Learning Algebraic Multigrid using Graph Neural Networks

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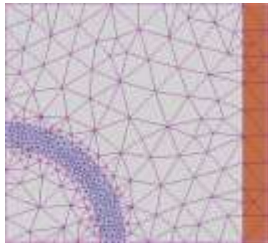
Goal: Large scale linear systems

- Solve $Ax = b$
- A is huge, need $O(n)$ solution!
- Some applications:
  - Discretization of PDEs



$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y)$$

  - Sparse graph analysis

Efficient linear solvers

- Decades of research on efficient iterative solvers for large-scale systems

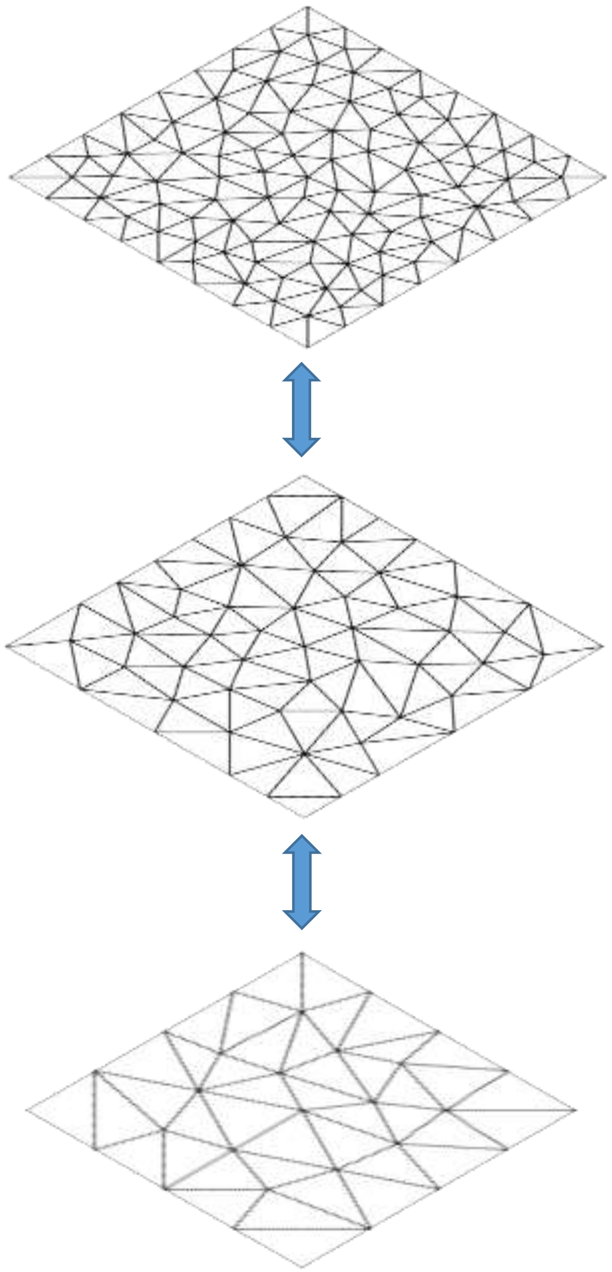
- We focus on Algebraic Multigrid (AMG) solvers

- Can we use machine learning to improve AMG solvers?

- Follow-up to Greenfeld et al. (2019) on *Geometric* Multigrid

What AMG does

- AMG works by successively **coarsening** the system of equations, and solving on multiple scales
- **Prolongation** operator P that creates the hierarchy
- We want to learn a mapping $P_\theta(A)$ with **fast convergence**



Learning P

- Unsupervised loss function over distribution $\mathcal{D}$:

$$\min_{\theta} \mathbb{E}_{A\sim\mathcal{D}}\, \rho\left(M\left(A, P_\theta(A)\right)\right)$$

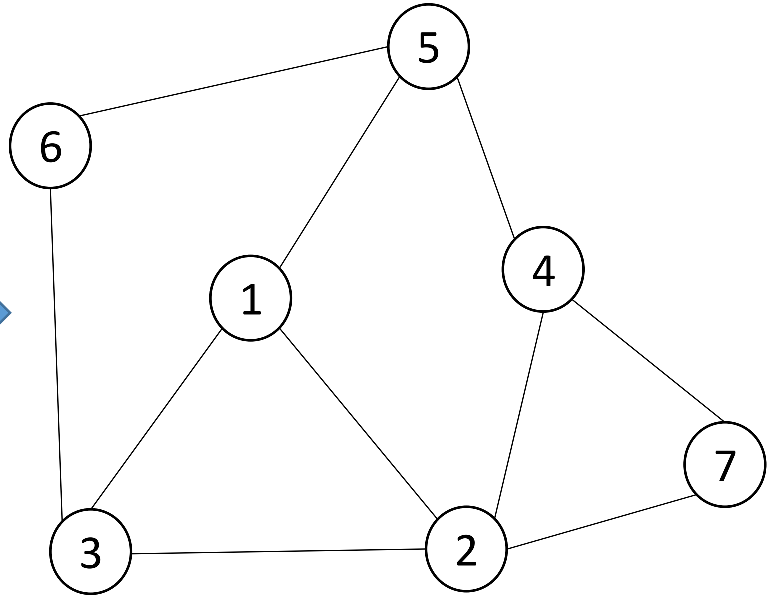
- $\rho\left(M\left(A, P_\theta(A)\right)\right)$ measures the convergence factor of the solver

- $P_\theta(A)$ is a NN mapping system A to prolongation operator P

Graph neural network

- Sparse matrices can be represented as graphs – we use a **Graph Neural Network** as the mapping $P_\theta(A)$

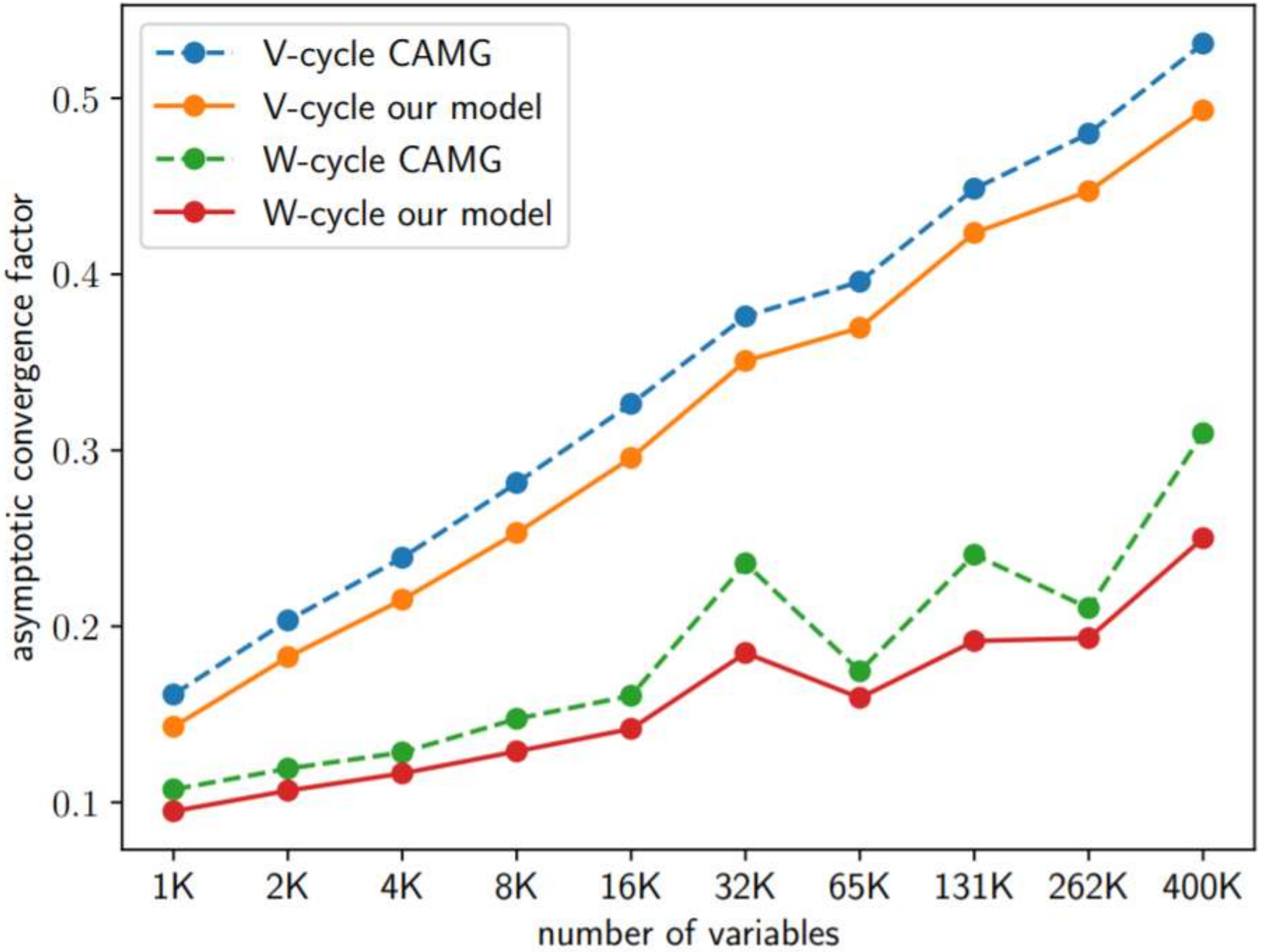
$$\begin{pmatrix} 2.7 & -0.5 & -0.5 & 0 & -1.7 & 0 & 0 \\ -0.5 & 7.7 & -4.9 & -0.6 & 0 & 0 & -1.7 \\ -0.5 & -4.9 & 6.2 & 0 & 0 & -0.8 & 0 \\ 0 & -0.6 & 0 & 2.9 & -0.6 & 0 & -1.7 \\ -1.7 & 0 & 0 & -0.6 & 13.1 & -10.8 & 0 \\ 0 & 0 & -0.8 & 0 & -10.8 & 11.6 & 0 \\ 0 & -1.7 & 0 & -1.7 & 0 & 0 & 3.4 \end{pmatrix}$$



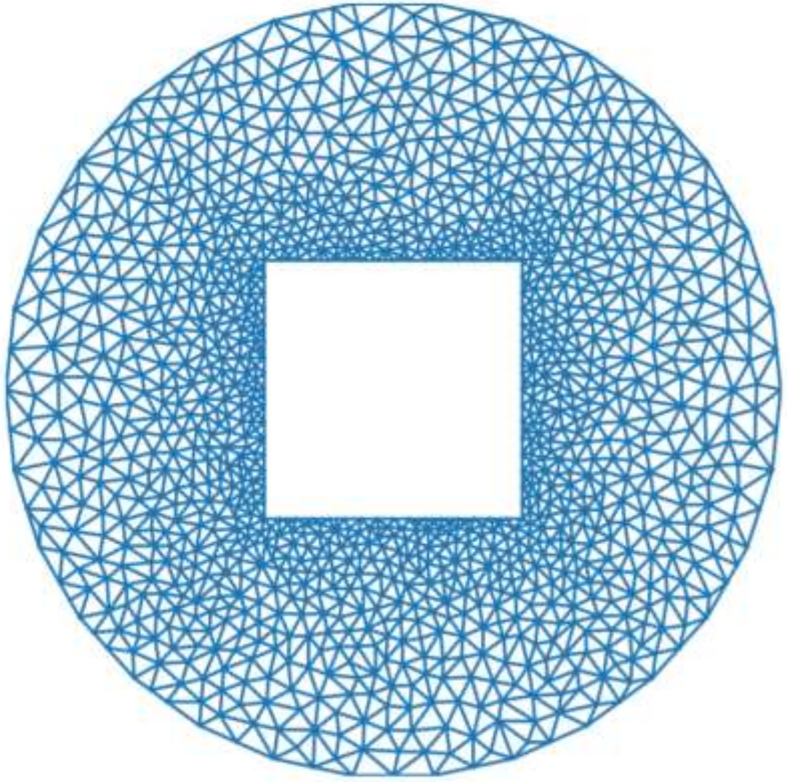
Benefits of our approach

- **Unsupervised training**– rely on algebraic properties
- **Generalization** –learn general *rules* for wide class of problems
- **Efficient training** – Fourier analysis reduces computational burden

Sample result; lower is better, ours is lower!



Finite Element PDE



Outline

- Overview of AMG
- Learning objective
- Graph neural network
- Results

1st ingredient of AMG: Relaxation

- System of equations: $a_{i1}x_1 + a_{i2}x_2 + \cdots a_{in}x_n = b_i$

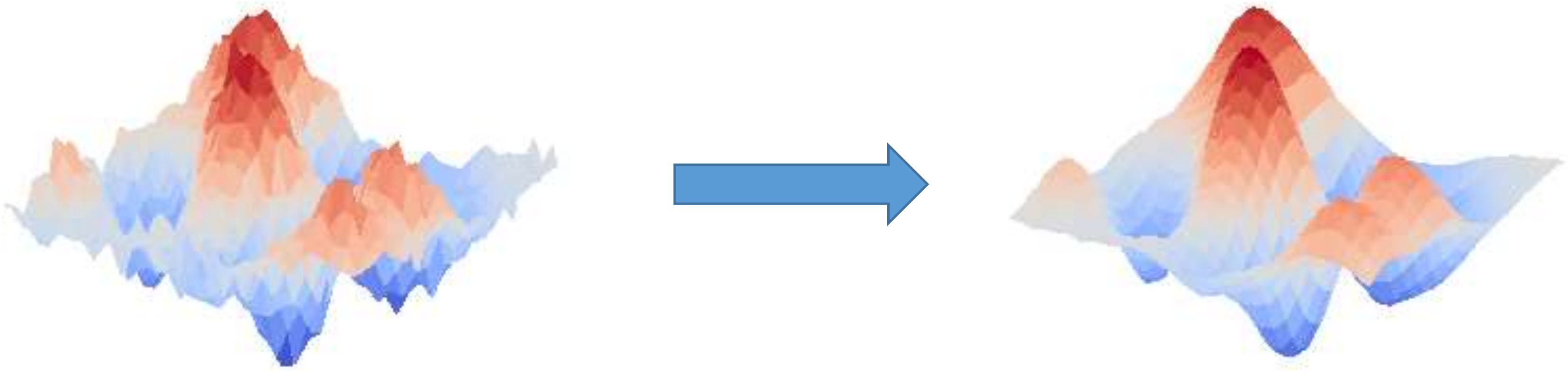
- Rearrange: $x_i = \frac{1}{a_{ii}}\left(b_i - \sum_{j \neq i} a_{ij}x_j\right)$

- Start with an **initial guess** $x_i^{(0)}$

- **Iterate** until convergence: $x_i^{(k+1)} = \frac{1}{a_{ii}}\left(b_i - \sum_{j \neq i} a_{ij}x_j^{(k)}\right)$

Relaxation smooths the error

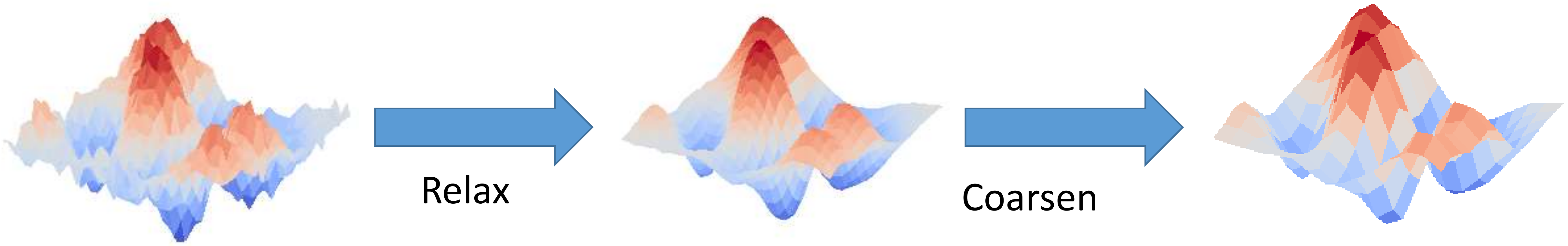
- Since relaxation is a local procedure, its effect is to **smooth out** the error



- How to accelerate relaxation by dealing with low-frequency errors?

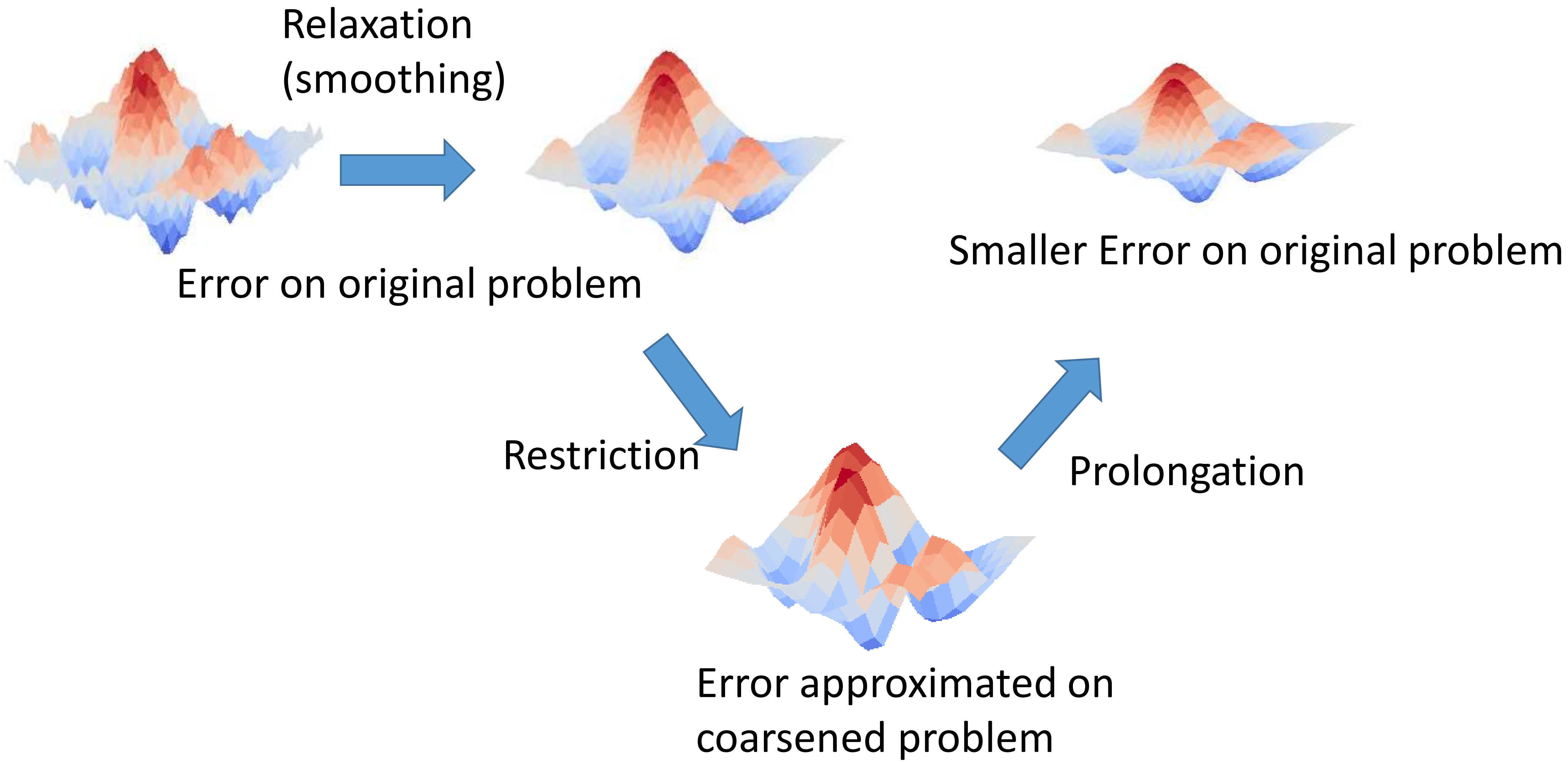
2nd ingredient of AMG: Coarsening

- Smooth error, and then **coarsen**



- Error is no longer smooth on coarse grid; relaxation is fast again!

Putting it all together

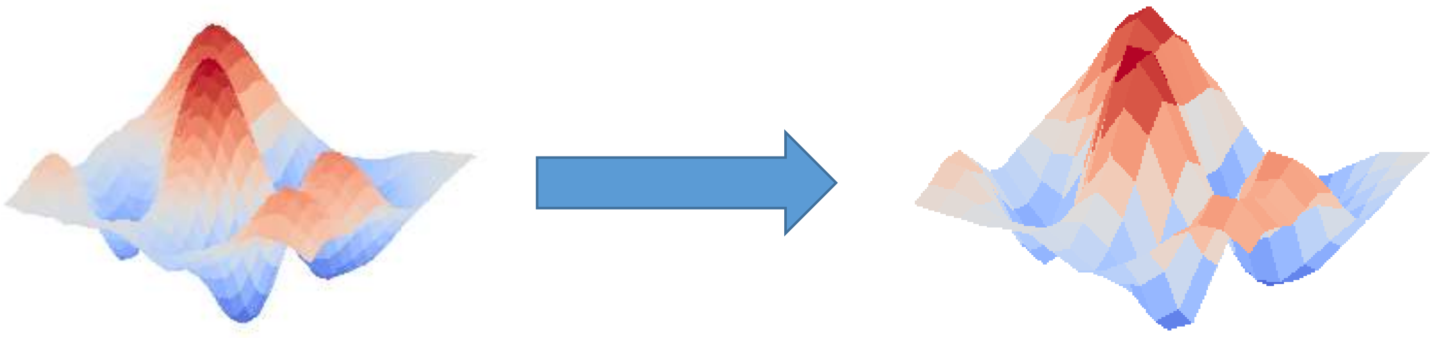


Learning objective

Prolongation operator

- Focus of AMG is prolongation operator P for defining scales and moving between them

- P needs to be sparse for efficiency, but also approximate well smooth errors



Learning P

- Quality can be quantified by estimating by how much the error is reduced each iteration:
  - $e^{(k+1)} = M(A,P)e^{(k)}$
  - $M(A,P) = S(I - P[P^T AP]^{-1}P^T A)S$
  - Asymptotically: $\|e^{(k+1)}\| \approx \rho(M)\|e^{(k)}\|$
  - Spectral radius: $\rho(M) = \max\{|\lambda_1|, \dots, |\lambda_n|\}$

- Our learning objective:

$$\min_\theta \mathbb{E}_{A\sim\mathcal{D}}\, \rho\left(M\left(A, P_\theta(A)\right)\right)$$

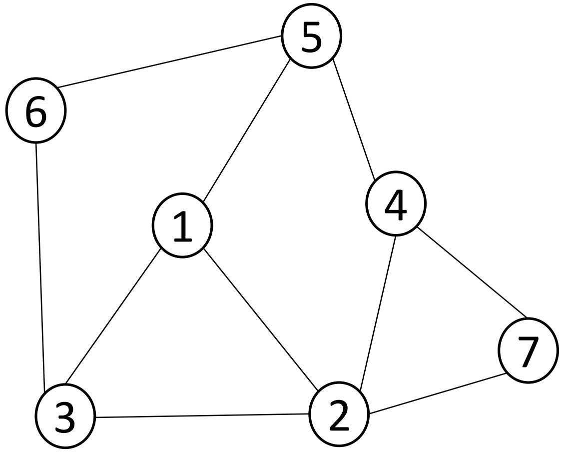
Graph neural network

Representing P_θ

- Sparse matrix $A \in \mathbb{R}^{n \times n}$ to sparse matrix $P \in \mathbb{R}^{n \times n_c}$
- Mapping should be **efficient**
- Matrices can be represented as graphs with edge weights

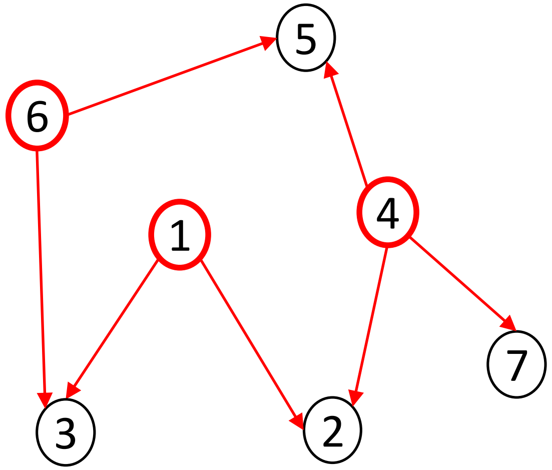
Representing P_θ

$$\begin{pmatrix} 2.7 & -0.5 & -0.5 & 0 & -1.7 & 0 & 0 \\ -0.5 & 7.7 & -4.9 & -0.6 & 0 & 0 & -1.7 \\ -0.5 & -4.9 & 6.2 & 0 & 0 & -0.8 & 0 \\ 0 & -0.6 & 0 & 2.9 & -0.6 & 0 & -1.7 \\ -1.7 & 0 & 0 & -0.6 & 13.1 & -10.8 & 0 \\ 0 & 0 & -0.8 & 0 & -10.8 & 11.6 & 0 \\ 0 & -1.7 & 0 & -1.7 & 0 & 0 & 3.4 \end{pmatrix}$$



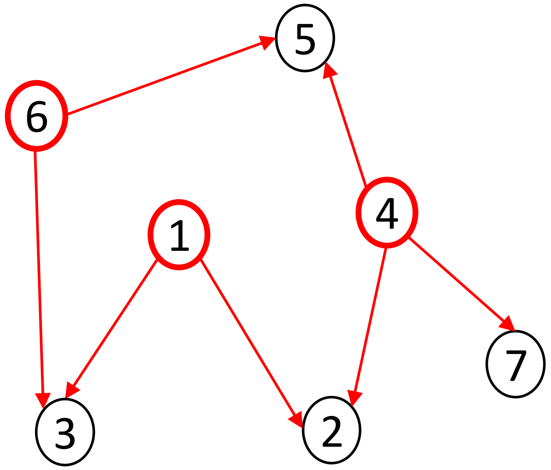
Input A

	1	4	6
1			
2			
3			
4			
5			
6			
7			



Sparsity pattern

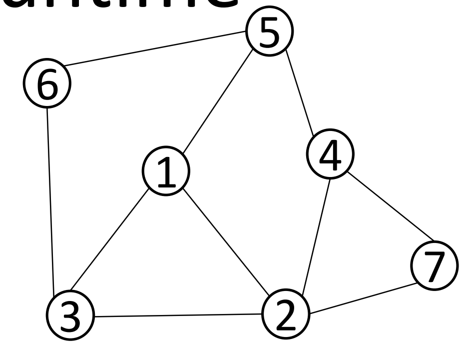
$$\begin{pmatrix} 1 & 0 & 0 \\ 0.3 & 0.7 & 0 \\ 0.9 & 0 & 0.1 \\ 0 & 1 & 0 \\ 0 & 0.2 & 0.8 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

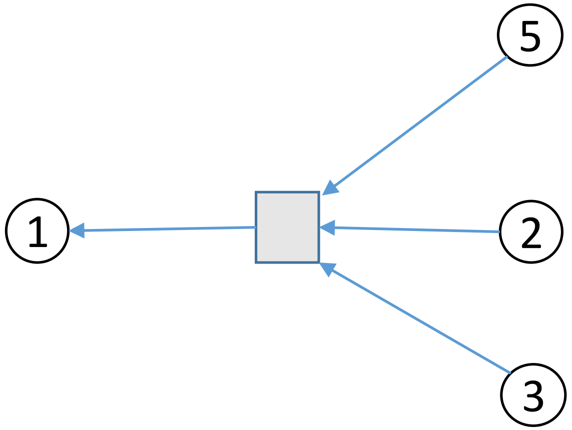


Output P

GNN architecture

- Message Passing architectures can handle any graph, and have $O(n)$ runtime





- Graph Nets framework from Battaglia et al. (2018) generalize many MP variants, handle edge features

Results

Spectral clustering

- Bottleneck is an iterative eigenvector algorithm that uses a linear solver

- Evaluate number of iterations required to reach convergence

- Train network on dataset of small 2D clusters, test on various 2D and 3D distributions

Conclusion

- Algebraic Multigrid is an **effective $\boldsymbol{O(n)}$ solver** for a wide class of linear systems $Ax = b$
- Main challenge in AMG is constructing **prolongation operator $\boldsymbol{P}$**, which controls how information is passed between grids
- We use an $O(n)$, **edge-based GNN** to learn a mapping $P_\theta(A)$, without supervision
- **GNN generalizes** to larger problems, with different distributions of sparsity pattern and elements

Take home messages

- In a well-developed field, might make sense to **apply ML to a part of the algorithm**

- Graph neural networks can be an effective tool for **learning sparse linear systems**