

ROBUST SDE-BASED VARIATIONAL FORMULATIONS FOR SOLVING LINEAR PDEs VIA DEEP LEARNING

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Solving Kolmogorov PDEs

- We want to solve *partial differential equations* (PDEs) of the following form:

$$\begin{cases} (\partial_t + \frac{1}{2}(\sigma\sigma^\top) : \nabla^2 + b \cdot \nabla) V(x, t) = 0, \\ V(x, T) = g(x), \quad (x, t) \in \mathbb{R}^d \times [0, T]. \end{cases}$$

- Applications:** modelling of diffusion processes in physics, pricing of financial derivatives, diffusion-based generative modeling, reinforcement learning, ...
- Idea:** minimize *variational formulations* using neural networks $u_\theta \in \mathcal{U}$ with parameters θ , i.e., consider losses

$$\mathcal{L} : \mathcal{U} \rightarrow \mathbb{R}_{\geq 0},$$

which shall be minimal iff $u \in \mathcal{U}$ fulfills the PDE.

Stochastic Representations

- Itô calculus* (cf. Feynman-Kac formula) shows that

$$\underbrace{g(X_T) - V(\xi, \tau)}_{:=\Delta_V} - \underbrace{\int_\tau^T \sigma(X_s)^\top \nabla V(X_s, s) \cdot dW_s}_{:=S_V} = 0,$$

where X is the solution to the associated *stochastic differential equation* (SDE)

$$dX_s = b(X_s) ds + \sigma(X_s) dW_s, \quad X_\tau = \xi.$$

- As the stochastic integral S_u has vanishing expectation, this motivates the two losses

$$\begin{aligned} \mathcal{L}_{\text{FK}}(u) &:= \mathbb{E} [\Delta_u^2], \\ \mathcal{L}_{\text{BSDE}}(u) &:= \mathbb{E} [(\Delta_u - S_u)^2], \end{aligned}$$

where $(\xi, \tau) \sim \text{Unif}(\mathbb{R}^d \times [0, T])$.

Robust Losses

- The stochastic integral S_u in $\mathcal{L}_{\text{BSDE}}$ can be interpreted as a *control variate*.
- It guarantees statistical advantages for the estimator versions $\mathcal{L}^{(K)}$ (with K samples) at the optimum $u_\theta = V$:

Proposition 1 (Variance of Losses).

$$\begin{aligned} \mathbb{V} [\mathcal{L}_{\text{FK}}^{(K)}(u_\theta)] &= \frac{1}{K} \mathbb{V} [S_V^2], \\ \mathbb{V} [\mathcal{L}_{\text{BSDE}}^{(K)}(u_\theta)] &= 0. \end{aligned}$$

Proposition 2 (Variance of Gradients).

$$\begin{aligned} \mathbb{V} [\nabla_\theta \mathcal{L}_{\text{FK}}^{(K)}(u_\theta)] &= \frac{4}{K} \mathbb{V} [S_V \nabla_\theta u_\theta(\xi, \tau)], \\ \mathbb{V} [\nabla_\theta \mathcal{L}_{\text{BSDE}}^{(K)}(u_\theta)] &= 0. \end{aligned}$$

- For $\mathcal{L}_{\text{BSDE}}$ we can expect small variances also close to the solution $u_\theta \approx V$:

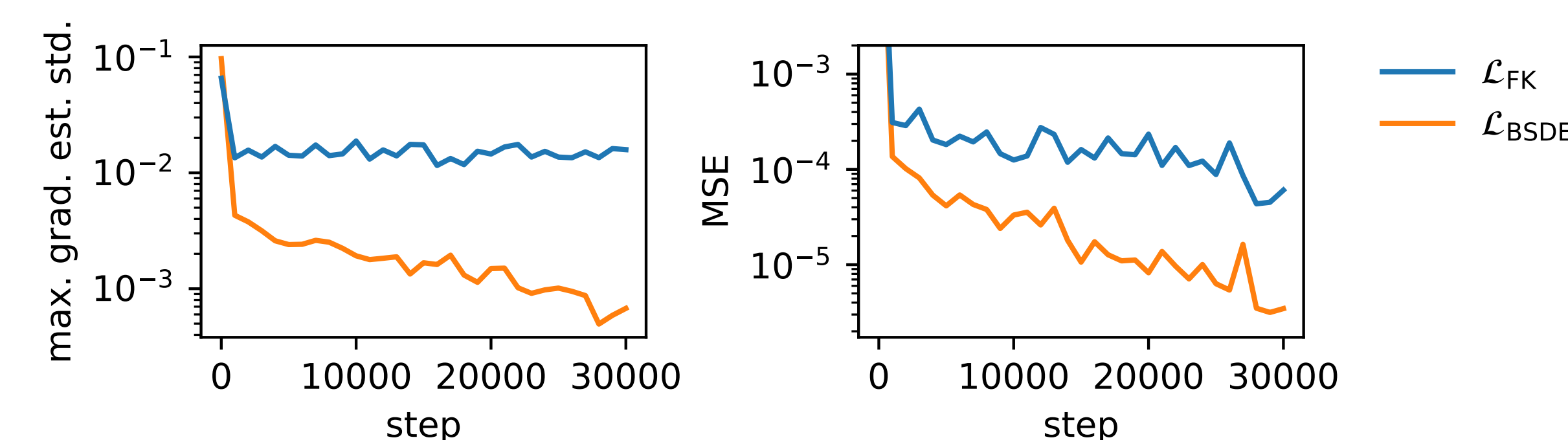
Proposition 3 (Stability Close to Solution). *Assume that*

$$|u_\theta(\xi, \tau) - V(\xi, \tau)| \leq \varepsilon, \quad \|\nabla_x(u_\theta - V)(x, t)\| \leq \varepsilon(1 + \|x\|^\gamma),$$

for some $\gamma \in \mathbb{R}_{>0}$. Then it holds that

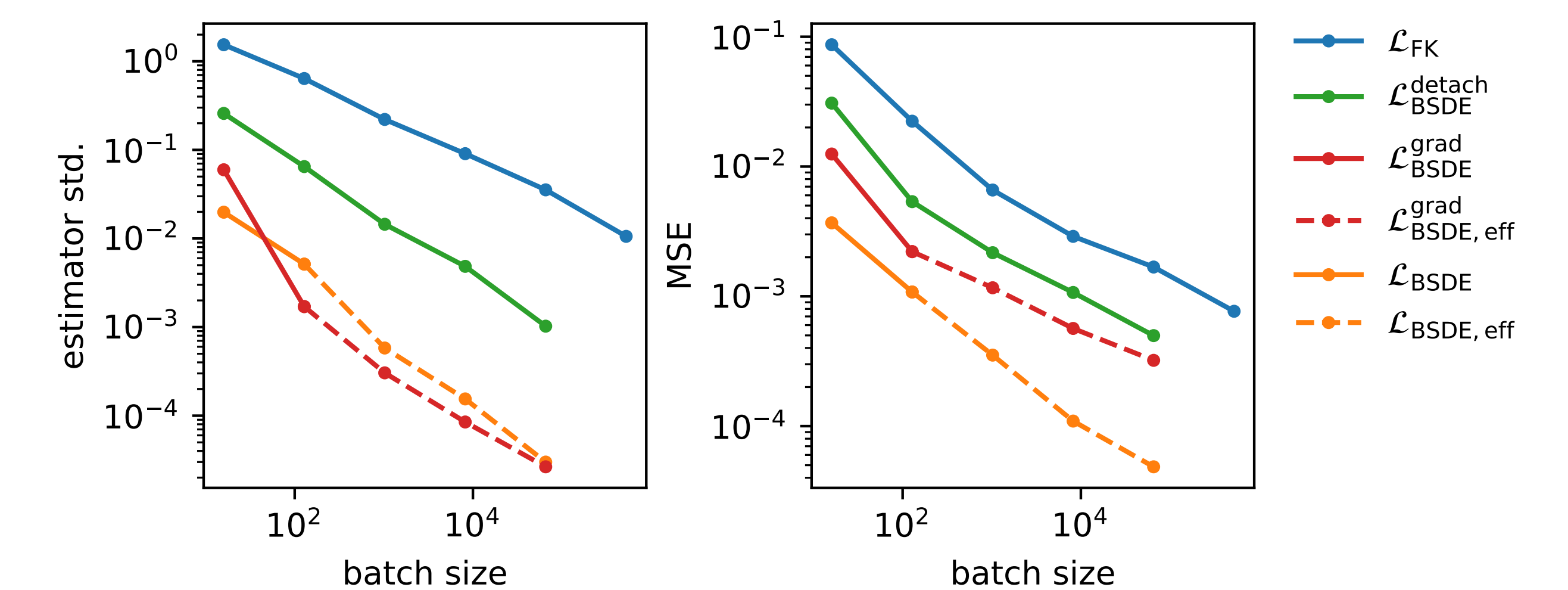
$$\mathbb{V} [\nabla_\theta \mathcal{L}_{\text{BSDE}}^{(K)}(u_\theta)] \lesssim \frac{\varepsilon^2}{K}.$$

- This can also be observed empirically:

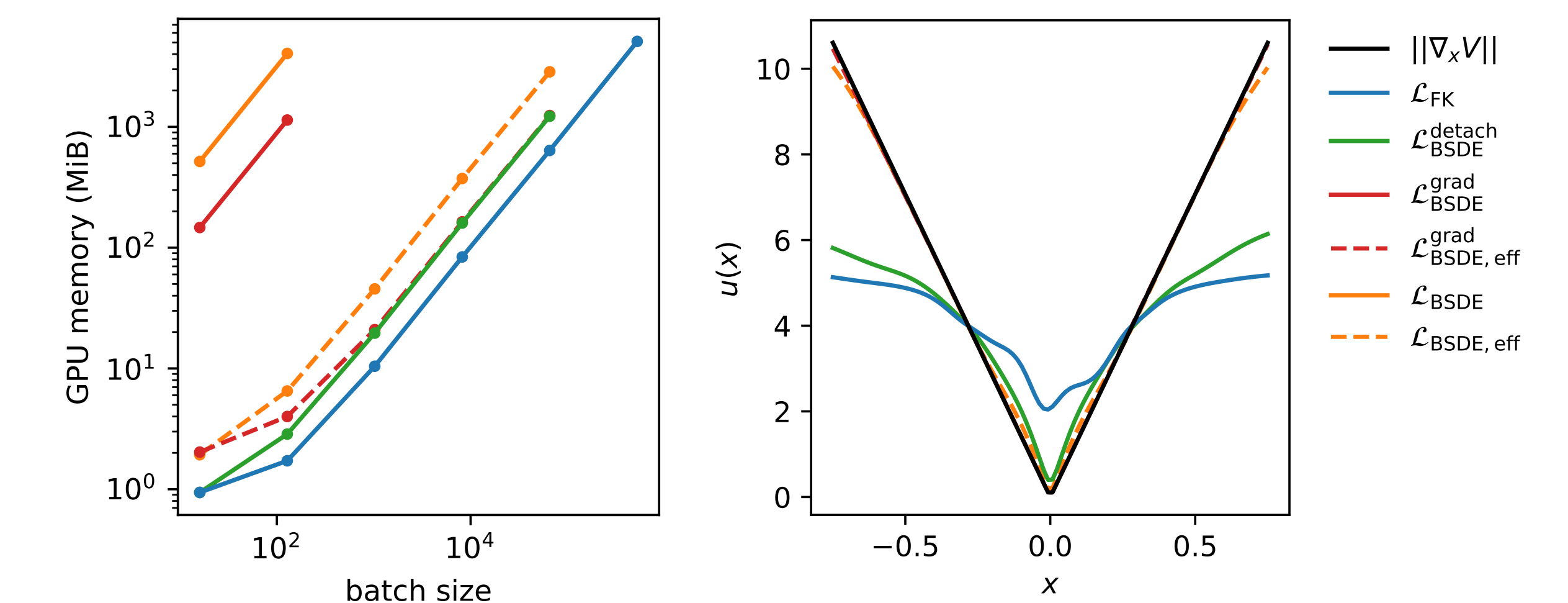


Numerical Experiments

- We propose various (more efficient) versions to include the control variate: $\mathcal{L}_{\text{BSDE}}^{\text{grad}}$, $\mathcal{L}_{\text{BSDE}}^{\text{detach}}$, and $\mathcal{L}_{\text{BSDE, eff}}$.
- We improve state-of-the-art performance and analyze trade-offs between accuracy and complexity:



- The efficient versions of the BSDE-based method combine accuracy and memory efficiency:



Takeaways and Reference

Our paper provides:

- variational formulations for (linear) PDEs,
- techniques for analyzing the variance of (gradient) estimators,
- novel estimators with reduced variance,
- empirical studies of complexity vs. performance.

arxiv.org/abs/2206.10588
github.com/juliusberner/robust_kolmogorov

