Learning aggregation for 3D anisotropic diffusion on a structured grid

$$-\nabla \cdot (\boldsymbol{D}\nabla u) = 0, \tag{1}$$

$$\boldsymbol{D} := \boldsymbol{R}^T \begin{bmatrix} \varepsilon_x & & \\ & \varepsilon_y & \\ & & 1 \end{bmatrix} \boldsymbol{R}, \tag{2}$$

$$\boldsymbol{R} := \begin{bmatrix} \cos\theta_z & -\sin\theta_z & 0 \\ \sin\theta_z & \cos\theta_z & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\theta_y & 0 & \sin\theta_y \\ 0 & 1 & 0 \\ -\sin\theta_y & 0 & \cos\theta_y \end{bmatrix}. \tag{3}$$

For both the *isotropic* and *anisotropic* cases we generate two sets each of:

- 500 training problems, and
- 250 testing problems

to train the ML method. For the anisotropic case, these problems randomly have the parameters $N_x = N_y = N_z = N \sim \mathcal{U}\{8, 14\}$; $\theta_z, \theta_y \sim \mathcal{U}(0, 2\pi)$; $\log_{10}\varepsilon_x, \log_{10}\varepsilon_y \sim \mathcal{U}(-4, 4)$. The isotropic problems have the same parameter distribution for N, while $\theta_z = \theta_y = 0$ and $\varepsilon_x = \varepsilon_y = 1$.

Each problem was discretized in Firedrake [1] using piecewise linear tetrahedral finite elements with homogeneous Dirichlet boundary conditions. Afterwards, the degrees-of-freedom corresponding to Dirichlet boundary conditions were removed from the system.

The network was then trained on the anisotropic problems with a coarsening ratio of $\alpha = 0.027 = (0.1)^3$, as opposed to the previous $\alpha = 0.1 \approx (0.1)^2$. This is the reason the convergence data in table 2 is higher than before. Existing results for the 2D diffusion problems are shown in table 1 for comparison purposes. Results for the untrained (existing 2D model) and trained (specifically on 3D) networks are given in table 2.

Problem Type	**Data Set**	**Random Conv.**	**Lloyd Conv.**	**Full ML Conv.**	**ML Agg.**	**ML Int.**
Isotropic	Train	0.4652	0.4208	0.3956	0.3974	0.4190
Isotropic	Test	0.4623	0.4177	0.3913	0.3922	0.4172
Anisotropic	Train	0.7680	0.7705	0.7462	0.7532	0.7614
Anisotropic	Test	0.7902	0.7978	0.7727	0.7776	0.7910

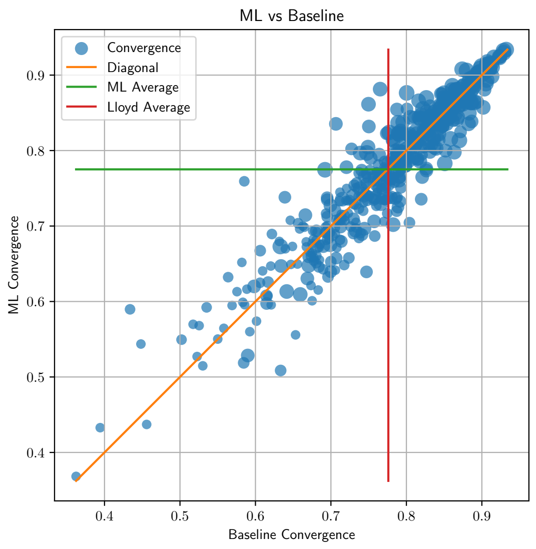
Table 1: Existing results for the 2D diffusion problems. This model has been trained on both isotropic and anisotropic diffusion in 2D. The column for *Full ML Conv.* is the method that uses the model for both aggregation and smoothing. *ML Agg.* and *ML Int.* refer to ML aggregation and Jacobi smoothing, Lloyd aggregation and ML smoothing, respectively.

Data Set	**Random Conv.**	**Lloyd Conv.**	**ML Conv.**
Iso., Train	0.5697	0.5855	0.5651
Iso., Test	0.5667	0.5780	0.5568
Aniso., Train	0.7761	0.7792	0.7751
Aniso., Test	0.7794	0.7834	0.7805

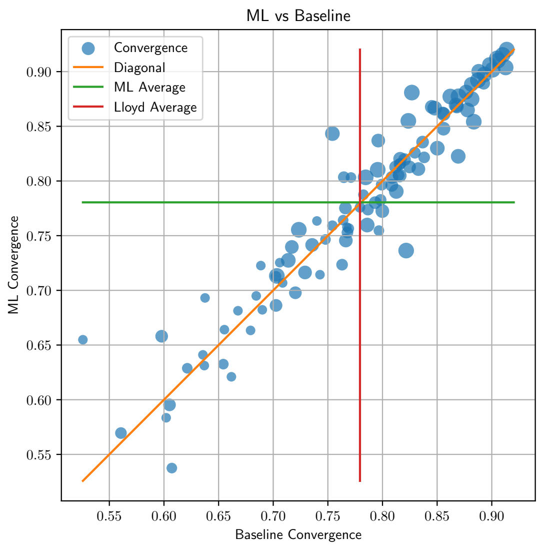
Table 2: Convergence of ML vs baseline, Lloyd methods on training, testing 3D datasets. This model was trained specifically on the 3D problems.

References

[1] F. Rathgeber, D. A. Ham, L. Mitchell, M. Lange, F. Luporini, A. T. T. McRae, G. Bercea, G. R. Markall, and P. H. J. Kelly, *Firedrake: automating the finite element method by composing abstractions*, CoRR, abs/1501.01809 (2015).

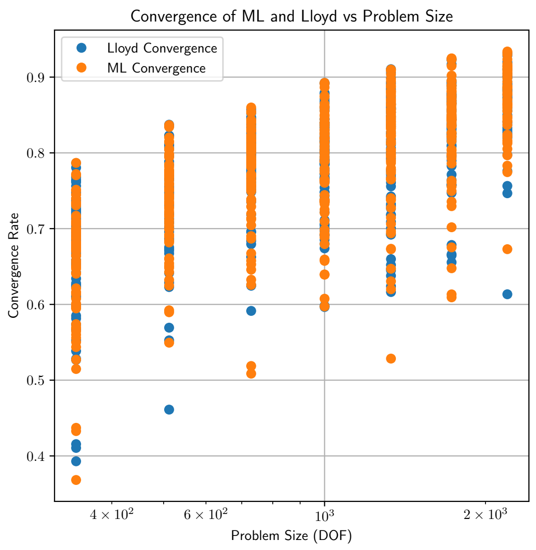


(a) Training convergence

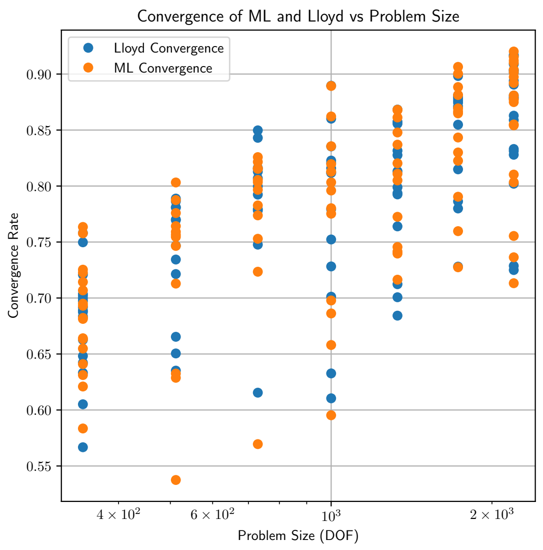


(b) Testing convergence

Figure 1: Convergence data for the ML AMG method vs a Lloyd and Jacobi SA method on the anisotropic datasets. Values below the diagonal indicate a better convergence for the ML. Markers are scaled by problem size.

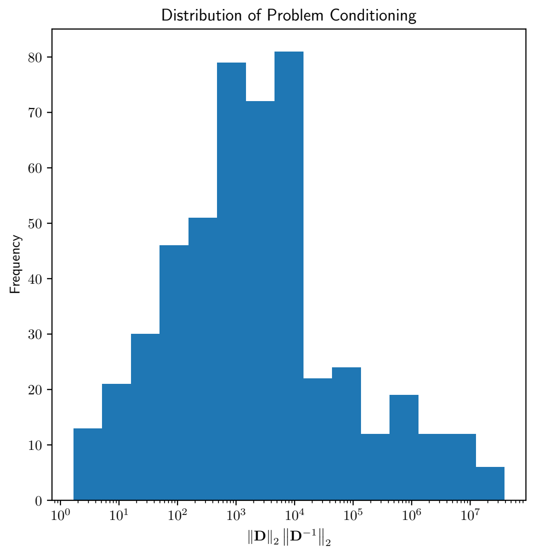


(a) Training convergence

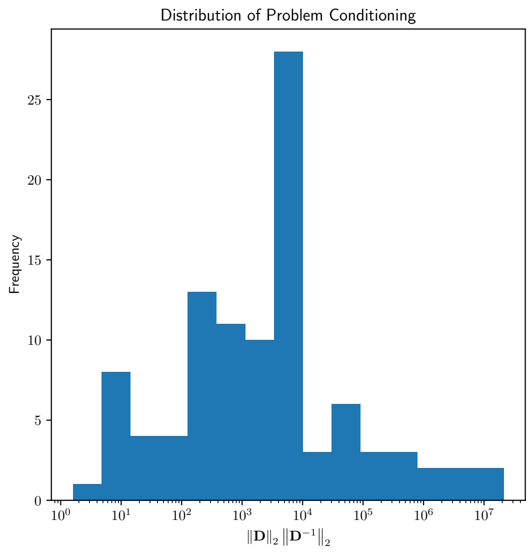


(b) Testing convergence

Figure 2: Convergence data for the two methods plotted against problem size (DOF) for anisotropic datasets.

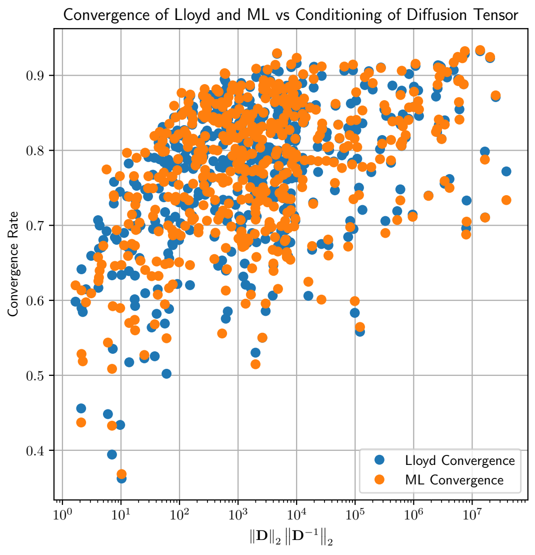


(a) Training Conditioning

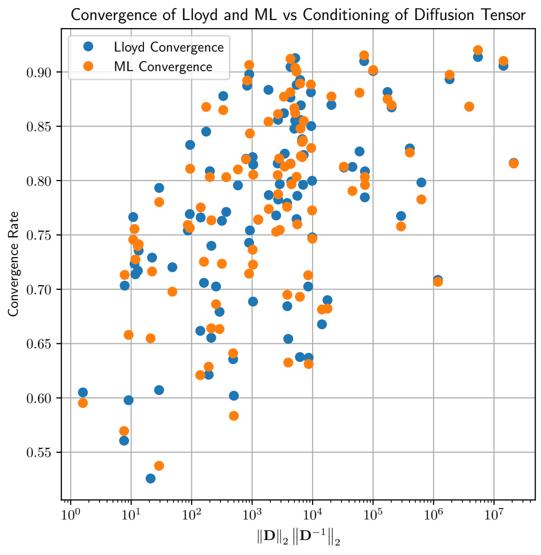


(b) Testing Conditioning

Figure 3: Histograms of problem conditioning for both anisotropic training and testing datasets.

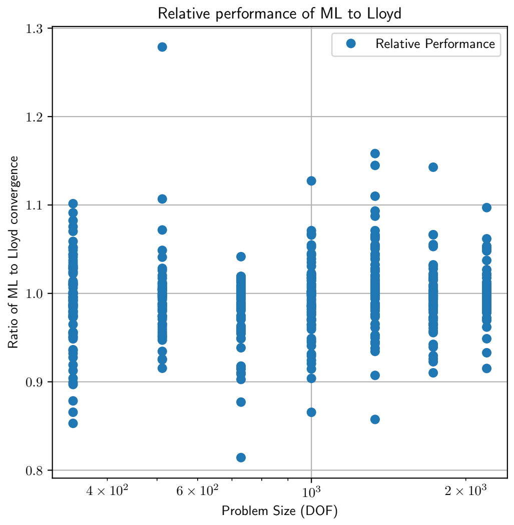


(a) Training Convergence

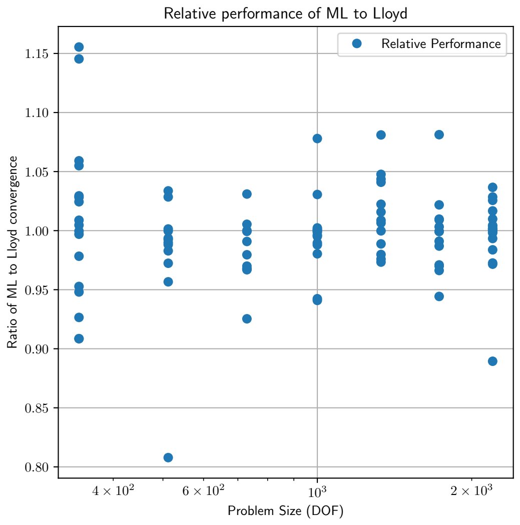


(b) Testing Convergence

Figure 4: Convergence on both anisotropic datasets per ratio of extremal eigenvalues of the diffusion tensor.



(a) Relative training performance



(b) Relative testing performance

Figure 5: Relative performance of the ML to the Lloyd method, plotted against problem size for the anisotropic datasets. Relative performance is obtained by dividing the ML convergence by the Lloyd convergence for each problem. Values below 1 indicate better ML performance, while values above 1 indicate better baseline performance.