Langevin dynamics with multiplicative noise: discretisation issues and path-integral representations

Leticia Cugliandolo[(1)], Vivien Lecomte[(2)], Frédéric van Wijland[(3)]

[(1)]LPTHE, Paris   [(2)]LIPhy, Grenoble   [(3)]MSC, Paris

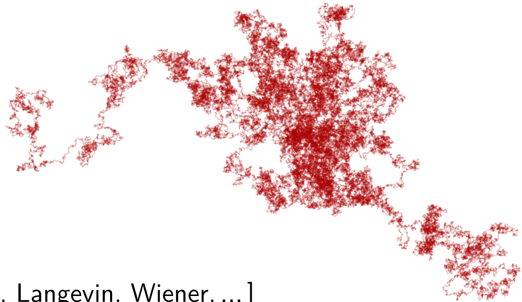
PSM Group Meeting — 10 January 2019

UNIVERSITÉ Grenoble Alpes

cnrs

LIPhy Laboratoire interdisciplinaire de Physique

Fluctuating trajectories – generic settings



[Brown, Einstein, Langevin, Wiener, ...]

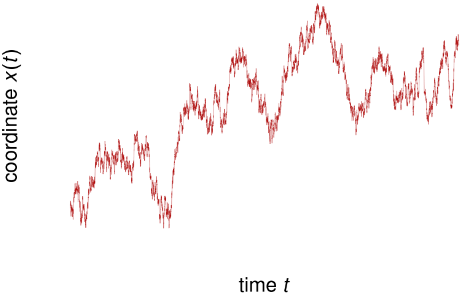
$$\underbrace{m\ddot{x}(t)}_{\text{inertia}} + \underbrace{\gamma\dot{x}(t)}_{\text{damping}} = \underbrace{f(x(t))}_{\text{force}} + \underbrace{\xi(t)}_{\text{noise}}$$

where

$x(t) =$ position, magnetisation, field, ...

$\xi(t) =$ result of from many small contributions (bath, ext. forces, ...)

Fluctuating trajectories – the case studied here



$$\underbrace{\dot{x}(t)}_{\text{damping}} = \underbrace{f(x(t))}_{\text{force}} + \underbrace{g(x(t))\,\eta(t)}_{\text{multiplicative noise}}$$

The *overdamped* dynamics has:

- one dimension
- "multiplicative noise" (*i.e.* configuration-dependent noise)
- with centered Gaussian $\eta(t)$

$$\langle \eta(t)\eta(t')\rangle = 2D\delta(t-t') \qquad \text{(white noise)}$$

Statement of the problem

Main issue: $x(t)$ is typically *not differentiable*.

Statement of the problem

Main issue: $x(t)$ is typically *not differentiable*.

Questions:

- How to define properly $\dot{x} = f(x) + g(x)\eta$?
  $\rightarrow$ OK, Mathematicians did it (stochastic calculus [Wiener, Itō, ...])
  $\rightarrow$ Corresponds to a careful scheme of time discretisation

Statement of the problem

Main issue: $x(t)$ is typically *not differentiable*.

Questions:

- How to define properly $\dot{x} = f(x) + g(x)\eta$?
  $\rightarrow$ OK, Mathematicians did it (stochastic calculus [Wiener, Itō, ...])
  $\rightarrow$ Corresponds to a careful scheme of time discretisation
  $\rightarrow$ For some choice: one can use the standard chain rule

$$\frac{d}{dt}\big[U(x(t))\big] = U'(x(t))\,\dot{x}(t)$$

For changes of variables: we call this property covariance

Statement of the problem

Main issue: $x(t)$ is typically *not differentiable*.

Questions:

- How to define properly $\dot{x} = f(x) + g(x)\eta$?
  $\rightarrow$ OK, Mathematicians did it (stochastic calculus [Wiener, Itō, ...])
  $\rightarrow$ Corresponds to a careful scheme of time discretisation
  $\rightarrow$ For some choice: one can use the standard chain rule

$$\frac{d}{dt}\big[U(x(t))\big] = U'(x(t))\,\dot{x}(t)$$

  For changes of variables: we call this property covariance

- Can one do the same for the **trajectory probability**?

$$\mathcal{D}x \;\; \mathbb{P}\big[(x(t))_{0<t<t_{\rm f}}\big] \;=\; \mathcal{D}x \;\exp\Big\{-\int_0^{t_{\rm f}} dt\,\mathcal{L}(x,\dot{x})\Big\}$$

Outline

- Introduction
- Discretising Langevin equations
  → Covariance in continuous time (Stratonovich scheme)
  → Covariance in discrete time
- Discretising path-integral trajectory probabilities $\mathbb{P}\big[(x(t))_{0<t<t_{\rm f}}\big]$
  → The Stratonovich scheme is **not** covariant
  → An "adaptive" covariant discretisation scheme

Outline

- Introduction
- Discretising Langevin equations
  → Covariance in continuous time (Stratonovich scheme)
  → Covariance in discrete time
- Discretising path-integral trajectory probabilities $\mathbb{P}\big[(x(t))_{0<t<t_{\mathrm{f}}}\big]$
  → The Stratonovich scheme is **not** covariant
  → An "adaptive" covariant discretisation scheme

What is discretisation?

Discretisation of $[0, t_{\mathrm{f}}]$:

$N = t_{\mathrm{f}}/\Delta t$ time steps of duration Δt

$x_t = x(t)$ at discrete times $t = 0, \Delta t, 2\Delta t, \dots$

Discretisation of Langevin: denoting $\Delta x = x_{t+\Delta t} - x_t$

$$\dot{x}(t) = f(x(t)) + g(x(t))\eta(t)$$

$$\updownarrow$$

$$\frac{\Delta x}{\Delta t} = f(\bar{x}_t) + g(\bar{x}_t)\eta_t \qquad \text{with} \quad x_t \le \bar{x}_t \le x_{t+\Delta t}$$

What is discretisation?

Discretisation of $[0, t_\mathrm{f}]$:

$N = t_\mathrm{f}/\Delta t$ time steps of duration Δt

$x_t = x(t)$ at discrete times $t = 0, \Delta t, 2\Delta t, \dots$

Discretisation of Langevin: denoting $\Delta x = x_{t+\Delta t} - x_t$

$$\dot{x}(t) = f(x(t)) + g(x(t))\eta(t)$$

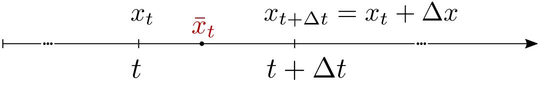
$$\updownarrow$$

$$\frac{\Delta x}{\Delta t} = f(\bar{x}_t) + g(\bar{x}_t)\eta_t \qquad \text{with} \;\; x_t \leq \bar{x}_t \leq x_{t+\Delta t}$$

Noise distribution: η_t's Gaussian i.i.d. with $\langle \eta_t \eta_{t'} \rangle = 2D\delta_{tt'}/\Delta t$

$$\mathbb{P}(\eta_t) = \left[\tfrac{\Delta t}{4\pi D}\right]^{\frac{1}{2}} \mathrm{e}^{-\frac{\Delta t}{4D}\eta_t^2} \quad \Longrightarrow \quad \boxed{\eta_t = O(\Delta t^{-1/2}) \implies \Delta x = O(\Delta t^{1/2})}$$

Do we need discretisation?



Discretisation of Langevin: with $\Delta x = x_{t+\Delta t} - x_t$

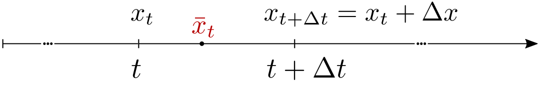
$$\frac{\Delta x}{\Delta t} = f(\bar{x}_t) + g(\bar{x}_t)\eta_t$$

Scheme: $\bar{x}_t = x_t + \alpha\Delta x$ (with $0 \le \alpha \le 1$)

Itō ($\alpha = 0$): $\bar{x}_t = x_t$ (simple for numerics)

Stratonovich ($\alpha = \frac{1}{2}$): $\bar{x}_t = (x_t + x_{t+\Delta t})/2$ (simple for time reversal)

Do we need discretisation? **YES**



Discretisation of Langevin: with $\Delta x = x_{t+\Delta t} - x_t$

$$\frac{\Delta x}{\Delta t} = f(\bar{x}_t) + g(\bar{x}_t)\eta_t$$

Scheme: $\bar{x}_t = x_t + \alpha \Delta x$ (with $0 \le \alpha \le 1$)

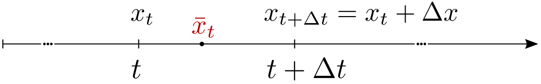
Itō ($\alpha = 0$): $\bar{x}_t = x_t$ (simple for numerics)

Stratonovich ($\alpha = \frac{1}{2}$): $\bar{x}_t = (x_t + x_{t+\Delta t})/2$ (simple for time reversal)

Fixing α is essential: upon Taylor expansion

$$\frac{\Delta x}{\Delta t} = f(\bar{x}_t) + g(\bar{x}_t)\eta_t = f(x_t) + g(x_t)\eta_t + \alpha \overbrace{\Delta x \, g'(x_t) \, \eta_t}^{=O(\Delta t^0)} + O(\Delta t^{\frac{1}{2}})$$

Do we need discretisation? **YES**



Discretisation of Langevin: with $\Delta x = x_{t+\Delta t} - x_t$

$$\frac{\Delta x}{\Delta t} = f(\bar{x}_t) + g(\bar{x}_t)\eta_t$$

Scheme: $\bar{x}_t = x_t + \alpha \Delta x$ (with $0 \le \alpha \le 1$)

Fixing α is essential: upon Taylor expansion

$$\frac{\Delta x}{\Delta t} = f(\bar{x}_t) + g(\bar{x}_t)\eta_t = f(x_t) + g(x_t)\eta_t + \alpha \overbrace{\Delta x\, g'(x_t)\, \eta_t}^{=O(\Delta t^0)} + O(\Delta t^{\frac{1}{2}})$$

Conclusion: the continuous-time writing $\dot{x} = f(x) + g(x)\eta$ $\quad [\Delta t \to 0]$
is *ambiguous* unless one specifies α

A covariant discretisation? $u(t) = U(x(t))$

Naive change of variables: apply the standard chain rule $\boxed{\dot{u} = U'(x)\,\dot{x}}$

$$\dot{u} = F(u) + G(u)\eta$$

with $F(u) = f(x)U'(x)$ and $G(u) = g(x)U'(x)$ ["covariance"]

A covariant discretisation? $u(t) = U(x(t))$

Naive change of variables: apply the standard chain rule $\boxed{\dot{u} = U'(x)\,\dot{x}}$

$$\dot{u} = F(u) + G(u)\eta$$

with $F(u) = f(x)U'(x)$ and $G(u) = g(x)U'(x)$ ["covariance"]

Is there an α-scheme for which it works?

$$\begin{aligned}\Delta u &= U(x_{t+\Delta t}) - U(x_t) = U(x_t + \Delta x) - U(x_t)\\ &= U'(x_t)\Delta x + \underbrace{\tfrac{1}{2}U''(x_t)\Delta x^2}_{=O(\Delta t)} + O(\Delta x^3)\end{aligned}$$

A covariant discretisation $u(t) = U(x(t))$

Naive change of variables: apply the standard chain rule $\dot{u} = U'(x)\,\dot{x}$

$$\dot{u} = F(u) + G(u)\eta$$

with $F(u) = f(x)U'(x)$ and $G(u) = g(x)U'(x)$ ["covariance"]

Is there an α-scheme for which it works?

$$\begin{aligned}\Delta u &= U(x_{t+\Delta t}) - U(x_t) = U(x_t + \Delta x) - U(x_t)\\ &= U'(x_t)\Delta x + \tfrac{1}{2}U''(x_t)\Delta x^2 + O(\Delta x^3)\end{aligned}$$

In Stratonovich $\bar{x}_t \overset{\mathsf{S}}{=} x_t + \frac{1}{2}\Delta x$:

$$\frac{\Delta u}{\Delta t} \overset{\mathsf{S}}{=} U'(\bar{x}_t)\frac{\Delta x}{\Delta t} + O(\Delta t^{1/2})$$

A covariant discretisation $u(t) = U(x(t))$

Naive change of variables: apply the standard chain rule $\boxed{\dot{u} = U'(x)\,\dot{x}}$

$$\dot{u} = F(u) + G(u)\eta$$

with $F(u) = f(x)U'(x)$ and $G(u) = g(x)U'(x)$ ["covariance"]

In Stratonovich $\bar{x}_t \overset{\mathsf{S}}{=} x_t + \frac{1}{2}\Delta x$:

$$\frac{\Delta u}{\Delta t} \overset{\mathsf{S}}{=} U'(\bar{x}_t)\frac{\Delta x}{\Delta t} + O(\Delta t^{1/2})$$

Conclusion: in Stratonovich, chain rule OK as $\Delta t \to 0$

$$\dot{u} \overset{\mathsf{S}}{=} U'(x)\,\dot{x} + O(\Delta t^{1/2})$$

A covariant discretisation $u(t) = U(x(t))$

Naive change of variables: apply the standard chain rule $\boxed{\dot u = U'(x)\,\dot x}$

$$\dot u = F(u) + G(u)\eta$$

with $F(u) = f(x)U'(x)$ and $G(u) = g(x)U'(x)$ ["covariance"]

In Stratonovich $\bar x_t \overset{\mathsf{S}}{=} x_t + \frac{1}{2}\Delta x$:

$$\frac{\Delta u}{\Delta t} \overset{\mathsf{S}}{=} U'(\bar x_t)\frac{\Delta x}{\Delta t} + O(\Delta t^{1/2})$$

Conclusion: in Stratonovich, chain rule OK as $\Delta t \to 0$

$$\dot u \overset{\mathsf{S}}{=} U'(x)\,\dot x + O(\Delta t^{1/2})$$

$$\dot u \overset{\mathsf{S}}{=} F(u) + G(u)\eta + O(\Delta t^{1/2})$$

A better covariant discretisation? $u(t) = U(x(t))$

In Stratonovich:

$$\dot{x} \overset{\mathsf{S}}{=} f(x) + g(x)\eta$$

$$\Downarrow$$

$$\dot{u} \overset{\mathsf{S}}{=} F(u) + G(u)\eta + O(\Delta t^{1/2})$$

A better covariant discretisation? $u(t) = U(x(t))$

In Stratonovich:

$$\dot{x} \stackrel{\mathsf{S}}{=} f(x) + g(x)\eta$$
$$\Downarrow$$
$$\dot{u} \stackrel{\mathsf{S}}{=} F(u) + G(u)\eta + O(\Delta t^{1/2})$$

Almost as if differentiable: if it were, the rest would be $O(\Delta t)$

A better covariant discretisation $u(t) = U(x(t))$

In Stratonovich:

$$\dot{x} \overset{\mathsf{S}}{=} f(x) + g(x)\eta$$
$$\Downarrow$$
$$\dot{u} \overset{\mathsf{S}}{=} F(u) + G(u)\eta + O(\Delta t^{1/2})$$

Almost as if differentiable: if it were, the rest would be $O(\Delta t)$

An improved scheme: $\bar{x}_t \overset{\beta_g}{=} x_t + \frac{1}{2}\Delta x + \beta_g(x_t)\Delta x^2$

$$\beta_g(x) = \frac{1}{24}\frac{g''(x)}{g'(x)} - \frac{1}{12}\frac{g'(x)}{g(x)}$$

improves covariance:

$$\dot{x} \overset{\beta_g}{=} f(x) + g(x)\eta$$
$$\Downarrow$$
$$\dot{u} \overset{\beta_G}{=} F(u) + G(u)\eta + O(\Delta t)$$

For enthusiasts: an **exact** covariant discretisation

Define the $\mathbb{T}_{f,g}$ operator:

$$\mathbb{T}_{f,g} h(x) = \frac{\mathrm{e}^{\mathcal{D}(x)\,\frac{\mathrm{d}}{\mathrm{d}x}} - \mathbf{1}}{\mathcal{D}(x)\,\frac{\mathrm{d}}{\mathrm{d}x}} h(x) = \sum_{n\geq 0} \frac{\left(\mathcal{D}(x)\frac{\mathrm{d}}{\mathrm{d}x}\right)^n}{(n+1)!} h(x)$$

$$\mathcal{D}(x) = f(x)\,\Delta t + g(x)\,\eta_t\,\Delta t$$ [acting as an operator in x]

For enthusiasts: an **exact** covariant discretisation

Define the $\mathbb{T}_{f,g}$ operator:

$$\mathbb{T}_{f,g} h(x) = \frac{\mathrm{e}^{\mathcal{D}(x)\,\frac{\mathrm{d}}{\mathrm{d}x}} - \mathbf{1}}{\mathcal{D}(x)\,\frac{\mathrm{d}}{\mathrm{d}x}} h(x) = \sum_{n\geq 0} \frac{\left(\mathcal{D}(x)\frac{\mathrm{d}}{\mathrm{d}x}\right)^n}{(n+1)!} h(x)$$

$$\mathcal{D}(x) = f(x)\,\Delta t + g(x)\,\eta_t\,\Delta t \qquad \text{[acting as an operator in } x\text{]}$$

Novel $\mathbb{T}_{f,g}$-scheme: $h(\bar{x}_t) \overset{\mathbb{T}_{f,g}}{=} \mathbb{T}_{f,g} h(x_t)$

For enthusiasts: an **exact** covariant discretisation

Define the $\mathbb{T}_{f,g}$ operator:

$$\mathbb{T}_{f,g} h(x) = \frac{\mathrm{e}^{\mathcal{D}(x)\,\frac{\mathrm{d}}{\mathrm{d}x}} - \mathbf{1}}{\mathcal{D}(x)\,\frac{\mathrm{d}}{\mathrm{d}x}} h(x) = \sum_{n\geq 0} \frac{\big(\mathcal{D}(x)\frac{\mathrm{d}}{\mathrm{d}x}\big)^n}{(n+1)!} h(x)$$

$$\mathcal{D}(x) = f(x)\,\Delta t + g(x)\,\eta_t\,\Delta t \qquad \text{[acting as an operator in } x\text{]}$$

Novel $\mathbb{T}_{f,g}$-scheme: $h(\bar{x}_t) \stackrel{\mathbb{T}_{f,g}}{=} \mathbb{T}_{f,g} h(x_t)$

Exact covariance:

$$\frac{\Delta x}{\Delta t} \stackrel{\mathbb{T}_{f,g}}{=} f(\bar{x}_t) + g(\bar{x}_t)\eta_t$$

$$\Updownarrow \qquad \text{at all orders in } \Delta t$$

$$\frac{\Delta u}{\Delta t} \stackrel{\mathbb{T}_{F,G}}{=} F(\bar{u}_t) + G(\bar{u}_t)\eta_t$$

For enthusiasts: an **exact** covariant discretisation

Define the $\mathbb{T}_{f,g}$ operator:

$$\mathbb{T}_{f,g} h(x) = \frac{\mathrm{e}^{\mathcal{D}(x)\,\frac{\mathrm{d}}{\mathrm{d}x}} - \mathbf{1}}{\mathcal{D}(x)\,\frac{\mathrm{d}}{\mathrm{d}x}} h(x) = \sum_{n\geq 0} \frac{\left(\mathcal{D}(x)\frac{\mathrm{d}}{\mathrm{d}x}\right)^n}{(n+1)!} h(x)$$

$$\mathcal{D}(x) = f(x)\,\Delta t + g(x)\,\eta_t\,\Delta t \qquad \text{[acting as an operator in } x\text{]}$$

Novel $\mathbb{T}_{f,g}$-scheme: $h(\bar{x}_t) \stackrel{\mathbb{T}_{f,g}}{=} \mathbb{T}_{f,g} h(x_t)$ $\quad \Longrightarrow \beta_g$-scheme at $O(\Delta t)$

Exact covariance:

$$\frac{\Delta x}{\Delta t} \stackrel{\mathbb{T}_{f,g}}{=} f(\bar{x}_t) + g(\bar{x}_t)\eta_t$$

$$\Updownarrow \qquad \text{at all orders in } \Delta t$$

$$\frac{\Delta u}{\Delta t} \stackrel{\mathbb{T}_{F,G}}{=} F(\bar{u}_t) + G(\bar{u}_t)\eta_t$$

Outline

- Introduction
- Discretising Langevin equations
  $\rightarrow$ Covariance in continuous time (Stratonovich scheme)
  $\rightarrow$ Improved covariance (β_g-scheme)
  $\rightarrow$ Covariance in discrete time ($\mathbb{T}_{f,g}$-scheme)
- Discretising path-integral trajectory probabilities $\mathbb{P}\big[(x(t))_{0<t<t_{\mathrm{f}}}\big]$
  $\rightarrow$ The Stratonovich scheme is **not** covariant
  $\rightarrow$ An "adaptive" covariant discretisation scheme

Aims

Path integral: $\langle \mathcal{O}(t_1,\ldots,t_k)\rangle = \int \mathcal{D}x\, O[x(t)]\,\mathbb{P}[x(t)]$

A very long history:

- Mathematics: PJ Daniell (1919), N Wiener ('20s)
- Quantum mechanics: R Feynman (1948), BS DeWitt (1957)
- Stoch. proc.: Stratonovich (1960), Horsthemke & Bach(1975),
  Graham (1977), Tirapegui & *al.* (70s-80s)
- Fields: Janssen ('70s), De Dominicis ('70s), Doi & Peliti ('80s)

Aims

Path integral: $\langle \mathcal{O}(t_1,\dots,t_k)\rangle = \int \mathcal{D}x\, O[x(t)]\, \mathbb{P}[x(t)]$

Hand-waving procedure:

$$\left.\begin{aligned} \mathbb{P}[\eta(t)] \propto \mathrm{e}^{-\int_0^{t_\mathrm{f}} \mathrm{d}t\, \frac{\eta(t)^2}{4D}} \\ \dot{x} = f(x) + g(x)\eta \end{aligned}\right\} \xrightarrow{\eta = \frac{\dot{x}-f(x)}{g(x)}} \mathbb{P}[x(t)] \propto \exp\left\{ -\underbrace{\int_0^{t_\mathrm{f}} \mathrm{d}t\, \frac{(\dot{x}-f(x))^2}{4Dg(x)^2}}_{\text{action } S[x(t)]} \right\}$$

Aims

Path integral: $\langle \mathcal{O}(t_1,\ldots,t_k)\rangle = \int \mathcal{D}x\, O[x(t)]\, \mathbb{P}[x(t)]$

Hand-waving procedure:

$$\left.\begin{array}{r}\mathbb{P}[\eta(t)] \propto \mathrm{e}^{-\int_0^{t_\mathrm{f}} \mathrm{d}t\, \frac{\eta(t)^2}{4D}} \\ \dot{x} = f(x) + g(x)\eta\end{array}\right\} \xrightarrow{\eta=\frac{\dot{x}-f(x)}{g(x)}} \mathbb{P}[x(t)] \propto \exp\Big\{ \underbrace{-\int_0^{t_\mathrm{f}} \mathrm{d}t\, \frac{(\dot{x}-f(x))^2}{4Dg(x)^2}}_{\text{action } S[x(t)]} \Big\}$$

Questions:

- Can we make sense of this procedure?
  - $\to$ How to discretise?
  - $\to$ Can we replace $\propto$ by $=$?

Aims

Path integral: $\langle \mathcal{O}(t_1, \ldots, t_k) \rangle = \int \mathcal{D}x \, O[x(t)] \, \mathbb{P}[x(t)]$

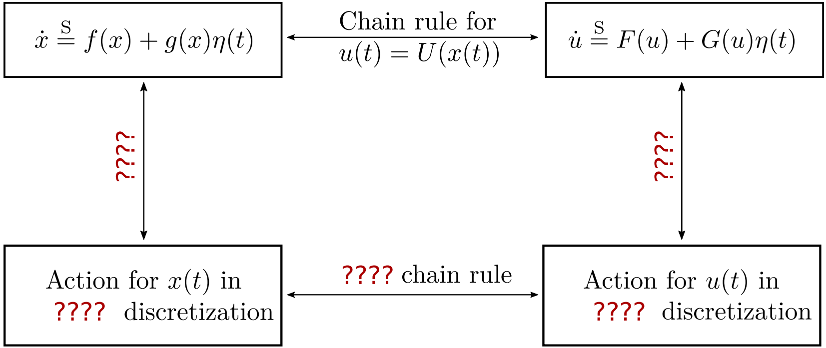
Hand-waving procedure:

$$\left.\begin{aligned} \mathbb{P}[\eta(t)] \propto \mathrm{e}^{-\int_0^{t_\mathrm{f}} \mathrm{d}t \, \frac{\eta(t)^2}{4D}} \\ \dot{x} = f(x) + g(x)\eta \end{aligned}\right\} \xrightarrow{\eta = \frac{\dot{x} - f(x)}{g(x)}} \mathbb{P}[x(t)] \propto \exp\Bigg\{ \underbrace{-\int_0^{t_\mathrm{f}} \mathrm{d}t \, \frac{(\dot{x} - f(x))^2}{4Dg(x)^2}}_{\text{action } S[x(t)]} \Bigg\}$$

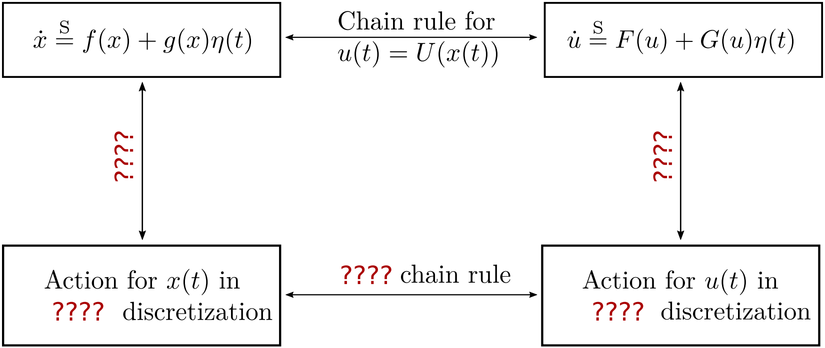
Questions:

- Can we make sense of this procedure?
  - $\rightarrow$ How to discretise?
  - $\rightarrow$ Can we replace $\propto$ by $=$?
- Can we ensure covariance?
  - $\rightarrow$ The action writes as $S[x] = \int_0^{t_\mathrm{f}} \mathrm{d}t \, \mathcal{L}(x, \dot{x})$
  - $\rightarrow$ Can we get $\mathcal{L}(u, \dot{u})$ by applying the chain rule in $\mathcal{L}(x, \dot{x})$?

Covariance

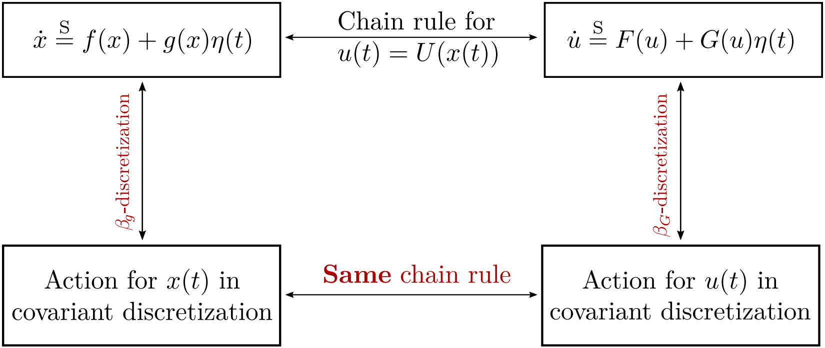

$\dot{x} \stackrel{\mathrm{S}}{=} f(x) + g(x)\eta(t)$
Chain rule for
$u(t) = U(x(t))$
$\dot{u} \stackrel{\mathrm{S}}{=} F(u) + G(u)\eta(t)$
????
????
Action for $x(t)$ in
???? discretization
???? chain rule
Action for $u(t)$ in
???? discretization

Covariance



Remark: the naive action $S[x(t)] = \int_0^{t_\mathrm{f}} \mathrm{d}t\, \frac{(\dot{x} - f(x))^2}{4Dg(x)^2}$ is **not** covariant

Covariance



Remark: the naive action $S[x(t)] = \int_0^{t_\text{f}} \mathrm{d}t \, \frac{(\dot{x}-f(x))^2}{4Dg(x)^2}$ is **not** covariant

From noise to path trajectory probability

Noise trajectory probability:

$$\mathbb{P}[\{\eta_\bullet\}] = \prod_{0\le t<t_{\mathrm{f}}} \left[\frac{\Delta t}{4\pi D}\right]^{\frac{1}{2}} \mathrm{e}^{-\frac{\Delta t}{4D}\eta_t^2}$$

Recursion at each time step:

$$\frac{x_{t+\Delta t} - x_t}{\Delta t} = f(\bar{x}_t) + g(\bar{x}_t)\eta_t \quad \Rightarrow \quad x_{t+\Delta t} = x_{t+\Delta t}(x_t, \eta_t)$$

Trajectory probability as a Feynman path integral

$$\mathbb{P}[\{x_\bullet\}] = \prod_{0\le t<t_{\mathrm{f}}} \mathbb{P}(x_{t+\Delta t}, t+\Delta t | x_t, t)$$

From noise to path trajectory probability

Noise trajectory probability:

$$\mathbb{P}[\{\eta_\bullet\}] = \prod_{0\leq t<t_\mathrm{f}} \Big[\frac{\Delta t}{4\pi D}\Big]^{\frac{1}{2}} \mathrm{e}^{-\frac{\Delta t}{4D}\eta_t^2}$$

Recursion at each time step:

$$\frac{x_{t+\Delta t} - x_t}{\Delta t} = f(\bar{x}_t) + g(\bar{x}_t)\eta_t \quad \Rightarrow \quad x_{t+\Delta t} = x_{t+\Delta t}(x_t, \eta_t)$$

Trajectory probability as a Feynman path integral

$$\mathbb{P}[\{x_\bullet\}] = \prod_{0\leq t<t_\mathrm{f}} \mathbb{P}(x_{t+\Delta t}, t+\Delta t | x_t, t) \equiv \mathcal{N}[\{x_\bullet\}]\,\mathrm{e}^{-S[\{x_\bullet\}]}$$

$\mathcal{N}[\{x_\bullet\}]$ = Normalisation prefactor

$S[\{x_\bullet\}]$ = Discrete-time action

A covariant normalisation prefactor

End-point discretised $\mathcal{N}[x(t)]$:

$$\mathcal{N}[\{x_\bullet\}] = \prod_{0\le k<t_\mathrm{f}} \frac{1}{\sqrt{4\pi D\Delta t}} \, \frac{1}{|g(x_{t+\Delta t})|}$$

Origin of the covariance: compensation of $U'(x_{t+\Delta t})$

- upon changing variables:

$$\mathbb{P}_X(x_{t+\Delta t}|x_t) = |U'(x_{t+\Delta t})| \, \mathbb{P}_U(u_{t+\Delta t}|u_t)$$

- upon changing between g and G:

$$g(x_{t+\Delta t}) = G(u_{t+\Delta t})/U'(x_{t+\Delta t})$$

A covariant normalisation prefactor

End-point discretised $\mathcal{N}[x(t)]$:

$$\mathcal{N}[\{x_\bullet\}] = \prod_{0\leq k<t_\mathrm{f}} \frac{1}{\sqrt{4\pi D\Delta t}} \frac{1}{|g(x_{t+\Delta t})|}$$

Origin of the covariance: compensation of $U'(x_{t+\Delta t})$

- upon changing variables:

$$\mathbb{P}_X(x_{t+\Delta t}|x_t) = |U'(x_{t+\Delta t})|\, \mathbb{P}_U(u_{t+\Delta t}|u_t)$$

- upon changing between g and G:

$$g(x_{t+\Delta t}) = G(u_{t+\Delta t})/U'(x_{t+\Delta t})$$

Conclusion:

this choice for $\mathcal{N}[\{x_\bullet\}]$ allows one to focus on the sole action

A Stratonovich-discretised action?

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \stackrel{\mathsf{S}}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

A Stratonovich-discretised action?

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \overset{\mathsf{S}}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

$$\delta S(\bar{x}) \overset{\mathsf{S}}{=} \frac{1}{2}\frac{\Delta t}{2D}\Big[\frac{\frac{\Delta x}{\Delta t} - f(\bar{x})}{g(\bar{x})}\Big]^2 + \frac{\Delta t}{2}\Big[f'(\bar{x}) - \frac{f(\bar{x})g'(\bar{x})}{g(\bar{x})}\Big] + \frac{D}{4}\big[2g'(\bar{x})^2 - g(\bar{x})g''(\bar{x})\big]\Delta t$$

A Stratonovich-discretised action?

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \overset{\mathsf{S}}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

$$\delta S(\bar{x}) \overset{\mathsf{S}}{=} \frac{1}{2}\frac{\Delta t}{2D}\Big[\frac{\frac{\Delta x}{\Delta t} - f(\bar{x})}{g(\bar{x})}\Big]^2 + \frac{\Delta t}{2}\Big[f'(\bar{x}) - \frac{f(\bar{x})g'(\bar{x})}{g(\bar{x})}\Big] + \frac{D}{4}\big[2g'(\bar{x})^2 - g(\bar{x})g''(\bar{x})\big]\Delta t$$

which encodes the continuous-time writing

$$S[x] \overset{\mathsf{S}}{=} \int_0^{t_\mathrm{f}}\mathrm{d}t\,\Big\{\frac{1}{4D}\Big[\frac{\dot{x} - f(x)}{g(x)}\Big]^2 + \frac{1}{2}f'(x) - \frac{f(x)g'(x)}{2g(x)} + \frac{D}{4}\big[2g'(x)^2 - g(x)g''(x)\big]\Big\}$$

A Stratonovich-discretised action **Not covariant!**

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \stackrel{\mathsf{S}}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

$$\delta S(\bar{x}) \stackrel{\mathsf{S}}{=} \frac{1}{2}\frac{\Delta t}{2D}\Big[\frac{\frac{\Delta x}{\Delta t}-f(\bar{x})}{g(\bar{x})}\Big]^2 + \frac{\Delta t}{2}\Big[f'(\bar{x}) - \frac{f(\bar{x})g'(\bar{x})}{g(\bar{x})}\Big] + \frac{D}{4}\big[2g'(\bar{x})^2 - g(\bar{x})g''(\bar{x})\big]\Delta t$$

which encodes the continuous-time writing

$$S[x] \stackrel{\mathsf{S}}{=} \int_0^{t_{\mathrm{f}}}\mathrm{d}t\,\Big\{\frac{1}{4D}\Big[\frac{\dot{x}-f(x)}{g(x)}\Big]^2 + \frac{1}{2}f'(x) - \frac{f(x)g'(x)}{2g(x)} + \frac{D}{4}\big[2g'(x)^2 - g(x)g''(x)\big]\ \Big\}$$

A Stratonovich-discretised action **Not covariant!**

Why?

A Stratonovich-discretised action **Not covariant!**

Why?

- Let's go from $u(t)$ to $x(t)$
- The dominant term (of order Δt^0) in $\delta S(\bar{u}_t)$ is

$$\frac{\Delta t}{4DG(\bar{u}_t)^2}\left[\frac{\Delta u}{\Delta t}\right]^2$$

A Stratonovich-discretised action **Not covariant!**

Why?

- Let's go from $u(t)$ to $x(t)$
- The dominant term (of order Δt^0) in $\delta S(\bar{u}_t)$ is

$$\frac{\Delta t}{4DG(\bar{u}_t)^2}\left[\frac{\Delta u}{\Delta t}\right]^2$$

- Changing variables, one uses the Stratonovich-discretised chain rule

$$\frac{\Delta u}{\Delta t} \overset{\text{S}}{=} U'(\bar{x}_t)\frac{\Delta x}{\Delta t} + O(\Delta t^{1/2})$$

A Stratonovich-discretised action **Not covariant!**

Why?

- Let's go from $u(t)$ to $x(t)$
- The dominant term (of order Δt^0) in $\delta S(\bar{u}_t)$ is

$$\frac{\Delta t}{4DG(\bar{u}_t)^2}\Big[\frac{\Delta u}{\Delta t}\Big]^2$$

- Changing variables, one uses the Stratonovich-discretised chain rule

$$\frac{\Delta u}{\Delta t} \overset{\mathsf{S}}{=} U'(\bar{x}_t)\frac{\Delta x}{\Delta t} + O(\Delta t^{1/2})$$

- The dominant term yields the expected $\frac{\Delta t}{4Dg(\bar{x}_t)^2}\big[\frac{\Delta x}{\Delta t}\big]^2$

A Stratonovich-discretised action **Not covariant!**

Why?

- Let's go from $u(t)$ to $x(t)$
- The dominant term (of order Δt^0) in $\delta S(\bar{u}_t)$ is

$$\frac{\Delta t}{4DG(\bar{u}_t)^2}\left[\frac{\Delta u}{\Delta t}\right]^2$$

- Changing variables, one uses the Stratonovich-discretised chain rule

$$\frac{\Delta u}{\Delta t} \stackrel{\mathsf{S}}{=} U'(\bar{x}_t)\frac{\Delta x}{\Delta t} + O(\Delta t^{1/2})$$

- The dominant term yields the expected $\frac{\Delta t}{4Dg(\bar{x}_t)^2}\left[\frac{\Delta x}{\Delta t}\right]^2$
- The rest $O(\Delta t^{1/2})$ yields a double-product contribution

$$\frac{\Delta t}{2Dg(\bar{x}_0)^2}\frac{\Delta x}{\Delta t} \times O(\Delta t^{1/2})$$

which is of order Δt and thus **cannot be neglected**.

A β_g-discretised action?

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \overset{\beta_g}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

A β_g-discretised action?

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \overset{\beta_g}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

$$\delta S(\bar{x}) \overset{\beta_g}{=} \frac{1}{2}\frac{\Delta t}{2D}\Big[\frac{\frac{\Delta x}{\Delta t} - f(\bar{x})}{g(\bar{x})}\Big]^2 + \frac{\Delta t}{2}\Big[f'(\bar{x}) - \frac{f(\bar{x})g'(\bar{x})}{g(\bar{x})}\Big]$$

A β_g-discretised action?

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \overset{\beta_g}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

$$\delta S(\bar{x}) \overset{\beta_g}{=} \frac{1}{2}\frac{\Delta t}{2D}\Big[\frac{\frac{\Delta x}{\Delta t}-f(\bar{x})}{g(\bar{x})}\Big]^2 + \frac{\Delta t}{2}\Big[f'(\bar{x}) - \frac{f(\bar{x})g'(\bar{x})}{g(\bar{x})}\Big]$$

which encodes the continuous-time writing

$$S[x] \overset{\beta_g}{=} \int_0^{t_{\mathrm{f}}}\mathrm{d}t\,\Big\{\frac{1}{4D}\Big[\frac{\dot{x}-f(x)}{g(x)}\Big]^2 + \frac{1}{2}f'(x) - \frac{f(x)g'(x)}{2g(x)}\Big\}$$

A β_g-discretised action **Covariant!**

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \stackrel{\beta_g}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

$$\delta S(\bar{x}) \stackrel{\beta_g}{=} \frac{1}{2}\frac{\Delta t}{2D}\Big[\frac{\frac{\Delta x}{\Delta t} - f(\bar{x})}{g(\bar{x})}\Big]^2 + \frac{\Delta t}{2}\Big[f'(\bar{x}) - \frac{f(\bar{x})g'(\bar{x})}{g(\bar{x})}\Big]$$

which encodes the continuous-time writing

$$S[x] \stackrel{\beta_g}{=} \int_0^{t_\mathrm{f}}\mathrm{d}t\,\Big\{\frac{1}{4D}\Big[\frac{\dot{x} - f(x)}{g(x)}\Big]^2 + \frac{1}{2}f'(x) - \frac{f(x)g'(x)}{2g(x)}\Big\}$$

A β_g-discretised action **Covariant!**

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \stackrel{\beta_g}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

$$\delta S(\bar{x}) \stackrel{\beta_g}{=} \frac{1}{2}\frac{\Delta t}{2D}\Big[\frac{\frac{\Delta x}{\Delta t}-f(\bar{x})}{g(\bar{x})}\Big]^2 + \frac{\Delta t}{2}\Big[f'(\bar{x}) - \frac{f(\bar{x})g'(\bar{x})}{g(\bar{x})}\Big]$$

which encodes the continuous-time writing

$$S[x] \stackrel{\beta_g}{=} \int_0^{t_\mathrm{f}}\mathrm{d}t\,\Big\{\frac{1}{4D}\Big[\frac{\dot{x}-f(x)}{g(x)}\Big]^2 + \frac{1}{2}f'(x) - \frac{f(x)g'(x)}{2g(x)}\Big\}$$

Remark:

- The writing is *different* than for the Stratonovich discretisation
- The action is thus more sensitive to discretisation details than the Langevin equation [Gulyaev & Edwards 1964, Tirapegui & *al.* 70s, ...]

A β_g-discretised action **Covariant!**

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \overset{\beta_g}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

$$\delta S(\bar{x}) \overset{\beta_g}{=} \frac{1}{2}\frac{\Delta t}{2D}\Big[\frac{\frac{\Delta x}{\Delta t} - f(\bar{x})}{g(\bar{x})}\Big]^2 + \frac{\Delta t}{2}\Big[f'(\bar{x}) - \frac{f(\bar{x})g'(\bar{x})}{g(\bar{x})}\Big]$$

which encodes the continuous-time writing

$$S[x] \overset{\beta_g}{=} \int_0^{t_\mathrm{f}} \mathrm{d}t \left\{ \frac{1}{4D}\Big[\frac{\dot{x} - f(x)}{g(x)}\Big]^2 + \frac{1}{2}f'(x) - \frac{f(x)g'(x)}{2g(x)} \right\}$$

Comparison:

- Same continuous-time writing as [de Witt'57] [Strato'60] [Graham'77]

A β_g-discretised action **Covariant!**

Using standard procedures:

$$\mathbb{P}(x_{t+\Delta t}|x_t) \stackrel{\beta_g}{=} \frac{1}{\sqrt{4\pi D\Delta t}\,|g(x_{t+\Delta t})|}\,\mathrm{e}^{-\delta S(\bar{x}_t)}$$

$$\delta S(\bar{x}) \stackrel{\beta_g}{=} \frac{1}{2}\frac{\Delta t}{2D}\Big[\frac{\frac{\Delta x}{\Delta t} - f(\bar{x})}{g(\bar{x})}\Big]^2 + \frac{\Delta t}{2}\Big[f'(\bar{x}) - \frac{f(\bar{x})g'(\bar{x})}{g(\bar{x})}\Big]$$

which encodes the continuous-time writing

$$S[x] \stackrel{\beta_g}{=} \int_0^{t_\mathrm{f}}\mathrm{d}t\,\Big\{\frac{1}{4D}\Big[\frac{\dot{x} - f(x)}{g(x)}\Big]^2 + \frac{1}{2}f'(x) - \frac{f(x)g'(x)}{2g(x)}\Big\}$$

Comparison:

- Same continuous-time writing as [de Witt'57] [Strato'60] [Graham'77]
- But **very different meaning**

Proof of covariance

- Let's go from $u(t)$ to $x(t)$

Proof of covariance

- Let's go from $u(t)$ to $x(t)$
- **Changing variables**, one uses the β_g-discretised chain rule

$$\frac{\Delta u}{\Delta t} \stackrel{\beta_g}{=} U'(\bar{x}_t)\frac{\Delta x}{\Delta t} + O(\Delta t)$$

$\rightarrow$ Now $O(\Delta t)$ does not interfere

Proof of covariance

- Let's go from $u(t)$ to $x(t)$
- **Changing variables**, one uses the β_g-discretised chain rule

$$\frac{\Delta u}{\Delta t} \overset{\beta_g}{=} U'(\bar{x}_t)\frac{\Delta x}{\Delta t} + O(\Delta t)$$

$\rightarrow$ Now $O(\Delta t)$ does not interfere

- **Find a lot of dust under the carpet**; for instance:

$$h(\bar{x}_k) \overset{\beta_g}{=} h(U^{-1}(\bar{u}_k)) + O(\Delta t) \qquad \forall \text{ function } h(x)$$

$\rightarrow$ This $O(\Delta t)$ does make trouble

Proof of covariance

- Let's go from $u(t)$ to $x(t)$
- **Changing variables**, one uses the β_g-discretised chain rule

$$\frac{\Delta u}{\Delta t} \stackrel{\beta_g}{=} U'(\bar{x}_t)\frac{\Delta x}{\Delta t} + O(\Delta t)$$

$\rightarrow$ Now $O(\Delta t)$ does not interfere

- **Find a lot of dust under the carpet**; for instance:

$$h(\bar{x}_k) \stackrel{\beta_g}{=} h(U^{-1}(\bar{u}_k)) + O(\Delta t) \qquad \forall \text{ function } h(x)$$

$\rightarrow$ This $O(\Delta t)$ does make trouble

- In the end, a mere **expansion in powers of Δt**
$\rightarrow$ See *Building a path-integral calculus* [arXiv:1806.09486]
Leticia Cugliandolo, VL, Frédéric van Wijland

Remark 1/2

Mathematician's view of Stochastic Calculus:

Give a well-defined meaning to

$$\int_0^{t_{\mathrm{f}}} \mathrm{d}t \left[h_1(x(t)) + h_2(x(t))\,\dot{x}\, \right]$$

i.e. go beyond Riemann sum (use a finer discretisation)

In Stratonovich: rules of ordinary calculus in this integral are **OK**

Remark 1/2

Mathematician's view of Stochastic Calculus:

Give a well-defined meaning to

$$\int_0^{t_\mathrm{f}} \mathrm{d}t \, \Big[h_1(x(t)) + h_2(x(t))\, \dot{x} \Big]$$

i.e. go beyond Riemann sum (use a finer discretisation)

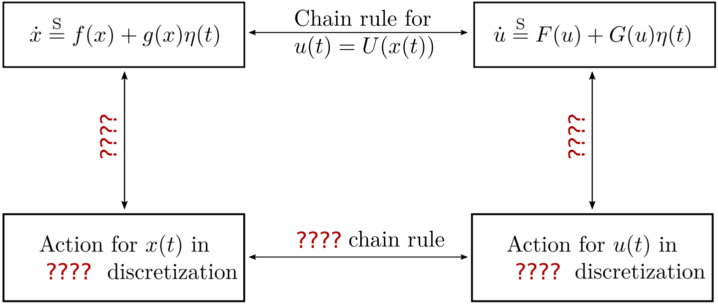
In Stratonovich: rules of ordinary calculus in this integral are **OK**

What the covariant discretisation brings:

Allow for the use of ordinary calculus in

$$\exp\bigg\{ -\int_0^{t_\mathrm{f}} \mathrm{d}t \, \Big[h_1(x(t)) + h_2(x(t))\, \dot{x} + h_3(x(t))\, \dot{x}^2 \Big] \bigg\}$$

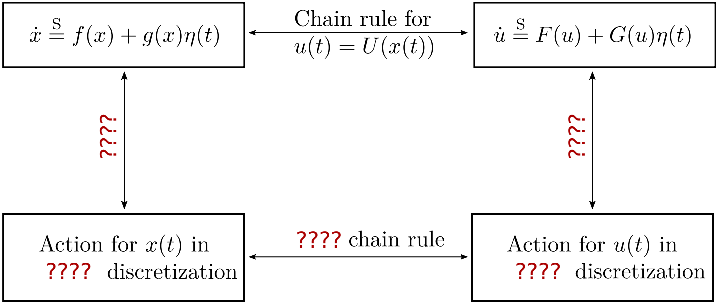
Remark 2/2



For an arbitrary ???? discretisation:

- The action is still correct
- The use of the ordinary chain rule in the action yields *wrong* results

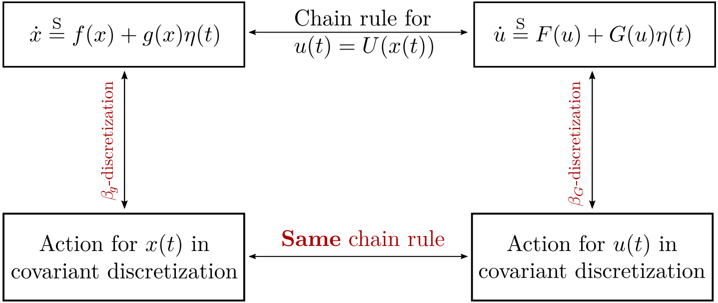
Remark 2/2



For an arbitrary ???? discretisation:

- The action is still correct
- The use of the ordinary chain rule in the action yields *wrong* results
- Changing variables in the time-discrete action is still possible
  But: yields intricate rules in the continuous-time limit
  See Leticia Cugliandolo & VL, JPhysA **50** 345001 (2017)

A graphical summary



An unequivocal meaning to $\mathbb{P}[x(t)] = \mathcal{N}[x(t)]\mathrm{e}^{-S[x(t)]}$ **and to**

$$S[x] \overset{\beta_g}{=} \int_0^{t_\mathrm{f}} \mathrm{d}t \left\{ \frac{1}{4D}\left[\frac{\dot{x} - f(x)}{g(x)}\right]^2 + \frac{1}{2}f'(x) - \frac{f(x)g'(x)}{2g(x)} \right\}$$

"Adaptive" covariant discretisation:

$$\bar{x}_t \overset{\beta_g}{=} x_t + \tfrac{1}{2}\Delta x + \beta_g(x_t)\Delta x^2$$

Perspectives

Extensions:

- Martin–Siggia–Rose–Janssen–de Dominicis action
- Higher dimensions; **non-trivial!** [w.i.p. Thibaut Arnoux de Pirey]

Perspectives

Extensions:

- Martin–Siggia–Rose–Janssen–de Dominicis action
- Higher dimensions; **non-trivial!** [w.i.p. Thibaut Arnoux de Pirey]
- Non-Gaussian noises
- Actions with higher powers of $\dot{x}$ than $\dot{x}^2$

Perspectives

Extensions:

- Martin–Siggia–Rose–Janssen–de Dominicis action
- Higher dimensions; **non-trivial!** [w.i.p. Thibaut Arnoux de Pirey]
- Non-Gaussian noises
- Actions with higher powers of $\dot{x}$ than $\dot{x}^2$

Applications:

- Quantum-mechanical action
- Improved numerical algorithms
- Obtaining correct actions for collective variables

Perspectives

Extensions:

- Martin–Siggia–Rose–Janssen–de Dominicis action
- Higher dimensions; **non-trivial!** [w.i.p. Thibaut Arnoux de Pirey]
- Non-Gaussian noises
- Actions with higher powers of $\dot{x}$ than $\dot{x}^2$

Applications:

- Quantum-mechanical action
- Improved numerical algorithms
- Obtaining correct actions for collective variables
- Supersymmetry for multiplicative noises
- Covariant WKB (small-noise expansion)

Supplementary material

Operator approach

From Fokker–Planck operator to path integrals

$$\begin{aligned} \partial_t P(x,t) &= \mathbb{W}\, P(x,t) \\ P(x_\mathrm{f},t_\mathrm{f}|x_\mathrm{i},t_\mathrm{i}) &= \langle x_\mathrm{f}|\mathrm{e}^{(t_\mathrm{f}-t_\mathrm{i})\mathbb{W}}|x_\mathrm{i}\rangle \\ &= \int_{x(t_\mathrm{i})=x_\mathrm{i}}^{x(t_\mathrm{f})=x_\mathrm{f}} \mathcal{D}x\, O[x(t)]\, \mathbb{P}[x(t)] \end{aligned}$$