

# Deep adaptive sampling: Algorithm, Theory, and Applications

Peng Cheng Laboratory

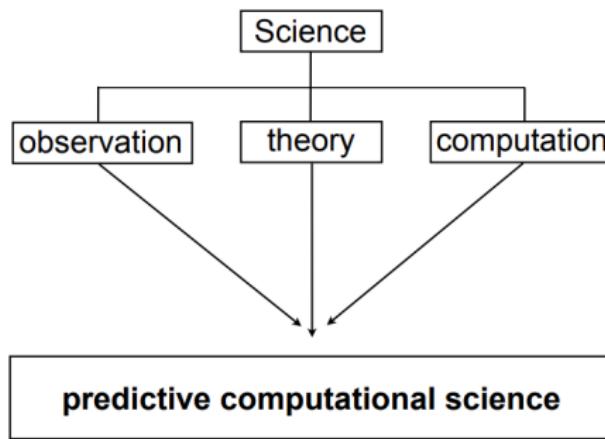
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Joint work with Xiaoliang Wan (Louisiana State University) and Chao Yang (Peking University)

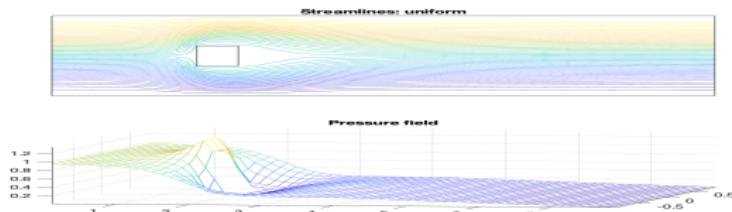
# Background



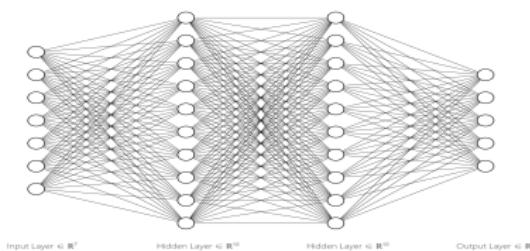
- Diffusion process
- Aerospace
- Molecular dynamics
- ...

# Background

- Mathematical (physical) model: PDEs or ODEs

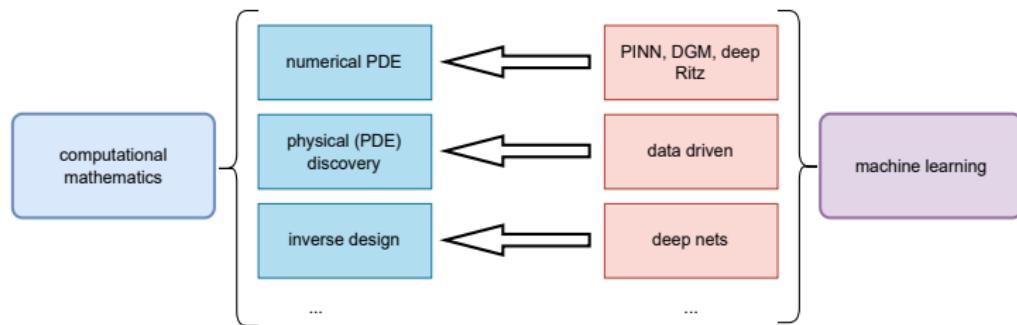
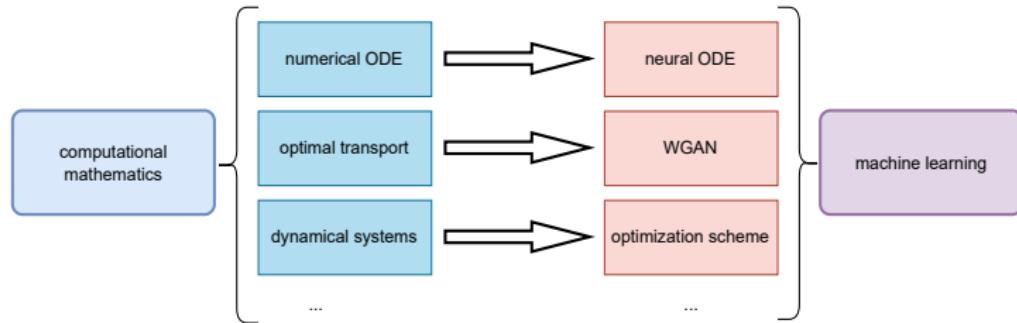


- Data-driven model (e.g., deep neural networks): no proper physical model but massive available data



- Numerical methods  
Both need numerical methods

# Machine learning & scientific computing (Scientific machine learning)



# Machine learning & scientific computing (Scientific machine learning)

- Uncertainty quantification (UQ): (Bayesian) Surrogate model, [Zhu and Zabaras, 2018]; Physical informed neural networks [Raissi, Perdikaris and Karniadakis, 2018]
- Density estimation and sampling method:  
Neural importance sampling, [Müller et.al, 2019]; Flow model for model reduction, [Wan and Wei, 2020]; Neural ODE, [Chen et.al , 2018]; Real NVP, [Dinh, Sohl-Dickstein and Bengio, 2016]; GAN, [Goodfellow et. al, 2014]; VAE, [Kingma and Welling, 2014]
- Deep neural networks for PDEs:  
Deep Ritz, [E and Yu, 2017] ; PDE-Net, [Long et. al, 2018]; PINN for PDE [Raissi, Perdikaris and Karniadakis, 2019]; Deep Galerkin [Sirignano and Spiliopoulos, 2018]; Physical constraint, [Zhu and Zabaras, 2019]; D3M, [Li, Tang, Wu and Liao, 2019]; PFNN, [Sheng and Yang, 2020]
- ...

# Big data era: data-driven

Using data to train a predictive model with parameters  $\Theta$

$$u(\mathbf{x}; \Theta)$$

e.g. deep neural networks

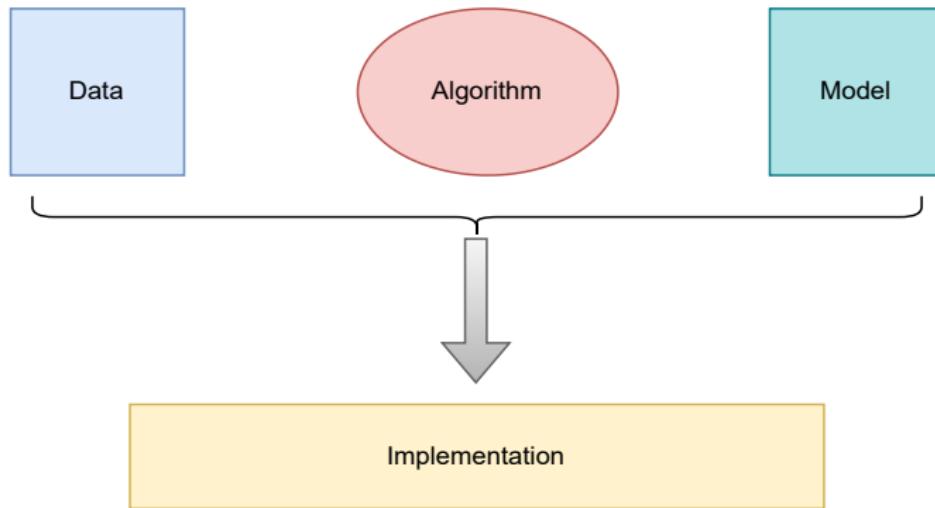
Training usually means an optimization problem

$$\min_{\Theta} \frac{1}{N} \sum_{i=1}^N J(x^{(i)}; \Theta).$$

where  $J$  is a proper loss function, e.g., mean square error, cross entropy etc.

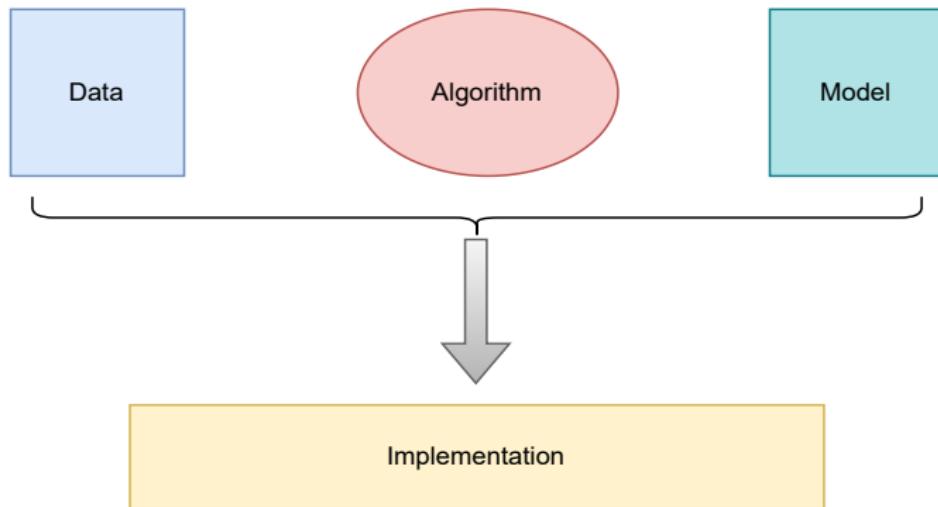
- machine learning
- computer vision
- signal processing
- ...

# Big data era: data-driven



- Model: deep neural networks, physical models, or coupling
- Data: labeled, unlabeled, random samples (our case) ....
- Algorithm: various optimization methods

# Big data era: data-driven



data is oil

- model is driven by data
- data has the influence on generalization

# Goal

## Traditional numerical methods

- high fidelity
- suffers from the curse of dimensionality

## Machine (deep) learning approaches

- low fidelity
- weaker dependence on dimensionality

our purpose:

Develop adaptive numerical methods by data-driven modes for high-dimensional scientific computing problems (e.g., Fokker-Planck equations, committor functions approximation)

- deep networks to alleviate the curse of dimensionality
- develop adaptive schemes using machine learning techniques

## Illustration of the statistical error

illustrate the statistical error of the machine learning technique from a function approximation perspective

Let  $\mathbf{X} \in \mathbb{R}^d$  and  $Y \in \mathbb{R}$  subject to a joint distribution  $\rho_{\mathbf{X}, Y}$ . Let  $\hat{Y} = m(\mathbf{X})$  be a model and  $y = h(\mathbf{x})$  be a function to be approximated. We know in the  $L_2$  sense the optimal model is

$$m^*(\mathbf{x}) = \arg \min_{m(\mathbf{x})} \left[ L(Y, \hat{Y}) = \int (y - m(\mathbf{x}))^2 \rho_{\mathbf{X}, Y}(\mathbf{x}, y) d\mathbf{x} dy \right].$$

$$m_{w^*}(\mathbf{x}) = \arg \min_{m_w \in W} \left[ L_N(Y, \hat{Y}) = \frac{1}{N} \sum_{i=1}^N (y^{(i)} - m_w(\mathbf{x}^{(i)}))^2 \right],$$

$L_N$ : a Monte Carlo approximation of  $L$  with dataset  $\{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$

# Illustration of the statistical error

illustrate the statistical error of the machine learning technique from a function approximation perspective

For a linear space  $V = \text{span}\{q_i(\mathbf{x})\}_{i=1}^n$

$$m_{\hat{\mathbf{v}}^*}(\mathbf{x}) = \arg \min_{m_{\hat{\mathbf{v}}} \in V} \left[ L_{V,N}(Y, \hat{Y}) = \frac{1}{N} \sum_{i=1}^N (m_{\hat{\mathbf{v}}}(\mathbf{x}^{(i)}) - h(\mathbf{x}^{(i)}))^2 \right],$$

Lemma (Tang, Wan and Yang, 2022)

Let  $h(\mathbf{x}) \in C(D)$  be a continuous function defined on a compact domain  $D \subset \mathbb{R}^d$  and  $\rho(\mathbf{x}) > 0$  be a PDF on  $D$ . Let  $V = \text{span}\{q_i(\mathbf{x})\}_{i=1}^n$  with  $q_i(\mathbf{x})$  being orthonormal polynomials in terms of  $\rho(\mathbf{x})$ . For any  $\delta > 0$  and with probability at least  $1 - 2\delta$ , we have for a sufficiently large  $N$

$$\|m_{\hat{\mathbf{v}}^*}(\mathbf{x}) - h(\mathbf{x})\|_{\rho} \leq C \sqrt{\frac{\ln \delta^{-1}}{N}} + \|m_V^*(\mathbf{x}) - h(\mathbf{x})\|_{\rho},$$

where  $C$  is a constant, and  $\|\cdot\|_{\rho}$  is the weighted  $L_2$  norm in terms of  $\rho(\mathbf{x})$ .

# Illustration of the statistical error

$$\|m_{V^*}(\mathbf{x}) - h(\mathbf{x})\|_\rho \leq C \sqrt{\frac{\ln \delta^{-1}}{N}} + \|m_V^*(\mathbf{x}) - h(\mathbf{x})\|_\rho,$$

statistical error

approximation error

- the hypothesis space  $V \rightarrow$  approximation error
- the training set  $\rightarrow$  statistical error

# Partial differential equations

$$\mathcal{L}(x; u(x)) = s(x) \quad \forall x \in \Omega,$$

$$\mathfrak{b}(x; u(x)) = g(x) \quad \forall x \in \partial\Omega.$$

$\mathcal{L}$  : partial differential operator,  $\mathfrak{b}$  : boundary operator.

FEM:

1. mesh
2. basis



Deep methods:

1. samples
2. neural networks

## Why deep methods

- fast inference
- tackle high dimensional problems

# Deep learning for PDEs

$$\begin{aligned}\mathcal{L}(x; u(x)) &= s(x) \quad \forall x \in \Omega, \\ \mathfrak{b}(x; u(x)) &= g(x) \quad \forall x \in \partial\Omega.\end{aligned}$$

$\mathcal{L}$  : partial differential operator,  $\mathfrak{b}$  : boundary operator.

How deep methods do: a deep net  $u(\mathbf{x}; \Theta) \rightarrow u(\mathbf{x})$

$$J(u(\mathbf{x}; \Theta)) = \|r(\mathbf{x}; \Theta)\|_{2,\Omega}^2 + \gamma \|b(\mathbf{x}; \Theta)\|_{2,\partial\Omega}^2,$$

where  $r(\mathbf{x}; \Theta) = \mathcal{L}u(\mathbf{x}; \Theta) - s(\mathbf{x})$ ,  $b(\mathbf{x}; \Theta) = \mathfrak{b}u(\mathbf{x}; \Theta) - g(\mathbf{x})$ , and

$$\|r(\mathbf{x}; \Theta)\|_{2,\Omega}^2 = \int_{\Omega} r^2(\mathbf{x}; \Theta) d\mathbf{x}$$

An optimization problem:  $\min_{\Theta} J(u(\mathbf{x}; \Theta))$

# Deep learning for PDEs

$$\begin{aligned}\mathcal{L}(x; u(x)) &= s(x) & \forall x \in \Omega, \\ \mathfrak{b}(x; u(x)) &= g(x) & \forall x \in \partial\Omega.\end{aligned}$$

$\mathcal{L}$  : partial differential operator,  $\mathfrak{b}$  : boundary operator.

How deep methods do: a deep net  $u(\mathbf{x}; \Theta) \rightarrow u(\mathbf{x})$

$$J_N(u(\mathbf{x}; \Theta)) = \frac{1}{N_r} \sum_{i=1}^{N_r} r^2(\mathbf{x}_\Omega^{(i)}; \Theta) + \hat{\gamma} \frac{1}{N_b} \sum_{i=1}^{N_b} b^2(\mathbf{x}_{\partial\Omega}^{(i)}; \Theta),$$

$\mathbf{x}_\Omega^{(i)}$  drawn from  $\Omega$  and  $\mathbf{x}_{\partial\Omega}^{(i)}$  drawn from  $\partial\Omega$

Key point:  $\min_{\Theta} J(u(\mathbf{x}; \Theta)) \rightarrow \min_{\Theta} J_N(u(\mathbf{x}; \Theta))$  discretize the loss by uniform sampling in general (or other quasi-random methods based on uniform samples)

# Deep learning for PDEs

$$u(\mathbf{x}; \Theta^*) = \arg \min_{\Theta} J(u(\mathbf{x}; \Theta)),$$

$$u(\mathbf{x}; \Theta_N^*) = \arg \min_{\Theta} J_N(u(\mathbf{x}; \Theta)).$$

$$\mathbb{E} (\|u(\mathbf{x}; \Theta_N^*) - u(\mathbf{x})\|_{\Omega}) \leq \underbrace{\mathbb{E} (\|u(\mathbf{x}, \Theta_N^*) - u(\mathbf{x}; \Theta^*)\|_{\Omega})}_{\text{statistical error}} + \underbrace{\|u(\mathbf{x}; \Theta^*) - u(\mathbf{x})\|_{\Omega}}_{\text{approximation error}}$$

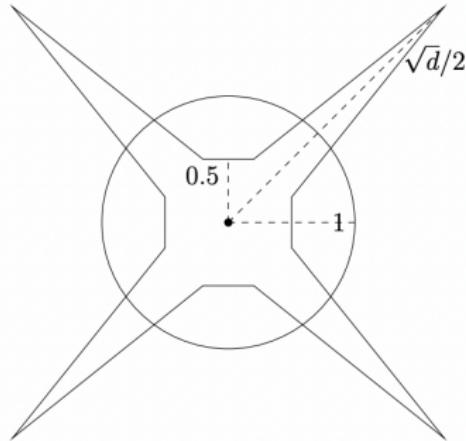
Our work: focus on how to reduce the statistical error

the capability of neural networks → approximation error  
the strategy of loss discretization → statistical error

Key point: how to sample?

# Geometric properties of high-dimensional spaces

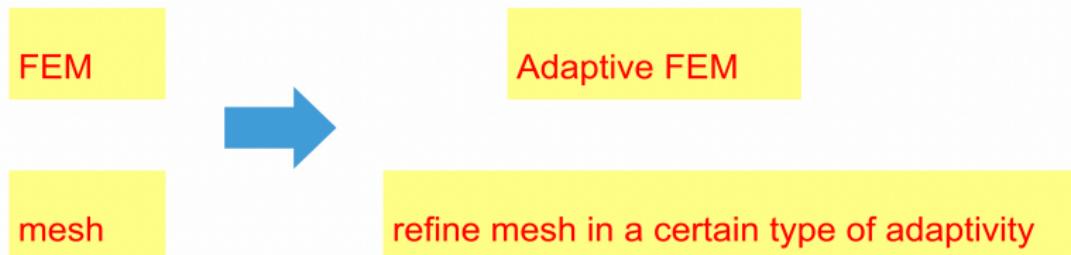
## uniformly distributed points in high-dimensional spaces



Most of the volume of a high-dimensional cube is located around its corner [Vershynin, High-Dimensional Probability, 2020]. Cube:  $[-1, 1]^d$

$$\mathbb{P}(\|\mathbf{x}\|_2^2 \leq 1) \leq \exp\left(-\frac{d}{10}\right).$$

Question: is uniform sampling optimal for deep methods?



Observation:

1. uniform mesh is not optimal for FEM
2. choosing uniform samples is not a good choice for high-dimensional problems

## Deep methods

lack of adaptivity → develop adaptive schemes

## Localized residual

Assume

$$\zeta = \int_{\Omega} 1_I(\mathbf{x}) d\mathbf{x} \approx \int_{\Omega} r^2(\mathbf{x}) d\mathbf{x} \ll 1.$$

A rare event!

Consider a Monte Carlo estimator of  $\zeta$  in terms of uniform samples

$$\hat{P}_{MC} = \frac{1}{N} \sum_{i=1}^N 1_I(\mathbf{x}^{(i)}).$$

The relative error of  $\hat{P}_{MC}$  is

$$\frac{\text{Var}^{1/2}(\hat{P}_{MC})}{\zeta} = N^{-1/2}((1 - \zeta)/\zeta)^{1/2} \approx (\zeta N)^{-1/2}.$$

sample size  $O(1/\zeta)$  → relative error  $O(1)$ .

# Adaptivity

- How does FEM do?

Error estimator

general framework: using an error estimator to refine mesh

- How does deep method do?

???

we need a general framework...

# Deep adaptive sampling method (DAS)

How deep methods do: a viewpoint of variance reduction

$$J_r(u(\mathbf{x}; \Theta)) = \int_{\Omega} r^2(\mathbf{x}; \Theta) d\mathbf{x} = \int_{\Omega} \frac{r^2(\mathbf{x}; \Theta)}{p(\mathbf{x})} p(\mathbf{x}) d\mathbf{x} \approx \frac{1}{N_r} \sum_{i=1}^{N_r} \frac{r^2(\mathbf{x}_{\Omega}^{(i)}; \Theta)}{p(\mathbf{x}_{\Omega}^{(i)})},$$

where  $\{\mathbf{x}_{\Omega}^{(i)}\}_{i=1}^{N_r}$  from  $p(\mathbf{x})$  instead of a uniform distribution.

or relax the definition of  $J_r(u)$

$$J_{r,p}(u(\mathbf{x}; \Theta)) = \int_{\Omega} r^2(\mathbf{x}; \Theta) p(\mathbf{x}) d\mathbf{x} \approx \frac{1}{N_r} \sum_{i=1}^{N_r} r^2(\mathbf{x}_{\Omega}^{(i)}; \Theta),$$

Importance sampling

$$p^* = \frac{r^2(\mathbf{x}; \Theta)}{\mu}, \quad \mu = \int_{\Omega} r^2(\mathbf{x}; \Theta) d\mathbf{x}$$

# Deep adaptive sampling method (DAS)

Sample from  $p(\mathbf{x})$  for a fixed  $\Theta$ : a deep generative model

$$p_{KRnet}(\mathbf{x}; \Theta_f) \approx \mu^{-1} r^2(\mathbf{x}; \Theta)$$

where  $p_{KRnet}(\mathbf{x}; \Theta_f)$  is a PDF induced by KRnet [Tang, Wan and Liao, 2020]; [Tang, Wan and Liao, 2021]

“Error estimator”:  $\hat{r}_X(\mathbf{x}) \propto r^2(\mathbf{x}; \Theta)$

$$D_{KL}(\hat{r}_X(\mathbf{x}) \| p_{KRnet}(\mathbf{x}; \Theta_f)) = \int_B \hat{r}_X \log \hat{r}_X d\mathbf{x} - \int_B \hat{r}_X \log p_{KRnet} d\mathbf{x}.$$

$$\min_{\Theta_f} H(\hat{r}_X, p_{KRnet}) = - \int_B \hat{r}_X \log p_{KRnet} d\mathbf{x}.$$

## Challenge

- design a valid PDF model for efficient sampling

## Deep adaptive sampling method (DAS)

Lemma (Tang, Wan and Yang, 2022)

Assume that  $|\Omega| = 1$  and  $p(\mathbf{x})$  is a PDF satisfying

$$D_{\text{KL}}(p\|p^*) \leq \varepsilon < \infty.$$

For any  $0 < a < \infty$ , we have

$$\mathbb{E} |Q_p[r^2] - \mathbb{E}[r^2]| \leq aN_r^{-1/2} + 2\|r^2/p\|_p \sqrt{\mathbb{P}(|r^2/p - \mu| > a; p)},$$

where

$$Q_p(r^2) = \frac{1}{N_r} \sum_{i=1}^{N_r} \frac{r^2(\mathbf{X}^{(i)})}{p(\mathbf{X}^{(i)})}, \quad \mathbf{X}^{(i)} \stackrel{i.i.d.}{\sim} p(\mathbf{x}),$$

and

$$\mathbb{P}(|r^2/p - \mu| > a; p) \leq \frac{\mu(2\varepsilon)^{1/2}}{a}.$$

# Deep adaptive sampling method (DAS)

## Deep generative models

- GAN [Goodfellow et.al, 2014] [Arjovsky, Chintala and Bottou, 2017]
  - VAE [Kingma and Welling, 2014]
  - NICE [Dinh, Krueger and Bengio, 2014], Real NVP [Dinh, Dickstein, and Bengio, 2016]
- 
- GAN & VAE generate sample efficiently
  - cannot get PDF

# Deep adaptive sampling method (DAS)

KRnet: construct a PDF model via Knothe-Rosenblatt rearrangement, [Tang, Wan and Liao, 2021]

$$\mathbf{z} = f_{KRnet}(\mathbf{x}) = L_N \circ f_{[K-1]}^{\text{outer}} \circ \cdots \circ f_1^{\text{outer}}(\mathbf{x}),$$

$$p_{KRnet}(\mathbf{x}) = p_{\mathbf{Z}}(f_{KRnet}(\mathbf{x})) |\det \nabla_{\mathbf{x}} f_{KRnet}|,$$

where  $f_{[i]}^{\text{outer}}$  is defined as

$$f_{[k]}^{\text{outer}} = L_S \circ f_{[k,L]}^{\text{inner}} \circ \cdots \circ f_{[k,1]}^{\text{inner}} \circ L_R.$$

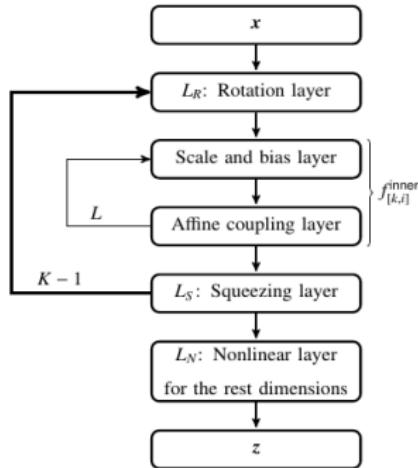
## Advantages

- GAN and VAE can not provide an explicit PDF though they can generate samples efficiently
- KRnet provides an explicit PDF
- KRnet can generate samples efficiently

# Deep adaptive sampling method (DAS)

## structure of KRnet

- squeezing layer
- rotation layer
- affine coupling layer
- nonlinear layer



## Deep adaptive sampling method (DAS)

The framework of DAS (see [Tang, Wan and Yang, 2022] for more details)  
1

// solve PDE

Sample  $m$  samples  $\mathbf{x}_{\Omega,k}^{(i)}$  and Sample  $m$  samples  $\mathbf{x}_{\partial\Omega,k}^{(j)}$ .

Update  $u(\mathbf{x}; \Theta)$  by descending the stochastic gradient of  $J_N(u(\mathbf{x}; \Theta))$ .

// Train KRnet

Sample  $m$  samples from  $\mathbf{x}_{\Omega,k}^{(i)}$ .

Update  $p_{KRnet}(\mathbf{x}; \Theta_f)$  by descending the stochastic gradient of  $H(\hat{r}_X, \hat{p}_{KRnet})$ .

// Refine training set (replace all points: DAS-R; the number of points increases gradually: DAS-G)

Generate  $\mathbf{x}_{\Omega,k+1}^{(i)} \subset \Omega$  through  $p_{KRnet}(\mathbf{x}; \Theta_f^{*,(k+1)})$ .

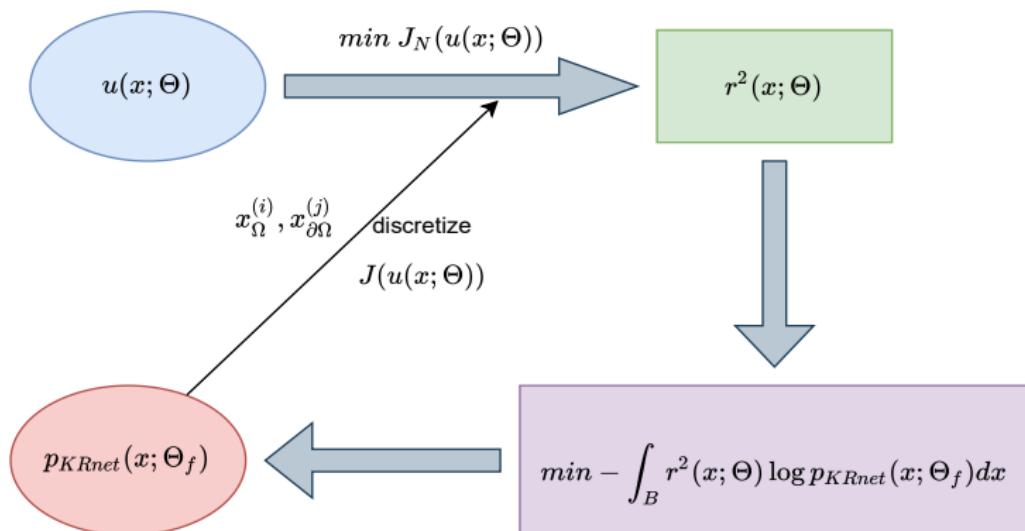
Repeat until stopping criterion satisfies

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<sup>1</sup>K. Tang, X. Wan and C. Yang, DAS: A deep adaptive sampling method for solving partial differential equations, arXiv preprint arXiv:2112.14038, (2022).

# Deep adaptive sampling method (DAS)

The framework of DAS. (see [Tang, Wan and Yang, 2022] for more details)<sup>2</sup>



<sup>2</sup>K. Tang, X. Wan and C. Yang, DAS: A deep adaptive sampling method for solving partial differential equations, arXiv preprint arXiv:2112.14038, (2022).

# Analysis of DAS for PDEs

## Theorem (Tang, Wan and Yang, 2022)

Let  $u(\mathbf{x}; \Theta_N^{*,(k)}) \in F$  be a solution of DAS at the  $k$ -stage where the collocation points are independently drawn from  $\hat{p}_{KRnet}(\mathbf{x}; \Theta_f^{*,(k-1)})$ . Given  $0 < \varepsilon < 1$ , the following error estimate holds under certain conditions

$$\left\| u(\mathbf{x}; \Theta_N^{*,(k)}) - u(\mathbf{x}) \right\|_{2,\Omega} \leq \sqrt{2} C_1^{-1} \left( R_k + \varepsilon + \left\| b(\mathbf{x}; \Theta_N^{*,(k)}) \right\|_{2,\partial\Omega}^2 \right)^{\frac{1}{2}}.$$

with probability at least  $1 - \exp(-2N_r\varepsilon^2/(\tau_2 - \tau_1)^2)$ .

## Corollary (Tang, Wan and Yang, 2022)

If the boundary loss  $J_b(u)$  is zero, then the following inequality holds

$$\mathbb{E}(R_{k+1}) \leq \mathbb{E}(R_k)$$

# Some progresses

## Fokker-Planck equations

- Develop adaptive deep learning techniques for solving Fokker-Planck equations

Adaptive deep density approximation for Fokker-Planck equations, Journal of Computational Physics, 2022.

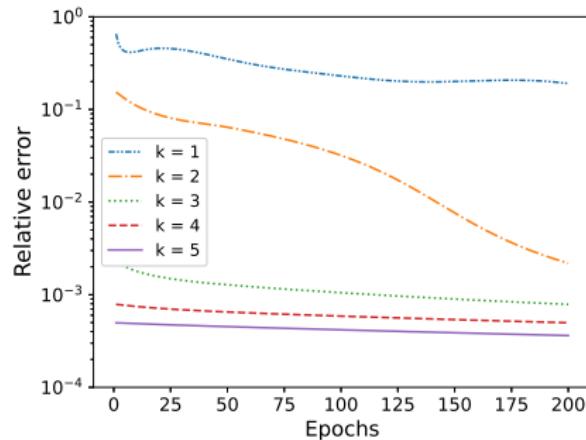
## General high-dimensional PDEs

- Develop adaptive deep learning techniques for solving general PDEs

DAS: A deep adaptive sampling method for solving partial differential equations, preprint, 2022.

# Fokker-Planck equations

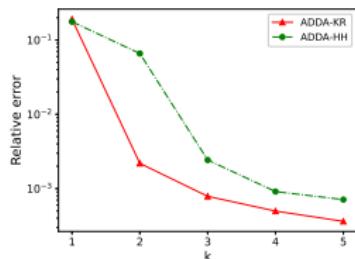
A special case:  $u(\mathbf{x}) = p(\mathbf{x})$



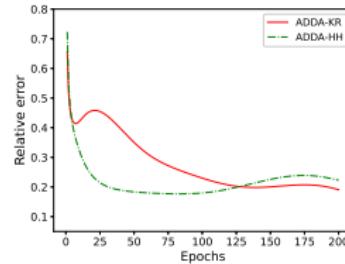
## setting

- $\frac{\partial p(\mathbf{x}, t)}{\partial t} = \nabla \cdot [p(\mathbf{x}, t) \nabla \log(\beta_1 p_1(\mathbf{x}) + \beta_2 p_2(\mathbf{x}))] + \nabla^2 p(\mathbf{x}, t)$
- stationary solution  
 $p_{st}(\mathbf{x}) = \beta_1 p_1(\mathbf{x}) + \beta_2 p_2(\mathbf{x}), \mathbf{x} \in \mathbb{R}^2, p_i(\mathbf{x}) : \text{Gaussian distribution}$

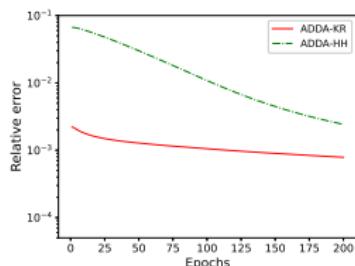
# Fokker-Planck equations



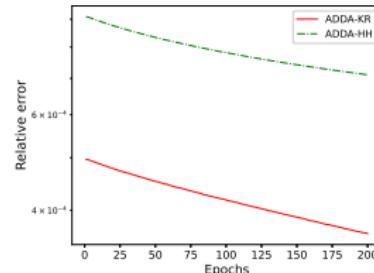
(a) KL divergence w.r.t.  
 $k$ -th model.



(b) The convergence  
behavior for  $k = 1$ .

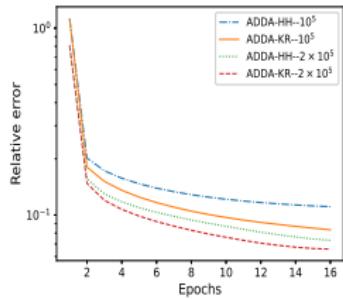


(c) The convergence  
behavior for  $k = 3$ .

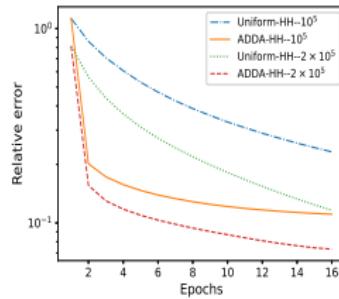


(d) The convergence  
behavior for  $k = 5$ .

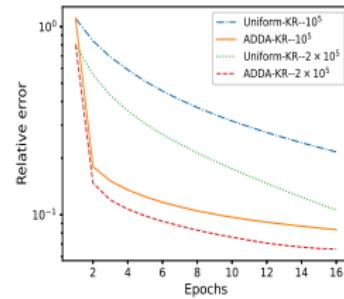
# Fokker-Planck equations



(e) Comparison of KR and HH: KL-divergence w.r.t epochs



(f) KL-divergence w.r.t epochs for HH

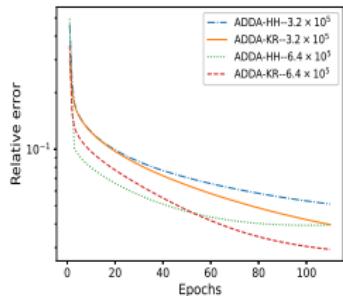


(g) KL-divergence w.r.t epochs for KR

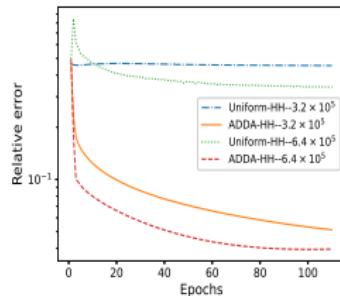
setting (HH: Real NVP)

- $\frac{\partial p(\mathbf{x}, t)}{\partial t} = \nabla \cdot [p(\mathbf{x}, t) \nabla \log(\beta_1 p_1(\mathbf{x}) + \beta_2 p_2(\mathbf{x}))] + \nabla^2 p(\mathbf{x}, t)$
  - stationary solution
- $$p_{st}(\mathbf{x}) = \beta_1 p_1(\mathbf{x}) + \beta_2 p_2(\mathbf{x}), \mathbf{x} \in \mathbb{R}^4, p_i(\mathbf{x}) : \text{Gaussian distribution}$$

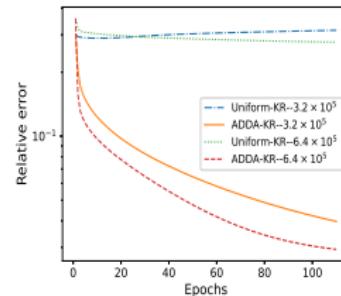
# Fokker-Planck equations



(h) Comparison of KR and HH: KL-divergence w.r.t epochs



(i) KL-divergence w.r.t epochs for HH



(j) KL-divergence w.r.t epochs for KR

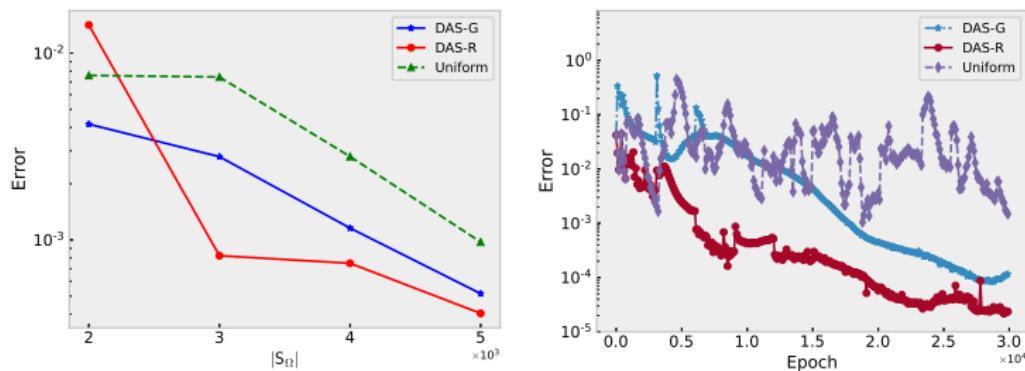
setting

- $\frac{\partial p(\mathbf{x}, t)}{\partial t} = \nabla \cdot [p(\mathbf{x}, t) \nabla \log(\beta_1 p_1(\mathbf{x}) + \beta_2 p_2(\mathbf{x}))] + \nabla^2 p(\mathbf{x}, t)$
- stationary solution  
 $p_{st}(\mathbf{x}) = \beta_1 p_1(\mathbf{x}) + \beta_2 p_2(\mathbf{x}), \mathbf{x} \in \mathbb{R}^8, p_i(\mathbf{x}) : \text{Gaussian distribution}$

# Elliptic PDEs: low-dimensional and low regularity cases

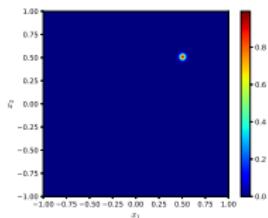
Two-dimensional peak problem

$$\begin{aligned}-\Delta u(x_1, x_2) &= s(x_1, x_2) \quad \text{in } \Omega, \\ u(x_1, x_2) &= g(x_1, x_2) \quad \text{on } \partial\Omega,\end{aligned}$$

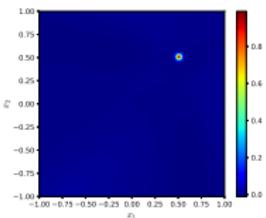


# Elliptic PDEs: low-dimensional and low regularity cases

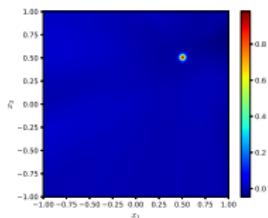
## Two-dimensional peak problem



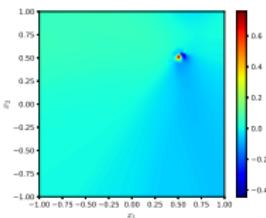
(k) The exact solution.



(l) DAS-R approximation.



(m) DAS-G approximation.

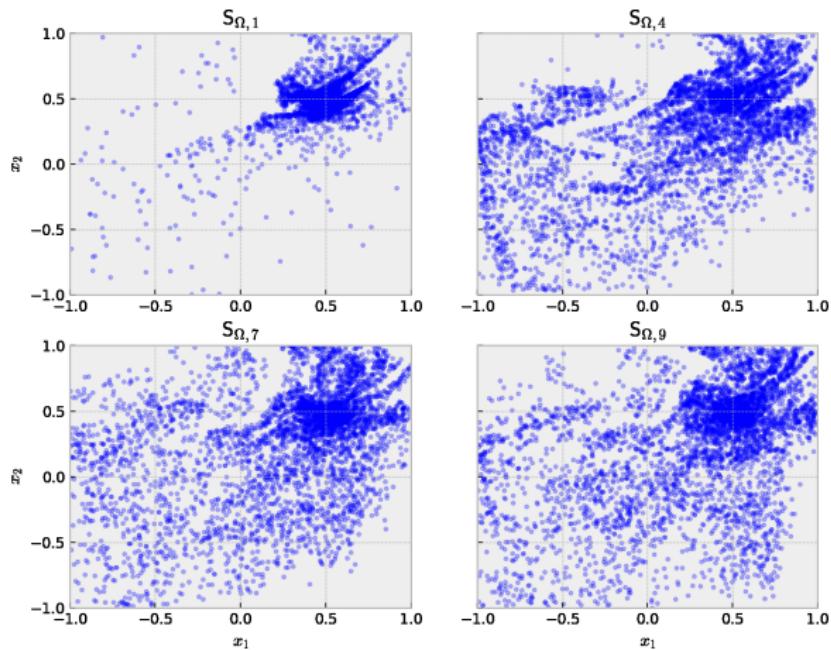


(n) Uniform sampling strategy.

# Elliptic PDEs: low-dimensional and low regularity cases

Two-dimensional peak problem

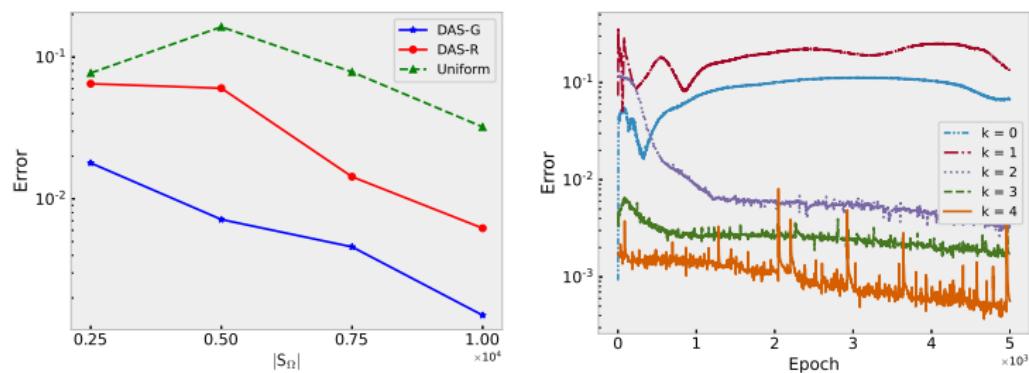
DAS-R samples



# Elliptic PDEs: low-dimensional and low regularity cases

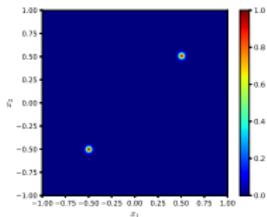
Two-dimensional problem with two peaks

$$\begin{aligned} -\nabla \cdot [u(x_1, x_2) \nabla(x_1^2 + x_2^2)] + \nabla^2 u(x_1, x_2) &= s(x_1, x_2) \quad \text{in } \Omega, \\ u(x_1, x_2) &= g(x_1, x_2) \quad \text{on } \partial\Omega, \end{aligned}$$

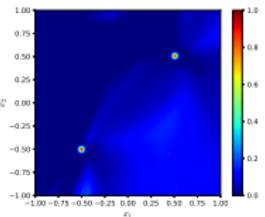


# Elliptic PDEs: low-dimensional and low regularity cases

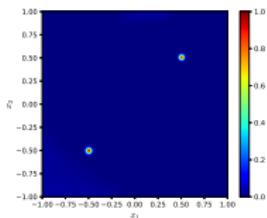
Two-dimensional problem with two peaks



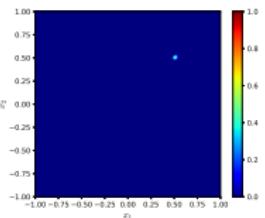
(o) The exact solution.



(p) DAS-R approximation.



(q) DAS-G approximation.

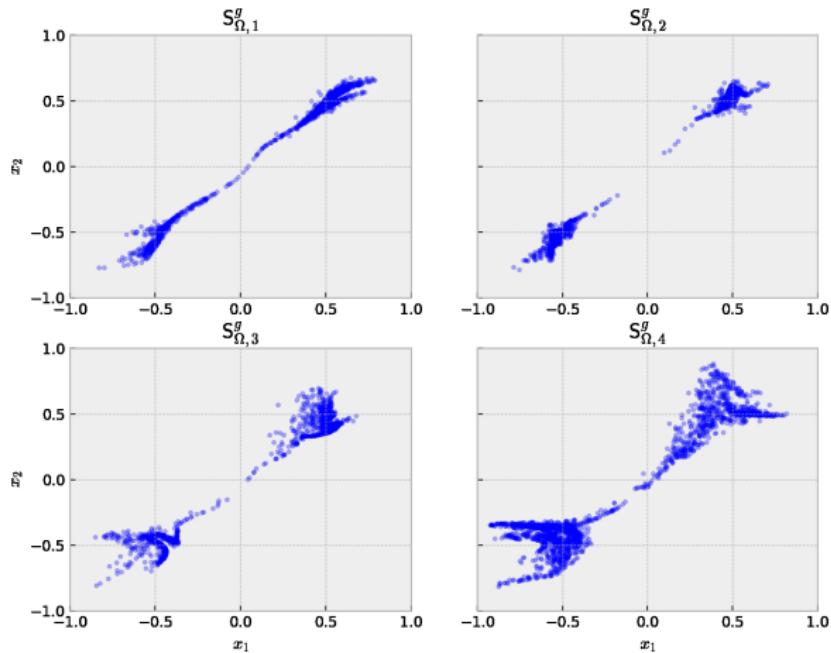


(r) Uniform sampling strategy.

# Elliptic PDEs: low-dimensional and low regularity cases

Two-dimensional problem with two peaks

DAS-G samples



# Linear PDEs: High-dimensional and low regularity cases

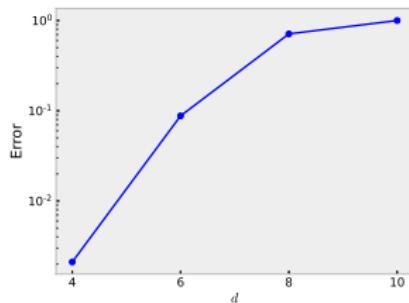
The  $d$ -dimensional linear equation

$$-\Delta u(\mathbf{x}) = s(\mathbf{x}), \quad \mathbf{x} \text{ in } \Omega = [-1, 1]^d,$$

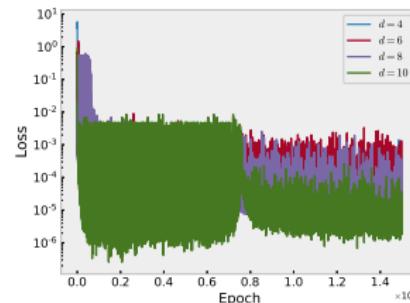
with an exact solution

$$u(\mathbf{x}) = e^{-10\|\mathbf{x}\|_2^2},$$

where the Dirichlet boundary condition on  $\partial\Omega$  is given by the exact solution. **The uniform sampling method becomes less effective as  $d$  increases**



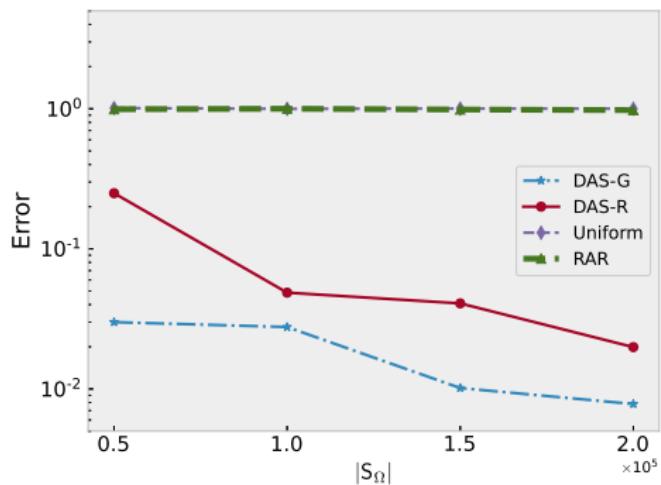
(s) Error



(t) Loss

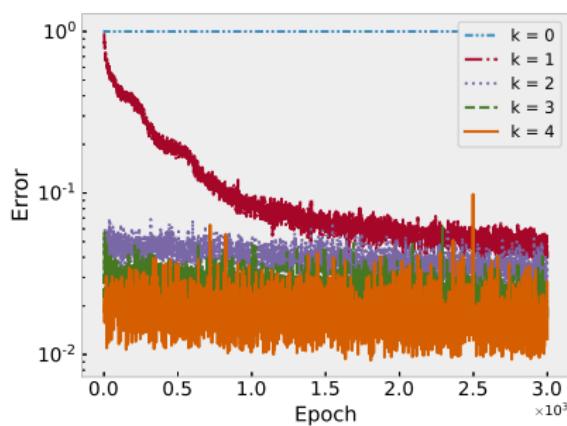
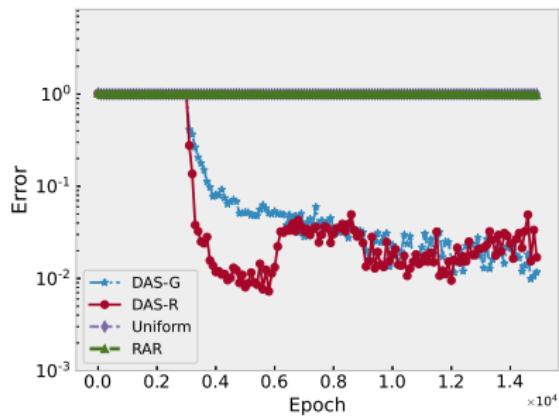
# Linear PDEs: High-dimensional and low regularity cases

The 10-dimensional linear equation



# Linear PDEs: High-dimensional and low regularity cases

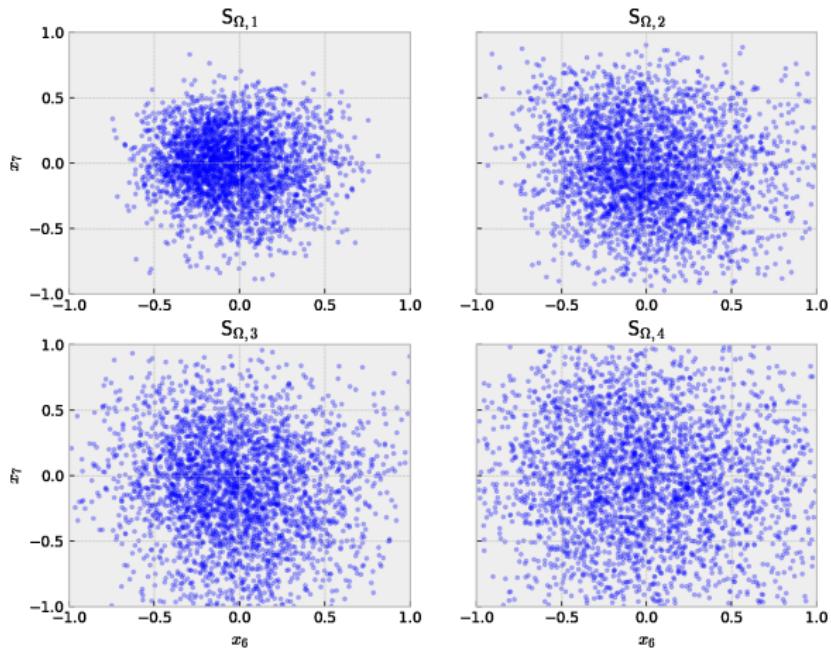
## The 10-dimensional linear equation



# Linear PDEs: High-dimensional and low regularity cases

The 10-dimensional linear equation

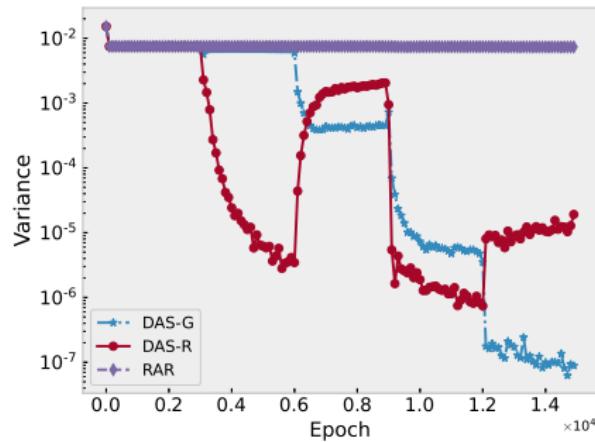
DAS-R samples



# Linear PDEs: High-dimensional and low regularity cases

The 10-dimensional linear equation

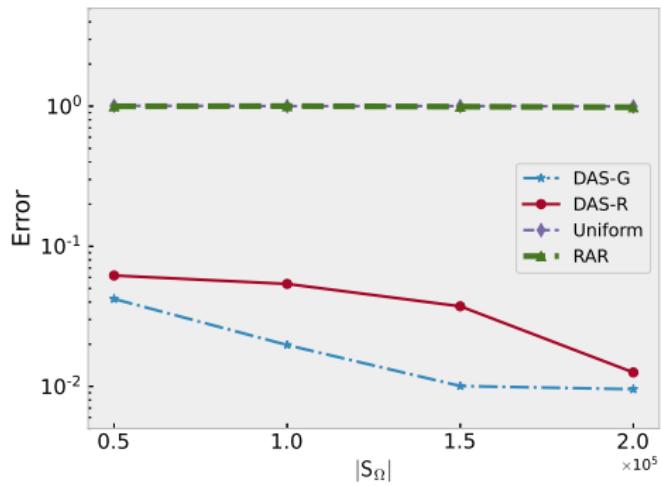
The evolution for the variance of residual



# Nonlinear PDEs: High-dimensional and low regularity cases

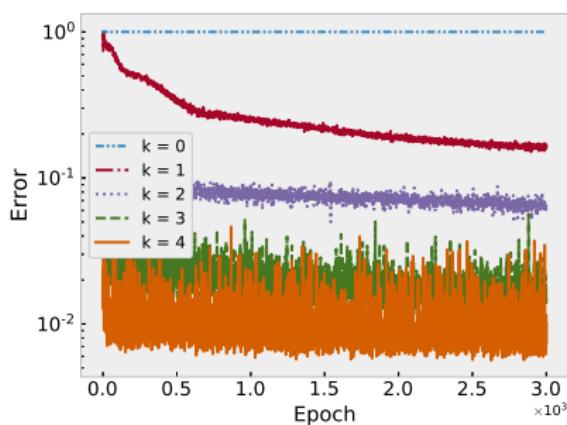
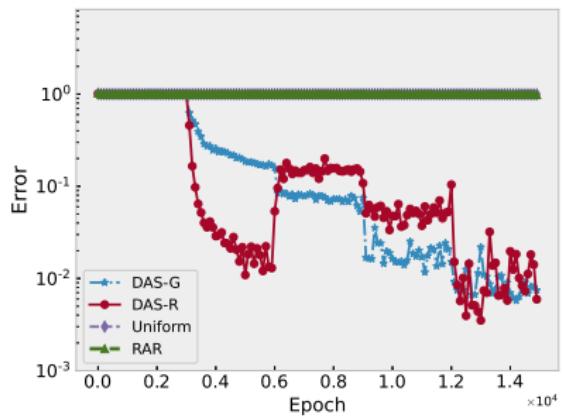
The 10-dimensional nonlinear equation

$$-\Delta u(\mathbf{x}) + u(\mathbf{x}) - u^3(\mathbf{x}) = s(\mathbf{x}), \quad \mathbf{x} \text{ in } \Omega = [-1, 1]^{10}.$$



# Nonlinear PDEs: High-dimensional and low regularity cases

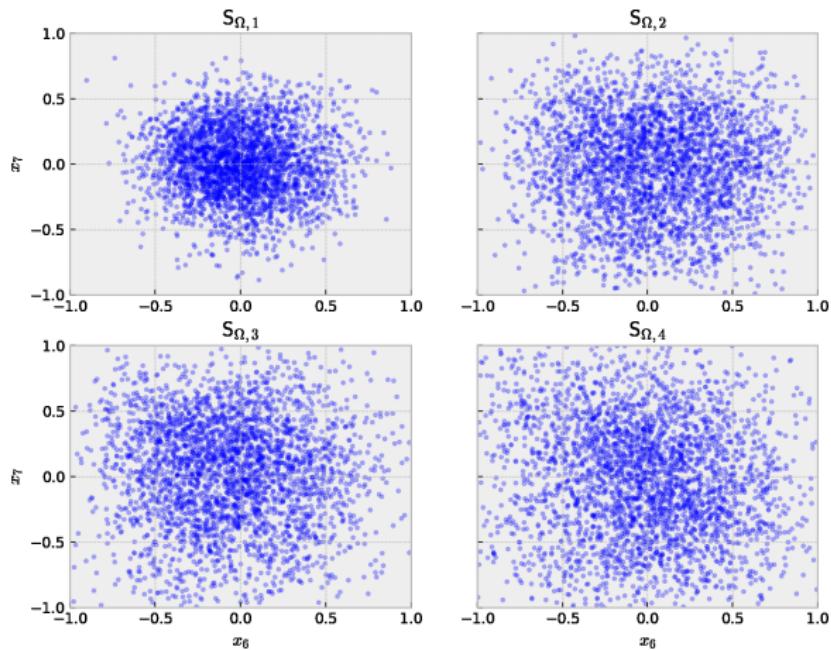
## The 10-dimensional nonlinear equation



# Nonlinear PDEs: High-dimensional and low regularity cases

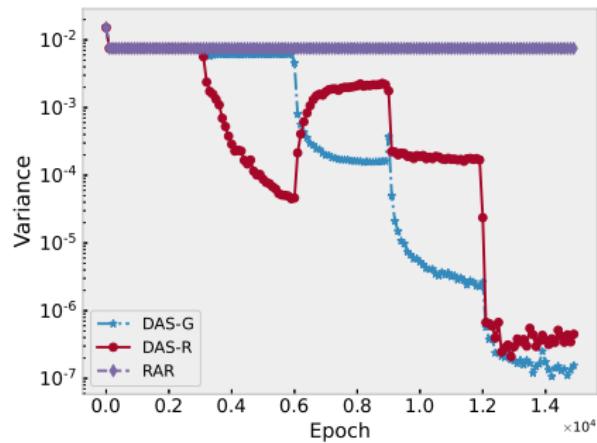
The 10-dimensional nonlinear equation

DAS-R samples



# Elliptic PDEs: High-dimensional and low regularity cases

The 10-dimensional nonlinear equation  
The evolution for the variance of residual



# Summary and outlook

## summary

- a general and flexible adaptive learning strategy using deep generative models for sample generation
- significantly improve the accuracy for PDEs with low regularity problems especially when the dimensionality is relatively large

## outlook

- large scale problems
- more robust and efficient PDF approximation and sample generation
- realistic applications