University of Colorado **Boulder**

Renormalization Group inspired inverse blocking with conditional normalizing flows

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Outline

Introduction

Perfect blocking implementation

Invertibility: The picture in momentum space

Upscaling flow (preliminary)

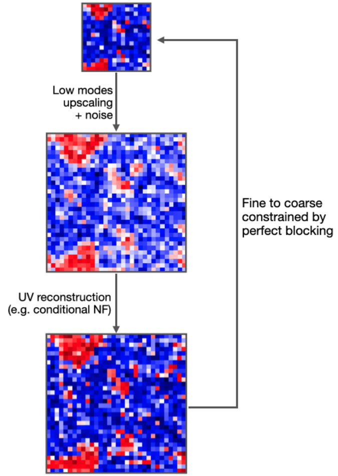
Conclusions

Introduction

Motivations

- Critical slowing down of MCMC near continuous phase transitions.
- Alternative ML-based sampling
  - Normalizing Flows (arXiv:1904.12072)
  - Multiscale / hierarchical generative models (arXiv:2604.10209)
  - Inverse RG upscaling (arXiv:2107.00466)
  - Diffusion and transport methods (arXiv:2311.03578; 2605.06134)
  - ...

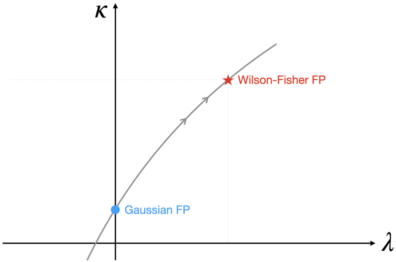
- Many existing generative models learn both infrared and ultraviolet degrees of freedom simultaneously.
- Investigate **perfect blocking** as a tool to reduce the learning task to the missing UV degrees of freedom.
  1. Upscale coarse MC-generated ensemble,
  2. Reconstruct the missing UV modes,
  3. Fine/coarse consistency enforced by perfect blocking.



The model: 2d ϕ^4

$$S[\phi] = -2\kappa \sum_{x,\mu} \phi_x \phi_{x+\hat{\mu}} + \sum_x \left[\phi_x^2 + \lambda(\phi_x^2 - 1)^2\right]$$

- Gaussian fixed point (no interactions).
- Wilson–Fisher fixed point (interacting critical point).
- $\lambda = 1,\ \kappa_c(\lambda) = 0.34$
- RG flow toward the Wilson–Fisher point.



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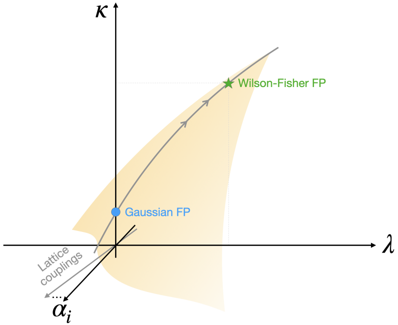

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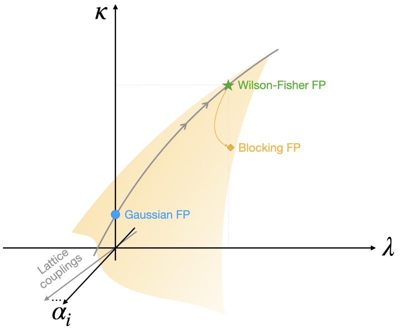
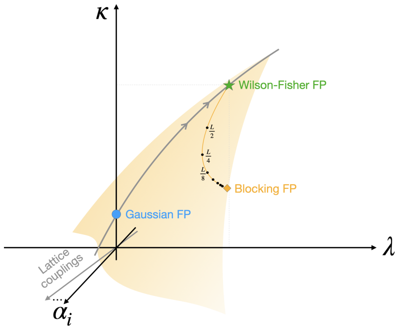


Perfect blocking

$$\langle \mathcal{O}_i(\Phi_L) \rangle = 2^{-\left(p+\frac{n\eta}{2}\right)} \langle \mathcal{O}_i(\phi_{L/2}) \rangle \;\; \forall \mathcal{O}_i \qquad \begin{cases} n = \# \text{ of fields, } p = \# \text{ of derivatives in } \mathcal{O}_i \\ \eta = 0.25 \end{cases}$$

- RG blocking changes the effective action: new couplings appear.
- Traditional route: perfect action for a fixed blocking transformation.
  (arXiv:2311.17816; 2502.03315; 2504.15870)
- Complementary route: perfect blocking for a fixed target action.
  - At this blocking FP, action is ≈ target one.
  - Upscaling flow ≈ in same parameter region



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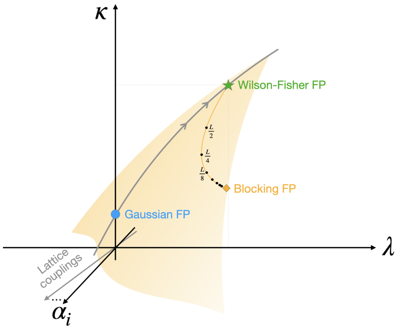

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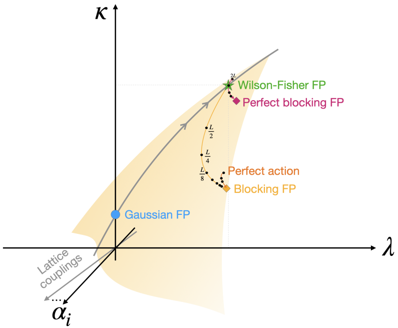
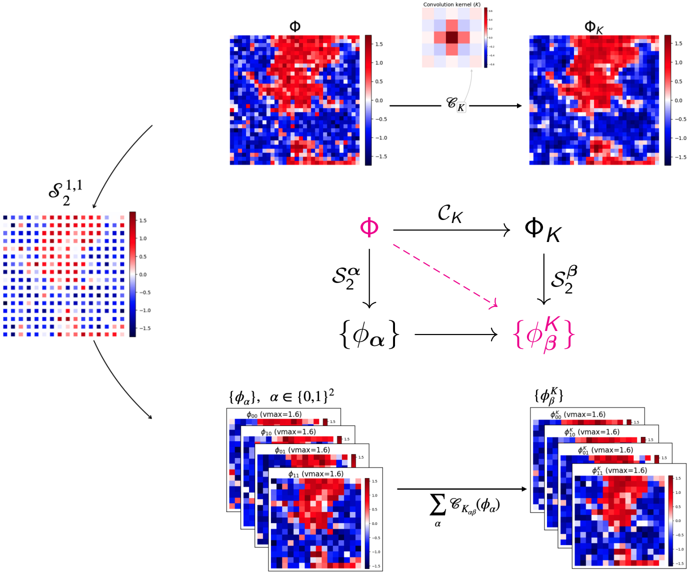


Perfect blocking implementation

Perfect blocking: Illustration

- Φ: $2L \times 2L$ configuration
- ϕ_α^K: $L \times L$ configurations with $\alpha \in \{00, 10, 01, 11\}$
- C_K: local stride-1 convolution
- S_2: stride-2 decimation
- $S_2 \circ C_K$: "perfect" blocking (after proper training of K)
- (!) Convolution might not be invertible, depending on K

$$\Phi \overset{?}{\leftarrow} \Phi^K$$



Perfect blocking: Training details

Kernel parametrization:

- D_4−symmetric local kernel K
- $\Rightarrow$ real in momentum space
- Normalized to $\sum_{\vec{r}} K(\vec{r}) = 2^{\eta/2}$
- η trained or fixed

Choice of observables:

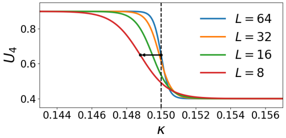
- Vol-averaged set of local operators[a]

$$\mathcal{O}_i(\phi) = \phi \prod_{m=1}^{M_{\max}-1} \left(\partial_1^{n_1(m)} \partial_2^{n_2(m)} \phi\right)$$

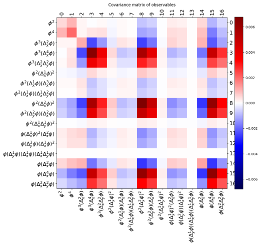
- $M_{\max}$ derivatives and $N_{\max}$ fields

[a] Symmetric derivatives, iterations of 1d discrete derivatives $\nabla^{(1)}\phi \equiv \frac{1}{2}(\phi_{x+1} - \phi_{x-1})$ and $\nabla^{(2)}\phi \equiv (\phi_{x+1} + \phi_{x-1} - 2\phi_x)$

Training ensembles: Blocked$_{(L\times L)}$ vs MC-gen$_{(L\times L)}$

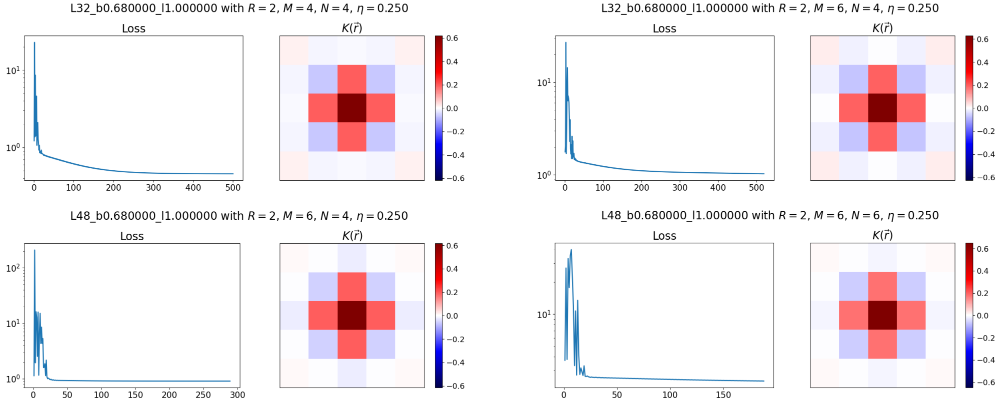


Loss $= \delta^T C^{-1} \delta$, w/ $\delta = \left(\langle \mathcal{O}(\phi^K_{00})\rangle - \langle \mathcal{O}(\Phi)\rangle\right)$



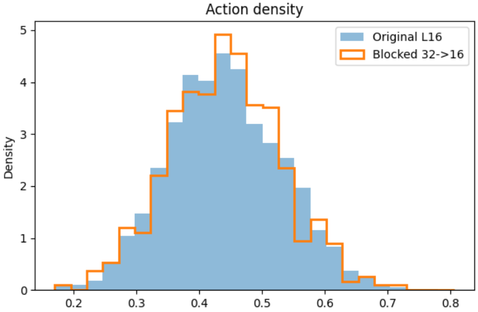
Perfect blocking: Training results at fixed $\eta = 0.25$

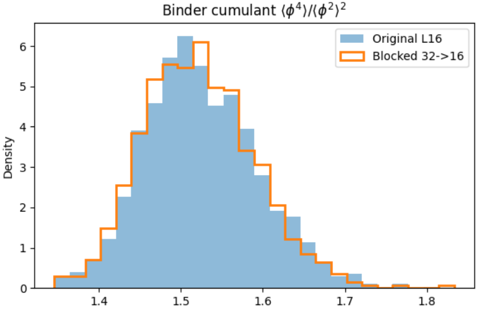
- Kernel parametrization in position space.
- Same R, increasing $M_{\max}$, $N_{\max}$ and lattice size L.



Action density and Binder cumulant

- $N_{\max} = 4$, $M_{\max} = 6$, $R = 2$, $\eta = 0.25$
- Blue: MC-gen $L = 16$ ensemble, orange line: blocked $L = 32 \to L = 16$
- Observables not in the loss.





Other $\langle \mathcal{O}_i \rangle$ histograms

0	ϕ^2
1	ϕ^4
2	$\phi^3(\Delta_y^2\phi) + \phi^3(\Delta_x^2\phi)$
3	$\phi^3(\Delta_y^4\phi) + \phi^3(\Delta_x^4\phi)$
4	$\phi^3(\Delta_y^6\phi) + \phi^3(\Delta_x^6\phi)$
5	$\phi^3(\Delta_x^2\Delta_y^2\phi)$
6	$\phi^3(\Delta_x^2\Delta_y^4\phi) + \phi^3(\Delta_x^4\Delta_y^2\phi)$
7	$\phi^2(\Delta_y^1\phi)^2 + \phi^2(\Delta_x^1\phi)^2$
8	$\phi^2(\Delta_y^1\phi)(\Delta_y^3\phi) + \phi^2(\Delta_x^1\phi)(\Delta_x^3\phi)$
9	$\phi^2(\Delta_y^1\phi)(\Delta_y^5\phi) + \phi^2(\Delta_x^1\phi)(\Delta_x^5\phi)$
10	$\phi^2(\Delta_y^1\phi)(\Delta_x^2\Delta_y^1\phi) + \phi^2(\Delta_x^1\phi)(\Delta_x^1\Delta_y^2\phi)$
11	$\phi^2(\Delta_y^1\phi)(\Delta_x^2\Delta_y^3\phi) + \phi^2(\Delta_x^1\phi)(\Delta_x^3\Delta_y^2\phi)$
12	$\phi^2(\Delta_y^1\phi)(\Delta_x^4\Delta_y^1\phi) + \phi^2(\Delta_x^1\phi)(\Delta_x^1\Delta_y^4\phi)$
13	$\phi^2(\Delta_y^2\phi)^2 + \phi^2(\Delta_x^2\phi)^2$
14	$\phi^2(\Delta_y^2\phi)(\Delta_y^4\phi) + \phi^2(\Delta_x^2\phi)(\Delta_x^4\phi)$
15	$\phi^2(\Delta_y^2\phi)(\Delta_x^2\phi)$
16	$\phi^2(\Delta_y^2\phi)(\Delta_x^2\Delta_y^2\phi) + \phi^2(\Delta_x^2\phi)(\Delta_x^2\Delta_y^2\phi)$
17	$\phi^2(\Delta_y^2\phi)(\Delta_x^4\phi) + \phi^2(\Delta_y^4\phi)(\Delta_x^2\phi)$
18	$\phi^2(\Delta_y^3\phi)^2 + \phi^2(\Delta_x^3\phi)^2$
19	$\phi^2(\Delta_y^3\phi)(\Delta_x^2\Delta_y^1\phi) + \phi^2(\Delta_x^1\Delta_y^2\phi)(\Delta_x^3\phi)$
20	$\phi^2(\Delta_x^1\Delta_y^1\phi)^2$
21	$\phi^2(\Delta_x^1\Delta_y^1\phi)(\Delta_x^1\Delta_y^3\phi) + \phi^2(\Delta_x^1\Delta_y^1\phi)(\Delta_x^3\Delta_y^1\phi)$
22	$\phi^2(\Delta_x^1\Delta_y^2\phi)^2 + \phi^2(\Delta_x^2\Delta_y^1\phi)^2$
23	$\phi(\Delta_y^1\phi)^2(\Delta_y^2\phi) + \phi(\Delta_x^1\phi)^2(\Delta_x^2\phi)$
24	$\phi(\Delta_y^1\phi)^2(\Delta_y^4\phi) + \phi(\Delta_x^1\phi)^2(\Delta_x^4\phi)$
25	$\phi(\Delta_y^1\phi)^2(\Delta_x^2\phi) + \phi(\Delta_y^2\phi)(\Delta_x^1\phi)^2$
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37	$\phi(\Delta_y^2\phi)^3 + \phi(\Delta_x^2\phi)^3$
38	$\phi(\Delta_y^2\phi)^2(\Delta_x^2\phi) + \phi(\Delta_y^2\phi)(\Delta_x^2\phi)^2$
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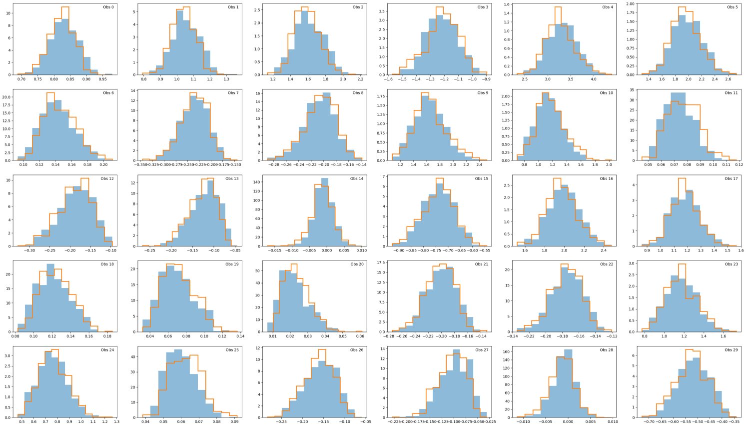
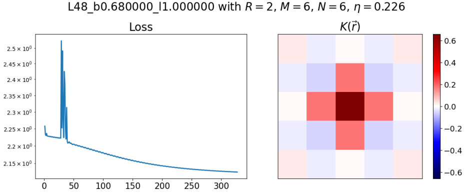
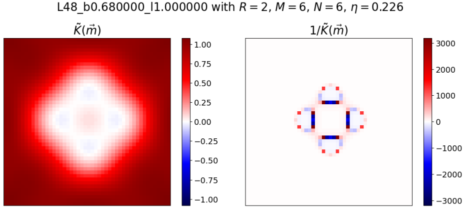


Blocking kernel in momentum space





- **D_4-symmetric parametrization**

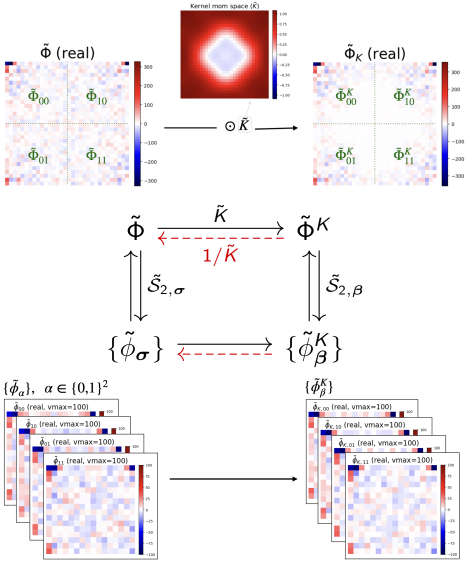
$$\tilde{K}(\vec{n} + \boldsymbol{s}L) = \sum_{\vec{r}} b(\vec{r}) \cos\left(\frac{\pi}{L}\vec{r}\cdot\vec{n}\right)(-1)^{\vec{r}\cdot\boldsymbol{s}}\,, \qquad b(g\vec{r}) = b(\vec{r})\ \forall g \in D_4$$

$n_i = 0, \ldots, L-1$ momenta on coarse lattice. Fine lattice: $\vec{n} + \vec{s}L$ with $\vec{s} \in \{0,1\}^2$

- Enforcing positivity worsens the cost function and η (when trained).
- Can we get away with a non–invertible kernel? Or do we need to sacrifice some freedom to impose invertibility?

Invertibility: The picture in momentum space

- Coarse lattice: $\vec{k} = \frac{2\pi}{L}\vec{n}, \quad n_i = 0, \ldots, L-1.$
- Fine lattice: $\vec{m} = \vec{n} + \vec{s}L, \quad \vec{s} \in \{0,1\}^2$
- $\Rightarrow \widetilde{\Phi}(\vec{m}) \equiv \widetilde{\Phi}_{\vec{s}}(\vec{n}).$
- Convolution: $\widetilde{\Phi}_K(\vec{m}) = \widetilde{K}(\vec{m})\,\widetilde{\Phi}(\vec{m}).$
- Define: $M_{\boldsymbol{\sigma}}(\vec{n} + \boldsymbol{s}L) = (-1)^{\boldsymbol{\sigma}\cdot\vec{s}} e^{i\pi\vec{n}\cdot\boldsymbol{\sigma}/L}.$
- (Note: $M_{\boldsymbol{\sigma}}(\vec{n} + \boldsymbol{s}L) = 1\ \forall \vec{n}$.)
- Stride-2: $\widetilde{\phi}^K_{\boldsymbol{\sigma}}(\vec{n}) = \frac{1}{4}\sum_{\vec{s}} M_{\boldsymbol{\sigma s}}(\vec{n})\,\widetilde{\Phi}^K(\vec{n} + \vec{s}L).$
- L.h.s.: Any chance of basis $P_{\boldsymbol{\sigma}}$ s.t. $\det P_{\boldsymbol{\sigma}} \neq 0$ and $P^{\dagger}_{\boldsymbol{\sigma}}(\vec{m}) = P_{\boldsymbol{\sigma}}(-\vec{m})$.
- E.g., low/high-mode basis $P_\alpha = \frac{1}{4} H_{\alpha\sigma} M_\sigma$.



Blocking in momentum space

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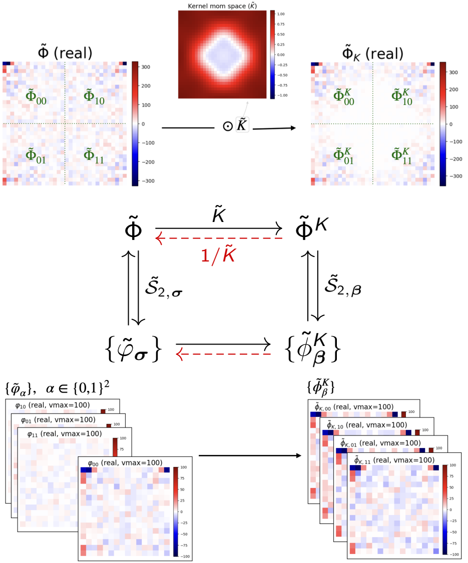
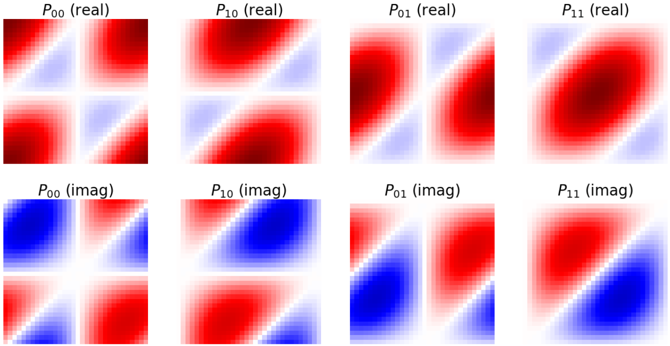


Low/high modes separation

- Choose $P_\sigma(\vec{m}) = \frac{1}{4} H_{\sigma\alpha} M_\alpha(\vec{m})$ with H the Hadamard matrix.
- $\tilde{\varphi}_\alpha(\vec{n}) = \frac{1}{4} \sum_s \Phi(\vec{n} + sL) P_\alpha(\vec{n} + sL)$
- $\Phi(\vec{n} + sL) = P^\dagger_\alpha(\vec{n} + sL)\, \tilde{\varphi}_\alpha(\vec{n})$

$$\begin{tikzcd} \tilde{\Phi} \arrow[r, shift left, "\tilde{K}"] \arrow[d, shift left, "\tilde{\mathcal{S}}_{2,\sigma}"] & \tilde{\Phi}^K \arrow[l, shift left, dashed, "\times"] \arrow[d, shift left, "\tilde{\mathcal{S}}_{2,\beta}"] \\ \{\tilde{\varphi}_\sigma\} \arrow[u, shift left] \arrow[r, shift left] & \{\tilde{\phi}^K_\beta\} \arrow[u, shift left] \arrow[l, shift left, dashed] \end{tikzcd}$$



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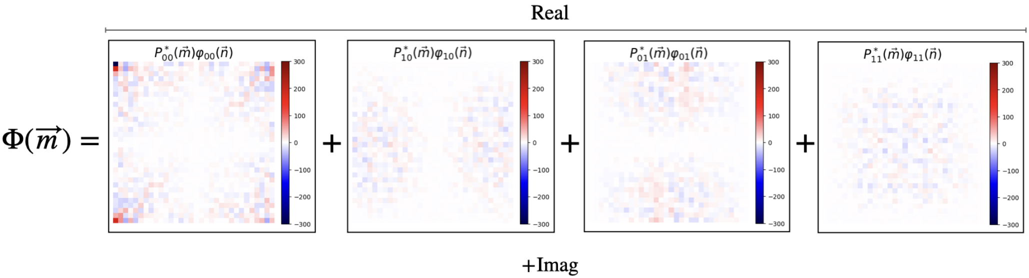
\end{tikzcd}$$

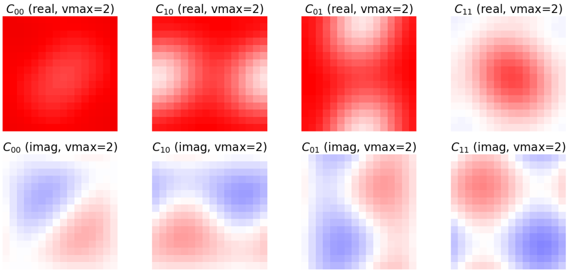


Maps between small volumes

- $\tilde{\phi}^K_\alpha(\vec{n}) = \sum_\beta A_{\alpha\beta}(\vec{n})\tilde{\varphi}_\beta(\vec{n})$,
- Focus on $C_\beta \equiv A_{00,\beta}$; $C_\beta(\vec{n}) = \frac{1}{4}\sum_s \tilde{K}(\vec{n} + \boldsymbol{s}L)P_\beta(\vec{n} + \boldsymbol{s}L)$
- $\Rightarrow \tilde{\phi}^K_{00} = \sum_\beta C_\beta \tilde{\varphi}_\beta$
- $\Rightarrow \tilde{\varphi}^K_{00} = C_{00}^{-1}\left(\tilde{\phi}^K_{00} - \sum_{\beta\neq 00} C_\beta \tilde{\varphi}_\beta\right)$

$$
\begin{tikzcd}
\tilde{\Phi} \arrow[r, shift left, "\tilde{K}"] \arrow[d, shift right] & \tilde{\Phi}^K \arrow[l, shift left, dashed, "\times"] \arrow[d, shift right] \\
\{\tilde{\varphi}_{\boldsymbol{\sigma}}\} \arrow[u, shift right, "\tilde{S}_{2,\sigma}"'] \arrow[r, shift left, "A_{\boldsymbol{\sigma\alpha}}"] & \{\tilde{\phi}^K_{\boldsymbol{\beta}}\} \arrow[u, shift right, "\tilde{S}_{2,\beta}"'] \arrow[l, shift left, dashed]
\end{tikzcd}
$$

Only $C_{00}(\vec{n})$ needs to be invertible!



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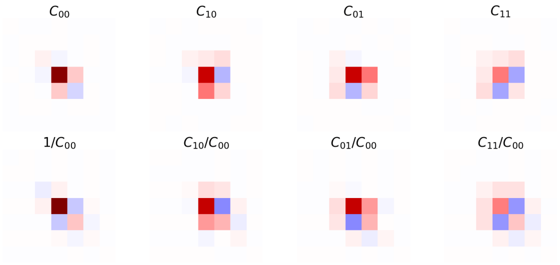
- $\tilde{\phi}^K_\alpha(\vec{n}) = \sum_\beta A_{\alpha\beta}(\vec{n})\tilde{\varphi}_\beta(\vec{n})$,
- Focus on $C_\beta \equiv A_{00,\beta}$; $C_\beta(\vec{n}) = \frac{1}{4}\sum_s \tilde{K}(\vec{n}+\boldsymbol{s}L)P_\beta(\vec{n}+\boldsymbol{s}L)$
- $\Rightarrow \tilde{\phi}^K_{00} = \sum_\beta C_\beta \tilde{\varphi}_\beta$
- $\Rightarrow \tilde{\varphi}^K_{00} = C_{00}^{-1}\left(\tilde{\phi}^K_{00} - \sum_{\beta\neq 00} C_\beta\tilde{\varphi}_\beta\right)$
- $\varphi_\beta(\vec{n})C_\beta(\vec{n})$ in position space correspond to local convolutions

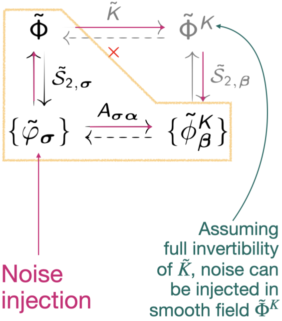
$$\begin{tikzcd}
\tilde{\Phi} \arrow[r, shift left, "\tilde{K}"] \arrow[d, shift left] & \tilde{\Phi}^K \arrow[l, shift left, dashed, "\times"'] \arrow[d, shift left] \\
\{\tilde{\varphi}_{\boldsymbol{\sigma}}\} \arrow[u, shift left, "\tilde{\mathcal{S}}_{2,\sigma}"'] \arrow[r, shift left, "A_{\boldsymbol{\sigma\alpha}}"] & \{\tilde{\phi}^K_{\boldsymbol{\beta}}\} \arrow[l, shift left, dashed] \arrow[u, shift left, "\tilde{\mathcal{S}}_{2,\beta}"']
\end{tikzcd}$$



Reconstruction strategy

- On *l.h.s.*, pick masks P_α, which sets $\tilde{\Phi} \xrightarrow[P_{\boldsymbol{\alpha}}]{} \{\tilde{\varphi}_{\boldsymbol{\sigma}}\}$.
- The choice of P_α determines the shape of $C_\beta(\vec{n})$ masks: if P_α separates low/high modes, then $C_{00}(\vec{n})$ becomes easily invertible.
- Training/reconstruction can be performed through the map

$$\tilde{\Phi} \longleftrightarrow \{\tilde{\varphi}_{\boldsymbol{\sigma}}\} \longleftrightarrow \{\tilde{\phi}^K_{\boldsymbol{\beta}}\}.$$



- Given an **input** coarse configuration $\tilde{\phi}^K_{00}$, only the three missing UV components $\tilde{\varphi}_{10}$, $\tilde{\varphi}_{01}$, $\tilde{\varphi}_{11}$ remain undetermined.
- $\tilde{\varphi}_{\beta\neq 00}$ natural latent space in which to inject trainable noise.

$$\boxed{\tilde{\phi}^K_{00},\ \tilde{\zeta}_{10}, \tilde{\zeta}_{01}, \tilde{\zeta}_{11}} \xrightarrow{f_\theta} \boxed{\tilde{\phi}^K_{00},\ \tilde{\eta}_{10}, \tilde{\eta}_{01}, \tilde{\eta}_{11}} \xrightarrow{\text{reconstruction}} \boxed{\tilde{\Phi}}$$

Upscaling flow (preliminary)

Conditional Normalizing Flow

Triangular conditional flow

$$\boxed{\begin{aligned}\eta_{10} &= f_{10}(\phi_{00}^K, \zeta_{10}),\\ \eta_{01} &= f_{01}(\phi_{00}^K, \eta_{10}, \zeta_{01}),\\ \eta_{11} &= f_{11}(\phi_{00}^K, \eta_{10}, \eta_{01}, \zeta_{11}).\end{aligned}}$$

Tested

- affine couplings,
- spline couplings,
- many orderings...

Affine flow

$$\eta_i = e^{s_i}\zeta_i + t_i$$

$$\log|\det J| = \sum_i s_i - \log C_{00}$$

Fixed reconstruction

$$\boxed{\Phi \to \begin{pmatrix}\varphi_{00}\\ \varphi_{10}\\ \varphi_{01}\\ \varphi_{11}\end{pmatrix} = \begin{pmatrix}\mathcal{C}_{00}^{-1} & -\mathcal{C}_{10} & -\mathcal{C}_{01} & -\mathcal{C}_{11}\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}\phi_{00}^K\\ \eta_{10}\\ \eta_{01}\\ \eta_{11}\end{pmatrix}}$$

$\mathcal{C}_{00}^{-1}$ and $\mathcal{C}_\beta$ are the position-space convolutions corresponding to the momentum-space kernels C_{00}^{-1} and $C_{00}^{-1}C_\beta$.

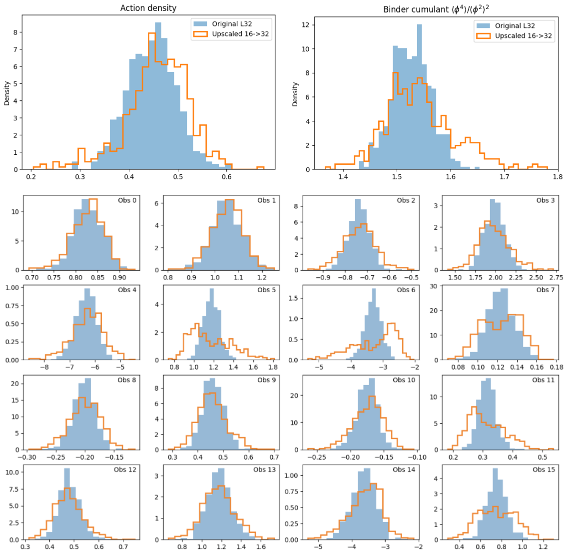
Metropolis-Hastings correction All info known to compute A/R

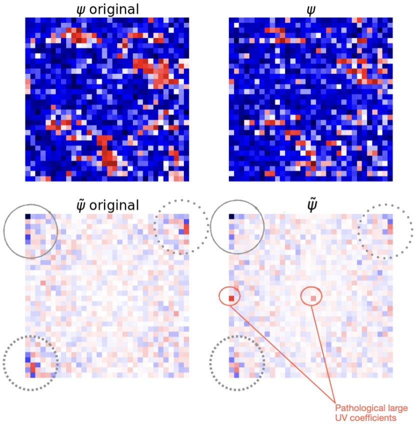
$$P_{\mathrm{acc}}(\Phi \to \Phi') = \min\left(1, \frac{\pi(\Phi')\, q(\Phi|\phi_{00}^K)}{\pi(\Phi)\, q(\Phi'|\phi_{00}^K)}\right),$$

$$q(\Phi|\phi_{00}^K) = \frac{p(\zeta)}{|\det J_{\zeta\to\eta}|\,|C_{00}|^{-1}},$$

$$p(\zeta) = \mathcal{N}(0, \mathbf{I}), \qquad \pi(\Phi) \propto e^{-S_{\phi^4}[\Phi]}.$$

Results (preliminary...)





Why doesn't it work yet?

- An upscaling flow is possible! (A. Hasenfratz poster at this conference).
- Work presented in the poster assumes **full invertibility** of blocking kernel,
- $\Rightarrow$ noise can be injected directly in smoothed Φ^K.

Possibility 1 : reconstruction tested until now not good enough:

Retrain blocking kernel
according to perfect blocking condition

$$\boxed{\Phi} \leftarrow \begin{pmatrix}\varphi_{00}\\ \varphi_{10}\\ \varphi_{01}\\ \varphi_{11}\end{pmatrix} = \boxed{\begin{pmatrix} \mathscr{C}_{00}^{-1} & -\mathscr{C}_{10} & -\mathscr{C}_{01} & -\mathscr{C}_{11}\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}} \begin{pmatrix} \boxed{\phi_{00}^K}\\ \eta_{10} = f_{10}(\phi_{00}^K, \zeta_{10})\\ \eta_{01} = f_{01}(\phi_{00}^K, \eta_{10}, \zeta_{01})\\ \eta_{11} = f_{11}(\phi_{00}^K, \eta_{10}, \eta_{01}, \zeta_{11})\end{pmatrix}$$

Change
noise
model

Improve conditional
flow model

Possibility 2 : Partial invertibility is indeed a limitation.

Conclusions

Conclusions and Outlook

- Perfect blocking: physically motivated framework for upscaling ensembles near criticality.
- The optimized blocking kernels appear to be
  - consistent across observables and training volumes,
  - effectively localized within a $\sim 5 \times 5$ stencil,
  - when trained, $\eta \approx 0.25 \pm 0.05$.
- The reconstruction explored here suggests full kernel invertibility may not be necessary $\rightarrow$ greater freedom for perfect blocking kernels.
- Under the assumption that the blocking kernel is fully invertible, successful upscaling (**A. Hasenfratz poster at this conference**).
- Future work:
  - clarify the minimal invertibility requirements,
  - extend the construction to other theories with infrared fixed points.