ETH zürich

First Optimize, Then Discretize for SciML

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Today's Talk

Part I – Function Space Optimization for SciML

Discretize function space algorithms in the tangent space of a neural network ansatz[1]

- Develop optimizers that provably mimic function space dynamics
- Design new algorithms and understand existing ones within this framework

Part II – Function Space Optimization at Scale

Scale the function space algorithms to millions of parameters[2]

- Leverage the Kronecker structure of linear layer Jacobians to approximate curvature matrices

[1] J. Müller and M. Zeinhofer (2024). "Position: Optimization in SciML Should Employ the Function Space Geometry". In: *Forty-first International Conference on Machine Learning*.

[2] F. Dangel, J. Müller, and M. Zeinhofer (2024). "Kronecker-Factored Approximate Curvature for Physics-Informed Neural Networks". In: *Advances in Neural Information Processing Systems*.

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Scientific Machine Learning

When referring to Scientific Machine Learning (SciML) we mean:

- Operator Learning[3]
- Variational Monte Carlo for Schrödinger's equation with NN ansatz[4]
- PINNs, Deep Ritz, etc.[5]
- Anything involving PDEs and neural networks

Observation

Introducing PDEs to objective functions complicates neural network training drastically.

[3] Z. Li, N. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, and A. Anandkumar (2021). "Fourier Neural Operator for Parametric Partial Differential Equations". In: *International Conference on Learning Representations*.

[4] D. Pfau, J. S. Spencer, A. G. Matthews, and W. M. C. Foulkes (2020). "Ab Initio Solution of the Many-Electron Schrödinger Equation with Deep Neural Networks". In: *Physical Review Research* 2.3, p. 033429.

[5] M. Raissi, P. Perdikaris, and G. E. Karniadakis (2019). "Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations". In: *Journal of Computational Physics* 378, pp. 686–707.

Optimization in SciML is a Challenge

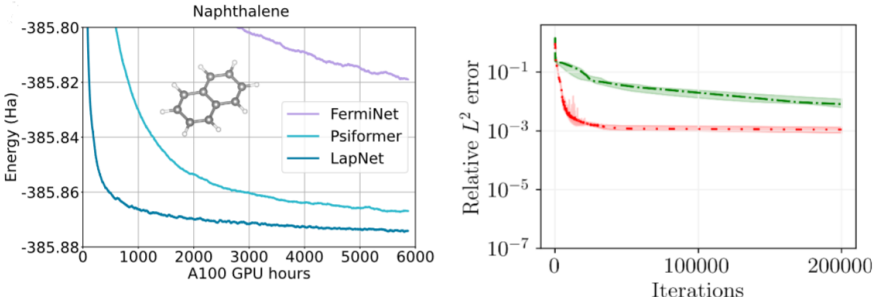


Figure: Illustration of neural network wavefunction optimization[6] and PINN optimization[7].

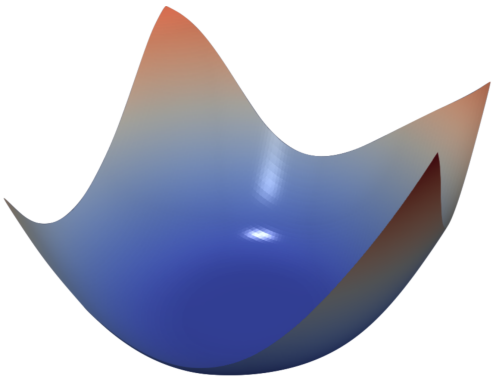
Proposition

Abandon first-order optimization. Exploit geometry in function space.

[6] R. Li et al. (2024). "A computational framework for neural network-based variational Monte Carlo with Forward Laplacian". In: *Nature Machine Intelligence*, pp. 1–11.

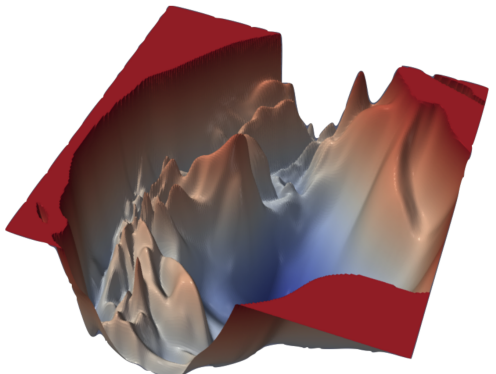
[7] J. Müller and M. Zeinhofer (2023). "Achieving High Accuracy with PINNs via Energy Natural Gradients". In: *International Conference on Machine Learning*.

Geometry in Function Space vs Paramter Space[8]



$u \mapsto E(u)$

"Function Space"



$\theta \mapsto L(\theta) = E(u_\theta)$

"Parameter Space"

[8] H. Li, Z. Xu, G. Taylor, C. Studer, and T. Goldstein (2018). "Visualizing the loss landscape of neural nets". In: *Advances in neural information processing systems* 31.

Abstract Function Space Optimization[9]

Informal Roadmap: "First Optimize, Then Discretize"

Given: "a SciML problem" and a neural network ansatz. We propose:

(i) **Continuous Formulation:** Formulate minimization/saddle point/... problem in a Hilbert space $\mathcal{H}$

$$E : \mathcal{H} \to \mathbb{R}.$$

(ii) **Optimize:** Decide for an appropriate iterative algorithm *in function space* $\mathcal{H}$

$$u_{k+1} = u_k + d_k, \quad k = 0, 1, 2, \dots$$

(iii) **Discretize:** Project update directions on the tangent space of neural network ansatz.

[9] J. Müller and M. Zeinhofer (2024). "Position: Optimization in SciML Should Employ the Function Space Geometry". In: *Forty-first International Conference on Machine Learning*.

Recap

Newton's Method for Minimization in Function Spaces

For (general) objective $E : \mathcal{H} \to \mathbb{R}$ do second-order Taylor expansion (in function space)

$$E(u + d) \approx E(u) + DE(u)d + \frac{1}{2}D^2E(u)(d, d).$$

Explicitly minimize in the variable d:

$$d = u - D^2E(u)^{-1}[DE(u)]$$

- Think of the expression $D^2E(u)^{-1}[DE(u)]$ as solving a PDE[10].

[10] The Euler-Lagrange equations of the Taylor expansion of E.

Newton: Continuous Formulation

- Suppose we aim to solve Poisson's equation

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega, \\ u &= g \quad \text{on } \partial\Omega \end{aligned}$$

- Reformulate as a minimization problem[11]

$$\min_{u \in H^2(\Omega)} E(u) = \frac{1}{2}\|\Delta u + f\|^2_{L^2(\Omega)} + \frac{1}{2}\|u - g\|^2_{L^2(\partial\Omega)}$$

- Ignore neural network ansatz classes.

[11] A formulation as a root finding problem or a variational formulation make sense, too.

Newton: Optimize

- For the quadratic minimization problem

$$u^* = \operatorname{argmin}_{u \in H^2(\Omega)} E(u) = \frac{1}{2}\|\Delta u + f\|^2_{L^2(\Omega)} + \frac{1}{2}\|u - g\|^2_{L^2(\partial\Omega)}$$

- Newton's method in function space has one step convergence

$$\begin{aligned} u^* &= u - D^2E(u)^{-1}[DE(u)] \\ &= u + \underbrace{(u^* - u)}_{=d}. \end{aligned}$$

Goal

Discretize such that we follow the optimal step $d = u^* - u$?

Newton: Discretize I – Bilinear Forms

Question

How to discretize the Newton step $D^2E(u)^{-1}[DE(u)]$?

- $D^2E(u) : H^2(\Omega) \times H^2(\Omega) \to \mathbb{R}$ is a *bilinear form*:

$$D^2E(u)(v, w) = \int_\Omega \Delta v \Delta w \, \mathrm{d}x + \int_{\partial\Omega} vw \mathrm{d}s$$

- $DE(u) : H^2(\Omega) \to \mathbb{R}$ is a *linear functional*:

$$DE(u)(v) = \int_\Omega (\Delta u + f)\Delta v \, \mathrm{d}x + \int_{\partial\Omega} (u - g)v \, \mathrm{d}s$$

- The expression $D^2E(u)^{-1}(DE(u))$ means: Find v such that

$$D^2E(u)(v, w) = DE(u)(w), \quad \text{for all} \quad w \in H^2(\Omega)$$

Newton: Discretize II – Galerkin Methods

Question

How to discretize an equation of the form: $D^2E(u)(v,w) = DE(u)(w), \quad$ for all $\quad w$?

- Choose basis functions $v_1, \ldots, v_n \in H^2(\Omega)$ and transfer to a matrix equation:

$$G_{ij} = D^2E(u)(v_j, v_i), \quad b_i = DE(u)(v_i)$$

- Solve the matrix equation

$$G\alpha = b$$

- Under suitable conditions, $v = \sum_{i=1}^{n} \alpha_i v_i$ is an approximate solution.

Naming convention

Discretizing a bilinear form with a finite dimensional vector space is a *Galerkin Method*.

Newton: Discretize III – Galerkin in Tangent Space

- Given a neural network ansatz $\{u_\theta \mid \theta \in \Theta\}$, as basis function choose

$$\partial_{\theta_1} u_\theta, \ldots, \partial_{\theta_p} u_\theta$$

- Discretize with a Galerkin ansatz using the basis functions $\partial_{\theta_1} u_\theta, \ldots, \partial_{\theta_p} u_\theta$:

$$G(\theta)_{ij} = D^2 E(u_\theta)(\partial_{\theta_j} u_\theta, \partial_{\theta_i} u_\theta), \qquad \nabla L(\theta)_i = DE(u_\theta)(\partial_{\theta_i} u_\theta)$$

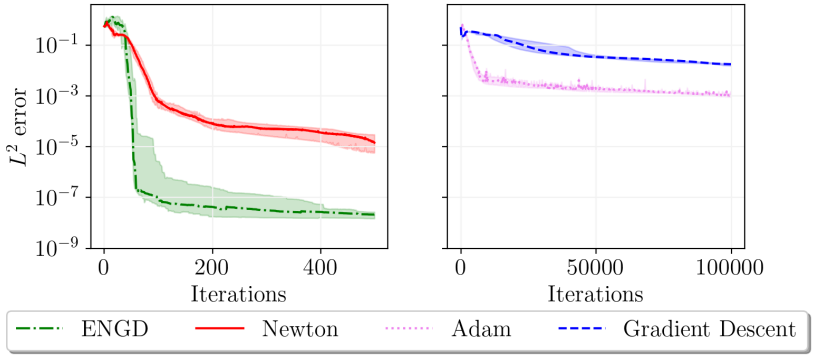
- This yields an optimization algorithm:

$$\theta_{k+1} = \theta_k - \eta_k G(\theta_k)^\dagger \nabla L(\theta_k).$$

- If $E(u) = \frac{1}{2}\|\Delta u + f\|^2_{L^2(\Omega)} + \frac{1}{2}\|u - g\|^2_{L^2(\partial\Omega)}$ we get:

$$G(\theta)_{ij} = \int_\Omega \Delta\partial_{\theta_i} u_\theta \Delta\partial_{\theta_j} u_\theta \,\mathrm{d}x + \int_{\partial\Omega} \partial_{\theta_i} u_\theta \partial_{\theta_j} u_\theta \mathrm{d}s$$

This Yields a Highly Efficient Method[12]



$$\theta_{k+1} = \theta_k - \eta_k G(\theta_k)^\dagger \nabla L(\theta_k), \quad k = 0, 1, 2 \dots$$

$$G(\theta)_{ij} = \int_\Omega \Delta \partial_{\theta_i} u_\theta \Delta \partial_{\theta_j} u_\theta \, \mathrm{d}x + \int_{\partial\Omega} \partial_{\theta_i} u_\theta \partial_{\theta_j} u_\theta \mathrm{d}s$$

[12] J. Müller and M. Zeinhofer (2023). "Achieving High Accuracy with PINNs via Energy Natural Gradients". In: *International Conference on Machine Learning*.

L^2 Gradient Flow for Rayleigh quotient: Cont. Form

- Suppose we want to minimize the Rayleigh quotient

$$R(\psi) = \frac{\langle H\psi, \psi \rangle}{\langle \psi, \psi \rangle},$$

  where H is the Hamiltonian (or any symmetric PDE operator).
- Rewrite the problem using $\tilde{\psi} = \psi / \|\psi\|_{L^2}$ as

$$\tilde{R}(\tilde{\psi}) = \langle H\tilde{\psi}, \tilde{\psi} \rangle$$

- The transformation $\psi / \|\psi\|_{L^2}$ is for mathematical convenience.

L^2 Gradient Flow for Rayleigh quotient: Optimize

- Do L^2 gradient flow with explicit Euler discretization on $\tilde{R}$

$$\tilde{\psi}_{k+1} = \tilde{\psi}_K - \eta_k T^{-1}(D\tilde{R}(\tilde{\psi}_k)),$$

- $T : L^2 \to (L^2)^*$ is the Riesz isometry[13] of L^2

$$T(\psi)(\phi) = \langle \psi, \phi \rangle$$

- $D\tilde{R}(\tilde{\psi})\phi = \langle H\tilde{\psi}, \phi \rangle$ is the Fréchet (functional) derivative of $\tilde{R}$.

[13] Can be viewed & discretized as bilinear form

L^2 Gradient Flow for Rayleigh quotient: Discretize

- The neural network ansatz and tangent space/Galerkin space are

$$\{\psi_\theta/\|\psi_\theta\|_{L^2} \mid \theta \in \Theta\}, \quad \operatorname{span}\{\partial_{\theta_1}\left(\frac{\psi_\theta}{\|\psi_\theta\|}\right), \ldots, \partial_{\theta_P}\left(\frac{\psi_\theta}{\|\psi_\theta\|}\right)\}$$

- Discretizing the Riesz map T yields

$$F_{ij} = T(\partial_{\theta_i}\left(\psi_\theta/\|\psi_\theta\|\right))(\partial_{\theta_j}\left(\psi_\theta/\|\psi_\theta\|\right)) = \langle \partial_{\theta_i}\left(\psi_\theta/\|\psi_\theta\|\right), \partial_{\theta_j}\left(\psi_\theta/\|\psi_\theta\|\right)\rangle$$

- Discretizing the functional derivative $D\tilde{R}$ yields the gradient of the loss $L(\theta) = R(\psi_\theta)$
- The final algorithm is $\theta_{k+1} = \theta_k - \eta_k F^\dagger \nabla L(\theta_k)$

Fact

One can compute that this is *stochastic reconfiguration*.

Translation: Function Space to Parameter Space

We can carry out the previous reasoning for different function space optimization methods[14]

Function Space	Parameter Space	Name in Literature
Newton	Generalized Gauss-Newton	ENGD[15]
Gradient Descent	Natural Gradient Descent[16]	—
Lagrange-Newton	Competitve Gradient Descent[17]	CPINNs[18]
Gauss-Newton	Gauss-Newton	GNNGD[19]

[14] J. Müller and M. Zeinhofer (2024). "Position: Optimization in SciML Should Employ the Function Space Geometry". In: *Forty-first International Conference on Machine Learning*.

[15] J. Müller and M. Zeinhofer (2023). "Achieving High Accuracy with PINNs via Energy Natural Gradients". In: *International Conference on Machine Learning*.

[16] S.-I. Amari (1998). "Natural Gradient Works Efficiently in Learning". In: *Neural Computation* 10.2, pp. 251–276.

[17] F. Schäfer and A. Anandkumar (2019). "Competitive gradient descent". In: *Advances in Neural Information Processing Systems* 32.

[18] Q. Zeng, S. H. Bryngelson, and F. T. Schaefer (2023). "Competitive Physics Informed Networks". In: *International Conference on Learning Representations*.

[19] A. Jnini, F. Vella, and M. Zeinhofer (2024). "Gauss-Newton Natural Gradient Descent for Physics-Informed Computational Fluid Dynamics". In: *arXiv preprint arXiv:2402.10680*.

A General Class of Minimization Algorithms

- Many optimization methods are of the form:

$$u_{k+1} = u_k + T_{u_k}^{-1}[DE(u_k)]$$

  where T_k is a linear, continuous, bijective map $T_{u_k} : \mathcal{H} \to \mathcal{H}^*$.
- Gradient Descent, Newton, Gauss-Newton, Lagrange-Newton, ...
- Assumption: T_{u_k} is coercive, i.e.,

$$\langle T_{u_k} v, v \rangle \geq \alpha \|v\|_{\mathcal{H}}^2$$

  for some $\alpha > 0$.

Projection Theorem

Theorem

For the discretized algorithm $\theta_{k+1} = \theta_k - \eta_k G(\theta_k)^\dagger \nabla L(\theta_k)$ *it holds*

$$u_{\theta_{k+1}} = u_{\theta_k} - \eta_k \Pi_{u_{\theta_k}} \underbrace{[T^{-1}_{u_{\theta_k}}(DE(u_{\theta_k}))]}_{=d_k} + \epsilon_k$$

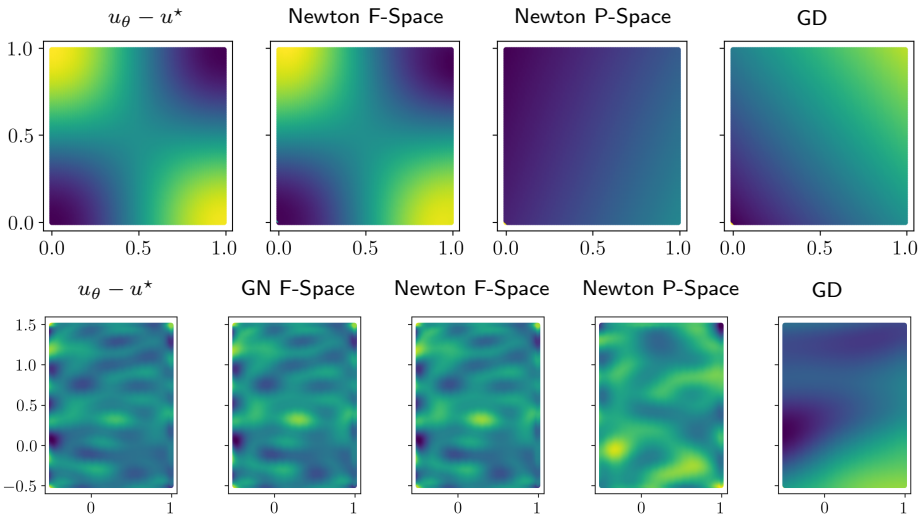
where Π_u *denotes the Galerkin projection onto the tangent space. The term* ϵ_k *corresponds to an error vanishing quadratically in the step and step size length*

$$\epsilon_k = O(\eta_k^2 \|G(\theta_k)^\dagger \nabla L(\theta_k)\|^2).$$

Proof.

Taylor expansion & Céa's Lemma. □

Visualization of the Projection Theorem



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The Price of Non-local Ansatz Functions

Recall the Structure of the ENGD Matrix

In every step of optimization the following matrix needs to be assembled and inverted

$$G(\theta)_{ij} = D^2 E(u_\theta)(\partial_{\theta_i} u_\theta, \partial_{\theta_j} u_\theta), \quad i, j = 1, \dots, p.$$

For neural network ansatz functions the matrix is dense, rank deficient and ill-conditioned.

- A direct solve works well for small networks.
- Naive application is doomed to fail, already for networks of modest size, say $p > 10^4$ trainable parameters.

What are our Options?

- Matrix-free solution methods for the system $G(\theta)d = \nabla L(\theta)$.
  - The matrix vector-product $G(\theta)v$ can be computed at comparable cost to the gradient $\nabla L(\theta)$[20, 21], hence use CG.
  - Drawback: CG iterates long due to ill-conditioning of $G(\theta)$.
- Derive cheap-to-invert approximations.
  - Derivatives of linear network layers yield Kronecker structure[22]. Leverage to build an approximation of $G(\theta)$!
  - The details fill the remaining talk.
- Combine both ideas, i.e., use preconditioned CG.

[20] N. N. Schraudolph (2002). "Fast curvature matrix-vector products for second-order gradient descent". In: *Neural computation* 14.7, pp. 1723–1738.

[21] A. Jnini, F. Vella, and M. Zeinhofer (2024). "Gauss-Newton Natural Gradient Descent for Physics-Informed Computational Fluid Dynamics". In: *arXiv preprint arXiv:2402.10680*.

[22] J. Martens (2020). "New Insights and Perspectives on the Natural Gradient Method". In: *The Journal of Machine Learning Research* 21.1, pp. 5776–5851.

Kronecker-Factor Approximation

- We discard cross-interactions between layers and use a Kronecker Approximation[23]:

$$\begin{aligned} G(\theta) &\approx \operatorname{diag}(G^{(1)}, \ldots, G^{(L)}) \\ &\approx \operatorname{diag}(A^{(1)} \otimes B^{(1)}, \ldots, A^{(L)} \otimes B^{(L)}). \end{aligned}$$

- Use the property of Kronecker product

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$$

- Ignoring bias terms, for layer l mapping from $\mathbb{R}^n \to \mathbb{R}^m$ the matrix $G^{(l)}(\theta)$ is of size (nm, nm) but the Kronecker factors are of size

$$A^{(l)} \in \mathbb{R}^{n \times n}, \quad B^{(l)} \in \mathbb{R}^{m \times m}$$

[23] We omit the θ dependency for brevity only.

Where does the Kronecker Structure Come From?

Structure of ENGD Matrix

Ignoring boundary terms, one can show that the ENGD matrix for Poisson is

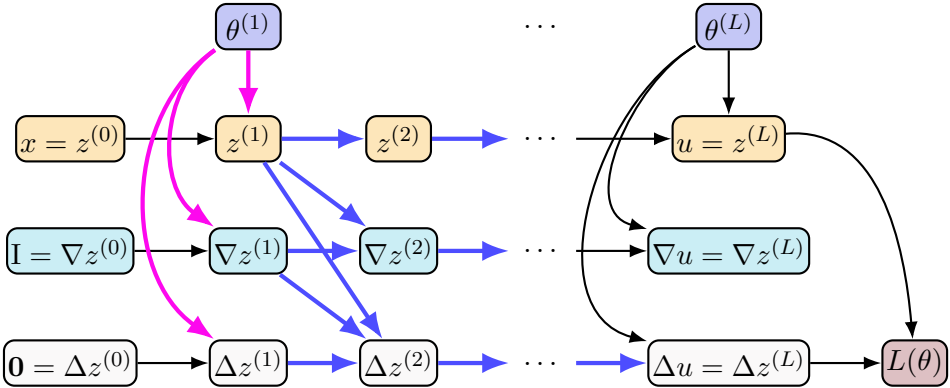
$$G^{(l)}(\theta) = \frac{1}{N_\Omega} \sum_{n=1}^{N_\Omega} \mathrm{J}_{\theta^{(l)}} \Delta u_\theta(x_n)^\top \, \mathrm{J}_{\theta^{(l)}} \Delta u_\theta(x_n)$$

- Key for Kronecker factors: Jacobian of $\theta \mapsto \theta x$, where θ is weight matrix

$$\mathrm{J}_\theta(\theta x) = x^\top \otimes \mathrm{Id}$$

- Need: children of $\theta^{(l)}$ in computational graph of $\theta^{(l)} \mapsto \Delta u_\theta(x_n)$.

Taylor Mode alias Forward Laplacian[24] Graph



$$\theta^{(l)} \mapsto \Delta u_\theta(x) = [(z^{(l)}, \nabla z^{(l)}, \Delta z^{(l)}) \mapsto \Delta u_\theta(x)] \circ [\theta^{(l)} \mapsto (z^{(l)}, \nabla z^{(l)}, \Delta z^{(l)})]$$

[24] R. Li et al. (2024). "A computational framework for neural network-based variational Monte Carlo with Forward Laplacian". In: *Nature Machine Intelligence*, pp. 1–11.

The Full K-FAC Approximation

Exact block of the ENGD matrix of a Laplace operator

$$G_\Omega^{(l)}(\theta) = \frac{1}{N} \sum_{n=1}^{N} \sum_{s=1}^{S} \sum_{s'=1}^{S} Z_{n,s}^{(l-1)} Z_{n,s'}^{(l-1)\top} \otimes g_{n,s}^{(l)} g_{n,s'}^{(l)\top}.$$

K-FAC for the ENGD matrix of a Laplace operator

$$G_\Omega^{(l)}(\theta) \approx \left(\frac{1}{NS} \sum_{n,s=1}^{N,S} Z_{n,s}^{(l-1)} Z_{n,s}^{(l-1)\top} \right) \otimes \left(\frac{1}{N} \sum_{n,s=1}^{N,S} g_{n,s}^{(l)} g_{n,s}^{(l)\top} \right) =: A_\Omega^{(l)} \otimes B_\Omega^{(l)}$$

$$Z_{n,1}^{(l)} \coloneqq z_n^{(l)}, \quad Z_{n,2}^{(l)} \coloneqq \partial_{x_1} z_n^{(l)}, \dots, Z_{n,1+d}^{(l)} = \partial_{x_d} z_n^{(l)}, \quad Z_{n,2+d}^{(l)} \coloneqq \Delta z_n^{(l)}$$

$$g_{n,s}^{(l)} \coloneqq \mathrm{J}_{Z_{n,s}^{(l)}} \Delta u_n$$

Further Details & Generalizations

- The K-FAC approximation works for more than just the Poisson equation:
  - general nonlinear PDEs using PINN formulation
  - Variational formulations (deep Ritz)
  - Neural Operators? Requires more work.
- Typically combined with
  - Trust-region methods for step-size choice
  - Exponential moving average for K-FAC-matrices
  - Infrequent updates of the K-FAC-matrices
  - Momentum on the natural gradient
- Find all details in the pre-print[25].

[25] F. Dangel, J. Müller, and M. Zeinhofer (2024). "Kronecker-Factored Approximate Curvature for Physics-Informed Neural Networks". In: *Advances in Neural Information Processing Systems*.

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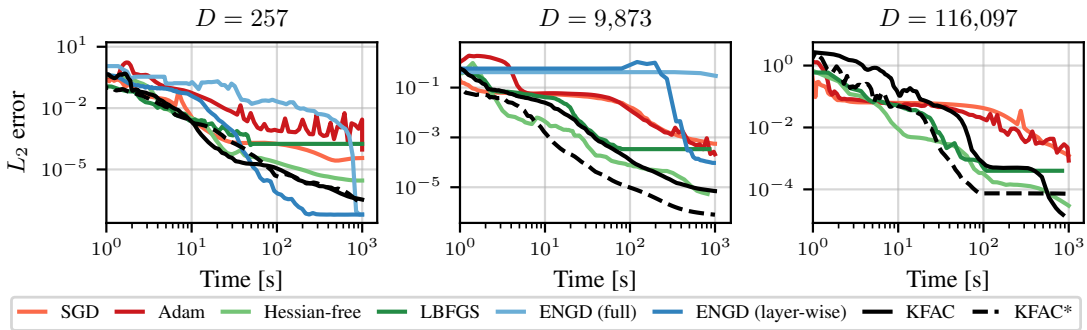
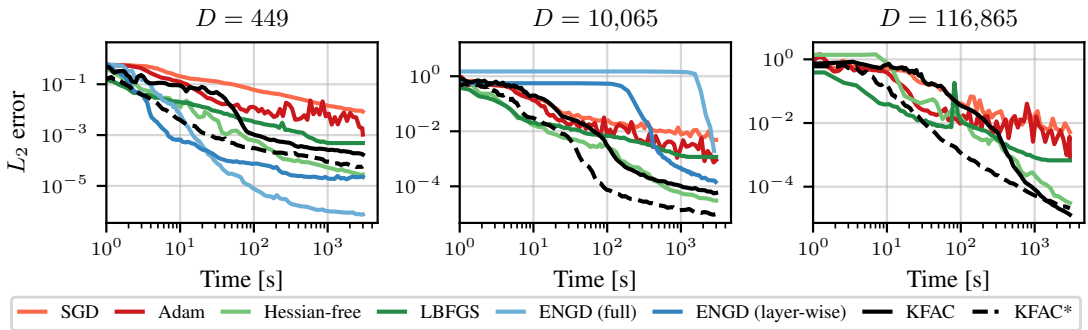
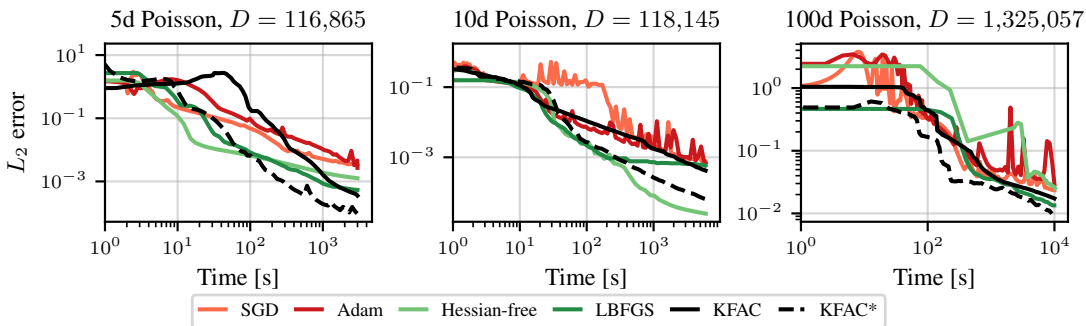
Poisson Equation Two Dimensions



Heat Equation Equation (4+1) Dimensions



High Dimensional Poisson Equation



Discussion

+ The K-FAC approximation allows to scale natural gradient methods to millions of parameters.
+ Even preliminary numerical experiments compare favorable to established optimizers.
+ The approximation generalizes to other PDEs (see pre-print[26] for details).
- The numerical experiments are preliminary, more equations need to follow.
- The K-FAC approximation is architecture dependent and complicated to handle.

[26] F. Dangel, J. Müller, and M. Zeinhofer (2024). "Kronecker-Factored Approximate Curvature for Physics-Informed Neural Networks". In: *Advances in Neural Information Processing Systems*.

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When is the Functional Viewpoint Useful?

- We discussed difficulty of NN optimization for loss functions including PDE operators.
- Infinite dimensional algorithms can exploit geometric structure.
- Obtain an algorithm by Galerkin discretization in tangent space.
- Scalability can be non-trivial.

When can this be useful?

The problem possesses a continuous formulation & contains PDE terms.

When does it not help?

First order methods are successful e.g., supervised deep learning applications.

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