The Signal to Noise problem and Stochastic Automatic Differentiation

[G.C., A. Ramos, EPJC 85 (2025) 9, 1037]

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The Signal to Noise problem

- Physical properties – Euclidean time behavior of 2-point functions

$$C(x_0) = \sum_{\vec{x}} \left\langle O^\dagger(x) O(0) \right\rangle_{\mathrm{c}} = \sum_n |\langle 0|O|n\rangle|^2 e^{-E_n x_0} \xrightarrow[x_0 \to \infty]{} |\langle 0|O|i\rangle|^2 e^{-E_i x_0}$$

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  - energy levels, matrix elements
  - variance problem for large x_0

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- Parisi/Lepage argument for the variance [Parisi 1984; Lepage 1989]
  - Case of a scalar interpolator

$$\sigma^2(x_0) \propto \left\langle O^2(x_0) O^2(0) \right\rangle - \langle O(x_0) O(0) \rangle^2$$

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  - Signal to Noise

$$\frac{\text{error}[C(x_0)]}{C(x_0)} \xrightarrow[x_0 \to \infty]{} \frac{e^{E_0 x_0}}{\sqrt{N_{\text{conf}}}}$$

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- More generally: apply the same argument to the variance

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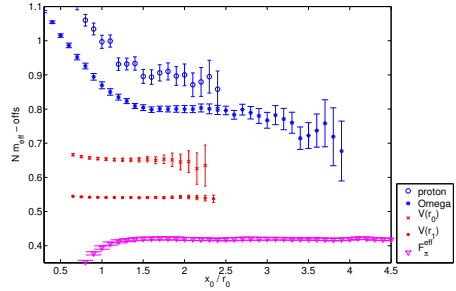
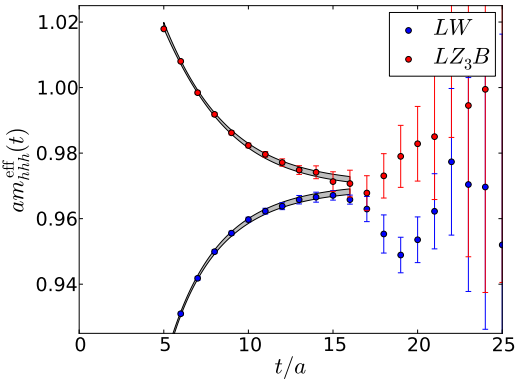
- Scalar: StN $\sim e^{E_0 x_0}$
- Pion: StN $\sim$ const.
- Proton: StN $\sim e^{(m_p - 3m_\pi)x_0}$



[Sommer 2014]

Solutions?

- Longstanding & ubiquitous problem in MC
- Typical solutions (smearing, GEVP, etc.)
  - Allow to extract information at earlier x_0
  - Excited state contamination
  - Do not solve the core of the StN problem



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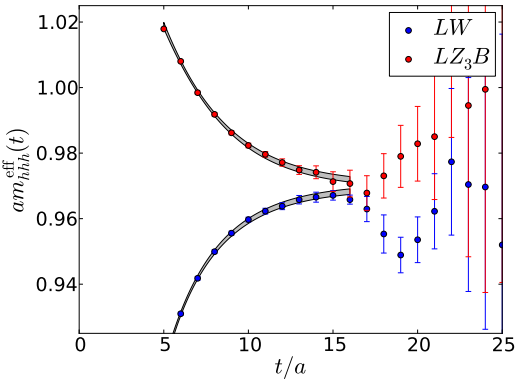

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Source:
2-point expectation value

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$$Z[J] = \int D\phi e^{-S[\phi]+JO(x_0=0)} \qquad \longrightarrow \qquad C(t) = \frac{\partial}{\partial J}\bigg|_{J=0} \langle O(x_0)\rangle$$

1-point function!

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- How to compute derivatives efficiently
  - Not with finite differences [Detmold 2005]
  - Stochastic automatic differentiation [G.C., A. Ramos, B. Zaldivar, 2024]

Automatic Differentiation

Automatic Differentiation – truncated polynomials

- Many flavour of AD – we choose truncated polynomials
- Power series $\mathcal{O}(\varepsilon^K)$

$$\tilde{x} \equiv x_0 + x_1\varepsilon + x_2\varepsilon^2 + \cdots + x_K\varepsilon^K$$

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- Define operations & elementary functions
  - Multiplication for $K = 2$

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- All operations are exact at each order

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- Compute Taylor expansion of any deterministic function

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- Practical example:

Code (Julia)

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julia> using FormalSeries
julia> f(x) = 1/(1-x)
julia> xs = Series((0.0,1.0,0.0,0.0,0.0))
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- This can be done for any existing program

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  - Fitting, Integration, ...
  - Error propagation and data analysis [ADerrors - A. Ramos 2018]
  - Ideal for systematic error estimates in, e.g., machine learning algorithms

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- Basis of Forward Automatic Differentiation

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Automatic Differentiation ruled out due to Stochastic elements

How to overcome this?

Extending Automatic Differentiation for Monte Carlo processes

Reweighting & Automatic Differentiation

[G.C., A. Ramos, B. Zaldivar, 2024]

Samples

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Expectation values w.r.t

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Reweighting & Automatic Differentiation

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- Expectation value with Taylor series coefficients

$$\frac{\sum_\alpha e^{S(\phi^\alpha,\theta)-S(\phi^\alpha,\tilde{\theta})} f(\phi)}{\sum_\alpha e^{S(\phi^\alpha,\theta)-S(\phi^\alpha,\tilde{\theta})}} = \sum_{n=0}^{K} f_n \varepsilon^n, \qquad f_n = \frac{1}{n!}\frac{\partial^n}{\partial\theta^n}\,\langle f(\phi)\rangle\Big|_\theta$$

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Conventional 2-point functions & Reweighting

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HMC & Automatic Differentiation (NSPT-inspired method)

1. Fictitious momenta π conjugate to ϕ

$$H(\phi, \pi) = \frac{1}{2}\pi^2 + S(\phi; \theta)$$

2. Solve EoM with initial random momenta $\pi(t = 0) \sim N(0, 1)$

$$\dot{\phi} = \frac{\partial H}{\partial \pi} = \pi, \qquad \dot{\pi} = -\frac{\partial H}{\partial \phi}$$

$$(\phi(0), \pi(0)) \longrightarrow (\phi(t), \pi(t))$$

3. Metropolis: Acc./Rej. with probability $e^{-\Delta H}$
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Cannot Acc./Rej.

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MC samples are truncated polynomials
$\tilde{\phi}^0, \tilde{\phi}^1, \ldots, \tilde{\phi}^N$

HMC & Automatic Differentiation

- HMC samples are truncated polynomials

$$\tilde{\phi} = \phi + \varepsilon\phi_{(1)}$$
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- Valid for similar sampling algorithm (Langevin, SMD, etc.)

Comparison & Change of variables

Reweighting

- $\{\phi^\alpha\}_{\alpha=1}^N \sim e^{-S(\phi;\theta)}$
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- Hamiltonian AD finds the exact transformation that leads to constant RW factors [G.C., A. Ramos, B. Zaldivar, 2024; G.C. 2025 (Thesis)]

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  - Exact – RW factors drop from the computation!

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  - Approximate – partially eliminate RW factors

4D Scalar field theory

$$S^{\text{4D}}_{\text{latt}}(\phi; m, \lambda) = \sum_x \left\{ \frac{1}{2} \sum_\mu [\phi(x+\mu) - \phi(x)]^2 + \frac{m^2}{2}\phi^2(x) + \lambda\phi^4(x) \right\}$$

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$$\dot{\tilde{\pi}}(x) = \frac{1}{2}\sum_\mu \left[\tilde{\phi}(x+\mu) + \tilde{\phi}(x-\mu)\right] - (4+\hat{m}^2)\tilde{\phi}(x) - 4\lambda\tilde{\phi}^3(x) + \epsilon\delta_{x_0,0}$$

HAD solution for the Signal to Noise problem

$$C(x_0)^{2-\text{point}} = \langle O(x_0) O(0) \rangle$$

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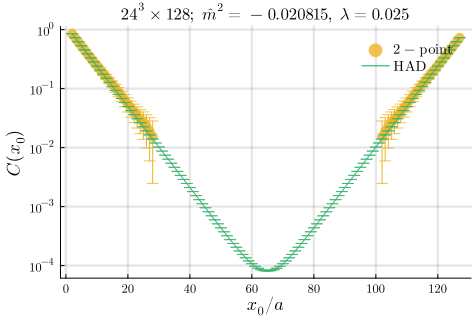

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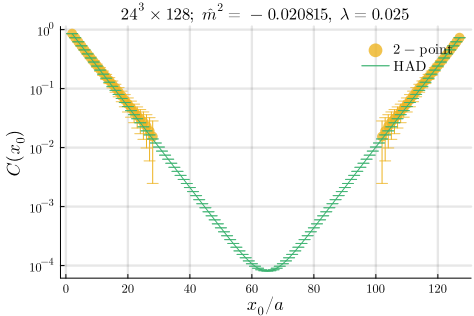

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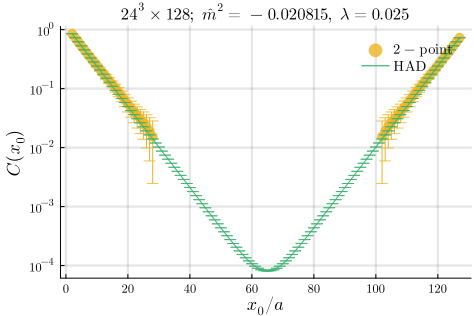

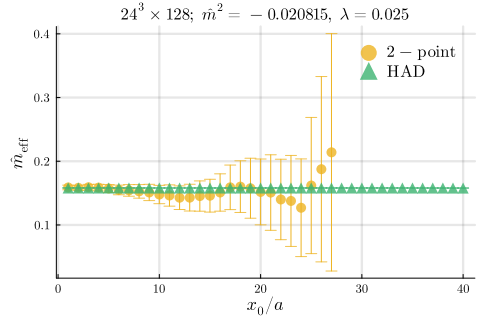

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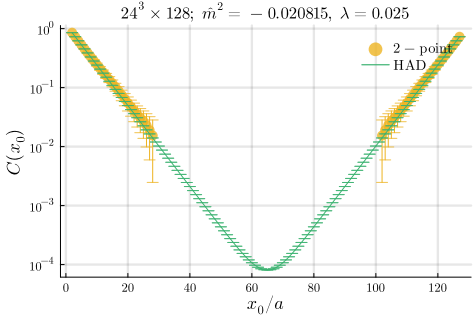

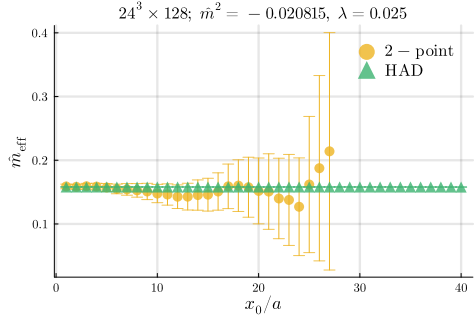

- HAD solves StN problem completely
  - convergence
  - compact variables, complex interpolators

Transformed Reweighting (TRW)

- Transformation?

$$S_{\text{latt}}(\phi_p; m) = \sum_p \phi_p^* \left[\sum_\mu \hat{p}_\mu^2 + m^2 \right] \phi_p + \mathcal{O}(\lambda), \qquad \hat{p} = 2\sin(ap/2)$$

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  - $\hat{m}_{\text{transf.}} = \hat{m}$
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- $\lambda \neq 0$: use the same (approximate) transformation
  - $\hat{m}_{\text{transf.}} = \hat{m}_R$

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- Conventional samples tuned to have $(am_R)^2 \sim 0.025$

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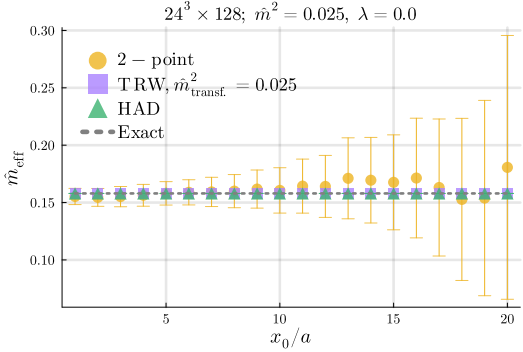

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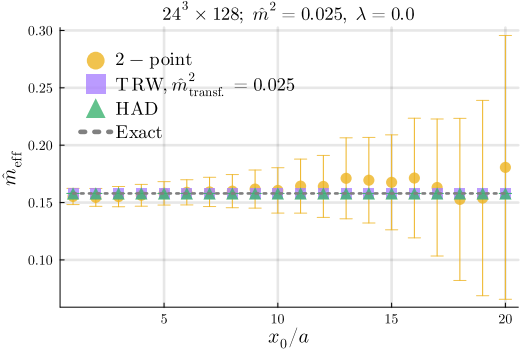

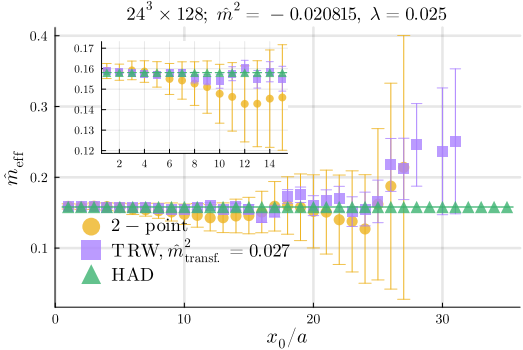

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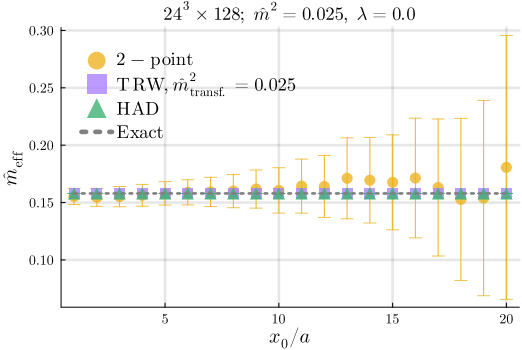

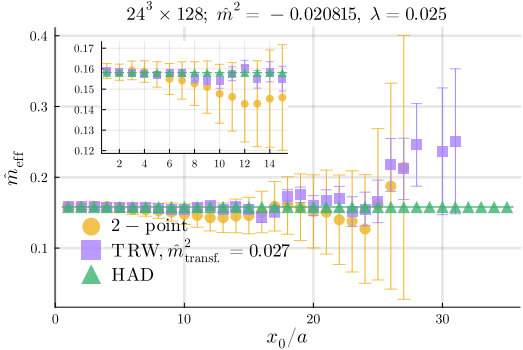

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- Approximate for $\lambda \neq 0$
- Still provides an improvement
  - But how do we choose $\hat{m}_{\text{transf.}}$?

Interacting case – transformation dependence

- Scan over $\hat{m}_{\text{trans.}}$ (cheap)

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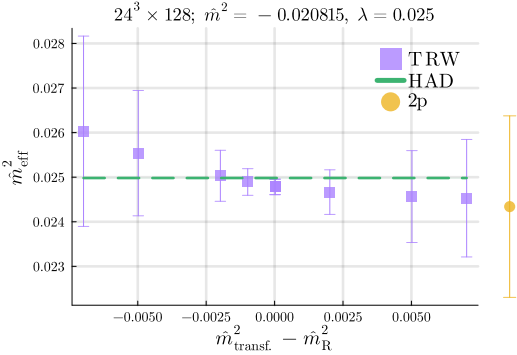

- Optimal $\hat{m}_{\text{trans.}} = \hat{m}_R$

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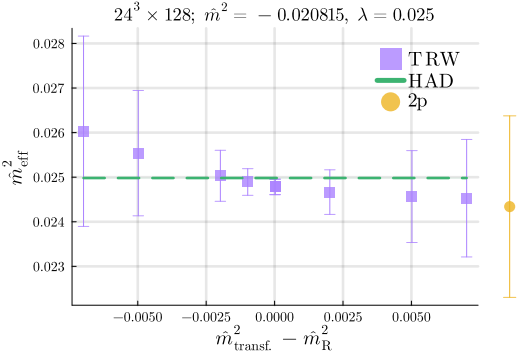

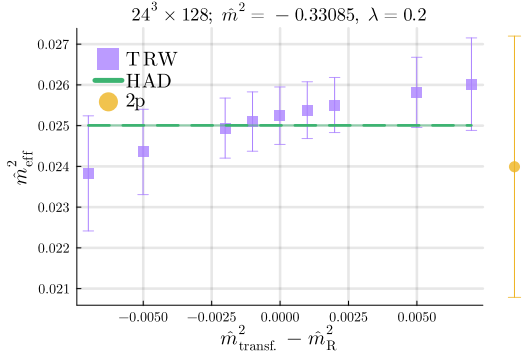

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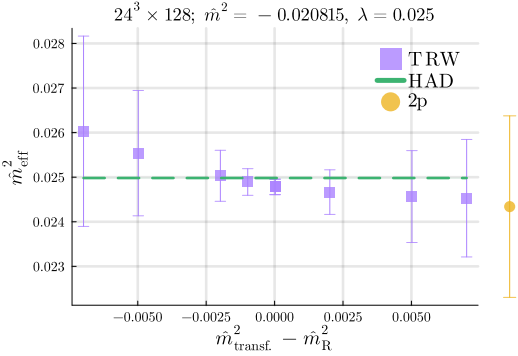

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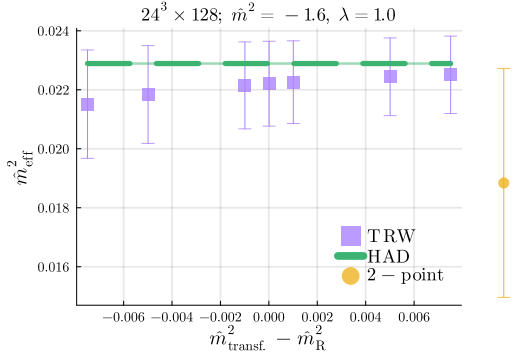

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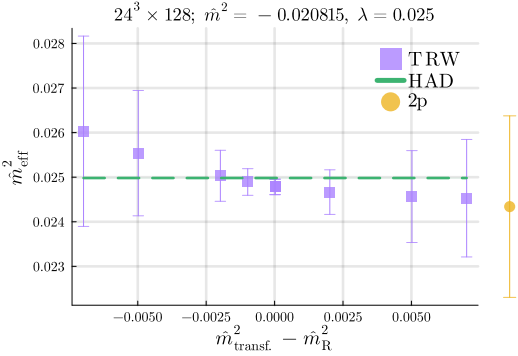

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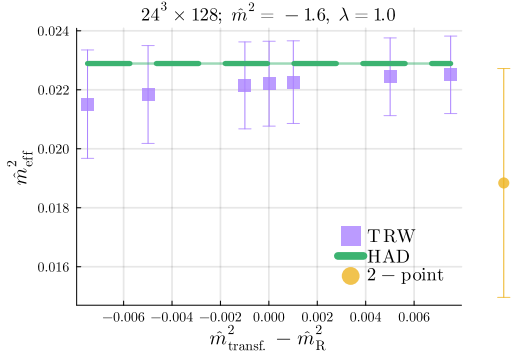

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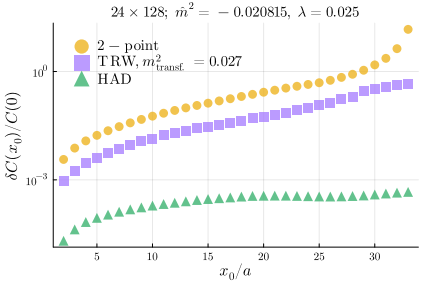

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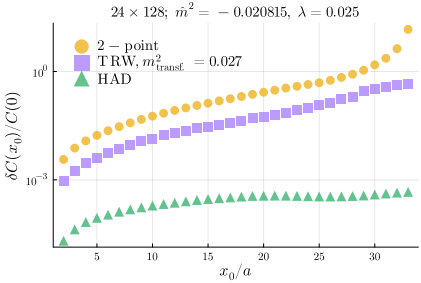

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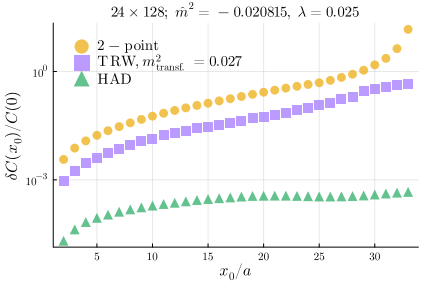

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Conclusions

- StN is an important problem for lattice field theory
- A change of perspective of the StN is possible:
  - The usual 2-point computation is a reweighting computation of a derivative
  - StN + RW leads to worse precision
  - Correlator as derivative of a 1PF – variance depends on how it is computed
- Key ingredient: Stochastic AD
  - Computes derivatives exactly
  - Single simulation, no need for finite-differences
- Hamiltonian method solves the StN exactly
  - not generally applicable (convergence, complex interpolators, etc.)
- Field transformations can reduce (or eliminate) the variance – solves the StN problem
  - Re-utilize samples – TRW is cheap
  - General (no problems with convergence, etc)

Future ideas

- Machine Learning to find changes of variables
  - P. Butti, G. C., A. Nada, L. Spatscheck
    Normalizing flows – attack the StN and not the sampling
    Parametrize transformation $f(\phi)$ as a norm. flow
    Reweighting factors $\longrightarrow$ KL divergence
  - Extensions for gauge theory
- Scalar-gauge theories
  - Scalar masses known to be noisy
  - Propagators are gauge-invariant (no gauge fixing needed)
  - Study the triviality problem

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$$f'(x) = \lim_{\varepsilon \to 0} \frac{f(x+\varepsilon) - f(x)}{\varepsilon}$$

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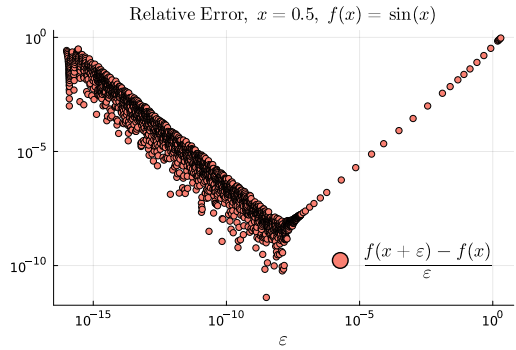

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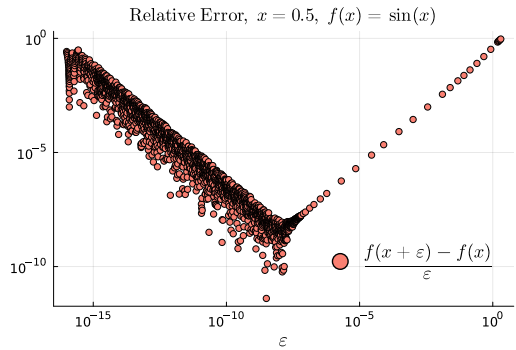

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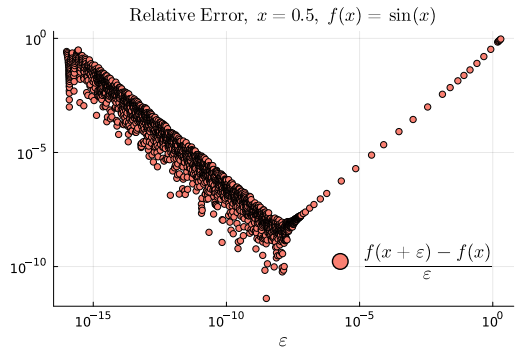

Comparison & Change of variables

Reweighting

- $\{\phi^\alpha\}_{\alpha=1}^N \sim e^{-S(\phi;\theta)}$
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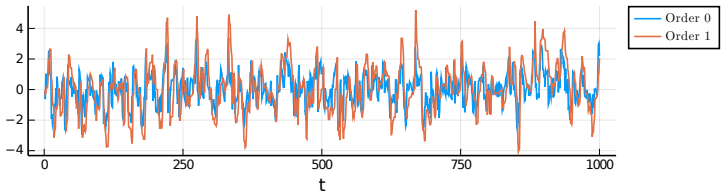

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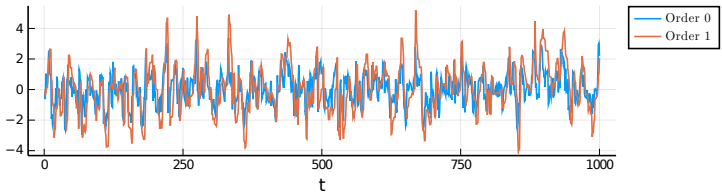

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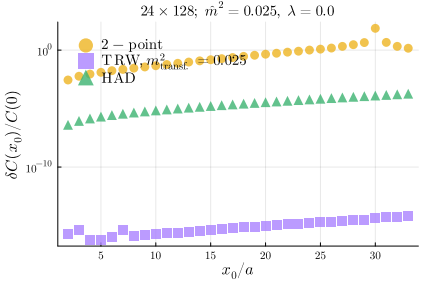

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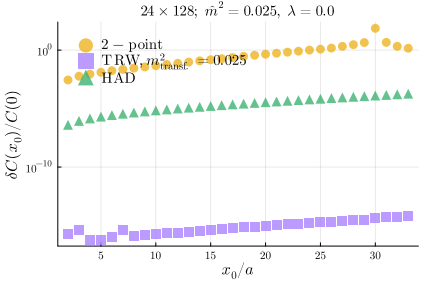

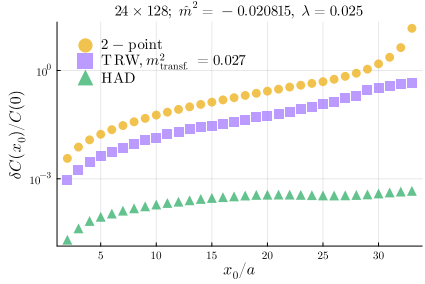

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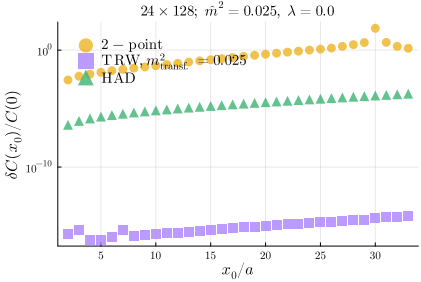

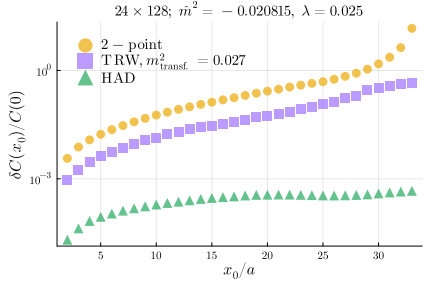

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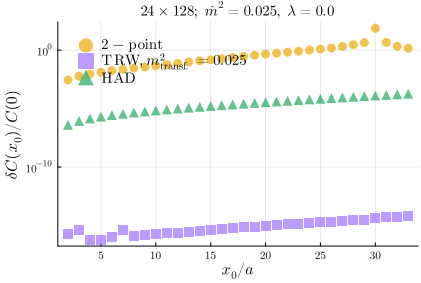

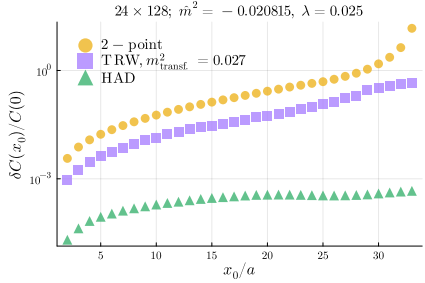

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