Non-Intrusive Parallel-in-Time Solvers for Challenging Problems

Research in Industry Projects for Students - On-site Presentation

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Institute for Pure & Applied Mathematics (IPAM)

Figure: Institute for Pure & Applied Mathematics (IPAM)

- IPAM is an NSF Math Institute located in the UCLA Campus
- IPAM fosters the interaction of mathematics with a broad range of science and technology, builds new interdisciplinary research communities, promotes mathematical innovation, and engages and transforms the world through mathematics.
- IPAM fulfills its mission through workshops and other programs that connect mathematics and other disciplines or multiple areas of mathematics.

Research in Industrial Projects (RIPS)

Figure: Research in Industrial Projects (RIPS)

- The RIPS Program provides an opportunity for undergraduates to work in teams on real-world research projects proposed by sponsors from industry or the public sector.
- RIPS offers stipend, travel allowance, housing and meals, site-visit with sponsors and support for participation in conferences
- 9 industry projects for 36 students, 12 of which are international
- 2024 projects: Aerospace Corporation, AMD, Analog Devices, LLNL, NASA Goddard, NASA Ames, RAND Corporation, Relay Therapeutics, SimCorp

Parallel-in-Time (PinT) Motivation

- Processor clock speeds are stagnant, while the number of cores is increasing.
- Need arises for parallel algorithms to take advantage of increasing cores.

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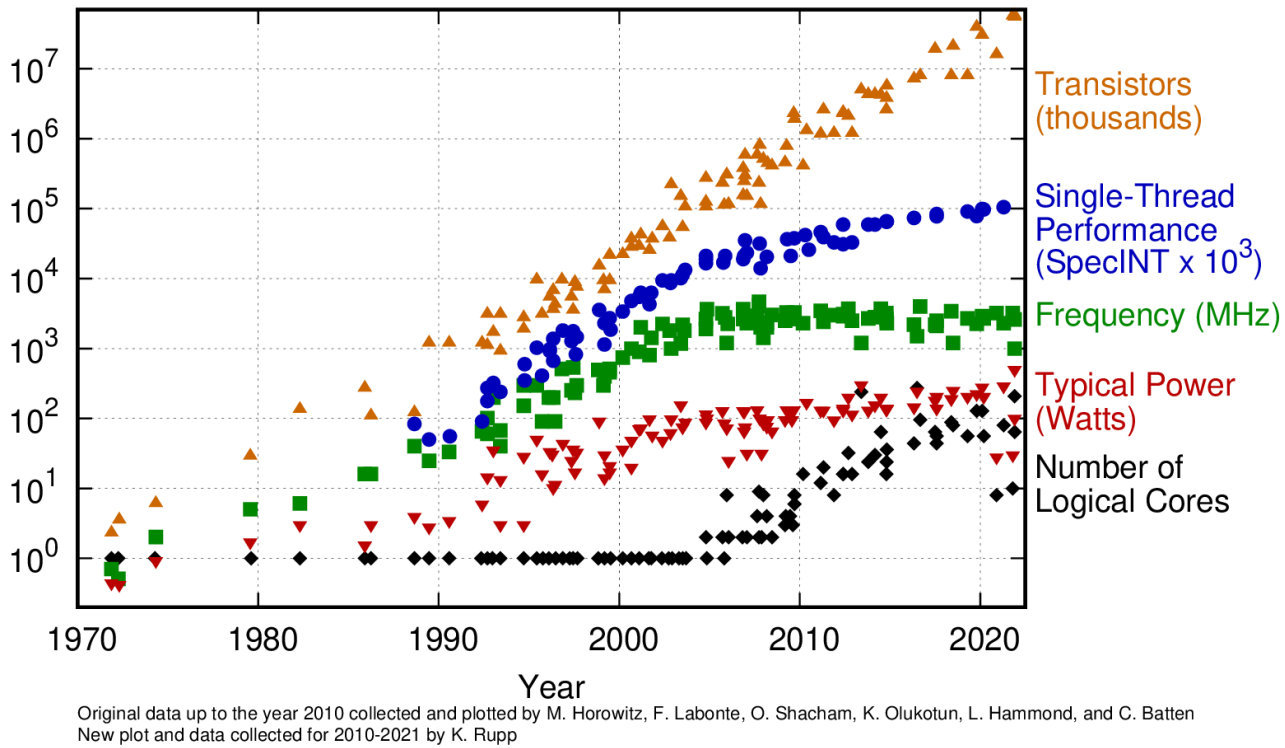

Figure: Stagnation of processor speed

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Non-Intrusive:

- Little effort and code are required
- More general approach and leverages experts on the library team

Discretization using finite difference

$$-u_{xx} = f$$

Let $u_i \approx u(x_i)$.
We can use the finite difference approximation

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Assuming Dirichlet boundary conditions, we can write this in a linear system $A\mathbf{u} = \mathbf{f}$:

$$\frac{1}{\delta x^2}\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & & \vdots \\ 0 & -1 & \ddots & & 0 \\ \vdots & & & & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix}\begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_M \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_M \end{pmatrix}.$$

Relaxation with splitting: Jacobi and Gauss-Seidel

$$\mathbf{x}_{k+1} = \mathbf{x}_k + M^{-1}(\mathbf{b} - A\mathbf{x}_k), \quad A = M + N$$

Let $A = L + D + U$, where L is lower triangular, D is diagonal, and U is upper triangular.

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Relaxation methods and Multigrid

Relaxation methods are better at correcting oscillatory errors.

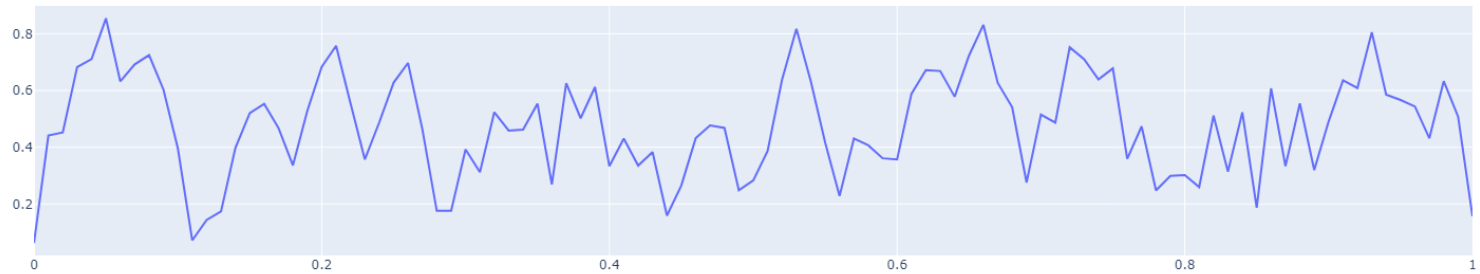

Figure: Fine Grid Iteration 0

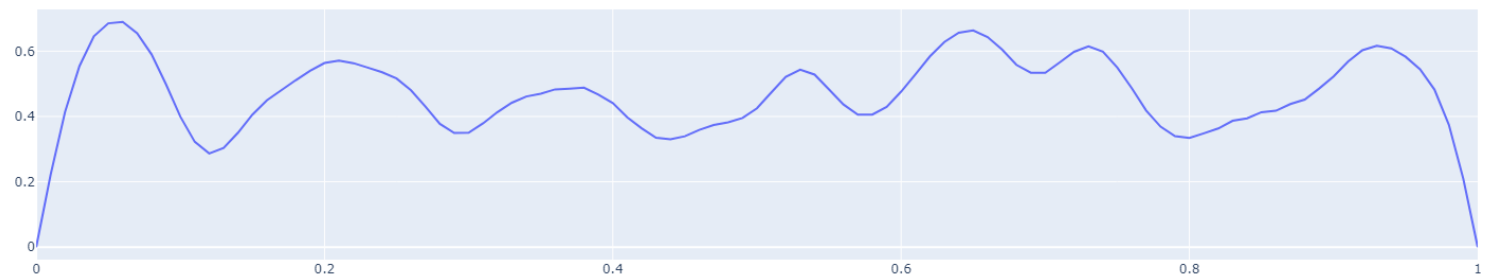

Figure: Fine Grid Iteration 5

Multigrid: the V-cycle

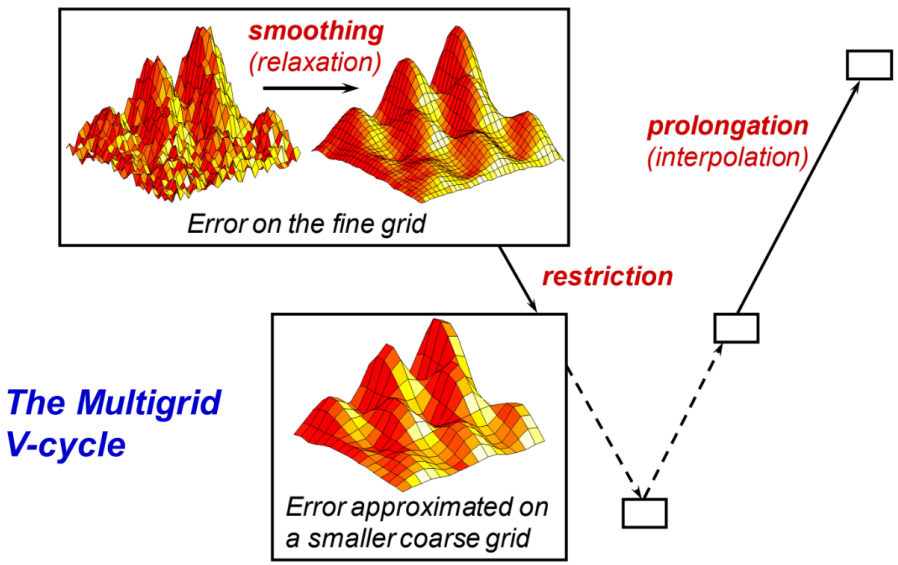

Figure: Multigrid V-cycle

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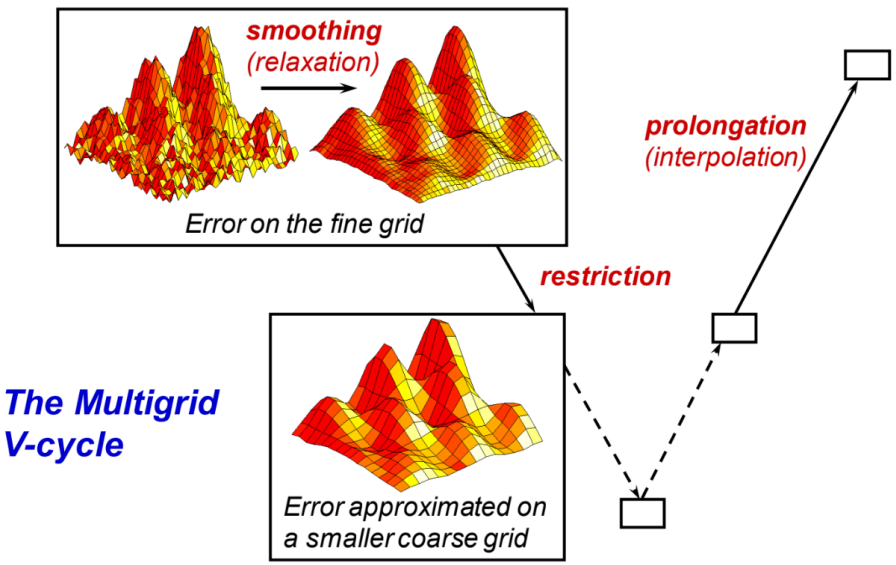

Figure: Multigrid V-cycle

- Multigrid attacks the weakness of relaxation methods by going through a hierarchy of grid sizes.
- Low-frequency (smooth) errors on the fine grid turn into high-frequency (oscillatory) error on the coarser grid and are corrected more effectively through relaxation.

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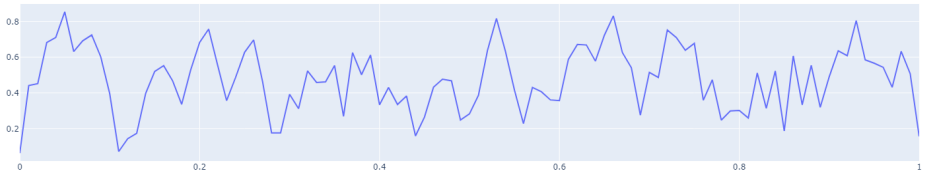

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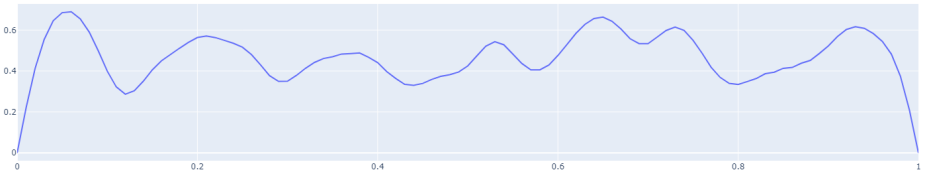

Figure: Fine Grid Iteration 5

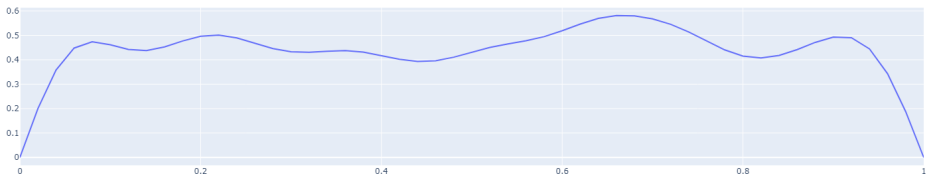

Figure: Coarse Grid Iteration 0

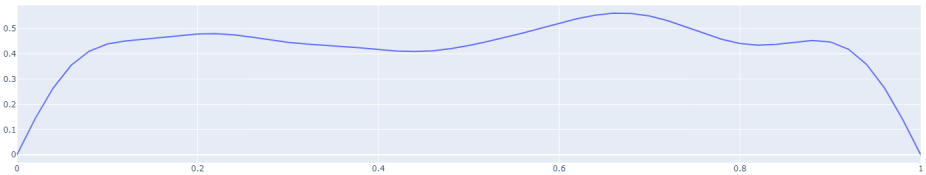

Figure: Coarse Grid Iteration 5

Multigrid reduction in time (MGRIT)

MGRIT algorithm is a parallel-in-time approach for solving time dependent problems that is designed to be non-intrusive.

MGRIT

Consider the diffusion equation $u_t - u_{xx} = f$ with the following discretization

$$u_t \approx \frac{u_j^{i+1} - u_j^i}{\delta t}, \quad -u_{xx} \approx \frac{-u_{j-1}^i + 2u_j^i - u_{j+1}^i}{\delta x^2}$$

where $u_j^i \approx u(x_j, t_i)$.

Using Forward Euler, we get the update rule

$$\mathbf{u}^i = \Phi \mathbf{u}^{i-1} + \delta t \mathbf{f}^{i-1} \text{ for } i = 1, 2 \ldots, n \text{ and } \mathbf{u}^0 = \mathbf{g}^0,$$

where $\mathbf{u}^i \approx \begin{bmatrix} u_0^i & u_1^i & \cdots & u_N^i \end{bmatrix}^T$ and Φ has the stencil $[\beta \;\; 1-2\beta \;\; \beta]$, where $\beta = \delta t / \delta x^2 \leq 1/2$ by the CFL constraint.

MGRIT: the coarse-grid operator

Using the partition below, we let $t_i = i\delta t$ for the fine time grid and $T_i = mi\delta t$ for the coarse time grid with coarsening factor m.

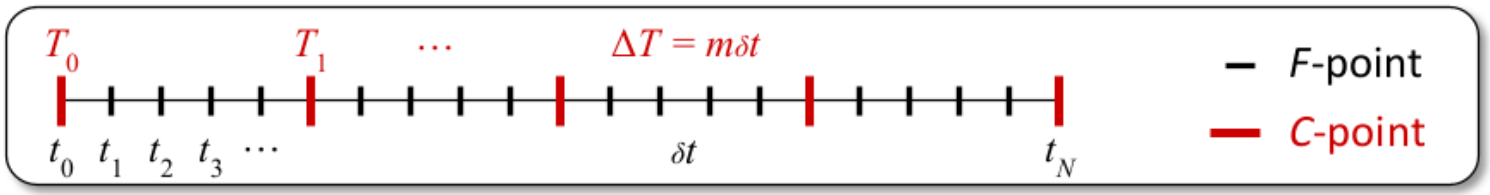

Figure: Coarse and fine time grids

Then to solve each coarse time step is to solve the following system

$$T(m)\mathbf{u} = \begin{pmatrix} I & & & & \\ -\Phi^m & I & & & \\ & -\Phi^m & I & & \\ & & \ddots & \ddots & \\ & & & -\Phi^m & I \end{pmatrix} \begin{pmatrix} u_0 \\ u_m \\ u_{2m} \\ \vdots \\ u_N \end{pmatrix} = \mathbf{f}.$$

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So we have the "target matrix" $T(m)$ which we want to approximate with some matrix A

$$T(m) = \begin{pmatrix} I & & & \\ -\Phi^m & I & & \\ & \ddots & \ddots & \\ & & -\Phi^m & I \end{pmatrix}, \quad A = \begin{pmatrix} I & & & \\ -\Psi & I & & \\ & \ddots & \ddots & \\ & & -\Psi & I \end{pmatrix}.$$

Approximating the coarse-grid operator (cont'd)

$$T(m) = \begin{pmatrix} I & & & \\ -\Phi^m & I & & \\ & \ddots & \ddots & \\ & & -\Phi^m & I \end{pmatrix}, \quad A = \begin{pmatrix} I & & & \\ -\Psi & I & & \\ & \ddots & \ddots & \\ & & -\Psi & I \end{pmatrix}$$

For a good approximation, we want A to be *spectrally equivalent* to $T(m)$, i.e. the following is bounded independent of problem size

$$\|I - AT^{-1}\|.$$

$$\begin{aligned} \|I - AT^{-1}\| &= \sup_x \frac{\|(I - AT^{-1})x\|}{\|x\|} \\ &= \sup_y \frac{\|(T - A)y\|}{\|Ty\|} \end{aligned}$$

Implementation of basic concepts

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- We worked on some examples of using neural networks to solve ODEs and matrix approximation.

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- By changing the step function, we have worked on the Forward Euler (explicit) version of the equation.
- We have integrated machine learning.

Why Machine Learning?

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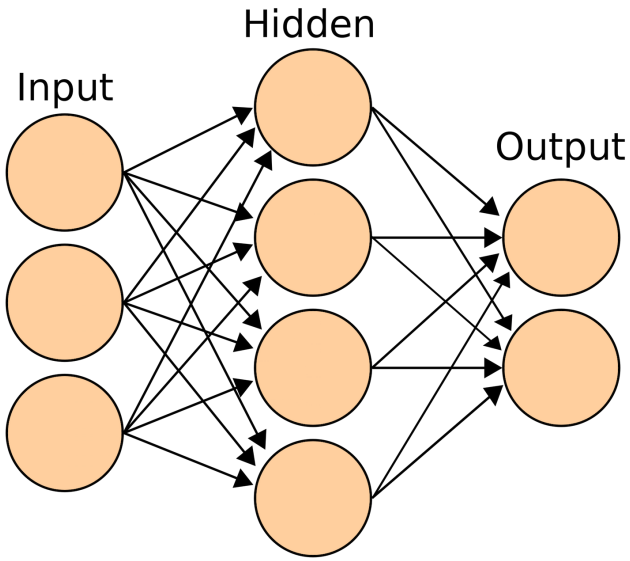
We want a "non-intrusive" way to estimate coarse-grid operators.
Machine learning is good at coming up at more general solutions.

Current Neural Network Architecture

For 1D diffusion problem:
Input: $(\phi, m) \in \mathbb{R}^3 \times \mathbb{R}$.
Output: $\psi \in \mathbb{R}^3$.



ϕ is the "stencil" of Φ. For example, in our periodic problem,

$$L = \frac{1}{\delta x^2} \begin{bmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{bmatrix},$$

and $\Phi = I - \delta t L$ has stencil
$\phi = \begin{bmatrix} \beta & 1 - 2\beta & \beta \end{bmatrix}$ where $\beta = \delta t / \delta x^2$

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- Recall, the ℓ^2 norm of a vector $v \in \mathbb{R}^d$ is $\|v\|_{\ell^2}^2 = v_1^2 + \cdots + v_d^2$.
- The norm of a matrix is defined as the induced 2-norm (or spectral norm)

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$$\|A\| = \sup_{0 \neq v \in \mathbb{R}^d} \frac{\|Av\|_{\ell^2}}{\|v\|_{\ell^2}}.$$

- Equivalently, this is the largest magnitude of eigenvalue of A.

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1st Loss function

$$\mathcal{L}_1 = \frac{\|Ty_k - Ay_k\|^2}{\|Ty_k\|^2} = \frac{\sum_r (T_r y_k - A_r y_k)^2}{\sum_r (T_r y_k)^2} \leq \sum_r \frac{(T_r y_k - A_r y_k)^2}{(T_r y_k)^2}$$

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where T_r, A_r denote row r of T and A respectively.

By focusing on one row, and letting $y_k(i)$ be the restriction of y_k to the coarse time point i, we obtain a simplified expression

$$\mathcal{L}_1' = \sum_{k=1}^K \frac{((\Phi^m)_r y_k - \Psi_r y_k(i))^2}{(1 - (\Phi^m)_r y_k(i))^2}.$$

Loss Function 2

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Let (λ_k, y_k) be the orthogonal eigenpairs of Φ^m, sorted such that $\lambda_i \geq \lambda_{i+1}$. Let $K \leq d$.
Then we get the following loss function

2nd Loss Function

$$\mathcal{L}_2 = \sum_{k=1}^{K} \|\Phi^m y_k - \Psi y_k\|_{\ell^2}^2.$$

Loss Function 3

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Consider (λ_k, y_k) be orthogonal eigenpairs of Φ, sorted such that $|\lambda_i| \geq |\lambda_{i+1}|$. Let $K \leq d$ be the number of testing vectors.
By expanding out the ℓ_2 norm of the vectors, if $M = N/m$ be the number of block rows of $T(V)$, then we have a new loss function.

3rd Loss Function

$$\mathcal{L}_3 = \sum_{k=1}^{K} \frac{(M-1)\|\Phi^m y_k - \Psi y_k\|_{\ell^2}^2.}{(1+(M-1)|\lambda_k^m - 1|)^2}$$

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- For example, for the equation $u_t = u_{xx}$, if we consider N gridpoints, then the eigenvalues are given by

$$\lambda_k = 1 - 2\beta\left(1 - \cos\left(\frac{k\pi}{N+1}\right)\right), 1 \leq k \leq N$$

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  where $\beta = \delta t/\delta x^2 \leq 1/2$.
- This makes approximation for Ψ easier as smaller eigenvalues' decay faster.
- However, the distribution of $|\lambda_k|$ varies between different types of PDEs (hyperbolic, elliptic, etc).

Loss Functions we are comparing

- $\mathcal{L}_1 = \sum_{k=1}^{K} \frac{((\Phi^m)_r y_k - \Psi_r y_k(i))^2}{(1-(\Phi^m)_r y_k(i))^2 + \epsilon}$ where y_k are random vectors with an additional constant vector of all 1's, and ϵ is added to avoid dividing by zero.
- $\mathcal{L}_1 = \sum_{k=1}^{K} \frac{((\Phi^m)_r y_k - \Psi_r y_k(i))^2}{(1-(\Phi^m)_r y_k(i))^2 + \epsilon}$ where y_k are largest eigenvectors of Φ.
- $\mathcal{L}_2 = \sum_{k=1}^{K} \|\Phi^m y_k - \Psi y_k\|_{\ell^2}^2$ where y_k are largest eigenvectors of Φ.
- $\mathcal{L}_3 = \sum_{k=1}^{K} \frac{(M-1)\|\Phi^m y_k - \Psi y_k\|_{\ell^2}^2.}{(1+(M-1)|\lambda_k^m - 1|)^2}$ where (λ_k, y_k) are largest pairs of eigenvalues and eigenvectors of Φ

Loss Functions we are comparing (cont'd)

We also consider modifications of the preceding loss functions, including:

- Using eigenvectors instead of random vectors for $\mathcal{L}_1$.
- Adding the constant vector of all 1s to the test vector list for $\mathcal{L}_2, \mathcal{L}_3$ and $\mathcal{L}_1$ with eigenvectors.

Loss Function Landscapes

Consider the problem set up with

$$\delta x = \frac{1}{16}, \quad \delta t = \frac{1}{4096}, \quad \beta = \frac{1}{16} \quad m = 4$$

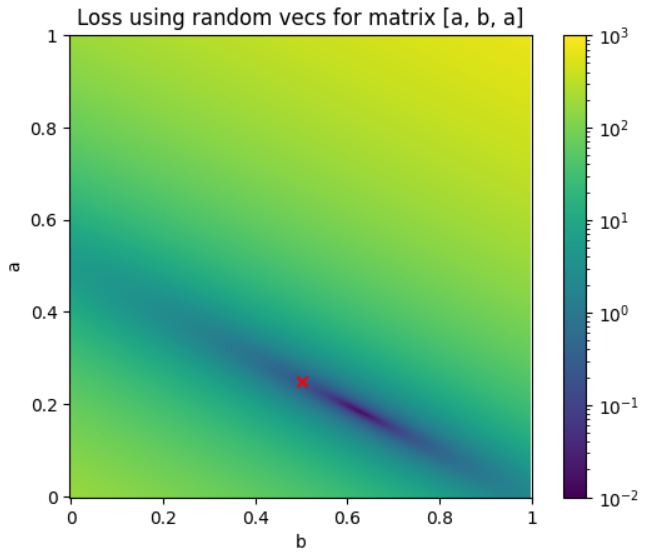
The stencil for $\Phi = \begin{bmatrix} 0.0625 & 0.8750 & 0.0625 \end{bmatrix}$, and our input to the loss function is $[0.0625, 0.8750, 0.0625, 4.0000]$.
The re-discretization stencil is $\begin{bmatrix} 0.2500 & 0.5000 & 0.2500 \end{bmatrix}$

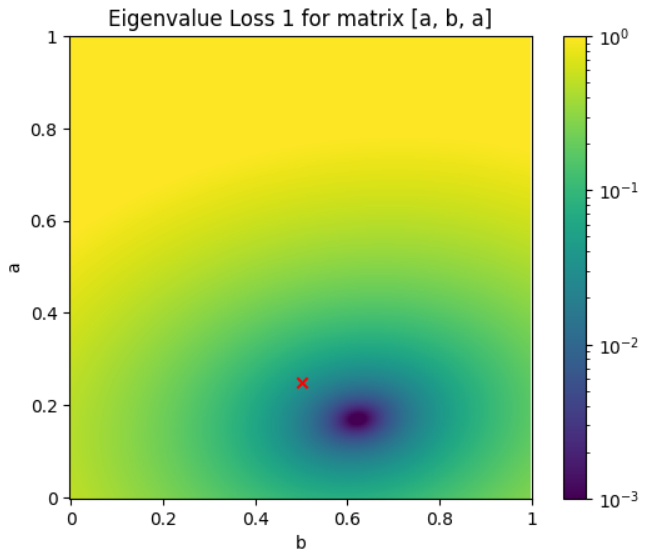
If we restrict the approximation Ψ to have stencil of the form $\begin{bmatrix} a & b & a \end{bmatrix}$, we can plot the loss at (a, b) for each loss function.

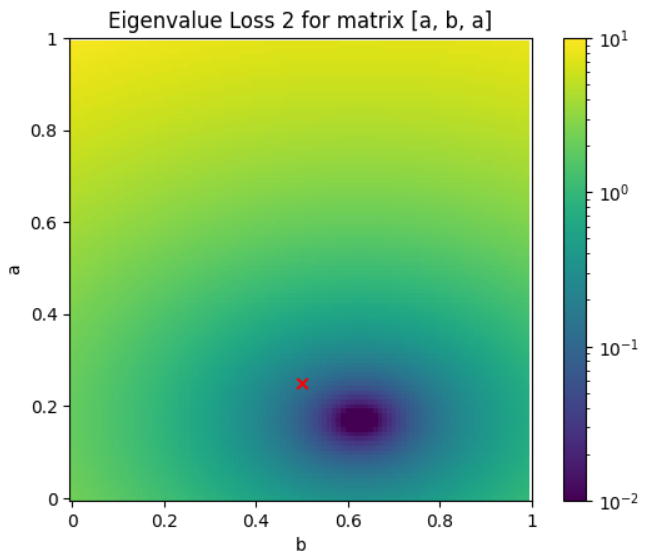
This allows us to observe the loss landscape for each loss function, as well as where the re-discretization stencil, which we know converges well in PyMGRIT, lies.

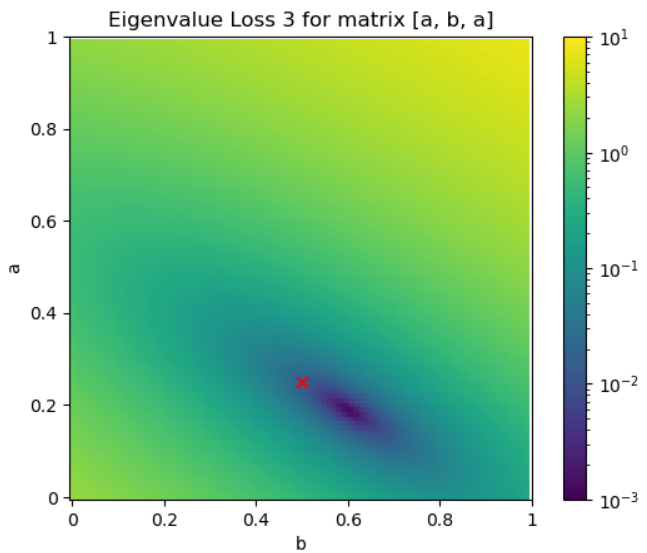
Loss Function Landscapes (cont'd)

x is the re-discretization stencil.









Loss Function Landscapes (cont'd)

$\mathcal{L}_1$ with eigenvectors vs eigenvectors and constant vector.

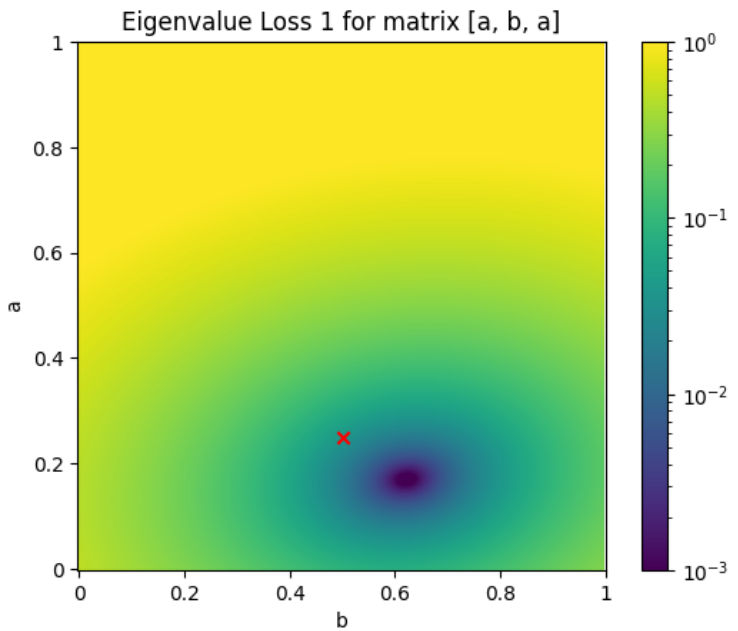


Figure: $\mathcal{L}_1$ with evecs

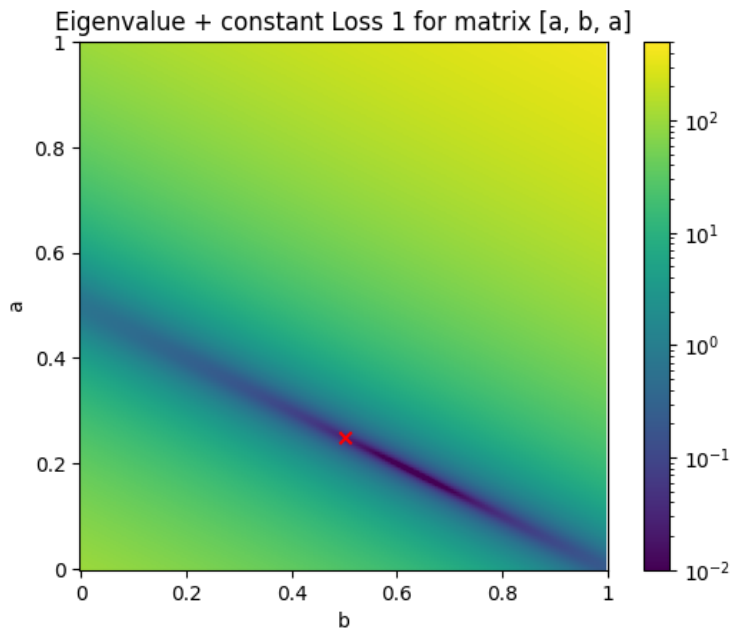


Figure: $\mathcal{L}_1$ with evecs and the constant vector

Loss Function Landscapes (cont'd)

$\mathcal{L}_2$ with eigenvectors vs eigenvectors and constant vector.

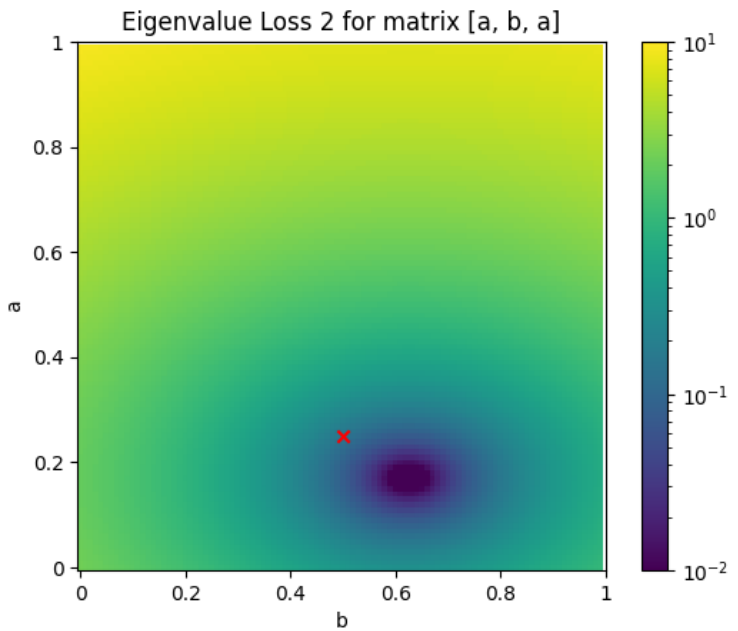


Figure: $\mathcal{L}_2$ with evecs

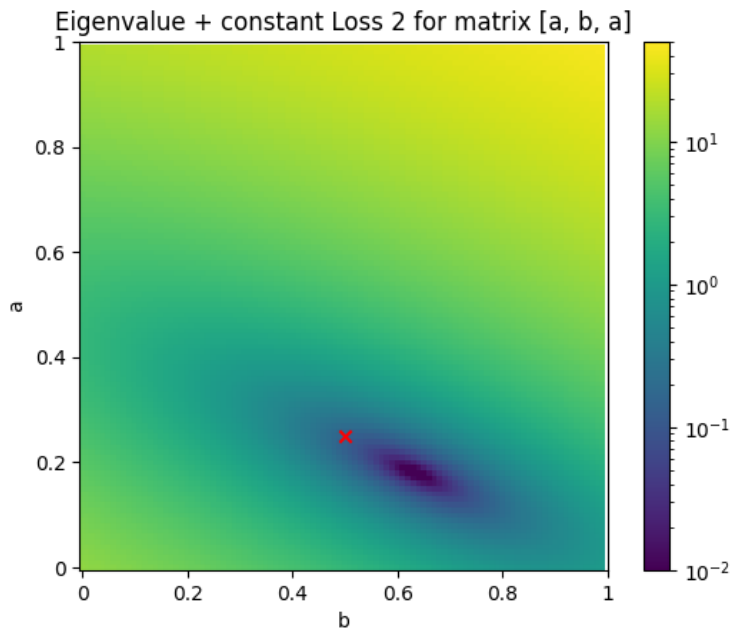


Figure: $\mathcal{L}_2$ with evecs and the constant vector

Loss Function Landscapes (cont'd)

$\mathcal{L}_3$ with eigenvectors vs eigenvectors and constant vector.

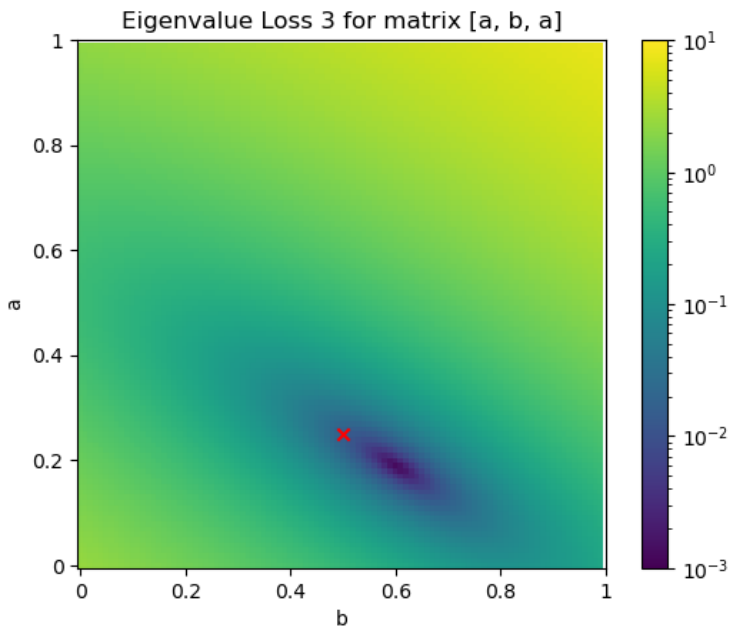


Figure: $\mathcal{L}_3$ with evecs

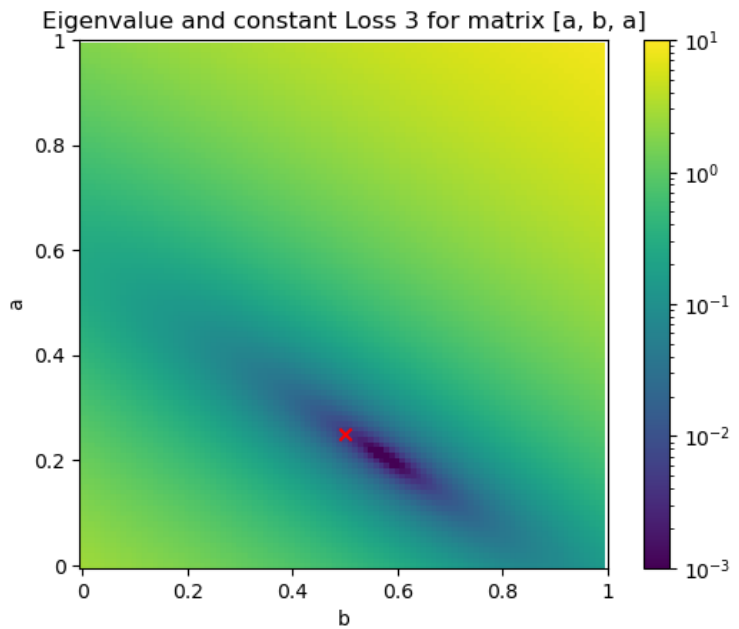


Figure: $\mathcal{L}_3$ with evecs and the constant vector

Performance of optimal stencil in PyMGRIT

$$\delta x = \frac{1}{16}, \quad \delta t = \frac{1}{4096}, \quad m = 4$$

Loss Function	optimal stencil			Residual	Conv. Factor
$\mathcal{L}_1$ Random	[0.1814	0.6324	0.1814]	6.60e-5	4.04e-1
$\mathcal{L}_1$ EVecs	[0.1700	0.6221	0.1700]	2.13e-2	9.40e-1
$\mathcal{L}_1$ EVecs, const.	[0.1824	0.6341	0.1824]	6.60e-6	2.82e-1
$\mathcal{L}_2$	[0.1705	0.6223	0.1705]	2.11e-2	9.59e-1
$\mathcal{L}_2$ const.	[0.1797	0.6346	0.1797]	1.55e-4	4.17e-1
$\mathcal{L}_3$	[0.1831	0.6105	0.1831]	9.33e-2	9.72e-1
$\mathcal{L}_3$ const.	[0.1990	0.5887	0.1990]	6.16e-2	8.80e-1
Re-disc	[0.2500	0.5000	0.2500]	1.73e-8	9.93e-2

Neural Network Testing Setup

Training set: $\beta \in \{1/8, 1/12, 1/16, 1/24\}$, $m = \{1, 2, 3, 4\}$ (4 stencils).
Test problem: $\beta = 1/10$, $\delta x = 1/16, \delta t = 1/2560$. In PyMGRIT, $n_t = 2561$, $n_x = 17$.

We use a feedforward neural network with 3 hidden layers of 50 neurons each with the LeakyReLU activation function.

Neural Network Results ($m = 2$)

Loss Function	Output Stencil	Output Loss	Redisc. Loss
$\mathcal{L}_1$ Random	$[0.131, 0.743, 0.131]$	0.177	0.143
$\mathcal{L}_1$ Evecs	$[0.127, 0.726, 0.121]$	6.75e-3	6.15e-3
$\mathcal{L}_1$ Evecs, const.	$[0.159, 0.693, 0.150]$	1.21e-3	4.83e-3
$\mathcal{L}_2$	$[0.128, 0.733, 0.120]$	4.03e-2	3.48e-2
$\mathcal{L}_2$ const.	$[0.130, 0.738, 0.125]$	4.15e-2	3.48e-2
$\mathcal{L}_3$	$[0.135, 0.720, 0.136]$	8.92e-3	1.31e-1
$\mathcal{L}_3$ const.	$[0.138, 0.716, 0.138]$	8.62e-3	3.62e-3
Re-disc.	$[0.200, 0.600, 0.200]$	—	—

PyMGRIT Results ($m = 2$)

Loss Function	Output Stencil	Residual	Conv. Factor
$\mathcal{L}_1$ Random	$[0.131, 0.743, 0.131]$	2.28	5.74e-1
$\mathcal{L}_1$ Evecs	$[0.127, 0.726, 0.121]$	1.85e-2	9.42e-1
$\mathcal{L}_1$ Evecs, const.	$[0.159, 0.693, 0.150]$	2.07e-4	4.03e-1
$\mathcal{L}_2$	$[0.128, 0.733, 0.120]$	1.13e-2	9.03e-1
$\mathcal{L}_2$ const.	$[0.130, 0.738, 0.125]$	1.69e-3	6.3e-1
$\mathcal{L}_3$	$[0.135, 0.720, 0.136]$	5.00e-2	8.86e-1
$\mathcal{L}_3$ const.	$[0.138, 0.716, 0.138]$	2.27e-2	7.21e-1
Re-disc.	$[0.200, 0.600, 0.200]$	7.60e-8	6.77e-2

Next steps

- 1D Diffusion only proof-of-concept – generalize to more types of PDEs, such as advection (which is harder for MGRIT).
- Currently, Ψ hard-coded to be tridiagonal. For larger coarsening factors, larger stencil may result in better convergence. Use second neural network to select nonzero entries of Ψ, following Ru Huang et als' paper.
- Use bootstrapping ideas:
  - Use the output to train the model.
  - Solve $A\mathbf{u} = \mathbf{0}$ to generate error vectors and update the training set with them.
- Work on periodic condition.

Acknowledgement

- Thank you for listening!
- Questions?