Automatic differentiation for stochastic processes

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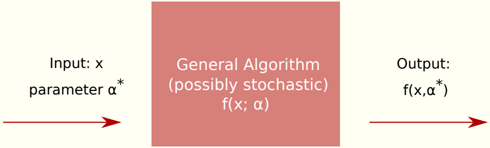
Objective



$$\frac{\partial \text{output}}{\partial \text{input}}$$

Algorithm involves a stochastic element:

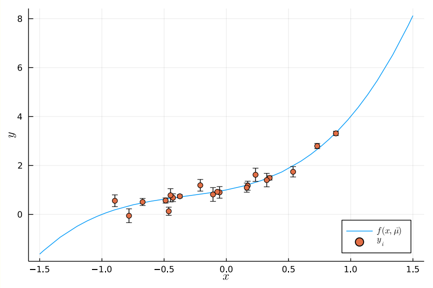
- Cannot be decomposed into basic operations
- How to extend Automatic Differentiation (AD)?
  - Multiple simulations
  - Reweighting
  - Generalized Series expansions

Examples:

- Bayesian inference with Monte-Carlo integration
- QED+QCD isospin breaking effects - Reweighting method [RM123 Collaboration]
- ...

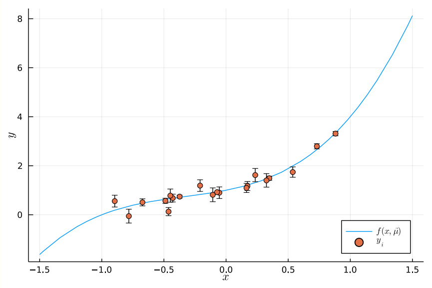
Bayesian inference as the toy model

Dataset: $D = \{x_i, y_i\}_{i=1}^{N}$



Basics of Bayesian inference

Dataset: $D = \{x_i, y_i\}_{i=1}^{N}$



- Assumes the data is obtained from a distribution:
  - $N(y_i|f(x_i,\vec{\phi}),\sigma_i)$
  - $f(x,\vec{\phi}) = \sum_{j=0}^{3}\phi_j x^j$
- Likelihood function:

$$p(\vec{y}|X,\vec{\phi}) = \prod_{i=1}^{N} N(y_i|f(x_i,\vec{\phi}),\sigma_i)$$

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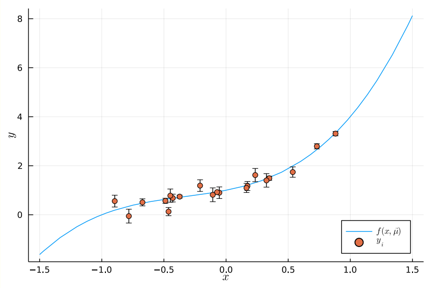

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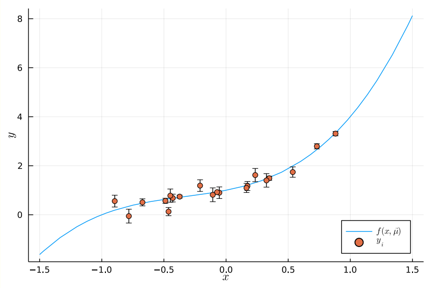

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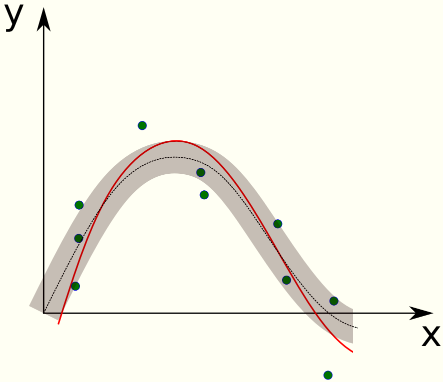
Bayes Theorem:

$$p(\vec{\phi}|D) \propto p(\vec{y}|X, \vec{\phi}) p(\vec{\phi})$$

Predictive distribution:

$$p(y_*|x_*, D) = \int \prod_i d\phi_i p(y_*|x_*, \vec{\phi}) \color{red}{p(\vec{\phi}|D)}$$

- Monte-Carlo integration:
  - Sample from $p(\vec{\phi}|D)$: $\{\phi_{i,j}\}_{j=1}^{N_{iter}}$
  - $\frac{1}{N}\sum_{j=1}^{N} p(y_*|x_*, \phi_{i,j})$
- Hybrid Monte-Carlo
  - Omelyan 4th order $\mathcal{O}(\varepsilon^4)$



Hamiltonian and Equations of Motion

$$S(\vec{\phi}) \propto -\log\Big(p(\vec{\phi}|D)\Big)$$

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$$\boxed{\mathrm{H}(\vec{\phi},\vec{\pi}) = \frac{\vec{\pi}^2}{2} + \frac{1}{2\sigma_{\mathrm{p}}^2}(\vec{\phi}-\vec{\mu})^2 + \sum_{\mathrm{i}=1}^{\mathrm{N}} \frac{1}{2}\left(\frac{\mathrm{y_i} - \mathrm{f}(\mathrm{x_i},\vec{\phi})}{\sigma_{\mathrm{i}}}\right)^2}$$

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Equations of motion:

$$\dot{\phi}_{\mathrm{j}} = \pi_{\mathrm{j}},$$

$$\dot{\pi}_{\mathrm{j}} = -\frac{1}{\sigma_{\mathrm{p}}^2}(\phi_{\mathrm{j}} - \mu_{\mathrm{j}}) + \sum_{\mathrm{i}=0}^{\mathrm{N}} \frac{1}{\sigma_{\mathrm{i}}^2}\left(\mathrm{y_i} - \mathrm{f}(\mathrm{x_i}, \vec{\phi})\right)(\mathrm{x_i})^{\mathrm{j}}$$

Estimate dependence on an input parameter

$$\frac{\partial \mathrm{output}}{\partial \mathrm{input}} \longrightarrow \frac{\partial \mathcal{O}}{\partial \sigma_{\mathrm{p}}} = \frac{\partial}{\partial \sigma_{\mathrm{p}}} \int \prod_{\mathrm{i}} \mathrm{d}\phi_{\mathrm{i}} \mathcal{O} \mathrm{p}(\vec{\phi}|\mathrm{D})$$

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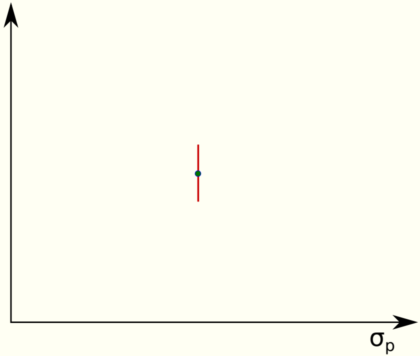

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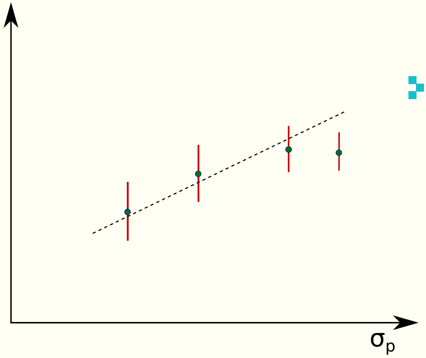

- Simulate multiple times?
  - Costly
  - Poor scaling with # of parameters
  - Discrete result
  - Step-size dependent

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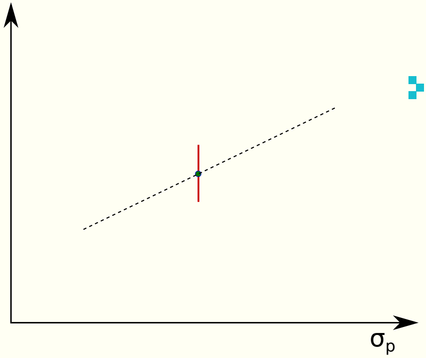

- Automatic Differentiation
  - MC integration not decomposable into basic operations

Typical approach - REWEIGHTING

$$\langle \mathcal{O} \rangle_{\mathrm{g}} = \frac{\left\langle \mathrm{e}^{-\Delta \mathrm{S}} \mathcal{O} \right\rangle_0}{\left\langle \mathrm{e}^{-\Delta \mathrm{S}} \right\rangle_0} = \langle \mathcal{O} \rangle_{\mathrm{g}} - \mathrm{g} \left\langle \mathrm{S}_1 \mathcal{O} \right\rangle_0^{\mathrm{con}}$$

Average in $\mathrm{S}_0 + \mathrm{g}\mathrm{S}_1$

Samples from S_0

Requires connected component

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Average in $S_0 + gS_1$

Samples from S_0

Requires connected component

- Averages with 'incomplete' action – recycle ensembles
  - QCD w/ degenerate quark masses
- Weighted average equivalent to full theory
- Requires subtraction of disconnected component
  - Noisy!
  - Systematic error if ignored

series expansion (NSPT)

Problem: How predictions change when changing σ_{p} around σ_{p}^{*}?

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Solution: Expand input fields/parameters around σ_p^*!

$$\phi_\mathrm{i}(\sigma_\mathrm{p}) = \sum_\mathrm{n} \phi_\mathrm{i}^{(\mathrm{n})}(\sigma_\mathrm{p} - \sigma_\mathrm{p}^*)^\mathrm{n} = \sum_\mathrm{n} \left.\frac{\partial^\mathrm{n}\phi_\mathrm{i}}{\partial\sigma_\mathrm{p}^\mathrm{n}}\right|_{\sigma_\mathrm{p}=\vec{\sigma}_\mathrm{p}^*}(\sigma_\mathrm{p} - \sigma_\mathrm{p}^*)^\mathrm{n}.$$

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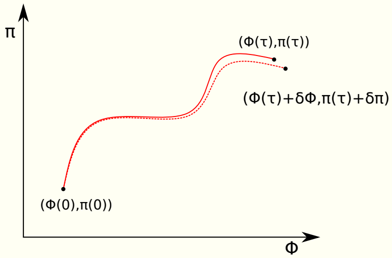
$$\dot{\phi}_\mathrm{i}^{(\mathrm{n})} = \left(\frac{\partial H}{\partial \pi_\mathrm{i}}\right)^{(\mathrm{n})} = \pi_\mathrm{i}^{(\mathrm{n})}$$

$$\dot{\pi}_\mathrm{i}^{(\mathrm{n})} = -\left(\frac{\partial H}{\partial \phi_\mathrm{i}}\right)^{(\mathrm{n})}$$

$$\phi_{\mathrm{i},0}^{(0)} \rightarrow \phi_{\mathrm{i},1}^{(0)} \rightarrow \phi_{\mathrm{i},2}^{(0)} \rightarrow \phi_{\mathrm{i},3}^{(0)} \rightarrow \phi_{\mathrm{i},4}^{(0)} \rightarrow$$

$$\phi_{\mathrm{i},0}^{(1)} \rightarrow \phi_{\mathrm{i},1}^{(1)} \rightarrow \phi_{\mathrm{i},2}^{(1)} \rightarrow \phi_{\mathrm{i},3}^{(1)} \rightarrow \phi_{\mathrm{i},4}^{(1)} \rightarrow$$

...



Numerical Implementation

- Overload operators (+, -, *,...) and basic function $(\sin, \cos, \log, ...)$ for the expansion objects:
  - Operations act order by order automatically
  - Exact to each order
  - 'Recicle' code

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Cannot perform Metropolis step to correct finite ε effects:

$$\Delta H^{(n)} \neq 0$$

$$H(\phi, p) = \sum_n H^{(n)} \delta\sigma_p^n$$

$$\dot{\phi}_i^{(n)} = \left(\frac{\partial H}{\partial p_i}\right)^{(n)},$$

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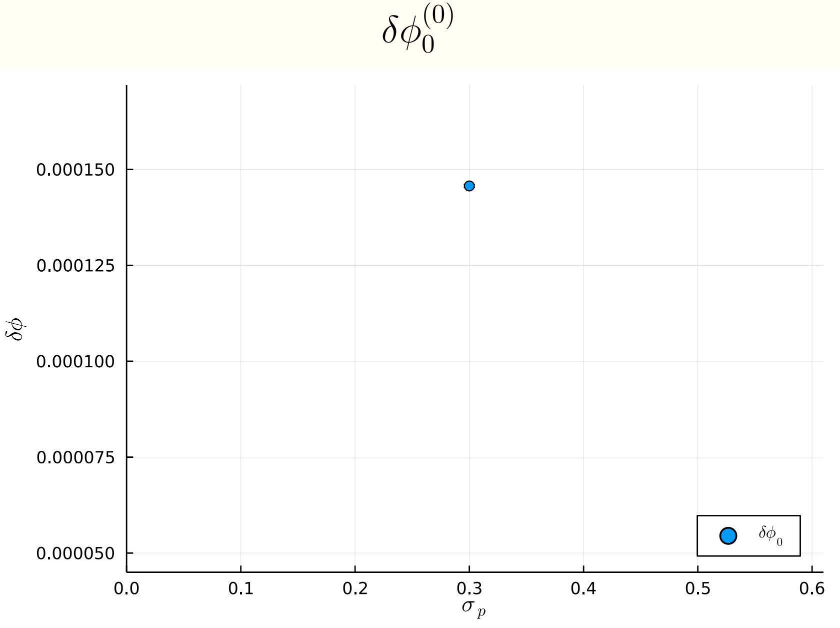
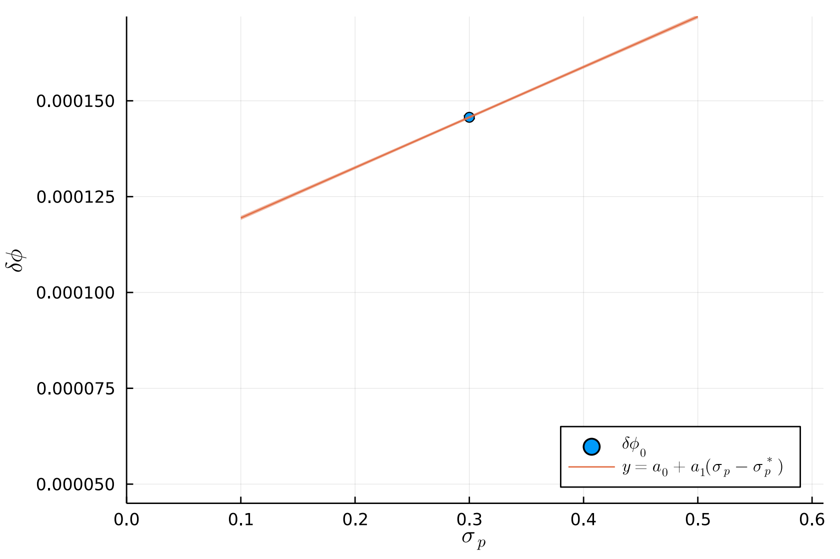
$$\langle \mathcal{O} \rangle = \langle \mathcal{O} \rangle^{(0)} + \langle \mathcal{O} \rangle^{(1)} (\sigma_p - \sigma_p^*) + \langle \mathcal{O} \rangle^{(2)} (\sigma_p - \sigma_p^*)^2 + ...$$

results

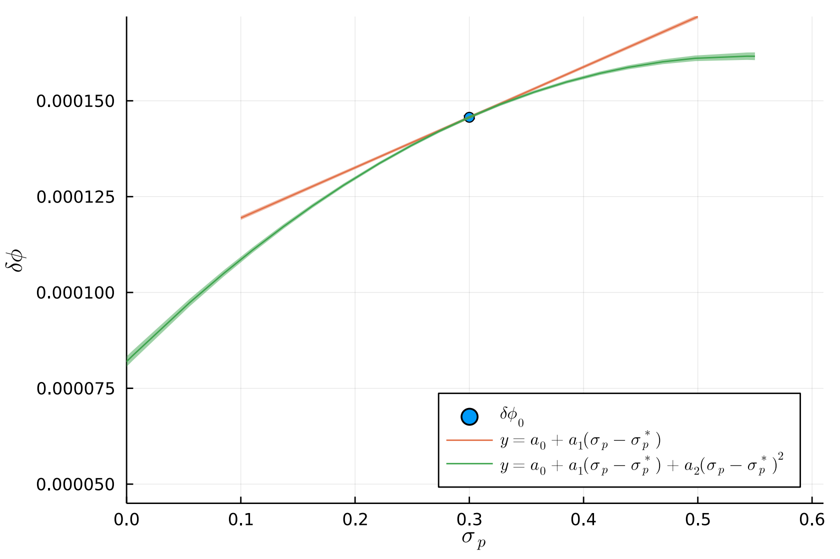
Local variance reconstruction



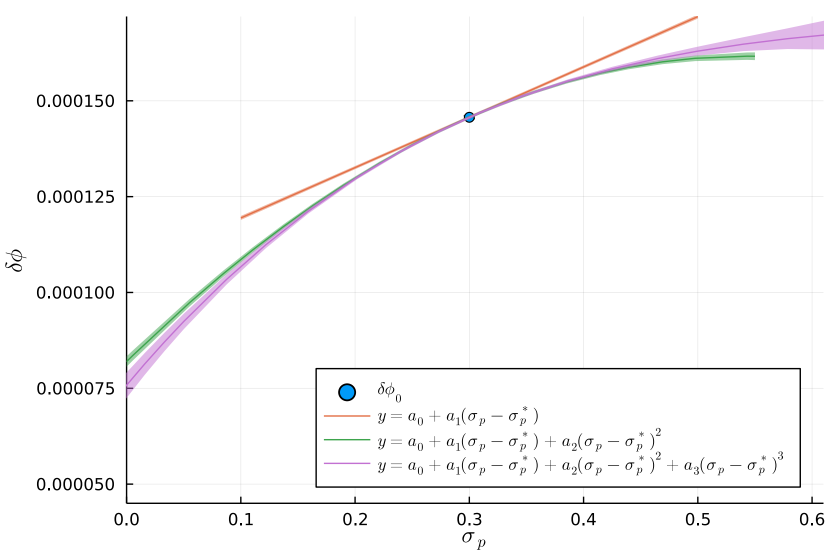
$$\delta\phi_0^{(0)} + \delta\phi_0^{(1)}(\sigma_{\mathrm{p}} - 0.3)$$



$$\delta\phi_0^{(0)} + \delta\phi_0^{(1)}(\sigma_\mathrm{p} - 0.3) + \delta\phi_0^{(2)}(\sigma_\mathrm{p} - 0.3)^2$$



$$\delta\phi_0^{(0)} + ... + \delta\phi_0^{(3)}(\sigma_\mathrm{p} - 0.3)^3$$



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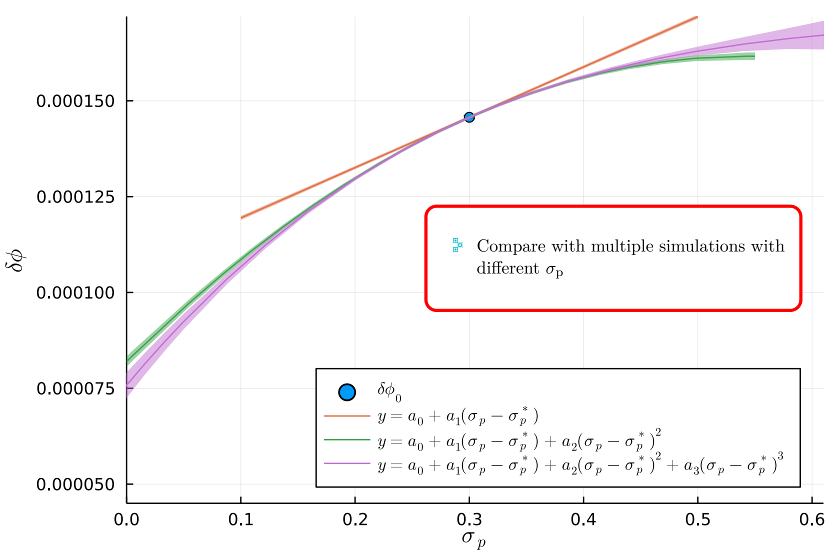
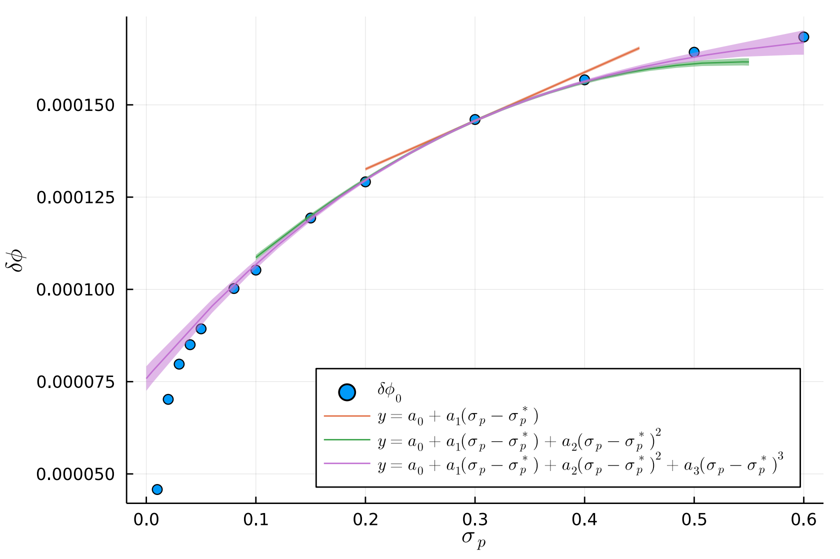


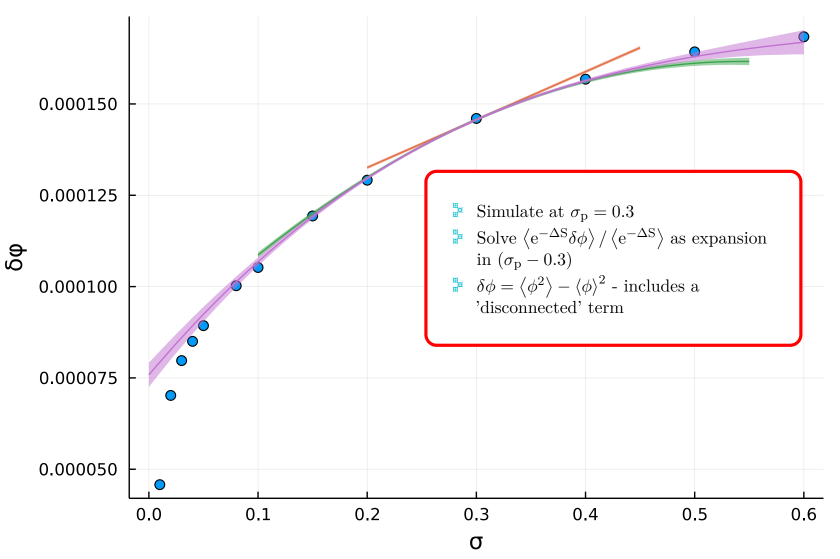
- Compare with multiple simulations with different σ_p

Local variance reconstruction

$$\delta\phi_0^{(0)} + ... + \delta\phi_0^{(3)}(\sigma_{\mathrm{p}} - 0.3)^3$$

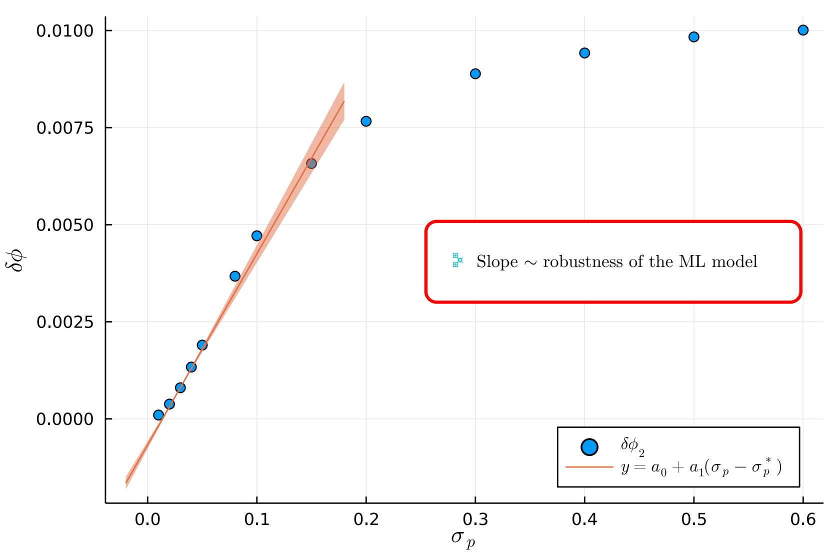


Use Series expansion in Reweighting!

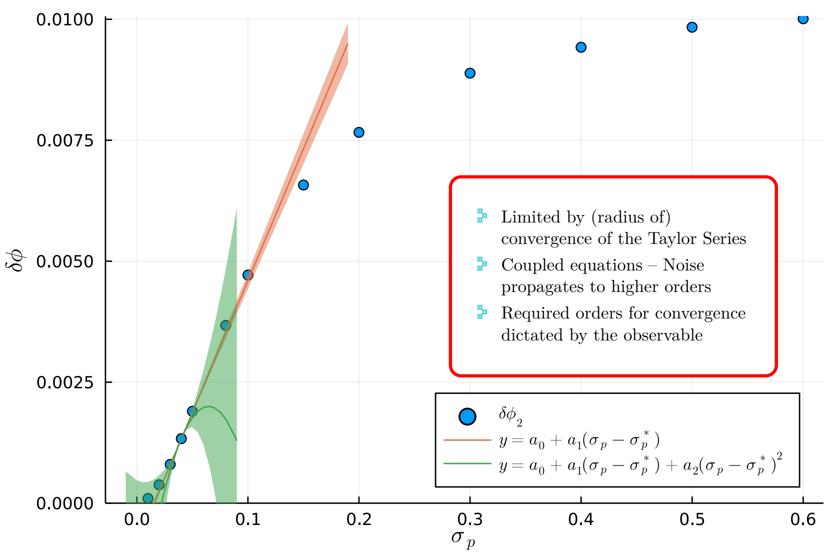


- Simulate at $\sigma_{\mathrm{p}} = 0.3$
- Solve $\left\langle \mathrm{e}^{-\Delta \mathrm{S}} \delta\phi \right\rangle / \left\langle \mathrm{e}^{-\Delta \mathrm{S}} \right\rangle$ as expansion in $(\sigma_{\mathrm{p}} - 0.3)$
- $\delta\phi = \left\langle \phi^2 \right\rangle - \left\langle \phi \right\rangle^2$ - includes a 'disconnected' term

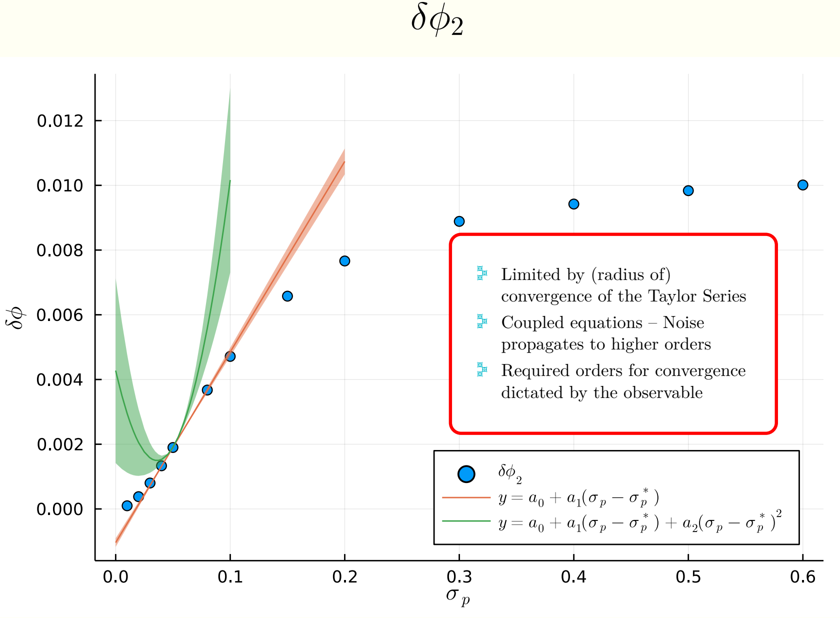
$\delta\phi_2$


0.0100
0.0075
0.0050
0.0025
0.0000
$\delta\phi$
0.0
0.1
0.2
0.3
0.4
0.5
0.6
σ_p
Slope ~ robustness of the ML model
$\delta\phi_2$
$y = a_0 + a_1(\sigma_p - \sigma_p^*)$

$\delta\phi_2$



- Limited by (radius of) convergence of the Taylor Series
- Coupled equations – Noise propagates to higher orders
- Required orders for convergence dictated by the observable



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Local variance reconstruction - Convergence

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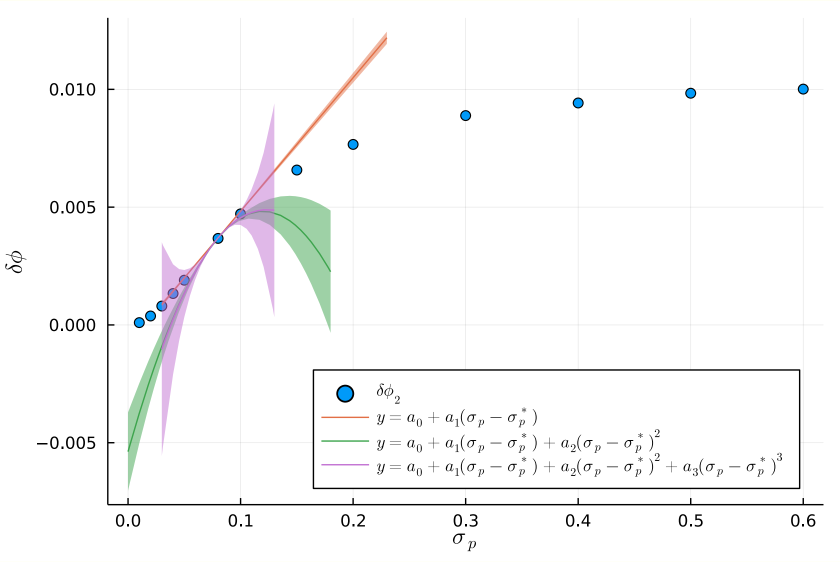

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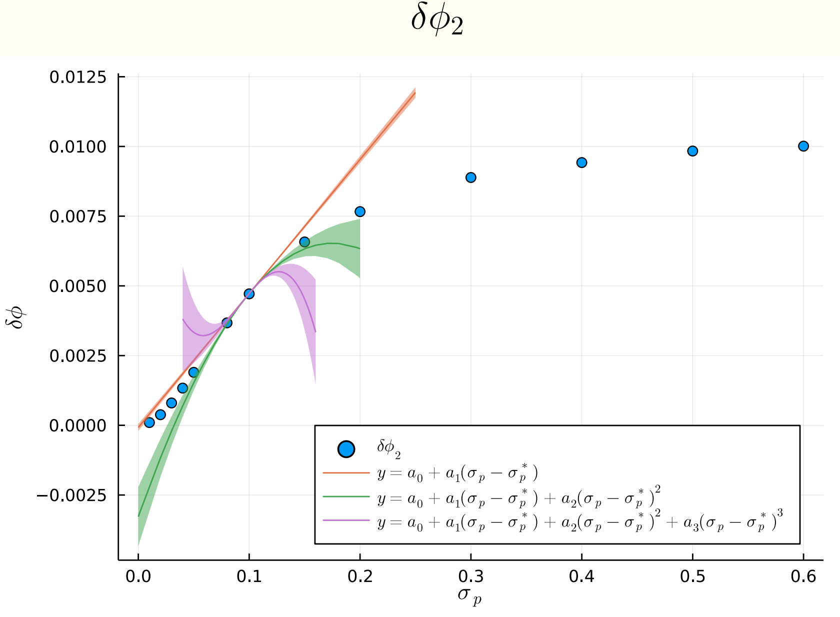

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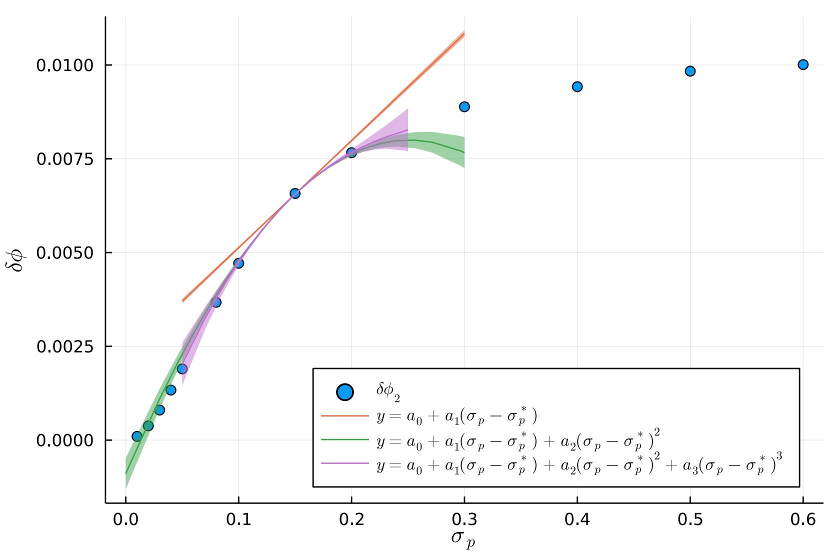
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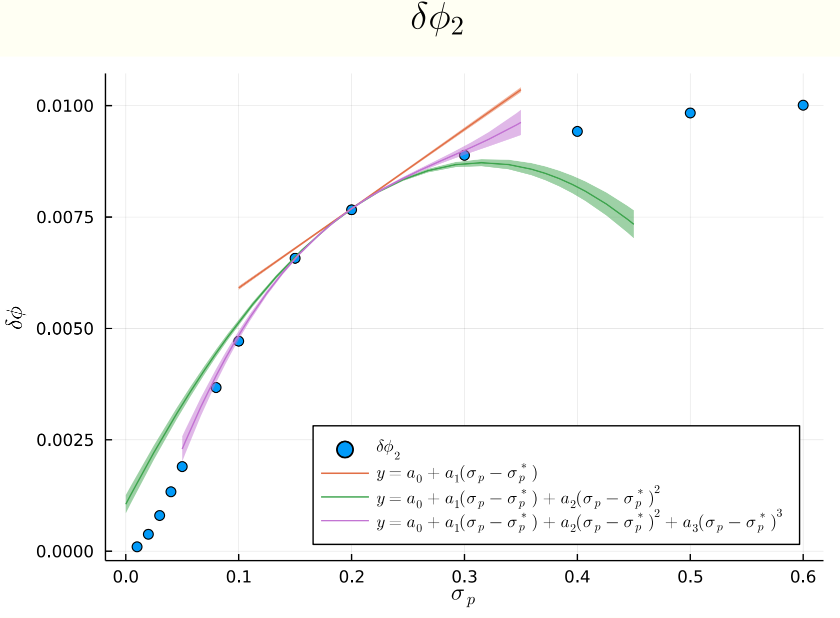

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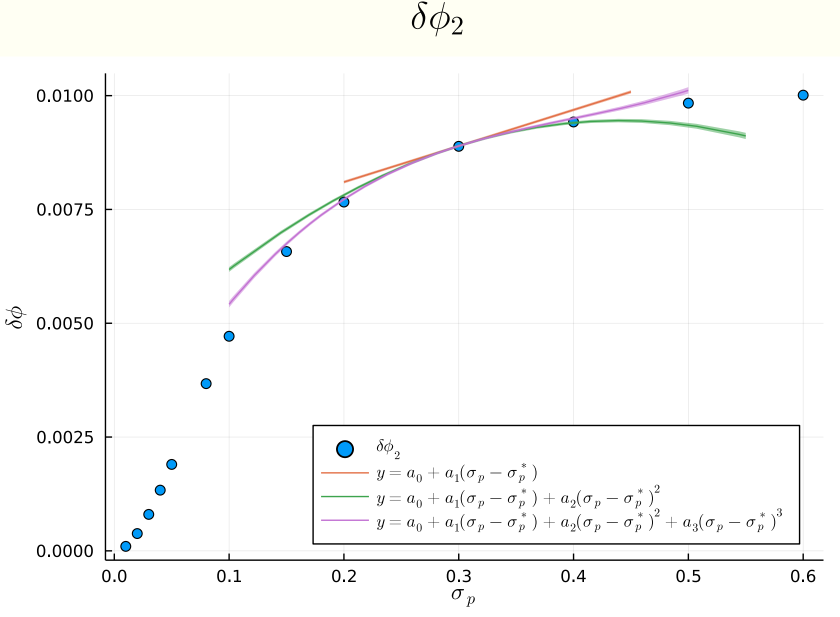

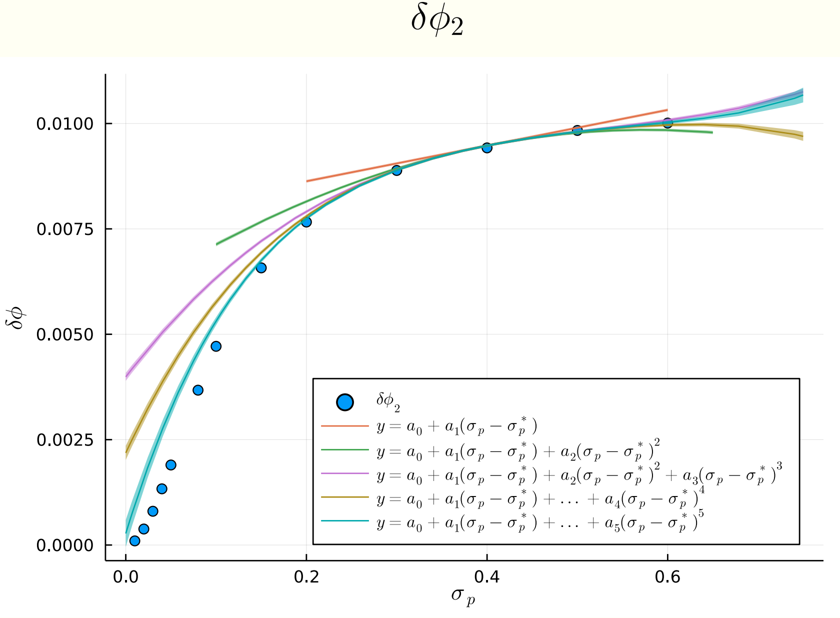
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$y = a_0 + a_1(\sigma_p - \sigma_p^*) + \ldots + a_5(\sigma_p - \sigma_p^*)^5$

Summary

Message for ML:

- A single simulation allows to estimate how the predictions are affected by hyper-parameters of the model;
  - Robustness of the model/assumptions
  - Allows to choose the optimal hyper-parameter
  - Estimate systematic uncertainty associated with this choice
- Not restricted to the prior – can be applied to any hyper-parameter of the model
- Allows to be used simultaneously for various hyper-parameters
- Equally good results for a Neural-Network (non-linear!)

Summary

Message for Lattice:

- No need of connected component $\longrightarrow$ increased precision
- Corrections of orders $n > 1$;
- Suitable for gauge theories:
  - Gauge suppression reduces fluctuations
  - QCD strongly coupled + QED $g_{QED} \neq 0$ correction: Expand in g_{QED}

extra

Stochastic Quantization – basics

The basic idea of stochastic quantization is to consider the Euclidean path integral measure $\exp\{-(1/\hbar)\, S_E\}/\int D\phi \exp\{-(1/\hbar)\, S_E\}$ *as the stationary distribution of a stochastic process.*

[Parisi1980ys] [DAMGAARD1987227]

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Start with Euclidean Field Theory

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Introduce a fictitious stochastic time

$$\phi(x) \rightarrow \phi(x, t)$$

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Introduce a fictitious stochastic time

$$\phi(\mathrm{x}) \to \phi(\mathrm{x}, \mathrm{t})$$

Choose stochastic dynamics in fictitious time, e.g. Langevin Equation

$$\frac{\mathrm{d}\phi(\mathrm{x}, \mathrm{t})}{\mathrm{dt}} = -\frac{\partial \mathrm{S}[\phi]}{\partial \phi(\mathrm{x}, \mathrm{t})} + \eta(\mathrm{x}, \mathrm{t})$$

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[Parisi1980ys] [DAMGAARD1987227]

Start with Euclidean Field Theory

$$\langle \mathrm{O}[\phi] \rangle = \frac{\int \mathrm{D}\phi \mathrm{O}[\phi] \mathrm{e}^{-\mathrm{S}[\phi]}}{\int \mathrm{D}\phi \mathrm{e}^{-\mathrm{S}[\phi]}}$$

Introduce a fictitious stochastic time

$$\phi(\mathrm{x}) \to \phi(\mathrm{x}, \mathrm{t})$$

Choose stochastic dynamics in fictitious time, e.g. Langevin Equation

$$\frac{\mathrm{d}\phi(\mathrm{x}, \mathrm{t})}{\mathrm{dt}} = -\frac{\partial \mathrm{S}[\phi]}{\partial \phi(\mathrm{x}, \mathrm{t})} + \eta(\mathrm{x}, \mathrm{t})$$

Gaussian noise:

$$\langle \ldots \rangle_\eta = \frac{\int \mathrm{D}\eta \ldots \mathrm{e}^{-\frac{1}{4} \int \mathrm{dzd}\tau \eta^2(\mathrm{z}, \tau)}}{\int \mathrm{D}\eta \mathrm{e}^{-\frac{1}{4} \int \mathrm{dzd}\tau \eta^2(\mathrm{z}, \tau)}}$$

$$\left\langle \eta(\mathrm{x}, \mathrm{t}) \eta(\mathrm{y}, \mathrm{t}') \right\rangle_\eta = 2\delta(\mathrm{x} - \mathrm{y}) \delta(\mathrm{t} - \mathrm{t}')$$

Key idea:

$$\langle \mathrm{O}[\phi_\eta(\mathrm{x}_1,\mathrm{t})...\phi_\eta(\mathrm{x}_\mathrm{n},\mathrm{t})]\rangle_\eta \rightarrow_{\mathrm{t}\rightarrow\infty} \langle \mathrm{O}[\phi(\mathrm{x}_1)...\phi(\mathrm{x}_\mathrm{n})]\rangle$$

Equal-time correlation functions

Stochastic Quantization – Convergence

$$\langle \mathrm{O}[\phi_\eta] \rangle_\eta = \frac{\int \mathrm{D}\eta \mathrm{O}[\phi_\eta] \mathrm{e}^{-\frac{1}{4}\int \mathrm{dzd}\tau \eta^2(\mathrm{z},\tau)}}{\int \mathrm{D}\eta \mathrm{e}^{-\frac{1}{4}\int \mathrm{dzd}\tau \eta^2(\mathrm{z},\tau)}} = \int \mathrm{D}\phi \mathrm{O}[\phi] \mathrm{P}(\phi, \mathrm{t})$$

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Proof by the Fokker-Planck equation:

$$\dot{\mathrm{P}}(\phi, \mathrm{t}) = \int \mathrm{dz} \frac{\delta}{\delta\phi(\mathrm{z})} \left(\frac{\delta \mathrm{S}}{\delta\phi(\mathrm{z})} + \frac{\delta}{\delta\phi(\mathrm{z})} \right) \mathrm{P}(\phi, \mathrm{t})$$

[FLORATOS1983392]

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The equilibrium limit is equivalent to

$$\lim_{\mathrm{t}\to\infty} = \mathrm{P}_{\mathrm{eq}}(\phi) = \frac{\mathrm{e}^{-\mathrm{S}[\phi]}}{\int \mathrm{D}\phi \mathrm{e}^{-\mathrm{S}[\phi]}}$$

Stochastic Quantization – Perturbation Theory

Perturbative action:

$$\mathrm{S} = \mathrm{S}_0 + \mathrm{g}\mathrm{S}_\mathrm{I} \quad \to \quad \mathrm{P}(\phi, \mathrm{t}) = \sum_{\mathrm{n}=0}^{\infty} \mathrm{g}^\mathrm{n} \mathrm{P}^{(\mathrm{n})}(\phi, \mathrm{t})$$

Fokker-Planck $\to$ hierarchy of equations

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Fokker-Planck $\rightarrow$ hierarchy of equations

Leading order P converges to free theory:

$$\mathrm{P}^{(0)}(\phi, \mathrm{t}) \rightarrow_{\mathrm{t}\rightarrow\infty} \frac{\mathrm{e}^{-\mathrm{S}_0}}{\mathrm{Z}_0}$$

Weak convergence for $\mathrm{n} > 0$

$$\mathrm{P}^{(\mathrm{n})}(\phi, \mathrm{t}) \rightarrow_{\mathrm{t}\rightarrow\infty} \mathrm{P}_{\mathrm{eq}}^{(\mathrm{n})}(\phi)$$

$\mathrm{P}_{\mathrm{eq}}^{(\mathrm{k})}$ are related by Dyson-Schwinger equivalent relations – recovers the standard field theoretic expansive

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Perturbative action:

$$S = S_0 + gS_I \quad \rightarrow \quad P(\phi, t) = \sum_{n=0}^{\infty} g^n P^{(n)}(\phi, t)$$

Fokker-Planck → hierarchy of equations

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Equivalently, expand the Langevin equation

$$\phi_\eta(x, t) = \phi_\eta^{(0)}(x, t) + \sum_{n=1}^{\infty} \phi_\eta^{(n)}(x, t) g^n$$

Local variance reconstruction

$$\delta\phi_{\mathrm{i}}^{(\mathrm{n})} = \frac{1}{\mathrm{n}!}\left.\frac{\partial^{\mathrm{n}}\delta\phi_{\mathrm{i}}}{\partial\sigma_{\mathrm{p}}^{\mathrm{n}}}\right|_{\sigma_{\mathrm{p}}=\vec{\sigma}_{\mathrm{p}}^{*}}$$

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Reconstruction:

$$\delta\phi_{\mathrm{i}} = \delta\phi_{\mathrm{i}}^{(0)} + \delta\phi_{\mathrm{i}}^{(1)}\left(\sigma_{\mathrm{p}} - \sigma_{\mathrm{p}}^{*}\right) + \delta\phi_{\mathrm{i}}^{(2)}\left(\sigma_{\mathrm{p}} - \sigma_{\mathrm{p}}^{*}\right)^{2} + \delta\phi_{\mathrm{i}}^{(3)}\left(\sigma_{\mathrm{p}} - \sigma_{\mathrm{p}}^{*}\right)^{3} + \ldots$$

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From MC average!

How to sample from the distribution function?

Molecular Dynamics Monte-Carlo

$$P \to e^{-S(\phi)}$$

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$$\mathrm{H}(\phi, \pi) = \frac{1}{2}\pi^2 + \mathrm{S}(\phi), \qquad \mathrm{P}' \to \mathrm{e}^{-\mathrm{H}(\phi)};$$

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$$\dot{\phi}_j = \frac{\partial H}{\partial \pi_j} = \pi_j, \qquad \dot{\pi}_j = -\frac{\partial H}{\partial \phi_j};$$

- Propose new configuration after time τ: $(\phi(\tau), \pi(\tau))$

Hamiltonian Monte-Carlo + Gaussian Momentum update
Exact method

Hybrid Monte-Carlo

Hamiltonian Monte-Carlo + Gaussian Momentum update

~~Exact~~ method

Numerical Integration $\rightarrow \Delta H \neq 0$

Hamiltonian Monte-Carlo + Gaussian Momentum update

~~Exact~~ method

Numerical Integration $\rightarrow \Delta \mathrm{H} \neq 0$

Metropolis Accept/Reject step:

$$\mathrm{P}_{\mathrm{acc}} = \min\left(1, \mathrm{e}^{-\Delta \mathrm{H}}\right)$$

$$\Delta \mathrm{H} = \mathrm{H}(\phi', \pi') - \mathrm{H}(\phi, \pi)$$

Algorithm Recap - HMC

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- Repeat.

Numerical Integration

Discretize time: $\tau = \mathrm{n}\varepsilon$

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Euler's Method:

$$\mathcal{I}_1(\varepsilon): \; \pi(\mathrm{t}+\varepsilon) = \pi(\mathrm{t}) + \varepsilon \frac{\mathrm{d}\pi(\mathrm{t})}{\mathrm{dt}}$$

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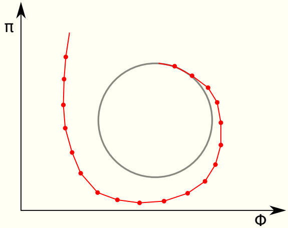

$\mathcal{O}(\varepsilon)$ global error

Discretize time: $\tau = \mathrm{n}\varepsilon$

Modified Euler's Method:

$$\pi(\mathrm{t}+\varepsilon) = \pi(\mathrm{t}) + \varepsilon\frac{\mathrm{d}\pi(\mathrm{t})}{\mathrm{dt}},$$

$$\phi(\mathrm{t}+\varepsilon) = \phi(\mathrm{t}) + \varepsilon\frac{\mathrm{d}\phi(\mathrm{t}+\varepsilon)}{\mathrm{dt}}$$

Numerical Integration

Discretize time: $\tau = \mathrm{n}\varepsilon$

Modified Euler's Method:

$$\mathcal{I}_2(\varepsilon)\mathcal{I}_1(\varepsilon)$$

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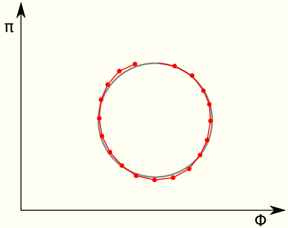

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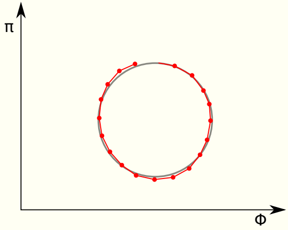
Leapfrog method:

$$\mathcal{I}_1(\varepsilon/2)\mathcal{I}_2(\varepsilon)\mathcal{I}_1(\varepsilon/2)$$



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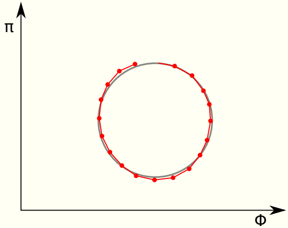

$\mathcal{O}(\varepsilon)$ global error

Leapfrog method:

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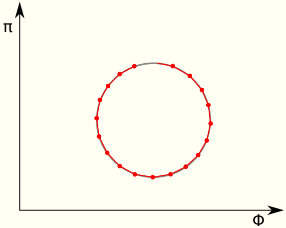

$\mathcal{O}\left(\varepsilon^2\right)$ global error

extra

Discretize time: $\tau = \mathrm{n}\varepsilon$

Omelyan $\mathcal{O}(\varepsilon^4)$

[Dallabrida2017]

$$\mathcal{I}_1(\mathrm{R}_1)\mathcal{I}_2(\mathrm{R}_2)\mathcal{I}_1(\mathrm{R}_3)\mathcal{I}_2(\mathrm{R}_4)\mathcal{I}_1(\mathrm{R}_5)\mathcal{I}_2(\mathrm{R}_6)\mathcal{I}_1(\mathrm{R}_5)\mathcal{I}_2(\mathrm{R}_4)\mathcal{I}_1(\mathrm{R}_3)\mathcal{I}_2(\mathrm{R}_2)\mathcal{I}_1(\mathrm{R}_1)$$

$$\mathrm{R}_\mathrm{i} = \varepsilon \mathrm{r}_\mathrm{i}$$

$$\mathrm{r}_1 = 0.08398315262876693, \qquad \mathrm{r}_2 = 0.2539785108410595$$

$$\mathrm{r}_3 = 0.6822365335719091, \qquad \mathrm{r}_4 = -0.03230286765269967$$

$$\mathrm{r}_5 = 1/2 - \mathrm{r}_1 - \mathrm{r}_3, \qquad \mathrm{r}_6 = 1 - 2(\mathrm{r}_2 + \mathrm{r}_4)$$

$\mathcal{O}\left(\varepsilon^4\right)$ global error

$\sim 300\times$ more precise than Leapfrog (for the same number of force evaluations)

Detour – Complicated free theories...

Markov chain – each element depends only on the previous one

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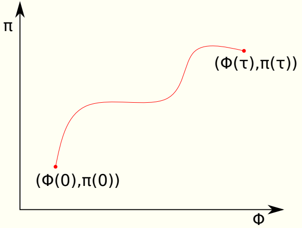

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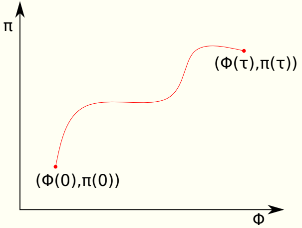

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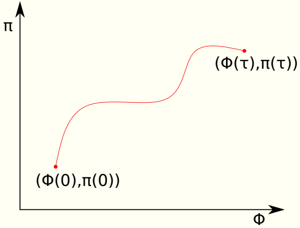

In general, larger τ decreases correlations

What if the system has a natural frequency?

Complicated free theories – Harmonic oscillator in disguise

Single harmonic oscillator

$$\mathrm{H}(\phi, \mathrm{p}) = \frac{\pi^2}{2} + \frac{\phi^2}{2\sigma^2}$$

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Equations of motion with gaussian update:

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Single trajectory:

$$\phi(\mathrm{t}_{\mathrm{n}+1}, \eta_{\mathrm{n}}, \delta\mathrm{t}_{\mathrm{n}}) = \phi(\mathrm{t}_{\mathrm{n}}, \eta_{\mathrm{n}-1}, \delta_{\mathrm{n}-1}) \cos(\delta\mathrm{t}_{\mathrm{n}}/\sigma) + \eta_{\mathrm{n}}\sigma \sin(\delta\mathrm{t}_{\mathrm{n}}/\sigma).$$

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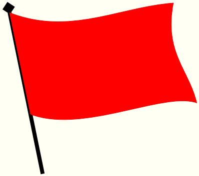

If trajectories are constant and

$$\delta\mathrm{t}/\sigma = \mathrm{k}\pi, \ \mathrm{k} \in \mathbb{Z}$$

$$\phi_{\mathrm{n}+1} = \pm\phi_{\mathrm{n}}$$

Non Ergodic!!!

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Multiple sequential trajectories

$$\phi_{\mathrm{n}} = \prod_{\mathrm{j}=1}^{\mathrm{n}-1} \cos(\delta\mathrm{t}_{\mathrm{j}}/\sigma)\phi_0 + \sum_{\mathrm{k}=0}^{\mathrm{n}-1} \eta_{\mathrm{k}}\sigma \sin(\delta\mathrm{t}_{\mathrm{k}}/\sigma) \prod_{\mathrm{j}=\mathrm{k}+1}^{\mathrm{n}-1} \cos(\delta\mathrm{t}_{\mathrm{k}}\sigma).$$

Chain Correlations

Correlation after n trajectories:

$$\langle \phi_0 \phi_\mathrm{n} \rangle \equiv \prod_{\mathrm{k}=0}^{\mathrm{n}-1} \int \mathrm{d}\eta_\mathrm{k} \mathrm{P}(\eta_\mathrm{k}) \int \mathrm{d}\delta \mathrm{t}_\mathrm{k} \mathrm{P}(\delta \mathrm{t}_\mathrm{k}) \int \mathrm{d}\phi_0 \mathrm{P}(\phi_0) \phi_0 \phi_\mathrm{n}.$$

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Gaussian: $\eta \sim \mathrm{N}(0, 1)$

Gaussian: $\phi_0 \sim \mathrm{N}(0, \sigma^2)$

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Gaussian: $\phi_0 \sim \mathrm{N}(0, \sigma^2)$

Exponential: $\mathrm{P}(\mathrm{t}, \lambda) = \Theta(\mathrm{t}) \exp(-\mathrm{t}/\lambda)/\lambda$

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Gaussian: $\phi_0 \sim N(0,\sigma^2)$

Exponential: $P(t,\lambda) = \Theta(t) \exp(-t/\lambda)/\lambda$

RHMC

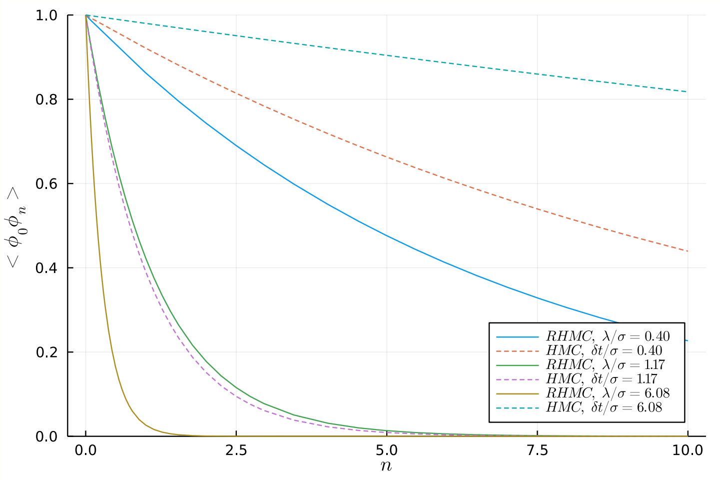
$$\langle \phi_0 \phi_n \rangle_\lambda = \sigma^2 \left(\frac{1}{1+\lambda^2/\sigma^2} \right)^n$$

HMC

$$\langle \phi_0 \phi_n \rangle_{\delta t} = \sigma^2 \left(\cos(\delta t/\sigma) \right)^n$$

[RHMC2017]

A red flag is never alone!



extra

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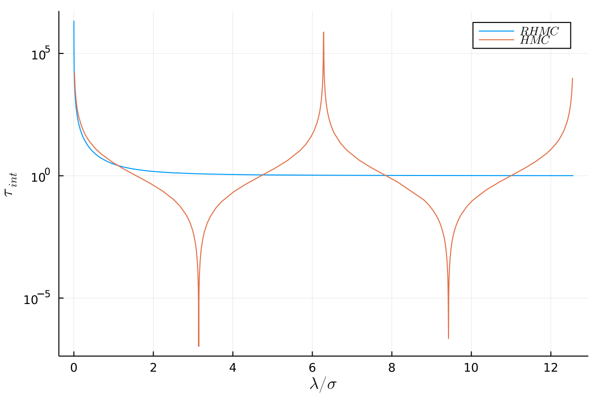
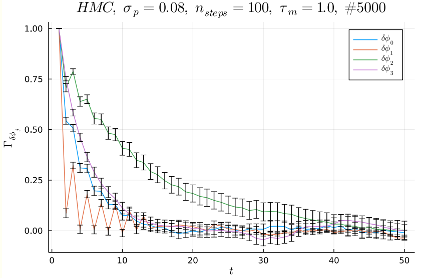
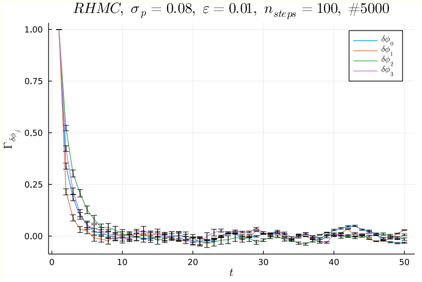


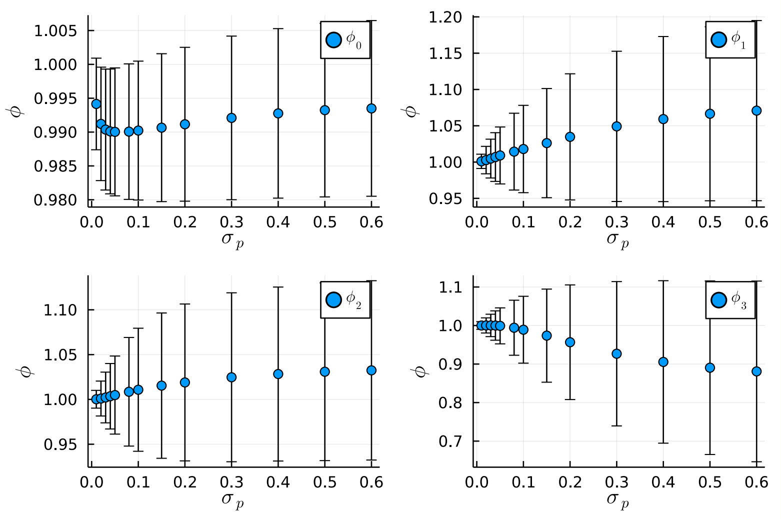
Testing Correlations





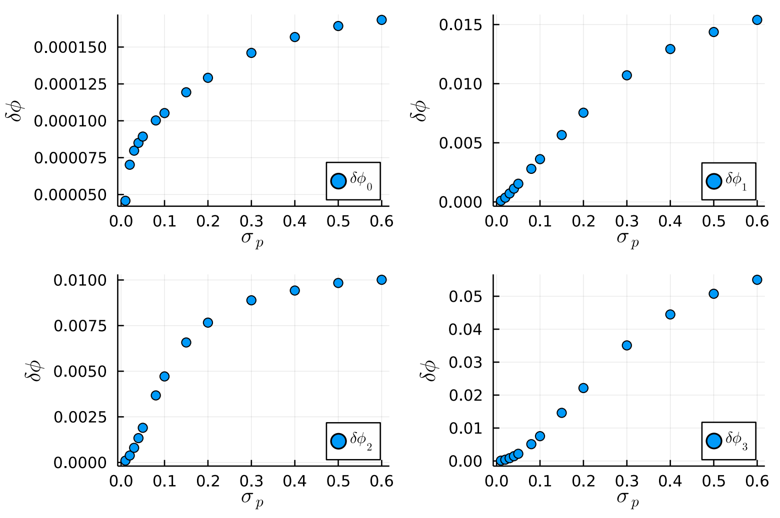
Simulate multiple times?

$\langle \phi_{\mathrm{j}} \rangle$:



Simulate multiple times?

$$\delta\phi_{\mathrm{j}} = \left\langle \phi_{\mathrm{j}}^2 \right\rangle - \left\langle \phi_{\mathrm{j}} \right\rangle^2 :$$



How to take σ_{p} into account for the prediction?

Model robustness

$$\delta\phi_{\mathrm{j}} = \delta\phi_{\mathrm{j}}^{(0)} + \delta\Delta\phi_{\mathrm{j}} \simeq \delta\phi_{\mathrm{j}}^{(0)} + \delta\phi_{\mathrm{j}}^{(1)}(\sigma_{\mathrm{p}} - \sigma_{\mathrm{p}}^{*})$$