Observifolds: path integral contour deformation

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2003.05914, 2101.12668 with <u>Tej Kanwar</u>, Hank Lamm, Mike Wagman, Neill Warrington
2106.01975 Kanwar thesis

ECT* “Machine Learning on and off the lattice”, Sep 29th 2021

Signal-to-noise

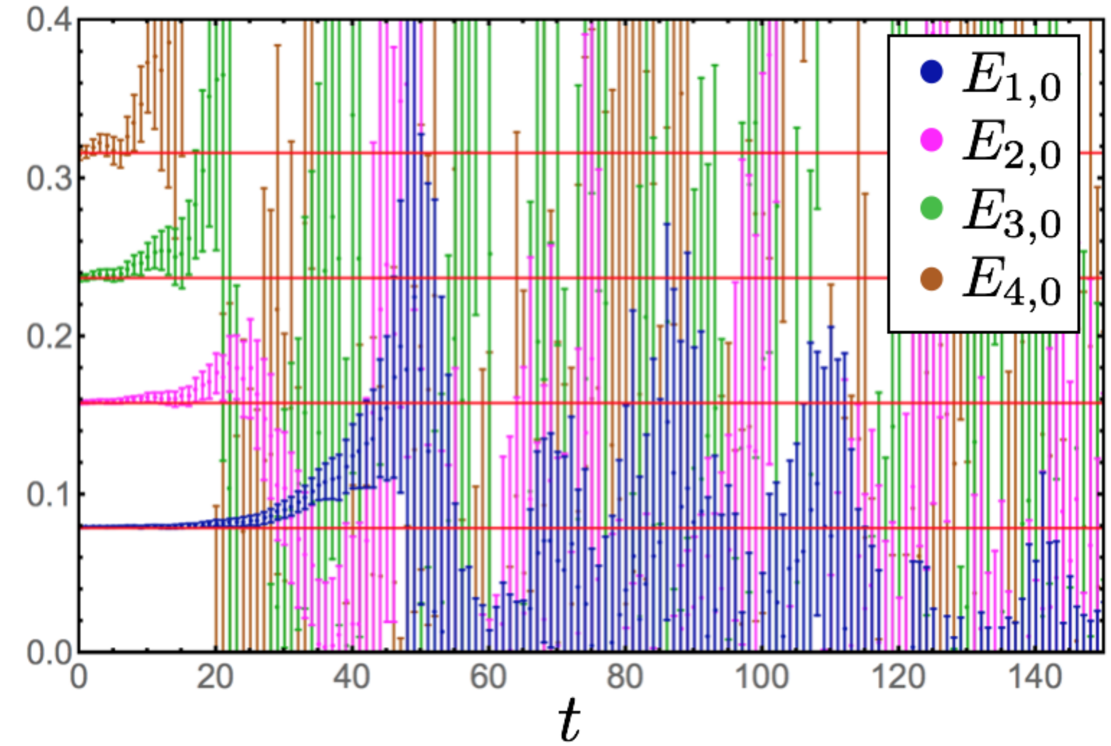
An exponential challenge

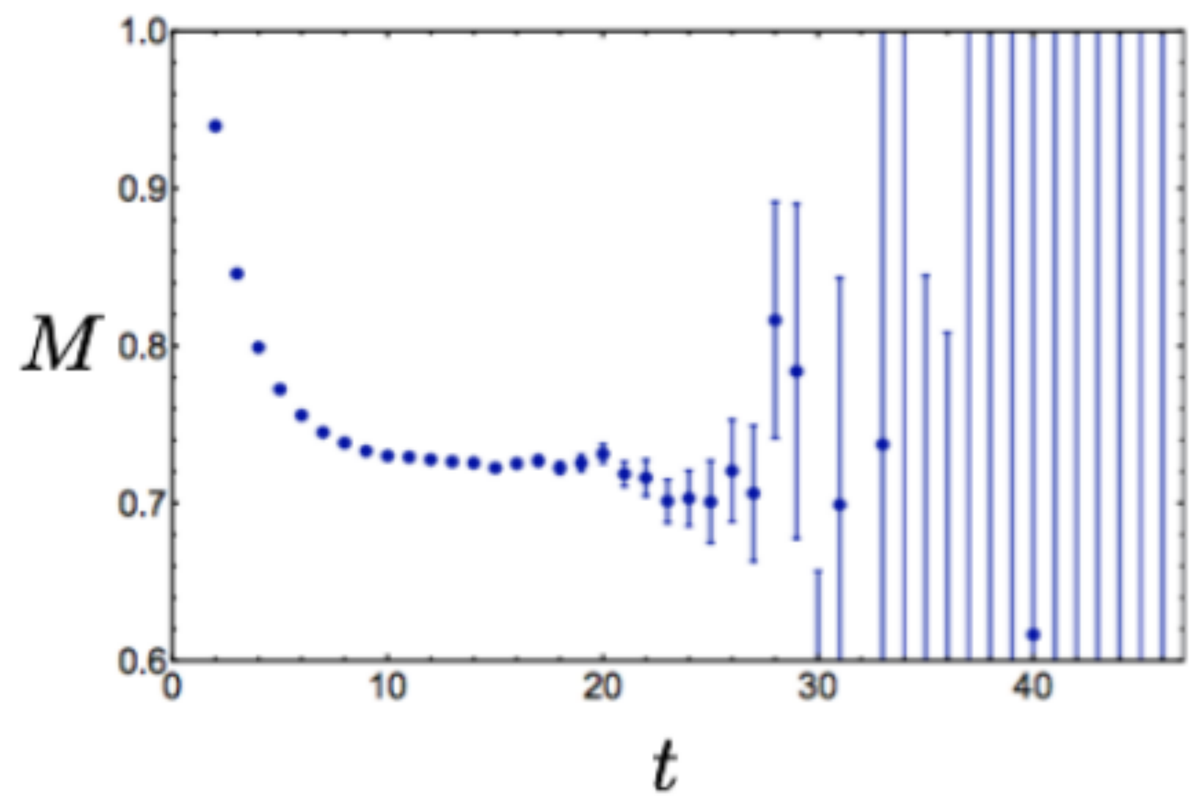
- Calculation of observables in QFT using Monte-Carlo methods are beset by noise

$$\sigma = \sqrt{\mathrm{Var}(\mathcal{O})/N}$$

$$\mathrm{StN} = \frac{\langle \mathcal{O} \rangle}{\sigma}$$

- StN problem: decays exponentially in some extensive quantity
    - 0+1D complex scalar field theory: effective energy of charge Q states
    - Proton effective mass in QCD
- Exponentially large numbers of MC samples required to overcome
- Generic issue hampering many physics analyses





Signal-to-noise

Parisi–Lepage

- Two point correlation function

$$\langle \mathcal{O}_2(t)\mathcal{O}_1(0)\rangle$$

- Variance

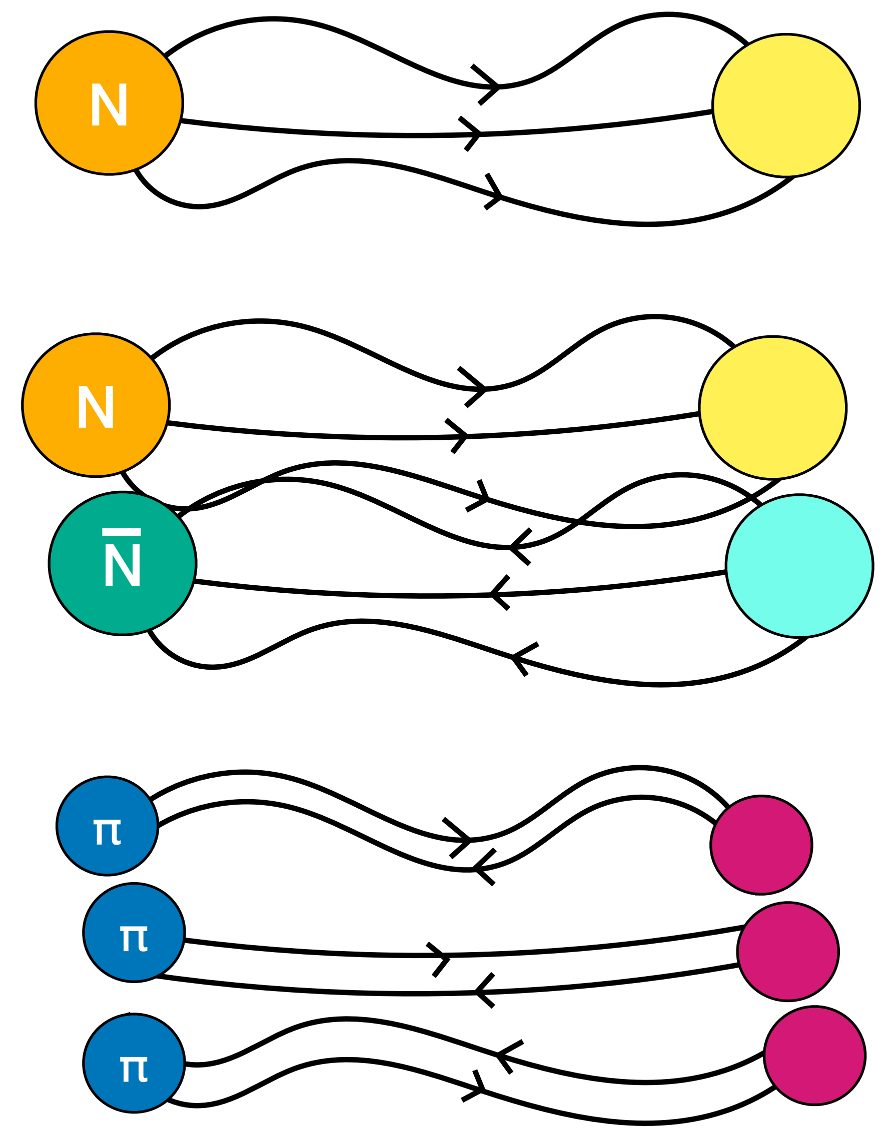
$$\mathrm{Var}[\mathrm{Re}[\mathcal{O}_2(t)\mathcal{O}_1(0)]] = \frac{1}{2}\langle \mathcal{O}_2(t)\mathcal{O}_2^*(t)\mathcal{O}_1^*(0)\mathcal{O}_1(0)\rangle + \ldots$$

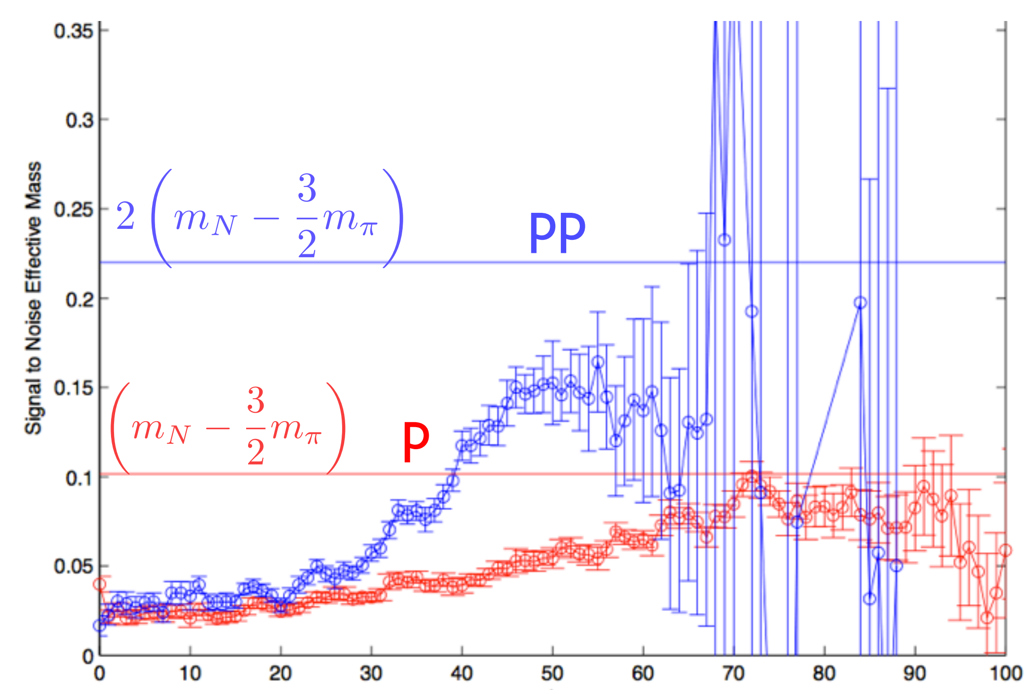
- Bosonic theory: first term dominated by vacuum state → constant in time

$$\mathrm{StN}[\mathrm{Re}[\mathcal{O}_2(t)\mathcal{O}_1(0)]] = \frac{|\,\mathrm{Re}\,\langle \mathcal{O}_2(t)\mathcal{O}_1(0)\rangle\,|}{\sqrt{\frac{1}{n}\mathrm{Var}[\mathrm{Re}[\mathcal{O}_2(t)\mathcal{O}_1(0)]]}} \sim \sqrt{n}e^{-Et}$$

- Fermions: slightly improved as fermions are integrated out and provide nonlocal structure

$$\mathrm{StN}(C_N) \sim \frac{e^{-M_N t}}{e^{-3m_\pi t/2}} \sim e^{-(M_N - \frac{3}{2}m_\pi)t}$$





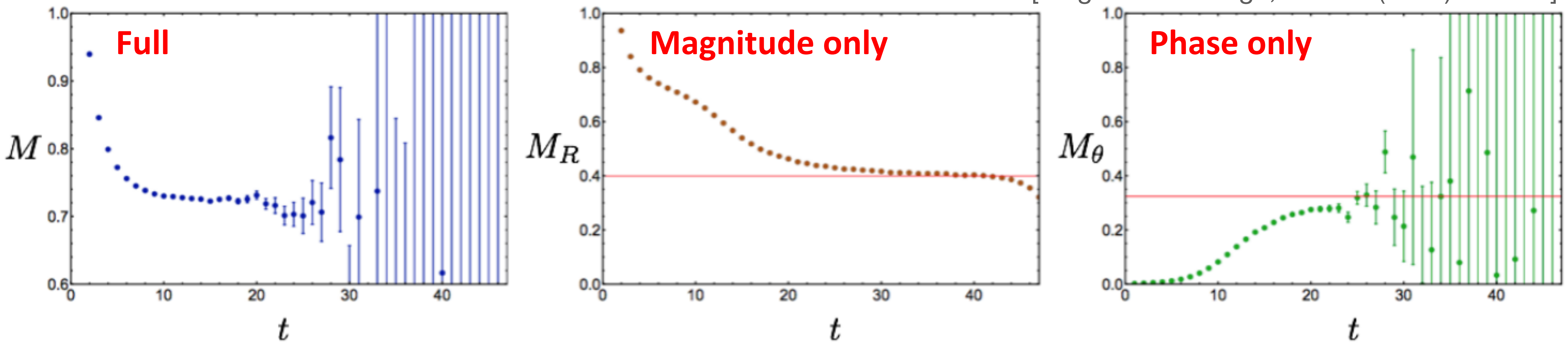
NPLQCD collaboration 2009

Phase fluctuations

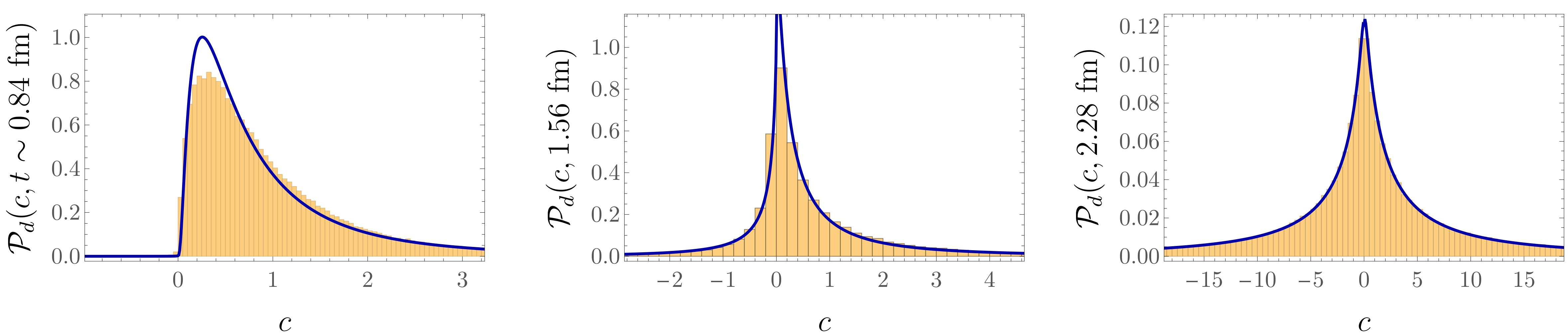
Wagman–Savage

- Wagman and Savage noted that the StN growth is due to fluctuations in the phase of a quantity (nucleon effective mass)

[Wagman & Savage, PRD96 (2017) 114508]



- Correlation function data for eg deuteron [NPLQCD] are reproduced by product of log-normal distribution (magnitude) and a wrapped-normal distribution (phase)



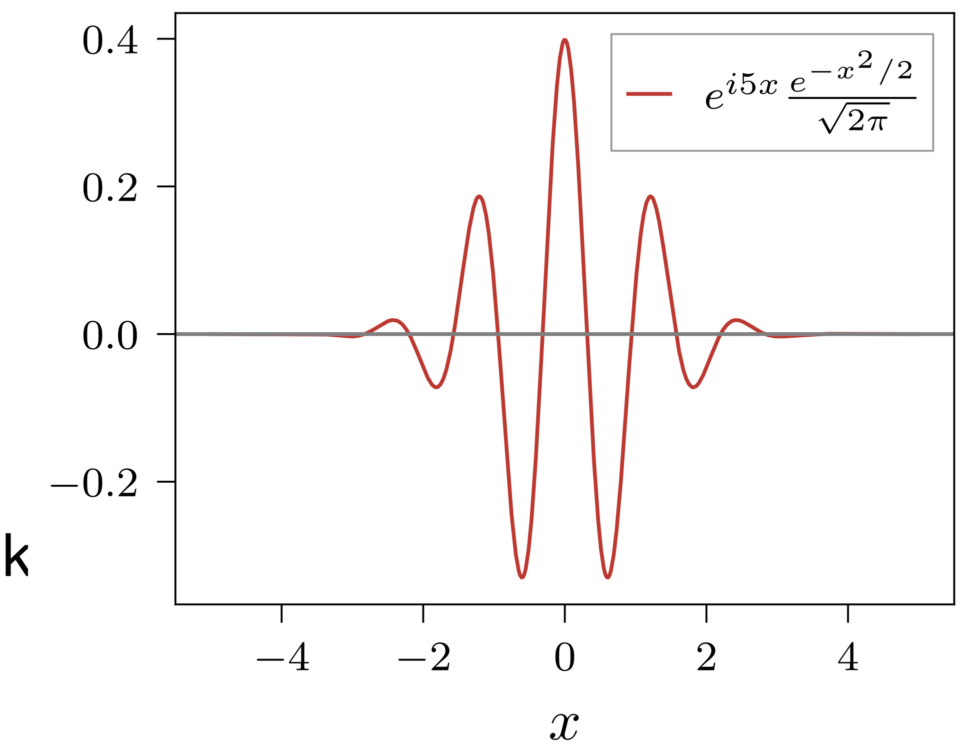
Contour deformation for observables

Goals

- Observables in QFT defined by path integrals that integrate field variables over a specified contour
- Variances of observables are also defined similarly
- What happens in contour is modified?
  - Holomorphic observables are unchanged (Cauchy's theorem)
  - Variance can change
- Look for deformations where variance is reduced
  - Use ML technologies to optimise such a contour

Oscillatory integrals

A simple example



- Consider Gaussian action for one degree of freedom
- Partition function and observables in Euclidean space

$$Z = \int dx e^{-x^2/2} = \sqrt{2\pi} \qquad \langle \mathcal{O} \rangle = \frac{1}{Z} \int dx \mathcal{O}(x) e^{-x^2/2}$$

- Average phase observable falls exponentially fast with k

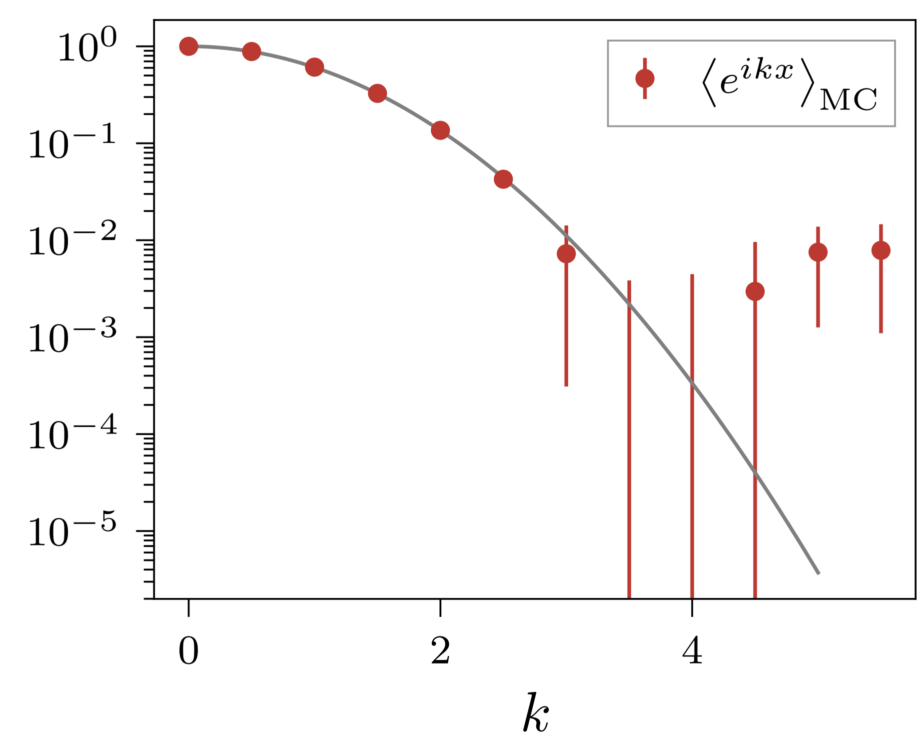
$$\left\langle e^{ikx} \right\rangle = \frac{1}{Z} \int dx\, e^{ikx} e^{-\frac{x^2}{2}} = e^{-k^2/2}$$

- Variance

$$\mathrm{Var}[\mathrm{Re}[e^{ikx}]] = \frac{1}{2}\left\langle |e^{ikx}|^2 \right\rangle + \frac{1}{2}\mathrm{Re}\left\langle (e^{ikx})^2 \right\rangle - \left\langle \mathrm{Re}[e^{ikx}] \right\rangle^2$$
$$= \frac{1}{2} + \frac{1}{2}\mathrm{Re}\left\langle e^{2ikx} \right\rangle - e^{-k^2} \sim \frac{1}{2},$$

- StN problem if we evaluate via Monte-Caro

$$\mathrm{StN}[\mathrm{Re}[e^{ikx}]] = \frac{\sqrt{n} e^{-k^2/2}}{\sqrt{\mathrm{Var}[\mathrm{Re}[e^{ikx}]]}} \sim \sqrt{n} e^{-k^2/2}$$

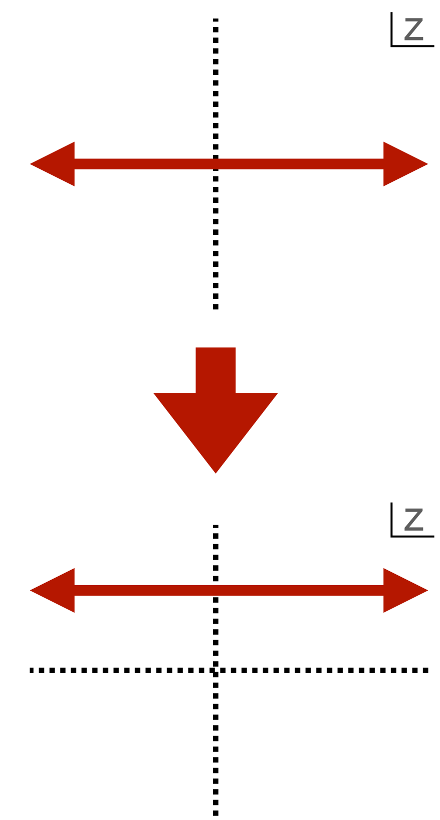


G Kanwar thesis

Contour deformation

A simple example

- Integrand is holomorphic so by Cauchy's theorem we can change the contour
    - Many possibilities: simple choice $z(x) = x + ik$
- Rewrite integral



$$\left\langle e^{ikx} \right\rangle = \frac{1}{Z} \int_{\mathbb{R}} dz\, e^{ikz} e^{-\frac{z^2}{2}} = \frac{1}{Z} \int_{\mathbb{R}+ik} dz\, e^{ikz} e^{-\frac{z^2}{2}}$$

$$= \frac{1}{Z} \int dx\, e^{ikz(x)} e^{-\frac{z(x)^2}{2}} = \frac{1}{Z} \int dx\, e^{ik(x+ik)} e^{-\frac{(x+ik)^2}{2}}$$

$$= \frac{1}{Z} \int dx\, e^{ikx} e^{-k^2} e^{-\frac{x^2}{2} - ikx + \frac{k^2}{2}}$$

$$= \frac{1}{Z} \int dx\, e^{-\frac{k^2}{2}} e^{-\frac{x^2}{2}} = \left\langle e^{-\frac{k^2}{2}} \right\rangle = e^{-\frac{k^2}{2}} \langle 1 \rangle$$

- No sign problem at all!
- Other contours will be worse

Path integrals in QFT

- Path integrals in QFT defined by integral over field values at every point

$$\langle \mathcal{O} \rangle \equiv \frac{1}{Z} \int_{\mathcal{M}} \mathcal{D}U \; e^{-S(U)} \; \mathcal{O}(U) \qquad\qquad Z \equiv \int_{\mathcal{M}} \mathcal{D}U \;\; e^{-S(U)}.$$

- With a lattice regulator, reduces to high dimensional integral over variables parameterising fields

$$\langle \mathcal{O} \rangle \simeq \frac{1}{Z} \int_{\mathbb{R}} dU_1 \int_{\mathbb{R}} dU_2 \ldots \int_{\mathbb{R}} dU_n J(\{U_i\}) e^{-S(\{U_i\})} \mathcal{O}(\{U_i\})$$

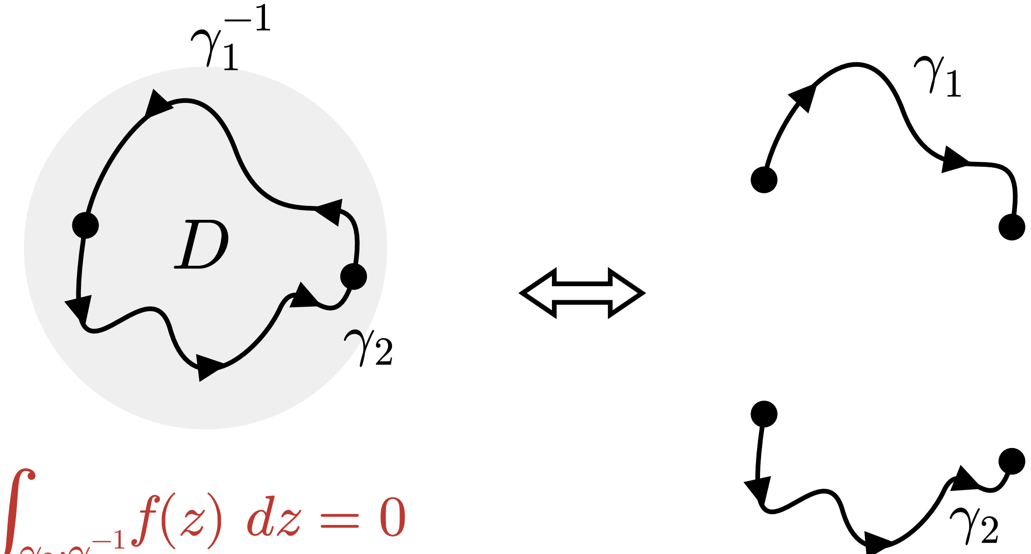
  (Jacobian present in general)

- Consider three cases
  - U(1) gauge theory in 1+1d
  - Complex scalar field theory in 0+1d
  - SU(N) gauge theory in 1+1d

Contour deformation of path integrals

Cauchy Theorem

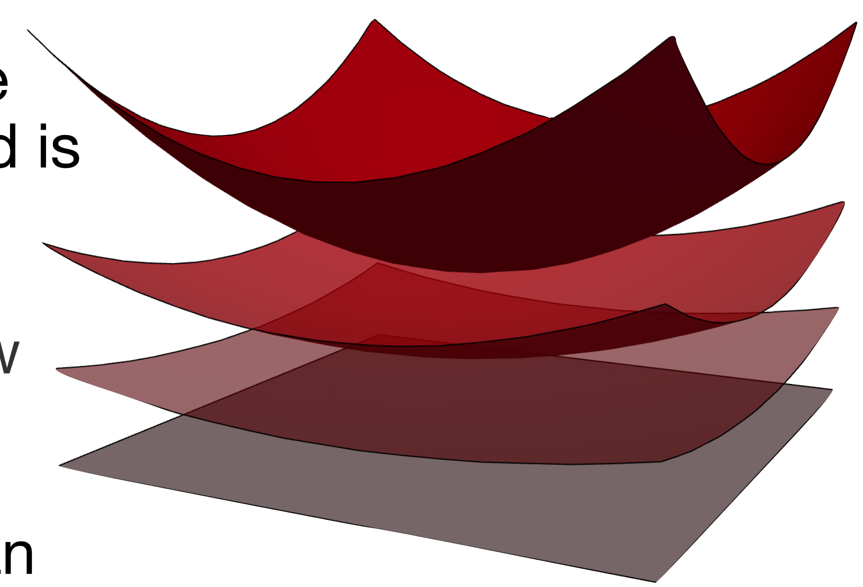
- Cauchy's Integral Theorem in pictures



$$\int_{\gamma_2 \cdot \gamma_1^{-1}} f(z)\ dz = 0$$

$$\int_{\gamma_1} f(z)\ dz \;=\; \int_{\gamma_2} f(z)\ dz$$

- Extends straightforwardly to higher dimensions: a contour deformation from manifold M_A to M_B leaves the integral value unchanged if $M_A \cup M_B$ bounds a region in which the integrand is holomorphic



- Non-zero density: see Alexandru et al. 2007.05436 for review

- Real-time evolution [Alexandru, et al. PRL117(081602), PRD95(114501); Mou, et al. JHEP11(135), Kanwar & Wagman PRD 104(014513)]

Contour deformation of path integrals

Holomorphic quantities

- Most observables we are interested in correspond to holomorphic (or even entire) integrands
- Action is polynomial in field variables so measure is holomorphic
- Observables are also polynomials in field
- Fermions are integrated analytically giving determinant of Dirac operator (an O(V) polynomial of fields)
    - The gauge field integration measure is a polynomial (det) x exponential
    - Quark propagators (inverse of Dirac operator) are O(V) polynomials of gauge field

Contour deformation of path integrals

Observifolds

- Observable $\langle \mathcal{O} \rangle \equiv \frac{1}{Z} \int_{\mathcal{M}} \mathcal{D}U \, e^{-S(U)} \, \mathcal{O}(U)$
- After contour deformation

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int_{\widetilde{\mathcal{M}}} \mathcal{D}\widetilde{U} \, e^{-S(\widetilde{U})} \, \mathcal{O}(\widetilde{U})$$

$$= \frac{1}{Z} \int_{\mathcal{M}} \mathcal{D}U \, J(U) \, e^{-S(\widetilde{U}(U))} \, \mathcal{O}(\widetilde{U}(U))$$

$$\widetilde{U} : \mathcal{M} \to \widetilde{\mathcal{M}}$$

bijective map

$$J(U) = \det \frac{\partial \widetilde{U}}{\partial U}$$

Jacobian

- Define deformed observable

$$\mathcal{Q}(U) \equiv e^{-[S_{\text{eff}}(U) - S(U)]} \mathcal{O}(\widetilde{U}(U))$$

where

$$S_{\text{eff}}(U) \equiv S(\widetilde{U}(U)) - \log J(U)$$

- Satisfies

$$\boxed{\langle \mathcal{O}(U) \rangle = \langle \mathcal{Q}(U) \rangle}$$

Contour deformation of path integrals

Observifolds

- Variance of deformed observable is

$$\mathrm{Var}(\mathrm{Re}\,\mathcal{Q}) = \left\langle (\mathrm{Re}\,\mathcal{Q})^2 \right\rangle - \left(\mathrm{Re}\,\langle \mathcal{Q} \rangle\right)^2$$

Have assumed here <O> is real

- First term has non-holomorphic integrand
  - Possible that $\mathrm{Var}(\mathrm{Re}\,\mathcal{Q}) \ll \mathrm{Var}(\mathrm{Re}\,\mathcal{O})$ for some deformed manifold
  - In which case StN(Re(Q)) > StN(Re(O))
- Parameterise manifold and find best parameters via gradient descent (no need for new ensemble generation)

$$\nabla_{\vec{\omega}}\,\mathrm{Var}(\mathrm{Re}\,\mathcal{Q}) = \left\langle \nabla_{\vec{\omega}} (\mathrm{Re}\,\mathcal{Q})^2 \right\rangle = 2\left\langle \mathrm{Re}\,\mathcal{Q}\,\mathrm{Re}\,\nabla_{\vec{\omega}}\,\mathcal{Q} \right\rangle$$
$$= 2\left\langle (\mathrm{Re}\,\mathcal{Q})\,\mathrm{Re}\left(\mathcal{Q}\left[-\nabla_{\vec{\omega}}\,S_{\mathrm{eff}} + \frac{\nabla_{\vec{\omega}}\,\mathcal{O}(\widetilde{U})}{\mathcal{O}(\widetilde{U})}\right]\right)\right\rangle .$$

Contour deformation of path integrals

Observifolds in practice

- Many possible deformations
  - Some guidance from physics
- Simple intuitive deformations such as constant vertical shifts in imaginary direction

$$z(x) = x + ik$$

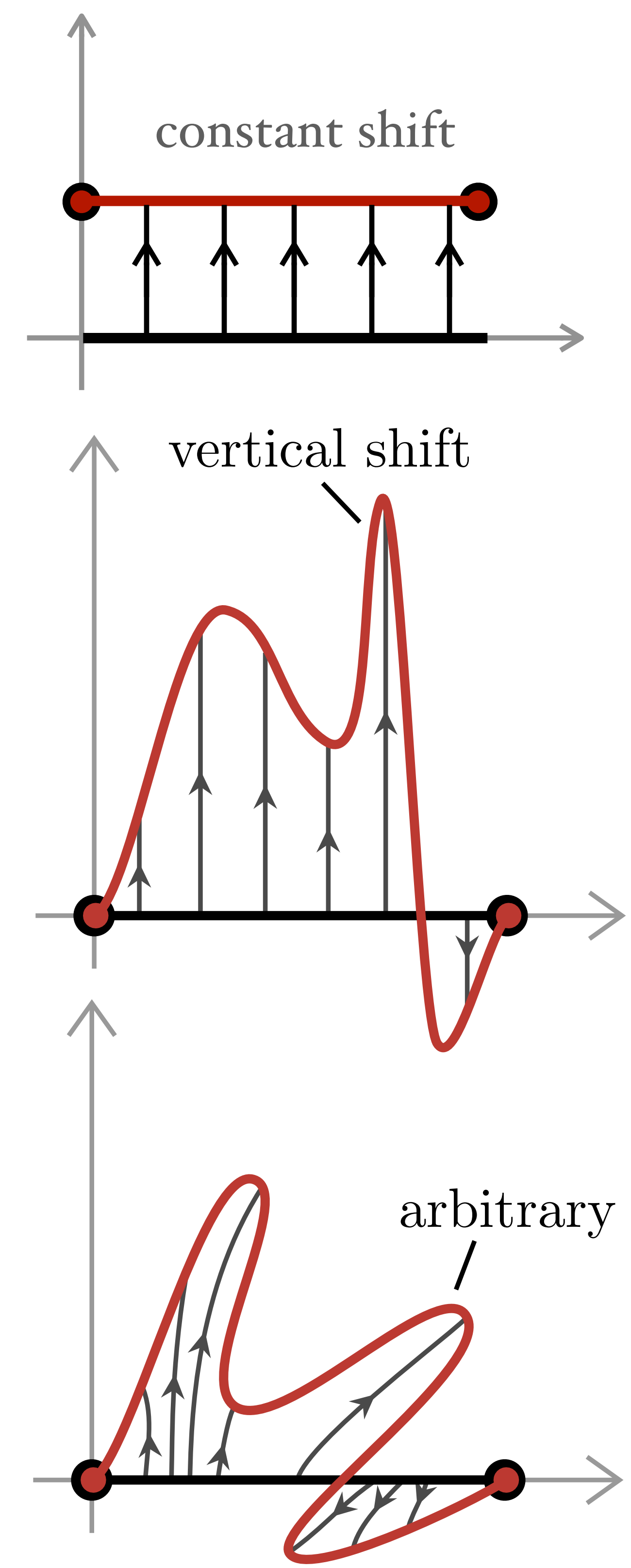
- More complex position dependent vertical shifts

$$z(x) = x + i\delta(x)$$

- Arbitrary (Cauchy-preserving) deformations

$$z(s) = x(s) + iy(s)$$

  - Can not use original coordinate to parameterise



Contour deformation of path integrals

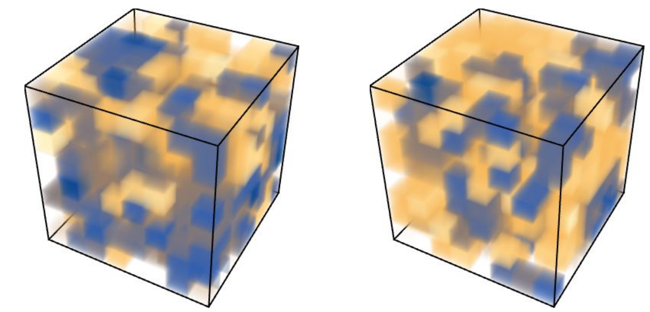
Observifolds in practice

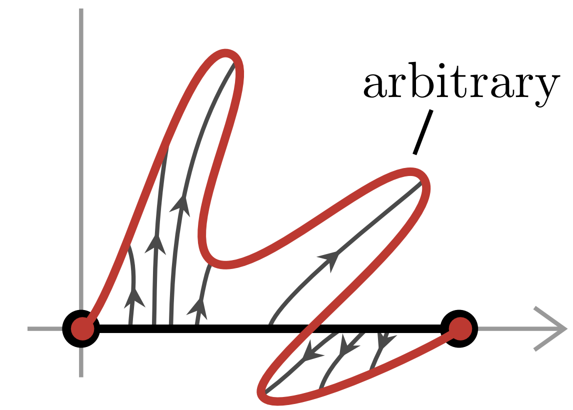
1. Generate ensemble of field configurations

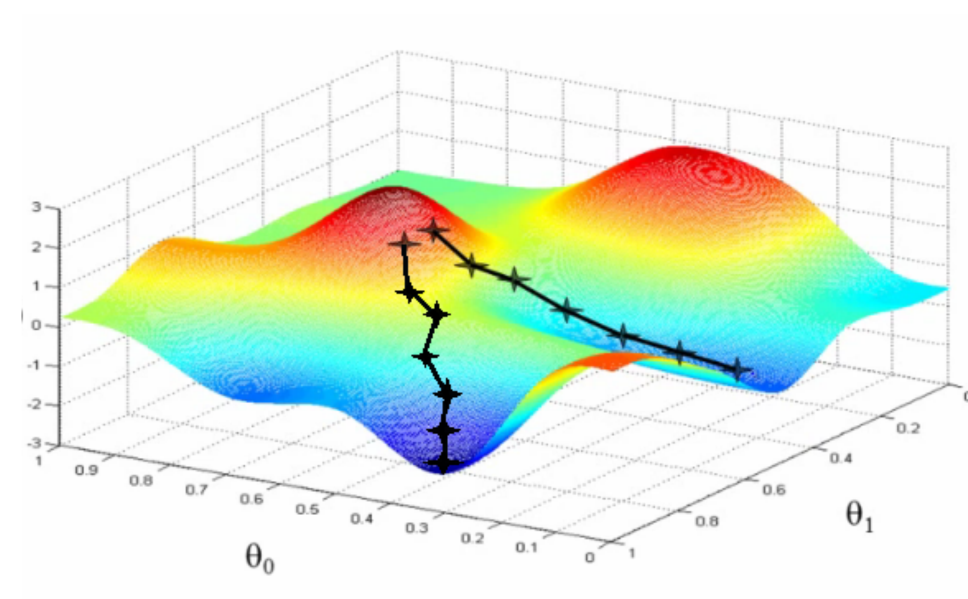
REPEAT

2. Define parameterisation of integration measure
3. Define class of deformations to explore
4. Perform stochastic gradient descent to minimise a loss function (variance)

5. Evaluate learned observable on ensemble

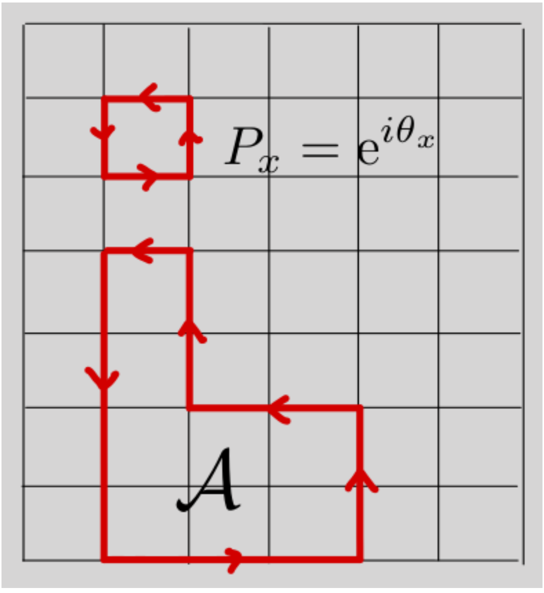






Abelian gauge theory in 1+1d

Simple example



- Wilson action (angles rather than plaquettes): $\theta_x \equiv \arg P_x$

$$S_G(\theta) \equiv -\beta \sum_x \cos\theta_x$$

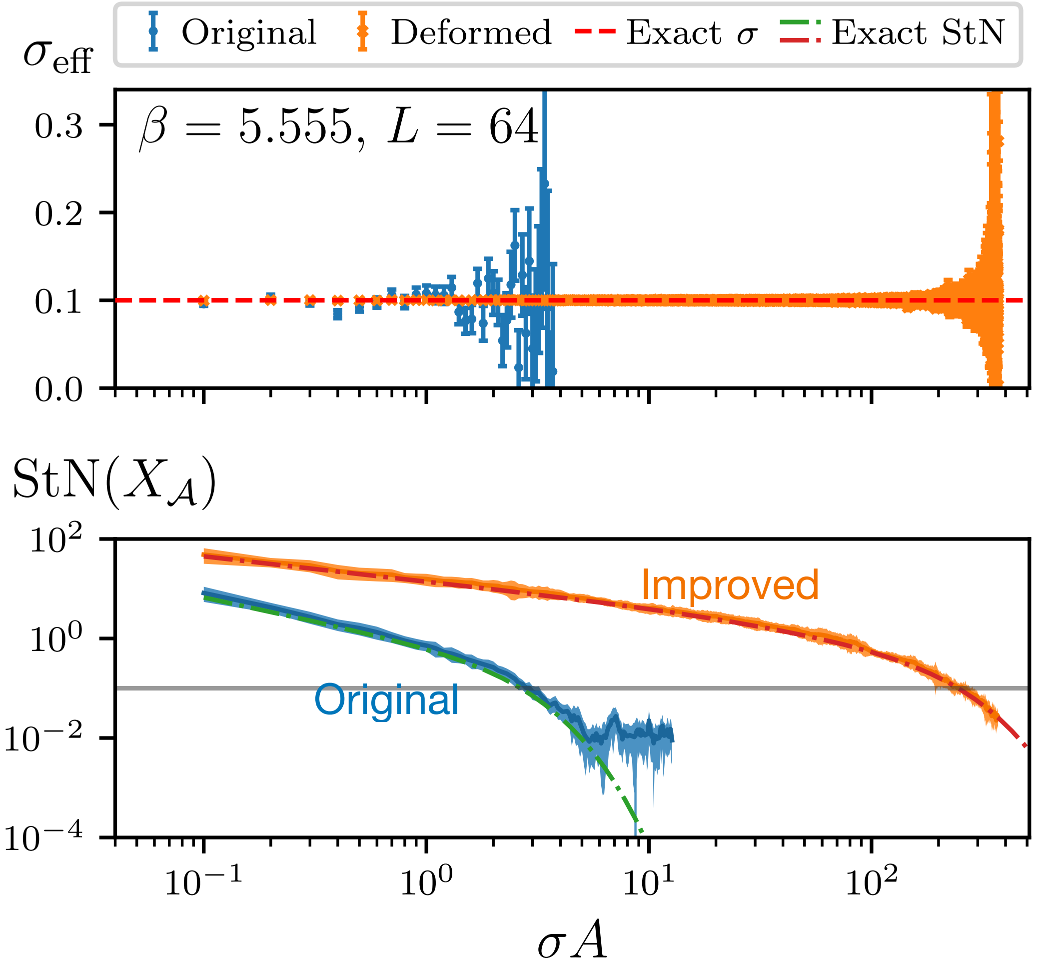
- Observables: Wilson loops of different areas

$$\langle W_\mathcal{A} \rangle \equiv \left\langle \prod_{x\in\mathcal{A}} e^{i\theta_x} \right\rangle = e^{-\sigma A}$$

- Deformation: $\widetilde{\theta}_x = \theta_x + i\delta_x$
- Improved observable for one parameter shift $\delta_x = \delta$ inside loop (zero outside)

$$X_\mathcal{A} \equiv J(\theta) e^{-\left[S_G(\widetilde{\theta}(\theta)) - S_G(\theta)\right]} W_\mathcal{A}(\widetilde{\theta}(\theta))$$
$$= e^{-\left[S_G(\widetilde{\theta}(\theta)) - S_G(\theta)\right]} e^{-\delta A} W_\mathcal{A}(\theta),$$

- By choosing delta can cancel phase of $W_\mathcal{A}(\theta)$ using $\mathrm{Im}(S_G(\widetilde{\theta}))$
  - Huge improvements found!
- NB: all quantities are analytically calculable in this case



Complex scalar theory in 0+1d

Contour learning

- Action in polar coordinates $\phi_t = R_t e^{i\theta_t}$

$$S = -2\sum_{t=0}^{L-1} R_t R_{t+1} \cos(\theta_{t+1} - \theta_t) + V(R)$$

$$V(R) \;=\; \sum_t (2+m^2)R_t^2 + \lambda R_t^4$$

- Deform only angles (unit Jacobian)

$$\tilde{\theta}_t = \theta_t + i\delta_t^{(1)} + i\delta_t^{(2)} f_c(R_t R_{t+1}) + i\delta_t^{(3)} f_c(R_{t-1}R_t)$$

$$f_c(x) = c\,\tanh((cx)^{-1})$$

- Deformed observable

$$D_t \equiv e^{-[S_{\rm eff}(\theta)-S(\theta)]} C_t(R,\widetilde{\theta}) = e^{-[S_{\rm eff}(\theta)-S(\theta)]} R_t R_0 e^{i\widetilde{\theta}_t - i\widetilde{\theta}_0}$$

- Deform 1:

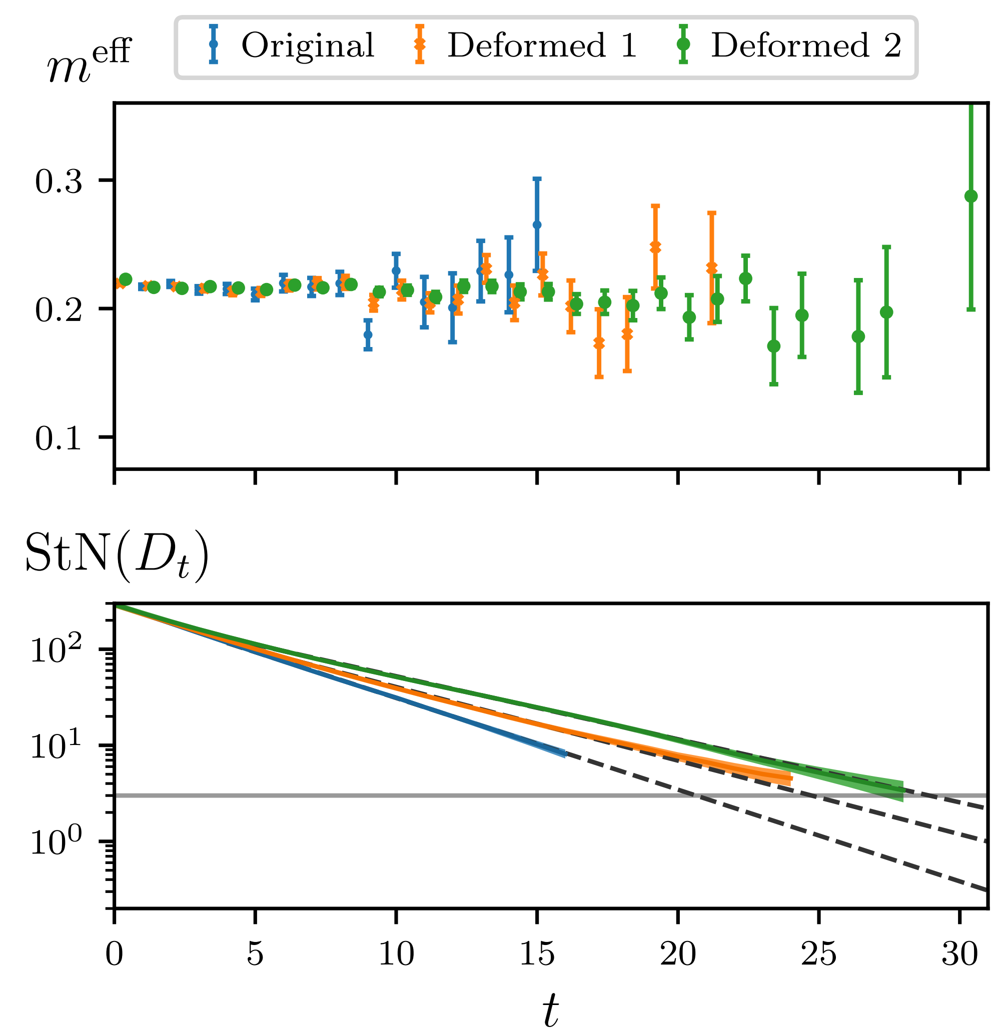
$$c = \delta_{t'}^{(2)} = \delta_{t'}^{(3)} = 0,\ \delta_{t'}^{(1)} = t'\delta \text{ for } |t'| < t$$

- Deform 2: full 3L+1 parameter optimisation
    - Order of magnitude gain in StN vs undeformed

- Observable

$$G_t \equiv \langle \phi_t \phi_0^\dagger \rangle = \left\langle R_t R_0 e^{i\theta_t - i\theta_0} \right\rangle \equiv \langle C_t(R,\theta)\rangle$$

$$m^{\rm eff}(t) \equiv \text{arccosh}\left(\frac{G_{t-1}+G_{t+1}}{2G_t}\right)$$



$m = 0.15,\ \lambda = 3\times 10^{-3},\ L = 64$

SU(N) gauge theory in 1+1d

Action

- Action is given by

$$S \equiv -\frac{1}{g^2} \sum_{x \in \mathcal{V}} \operatorname{tr}\left(P_x + P_x^{-1}\right)$$

  where

$$P_x \equiv U_{x,1} U_{x+\hat{1},2} U^{-1}_{x+\hat{2},1} U^{-1}_{x,2}$$

  NB: P_x^{-1} is complexification of $P_x^\dagger$

- With open BCs, can choose a maximal tree gauge such that plaquettes and links have 1-to-1 correspondence

$$U_{x,1} = \left[\prod_{k=0}^{x_2-1} P_{x+k\hat{2}}\right]^{-1} \qquad P_x = U_{x,1} U^{-1}_{x+\hat{2},1}$$

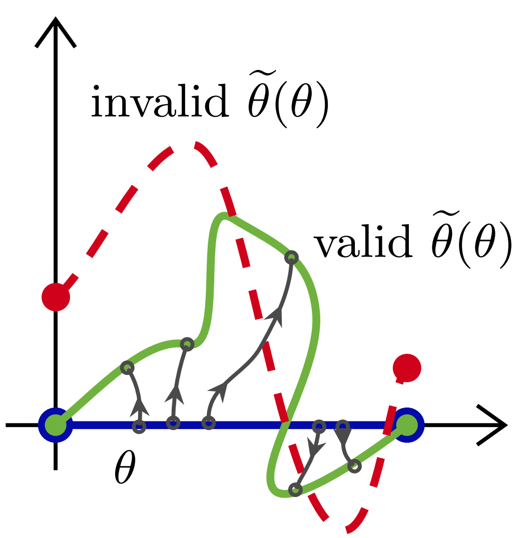
- Path integral factorises in this gauge

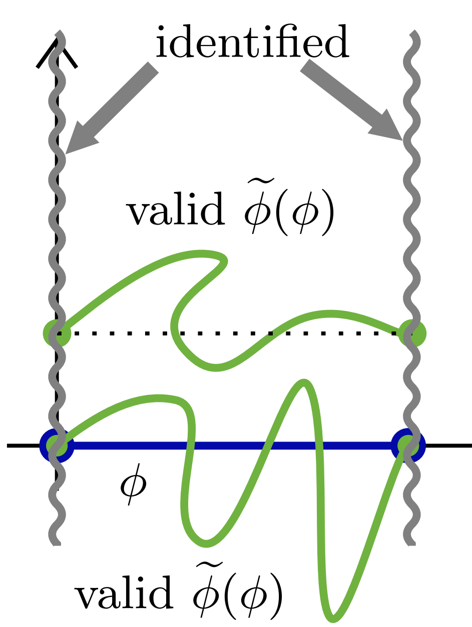
- Observables can be determined semi-analytically from single site SU(N) integrals

SU(N) gauge theory in 1+1d

Defining coordinates

- SU(N) can be coordinatised (Bronzan 1988) using a set of angular variables (not unique choice)
  - Azimuthal angles: $\phi_1, \ldots, \phi_J \in [0, 2\pi]$ $\quad J = (N^2 + N - 2)/2$
  - Zenith angles: $\theta_1, \ldots, \theta_K \in [0, \pi/2]$ $\quad K = (N^2 - N)/2$
  - Together write as $\Omega \equiv (\phi_1, \ldots, \phi_J, \theta_1, \ldots, \theta_K).$
- Action and relevant observables holomorphic in these angles
- Deformations of angular contours
  - Azimuthal identified at boundaries
  - Zenith angles preserve endpoints at boundary





SU(N) gauge theory in 1+1d

Defining coordinates

- SU(2): 2 azimuthal and 1 zenith angles

$$
\begin{aligned}
P_x^{11} &= \sin\theta_x \, e^{i\phi_x^1}, \\
P_x^{12} &= \cos\theta_x \, e^{i\phi_x^2}, \\
P_x^{21} &= -\cos\theta_x \, e^{-i\phi_x^2}, \\
P_x^{22} &= \sin\theta_x \, e^{-i\phi_x^1},
\end{aligned}
$$

$$
\begin{aligned}
\theta_x &= \arcsin(|P_x^{11}|), \\
\phi_x^1 &= \arg(P_x^{11}), \\
\phi_x^2 &= \arg(P_x^{12}),
\end{aligned}
$$

- SU(3): 5 azimuthal and 3 zenith angles

$$
\begin{aligned}
P_x^{11} &= \cos\theta_x^1 \cos\theta_x^2 e^{i\phi_x^1}, \\
P_x^{12} &= \sin\theta_x^1 e^{i\phi_x^3}, \\
P_x^{13} &= \cos\theta_x^1 \sin\theta_x^2 e^{i\phi_x^4}, \\
P_x^{21} &= \sin\theta_x^2 \sin\theta_x^3 e^{-i(\phi_x^4+\phi_x^5)} \\
&\quad - \sin\theta_x^1 \cos\theta_x^2 \cos\theta_x^3 e^{i(\phi_x^1+\phi_x^2-\phi_x^3)}, \\
P_x^{22} &= \cos\theta_x^1 \cos\theta_x^3 e^{i\phi_x^2}, \\
P_x^{23} &= -\cos\theta_x^2 \sin\theta_x^3 e^{-i(\phi_x^1+\phi_x^5)} \\
&\quad - \sin\theta_x^1 \sin\theta_x^2 \cos\theta_x^3 e^{i(\phi_x^2-\phi_x^3+\phi_x^4)}, \\
P_x^{31} &= -\sin\theta_x^1 \cos\theta_x^2 \sin\theta_x^3 e^{i(\phi_x^1-\phi_x^3+\phi_x^5)} \\
&\quad - \sin\theta_x^2 \cos\theta_x^3 e^{-i(\phi_x^2+\phi_x^4)}, \\
P_x^{32} &= \cos\theta_x^1 \sin\theta_x^3 e^{i\phi_x^5}, \\
P_x^{33} &= \cos\theta_x^2 \cos\theta_x^3 e^{-i(\phi_x^1+\phi_x^2)} \\
&\quad - \sin\theta_x^1 \sin\theta_x^2 \sin\theta_x^3 e^{-i(\phi_x^3-\phi_x^4-\phi_x^5)},
\end{aligned}
$$

$$
\begin{aligned}
\theta_x^1 &= \arcsin(|P_x^{12}|), \\
\theta_x^2 &= \arccos\left(|P_x^{11}|/\cos(\theta_x^1)\right), \\
\theta_x^3 &= \arccos\left(|P_x^{22}|/\cos(\theta_x^1)\right), \\
\phi_x^1 &= \arg(P_x^{11}), \\
\phi_x^2 &= \arg(P_x^{22}), \\
\phi_x^3 &= \arg(P_x^{12}), \\
\phi_x^4 &= \arg(P_x^{13}), \\
\phi_x^5 &= \arg(P_x^{32}).
\end{aligned}
$$

SU(2) gauge theory in 1+1d

Defining deformations

SU(3) more complicated!

- SU(2) deformed coordinates given by

$$\tilde{\theta}_x \equiv \theta_x + i \sum_{y \le x} f_\theta \left(\theta_y, \phi_y^1, \phi_y^2; \kappa^{xy}, \lambda^{xy}, \eta^{xy}, \chi^{xy}, \zeta^{xy}\right)$$

$$\tilde{\phi}_x^1 \equiv \phi_x^1 + i\kappa_0^{x;\phi^1} + i \sum_{y \le x} f_{\phi^1} \left(\theta_y, \phi_y^1, \phi_y^2; \kappa^{xy}, \lambda^{xy}, \eta^{xy}, \chi^{xy}, \zeta^{xy}\right)$$

$$\tilde{\phi}_x^2 \equiv \phi_x^2 + i\kappa_0^{x;\phi^2} + i \sum_{y \le x} f_{\phi^2} \left(\theta_y, \phi_y^1, \phi_y^2; \kappa^{xy}, \lambda^{xy}, \eta^{xy}, \chi^{xy}, \zeta^{xy}\right)$$

- with many parameters defining the deformation

$$f_\theta = \sum_{m=1}^{\Lambda} \kappa_m^{xy;\theta} \sin\left(2m\theta_y\right) \left\{1 + \sum_{n=1}^{\Lambda} \left[\eta_{mn}^{xy;\theta,\phi^1} \sin(n\phi_y^1 + \chi_{mn}^{xy;\theta,\phi^1}) + \eta_{mn}^{xy;\theta,\phi^2} \sin(n\phi_y^2 + \chi_{mn}^{xy;\theta,\phi^2})\right]\right\},$$

$$f_{\phi^1} = \sum_{m=1}^{\Lambda} \kappa_m^{xy;\phi^1} \sin(m\phi_y^1 + \zeta_m^{xy;\phi^1}) \left\{1 + \sum_{n=1}^{\Lambda} \left[\lambda_{mn}^{xy;\phi^1,\theta} \sin(2n\theta_y) + \eta_{mn}^{xy;\phi^1,\phi^2} \sin(n\phi_y^2 + \chi_{mn}^{xy;\phi^1,\phi^2})\right]\right\}$$

$$f_{\phi^2} = \sum_{m=1}^{\Lambda} \kappa_m^{xy;\phi^2} \sin(m\phi_y^2 + \zeta_m^{xy;\phi^2}) \left\{1 + \sum_{n=1}^{\Lambda} \left[\lambda_{mn}^{xy;\phi^2,\theta} \sin(2n\theta_y) + \eta_{mn}^{xy;\phi^2,\phi^1} \sin(n\phi_y^1 + \chi_{mn}^{xy;\phi^2,\phi^1})\right]\right\}$$

- Jacobian triangular so calculable in O(V)

SU(N) gauge theory in 1+1d

Defining observables

- Focus on Wilson loop observables for various areas
- Advantageous to fix the gauge and focus on one component of the untraced loop

$$W_{\mathcal{A}}^{11} = \left(\prod_{x \in \mathcal{A}} P_x \right)^{11} \qquad \langle W_{\mathcal{A}}^{11} \rangle = \frac{1}{N} \mathrm{tr} \langle W_{\mathcal{A}} \rangle \sim e^{-\sigma A}$$

ordered product

- StN is exponentially degrading since $\mathrm{Var}(W_{\mathcal{A}}^{11}) \sim 1$
- Deformed observable with previous parameterisation

$$Q(\{P_x\}) \equiv \mathcal{O}(\{\widetilde{P}_x\}) \frac{e^{-S(\{\widetilde{P}_x\})}}{e^{-S(\{P_x\})}} \prod_x j_x \left[\frac{\sin(2\tilde{\theta}_x)}{\sin(2\theta_x)} \right]$$

where

$$\widetilde{P}_x = \begin{pmatrix} \sin\widetilde{\theta}_x e^{i\widetilde{\phi}_x^1} & \cos\widetilde{\theta}_x e^{i\widetilde{\phi}_x^2} \\ -\cos\widetilde{\theta}_x e^{-i\widetilde{\phi}_x^2} & \sin\widetilde{\theta}_x e^{-i\widetilde{\phi}_x^1} \end{pmatrix} \in SL(2, \mathbb{C})$$

SU(N) gauge theory in 1+1d

Ensembles

- Studies in 1+1d SU(2) and SU(3) with the following parameters

		$SU(2)$		$SU(3)$	
σ	V	g	β	g	β
0.4	16	0.98	4.2	0.72	11.7
0.2	32	0.71	8.0	0.53	21.7
0.1	64	0.51	15.5	0.38	41.8

- Dimensionless string tension σV held fixed

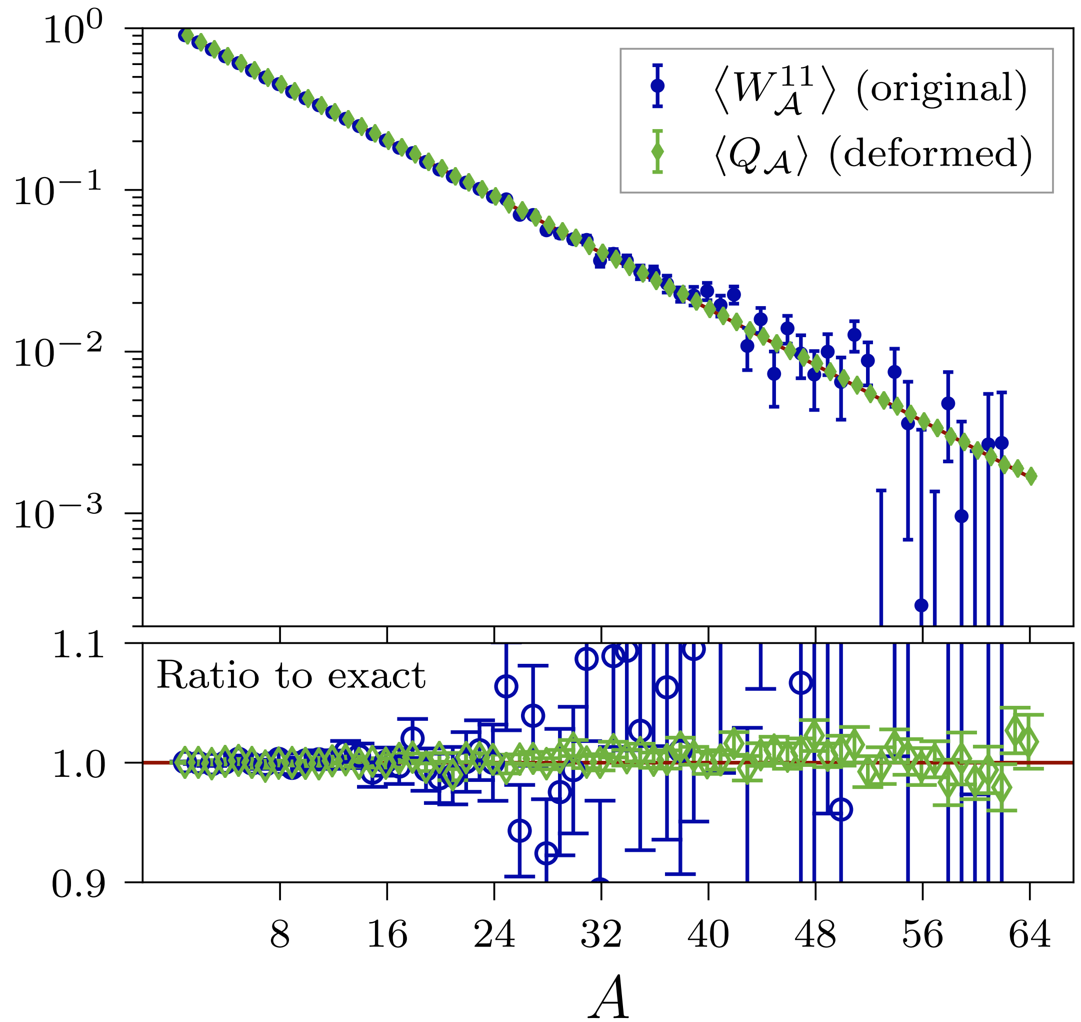
$$\sigma \equiv -\lim_{A\to\infty} \partial_A \ln W_{\mathcal{A}} \qquad W_{\mathcal{A}} \equiv \prod_{x,\mu\in\partial\mathcal{A}} U_{x,\mu}$$

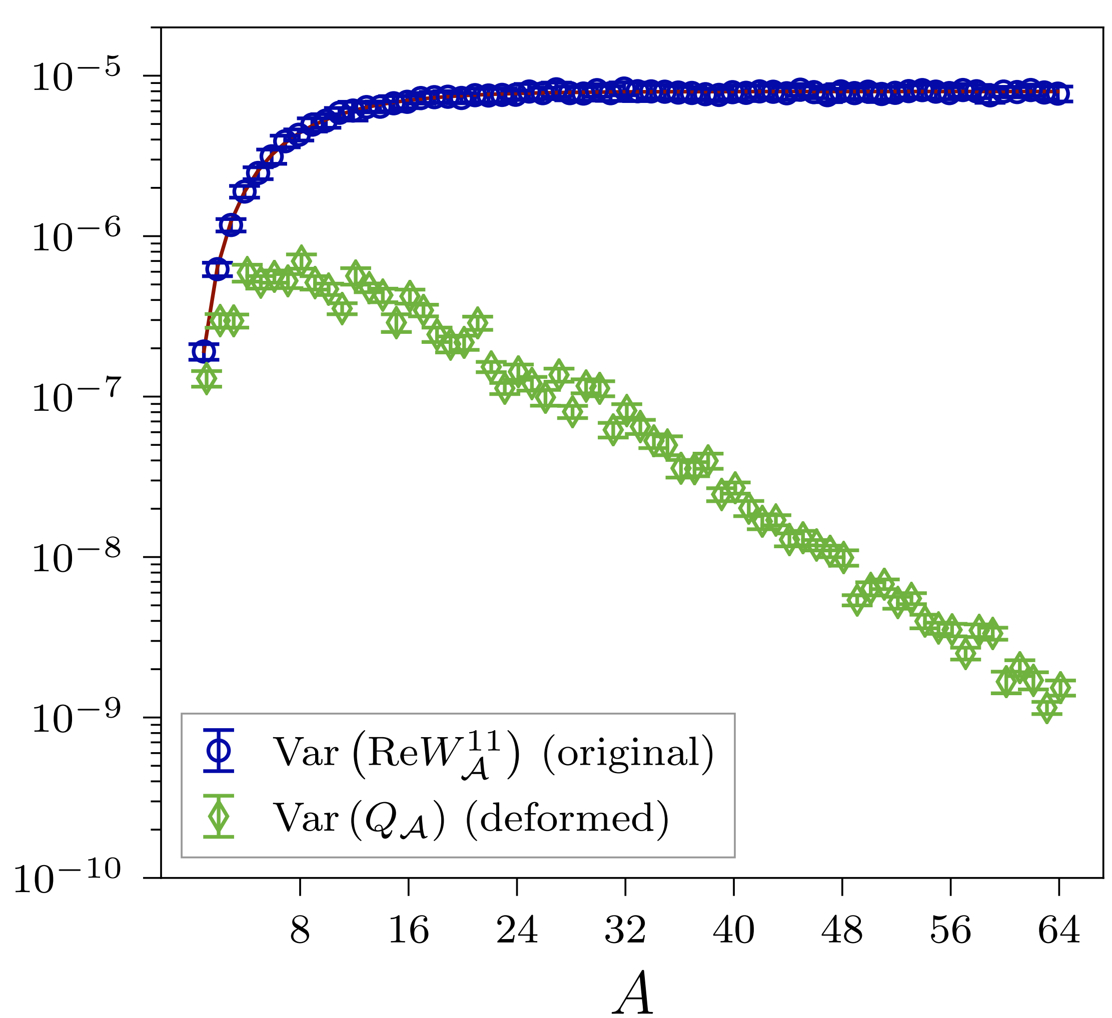
- N=32000 decor related configurations generated using HMC
    - Optimisation: 320/320/32360 configurations used for training/testing/measurement

SU(2) gauge theory in 1+1d

Results

- Expectation values and variances of SU(2) Wilson loops of various sizes on finest ensemble

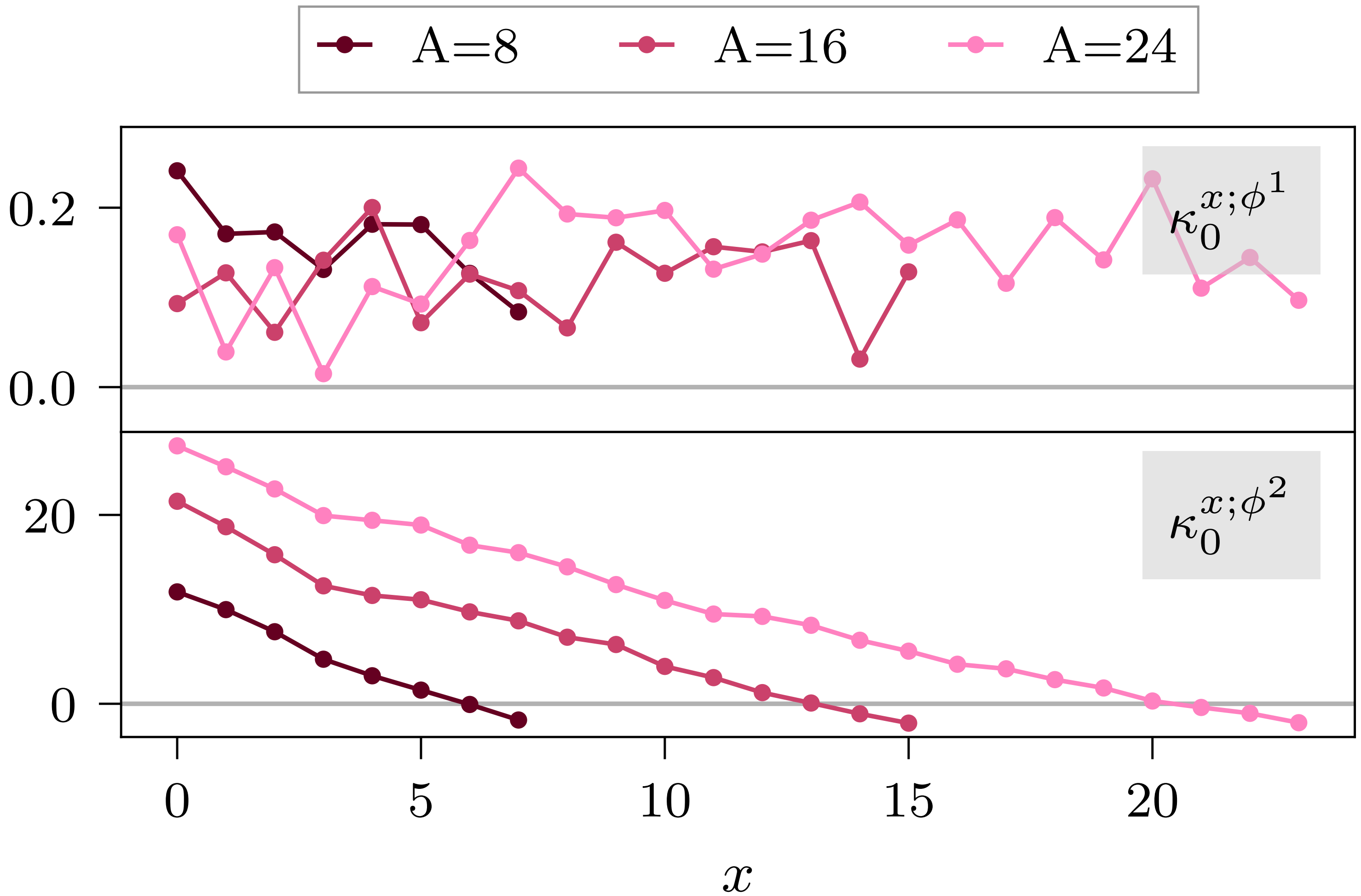




SU(2) gauge theory in 1+1d

Results

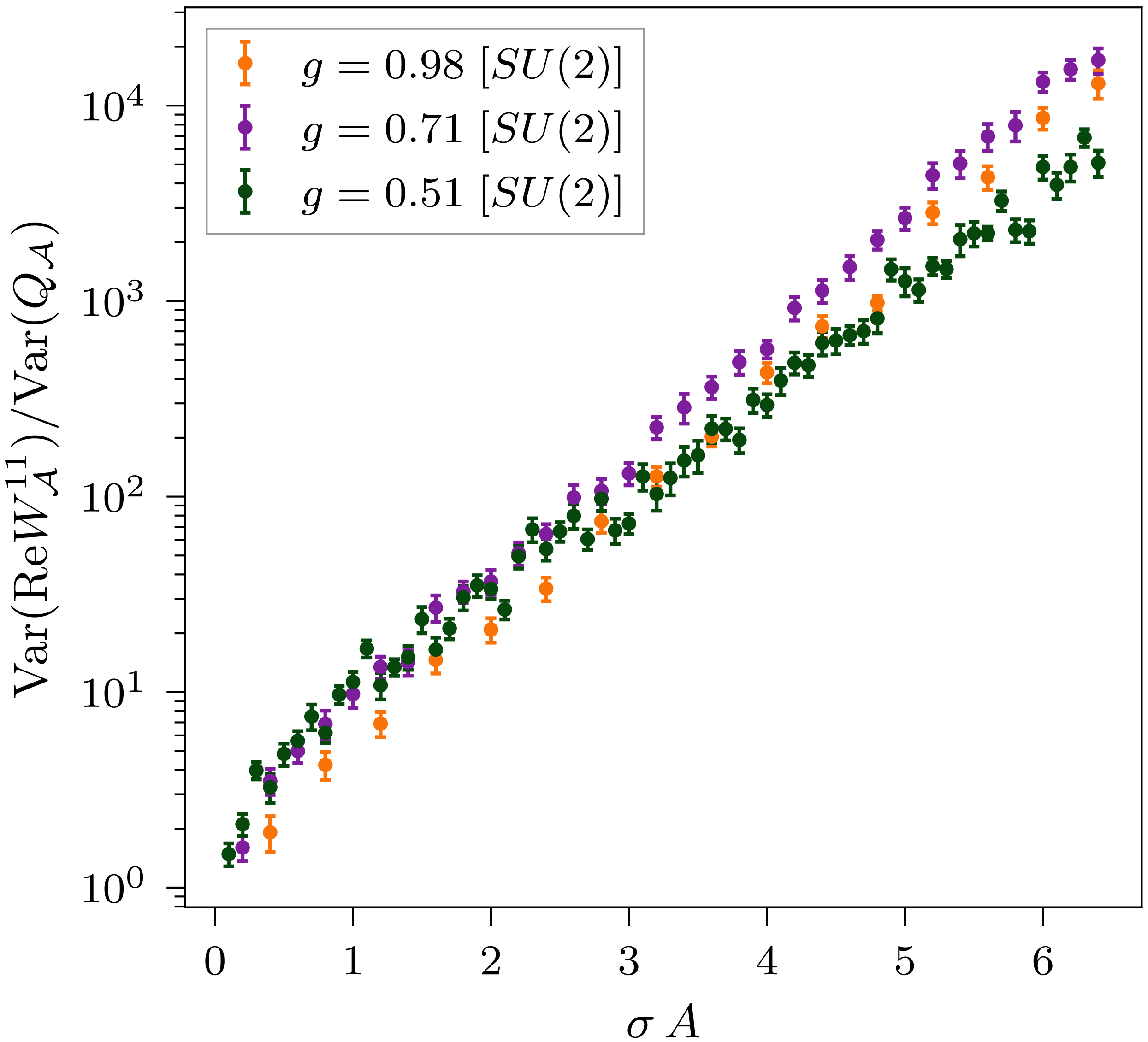
- What path is learnt?
- A ramped shift of one angle and small constant shift of another



SU(2) gauge theory in 1+1d

Results

- Continuum limit
  - Similar results seen all three lattice spacings
  - Fairly similar scaling for each coupling with differences likely due to training



SU(2) gauge theory in 1+1d

Results

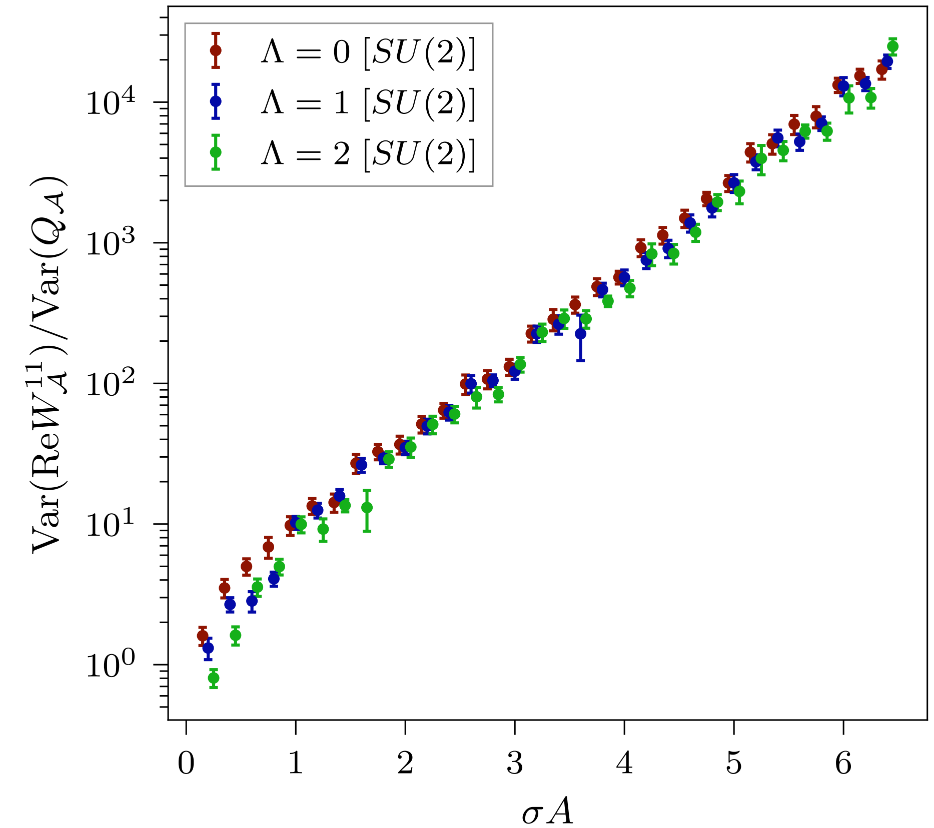
- Increasing cutoff on Fourier series does not improve

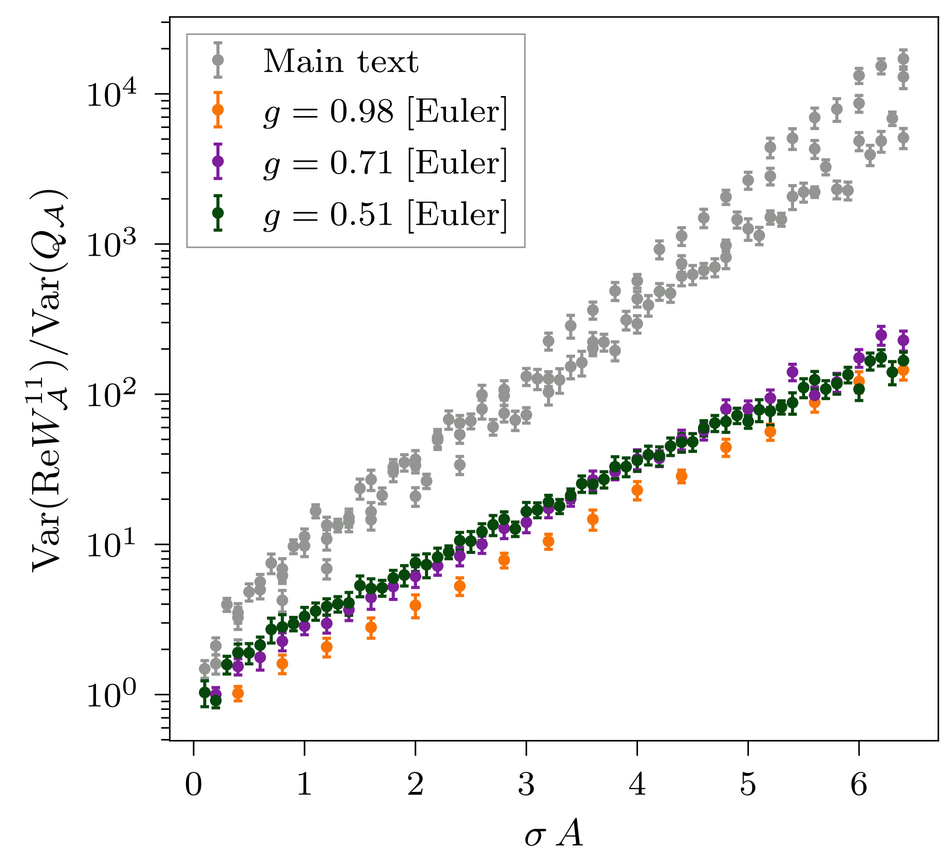
$$
\begin{aligned}
f_\theta &= \sum_{m=1}^{\Lambda} \kappa_m^{xy;\theta} \sin(2m\theta_y) \left\{ 1 + \sum_{n=1}^{\Lambda} \left[\eta_{mn}^{xy;\theta,\phi^1} \sin(n\phi_y^1 + \chi_{mn}^{xy;\theta,\phi^1}) + \eta_{mn}^{xy;\theta,\phi^2} \sin(n\phi_y^2 + \chi_{mn}^{xy;\theta,\phi^2}) \right] \right\}, \\
f_{\phi^1} &= \sum_{m=1}^{\Lambda} \kappa_m^{xy;\phi^1} \sin(m\phi_y^1 + \zeta_m^{xy;\phi^1}) \left\{ 1 + \sum_{n=1}^{\Lambda} \left[\lambda_{mn}^{xy;\phi^1,\theta} \sin(2n\theta_y) + \eta_{mn}^{xy;\phi^1,\phi^2} \sin(n\phi_y^2 + \chi_{mn}^{xy;\phi^1,\phi^2}) \right] \right\} \\
f_{\phi^2} &= \sum_{m=1}^{\Lambda} \kappa_m^{xy;\phi^2} \sin(m\phi_y^2 + \zeta_m^{xy;\phi^2}) \left\{ 1 + \sum_{n=1}^{\Lambda} \left[\lambda_{mn}^{xy;\phi^2,\theta} \sin(2n\theta_y) + \eta_{mn}^{xy;\phi^2,\phi^1} \sin(n\phi_y^1 + \chi_{mn}^{xy;\phi^2,\phi^1}) \right] \right\}
\end{aligned}
$$

  - Could be a training issue due to larger number of parameters?

- Alternative SU(2) parameterisation does less well

- Interesting to explore alternative parameterisations

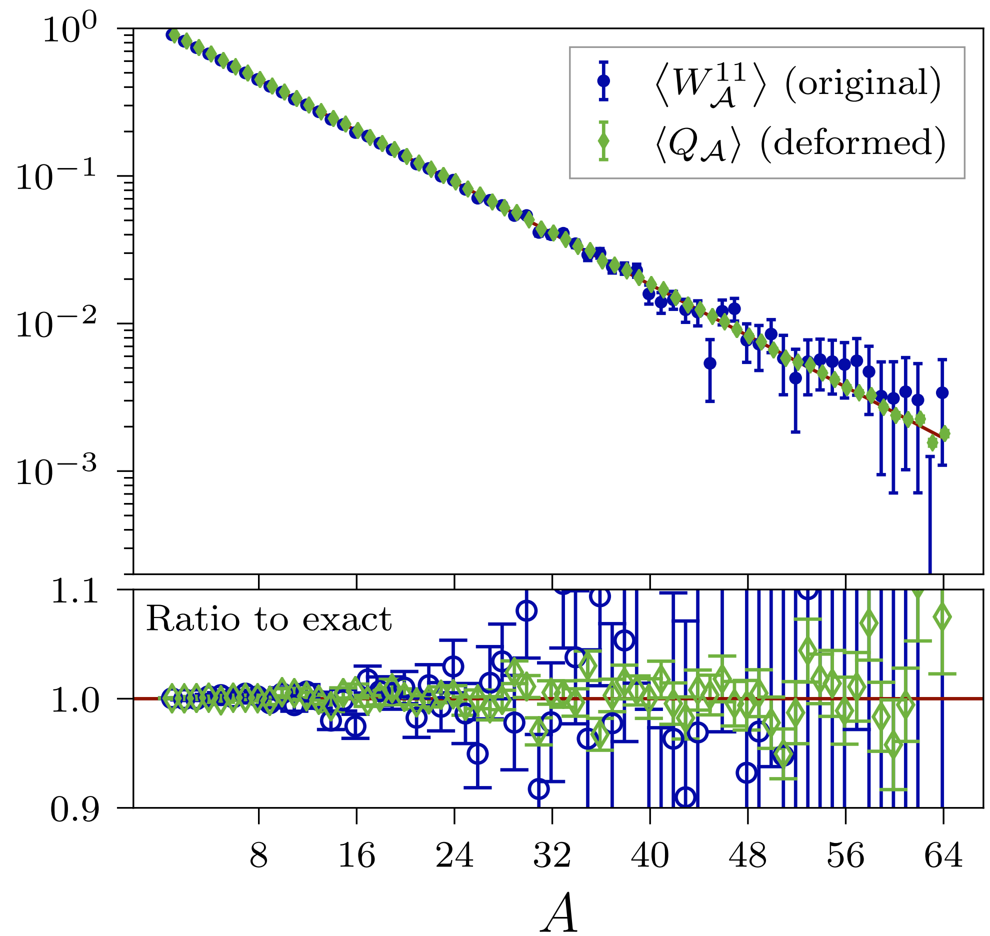


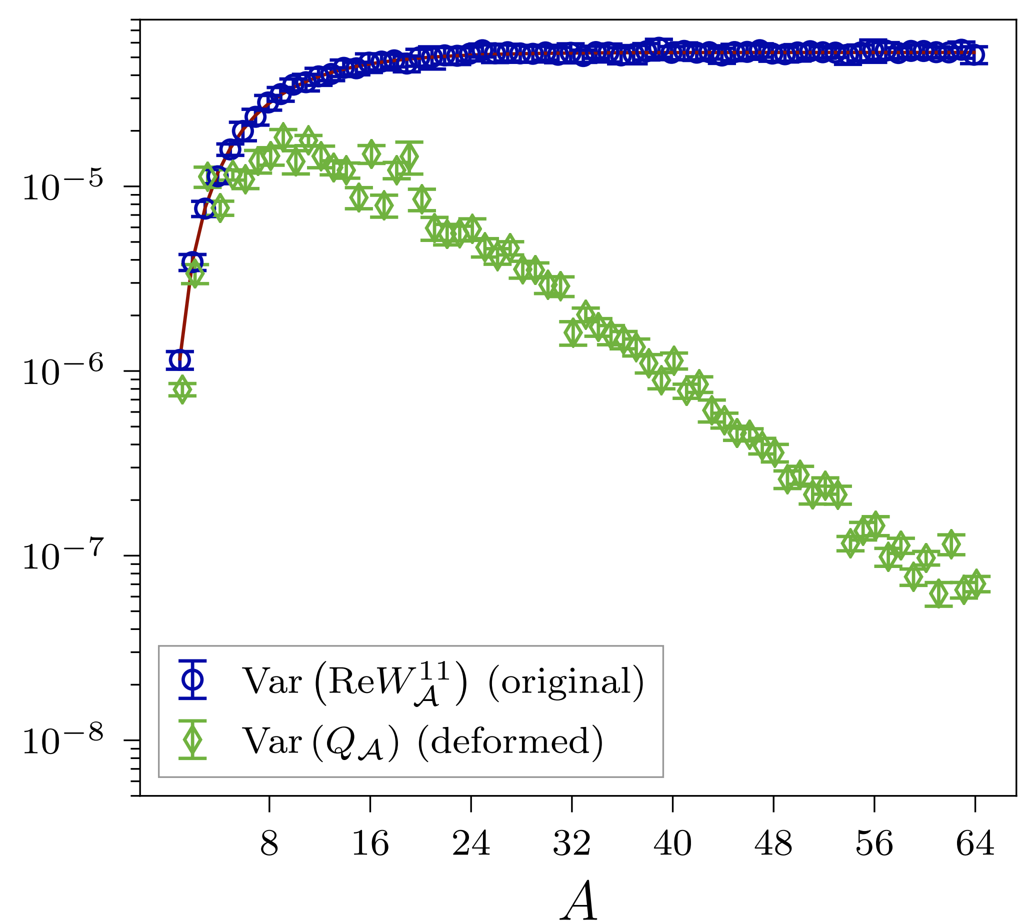


SU(3) gauge theory in 1+1d

Results

- SU(3) results show very similar improvements

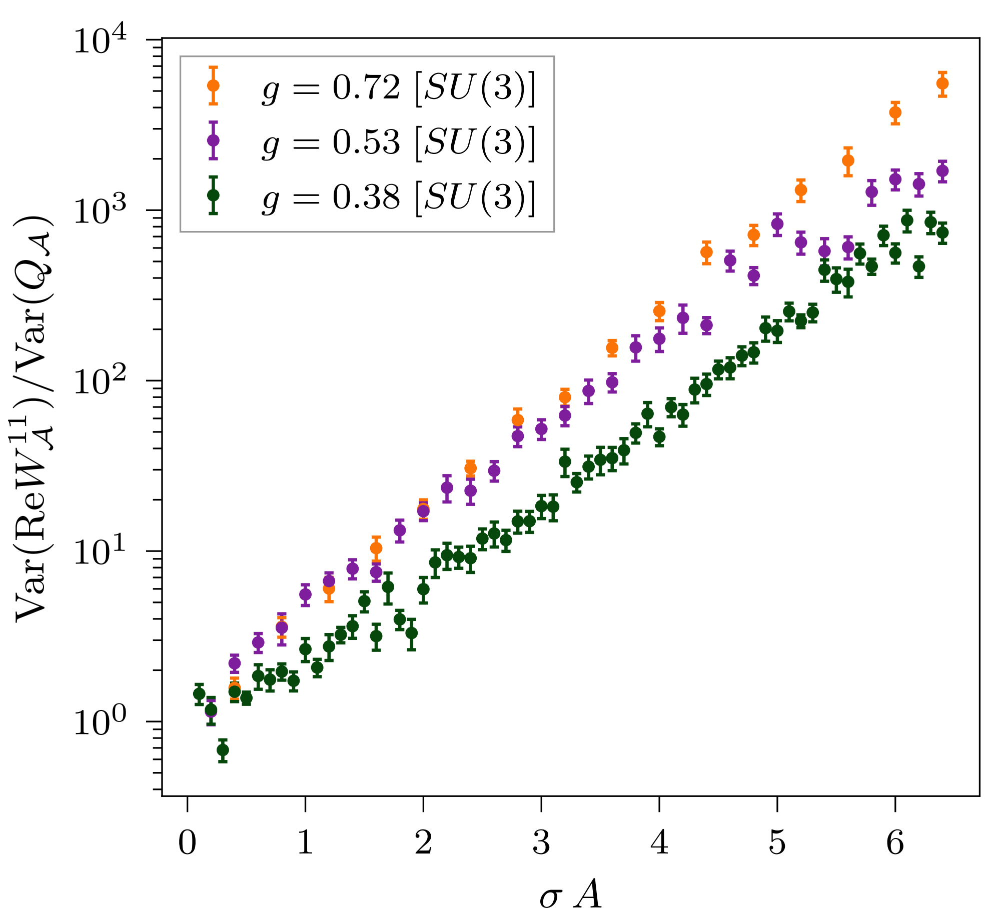


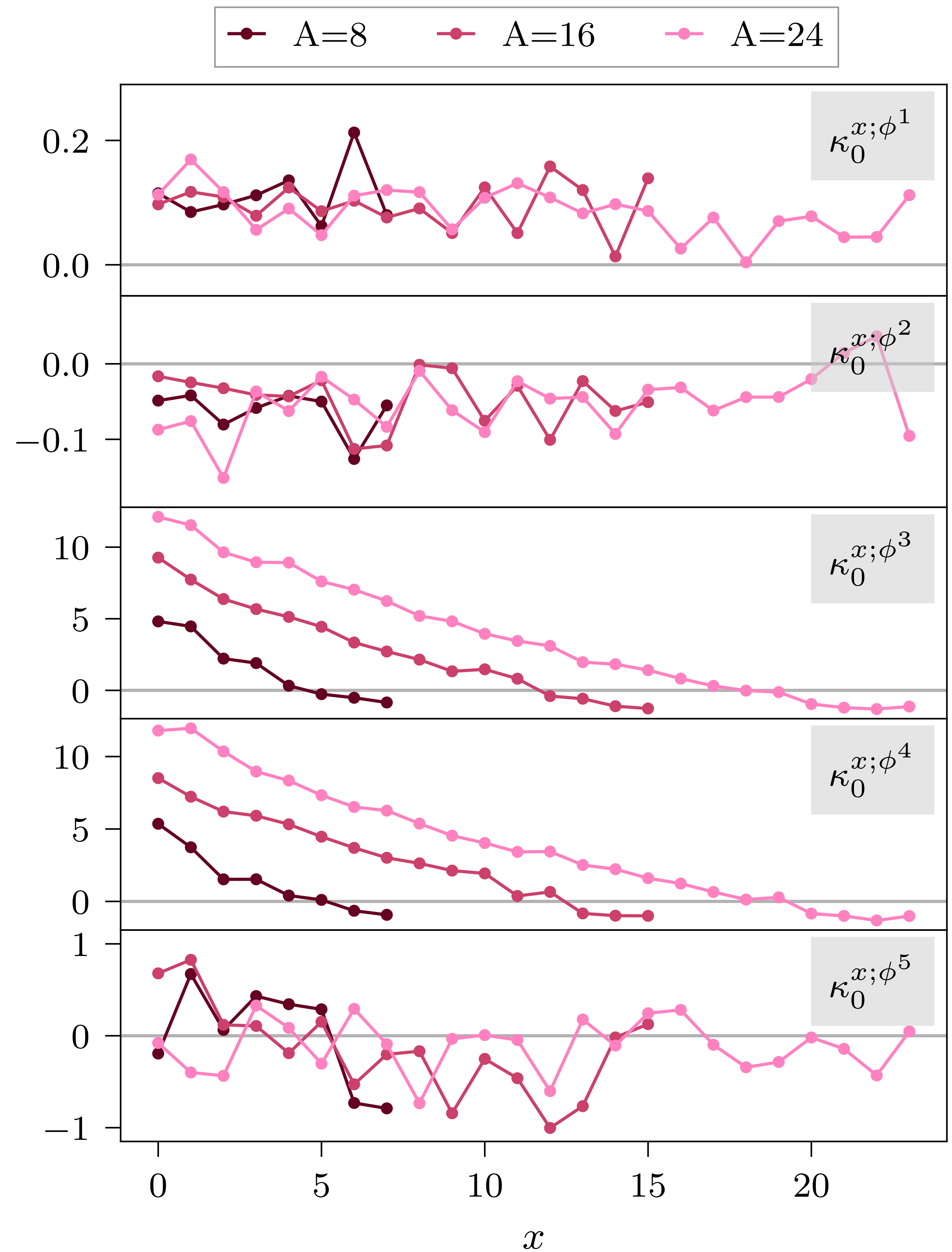


SU(3) gauge theory in 1+1d

Results

- Deformations of contours show similar ramp structures
- Slight decrease in improvement as continuum limit approached





Contour deformation of path integrals

Machine learning tools

- Stochastic gradient descent performed using ADAM optimiser
- Loss function given by variance

$$\mathcal{L} \equiv \left\langle (\mathrm{Re}\, Q_{\mathcal{A}})^2 \right\rangle = \frac{1}{2} \left\langle |Q_{\mathcal{A}}^2| \right\rangle + \frac{1}{2} \left\langle Q_{\mathcal{A}}^2 \right\rangle$$

- Gradient calculated from explicit form using JAX autodifferentiation

$$\nabla \mathcal{L} = \langle 2\, \mathrm{Re}\, Q_{\mathcal{A}} \nabla\, \mathrm{Re}\, Q_{\mathcal{A}} \rangle$$

- Evaluated stochastically on batches of training data

$$\nabla \mathcal{L} \approx \frac{1}{n} \sum_{i=1}^{n} \left[2\, \mathrm{Re}\, Q_{\mathcal{A}}(\{P_x^i\}) \nabla\, \mathrm{Re}\, Q_{\mathcal{A}}(\{P_x^i\}) \right]$$

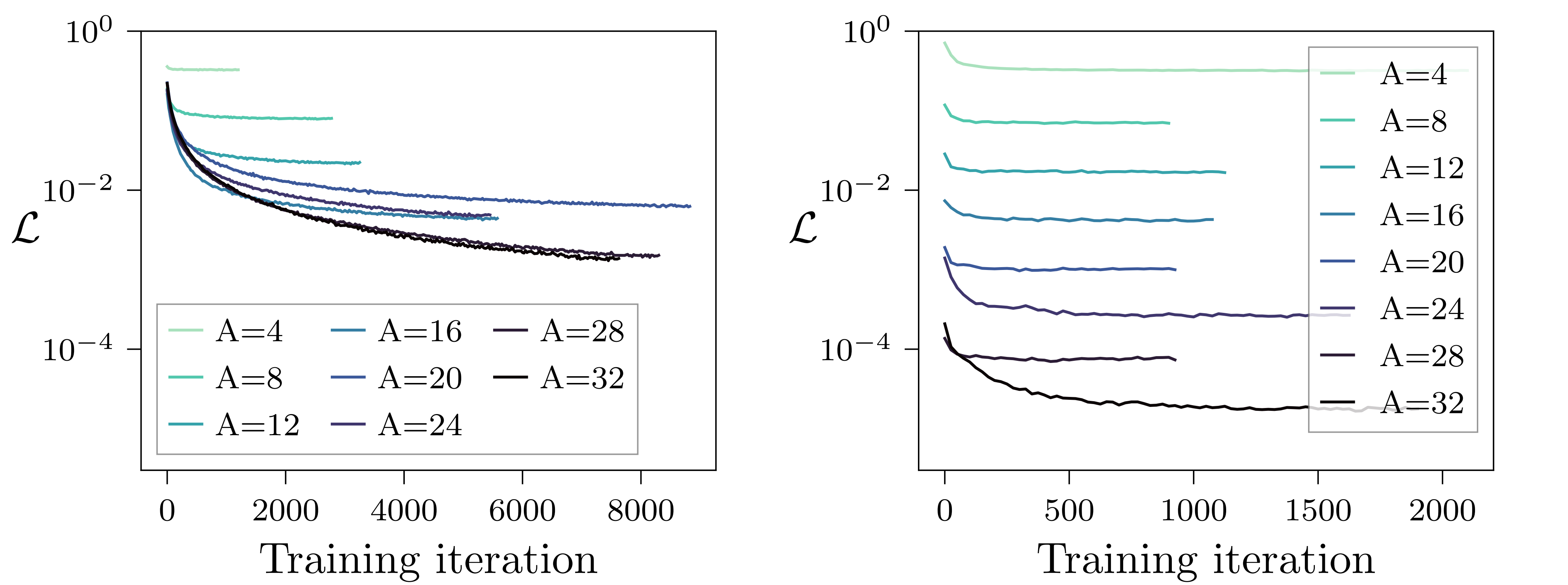
- Dynamic schedule reducing step size over once loss failed to improve sufficiently
- Optimisation halted once step size reduced twice
- Investigated adding various regularisation terms (not necessary)

$$\mathcal{L}_{\mathrm{L2}} \equiv \epsilon \sum_i |\lambda_i|^2 \qquad\qquad \mathcal{L}_{\mathrm{act}} \equiv \epsilon \frac{1}{Z} \int dx\, e^{-S(x)} \left| S(x) - \mathrm{Re}\, \tilde{S}(x) \right|$$

Contour deformation of path integrals

Machine learning ideas

- Transfer learning: use one observable to initialise deformation for other observables (area A → area A+1)
- SU(2) Wilson loops of various areas
- RH, smaller loop initialises larger loop (note horizontal scales)



Contour deformation for observables

Ongoing/future work

- Promising results in multiple theories
- Further exploration of possible/practical deformations
    - Fourier basis seems inefficient/hard to train
    - Possible ML approaches to defining deformation
- Extensions to higher dimensions
    - Requires working with links rather than plaquettes
    - In 2D, see similar performance in both formulations
- Extensions to fermionic theories
- Onward to QCD!