

Toward Contour Deformation for 4d Gauge Theories

Yin Lin 林胤 yin01@mit.edu

Aug 2, 2023 Lattice 2023
Fermilab



Gurtej Kanwar



Michael Wagman



Phiala Shanahan



William Detmold

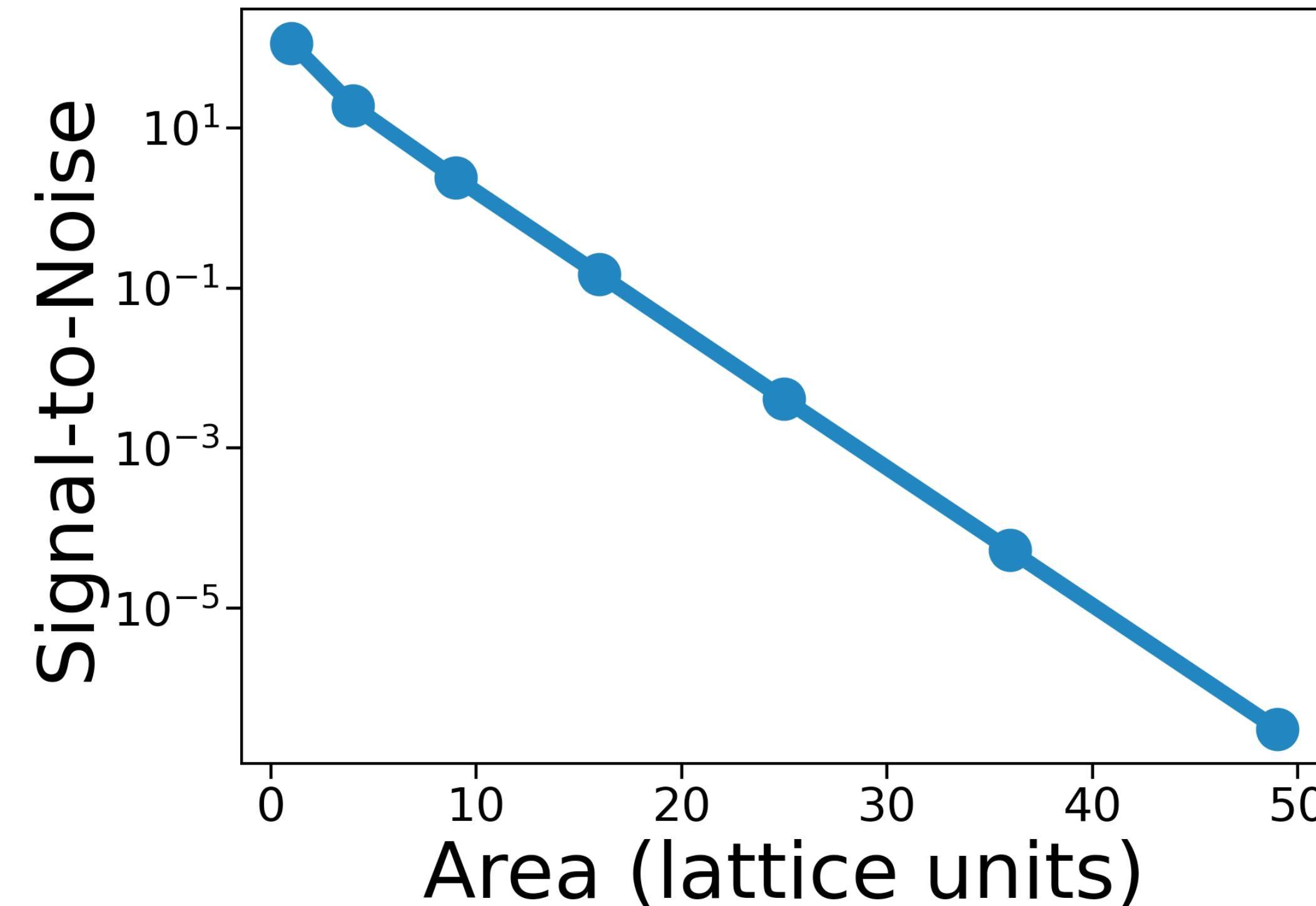


Massachusetts
Institute of
Technology



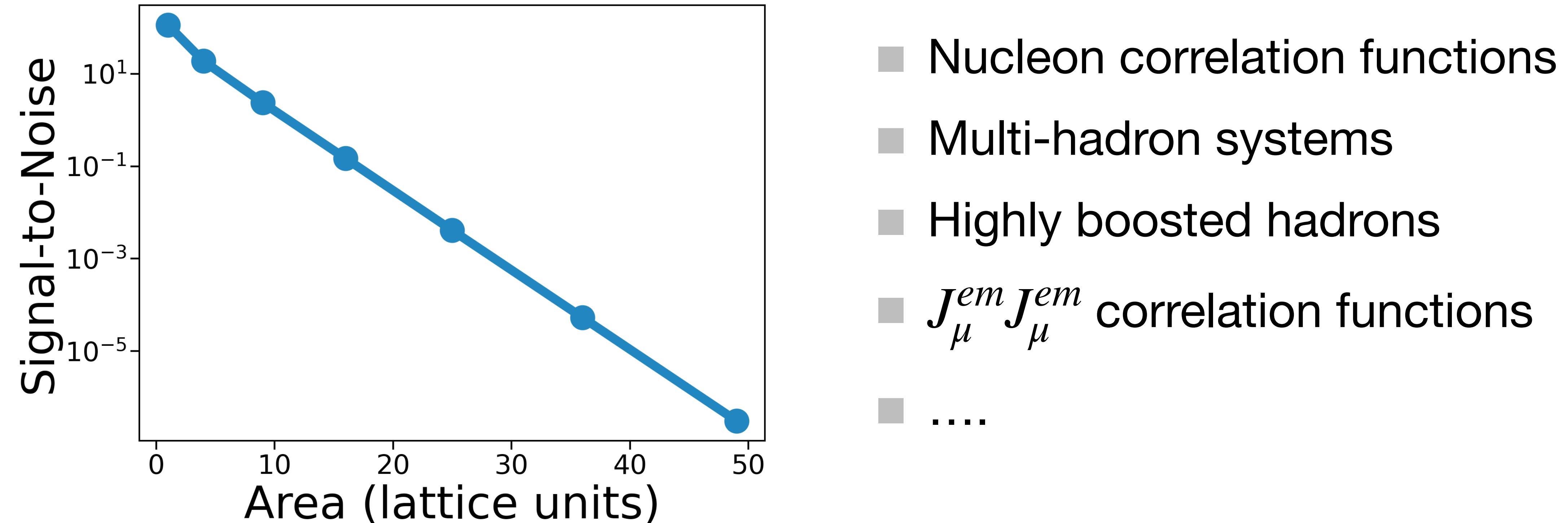
Signal-to-noise problems in LGT

Ubiquitous exponential signal-to-noise problems



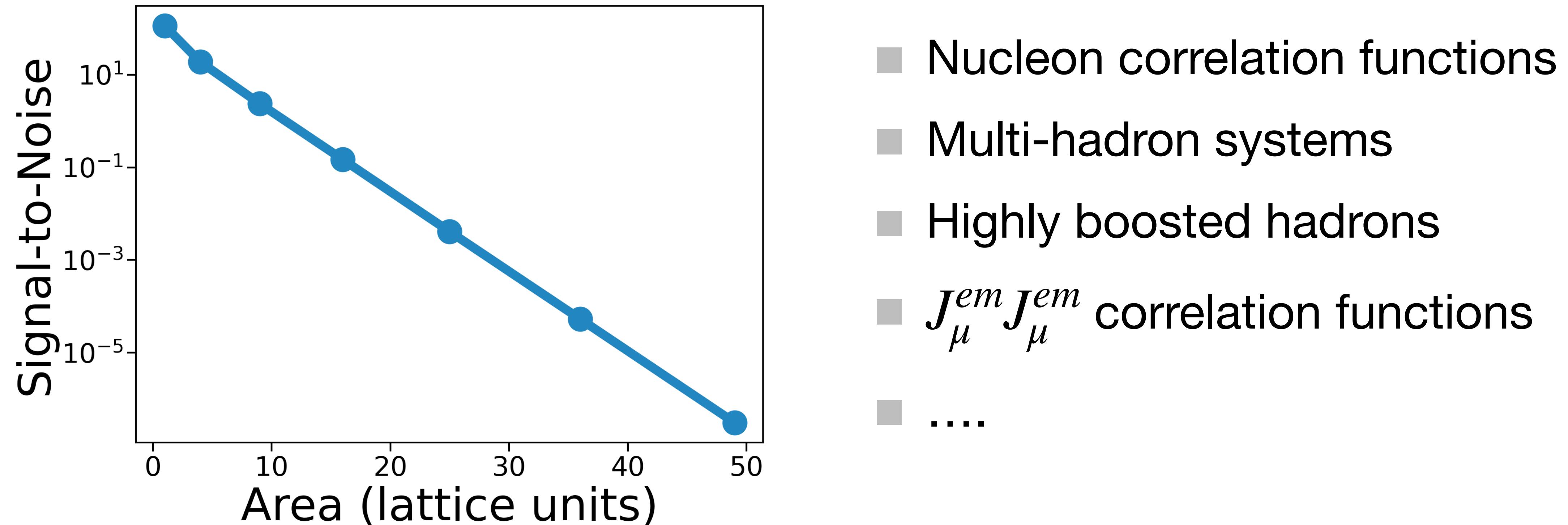
Signal-to-noise problems in LGT

Ubiquitous exponential signal-to-noise problems



Signal-to-noise problems in LGT

Ubiquitous exponential signal-to-noise problems



Monte Carlo measurements are complex-valued → Sign problems

[M. Wagman, M. Savage [hep-lat/1611.07643](https://arxiv.org/abs/1611.07643)]

Cauchy theorem and contour deformation

Can we design a “better” observable to alleviate the sign problem?

[A. Alexandru, G. Basar, P. Bedaque, N. Warrington [hep-lat/2007.05436](https://arxiv.org/abs/hep-lat/2007.05436)]

Cauchy theorem and contour deformation

Can we design a “better” observable to alleviate the sign problem?

[A. Alexandru, G. Basar, P. Bedaque, N. Warrington [hep-lat/2007.05436](https://arxiv.org/abs/hep-lat/2007.05436)]

For holomorphic $f(z)$ in some domain

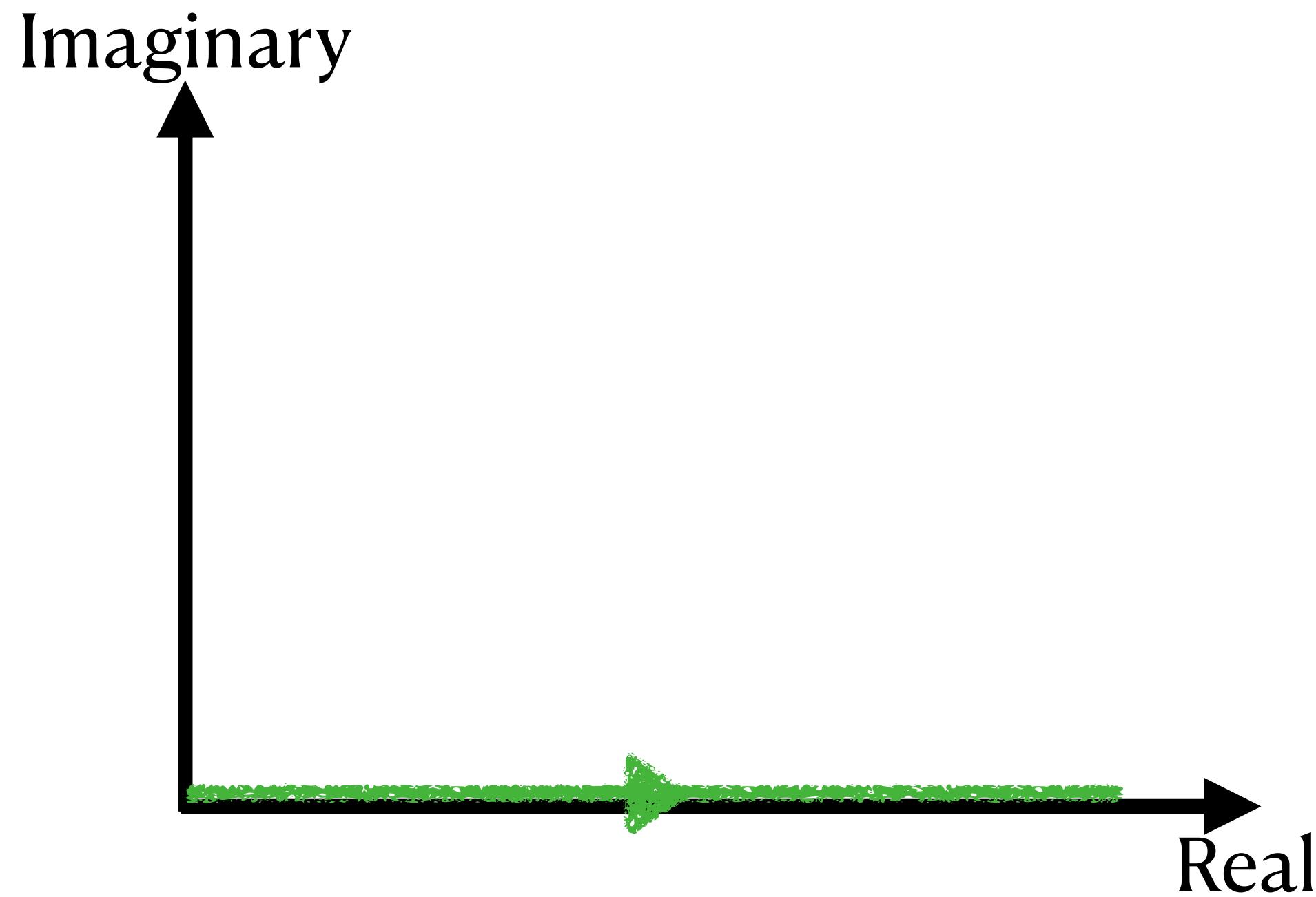
$$\oint f(z) \, dz = 0$$

Cauchy theorem and contour deformation

Can we design a “better” observable to alleviate the sign problem?

[A. Alexandru, G. Basar, P. Bedaque, N. Warrington [hep-lat/2007.05436](https://arxiv.org/abs/hep-lat/2007.05436)]

For holomorphic $f(z)$ in some domain



$$\oint f(z) \, dz = 0$$

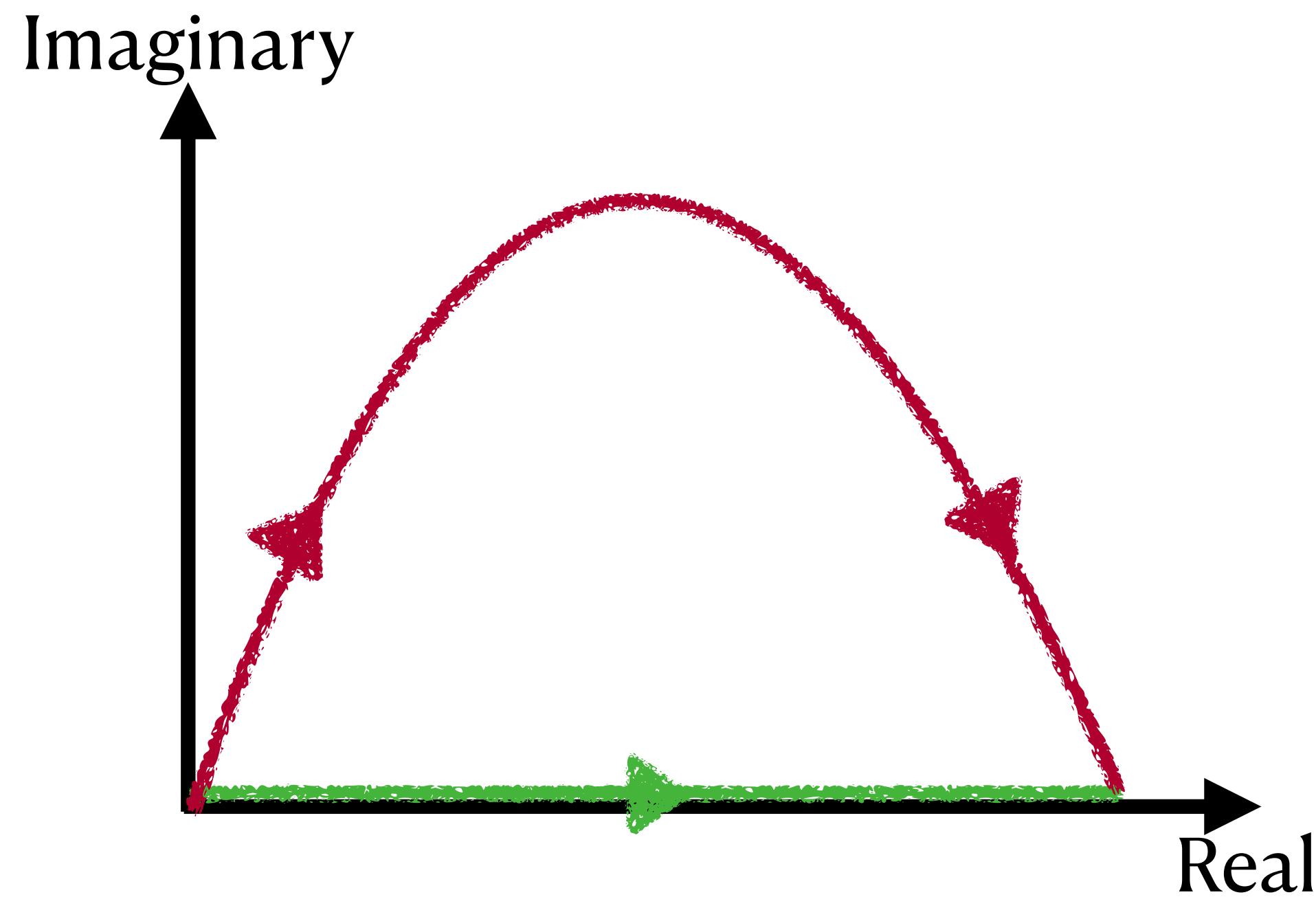
Cauchy theorem and contour deformation

Can we design a “better” observable to alleviate the sign problem?

[A. Alexandru, G. Basar, P. Bedaque, N. Warrington [hep-lat/2007.05436](https://arxiv.org/abs/hep-lat/2007.05436)]

For holomorphic $f(z)$ in some domain

$$\oint f(z) dz = 0$$

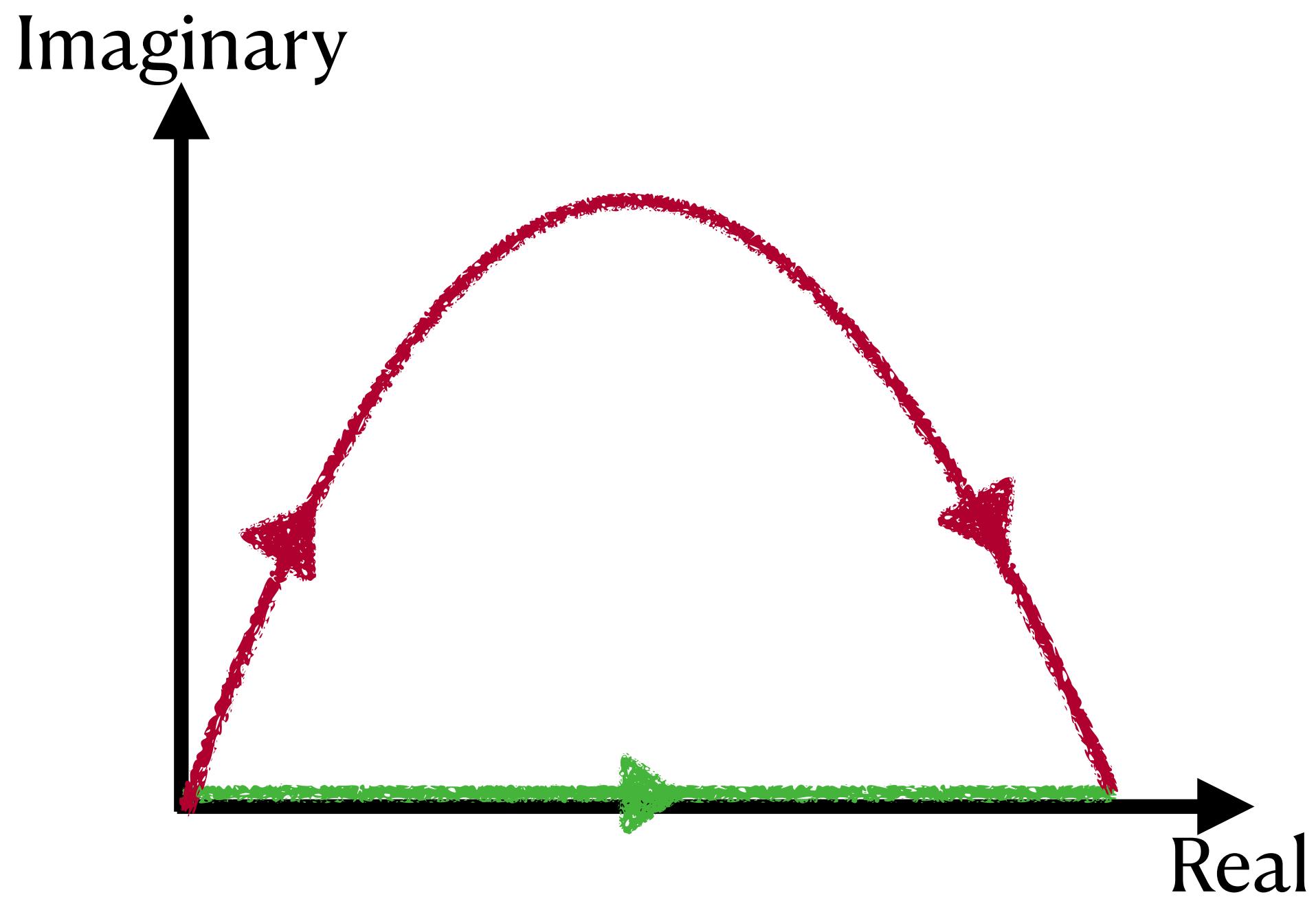


Cauchy theorem and contour deformation

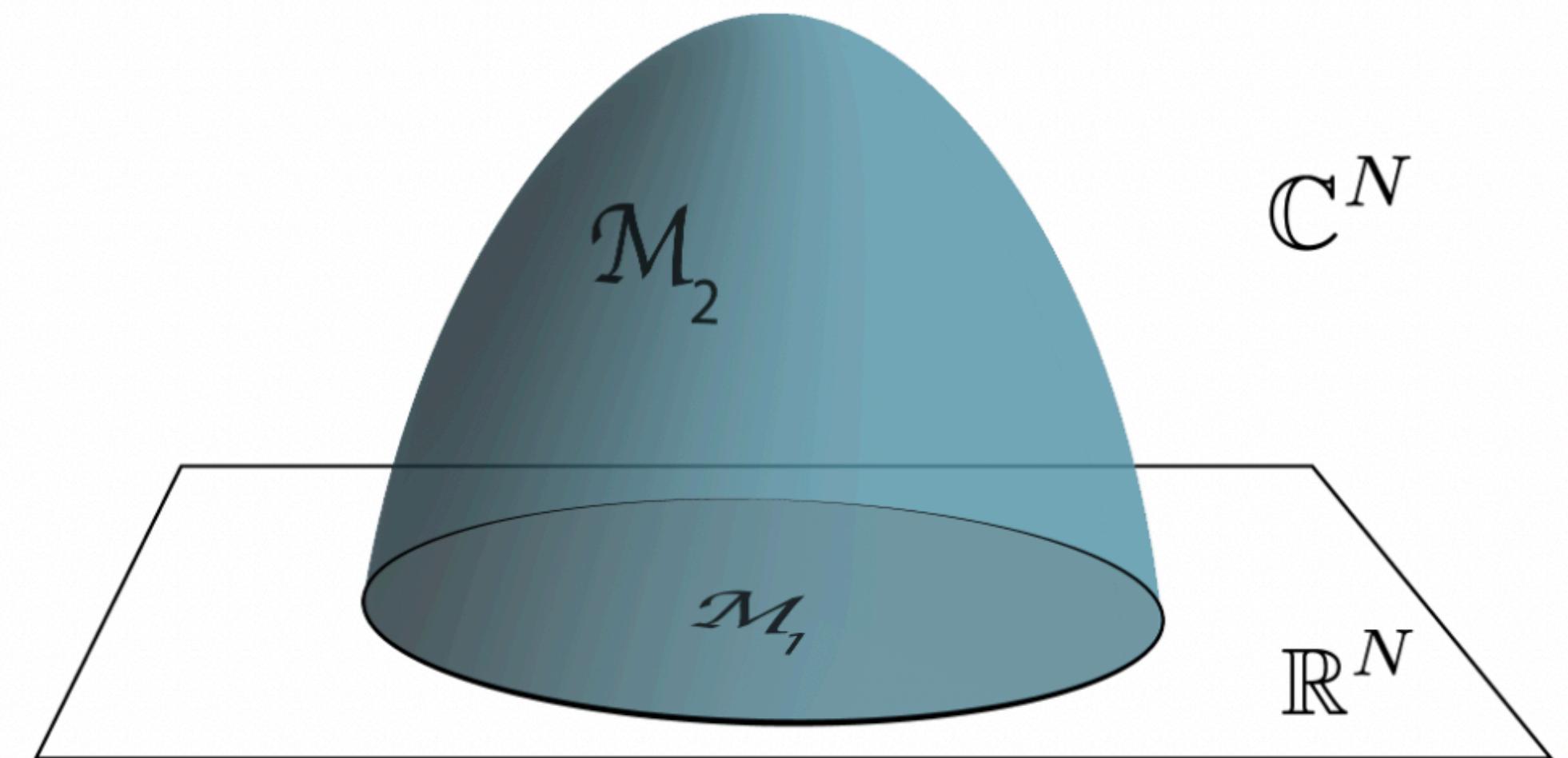
Can we design a “better” observable to alleviate the sign problem?

[A. Alexandru, G. Basar, P. Bedaque, N. Warrington [hep-lat/2007.05436](https://arxiv.org/abs/hep-lat/2007.05436)]

For holomorphic $f(z)$ in some domain



$$\oint f(z) \, dz = 0$$



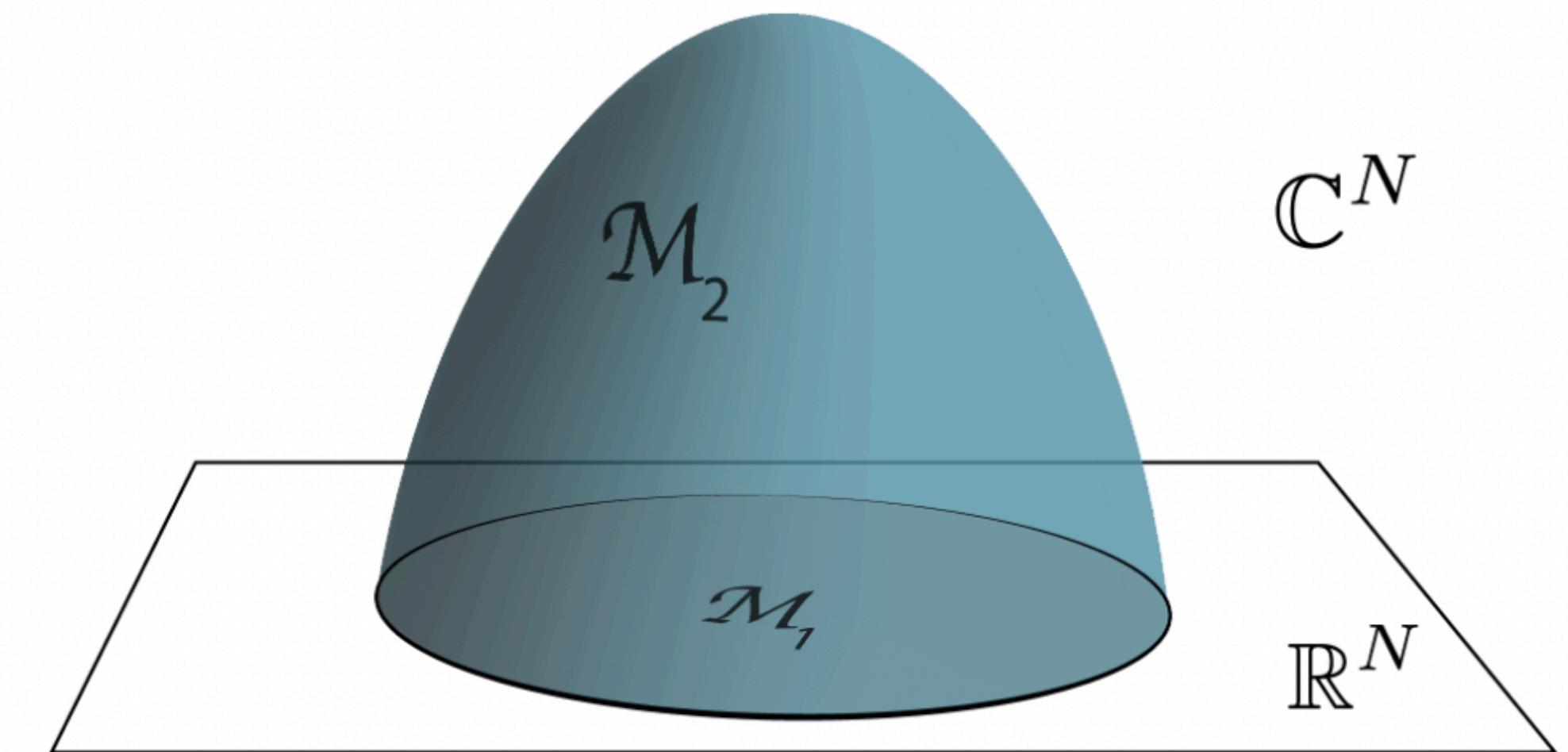
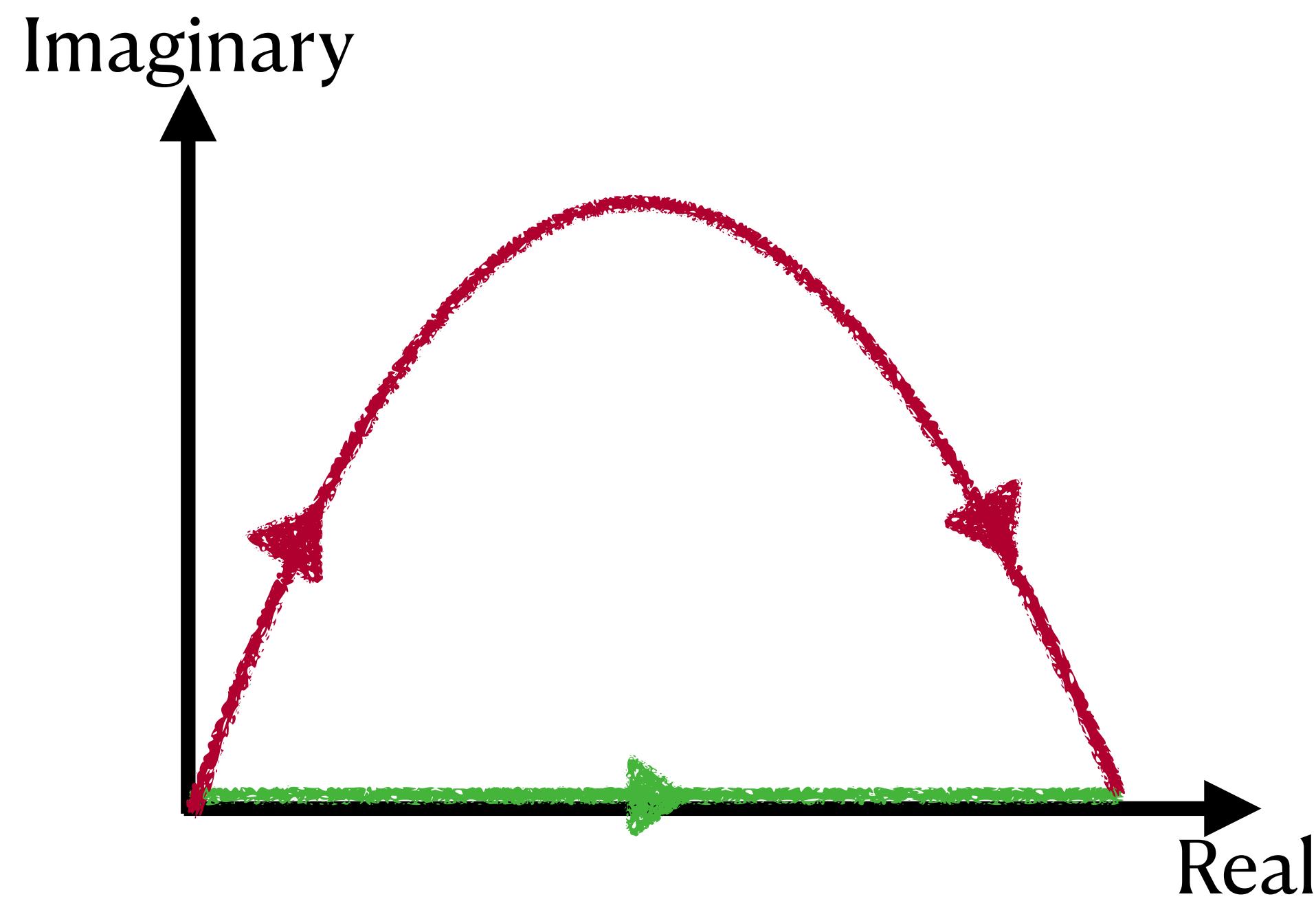
Cauchy theorem and contour deformation

Can we design a “better” observable to alleviate the sign problem?

[A. Alexandru, G. Basar, P. Bedaque, N. Warrington [hep-lat/2007.05436](https://arxiv.org/abs/hep-lat/2007.05436)]

For holomorphic $f(z)$ in some domain

$$\oint f(z) dz = 0$$



Expectation values are **holomorphic**, while variances are **not**

Contour deforming Wilson loops

Given a deformation on gauge field $U \rightarrow \widetilde{U}$



Contour deforming Wilson loops

Given a deformation on gauge field $U \rightarrow \widetilde{U}$

Wilson loop means are **holomorphic**

$$\begin{aligned}\langle \text{Re}W \rangle \\ = \text{Re} \int \prod_n dU_n \ p[U] \ W[U] \\ = \text{Re} \int \prod_n d\widetilde{U}_n \ p[\widetilde{U}] \ W[\widetilde{U}]\end{aligned}$$

Contour deforming Wilson loops

Given a deformation on gauge field $U \rightarrow \widetilde{U}$

Wilson loop means are **holomorphic**

$$\begin{aligned}\langle \text{Re}W \rangle \\ = \text{Re} \int \prod dU_n p[U] W[U] \\ = \text{Re} \int \prod_n d\widetilde{U}_n p[\widetilde{U}] W[\widetilde{U}]\end{aligned}$$

Variances are **not holomorphic**

$$\begin{aligned}\text{Var}(\text{Re}W[U]) &\neq \text{Var}(\text{Re}W[\widetilde{U}]) \\ \langle (\text{Re}W[U])^2 \rangle - \langle (\text{Re}W[U]) \rangle^2\end{aligned}$$

Contour deforming Wilson loops

Given a deformation on gauge field $U \rightarrow \widetilde{U}$

Wilson loop means are **holomorphic**

$$\begin{aligned}\langle \text{Re}W \rangle \\ = \text{Re} \int \prod dU_n p[U] W[U] \\ = \text{Re} \int \prod_n d\widetilde{U}_n p[\widetilde{U}] W[\widetilde{U}]\end{aligned}$$

Variances are **not holomorphic**

$$\text{Var}(\text{Re}W[U]) \neq \text{Var}(\text{Re}W[\widetilde{U}])$$
$$\langle (\text{Re}W[U])^2 \rangle - \langle (\text{Re}W[U]) \rangle^2$$

Deform $U \rightarrow \widetilde{U}$ to minimize the variances while guaranteeing exactness!

Constant deformations of $SU(2)$ and $SU(3)$

$SU(2)$ Euler angles

$$U = U(\theta_1, \phi_1, \phi_2)$$

$$\theta_i \in [0, \pi/2], \phi_i \in [0, 2\pi)$$

[W. Detmold, G. Kanwar, H. Lamm, M. Wagman, N. Warrington, [hep-lat/2101.12668](https://arxiv.org/abs/hep-lat/2101.12668)]

$SU(3)$ Euler angles

$$U = U(\theta_1, \theta_2, \theta_3, \phi_1, \phi_2, \phi_3, \phi_4, \phi_5)$$

Constant deformations of SU(2) and SU(3)

SU(2) Euler angles

$$U = U(\theta_1, \phi_1, \phi_2)$$

$$\theta_i \in [0, \pi/2], \phi_i \in [0, 2\pi)$$

[W. Detmold, G. Kanwar, H. Lamm, M. Wagman, N. Warrington, [hep-lat/2101.12668](https://arxiv.org/abs/hep-lat/2101.12668)]

SU(3) Euler angles

$$U = U(\theta_1, \theta_2, \theta_3, \phi_1, \phi_2, \phi_3, \phi_4, \phi_5)$$

Constant deformations

$$U(\theta_i, \phi_i) \rightarrow \widetilde{U} = U(\theta_i, \phi_i + i\Delta_i)$$

Δ_i are independent of the values of ϕ_i and θ_i

Constant deformations of SU(2) and SU(3)

SU(2) Euler angles

$$U = U(\theta_1, \phi_1, \phi_2)$$

$$\theta_i \in [0, \pi/2], \phi_i \in [0, 2\pi)$$

[W. Detmold, G. Kanwar, H. Lamm, M. Wagman, N. Warrington, [hep-lat/2101.12668](https://arxiv.org/abs/hep-lat/2101.12668)]

SU(3) Euler angles

$$U = U(\theta_1, \theta_2, \theta_3, \phi_1, \phi_2, \phi_3, \phi_4, \phi_5)$$

Constant deformations

$$U(\theta_i, \phi_i) \rightarrow \widetilde{U} = U(\theta_i, \phi_i + i\Delta_i)$$

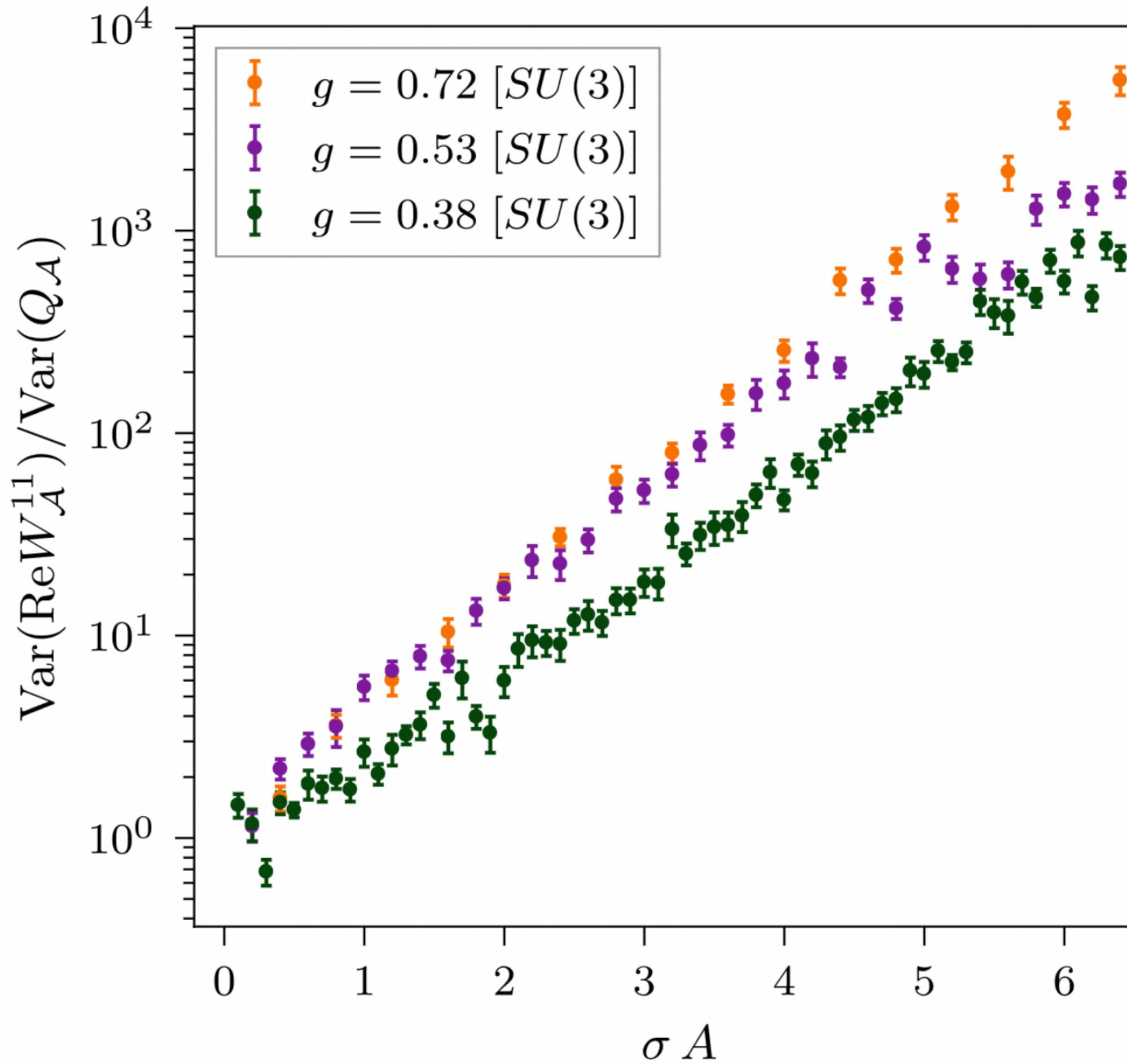
Δ_i are independent of the values of ϕ_i and θ_i

When we put a bunch of SU(N) matrices on a lattice...

Optimize $\Delta_{i,\mu}(x, y, z)$ to minimize the observable variance

Success story so far: SU(N) in 2d

Constant deformation work **extremely** well for U(1), SU(2), and SU(3) in 2d!

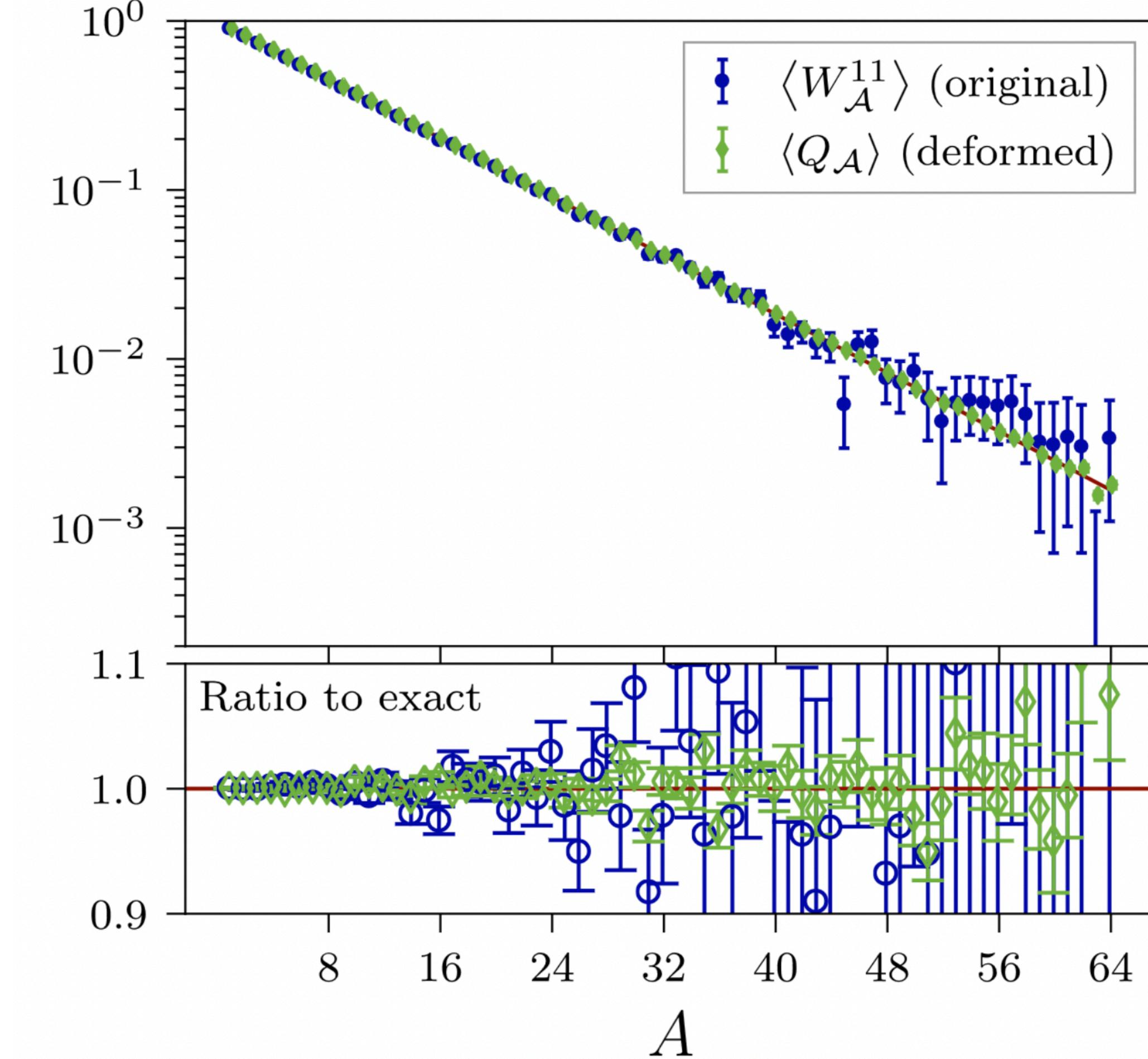
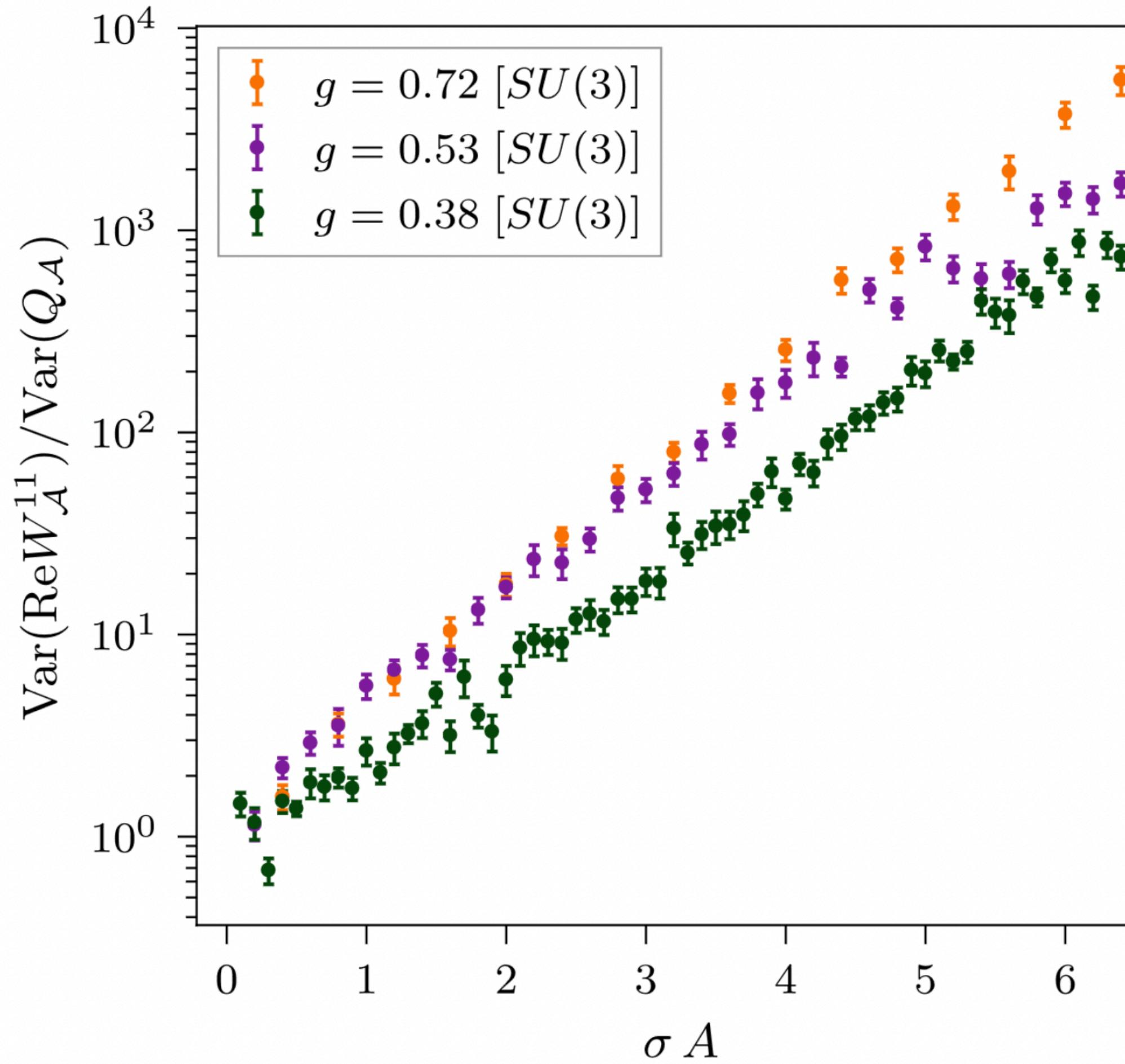


[W. Detmold, G. Kanwar, M. Wagman, N. Warrington, [hep-lat/2003.05914](https://arxiv.org/abs/hep-lat/2003.05914)]

[W. Detmold, G. Kanwar, H. Lamm, M. Wagman, N. Warrington, [hep-lat/2101.12668](https://arxiv.org/abs/hep-lat/2101.12668)]

Success story so far: SU(N) in 2d

Constant deformation work **extremely** well for U(1), SU(2), and SU(3) in 2d!



[W. Detmold, G. Kanwar, M. Wagman, N. Warrington, [hep-lat/2003.05914](https://arxiv.org/abs/hep-lat/2003.05914)]

[W. Detmold, G. Kanwar, H. Lamm, M. Wagman, N. Warrington, [hep-lat/2101.12668](https://arxiv.org/abs/hep-lat/2101.12668)]

Troubles of going beyond 2d

- ▶ 2d SU(N) gauge theories are special
 - ▶ With **open boundary condition** and **gauge fixing**, we can use **plaquette degrees of freedom**

Troubles of going beyond 2d

- ▶ 2d SU(N) gauge theories are special
 - ▶ With **open boundary condition** and **gauge fixing**, we can use **plaquette degrees of freedom**
- ▶ No such formulation exist for SU(N) gauge theories in **higher dimensions** and/or with **periodic boundary condition**

Troubles of going beyond 2d

- ▶ 2d SU(N) gauge theories are special
 - ▶ With **open boundary condition** and **gauge fixing**, we can use **plaquette degrees of freedom**
- ▶ No such formulation exist for SU(N) gauge theories in **higher dimensions** and/or with **periodic boundary condition**
 - ▶ Need to use **link degrees of freedom** for deformation

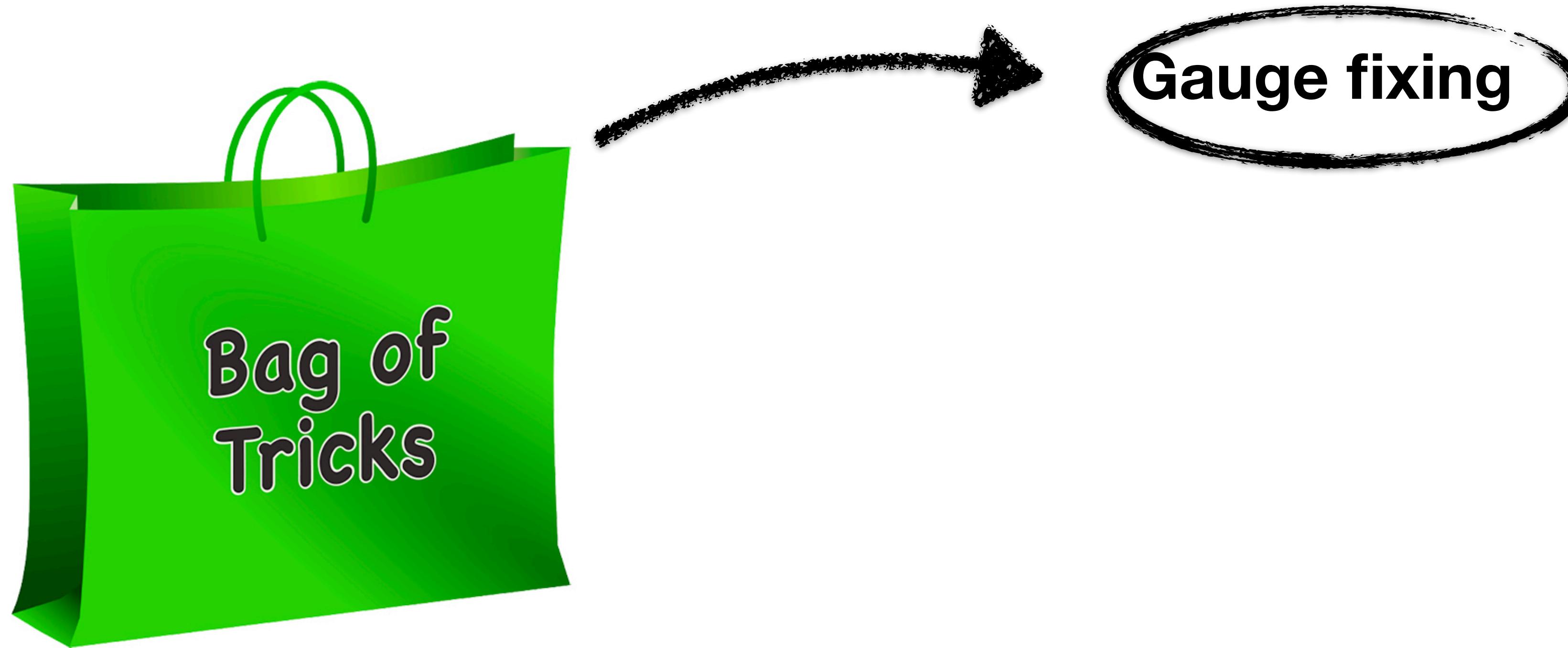
Troubles of going beyond 2d

- ▶ 2d SU(N) gauge theories are special
 - ▶ With **open boundary condition** and **gauge fixing**, we can use **plaquette degrees of freedom**
- ▶ No such formulation exist for SU(N) gauge theories in **higher dimensions** and/or with **periodic boundary condition**
 - ▶ Need to use **link degrees of freedom** for deformation
 - ▶ Fail to decrease variance for SU(N) gauge theories if directly applying the contour deformation, $\Delta_{i,\mu}(x, y, z)$

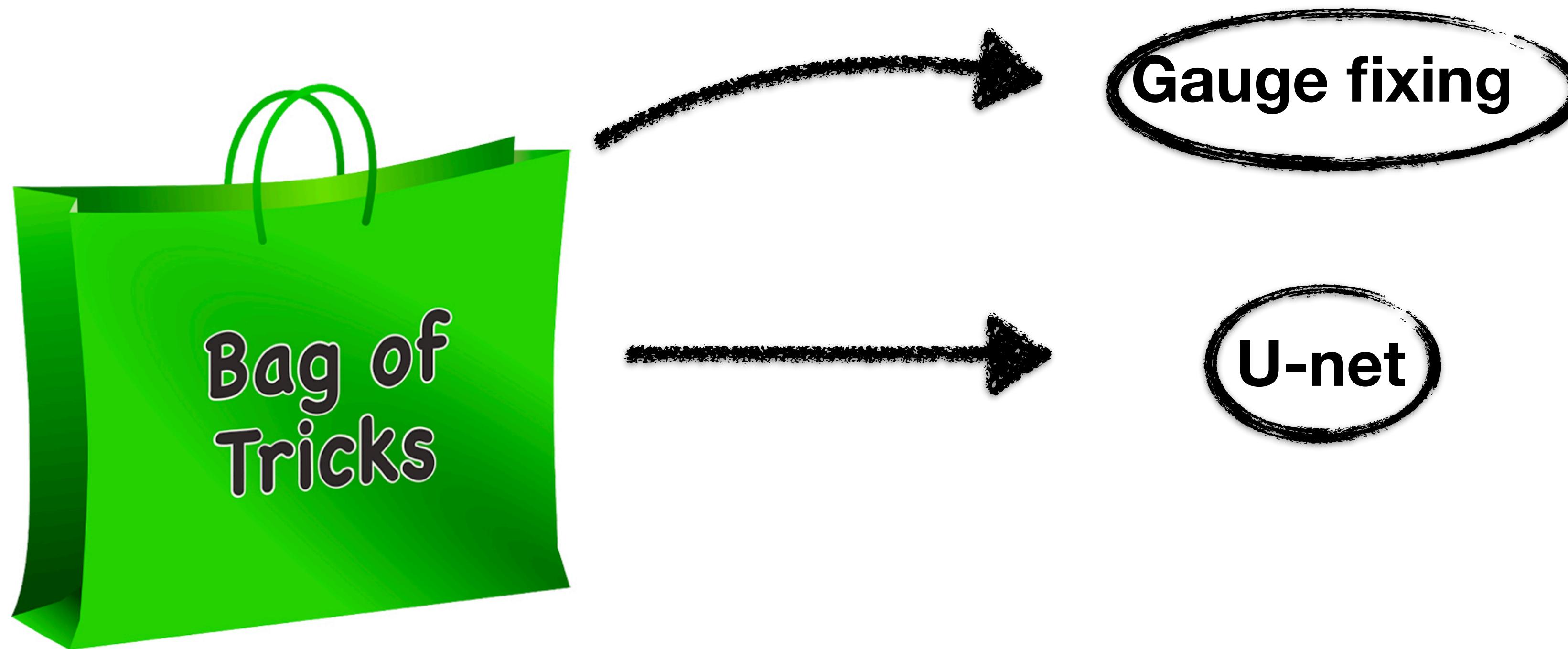
Contour deformation beyond 2d



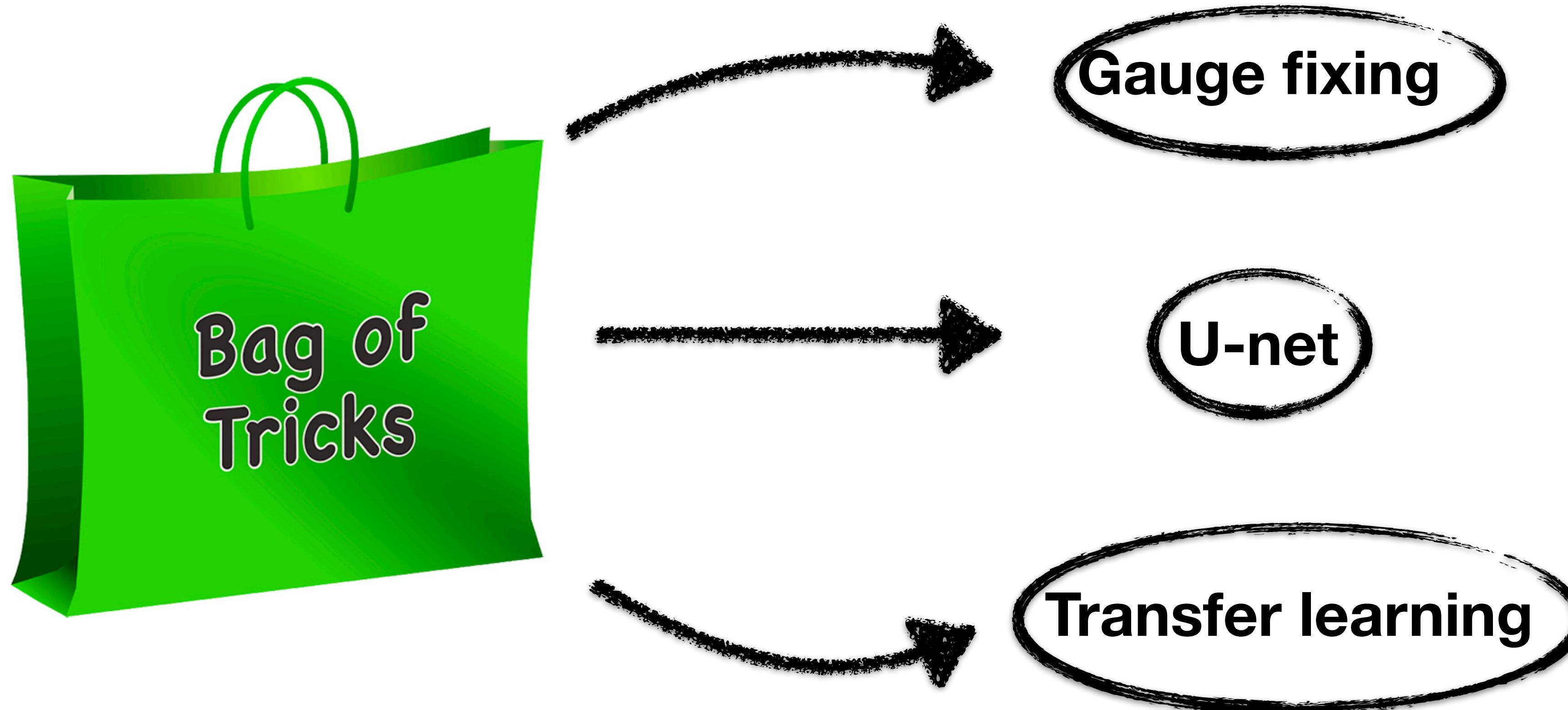
Contour deformation beyond 2d



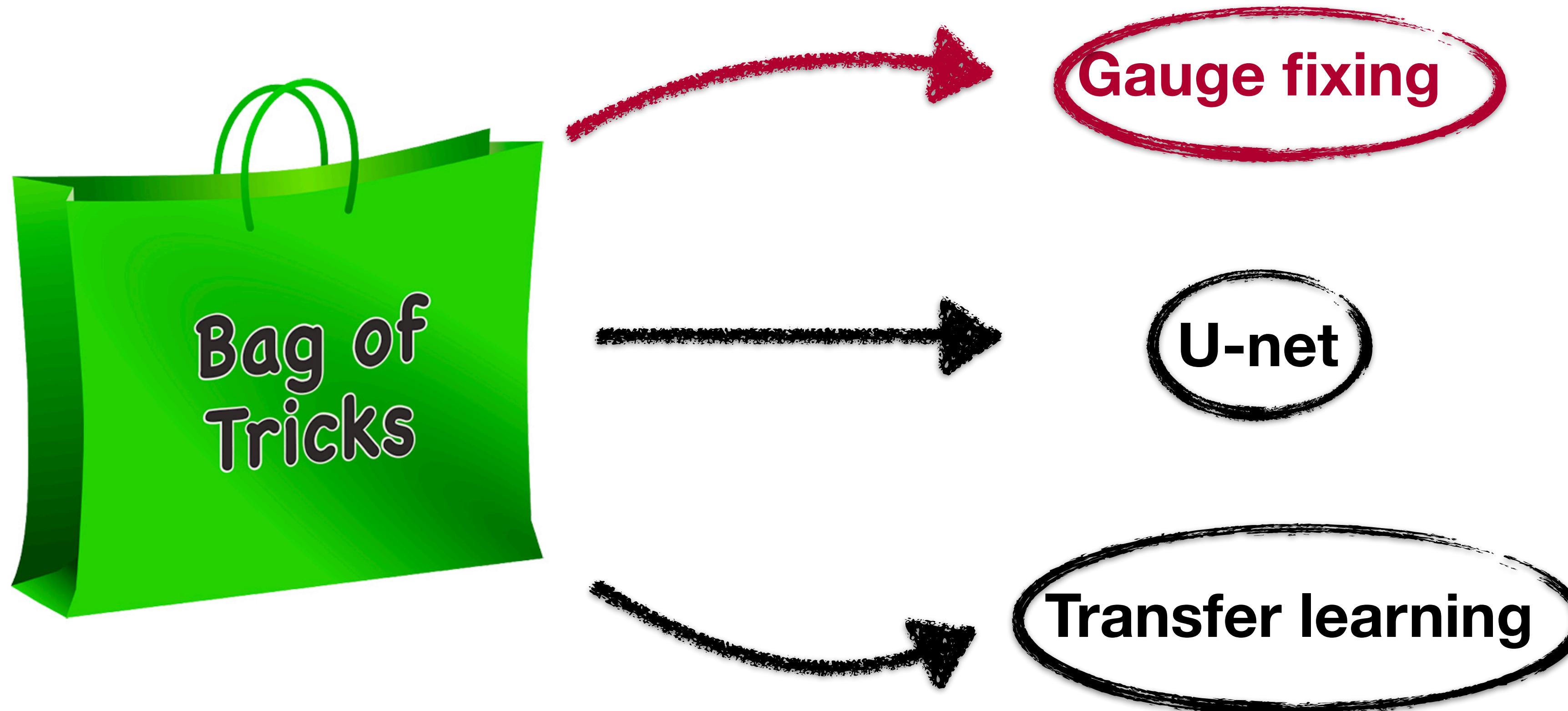
Contour deformation beyond 2d



Contour deformation beyond 2d

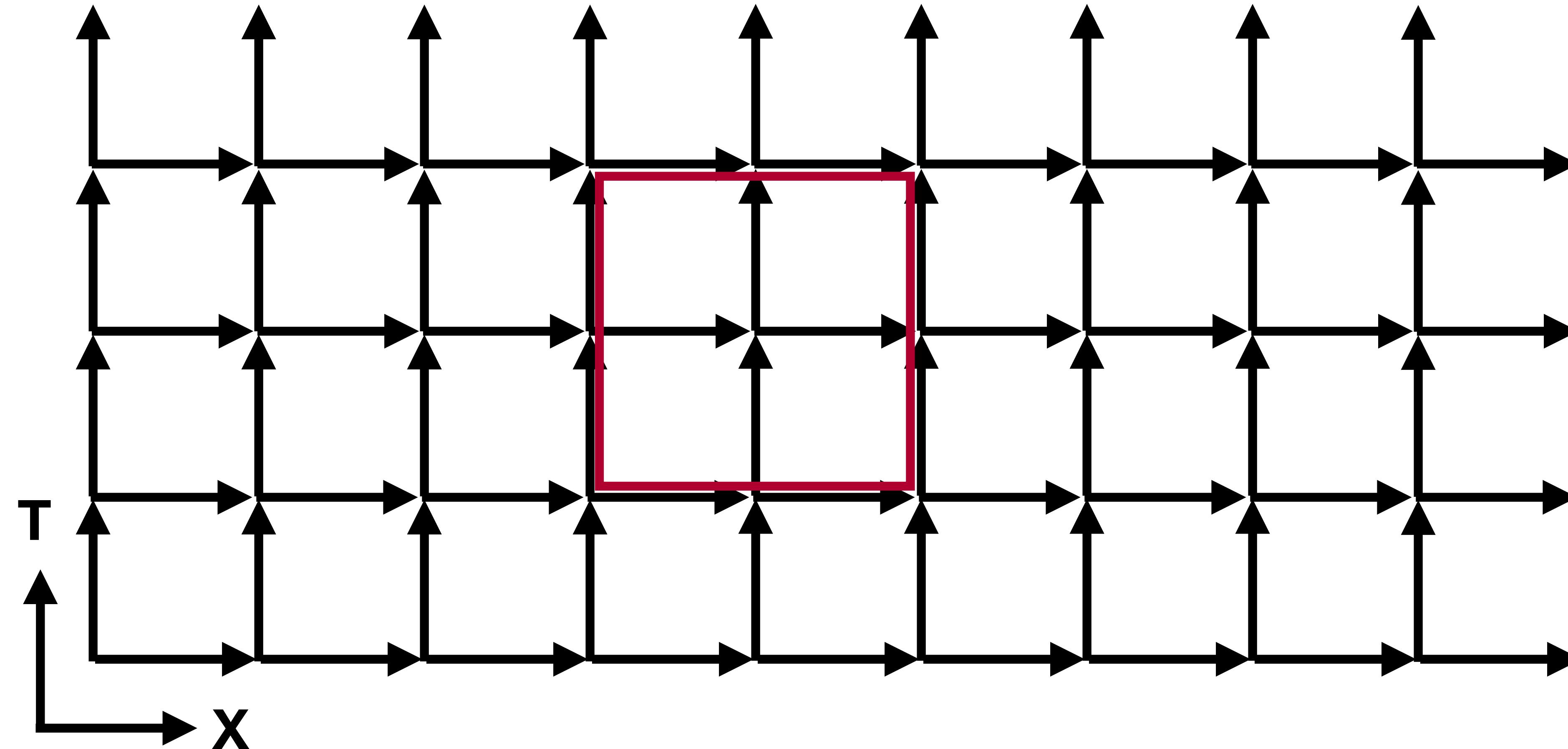


Contour deformation beyond 2d



Gauge fixing for contour deformation

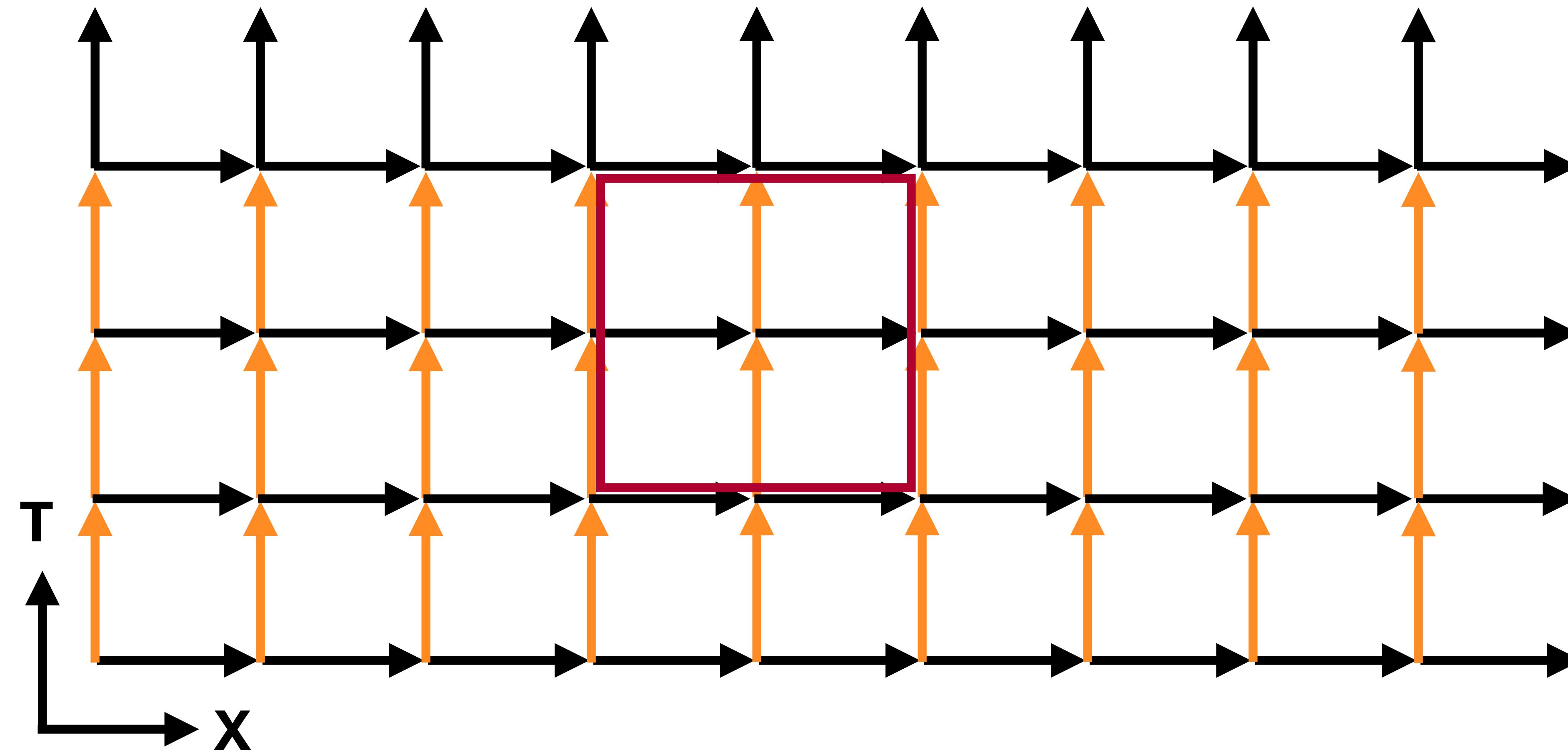
Heuristics: Reduce redundant degrees of freedom



Gauge fixing for contour deformation

Heuristics: Reduce redundant degrees of freedom

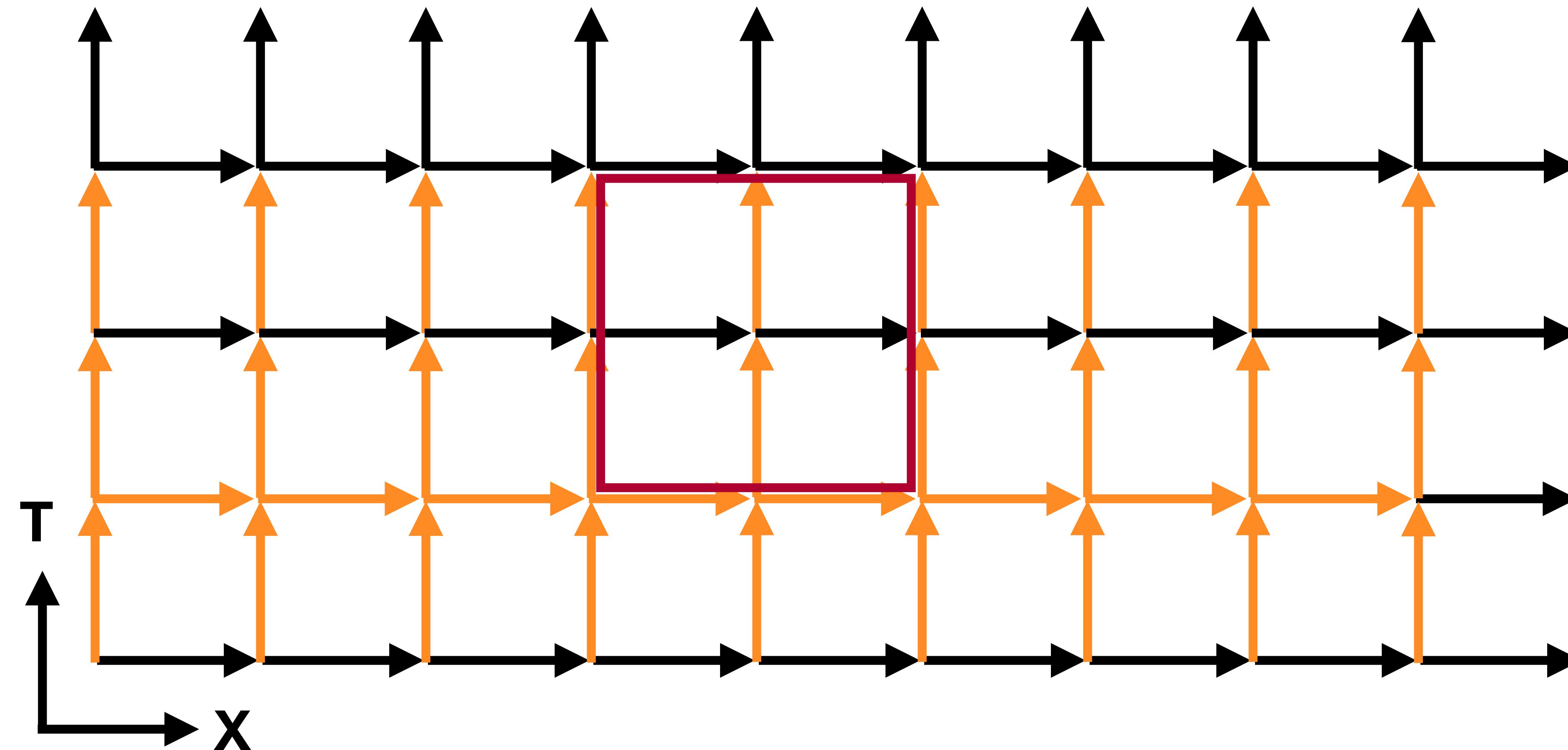
(orange links are gauge-fixed and black links are active)



Gauge fixing for contour deformation

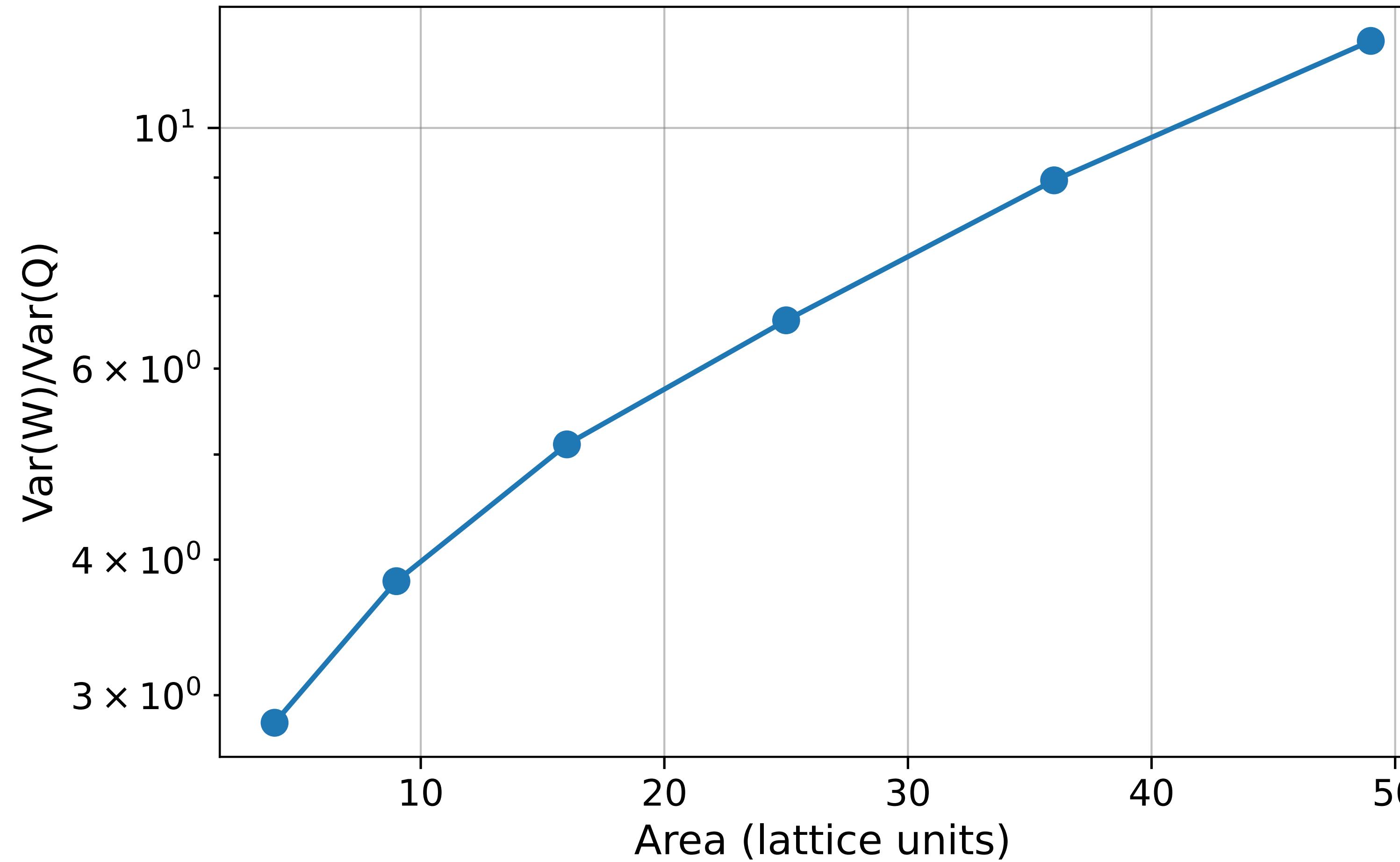
Heuristics: Reduce redundant degrees of freedom

(orange links are gauge-fixed and black links are active)



Results with direct parametrization

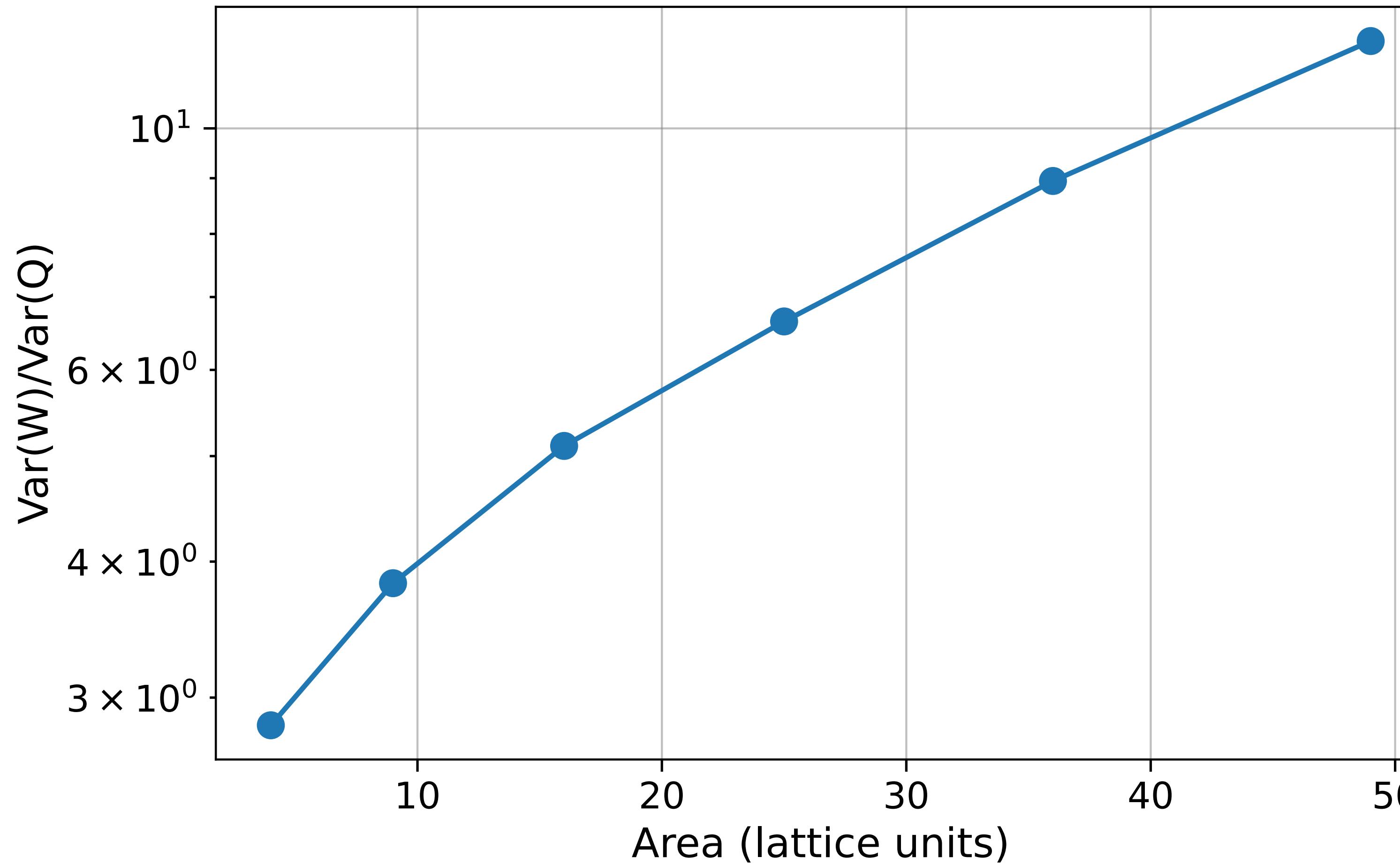
Example: $SU(2)$, $\beta=3.75$, 8^3



▶ Optimizing $\Delta_{i,\mu}(x, y, z)$
by minimizing the
variance of Wilson
loops

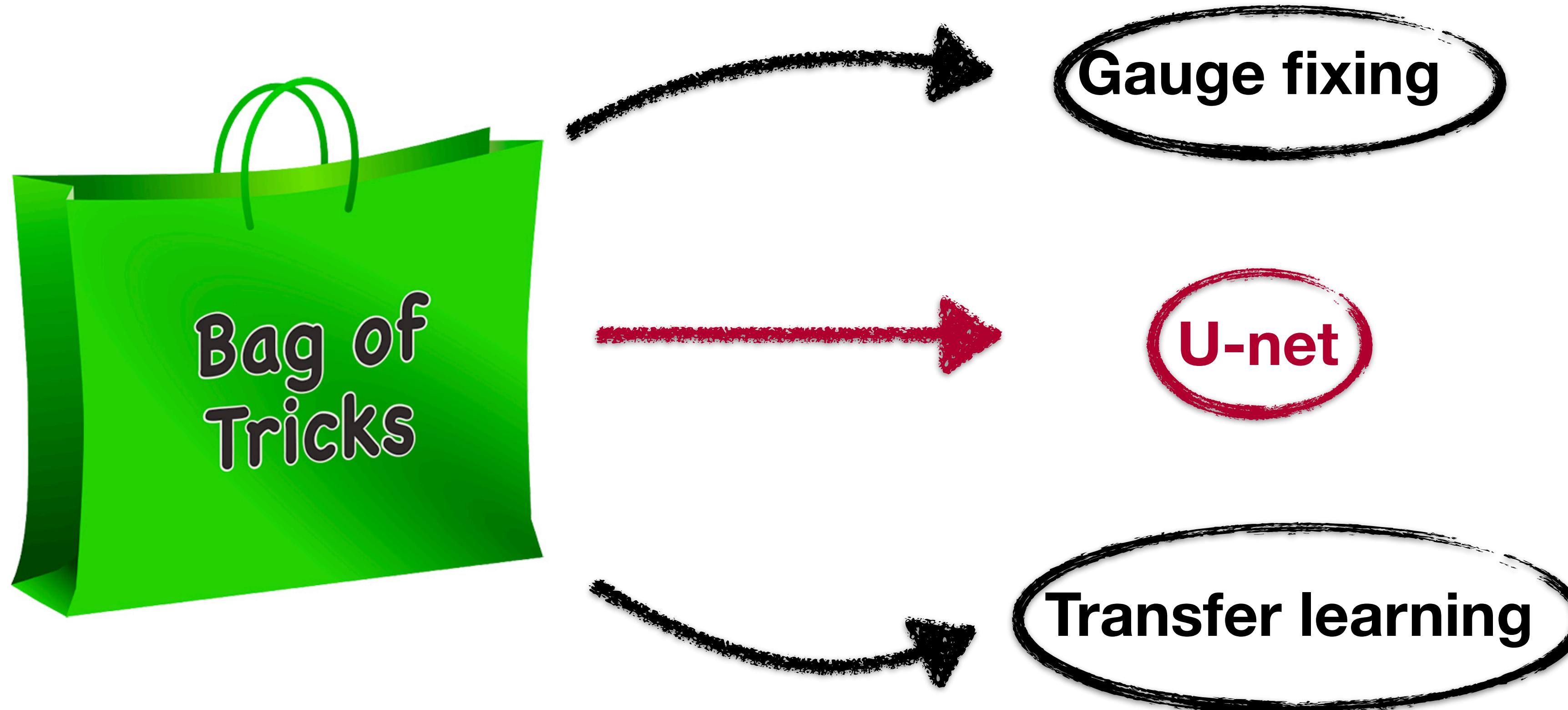
Results with direct parametrization

Example: $SU(2)$, $\beta=3.75$, 8^3



- ▶ Optimizing $\Delta_{i,\mu}(x, y, z)$ by minimizing the variance of Wilson loops
- ▶ Smaller improvements on larger lattices

Contour deformation beyond 2d



U-net for contour deformation

U-net is an alternative parametrization of $\Delta_{i,\mu}(x, y, z)$

[O. Ronneberger, P. Fischer, T. Brox, [cs/1505.04597](https://arxiv.org/abs/1505.04597)]



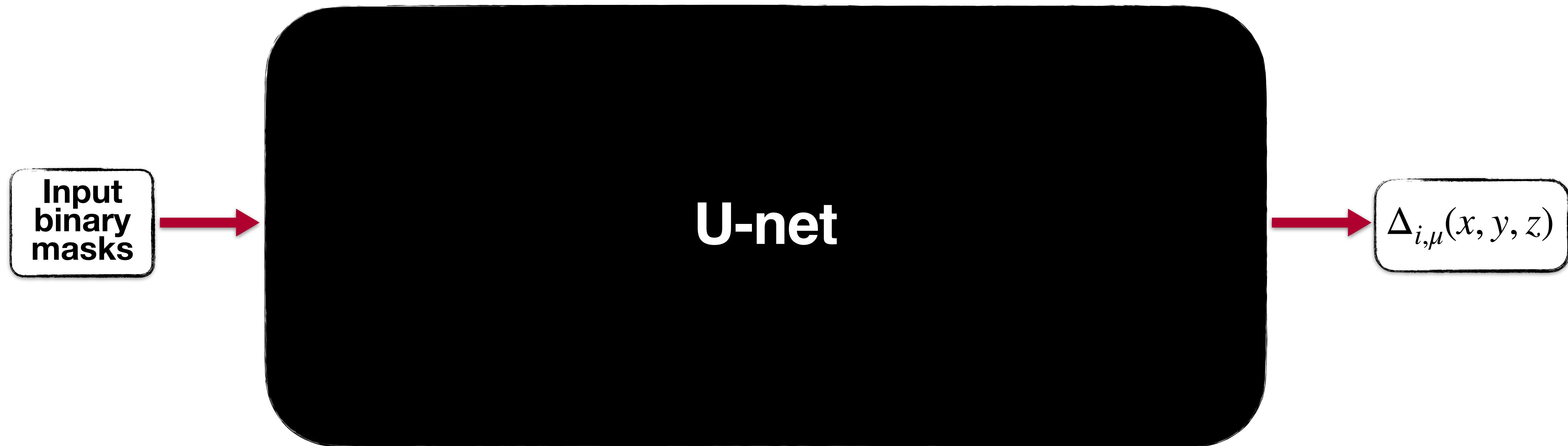
Massachusetts Institute of Technology

yin01@mit.edu Yin Lin 林胤

U-net for contour deformation

U-net is an alternative parametrization of $\Delta_{i,\mu}(x, y, z)$

[O. Ronneberger, P. Fischer, T. Brox, [cs/1505.04597](https://arxiv.org/abs/cs/1505.04597)]

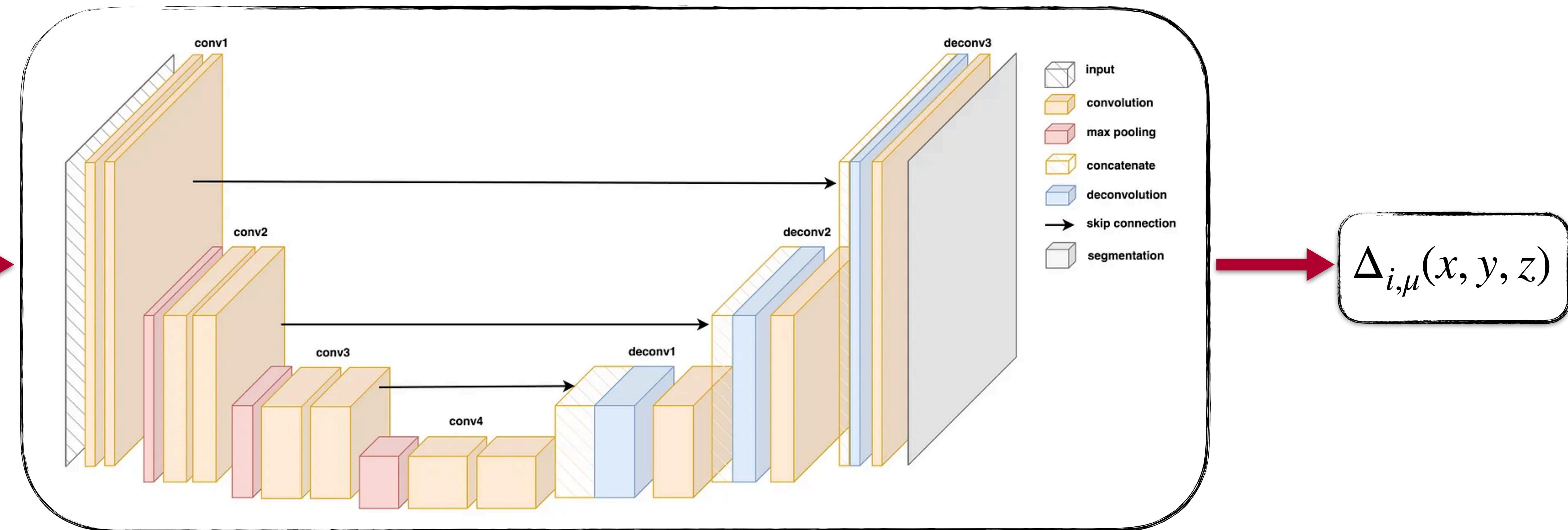


Input binary masks: encode the information of which links are **gauge fixed** and which links **lie on the Wilson loop** we aim to deform.

U-net for contour deformation

U-net is an alternative parametrization of $\Delta_{i,\mu}(x, y, z)$

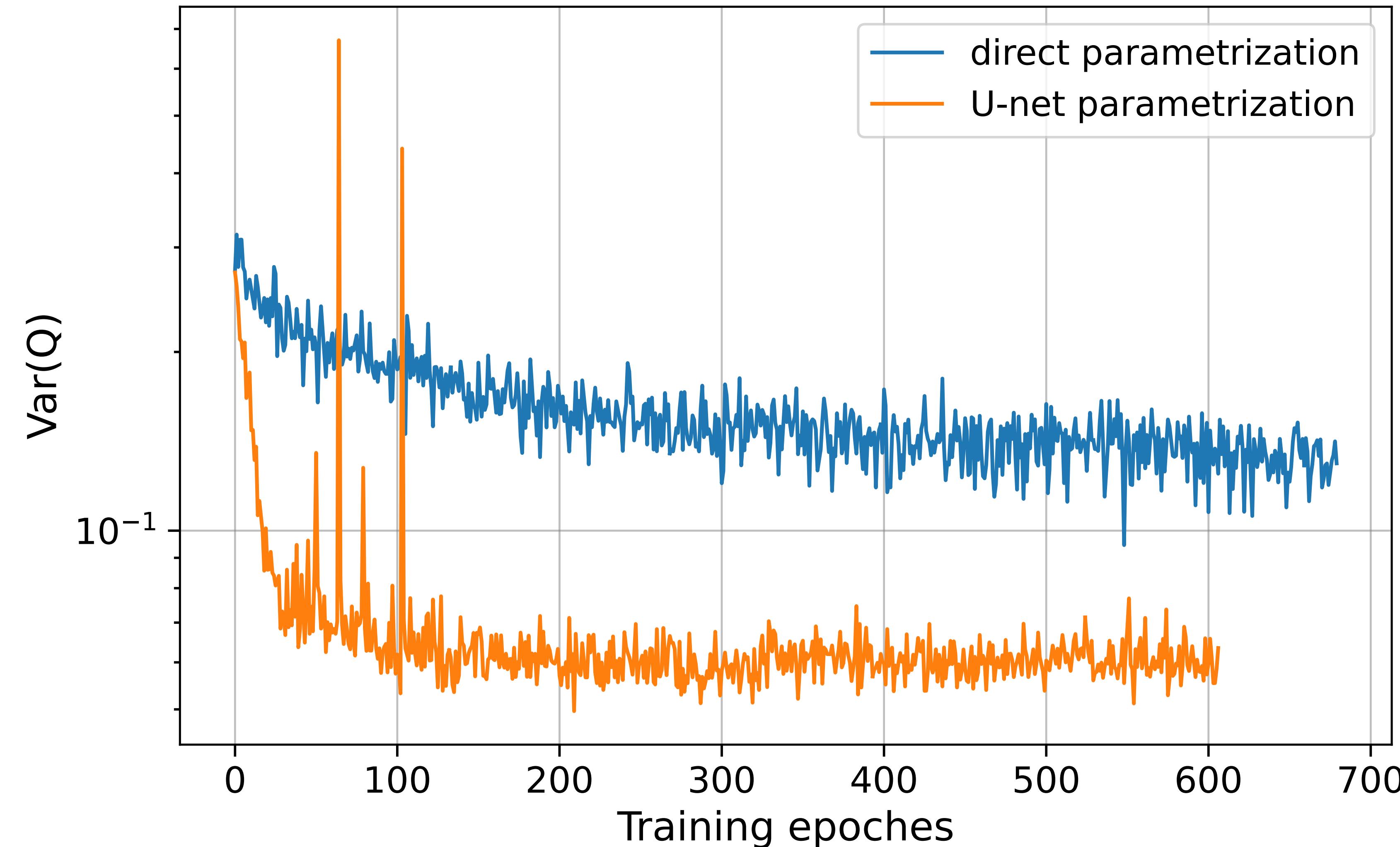
[O. Ronneberger, P. Fischer, T. Brox, [cs/1505.04597](https://arxiv.org/abs/1505.04597)]



Input binary masks: encode the information of which links are **gauge fixed** and which links **lie on the Wilson loop** we aim to deform.

U-net for contour deformation

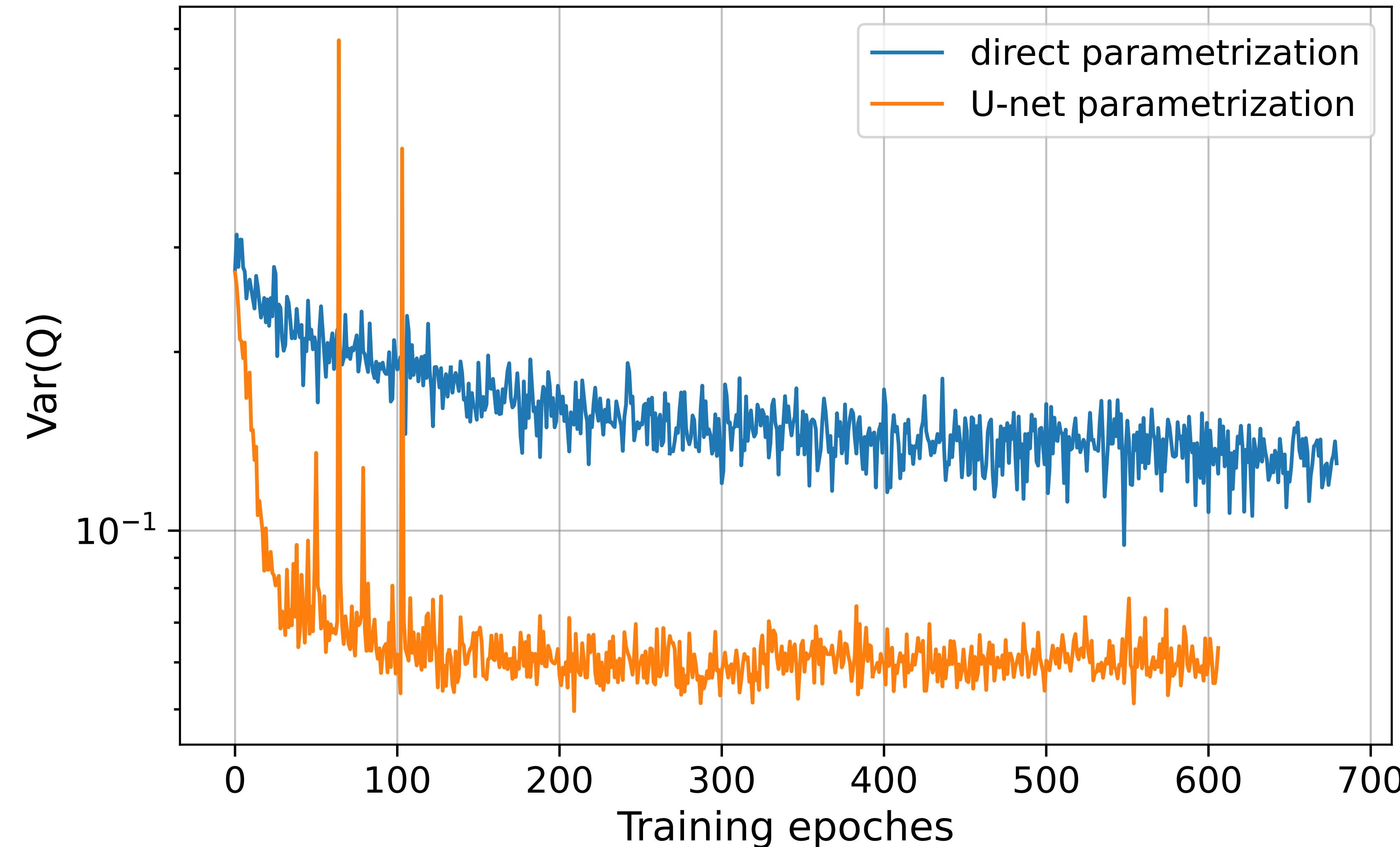
Example: SU(2), 16^3 , 4-by-4 Wilson loops



▶ Enable training with deeper networks, hence, larger lattices

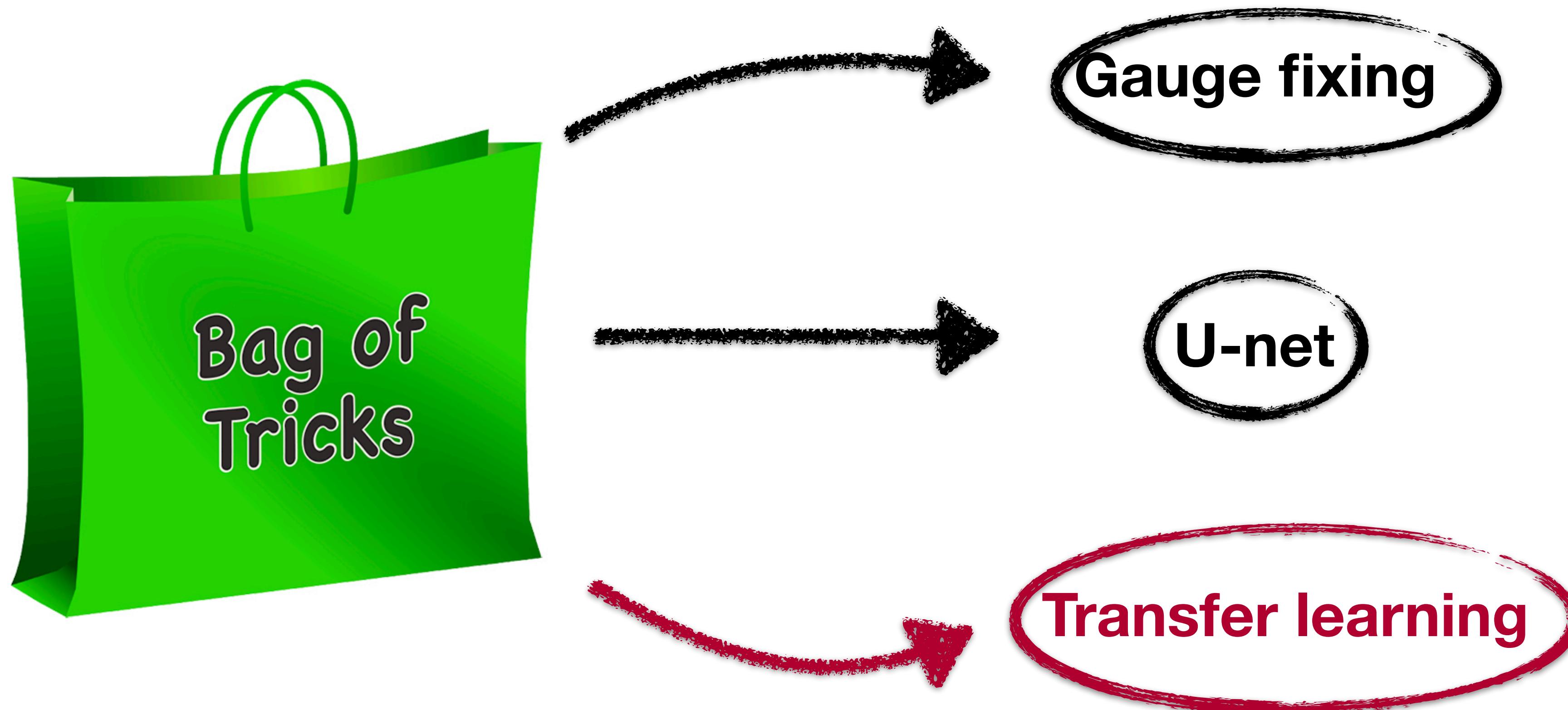
U-net for contour deformation

Example: SU(2), 16^3 , 4-by-4 Wilson loops

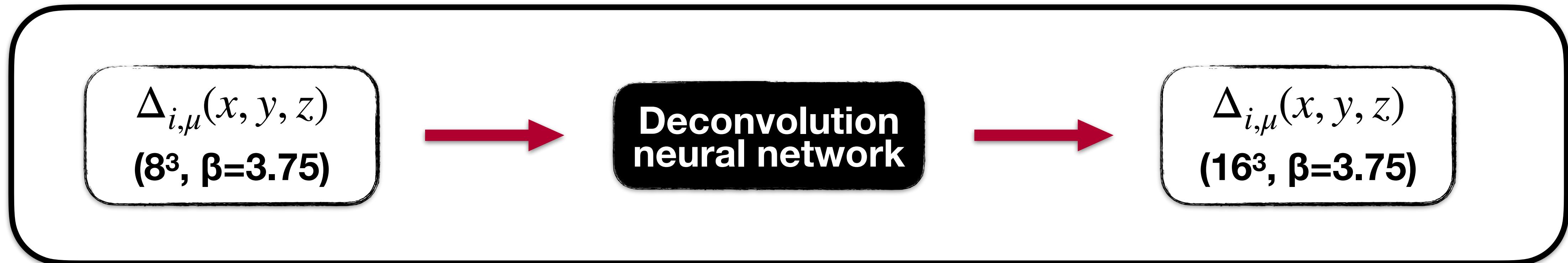


- ▶ Enable training with deeper networks, hence, larger lattices
- ▶ Required a lot of gauge configurations to avoid overtraining ($\sim 10^5$). Unfeasible for even larger lattices

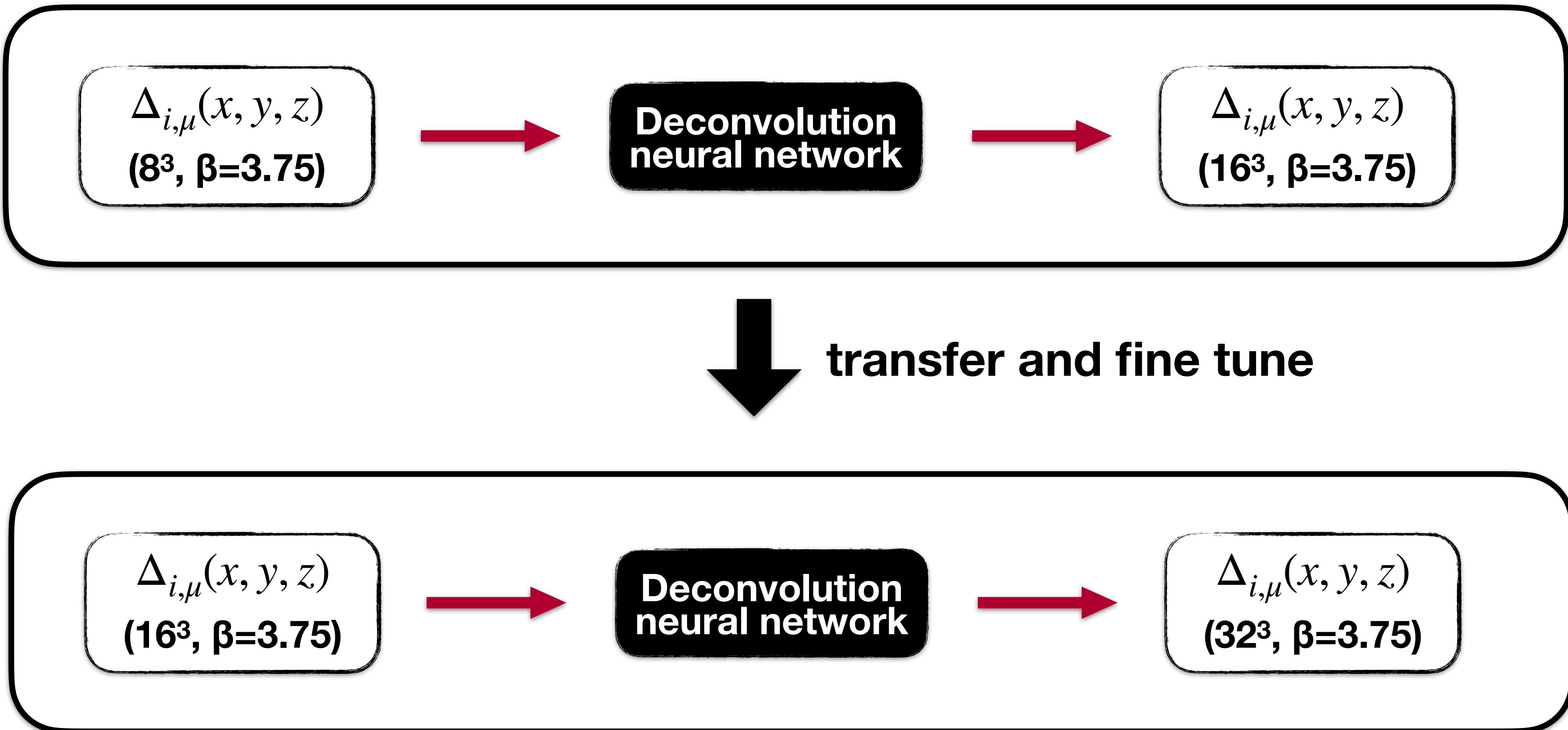
Contour deformation beyond 2d



Transfer learning for contour deformation

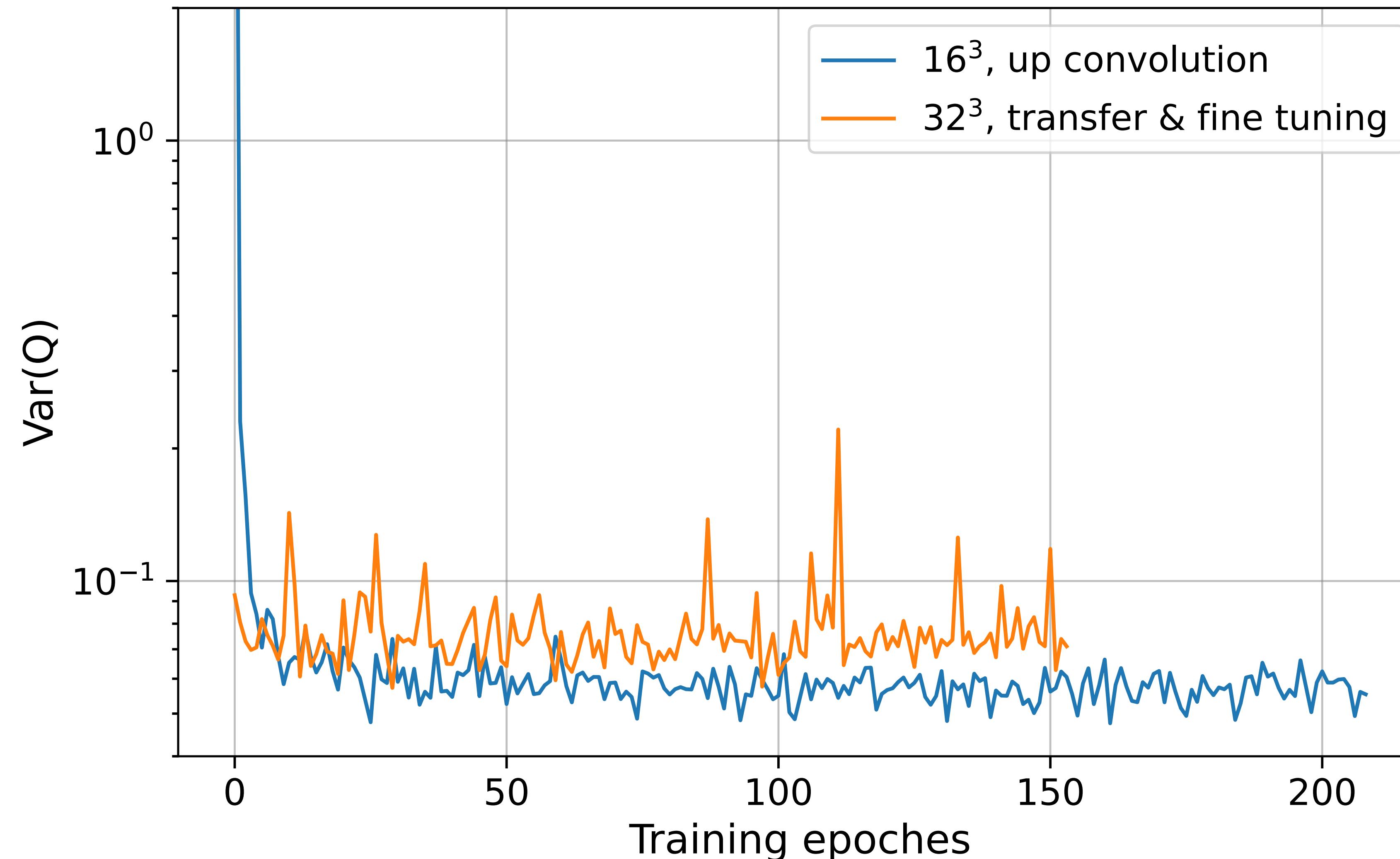


Transfer learning for contour deformation

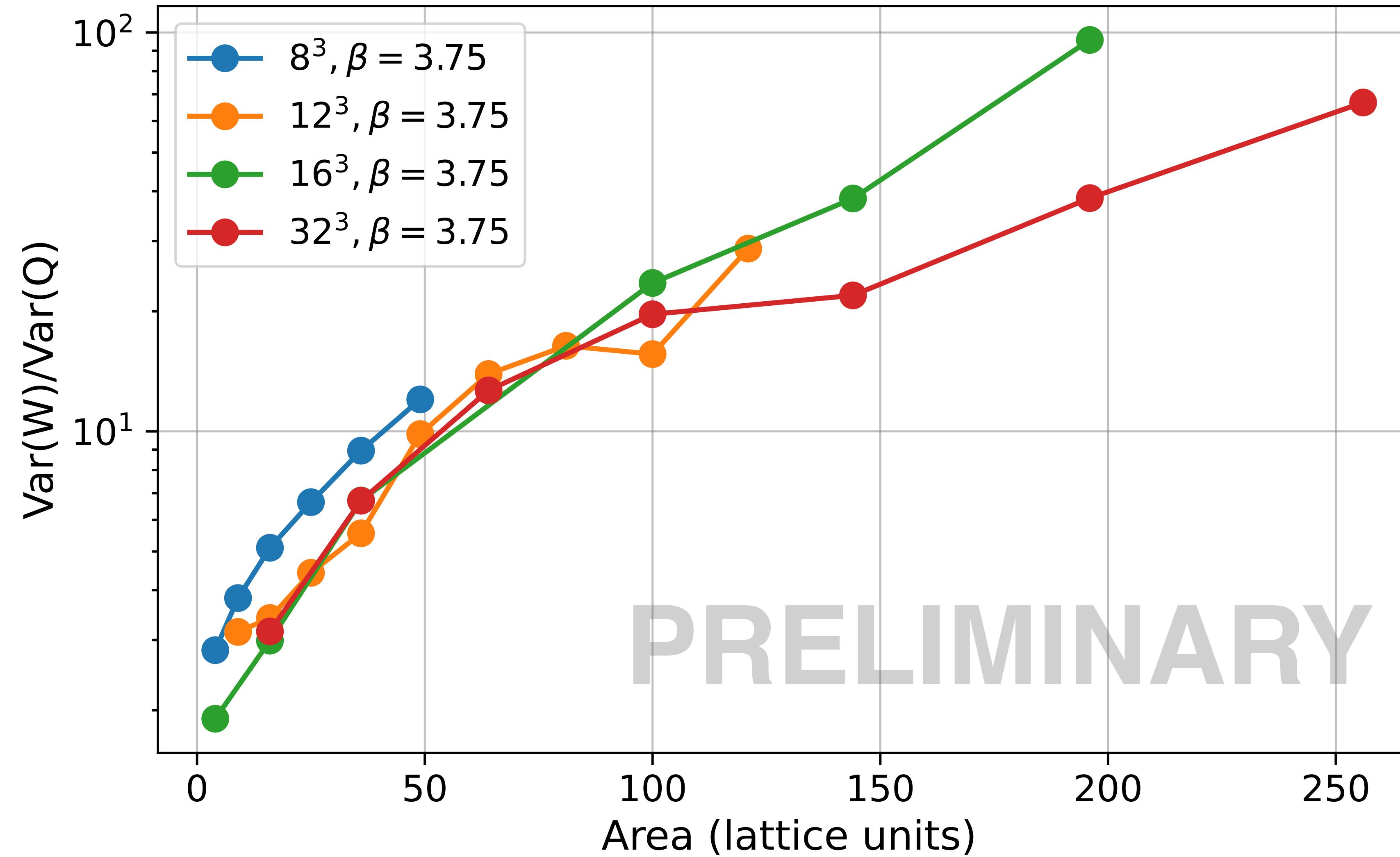


Volume transfer for contour deformation

Example: SU(2), $\beta=3.75$, 4-by-4 Wilson loops



SU(2) preliminary results



Where we are and where we are going

- **Exponential improvement** in the variance for SU(2), SU(3) gauge theories in 3d



Where we are and where we are going

- **Exponential improvement** in the variance for SU(2), SU(3) gauge theories in 3d
 - Can we gain **more improvement** with constant deformation?



Where we are and where we are going

- **Exponential improvement** in the variance for SU(2), SU(3) gauge theories in 3d
 - Can we gain **more improvement** with constant deformation?
 - Can we gain improvement **without gauge fixing**?



Where we are and where we are going

- **Exponential improvement** in the variance for SU(2), SU(3) gauge theories in 3d



- Can we gain **more improvement** with constant deformation?
- Can we gain improvement **without gauge fixing**?
- Can we perform **non-constant deformation**?

Where we are and where we are going

- **Exponential improvement** in the variance for SU(2), SU(3) gauge theories in 3d



- Can we gain **more improvement** with constant deformation?
- Can we gain improvement **without gauge fixing**?
- Can we perform **non-constant deformation**?
- Can we reduce the variance of **other gauge observables**?

Where we are and where we are going

- **Exponential improvement** in the variance for SU(2), SU(3) gauge theories in 3d
 - Can we gain **more improvement** with constant deformation?
 - Can we gain improvement **without gauge fixing**?
 - Can we perform **non-constant deformation**?
 - Can we reduce the variance of **other gauge observables**?
- **4d** work in progress — results soon!



Where we are and where we are going

- **Exponential improvement** in the variance for SU(2), SU(3) gauge theories in 3d
 - Can we gain **more improvement** with constant deformation?
 - Can we gain improvement **without gauge fixing**?
 - Can we perform **non-constant deformation**?
 - Can we reduce the variance of **other gauge observables**?
- **4d** work in progress — results soon!
- Putting **fermions** back to the theory



Where we are and where we are going

- **Exponential improvement** in the variance for SU(2), SU(3) gauge theories in 3d
 - Can we gain **more improvement** with constant deformation?
 - Can we gain improvement **without gauge fixing**?
 - Can we perform **non-constant deformation**?
 - Can we reduce the variance of **other gauge observables**?
- **4d** work in progress — results soon!
- Putting **fermions** back to the theory
 - **Gauge observables** on unquenched observables



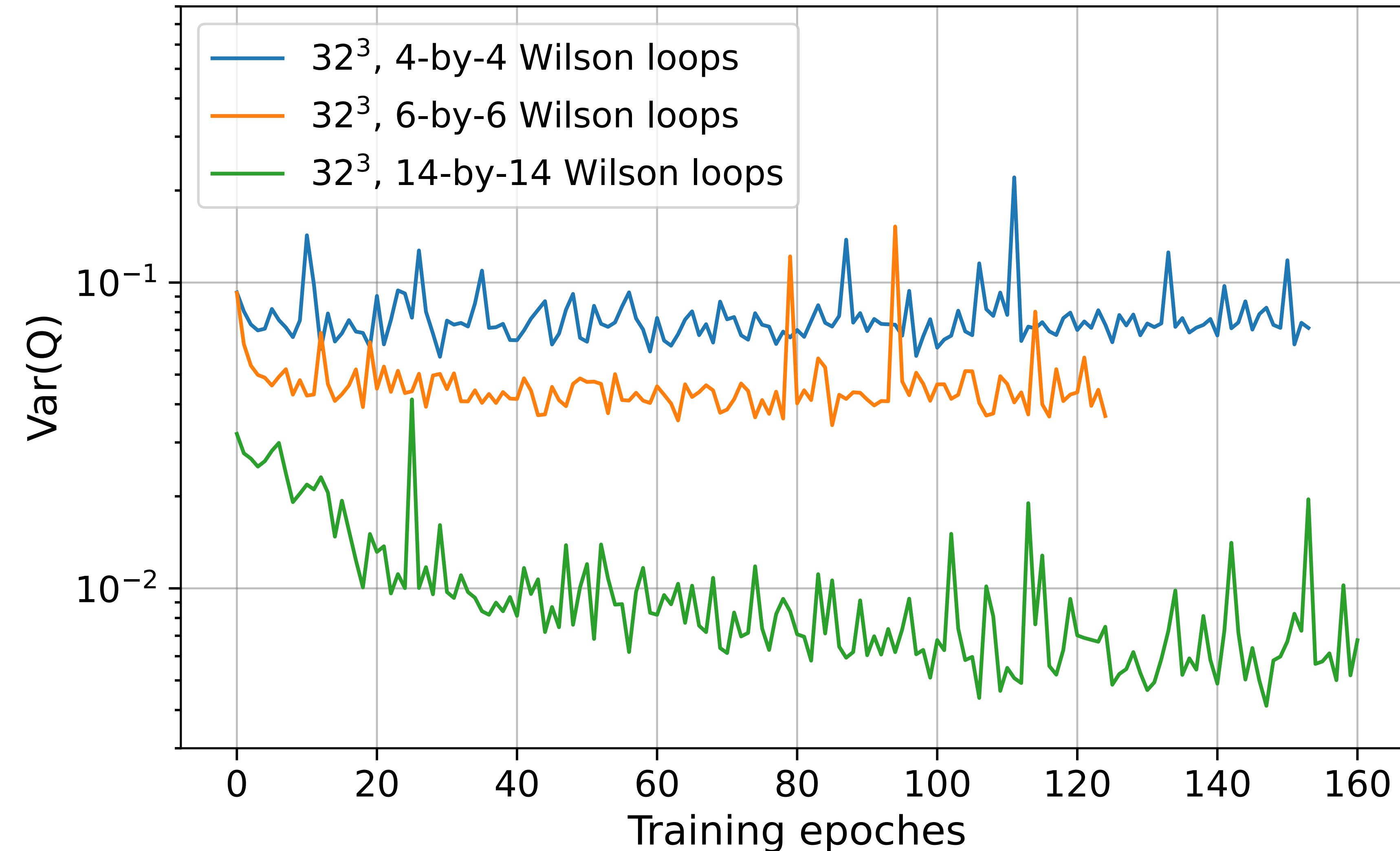
Where we are and where we are going

- **Exponential improvement** in the variance for SU(2), SU(3) gauge theories in 3d
 - Can we gain **more improvement** with constant deformation?
 - Can we gain improvement **without gauge fixing**?
 - Can we perform **non-constant deformation**?
 - Can we reduce the variance of **other gauge observables**?
- **4d** work in progress – results soon!
- Putting **fermions** back to the theory
 - **Gauge observables** on unquenched observables
 - **Fermionic observables** on unquenched observables

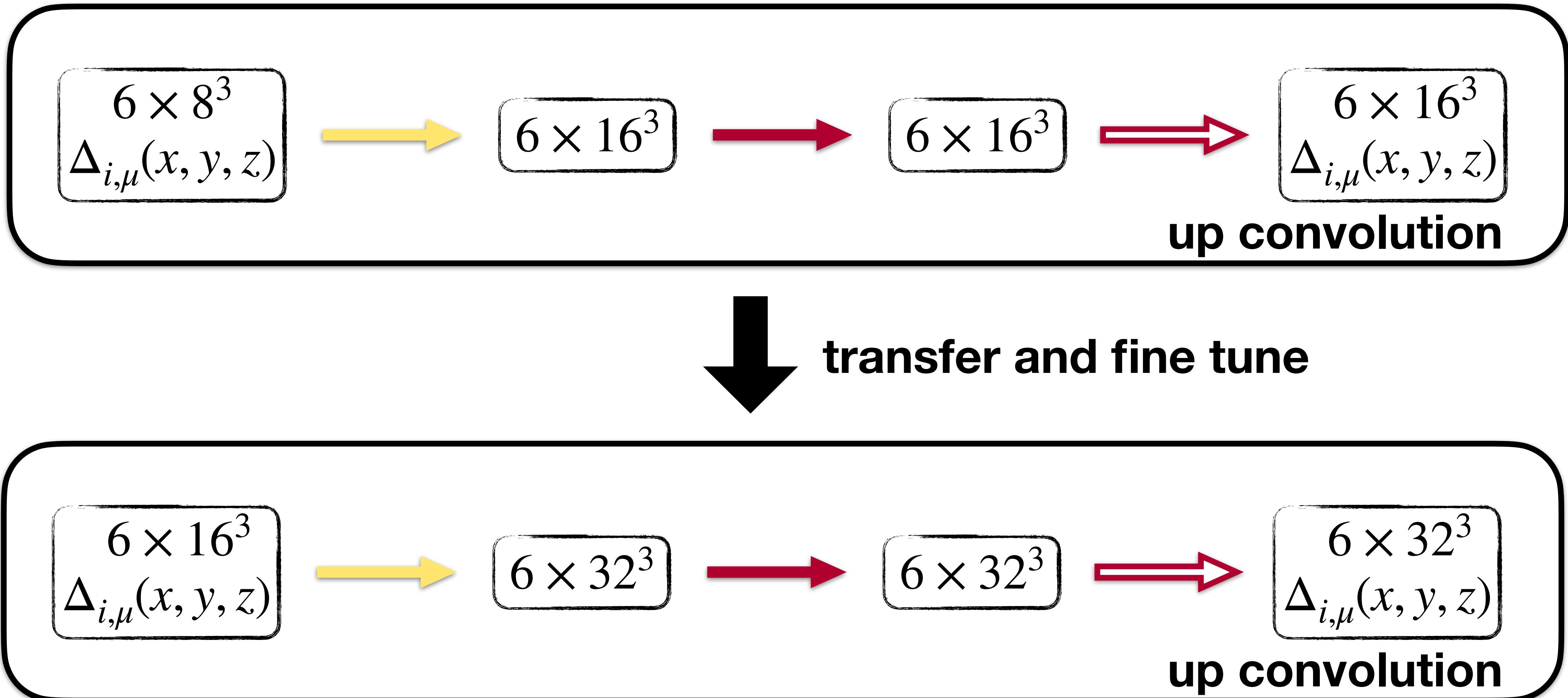


Area transfer for contour deformation

Example: SU(2), $\beta=3.75$



Transfer learning for contour deformation



→ = conv. , batch norm., ReLU

→ = up conv.

→ = gauge fix

Reweighting complex action

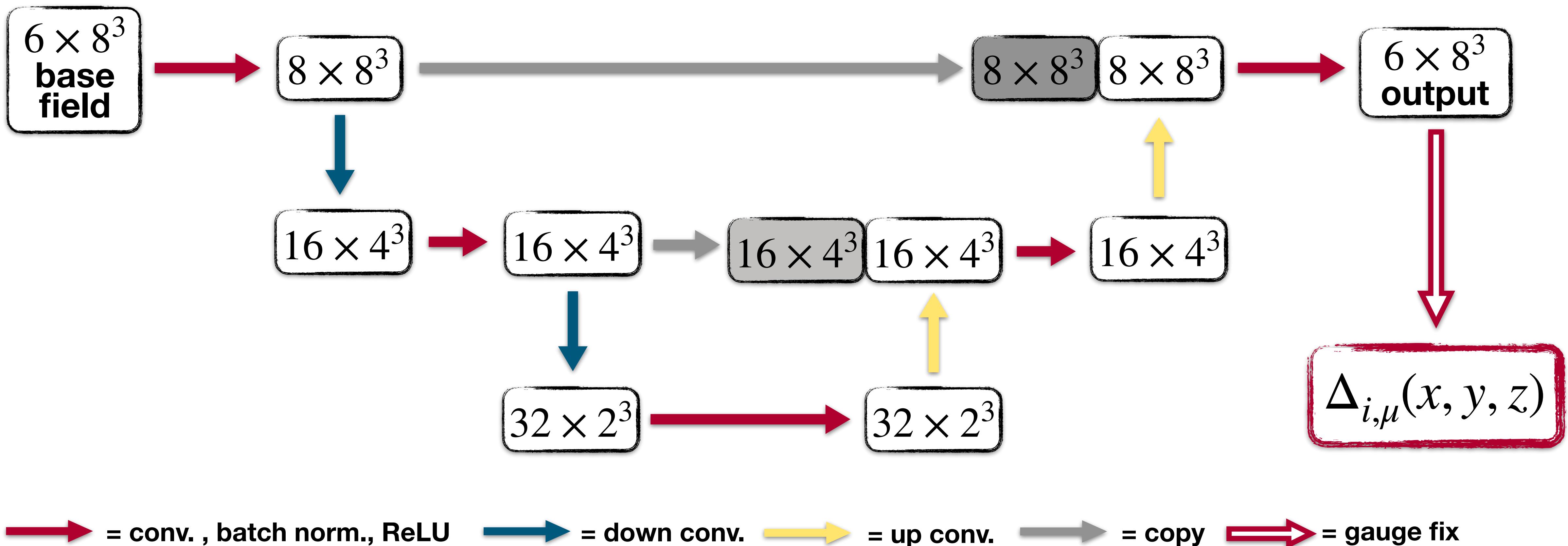
$$\begin{aligned}\langle \text{Re}W \rangle &= \text{Re} \int \prod_n \left[h(\tilde{\theta}_n) d\tilde{\theta}_n d\tilde{\phi}_{1,n} d\tilde{\phi}_{2,n} \right] p[\tilde{U}] W[\tilde{U}] \\ &= \text{Re} \int \prod_n \left[h(\theta) d\theta_n d\phi_{1,n} d\phi_{2,n} \right] p[U] \left(\frac{h(\tilde{\theta}_n)p[\tilde{U}]}{h(\theta_n)p[U]} W[\tilde{U}] \right) \\ &= \text{Re} \int \prod_n dU_n p[U] Q[U] = \langle Q \rangle\end{aligned}$$

U-net for contour deformation

U-net is an alternative parametrization of $\Delta_{i,\mu}(x, y, z)$

[O. Ronneberger, P. Fischer, T. Brox, [cs/1505.04597](https://arxiv.org/abs/1505.04597)]

Example: SU(2), 16^3



Errors on reweighting factors

