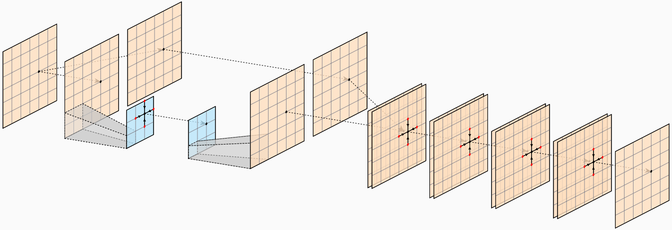


Gauge-equivariant multigrid neural networks

Christoph Lehner and Tilo Wettig (University of Regensburg)

arXiv:2302.05419 [hep-lat]
arXiv:2304.10438 [hep-lat]

ECT* Trento, June 28, 2023

Machine learning for lattice field theory and beyond

Outline

Introduction

Preconditioning

- In lattice QCD, wall-clock time is typically dominated by solution of Dirac equation

$$Du = b$$

  - Usually done by an iterative solver (here, GMRES)

- Time to solution is determined by condition number of Dirac matrix
  - Condition number increases dramatically in continuum limit and for physical quark mass
  - Thus number of iterations also increases dramatically (“Critical slowing down”)

- Way out: Preconditioning
  - Find a preconditioner M such that $M \approx D^{-1}$
  - Define $v = M^{-1}u$ and use

$$DMM^{-1}u = (DM)v = b$$

    to solve for v with preconditioned matrix DM (smaller condition number)
  - Then $u = Mv$

Measure of performance

$$\text{Iteration count gain} = \frac{\text{Iteration count without preconditioner}}{\text{Iteration count with preconditioner}}$$

- Iteration count refers to outer solver (here, GMRES)

Low and high modes

- Consider the eigendecomposition of D^{-1}

$$D^{-1} = \sum_n \lambda_n^{-1} |n\rangle\langle n|$$

- Preconditioner should approximate low-mode and high-mode components of D^{-1}
- Iterative solution of $Du = b$

$$u_{k+1} = f(D, b, u_k) \quad \text{with} \quad u_k \to u \quad \text{(true solution)}$$

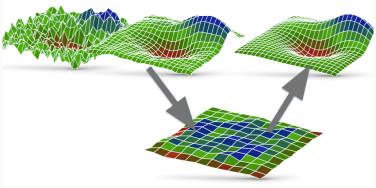
- Residual

$$r_k = b - Du_k \quad \text{with} \quad r_k \to 0$$

- Residual r_k can formally be expanded in the eigenmodes $|n\rangle$ of D
  → Preconditioner should reduce low- and high-mode contributions to r_k
- State-of-the-art algorithms (multigrid) are designed to do this
- We follow this paradigm, but here we learn the preconditioner

Multigrid in a nutshell

- Multigrid has two components
  - Smoother: Reduces error from high modes
  - Coarse-grid correction: Reduces error from low modes
    - “Restriction” to a coarse grid
    - Approximate solution of Dirac equation on coarse grid
    - “Prolongation” of solution vector from coarse to fine grid
  - Can be done on multiple levels



https://summerofhpc.prace-ri.eu/multithreading-the-multigrid-solver-for-lattice-qcd

- Multigrid setup
  - The art of multigrid: How to construct suitable restriction and prolongation operators?
  - Observation: Low eigenmodes are “locally coherent” Lüscher, arXiv:0706.2298 [hep-lat]
    (i.e., they are locally well approximated by a relatively small number of vectors)
    → Construct vectors that approximately span the near-null space
    Block these vectors to define the restriction operator (and use $P = R^\dagger$)
  - Setup is expensive but needs to be done only once per gauge-field configuration
    (can then be reused for multiple RHS)

Related work

1. Multigrid algorithms in lattice QCD
    - Brannick, Brower, Clark, Osborn, Rebbi arXiv:0707.4018 [hep-lat]
    - R. Babich et al. arXiv:1005.3043 [hep-lat]
    - Frommer et al. arXiv:1303.1377 [hep-lat]
    - Boyle arXiv:1402.2585 [hep-lat]
    - Brannick et al. arXiv:1410.7170 [hep-lat]
    - Brower, Clark, Strelchenko, Weinberg arXiv:1801.07823 [hep-lat]
    - Brower, Clark, Howarth, Weinberg arXiv:2004.07732 [hep-lat]
2. Neural networks for multigrid (but not for gauge theories), e.g.,
    - Katrutsa, Daulbaev, Oseledets arXiv:1711.03825 [math.NA]
    - He & Xu arXiv:1901.10415 [cs.CV]
    - Greenfeld, Galun, Basri, Yavneh, Kimmel arXiv:1902.10248 [cs.LG]
    - Eliasof, Ephrath, Ruthotto, Treister arXiv:2011.09128 [cs.CV]
    - Huang, Li, Xi arXiv:2102.12071 [math.NA]

Related work

3. Gauge-equivariant neural networks (but not for solving Dirac equation), e.g.,
    - Cohen, Weiler, Kicanaoglu, Welling arXiv:1902.04615 [cs.LG]
    - Finzi, Stanton, Izmailov, Wilson arXiv:2002.12880 [stat.ML]
    - Luo, Carleo, Clark, Stokes arXiv:2012.05232 [cond-mat.str-el]
    - Kanwar et al. arXiv:2003.06413 [hep-lat]
    - Boyda et al. arXiv:2008.05456 [hep-lat]
    - Favoni, Ipp, Müller, Schuh arXiv:2012.12901 [hep-lat]
    - Abbott et al. arXiv:2207.08945 [hep-lat]
    - Bacchio, Kessel, Schäfer, Vaitl arXiv:2212.08469 [hep-lat]
    - Aronsson, Müller, Schuh arXiv:2303.11448 [hep-lat]
4. Neural-network preconditioners for Schwinger model
    - Calì et al. arXiv:2208.02728 [hep-lat]

Related work

5. Gauge-equivariant multigrid setup and coarse gauge fields (late 1980s/early 1990s)
    - Amsterdam group (Hulsebos, Smit, Vink)
      e.g., Nucl. Phys. B Proc. Suppl. 9, 512 (1989), Nucl. Phys. B Proc. Suppl. 20, 94 (1991), Nucl. Phys. B 368, 379 (1992)
    - Israel group (Ben-Av et al.)
      e.g., Nucl. Phys. B 329, 193 (1990), Phys. Lett. B 253, 185 (1991), Nucl. Phys. B 405, 623 (1993)
    - Boston group (Brower et al.)
      e.g., Phys. Rev. D 43, 1965 (1991), Phys. Rev. D 43, 1974 (1991), Phys. Rev. Lett. 66, 1263 (1991)
    - Hamburg group (Kalkreuter et al.)
      e.g., Nucl. Phys. B 376, 637 (1992), Int. J. Mod. Phys. C 5, 629 (1994)

Parallel-transport convolution layers

Parallel transport

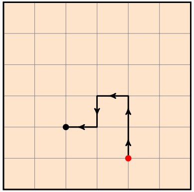
- Consider a field $\varphi(x)$ with $x \in S$ (space-time lattice, dim $= d$) and $\varphi \in V_I = V_G \otimes V_{\bar{G}}$ (gauge space: $V_G = \mathbb{C}^N$, non-gauge space: $V_{\bar{G}} = \mathbb{C}^{\bar{N}}$)
- Also consider an SU(N) gauge field $U_\mu(x)$ acting on V_G
- Define the parallel-transport operator for a path $p = p_1, \ldots, p_{n_p}$ with $p_i \in \{\pm 1, \ldots, \pm d\}$

$$T_p = H_{p_{n_p}} \cdots H_{p_2} H_{p_1}$$

with

$$H_\mu \varphi(x) = U_\mu^\dagger(x - \hat{\mu}) \varphi(x - \hat{\mu})$$

- H_μ transports information by a single hop in direction $\hat{\mu}$
- H_μ acts on field; new field $H_\mu \varphi$ is evaluated at x
- Example: $T_p = H_{-1} H_{-2} H_{-1} H_2 H_2$



Gauge equivariance

- A gauge transformation by $\Omega(x) \in \mathrm{SU}(N)$ acts in the usual way

$$\varphi(x) \to \Omega(x)\varphi(x)$$
$$U_\mu(x) \to \Omega(x)U_\mu(x)\Omega^\dagger(x+\hat{\mu})$$

- Such gauge transformations commute with T_p for any path p

$$T_p\varphi(x) \to \Omega(x)T_p\varphi(x)$$

- This is an example of gauge equivariance (a.k.a. gauge covariance):

> An object (here: φ) and the transformed object (here: $T_p\varphi$) transform in the same way under a gauge transformation.

- Building gauge equivariance into the model implies that the model does not have to learn the gauge symmetry → Same expressivity with fewer weights

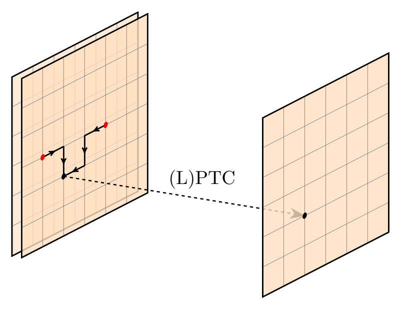
Parallel-transport convolutions

- Parallel-transport convolution layer and local parallel-transport convolution layer

$$\psi_a(x) \overset{\text{PTC}}{=} \sum_b \sum_{p \in P} W^p_{ab} T_p \varphi_b(x)$$

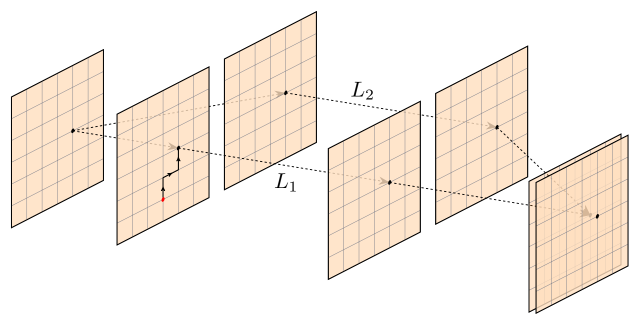
$$\psi_a(x) \overset{\text{LPTC}}{=} \sum_b \sum_{p \in P} W^p_{ab}(x) T_p \varphi_b(x)$$

  - $a =$ output feature index
  - $b =$ input feature index
  - $P =$ set of paths
  - W^p_{ab} acts on $V_{\bar{G}}$ (here: 4×4 spin matrix)
  - Elements of W: trainable layer weights
- Layers are gauge-equivariant
- No activation function since we want to learn a linear preconditioner
- Graphical conventions
  - Feature = Plane
  - Layer = Paths + Arrow



Parallel and identity layers

- Parallel layers act on the same input feature in parallel
- Identity layer (dashed arrow w/o paths): simple copy operation, i.e., output = input
- Example: (All layers except L_1 are identity layers)



Communication avoidance

- On machines with many nodes, subvolumes are assigned to different MPI processes
- We also consider models where no information is communicated between subvolumes (by setting the links $U_\mu(x)$ connecting subvolumes to zero)
- We find that the performance of these models (in terms of iteration count gain) is only slightly worse compared to those with communication
  $\rightarrow$ Overall wall-clock time could be lower since no time is spent on communication

Wilson-clover Dirac operator

Dirac operator

- The Wilson Dirac operator can be written in terms of single hops:

$$D_{\mathrm{W}} = \frac{1}{2}\sum_{\mu=1}^{4}\gamma_\mu(H_{-\mu} - H_{+\mu}) - \frac{1}{2}\sum_{\mu=1}^{4}(H_{-\mu} + H_{+\mu} - 2) + m$$

- For Wilson-clover, consider closed paths with four hops and define

$$Q_{\mu\nu} = H_{-\mu}H_{-\nu}H_{+\mu}H_{+\nu} + H_{-\nu}H_{+\mu}H_{+\nu}H_{-\mu} + H_{+\nu}H_{-\mu}H_{-\nu}H_{+\mu} + H_{+\mu}H_{+\nu}H_{-\mu}H_{-\nu}$$

Then

$$D_{\mathrm{WC}} = D_{\mathrm{W}} - \frac{c_{\mathrm{sw}}}{4}\sum_{\mu,\nu=1}^{4}\sigma_{\mu\nu}F_{\mu\nu}$$

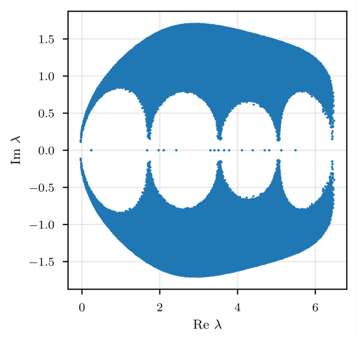
with

$$F_{\mu\nu} = \frac{1}{8}(Q_{\mu\nu} - Q_{\nu\mu}) \qquad \sigma_{\mu\nu} = \frac{1}{2}(\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu)$$

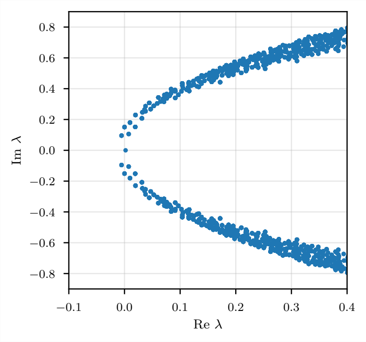
Numerical details and eigenvalue spectrum

- $V = 8^3 \times 16$, $\beta = 6.0$ (pure gauge), $c_{SW} = 1$, periodic boundary conditions for all fields
- Quark mass m is tuned so that D_{WC} is near criticality
  (i.e., real part of smallest nonzero eigenvalue ≈ 0)
  $\rightarrow$ Solution of $Du = b$ is challenging problem

$Q = 0 \quad (m = -0.6)$



$Q = 1 \quad (m = -0.5645)$



High-mode preconditioners

Model setup and training strategy

- High-mode part of Dirac spectrum is related to short-distance behavior
  $\rightarrow$ Expect one or two layers with small number of hops to show gain in iteration count
- Consider a linear model M mapping a vector x to Mx
- Supervised learning approach with training step as follows:
  - Pick random vector v from Gaussian distribution (mean zero, standard deviation 1)
  - Compute training tuple $(D_{\text{WC}}v, v)$ and optimize cost function

$$C = |MD_{\text{WC}}v - v|^2$$

    $\rightarrow$ Model learns to map $D_{\text{WC}}v$ to v (and hence $M \approx D_{\text{WC}}^{-1}$)
  - Optimizer is Adam — Kingma & Ba, arXiv:1412.6980 [cs.LG]
  - Derivatives w.r.t. model weights computed using backpropagation
- Training data set is unbounded in size $\rightarrow$ No need to add a regulator
- Cost function is dominated by high modes

Models chosen for high-mode preconditioner

- One layer, one hop (i.e., 9 paths)

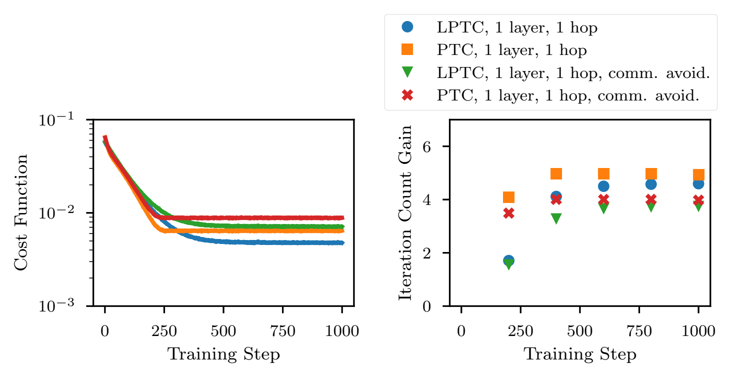
$$T_0 = \mathbb{1}\,,\ T_1 = H_1\,,\ T_2 = H_2\,,\ T_3 = H_3\,,\ T_4 = H_4\,,\ T_5 = H_{-1}\,,\ T_6 = H_{-2}\,,\ T_7 = H_{-3}\,,\ T_8 = H_{-4}$$

- One layer, two hops: extend the above by 56 two-hop paths

$$H_a H_b \qquad \text{with} \qquad a, b \in \{-4, -3, -2, -1, 1, 2, 3, 4\} \qquad (a \neq -b)$$

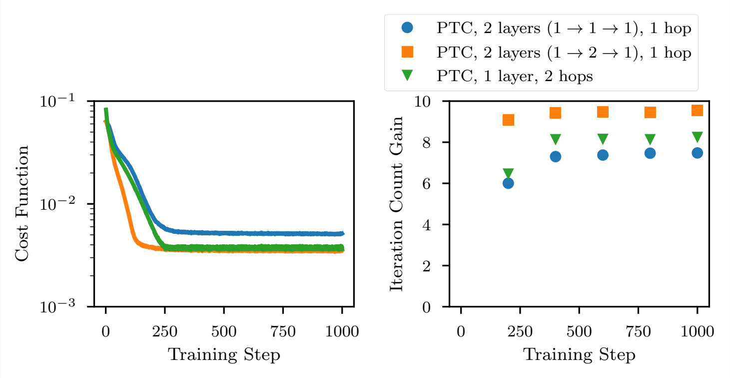
- "Deep" network of two one-hop layers:
  - $1 \to 1 \to 1$: Two successive layers with one hop each
  - $1 \to 2 \to 1$: Two output features in first layer, two input features in second layer
- PTC (layer weights constant) and LPTC (layer weights depend on x)
- Communication avoidance: $U_\mu(x) \equiv 0$ between subvolumes of size $4^3 \times 8$

Results for high-mode preconditioner (one layer, one hop)

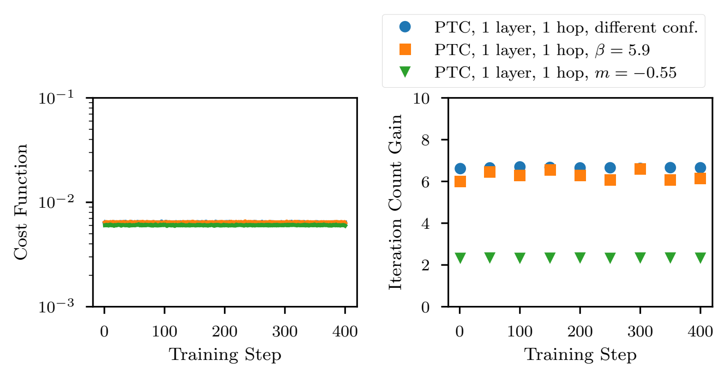


- No gain from LPTC (and they require more training)
- Communication-avoiding version only slightly worse (could be amortized)

Results for high-mode preconditioner (“deep” network or multiple hops)



- $1 \rightarrow 2 \rightarrow 1$ model performs best (and gives $\sim$ twice the gain of 1 layer/1 hop model)
- Since layers are linear, deep models are not more expressive than shallow models with same number of hops (but easier to train b/o smaller number of weights) $\rightarrow$ 2-hop model should reach similar performance with improved training procedure



- No retraining required for (i) different configuration from same ensemble, (ii) configuration with different β, (iii) different mass
- $m = -0.55$ is not tuned to criticality → Easier initial problem → Smaller gain
- Performance varies slightly between configurations

Low-mode preconditioners

Possible approaches

- Low-mode part of Dirac spectrum is related to long-distance behavior
  $\rightarrow$ Need deep network of (L)PTC layers to propagate information over long distances
- Alternative: Use multigrid paradigm
  - Define coarse version of the lattice
  - Define restriction and prolongation operations (= layers)
  - Preserve low-mode part of Dirac spectrum

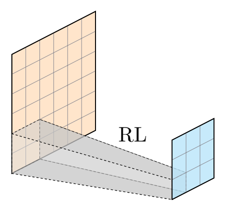
Low-mode preconditioners

Standard construction

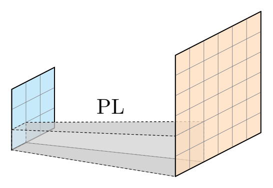
Standard approach: No gauge degrees of freedom on the coarse grid

- Define a coarse grid $\tilde{S}$ with fields $\tilde{\varphi}(y)$, where $y \in \tilde{S}$ and $\tilde{\varphi} \in \tilde{V}_I$
- $\tilde{V}_I$ has no gauge degrees of freedom → No gauge transformations on $\tilde{V}_I$
- $B =$ block map from $\tilde{S}$ to S (i.e., sites $B(y)$ on fine grid correspond to y on coarse grid)
- Restriction and prolongation layer (with $R = P^\dagger$)

$$\tilde{\psi}(y) \stackrel{\text{RL}}{=} \sum_{x \in B(y)} W(y,x)\varphi(x)$$



$$\psi(x) \stackrel{\text{PL}}{=} W(y,x)^\dagger \tilde{\varphi}(y)$$



Restriction and prolongation layers

- Find s vectors in the near-null space of D

$$Du_i \approx 0 \qquad (i = 1, \ldots, s)$$

  - Apply GMRES for D with source vector $= 0$ and random initial guess (solve to 10^{-8})
  - This removes high-mode components and leaves linear combination of low modes
- Block the u_i
  - One site $y \in \tilde{S}$ corresponds to a set of sites (or block) $B(y) \in S$
  - Blocked vector u_i^y lives on the sites of $B(y)$
- Orthonormalize the u_i^y within each block $\to \bar{u}_i^y$
- Then the prolongation map is defined by

$$W(y,x)^\dagger = \sum_{i=1}^{s} \bar{u}_i^y(x)\hat{e}_i^\dagger \qquad \text{no trainable weights}$$

with $x \in B(y)$ and $\hat{e}_i$ the canonical unit vectors of $\tilde{V}_I$

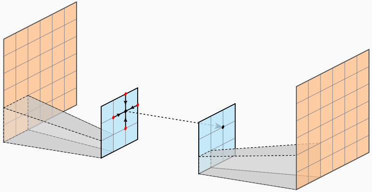
Model setup and training strategy

- Coarse-grid operator is defined as

$$\tilde{D} = R D_{\mathrm{WC}} P$$

  with R and P defined by restriction and prolongation layers

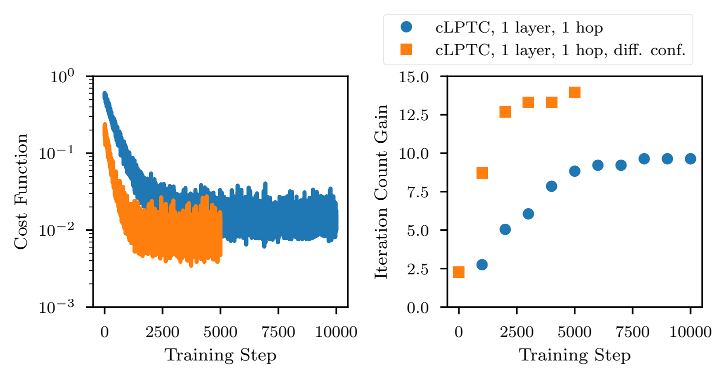
- Now need approximate solution of Dirac equation involving $\tilde{D}$
- Coarse-grid model for preconditioner $\tilde{M}$ contains single LPTC layer with zero- and one-hop paths and gauge fields replaced by $\mathbb{1}$ (layer is denoted by cLPTC)



- Same training strategy as before, with cost function

$$C = |\tilde{M}\tilde{D}v - v|^2$$

Results for low-mode preconditioner (cLPTC layer)

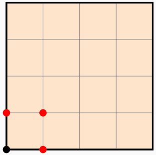


- Iteration count gain refers to inversion of $\tilde{D}$ (we use $\tilde{S} = 2^3 \times 4$ and $s = 12$)
- Longer training period compared to high-mode preconditioner
- Transfer learning works with moderate retraining

Low-mode preconditioners

Gauge-equivariant construction

Now: Explicit gauge degrees of freedom on the coarse grid



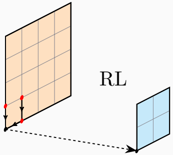
$B(y) = \{\bullet, {\color{red}\bullet}\}$

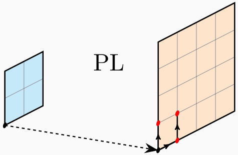
$B_r(y) = \bullet$

- Same coarse grid $\tilde{S}$ as before, but now $\tilde{\varphi}(y) \in V_G \otimes \tilde{V}_{\bar{G}}$ ($V_G =$ same local gauge space as on fine grid)
- Define a reference site $B_r(y) \subset B(y)$ on the fine grid
- Goal: Find restriction and prolongation layers such that $\tilde{\varphi}(y) \to \tilde{\Omega}(y)\tilde{\varphi}(y)$ under gauge transformations Ω, where

$$\tilde{\Omega}(y) = \Omega(B_r(y))$$

Restriction and prolongation layers





- Define RL/PL by pooling and subsampling layers

$$\mathrm{RL} = \mathrm{SubSample} \circ \mathrm{Pool} \qquad \mathrm{PL} = \mathrm{Pool}^{\dagger} \circ \mathrm{SubSample}^{\dagger}$$

- Pooling layer

$$\mathrm{Pool}\, \varphi(x) = \sum_{q \in Q} W_q(x) T_q \varphi(x)$$

gauge-invariant weights (now trainable)

with $q = (p, \bar{U})$, path p, gauge field $\bar{U}$, $T_q = T_p(\bar{U})$, and $W_q(x) \in \mathrm{End}(V_{\bar{G}})$ (spin matrices)
(in practice, we use a variety of differently smeared links $\bar{U}$)

- Subsampling layer

$$\mathrm{SubSample}\, \varphi(y) = \varphi(B_r(y))$$

Training setup: How to train RL/PL?

- Obvious idea: Train $\mathrm{PL} \circ \mathrm{RL}$ as an autoencoder that preserves the low modes
  - Use cost function $C = |\mathrm{PL} \circ \mathrm{RL}\, v_\ell - v_\ell|^2$ with fine-grid vectors v_ℓ from near-null space
  - Result: Did not perform well in multigrid preconditioner!
- What was missing?
  - $\mathrm{PL} \circ \mathrm{RL}$ should also project high eigenmodes to zero
  - Also encourage $\mathrm{RL} \circ \mathrm{PL} = \mathbb{1}$ (so that $P = \mathrm{PL} \circ \mathrm{RL}$ is proper projection operator with $P^2 = P$)
- Combined cost function

$$C = |\mathrm{PL} \circ \mathrm{RL}\, v_\ell - v_\ell|^2 + |\mathrm{PL} \circ \mathrm{RL}\, v_h - P_\ell v_h|^2 + |\mathrm{RL} \circ \mathrm{PL}\, v_c - v_c|^2$$

  - v_h and v_c are random vectors on fine and coarse grid, respectively
  - P_ℓ is blocked low-mode projector

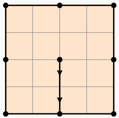
$$P_\ell = W^\dagger W \qquad \text{with} \qquad W(y,x)^\dagger = \sum_{i=1}^{s} \bar{u}_i^y(x)\hat{e}_i^\dagger$$

  - Still costly since we need near-null space vectors, but see Outlook

For gauge-equivariant coarse layers we need coarse gauge field

- Option 1: Plain coarse-gauge-field construction
  - Let y and y' be neighboring points on the coarse grid with $B_r(y') - B_r(y) = b\hat{\mu}$
  - The corresponding coarse-grid gauge field is then

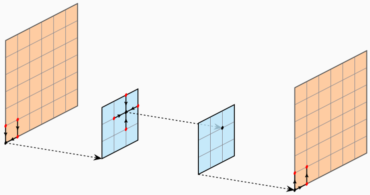
$$\tilde{U}_\mu(y) = U_\mu(B_r(y)) \cdots U_\mu(B_r(y) + (b-1)\hat{\mu})$$



- Option 2: Galerkin coarse-gauge-field construction

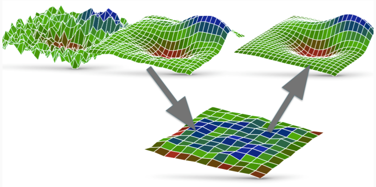
$$\tilde{U}_\mu(y) = \tilde{D}(y, y+\mu) \qquad \text{with} \qquad \tilde{D} = \mathrm{RL} \circ D_{\mathrm{WC}} \circ \mathrm{PL}$$

- Both options transform correctly under gauge transformations (on coarse grid)
- Coarse-grid model for preconditioner $\tilde{M}$ similar to standard version but with coarse gauge fields (instead of $\mathbb{1}$)



Multigrid preconditioners

Model setup



https://summerofhpc.prace-ri.eu/multithreading-the-multigrid-solver-for-lattice-qcd

- Combine the high- and low-mode models to learn a model M that approximates the short- and long-distance features of D^{-1}
- First create a short-distance model that accepts a second input feature (initial guess)
  - Model plays role of smoother in multigrid method
  - Initial guess from long-distance model acting on coarse grid

Smoother

- Recall: Iterative solver finds a sequence of u_k that approximately solve $Du = b$ (exact solution for large k)
- Assume we have a high-mode model M_h that approximates D^{-1}
- Smoother maps the tuple (u_k, b) to u_{k+1}

$$
\begin{aligned}
u_{k+1} &= (\mathbb{1} - M_\mathrm{h} D) u_k + M_\mathrm{h} b \\
&= u_k + M_\mathrm{h}(b - D u_k)
\end{aligned}
$$

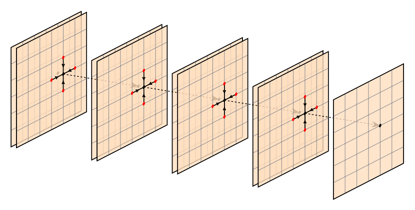
("iterative relaxation approach" or "defect correction" with defect $b - Du$)

Smoother model setup and training strategy

- In smoother iteration

$$u_{k+1} = u_k + M_\mathrm{h}(b - Du_k) \qquad (*)$$

  both D and high-mode model M_h can be represented by (L)PTC layers
  $\rightarrow$ Train a model M_s to map (u_k, b) to a u_{k+r} (with $r \in \mathbb{N}^+$)
  - Model must have two input features and one output feature
  - Every smoother iteration $(*)$ corresponds to two (L)PTC layers
    $\rightarrow$ Construct M_s using $2r$ successive layers (here with up to one hop each)
  - We use $r = 2$ since it performed better than $r = 1$ in full multigrid model

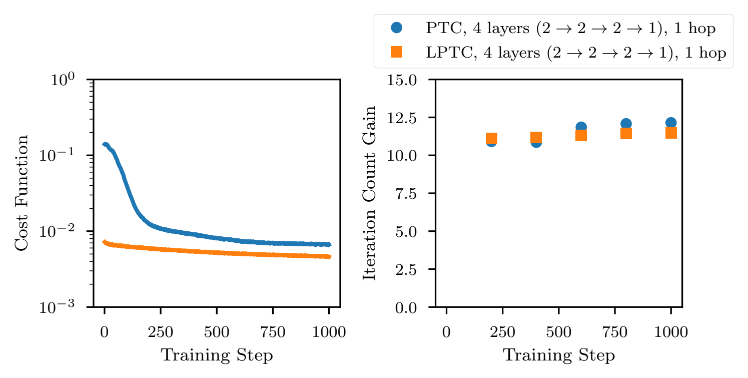


- Cost function

$$C = |M_s(u_k, b) - u_{k+r}|^2$$

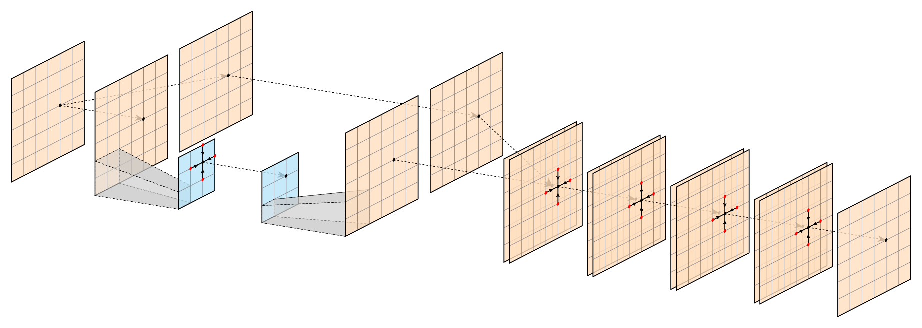
  For training, use random vectors u_k, b and u_{k+r} given by $(*)$

Results for smoother



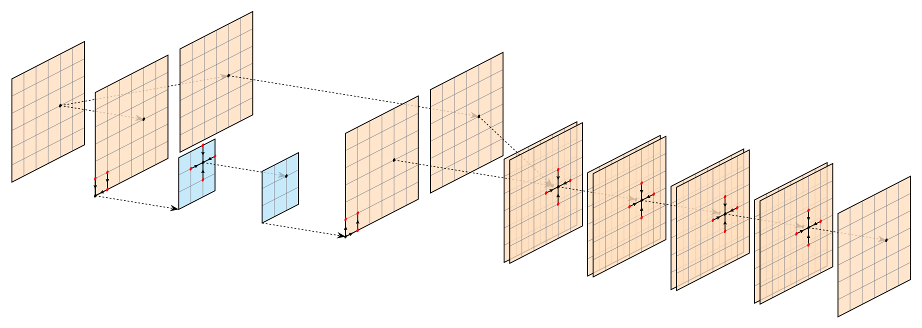
- Iteration count gain from using M_s as preconditioner for $Du = b$ with initial guess zero
- Performance is $\sim$ twice that of M_h with 1 layer/1 hop (since $r = 2$)
- Trained PTC model is used as initial weights for LPTC model (but no benefit from LPTC)

Combined two-level multigrid model (standard version)



- Duplicate the input feature and preserve one copy for smoother
- Restrict other copy to coarse grid and apply our coarse-grid model
- Prolongate result to fine grid
- Combine copy of initial feature and result of coarse-grid model to two input features for smoother (= last four layers)
- Additional multigrid levels: Recursively replace coarse-grid layer by entire model

Combined two-level multigrid model (gauge-equivariant version)



- Duplicate the input feature and preserve one copy for smoother
- Restrict other copy to coarse grid and apply our coarse-grid model
- Prolongate result to fine grid
- Combine copy of initial feature and result of coarse-grid model to two input features for smoother (= last four layers)
- Additional multigrid levels: Recursively replace coarse-grid layer by entire model

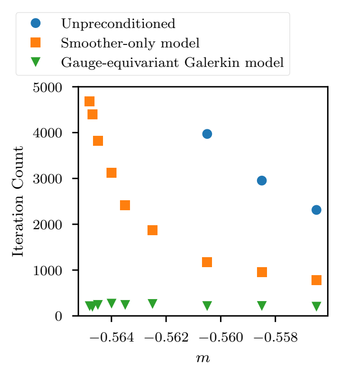
Training strategy for multigrid model

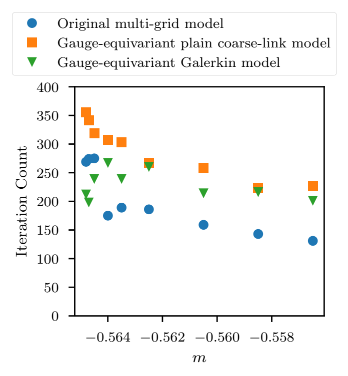
- First train layer weights of individual models
- Performance can be further improved by continued training with cost function

$$C = |M\,b_h - u_h|^2 + |M\,b_\ell - u_\ell|^2$$

  - $b_h = D_{\mathrm{WC}} v_1$, $u_h = v_1$, $b_\ell = v_2$, $u_\ell = D_{\mathrm{WC}}^{-1} v_2$
  - v_1 and v_2 are random vectors with $|b_h| = |b_\ell| = 1$

Results: Critical slowing down (CSD) for $Q = 1$





- Iteration count of GMRES to 10^{-8} precision with and without preconditioner
- CSD eliminated by standard multigrid model and model with Galerkin gauge fields
- Small remnants of CSD with plain coarse gauge fields

Summary and outlook

Summary

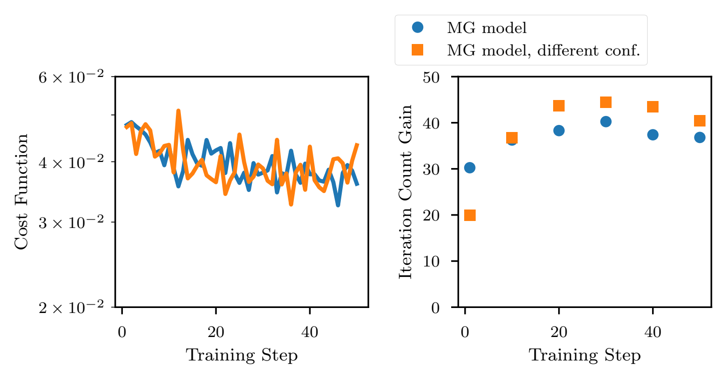
- We reformulate the problem of constructing a (multigrid) preconditioner in the language of gauge-equivariant neural networks.
- We find that such networks can learn the general paradigms of multigrid, significantly reduce the iteration count of the outer solver, and eliminate critical slowing down.
  - Both for standard and gauge-equivariant construction of restriction/prolongation.
- Transfer learning: If we change the gauge-field configuration or system parameters like κ and β, only very little or no extra training is needed.
- We can implement communication avoidance naturally.
- We provide a flexible implementation interface (GPT) for experimentation and further studies.

Outlook

- Setup (determination of spin matrices for restriction/prolongation layers) currently still costly because near-null space is needed
  - Future: Remove this cost by gauge-invariant models with these spin matrices as output
  - Use energy density, topological-charge density, Wilson loops
  - Useful for ensemble generation (where setup cost cannot be amortized)
- Apply our methods to Dirac operators whose spectrum encircles the origin (e.g., DWF)
- Directly approximate complex hadronic correlation functions without constructing them from intermediate approximations of propagators
- Benchmarking on large lattices and comparison to state-of-the-art multigrid (larger volumes should lead to larger iteration count gain)

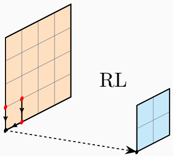
Backup slides

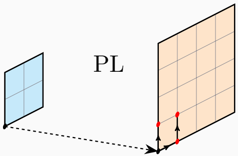
Results for full multigrid model (standard version)



- Performance greatly improved over individual high-/low-mode models
- Continued training converges very quickly
- Transfer learning works again after brief retraining

More details on the pooling layer





- Gauge field $\bar{U}$ in $T_p(\bar{U})$ needs to satisfy

$$\bar{U}_\mu(x) \to \Omega(x)\bar{U}_\mu(x)\Omega^\dagger(x+\hat{\mu})$$

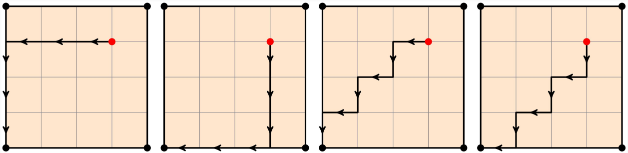
  In practice, we use a variety of differently smeared links
- Complete set of paths P transports every element of $B(y)$ exactly once to $B_r(y)$ $\to |P| = |B(y)|$
- $\tilde{\varphi} = \mathrm{RL}\,\varphi$ yields $\tilde{\varphi}(y) \to \tilde{\Omega}(y)\tilde{\varphi}(y)$ under gauge transformations $\varphi(x) \to \Omega(x)\varphi(x)$

More details

- Need prescription for q in

$$\text{Pool}\,\varphi(x) = \sum_{q \in Q} W_q(x) T_q \varphi(x)$$

  with $q = (p, \bar{U})$, path p, gauge field $\bar{U}$, $T_q = T_p(\bar{U})$
- For fixed i, we define paths $p^{(ij)}$ that connect all elements of $B(y)$, enumerated by $j = 1, \ldots, |B(y)|$, to the reference site $B_r(y)$. For different i we use different prescriptions for the paths $p^{(ij)}$, and then use the couples $q_{ij} = (p^{(ij)}, \bar{U}^{(i)})$.
- We define four different prescriptions $\hat{p}_1, \ldots, \hat{p}_4$ (depth first, breadth first, lexicographic, reverse lexicographic)



  and set $p^{(ij)} = p^{(j)}_{i \bmod 4}$

More details

- Concretely, we use 9 different gauge fields $\bar{U}^{(i)}$ with $i = 1, \ldots, 9$. We construct the $\bar{U}^{(i)}$ by applying $i(i-1)/2$ steps of $\rho = 0.1$ stout smearing to the unsmeared gauge fields U. Smearing radius proportional to $\sqrt{i(i-1)}$.
- Hence we have 9 different spin-matrix fields $W_1(x), \ldots, W_9(x)$.
- In practice, it is sufficient to use the same weights in PL and RL so that $\mathrm{PL} = \mathrm{RL}^\dagger$. Found no benefits from general case.
- Coarse-grid size $2^3 \times 4$