(U, G)$$

- **Learning Goal:** Because the above optimization problem is not easy to solve, we want to learn a single solver that best approximates the mapping $G \rightarrow U^*(G)$ for all G.

$$\hat{U}(G) = Solver(G) \quad \text{where, } \hat{U} \text{ is an approximation is } U^*$$

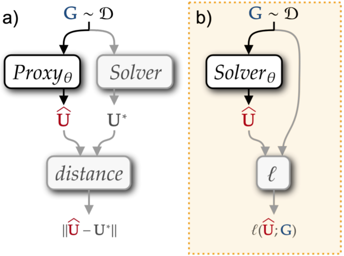


Figure: Proxy approach (a) vs. DSS (b)

Graph Neural Network implementation of a DSS

- **Node Embedding**: For each node, H_i is an embedding of actual state U_i, which is used for training and prediction

- **Message passing**: This step performs $\bar{k}$ updates on the latent state variable $\mathbf{H}$ using an **UPDATE** function M_θ^k and **AGGREGATE** function $\mathbf{\Psi}$

$$
\begin{aligned}
\phi^k_{\rightarrow,i} &= \sum_{j \in \mathcal{N}^\star(i;\mathbf{G})} \Phi^k_{\rightarrow,\theta}(H_i^{k-1}, A_{ij}, H_j^{k-1}) && \textit{outgoing edges} \\
\phi^k_{\leftarrow,i} &= \sum_{j \in \mathcal{N}^\star(i;\mathbf{G})} \Phi^k_{\leftarrow,\theta}(H_i^{k-1}, A_{ji}, H_j^{k-1}) && \textit{ingoing edges} \\
\phi^k_{\circlearrowleft,i} &= \Phi^k_{\circlearrowleft,\theta}(H_i^{k-1}, A_{ii}) && \textit{self loop}
\end{aligned}
$$

Latent states H_i^k are then computed using trainable mapping Ψ_θ^k, in a ResNet-like fashion:

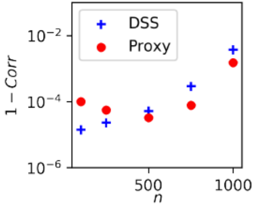
$$
\mathbf{H}^k = \mathbf{M}_\theta^k(\mathbf{H}^{k-1}, \mathbf{G}) := (H_i^k)_{i \in [n]}, \text{ with } H_i^k = H_i^{k-1} + \Psi_\theta^k(H_i^{k-1}, B_i, \phi^k_{\rightarrow,i}, \phi^k_{\leftarrow,i}, \phi^k_{\circlearrowleft,i})
$$

Linear Solver Experiment

- We had seen how tempetrature distribution for a 2D domain can be obtined by solving Poisson equation using the DSS
- Following were its results

Method	**DSS**	Proxy	LU
Correlation w/ LU	$>$**99.99%**	$>$**99.99%**	-
NRMSE w/ LU	1.6e-3	**1.1e-3**	-
Time per instance (ms) * Inference time divided by batch size	1.8*	1.8*	2.4
Loss 10^{th} percentile	**3.9e-4**	7.0e-3	4.5e-27
Loss 50^{th} percentile	**1.2e-3**	1.6e-2	6.1e-26
Loss 90^{th} percentile	**4.1e-3**	4.0e-2	6.3e-25

- Next we had analyzed how well trained model is able to generalize to a distribution that is different from the training distribution



Comments on Midterm Presentation

- Motivation could have been more elaborate and clear
- For the past work only the name of the approach or method is mentioned, could have covered a brief theme of these approaches
- Skipped a part on universal approximation property
- More emphasis regarding the performance metric (correlation between two solvers) could have been discussed as it is not a common performance metric.
- For future work: Include a code walkthrough of replication of work.

Addressing the Comments

- **Universal approximation property** now explained in detail
- The performance metrics used **Pearson Correlation Coefficient** and NRMSE have been discussed in detail and also explained during the code demonstration
- Code has now been discussed properly and a code walkthorugh has been included
- We learnt about **GRNN** and made an attempt to incorporate it in the code

Universal Approximation Property

Let us say that all the interaction graphs, G are sampled from a given distribution $\mathcal{D}$. Let $supp(\mathcal{D})$ (support of $\mathcal{D}$) follow four hypotheses:

- **Permutation Invariance:** For any $G \in supp(\mathcal{D})$ and $\sigma \in \Sigma_n$, $\sigma \star G \in supp(\mathcal{D})$
- **Compactness:** $supp(\mathcal{D})$ is a compact subset
- **Connectivity:** For any $G \in supp(\mathcal{D})$, $\tilde{G}$ has only one connected component.
- **Seperability of external inputs:** There exist $\delta > 0$ such that for any $G = (n, A, B) \in supp(\mathcal{D})$ and any $i \neq j \in \{1, 2, ..., n\}, ||B_i - B_j|| \geq \delta$

and let l be a continuous and permutation-invariant loss function such that for any $G \in supp(\mathcal{D})$, our problem has a unique minimizer $U^*(G)$, continuous w.r.t G. Then $\forall\, \epsilon > 0\, \exists\, Solver_\theta$, such that

$$||Solver_\theta(G) - U^*(G)|| \leq \epsilon$$

Normalization - Change of Variables (For Poisson Equation)

- In the Poisson case study, the nodes at the boundary are constrained (i.e. $A_{ii} = 1$ and $A_{ij} = 0$ if $i \neq j$), and the interior nodes are not
- Also, the coefficients of matrix A at these interior nodes satisfy a conservation equality ($A_{ii} = -\sum_{j \in [n] \setminus i} A_{ij}$)
- Due to this, the distributions of their respective B_i are very different

To overcome this issue we use change of variables as follows:

$$B_i' = \begin{cases} [B_i, 0, 0], & \text{if node } i \text{ is not constrained} \\ [0, 1, B_i], & \text{otherwise} \end{cases}$$

$$A_{ij}' = \begin{cases} A_{ij}, & \text{if } i \neq j \\ 0, & \text{otherwise} \end{cases}$$

Normalization and Evaluation Metric

So the now the loss function $l(U, G) = \sum_{i=1}^{n}(-B_i + \sum_{j=1}^{n} A_{ij} U_j)^2$ takes the form,

$$l^{'}(U, G^{'}) = \sum_{i=1}^{n} \left((1 - B_i^{'2})(-B_i^{'1}) + B_i^{'2}(U_i - B_i^{'3}) + \sum_{j=1}^{n} A_{ij}^{'}(U_j - U_i) \right)^2$$

where $B_i^{'p}$ denotes the p^{th} component of vector B_i

Pearson Correlation Metric: The correlation metric used by the authors is known as the Pearson correlation. It is defined as follows,

$$r_{12} = \frac{\sum_{i=1}^{n}(U_i^1 - \bar{U}^1)(U_i^2 - \bar{U}^2)}{\sqrt{\sum_{i=1}^{n}(U_i^1 - \bar{U}^1)^2}\sqrt{\sum_{i=1}^{n}(U_i^2 - \bar{U}^2)^2}}$$

AC power flow experiments

The second SSP example is the AC power flow prediction. Here, We know

- The amount of power being produced & consumed throughout the grid - encoded into B
- The way power lines are interconnected and their physical properties - encoded into A
- Our goal is to compute the voltage defined at each electrical node - encoded in state U

Let's consider a power grid with n nodes. We define the complex voltage at node i

$$V_i = |V_i| e^{j\theta_i}$$

The real part of the power consumed is denoted by $P_{d,i}$ and the imaginary part by $Q_{d,i}$.

Current State-of-the-art AC power flow computation uses the **Newton-Raphson** method

Loss Function : Kirchhoff's laws

The system of equations that govern the power grid are the following:

$$\begin{aligned}
\forall i \in [n] \setminus \{i_s\}, \quad & P_{g,i} - P_{d,i} = \sum_{j\in[n]} |V_i||V_j|(\mathrm{Re}(Y_{ij})\cos(\theta_i-\theta_j) + \mathrm{Im}(Y_{ij})\sin(\theta_i-\theta_j)) \\
\forall i \in I_{PQ}, \quad & -Q_{d,i} = \sum_{j\in[n]} |V_i||V_j|(\mathrm{Re}(Y_{ij})\sin(\theta_i-\theta_j) - \mathrm{Im}(Y_{ij})\cos(\theta_i-\theta_j)) \\
\forall i \in I_{PV}, \quad & |V_i| = V_{g,i}
\end{aligned}$$

This set of complex equations can be converted into a SSP using A, B and U and loss function-

$$\begin{aligned}
\ell(\mathbf{U},\mathbf{G}) = & \textstyle\sum_{i\in[n]}(1-B_i^5)\big(-B_i^1+U_i^1\sum_{j\in[n]} A_{ij}^1 U_j^1 \cos(U_i^2-U_j^2-A_{ij}^2)\big)^2 \\
& +\textstyle\sum_{i\in[n]} B_i^3\big(-B_i^2+U_i^1\sum_{j\in[n]} A_{ij}^1 U_j^1 \sin(U_i^2-U_j^2-A_{ij}^2)\big)^2 + \lambda\sum_{i\in[n]}(1-B_i^3)\big(U_i^1-B_i^4\big)^2
\end{aligned}$$

Details of Experiments

- Experiments are conducted on two standard benchmarks ($n = 14$) and ($n = 118$).
- For case 14 (resp. case 118), the dataset is split into 16064/2008/2008 (resp. 18432/2304/2304).

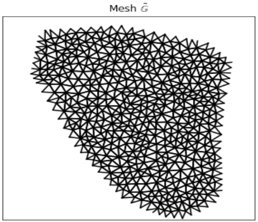
Neural Network Details

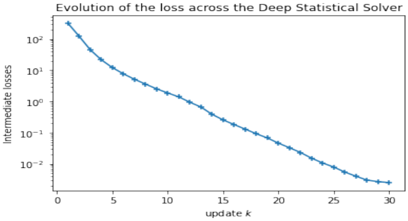
- Each NN block : single hidden layer of dimension $d = 10$ & leaky-ReLU non linearity
- Xavier Initialization, Adam Optimizer and Gradient Clipping were used
- For case $n = 14$, $\overline{k}$ was set to 10 ; we have $\alpha = 10^{-2}$, $lr = 3 * 10^{-3}$ and $\gamma = 0.9$
- For case $n = 118$, $\overline{k}$ was set to 30 ; we have $\alpha = 3 * 10^{-4}$, $lr = 3 * 10^{-3}$ and $\gamma = 0.9$)
- The number of weights is 1,722 for each of the $\overline{k}$ (M, D) blocks

Results

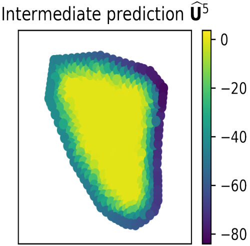
Dataset		IEEE 14 nodes			IEEE 118 nodes		
Method		**DSS**	Proxy	NR	**DSS**	Proxy	NR
Corr. w/ NR	$\lvert V_i \rvert$	99.93%	**>99.99%**	-	99.79%	**>99.99%**	-
	θ_i	99.86%	**>99.99%**	-	81.31%	**>99.99%**	-
	P_{ij}	**>99.99%**	**>99.99%**	-	**>99.99%**	**>99.99%**	-
	Q_{ij}	**>99.99%**	**>99.99%**	-	**>99.99%**	**>99.99%**	-
NRMSE w/ NR	$\lvert V_i \rvert$	2.0e-3	**4.9e-4**	-	1.4e-3	**1.2e-3**	-
	θ_i	7.1e-3	**1.7e-3**	-	5.7e-2	**4.5e-3**	-
	P_{ij}	6.2e-4	**2.6e-4**	-	1.0e-3	**3.9e-4**	-
	Q_{ij}	4.2e-4	**2.0e-4**	-	1.1e-4	**1.7e-4**	-
Time per instance (ms) * Inference time divided by batch size		**1e-2***	**1e-2***	2e1	**2e-1***	2e-1*	2e1
Loss 10^{th} percentile		**4.2e-6**	2.3e-5	1.4e-12	**1.3e-6**	6.2e-6	2.9e-14
Loss 50^{th} percentile		**1.0e-5**	4.0e-5	2.1e-12	**1.7e-6**	8.3e-6	4.2e-14
Loss 90^{th} percentile		**4.4e-5**	1.2e-4	3.3e-12	**2.5e-6**	1.3e-5	6.4e-14

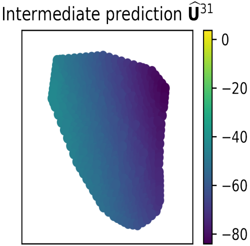
Replication of results -Linear Systems

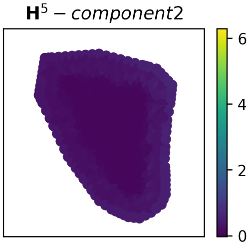


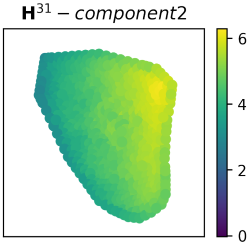


Intermediate predictions of State U and latent state H evolution

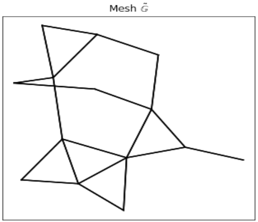


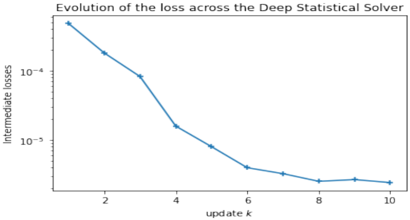




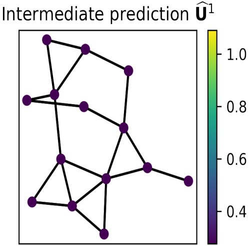


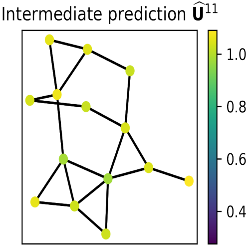
Replication of results - AC Power Flow Prediction

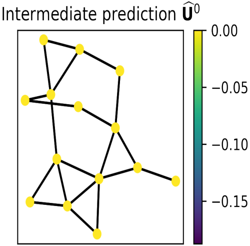


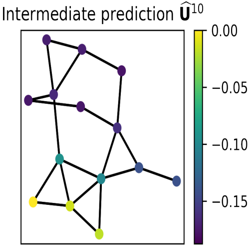


Intermediate predictions of Voltage and Phase Angle







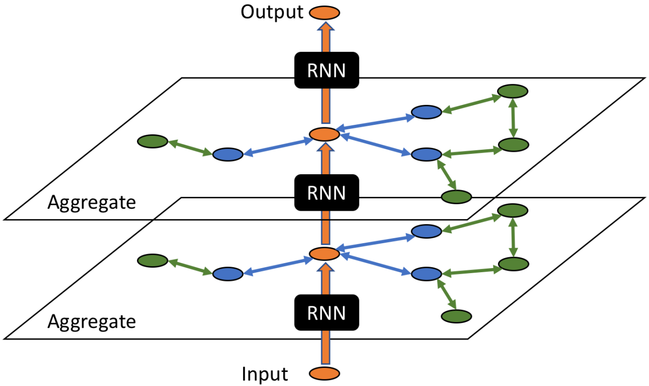


Conclusions

- We have performed an in-depth analysis of the Deep Statistical Solvers and in doing so we also learnt about Graph Neural Networks(GNN) which are widely used for physics based simulations.
- We covered the Universal Approximation Property of DSS. This property gives a theoretical backup to the network hence justifying its use in various domains.
- The effectiveness of DSSs was also experimentally demonstrated on two problems. We saw that the accuracy on power flow computations matches that of state-of-the-art approaches while speeding up calculations by 2 to 3 orders of magnitude.
- Another application of DSS is that it can be used as an initialization heuristic for classical optimization algorithms.

Extensions to the Work

- **Modification - Using Recurrent Graph Neural Networks (GRNN)** :
  In the paper authors have used GNN model of a limited depth. Instead, we can use **GNN with recurrent graph layers**. This will help in building deeper GNNs, without increasing the complexity of the training phase, while improving on the predictive performances.



References

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