High-dimensional Bayesian filtering through deep density approximation:

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February 11, 2026

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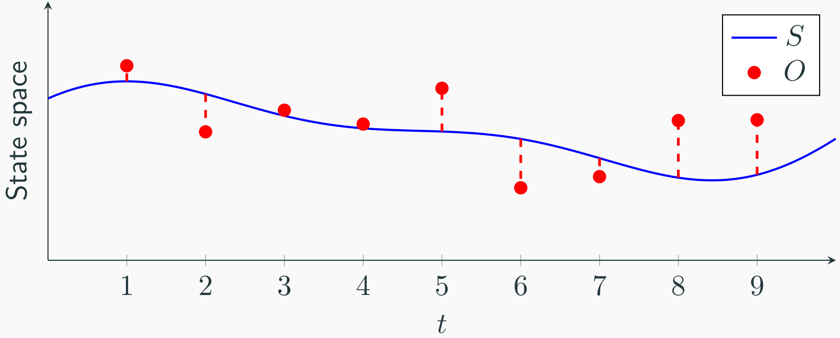
WASP WALLENBERG AI, AUTONOMOUS SYSTEMS AND SOFTWARE PROGRAM

Outline

1. Problem formulation and classical filters
2. The Fokker–Planck PDE
3. Feynman–Kac representations - Optimization formulations
4. Experiments

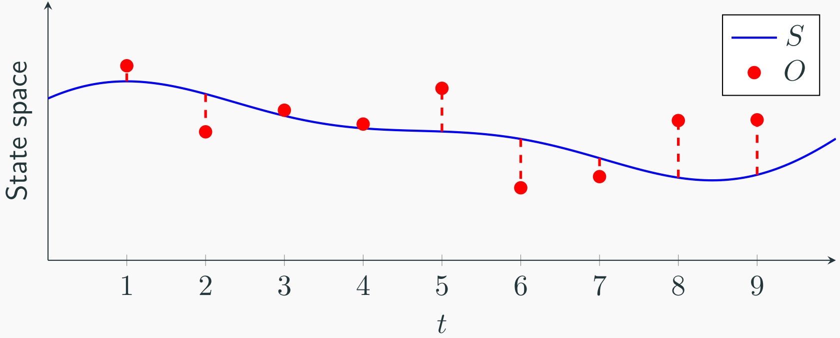
Introduction

The filtering problem



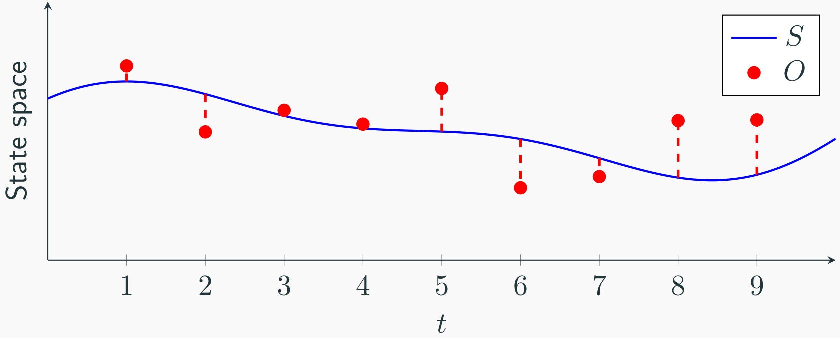
- What is S if we know O?

The filtering problem



- What is $\mathbb{P}(S_{t_k} \mid O_{1:k})$?

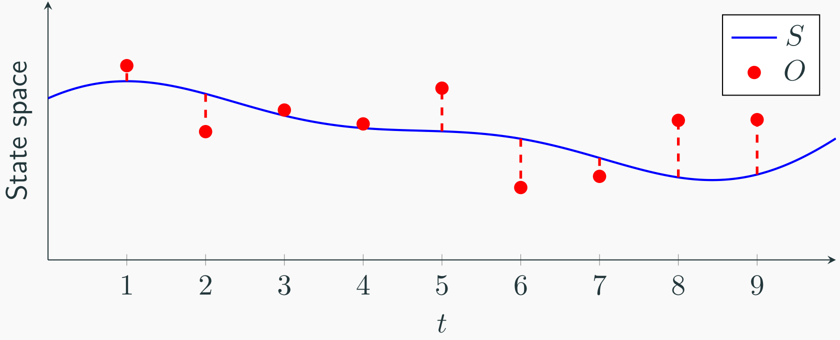
The filtering problem



- The filtering density p_{t_k} satisfies, for $B \subset \mathbb{R}^d$

$$\mathbb{P}(S_{t_k} \in B \mid O_{1:k}) = \int_B p_{t_k}(x \mid O_{1:k})\,\mathrm{d}x$$

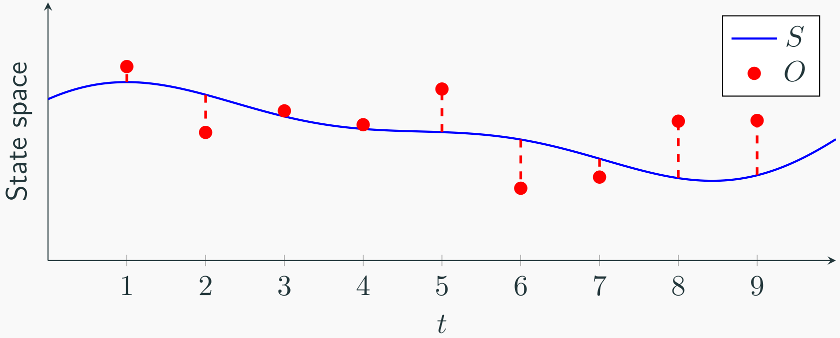
The filtering problem



- Goal: Find the density p_{t_k}

$$\mathbb{P}(S_{t_k} \in B \mid O_{1:k}) = \int_B p_{t_k}(x \mid O_{1:k})\,\mathrm{d}x$$

The filtering problem

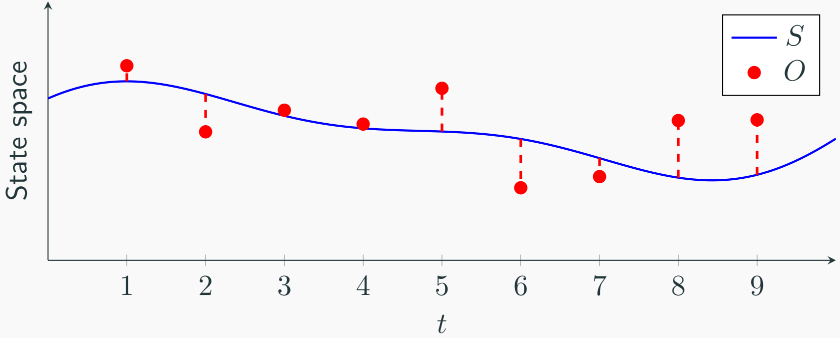


- Goal: Find the density p_{t_k}

$$\mathbb{P}(S_{t_k} \in B \mid O_{1:k}) = \int_B p_{t_k}(x \mid O_{1:k})\,\mathrm{d}x$$

Nonlinear dynamics: Particle filters (PF) $\sim O(n^d), \quad S_t \in \mathbb{R}^d$

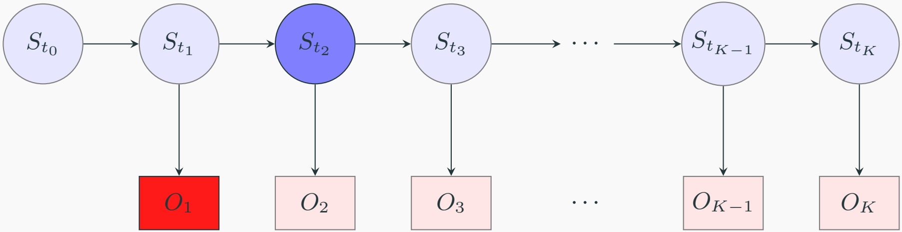
The filtering problem



- **Rephrased Goal:** Find p_t without the curse of dimensionality

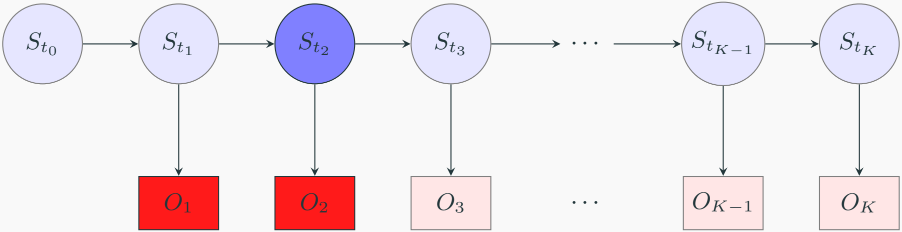
Setting

Prediction: $\mathbb{P}(S_{t_2} \mid O_1)$



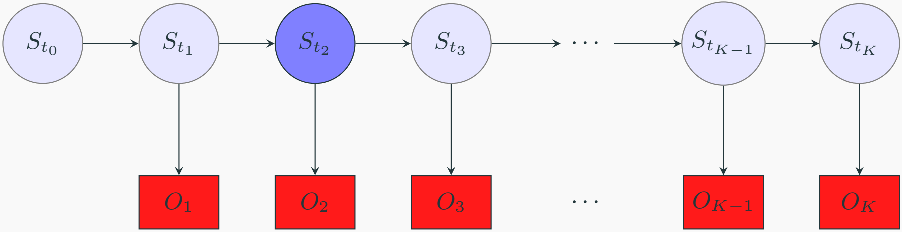
Prediction - Filtering - Smoothing

Filtering: $\mathbb{P}(S_{t_2} \mid O_{1:2})$



Prediction - Filtering - Smoothing

Smoothing: $\mathbb{P}(S_{t_2} \mid O_{1:K})$



Continuous-discrete setting

S solves the d-dimensional Stochastic Differential Equation (SDE)

$$S_t = S_0 + \int_0^t \mu(S_s)\,\mathrm{d}s + \int_0^t \sigma(S_s)\,\mathrm{d}B_s, \quad t \in [0,T].$$

Infinitesimal generator A, with $a := \sigma\sigma^\top$, given by

$$(A\varphi)(x) = \frac{1}{2}\sum_{i,j=1}^{d} a_{ij}(x)\,\frac{\partial^2\varphi(x)}{\partial x_i \partial x_j} + \sum_{i=1}^{d} \mu_i(x)\,\frac{\partial\varphi(x)}{\partial x_i}$$

- **Measurement model**:

$$O_k = h(S_{t_k}) + U_k, \quad k = 1,\ldots,K,$$

where $h\colon \mathbb{R}^d \to \mathbb{R}^{d'}$ and $U_k \sim \mathcal{N}(0, R_k)$.

- **Goal**: Find $p(S_{t_k} \mid O_{1:k})$ for $k = 1,\ldots,K$.

PDE formulation

Density equations:

- **Unconditional**: The (unconditional) density $\rho(t) = p(S_t)$, solves the Fokker–Planck equation (PDE)

$$\rho(t) = \rho(0) + \int_0^t A^* \rho(s)\, \mathrm{d}s, \quad t \in (0, T]$$

- **Filtering (conditional)**: The (unnormalized) filtering density $p_k(t_k) \propto p(S_{t_k} \mid O_{1:k})$ satisfies

$$\text{(Prior)} \quad p_0(0) = p(S_0)$$

$$\text{(Prediction)} \quad p_k(t) = g_k + \int_{t_k^+}^t A^* p_k(s)\, \mathrm{d}s, \quad t \in (t_k, t_{k+1}]$$

$$\text{(Update)} \quad g_k = \begin{cases} p(O_k \mid S_{t_k}) p_{k-1}(t_k), & k \geq 1, \\ p_0(0), & k = 0. \end{cases}$$

Feynman–Kac representations

Backward Kolmogorov

Define f such that for $\varphi \in D(A^*)$ we have

$$A^*\varphi - A\varphi = f(\varphi, \nabla\varphi).$$

Then for $q(t) = p_k(t_k + t_{k+1} - t)$, $t \in [t_k, t_{k+1}]$ it holds

$$\frac{\partial}{\partial t} q(t) + Aq(t) = -f(q(t), \nabla q(t)), \quad t \in [t_k, t_{k+1}],$$

$$q(t_{k+1}) = g_k.$$

Let X be an auxiliary process with the generator A,

$$X_t = X_0 + \int_0^t \mu(X_s)\,\mathrm{d}s + \int_0^t \sigma(X_s)\,\mathrm{d}W_s, \quad X_0 \sim p_0.$$

By Feynman–Kac formulas we derive two optimization schemes:

- Deep Splitting
- Deep Backward SDE

Deep Splitting

Deep splitting

Feynman–Kac on a time partition $t_k = t_{k,0} < \cdots < t_{k,N} = t_{k+1}$, recursively defined for $n = 0, 1 \ldots, N-1$

$$p_k(t_{k,n+1}, x) = \mathbb{E}\Big[p_k(t_{k,n}, X^{t_{k,n},x}_{t_{k,nn+1}}) + \int_{t_{k,n}}^{t_{k,n+1}} f\big(p_k(s, X^{t_{k,n},x}_{t_{k,n+1}+t_{k,n}-s}), \nabla p_k(s, X^{t_{k,n},x}_{t_{k,n+1}+t_{k,n}-s})\big)\,\mathrm{d}s\Big]$$

where for $t \in [t_{k,n}, t_{k,n+1}]$

$$X^{t_{k,n},x}_t = x + \int_{t_{k,n}}^{t} \mu(X^{t_{k,n},x}_s)\,\mathrm{d}s + \int_{t_{k,n}}^{t} \sigma(X^{t_{k,n},x}_s)\,\mathrm{d}W_s$$

Deep splitting

Feynman–Kac on a time partition $t_k = t_0 < \cdots < t_N = t_{k+1}$, recursively defined for $n = 0, 1 \ldots, N-1$

$$p_k(t_{n+1}, x) = \mathbb{E}\Big[p_k(t_n, X^x_{t_{n+1}}) + \int_{t_n}^{t_{n+1}} f\big(p_k(s, X^x_{t_{n+1}+t_n-s}), \nabla p_k(s, X^x_{t_{n+1}+t_n-s})\big)\,\mathrm{d}s\Big]$$

where for $t \in [t_n, t_{n+1}]$

$$X^x_t = x + \int_{t_n}^{t} \mu(X^x_s)\,\mathrm{d}s + \int_{t_n}^{t} \sigma(X^{t_n,x}_s)\,\mathrm{d}W_s$$

Deep splitting

Feynman–Kac on a time partition $t_k = t_0 < \cdots < t_N = t_{k+1}$, recursively defined for $n = 0, 1 \ldots, N-1$

$$p_k(t_{n+1}, x) \approx \mathbb{E}\Big[p_k(t_n, X^x_{t_{n+1}}) + f\big(p_k(t_n, X^x_{t_{n+1}}), \nabla p_k(t_n, X^x_{t_{n+1}})\big)\Delta t\Big]$$

where for $t \in [t_n, t_{n+1}]$

$$X^x_t = x + \int_{t_n}^t \mu(X^x_s)\,\mathrm{d}s + \int_{t_n}^t \sigma(X^x_s)\,\mathrm{d}W_s$$

Deep splitting

Feynman–Kac on a time partition $t_k = t_0 < \cdots < t_N = t_{k+1}$, recursively defined for $n = 0, 1 \ldots, N-1$

$$p_k(t_{n+1}, x) \approx \mathbb{E}\Big[p_k(t_n, \mathcal{X}^x_{n+1}) + f\big(p_k(t_n, \mathcal{X}^x_{n+1}), \nabla p_k(t_n, \mathcal{X}^x_{n+1})\big)\Delta t\Big]$$

where

$$\mathcal{X}^x_{n+1} = x + \mu(\mathcal{X}^x_n)\Delta t + \sigma(\mathcal{X}^x_n)(W_{t_{n+1}} - W_{t_n})$$

Deep splitting

Feynman–Kac on a time partition $t_k = t_0 < \cdots < t_N = t_{k+1}$, recursively defined for $n = 0, 1 \ldots, N-1$

$$\overline{\pi}_{k,n+1} = \underset{\phi \in C(\mathbb{R}^d;\mathbb{R})}{\arg\min}\, \mathbb{E}\Bigg[\bigg|\phi(\mathcal{X}_n) - \Big(\overline{\pi}_{k,n}(\mathcal{X}_{n+1}) + f\big(\overline{\pi}_{k,n}(\mathcal{X}_{n+1}), \nabla\overline{\pi}_{k,n}(\mathcal{X}_{n+1})\big)\Delta t\Big)\bigg|^2\Bigg]$$

where

$$\mathcal{X}_{n+1} = \mathcal{X}_n + \mu(\mathcal{X}_n)\Delta t + \sigma(\mathcal{X}_n)(W_{t_{n+1}} - W_{t_n})$$

Deep splitting

Feynman–Kac on a time partition $t_k = t_0 < \cdots < t_N = t_{k+1}$, recursively defined for $n = 0, 1 \ldots, N-1$

$$\pi_{k,n+1} = \underset{\phi \in C(\mathbb{R}^d \times \mathbb{R}^{d' \times k}; \mathbb{R})}{\arg\min} \mathbb{E}\Big[\Big|\phi(\mathcal{X}_n, O_{1:k}) - \Big(\pi_{k,n}(\mathcal{X}_{n+1}, O_{1:k}) + f\big(\pi_{k,n}(\mathcal{X}_{n+1}, O_{1:k}), \nabla\pi_{k,n}(\mathcal{X}_{n+1}, O_{1:k})\big)\Delta t\Big)\Big|^2\Big]$$

where

$$\mathcal{X}_{n+1} = \mathcal{X}_n + \mu(\mathcal{X}_n)\Delta t + \sigma(\mathcal{X}_n)(W_{t_{n+1}} - W_{t_n})$$

Deep Backward SDE

Deep Backward SDE

Nonlinear Feynman–Kac:

$$p_k(t_{k+1}, x) = \mathbb{E}\left[g_k(X^x_{t_{k+1}}) + \int_{t_k}^{t_{k+1}} f(X^x_s, Y_s, Z_s)\,\mathrm{d}s\right],$$

where (X, Y, Z), with $t \in [t_k, t_{k+1}]$, satisfies

$$X^x_t = x + \int_{t_k}^{t} \mu(X^x_s)\,\mathrm{d}s + \int_{t_k}^{t} \sigma(X^x_s)\,\mathrm{d}W_s,$$

$$Y_t = g_k(X^x_{t_{k+1}}, o_{1:k}) + \int_t^{t_{k+1}} f(X^x_s, Y_s, Z_s)\,\mathrm{d}s - \int_t^{t_{k+1}} Z_s^\top\,\mathrm{d}W_s.$$

Deep Backward SDE

Nonlinear Feynman–Kac:

$$p_k = \underset{u \in C([t_k, t_{k+1}] \times \mathbb{R}^d \times \mathbb{R}^{d' \times k}; \mathbb{R})}{\arg\min} \mathbb{E}\left[\left|Y_{t_{k+1}}^{(u, o_{1:k})} - g_k(X_{t_{k+1}}, O_{1:k})\right|^2\right]$$

where (X, Y, Z), with $t \in [t_k, t_{k+1}]$, satisfies

$$X_t^x = x + \int_{t_k}^{t} \mu(X_s^x)\,\mathrm{d}s + \int_{t_k}^{t} \sigma(X_s^x)\,\mathrm{d}W_s,$$

$$Y_t = g_k(X_{t_{k+1}}^x, o_{1:k}) + \int_t^{t_{k+1}} f(X_s^x, Y_s, Z_s)\,\mathrm{d}s - \int_t^{t_{k+1}} Z_s^\top\,\mathrm{d}W_s.$$

Deep Backward SDE

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where (X, Y, Z), with $t \in [t_k, t_{k+1}]$, satisfies

$$X_t = X_{t_k} + \int_{t_k}^{t} \mu(X_s) \, \mathrm{d}s + \int_{t_k}^{t} \sigma(X_s) \, \mathrm{d}W_s,$$

$$Y_t = u(t_k, X_{t_k}) - \int_{t_k}^{t} f(X_s, Y_s, Z_s) \, \mathrm{d}s + \int_{t_k}^{t} Z_s^{\top} \, \mathrm{d}W_s,$$

$$Z_t = \nabla u(t, X_t).$$

Deep Backward SDE

Nonlinear Feynman–Kac:

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where $(\mathcal{X}, \mathcal{Y}, \mathcal{Z})$, with $n = 0, \ldots, N-1$, satisfies

$$\mathcal{X}_{k,n+1} = \mathcal{X}_{k,n} + \mu(\mathcal{X}_{k,n})(t_{k,n+1} - t_{k,n}) + \sigma(\mathcal{X}_n)(W_{t_{k,n+1}} - W_{t_{k,n}})$$

$$Y_t = u(t_k, X_{t_k}) - \int_{t_k}^{t} f(X_s, Y_s, Z_s)\, \mathrm{d}s + \int_{t_k}^{t} Z_s^\top\, \mathrm{d}W_s,$$

$$Z_t = \nabla u(t, X_t).$$

Deep Backward SDE

Nonlinear Feynman–Kac:

$$p_k = \underset{u \in C([t_k, t_{k+1}] \times \mathbb{R}^d \times \mathbb{R}^{d' \times k}; \mathbb{R})}{\arg\min} \mathbb{E}\left[\left| Y_{t_{k+1}}^{(u, o_{1:k})} - g_k(X_{t_{k+1}}, O_{1:k}) \right|^2 \right]$$

where $(\mathcal{X}, \mathcal{Y}, \mathcal{Z})$, with $n = 0, \ldots, N-1$, satisfies

$$\mathcal{X}_{k,n+1} = \mathcal{X}_{k,n} + \mu(\mathcal{X}_{k,n})(t_{k,n+1} - t_{k,n}) + \sigma(\mathcal{X}_n)(W_{t_{k,n+1}} - W_{t_{k,n}})$$

$$\mathcal{Y}_{k,n+1} = u(t_k, \mathcal{X}_{k,0}) - \sum_{\ell=0}^{n} f\big(\mathcal{X}_{k,\ell}, \mathcal{Y}_{k,\ell}, \mathcal{Z}_{k,\ell}\big)\Delta t + \sum_{\ell=0}^{n} \mathcal{Z}_{k,\ell}^{\top}(W_{t_{k,\ell+1}} - W_{t_{k,\ell}})$$

$$\mathcal{Z}_{k,\ell} = \nabla u(t_{k,\ell}, \mathcal{X}_{k,\ell}).$$

Deep Backward SDE

Nonlinear Feynman–Kac:

$$p_k \approx \underset{u \in C([t_k, t_{k+1}] \times \mathbb{R}^d \times \mathbb{R}^{d' \times k}; \mathbb{R})}{\arg\min} \mathbb{E}\left[\left| \mathcal{Y}_{k,N} - g_k(\mathcal{X}_{k,N}, O_{1:k}) \right|^2 \right]$$

where $(\mathcal{X}, \mathcal{Y}, \mathcal{Z})$, with $n = 0, \ldots, N-1$, satisfies

$$\mathcal{X}_{k,n+1} = \mathcal{X}_{k,n} + \mu(\mathcal{X}_{k,n})(t_{k,n+1} - t_{k,n}) + \sigma(\mathcal{X}_n)(W_{t_{k,n+1}} - W_{t_{k,n}})$$

$$\mathcal{Y}_{k,n+1} = u(t_k, \mathcal{X}_{k,0}) - \sum_{\ell=0}^{n} f\left(\mathcal{X}_{k,\ell}, \mathcal{Y}_{k,\ell}, \mathcal{Z}_{k,\ell}\right)\Delta t + \sum_{\ell=0}^{n} \mathcal{Z}_{k,\ell}^{\top}(W_{t_{k,\ell+1}} - W_{t_{k,\ell}})$$

$$\mathcal{Z}_{k,\ell} = \nabla u(t_{k,\ell}, \mathcal{X}_{k,\ell}).$$

Deep Backward SDE

Nonlinear Feynman–Kac:

$$\pi_k = \mathop{\arg\min}_{\substack{w \in C(\mathbb{R}^d \times \mathbb{R}^{d' \times k}; \mathbb{R}) \\ (v_n)_{n=0}^{N-1} \in C(\mathbb{R}^d \times \mathbb{R}^{d' \times k}; \mathbb{R}^d)^N}} \mathbb{E}\left[\left|\mathcal{Y}_{k,N} - g_k(\mathcal{X}_{k,N}, O_{1:k})\right|^2\right]$$

where $(\mathcal{X}, \mathcal{Y}, \mathcal{Z})$, with $n = 0, \ldots, N-1$, satisfies

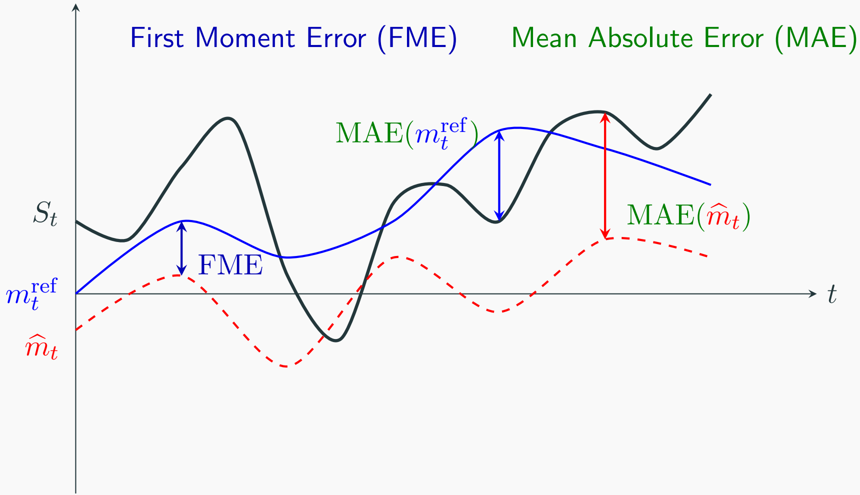
$$\mathcal{X}_{k,n+1} = \mathcal{X}_{k,n} + \mu(\mathcal{X}_{k,n})(t_{k,n+1} - t_{k,n}) + \sigma(\mathcal{X}_n)(W_{t_{k,n+1}} - W_{t_{k,n}})$$

$$\mathcal{Y}_{k,n+1} = w(\mathcal{X}_{k,0}) - \sum_{\ell=0}^{n} f\big(\mathcal{X}_{k,\ell}, \mathcal{Y}_{k,\ell}, \mathcal{Z}_{k,\ell}\big)\Delta t + \sum_{\ell=0}^{n} \mathcal{Z}_{k,\ell}^\top (W_{t_{k,\ell+1}} - W_{t_{k,\ell}})$$

$$\mathcal{Z}_{k,\ell} = v_\ell(\mathcal{X}_{k,\ell}).$$

Numerical experiments

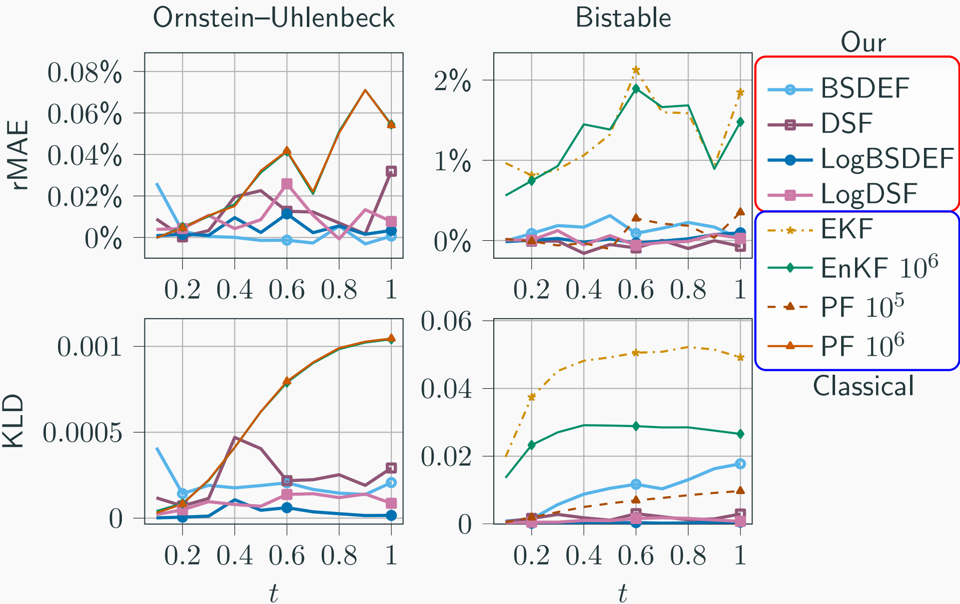
Moment errors



Tons of abbreviations ending with "F"

- BSDEF - deep Backward SDE Filter
- DSF - Deep Splitting Filter
- LogBSDEF and LogDSF - log versions
- EKF - Extended Kalman Filter
- EnKF - Ensemble Kalman Filter
- PF - bootstrap Particle Filter

Toy example



Ornstein–Uhlenbeck
Bistable
rMAE
KLD
0.08%
0.06%
0.04%
0.02%
0%
2%
1%
0.001
0.0005
0
0.06
0.04
0.02
0.2 0.4 0.6 0.8 1
t
Our
BSDEF
DSF
LogBSDEF
LogDSF
EKF
EnKF 10^6
PF 10^5
PF 10^6
Classical

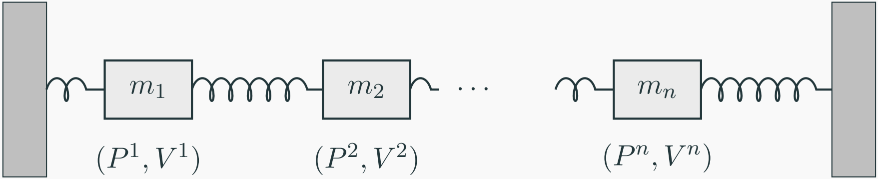
Linear spring-mass - model

Let the state S be split into position P and velocity V so that

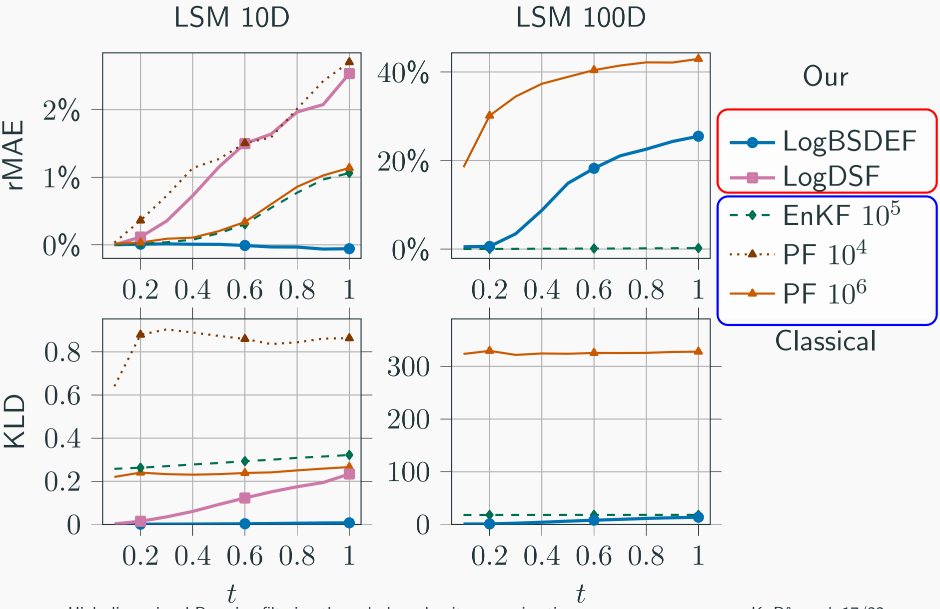
$$P_t = P_0 + \int_0^t V_s \, \mathrm{d}s + \int_0^t \sigma \, \mathrm{d}B_s^{(1)}$$
$$V_t = V_0 + \int_0^t (A_{21} P_s + A_{22} V_s) \, \mathrm{d}s + \int_0^t \sigma \, \mathrm{d}B_s^{(2)}$$

where A_{21} and A_{22} are stiffness and damping matrices with uniform sampled parameters, and we have partial observations:

$$O_k = P_{t_k} + \eta_k, \quad \eta_k \sim N(0, R)$$



Linear spring-mass - results



Lorenz-96 - model

$$\frac{\mathrm{d}x_i(t)}{\mathrm{d}t} = (x_{i+1}(t) - x_{i-2}(t))x_{i-1}(t) - x_i(t) + F, \quad i = 1, \ldots, d$$

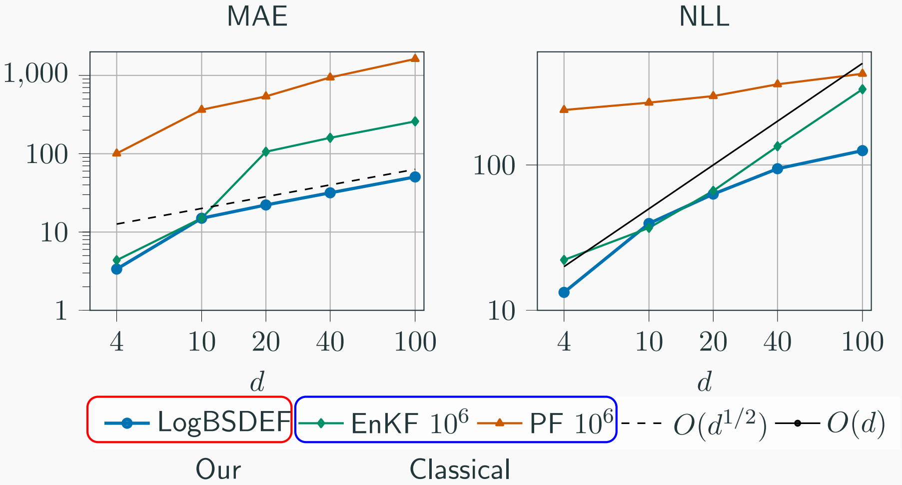
where $x_0 = x_d$ and $x_{-1} = x_{d-1}$

We consider an SDE extension with additive noise given by $\sigma(x) = \sigma I$

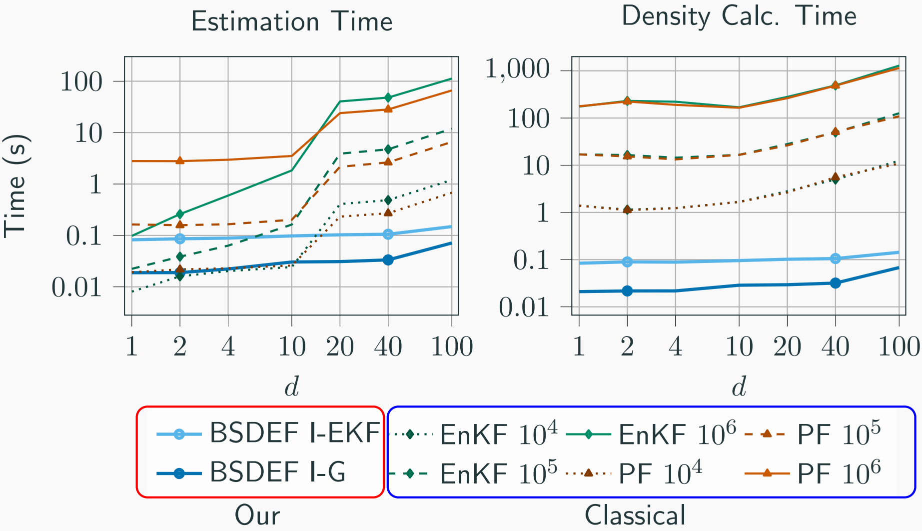
Let $d = [4, 10, 20, 40, 100]$ and consider partial observations in $d' = [4, 5, 5, 10, 25]$-dimensions through the measurement function

$$\big(h(x)\big)_i = \begin{cases} x_i, & (d, d') = (4, 4), \\ x_{2i}, & (d, d') = (10, 5), \\ x_{4i}, & (d, d') = (20, 5),\ (40, 10),\ (100, 25). \end{cases} \tag{1}$$

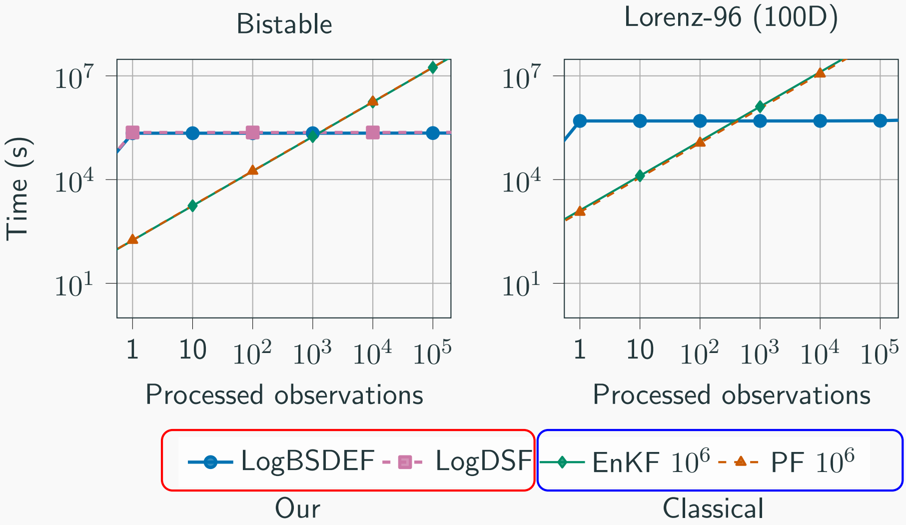
Lorenz-96 - results



Computational inference time



Trade-off including training time



What did we learn?

- The deep BSDE approach outperforms the splitting method
- Solving the log-density Fokker–Planck improves performance
- Satisfactory performance for nonlinear and high-dimensional problems without curse of dimensionality

Outlook:

- Parameter inference, introduce a probability measure over a set Θ of parameters modelling μ, σ, h, p_0
- Explore other architectures

See the paper