Tackling the Signal to Noise problem with Stochastic Automatic Differentiation

[G.C., A. Ramos, arXiv:2502.15570]

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The Signal to Noise problem

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

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

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

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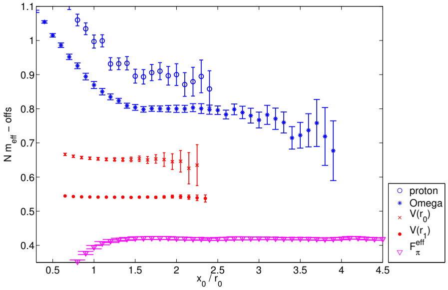

[Sommer 2014]

Solutions?

- Longstanding & ubiquitous problem in MC
- Typical solutions (smearing, GEVP, etc.)
  - Allow to extract information at earlier x_0
  - Excited state contamination
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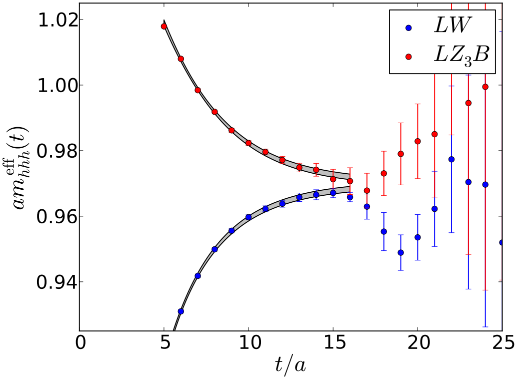

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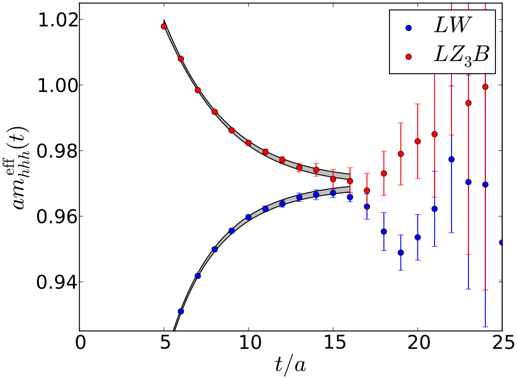

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Source:
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- How to compute derivatives efficiently
  - Not with finite differences [Detmold 2005]
  - Stochastic automatic differentiation [G.C., A. Ramos, B. Zaldivar, 2024]

Automatic Differentiation – truncated polynomials

- Extend AD to MC methods
- Power series $\mathcal{O}\left(\varepsilon^K\right)$

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

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Evaluate function at $\tilde{x} = x_0 + \varepsilon$ (Taylor theorem)

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Julia implementation:
https://igit.ific.uv.es/alramos/formalseries.jl

Code (Julia)

```
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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- Multiple expansions $\varepsilon \longrightarrow \varepsilon_i$
- Basis of Forward Automatic Differentiation

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Automatic Differentiation ruled out due to Stochastic elements

How to overcome this?

Reweighting & Automatic Differentiation

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

Samples

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

Expectation values w.r.t

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- Expectation value an Taylor series coefficients

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

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  - Conventional computation of a 2-point function can be seen as reweighting
  - Signal to Noise can be seen as a reweighting variance problem

HMC & Automatic Differentiation

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 $\pi(t=0) \sim N(0,1)$

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

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MC average as Taylor series

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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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- Find transformation that eliminates RW factors
  - Exact – RW factors drop from the computation!

$$-\tilde{S}_J[\tilde{\phi}] + \log\left|\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}\phi}\right| + S[\phi] = \text{const.}$$

  - Approximate – partially eliminate RW factors

4D Scalar field theory

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

$$\text{Operator:} \quad O(x_0) = \sum_{\vec{x}} \phi(x_0, \vec{x})$$

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

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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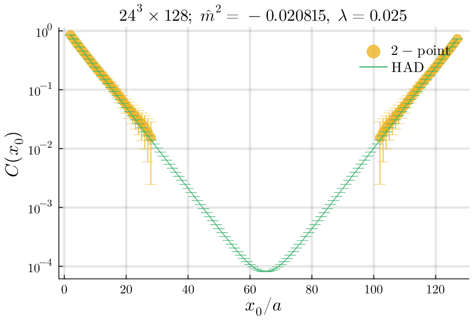

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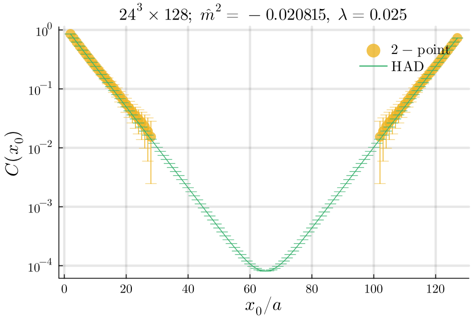

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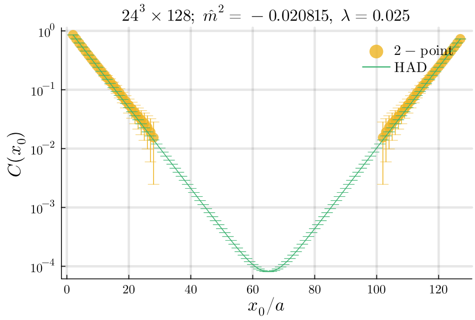

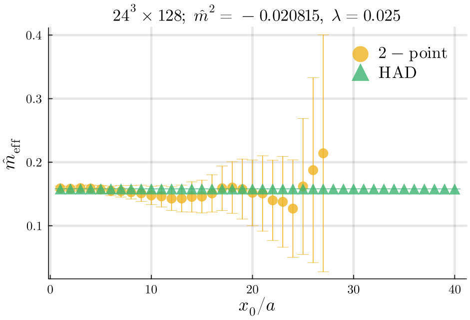

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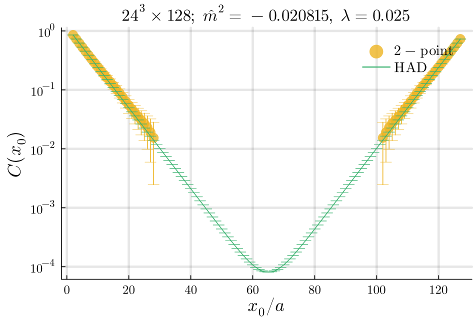

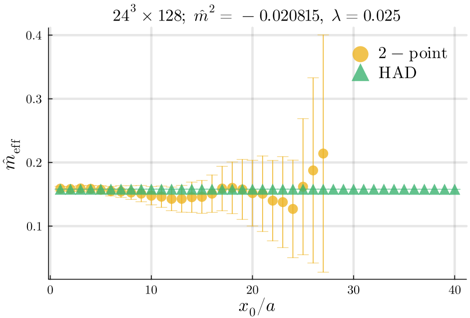

- HAD solves StN problem completely
  - convergence
  - compact variables, complex interpolators

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

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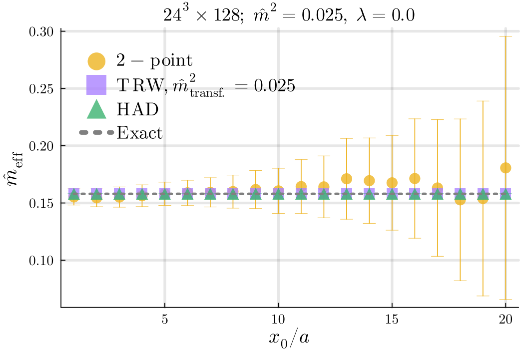

- Exact for $\lambda = 0$
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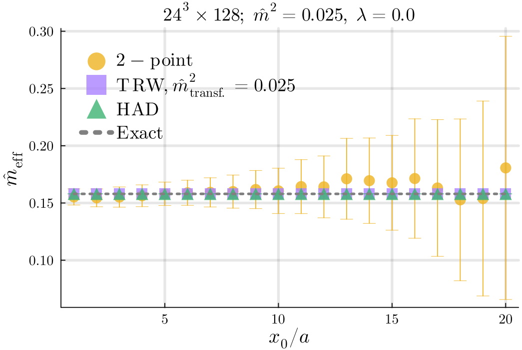

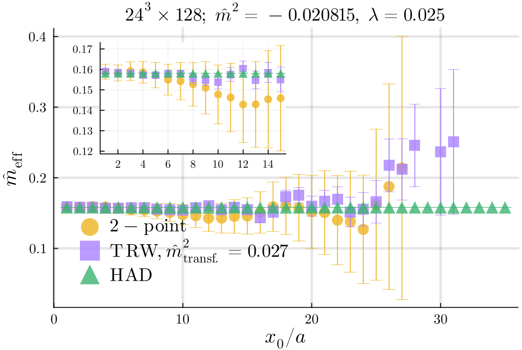

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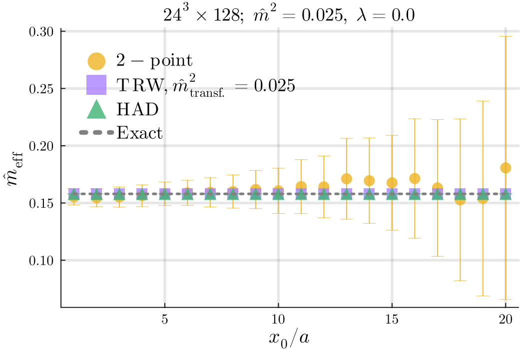

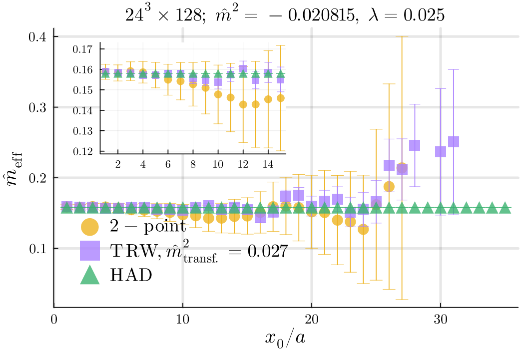

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- Approximate for $\lambda \neq 0$
- Still provides an improvement
  - But how do we choose $\hat{m}_{\text{transf.}}$?

Interacting case – transformation dependence

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

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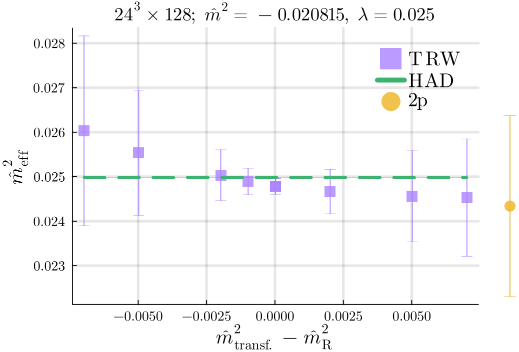

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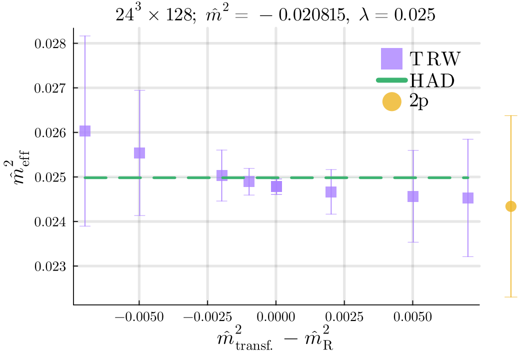

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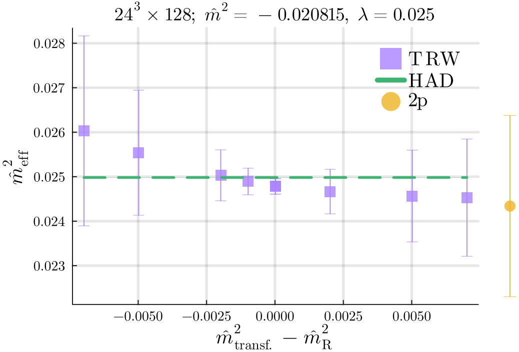

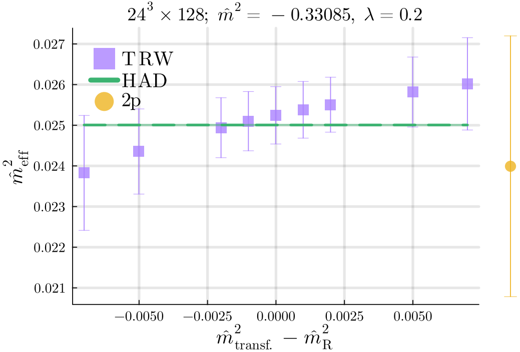

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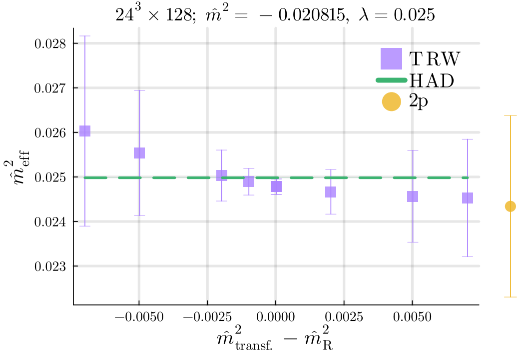

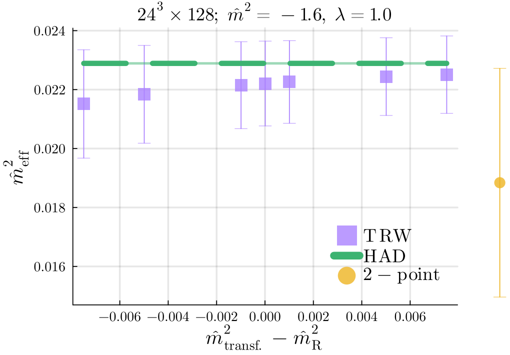

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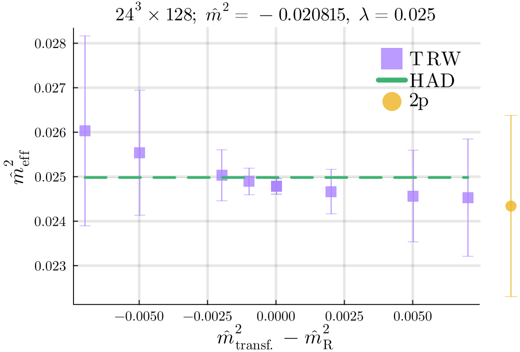

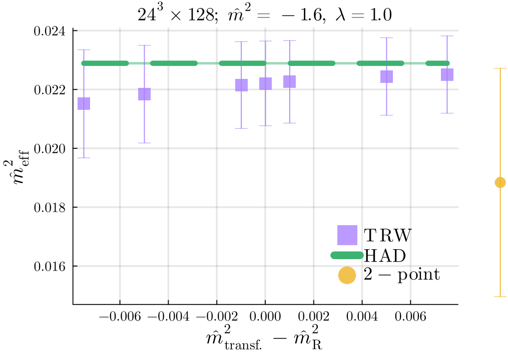

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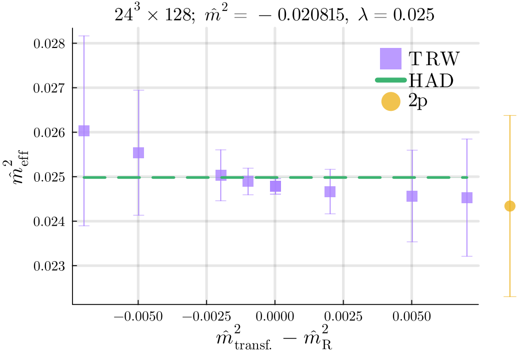

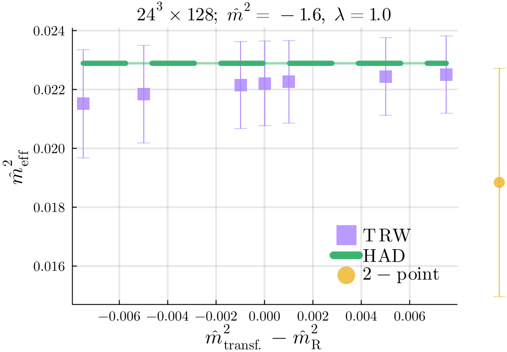

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- Precision degrades with λ
- $\hat{m}_{\text{trans.}} \neq \hat{m}_R$ still provides an improvement w.r.t. 2-point

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
  - the StN problem stems from the variance of the RW factors
  - Correlator as derivative of a 1-point function – variance depends on how it is computed (RW is just one possible way)
- 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)
  - Normalizing flows/Trivializing maps – attack the StN and not the sampling

Comparison & Change of variables

Reweighting

- $\{x^\alpha\}_{\alpha=1}^N \sim e^{-S(x;\theta)}$
- Weights $w^\alpha = e^{S(x^\alpha;m,\lambda)-S(x^\alpha;\tilde{m},\tilde{\lambda})}$ take into account dependence on parameters θ

HMC

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How are these methods related?

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Transformation:	$y^\alpha = \sigma x^\alpha$,	$\{y^\alpha\} \sim p_\sigma$
$\sigma^* = 1 \longrightarrow \sigma$	$w^\alpha(y) = y -$ independent	'No Reweighting'

Comparison & Change of variables

$$y^\alpha = \sigma x^\alpha$$

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What about HMC?
Equations of motion

$$\ddot{x}_0 = -\frac{x_0}{\sigma^2}, \qquad \langle x_0 \rangle$$

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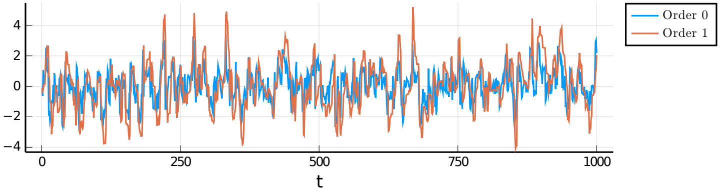

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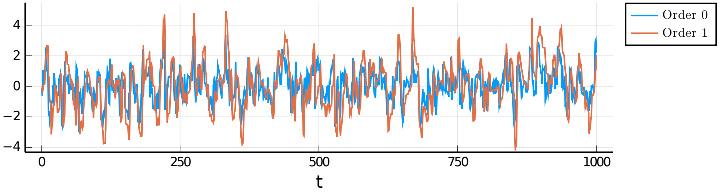

- Hamiltonian method finds the change of variables $x \to \tilde{y}$ that lead to constant reweighting factors