Deep learning for large time-step simulations of stochastic differential equations

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Outline

1. Introduction

- Stochastic differential equations (SDEs) describe uncertainty in finance, physics, epidemics, etc.
- Accurate numerical schemes are needed to carry out large time step Monte Carlo simulations, but difficult to develop.
- Deep learning techniques have been used to solve PDEs, especially with a physics-informed neural network(Raissi 2017, Yohai 2019, etc) .
- Can deep neural networks learn high-order numerical schemes to solve SDEs?

1.1 Stochastic differential equations

- Considering a generic scalar Itô SDE,

$$dY_t = a(Y_t,t)dt + b(Y_t,t)dW_t, 0 \leq t \leq T, \tag{1}$$

  where Y_t is the random variable with drift $a(Y_t,t)$, variance $b(Y_t,t)$, Wiener process W_t, given initial value $Y_0 := Y_{t=0}$.

- The real-valued random variable Y is defined on the probability space $(\Omega, \Sigma, \mathbb{P})$, with sample space Ω, σ-algebra Σ and probability measure $\mathbb{P}$.

1.2 Strong convergence of numerical solution

Solution in the integral form

$$Y_{t+\Delta t} = Y_t + \int_t^{t+\Delta t} a(Y_s, s)ds + \int_t^{t+\Delta t} b(Y_s, s)dW_s$$

Definition

Let the exact solution of an SDE at time t_i be given by Y_{t_i}, its discrete approximation $\hat{Y}_i$ with time step Δt converges in the strong sense, with order $\beta_s \in \mathbb{R}^+$, if there exists a constant C such that

$$E|Y_{t_i} - \hat{Y}_i| \le C(\Delta t)^{\beta_s}. \tag{2}$$

1.3 Numerical discretization

Classical Numerical schemes

Euler-Maruyama (strong order β_s = 0.5):

$$Y_{t+\Delta t} = Y_t + a(Y_t)\Delta t + b(Y_t)\sqrt{\Delta t}Z$$

Milstein (strong order β_s = 1.0):

$$Y_{t+\Delta t} = Y_t + a(Y_t)\Delta t + b(Y_t)\sqrt{\Delta t}Z + \frac{1}{2}b'(Y_t)b(Y_t)\Delta t(Z^2 - 1),$$

where $b'(Y)$ is the first derivative of $b(Y)$, $Z \sim N(0, 1)$.

1.4 Higher-order numerical approximation

How to improve numerical accuracy?

- Include higher-order terms[1]: ODE Runge-Kutta schemes plus high-order random terms of Itô calculus. There are 8 terms when β_s = 1.5, and 12 terms when β_s = 2.0.

$$Y_{t+\Delta t} = \underbrace{Y_t + a(Y_t)\Delta t + b(Y_t)\sqrt{\Delta t} Z + \frac{1}{2} b'(Y_t) b(Y_t) \Delta t (Z^2 - 1) + \ldots}_{\text{12 terms}}$$

High-order schemes are expensive to develop and implement.

- Reduce time step Δt, e.g., finer time grid.
The computational cost grows rapidly with more time points.

[1] Eckhard Platen (1999). An introduction to numerical methods for stochastic differential equations. Acta Numerica.

1.5 Coefficients of numerical schemes

- Euler-Maruyama, $Y_{t+\Delta t} = \underbrace{Y_t + a(Y_t)\Delta t}_{\alpha_0} + \underbrace{b(Y_t)\sqrt{\Delta t}}_{\alpha_1} Z$, where,

$$\begin{cases} \alpha_0 := Y_t + a(Y_t, t)\Delta t, \\ \alpha_1 := b(Y_t, t)\sqrt{\Delta t}, \end{cases} \tag{3}$$

The coefficients are a function of model parameters and time.

$$\alpha_j = \bar{H}_j \left(Y_t, a(Y_t, t), b(Y_t, t), t, \Delta t\right). \tag{4}$$

$\Rightarrow$Is it possible to learn these functions using machine learning?

2. Stochastic collocation method

Stochastic collocation Monte Carlo sampler (SCMC)[2]:

- Two scalar random variables, Y and X, are connected by,

$$F_Y(Y) \overset{d}{=} U \overset{d}{=} F_X(X), \tag{5}$$

where $U \sim \mathcal{U}([0,1])$ uniform distribution, cumulative distribution functions (CDF) $F_Y(\bar{y}) := P(Y \leq \bar{y})$ and $F_X(\bar{x}) := P(X \leq \bar{x})$.

- When $F_Y(\bar{y})$ and $F_X(\bar{x})$ are strictly monotonic, we have

$$\bar{y} = F_Y^{-1}(F_X(\bar{x})) := g(\bar{x}). \tag{6}$$

where the function $g(\cdot)$ maps sample $\bar{x}$ from X to sample $\bar{y}$ from Y, in the sense of both distribution and element-wise.

[2] L. A. Grzelak, etc (2019). The stochastic collocation Monte Carlo sampler. Quantitative Finance.

2.1 Stochastic collocation method

- Choosing optimal collocation points $(\hat{x}_j, \hat{y}_j)$ to approximate,

$$\bar{y} = g(\bar{x}) \approx \hat{g}_m(\bar{x}) = \sum_{j=1}^{m} \hat{y}_j \ell_j(\bar{x}),$$

  where $\hat{y}_j = F_Y^{-1}(F_X(\hat{x}_j))$, $\ell_j(\bar{x})$ interpolation basis functions.
- The polynomial chaos expansion reads

$$Y = \sum_{j=1}^{m} \alpha_{j-1} X^{j-1} = \alpha_0 + \alpha_1 X + ... + \alpha_{m-1} X^{m-1}, \qquad (7)$$

  where the coefficients are computed by

$$\mathbf{A}\boldsymbol{\alpha} = \hat{\mathbf{y}}$$

$$\begin{pmatrix} 1 & \hat{x}_1^1 & \hat{x}_1^2 & \dots & \hat{x}_1^{m-1} \\ 1 & \hat{x}_2^1 & \hat{x}_2^2 & \dots & \hat{x}_2^{m-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \hat{x}_m^1 & \hat{x}_m^2 & \dots & \hat{x}_m^{m-1} \end{pmatrix} \begin{pmatrix} \hat{\alpha}_0 \\ \hat{\alpha}_1 \\ \vdots \\ \hat{\alpha}_{m-1} \end{pmatrix} = \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_m \end{pmatrix}$$

2.2 SCMC algorithm

- The Cameron-Martin Theorem (1947) states that polynomial chaos approximations based on the normal distribution converge to any distribution.
- An increasing polynomial order in SCMC leads to exponential convergence.

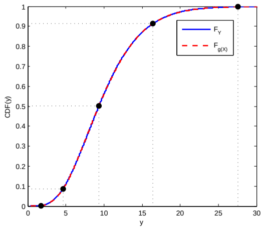
SCMC algorithm

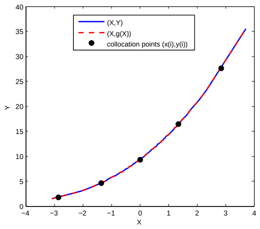
1. Calculate the CDF $F_X(\hat{x}_j)$ on m collocation points $(\hat{x}_1, \hat{x}_2, ..., \hat{x}_m)$ to obtain m pairs $(\hat{x}_j, F_X(\hat{x}_j))$;
2. Invert the CDF by $\hat{y}_j = F_Y^{-1}(F_X(\hat{x}_j))$ to form m triples $(\hat{x}_j, F_X(\hat{x}_j), \hat{y}_j)$;
3. Compute the interpolation function $\bar{y} = \hat{g}(\bar{x})$ on m pairs $(\hat{x}_j, \hat{y}_j)$.

2.3 An example of SCMC

Cheap distribution $X \sim \mathcal{N}(0,1)$, Gauss quadrature points $\hat{x}_i$; expensive distribution $Y \sim \Gamma(5,2)$, optimal collocation points $\hat{y}_i = F_Y^{-1}(F_X(\hat{x}_i))$, m=5 collocation points.

	$\hat{x}_1$	$\hat{x}_2$	$\hat{x}_3$	$\hat{x}_4$	$\hat{x}_5$
$\hat{x}_i$	-2.8570	-1.3556	0.0	1.3556	2.8570
$F_X(\hat{x}_i)$	0.0021	0.0876	0.50	0.9124	0.9979
$F_Y^{-1}(F_X(\hat{x}_i))$	1.7543	4.6651	9.3418	16.4443	27.5888





Stochastic collocation points parameterize the CDFs.

2.4 Connection between classical MC and SCMC

We aim to draw a conditional sample from the distribution,

$$F_{Y_{t+\Delta t}}(\bar{y}|Y_t = Y_i) \sim P(Y_{t+\Delta t} < \bar{y}|Y_t = Y_i).$$

For example, when there are three collocation points $m = 3$,

- SCMC reads

$$Y_{t+\Delta t} = \sum_{j=1}^{3} \alpha_{j-1} X^{j-1} = \alpha_0 + \alpha_1 X + \alpha_2 X^2,$$

- The Milstein scheme reads,

$$\begin{cases} X := Z \\ \alpha_0 := Y_i + a(Y_i, t_i)\Delta t + \frac{1}{2} b'(Y_i, t_i) b(Y_i, t_i), \\ \alpha_1 := b(Y_i, t_i)\sqrt{\Delta t}, \\ \alpha_2 := \frac{1}{2} b'(Y_i, t_i) b(Y_i, t_i). \end{cases}$$

2.5 Connection between classical MC and SCMC

$\Rightarrow$ These coefficients vary at different time points,

$$\boldsymbol{\alpha}_{i+1} = \bar{\mathbf{H}}_j \left(Y_i, a(Y_i, t_i), b(Y_i, t_i), t_i, \Delta t\right). \tag{8}$$

$$\mathbf{A}\boldsymbol{\alpha}_{\mathbf{i+1}} = \hat{\mathbf{y}}_{\mathbf{i+1}}$$

$$\begin{pmatrix} 1 & \hat{x}_1^1 & \hat{x}_1^2 & \dots & \hat{x}_1^{m-1} \\ 1 & \hat{x}_2^1 & \hat{x}_2^2 & \dots & \hat{x}_2^{m-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \hat{x}_m^1 & \hat{x}_m^2 & \dots & \hat{x}_m^{m-1} \end{pmatrix} \begin{pmatrix} \hat{\alpha}_{i+1,0} \\ \hat{\alpha}_{i+1,1} \\ \vdots \\ \hat{\alpha}_{i+1,m} \end{pmatrix} = \begin{pmatrix} \hat{y}_{i+1,1} \\ \hat{y}_{i+1,2} \\ \vdots \\ \hat{y}_{i+1,m} \end{pmatrix},$$

$$\hat{\mathbf{y}}_{i+1} = \hat{\mathbf{H}} \left(Y_i, a(Y_i, t_i), b(Y_i, t_i), t_i, \Delta t\right). \tag{9}$$

$\Rightarrow$ Stochastic collocation points vary at different time points.

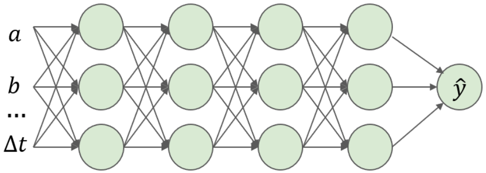
PS: for Markov processes, $\hat{\mathbf{y}}_{i+1} = \hat{\mathbf{H}} \left(Y_i, a(Y_i, t_i), b(Y_i, t_i), \Delta t\right)$ does not depend time t_i.

2.6 Learn stochastic collocation points

There are two options to determine these coefficients at time t_i,

- Output the coefficients inferred from SC points;
- Output SC points, inferring coefficients $\boldsymbol{\alpha}_{i+1} = \mathbf{A}^{-1}\hat{\mathbf{y}}_{\mathbf{i+1}}$.

  $\Rightarrow$ SC points have physical meaning and are interpretable.



$$\hat{\mathbf{y}}_{i+1} = \hat{\mathbf{H}}\left(Y_i, a(Y_i, t_i), b(Y_i, t_i), t_i, \Delta t\right).$$

3. Deep Neural Networks

Artificial neural networks are used as function approximators.

- Fully connected neural networks are a composite function,

$$H(x|\theta) = h^{(L)}(...h^{(2)}(h^{(1)}(x;\theta^{(1)});\theta^{(2)});...\theta^{(L)})$$

where $\theta = (\mathbf{W}_i, \mathbf{b}_i)$, $\mathbf{W}_i$ weights and $\mathbf{b}_i$ bias each hidden layer.

- Supervised learning to approximate the target function,

$$\operatorname*{argmin}_{\theta} \text{Loss}(\theta) := \operatorname*{argmin}_{\theta} \sum D(F(x_i|\theta), y_i),$$

where $D(\cdot,\cdot)$ measures the difference between $H(x_i|\theta)$ and y_i.

3.1 Approximation capacity

Why deep neural networks?

- Universal approximation theorem.
- Expressive power grows exponentially with the depth of ANN.

Deep neural networks[3]

Give any $\hat{\epsilon} \in (0,1)$, there exists a neural network which is capable of approximating any function from $F_{d,n}$ (d inputs, up to n-th derivatives) with error $\hat{\epsilon}$, using the following configurations:

- at least piece-wise activation functions,
- at least $c(\ln(1/\hat{\epsilon})+1)$ hidden layers and $c\hat{\epsilon}^{-d/n}(\ln(1/\hat{\epsilon})+1)$ weights and computation units, where $c := c(d,n)$ is constant, depending two parameters d and n.

$\Rightarrow$ An arbitrary approximation error can always be achieved with a sufficient bounded number of hidden layers and nodes.

[3] Dmitry Yarotsky (2017). Error bounds for approximations with deep ReLU networks.

3.2 Error from SCMC

When Gauss-Hermite quadrature is used, let $f_X(x)$ represent weight function, ω_i quadrature weights, $\Psi(x) = (g(x) - \hat{g}(x))^2$ the difference of distribution functions, M collocation points,

$$\int_R \Psi(x) f_X(x) = \sum_{i=1}^{M} \Psi(x_i)\omega_i + \epsilon_M,$$

where the approximation error is

$$\epsilon_M = \frac{M!\sqrt{\pi}}{2^M} \frac{\Psi^{(2M)}(\hat{\xi}_1)}{(2M)!}, \tag{10}$$

$\Rightarrow$ The error of SCMC exponentially converges to zero when the number of stochastic collocation points grows.

3.3 Estimating strong error of ANN-SCMC

ANN-SCMC strong convergence

When the approximation errors from ANN and SCMC are zero, ANN-SCMC has a strong convergence,

$$E|Y_{t_i} - \hat{Y}_i| \leq \epsilon(\Delta\tau) \leq C(\Delta t)^{\beta_s},$$

where time step $\Delta\tau$ is used to create (off-line) training data, and actual time step Δt is for prediction (on-line), $\Delta\tau << \Delta t$.

- During off-line training, small $\Delta\tau$ guarantees small error $\epsilon(\Delta\tau)$.
- When using the trained ANN-SCMC to solve SDEs, strong error $\epsilon(\Delta\tau)$ stays regardless of actual time step Δt.

3.4 ANN-SCMC numerical solver

1. Train ANN-SCMC off-line for $\hat{\mathbf{y}} = \hat{\mathbf{H}}\left(\cdot\right)$ based on generated data (e.g., using any classical MC with time step $\Delta\tau$).
2. Compute collocation points at time $t_{i+1} = t_i + \Delta t$, given $Y_i, a(Y_i, t_i), b(Y_i, t_i)$ at time t_i,

$$\hat{\mathbf{y}}_{i+1} = \hat{\mathbf{H}}\left(Y_i, a(Y_i, t_i), b(Y_i, t_i), t_i, \Delta t\right).$$

3. Calculate the coefficients $\boldsymbol{\alpha}_{i+1}$ through $\boldsymbol{\alpha}_{i+1} = \mathbf{A}^{-1}\hat{\mathbf{y}}_{\mathbf{i+1}}$.
4. Implement the polynomial expansion for all sample paths,

$$Y_{i+1} = \sum_{j=1}^{m} \alpha_{i+1,j-1} Z^{j-1}.$$

5. Return to Step 2 by $t_{i+1} \to t_i$, iterating until terminal time T.

4. Numerical experiments

When $a(Y_t, t) = \mu Y_t$ and $b(Y_t, t) = \sigma Y_t$, we have Geometric Brownian Motion (GBM),

$$dY_t = \mu Y_t dt + \sigma Y_t dW_t, 0 \leq t \leq T,$$

where drift μ and volatility σ are constant, with initial value Y_0.

- The Milstein scheme,

$$Y_{i+1,j} = Y_{ij}\left(1 + \mu\Delta t + \frac{1}{2}\sigma^2\Delta t\right) + \left(\sigma Y_{ij}\sqrt{\Delta t}\right) Z + \left(\frac{1}{2}\sigma^2 Y_{ij}\Delta t\right) Z^2,$$
$$\begin{cases} \alpha_{i+1,0} := Y_{ij} + Y_{ij}\mu\Delta t + \frac{1}{2}\sigma^2 Y_{ij}\Delta t, \\ \alpha_{i+1,1} := \sigma Y_{ij}\sqrt{\Delta t}, \\ \alpha_{i+1,2} := \frac{1}{2}\sigma^2 Y_{ij}\Delta t. \end{cases}$$

- For GBM, the conditional collocation points of ANN-SCMC, $\hat{\mathbf{y}}_{i+1} = \hat{\mathbf{H}}(\mu, \sigma, Y_i, \Delta t)$, are independent of time t.

4.1 ANN settings and off-line training

Hyper-parameters	Options
Hidden layers	4
Neurons (each layer)	50
Activation	Softplus
Initialization	Glorot_uniform
Optimizer	Adam
Batch size	1024
Training epochs	1700
Initial Learning rate	1e-3

ANN	Parameters	Value range	Method
input	drift, μ	[0.05, 0.50]	LHS
	volatility, σ	(0.0, 0.60]	LHS
	initial value, Y_0	(0.0, 15.0]	LHS
	time horizon, τ_{max}	(0, 4.0]	Equally
$\hat{H}_0(\cdot)$ output	point, $\hat{y}_0$	$(0.0, 15.5)$	SCMC
$\hat{H}_1(\cdot)$ output	point, $\hat{y}_1$	$(0.0, 15.5)$	SCMC
$\hat{H}_2(\cdot)$ output	point, $\hat{y}_2$	$(0.0, 17.5)$	SCMC
$\hat{H}_3(\cdot)$ output	point, $\hat{y}_3$	$(0.0, 20.0)$	SCMC
$\hat{H}_4(\cdot)$ output	point, $\hat{y}_4$	$(0.0, 32.5)$	SCMC
$\hat{H}_5(\cdot)$ output	point, $\hat{y}_5$	$(0.0, 55.0)$	SCMC

Training data, $\Delta\tau \to 0.0$ means using analytic solution of GBM.

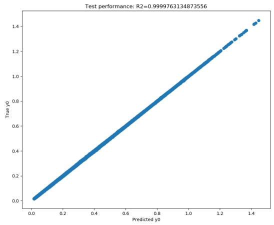
4.2 Performance of ANN-SCMC

- Approximation performance on the test dataset.

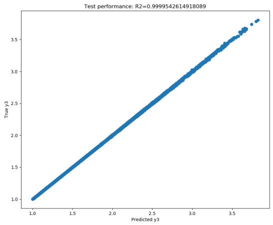
  $\hat{y}_i^a =$ ANN-SCMC, $\hat{y}_i =$ ground truth. $\hat{x}_i$ independent of time. $R^2(\hat{y}_i, \hat{y}_i^a)$ goodness of fit.

	$\hat{x_1}$	$\hat{x_2}$	$\hat{x_3}$	$\hat{x_4}$	$\hat{x_5}$
$\hat{x}_i$	-2.8570	-1.3556	0.0	1.3556	2.8570
$F_X(\hat{x}_i)$	0.0021	0.0876	0.50	0.9124	0.9979
$R^2(\hat{y}_i, \hat{y}_i^a)$	0.99997	0.99999	0.99997	0.99995	0.99951

- Predicted vs true collocation points, for example,



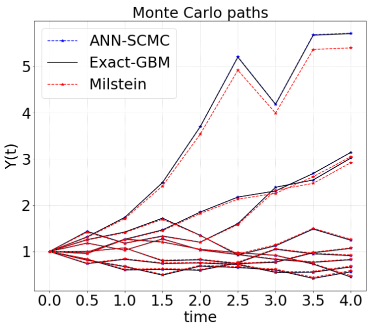
(a) $\hat{y}_2^a$ vs $\hat{y}_2$



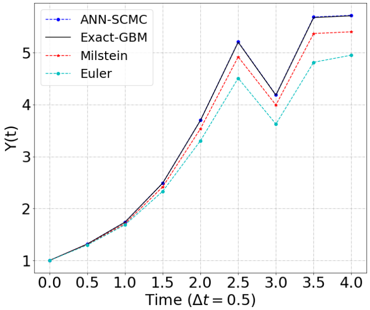
(b) $\hat{y}_3^a$ vs $\hat{y}_3$

4.3 Path-wise error

- Monte Carlo path-wise error:



(c) Monte Carlo paths

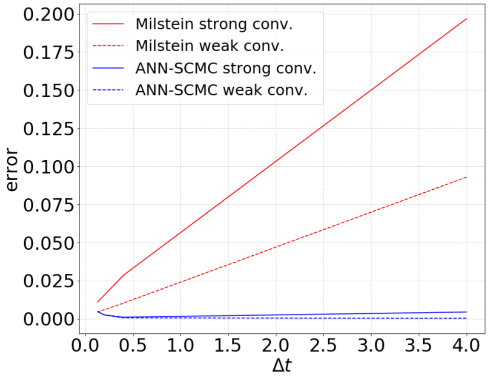


(d) Comparing Euler

$$\sigma = 0.3,\ r = 0.1,\ S_0 = 1.0,\ \Delta t = 0.5.$$

4.4 Convergence error

- Comparing strong convergences based on the closed-form solution of GBM.



Varying time step size, the averaged error over 1000 samples.

4.5 Application: Option pricing

- For Bermudan options, the holder has the right to exercise the contract at pre-specified dates up to maturity.
- Price Bermudan put options via Longstaff-Schwartz approach.
- Setting: under the risk-neutral measure, stock price $Y_0 = 1.0$, risk-less interest rate $r = 0.1$, strike $K = 1.1$, terminal time $T = \Delta t \times M_B$, the number of monitoring dates M_B, time step Δt, the number of sample paths $N = 100000$.

4.6 Bermudan option with big time steps

- Reference value V_{ref}=Analytic MC, from analytical paths of GBM; Relative error $|\frac{V_{ref}-V}{V_{ref}}|$; Time step $\Delta t = 0.4$.

	method	M_B=5	M_B=10	M_B=20
	Analytic MC	0.14806 (0.00%)	0.16313 (0.00%)	0.17338 (0.00%)
	Milstein MC	0.14353 (3.06%)	0.15734 (3.55%)	0.16642 (4.01%)
σ=0.30	ANN-SCMC	0.14780 (0.04%)	0.16305 (0.05%)	0.17322 (0.09%)
	Analytic MC	0.19716 (0.00%)	0.22464 (0.00%)	0.24454 (0.00 %)
	Milstein MC	0.19069 (3.29%)	0.21616 (3.78%)	0.23448 (4.11 %)
σ=0.40	ANN-SCMC	0.19711 (0.03%)	0.22454 (0.04%)	0.24438 (0.06%)

5. Summary and Outlook

Conclusions:

- ANN-SCMC provides a data-driven numerical solver for SDEs;
- Implement large time-step simulations with a small error in strong convergence;
- More accurate than classical schemes.

Ongoing work:

- Test ANN-SCMC on more complicated SDEs;
- Increase the computation speed.

References

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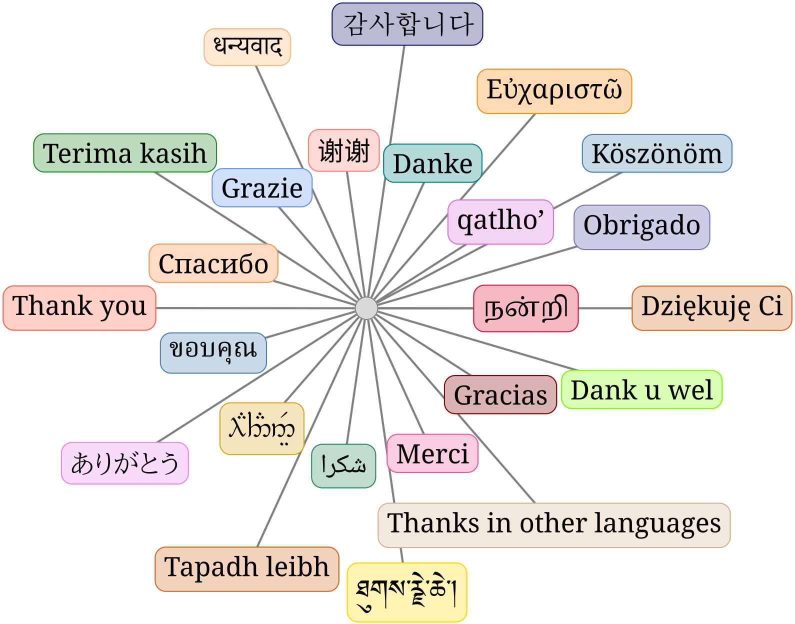
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Εὐχαριστῶ
Terima kasih
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Danke
Köszönöm
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Спасибо
Thank you
நன்றி
Dziękuję Ci
ขอบคุณ
Gracias
Dank u wel
ありがとう
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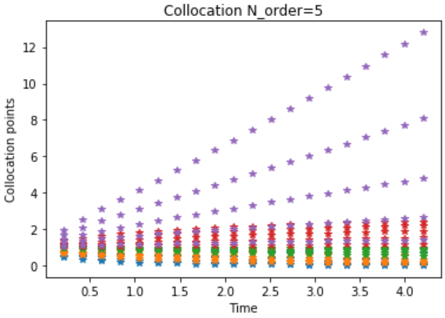
Backup: Stochastic collocation points



(e) Order-5