Algorithms and Scientific Software for Quasi-Monte Carlo, Fast Gaussian Process Regression, and Scientific Machine Learning

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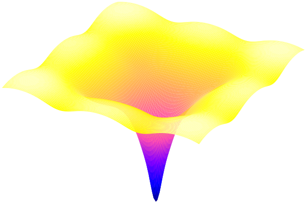
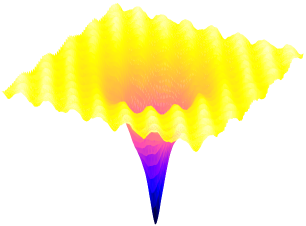
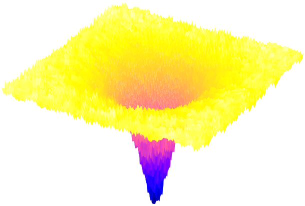
PhD Defense. Illinois Institute of Technology, Department of Applied Mathematics. 2025.

SE grid	SI lattice	DSI digital net
error = 3.7e-2	error = 2.8e-2	error = 2.6e-2
time = 1.6e0	time = 8.0e-4	time = 1.5e-3
MLL = 6.3e3	MLL = -3.8e2	MLL = -4.5e3







Quasi-Monte Carlo (QMC) Background

Efficient algorithms for high-dimensional numerical integration

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Efficient algorithms for high-dimensional numerical integration

Motivation

- QMC methods replace independent points with low-discrepancy (LD) points
- LD sequences evenly cover the unit cube in high dimensions
- QMC has faster convergence for "smooth" functions [81, 23, 63, 25, 72, 105, 24]
- Randomizing LD sequences [22, 83, 70, 71, 84, 78, 119] helps to
  - Enable QMC error estimation, e.g., using randomizations of LD points for IID estimates
  - Avoid boundary observations, as randomized LD points lie in $(0, 1)$ almost surely
  - Avoid fooling functions, which are theoretically possible for deterministic LD sequences

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Applications

- Financial modeling, especially for option pricing [53, 67, 68, 69, 126, 38]
- Solving PDEs (partial differential equations) [41, 65, 66, 42, 64, 101]
- Ray tracing, for simulating light transport in graphics rendering [51, 91, 121]

IID Points versus Randomized Low-Discrepancy (LD) Sequences

IID (independent identically distributed) points have gaps and clusters. LD points have more even coverage.

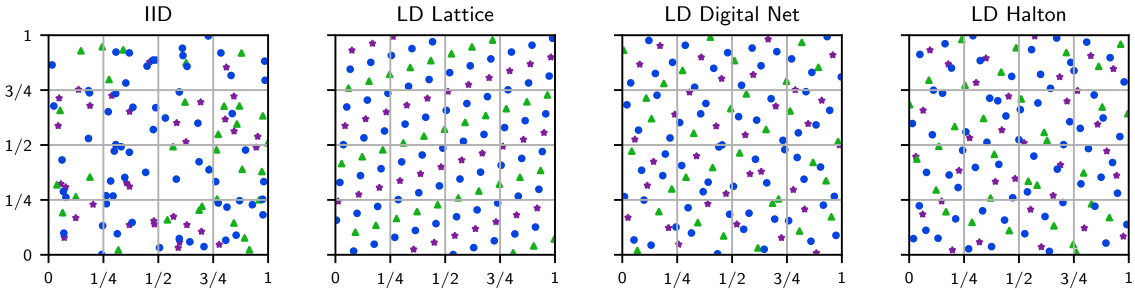

Figure: Purple stars for the first 32 points, green triangles for the next 32, and blue circles for the subsequent 64. Extensible constructions of a lattice with a random shift, a digital net with a nested uniform scramble, and a Halton point set with a linear matrix scramble and permutation scramble.

Quasi-Monte Carlo with LD Points vs IID Monte Carlo

The more even coverage of LD points enables QMC to converge faster for "smooth" functions

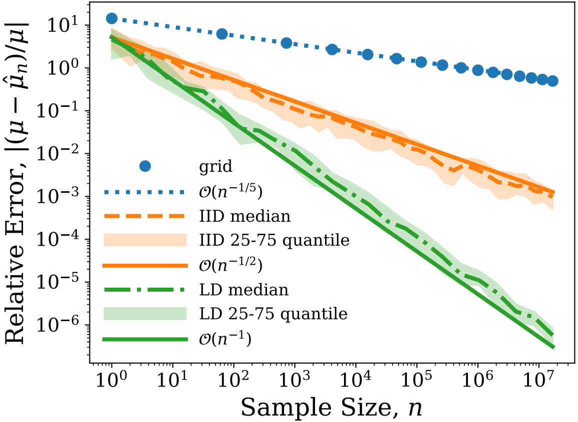

Figure: Approximation of the 6-dimensional Keister function [58].

Gaussian Process (GP) Regression Background

Flexible interpolation models with built-in uncertainty quantification (UQ) [94, 31]

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Advantages

- UQ from (computable) posterior distribution conditioned on observations
- Equivalent to kernel interpolation in a RKHS (reproducing kernel Hilbert space)

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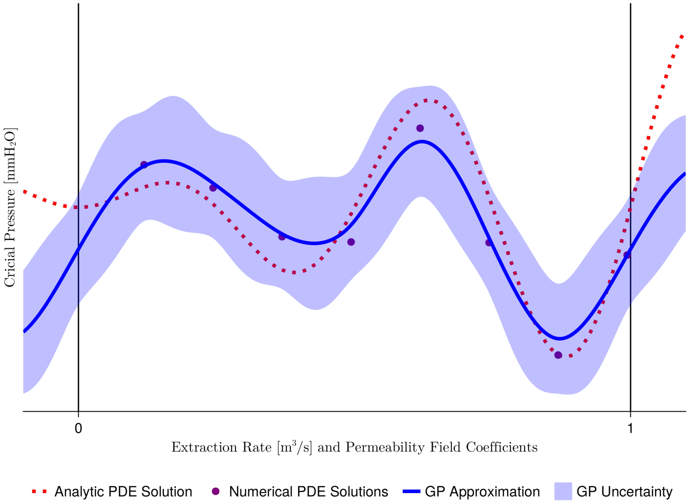
- Bayesian optimization, for finding global minima of expensive simulations [32, 106, 125].
- Solving PDEs, with deterministic [18, 14, 15, 6, 75] or random coefficients [54, 55, 5, 114]
- Bayesian cubature, possible since the integral of a GP is still Gaussian [9, 82, 36, 96, 97, 95]
- Reliability analysis, to efficiently predict the probability of system failure [92, 98, 28, 3, 127, 109]

Gaussian Processes (GPs) for Interpolation with Uncertainty Quantification



Multitask Gaussian Processes (MTGPs)

For modeling correlated simulations which capture inter-task and intra-task covariance [7, 10]

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Applications

- Multitask Bayesian optimization, for multi-objective- or meta-learning [118, 60, 49, 20, 112]
- Medical treatment analysis, for modeling correlated treatment effects [1, 29, 33, 13]
- Engineering applications, for performance metrics under design controls [11, 74]

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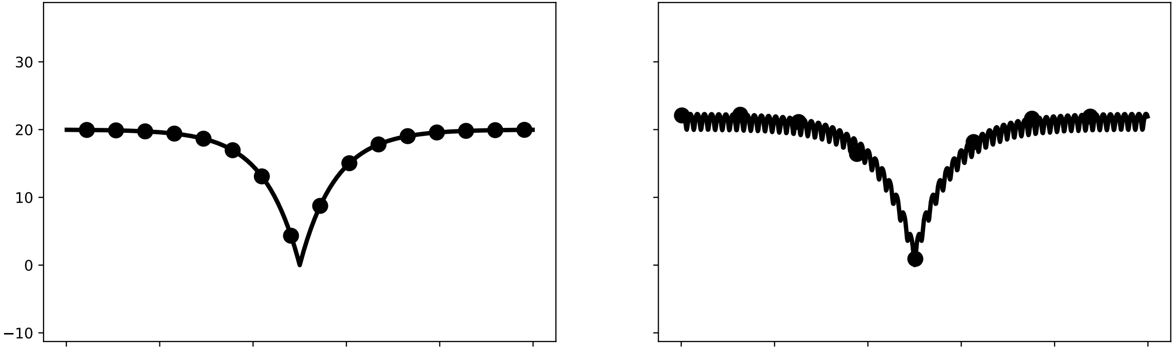
Applications of GPs with derivatives observations [94, Chapter 9.4]

- Bayesian optimization, for surface terrain reconstruction [30] and training ML models [89]
- Bayesian cubature, where derivative information enhances GP predictions [124]
- Modeling dynamical systems, with connected function and derivative observations [107]
- Solving PDEs, where the function and derivative observations are optimized to satisfy the governing equation and minimize the RKHS norm [14, 15]

Independent GPs vs a Multitask GP (MTGP)

Low Fidelity Left, High Fidelity Right



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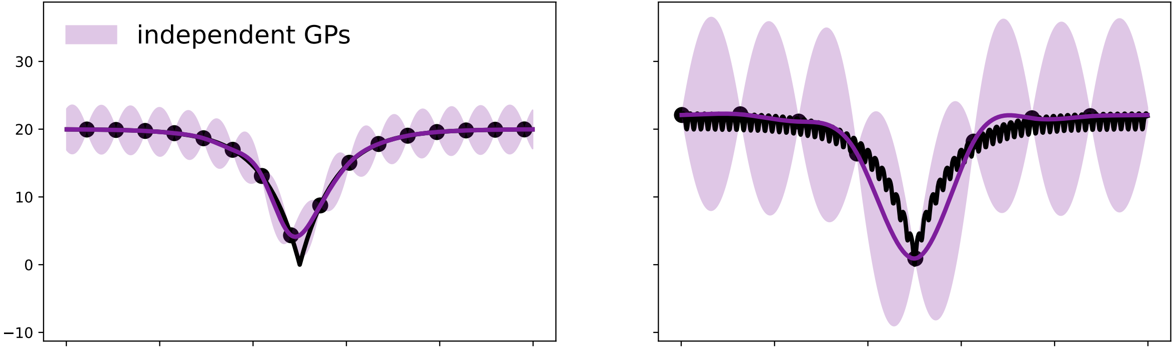

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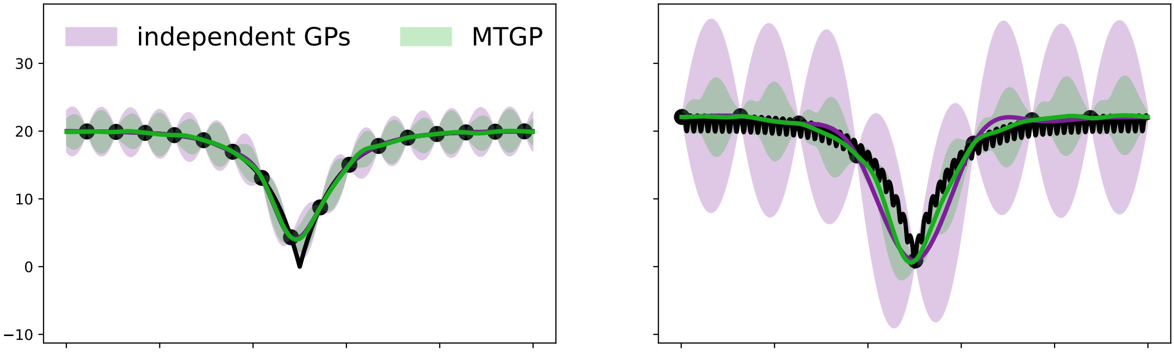

Accelerated GPs for Controlled Experiments

GP fitting requires solving a linear system in an $n \times n$ Gram matrix which is symmetric-positive-definite (SPD)

Classic GPs fitting and optimization requires $\mathcal{O}(n^3 + n^2 d)$ computations and $\mathcal{O}(n^2)$ storage

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Existing acceleration methods (not explored here)

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  - Reduces computations to $\mathcal{O}(n^2 d)$
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  - Reduces computations to $\mathcal{O}(n^2 d)$
  - Requires well-conditioned Gram matrices
- Structured kernel interpolation [103, 35, 122, 123], which uses grid points and product kernels
  - Creates Kronecker (or Toeplitz) Gram matrices
  - Reduces storage to $\mathcal{O}(n^{2/d} d)$
  - Reduces computations to $\mathcal{O}(n^{2/d} d^2 + n^{3/d} d)$

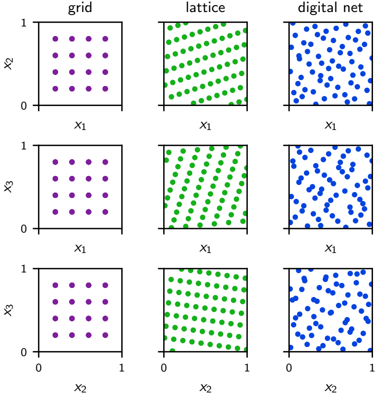

Figure: Projections of $n = 64$ points in $d = 3$ dimensions from a grid, an LD lattice, and an LD digital net.

Fast GPs Pairing Low-Discrepancy (LD) Points with Special Kernels

Reduce high GP costs by forcing structure into the Gram matrix [129, 128]

- $\mathcal{O}(n \log n + nd)$ computations, compared to standard $\mathcal{O}(n^3 + n^2 d)$ requirement, and
- $\mathcal{O}(n)$ memory, compared to standard $\mathcal{O}(n^2)$ requirement

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- Shift-invariant (SI) or digitally-SI (DSI) kernels, of varying smoothness

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- Using uncommon kernels, either the SI or DSI kernels, which are practically performant

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Applications

- Solving PDEs, often with random coefficients sampled at LD locations [54, 55, 114, 116]
- Fast Bayesian cubature, which enables error estimation for QMC [96, 97, 95]
- Discrepancy computation, for terms appearing in cubature error bounds [43, 44]

Fast GPs using LD points and SI/DSI kernels

Maintain accuracy with reduced compute from $\mathcal{O}(n^3+n^2d)$ to $\mathcal{O}(n\log n+nd)$ and storage from $\mathcal{O}(n^2)$ to $\mathcal{O}(n)$

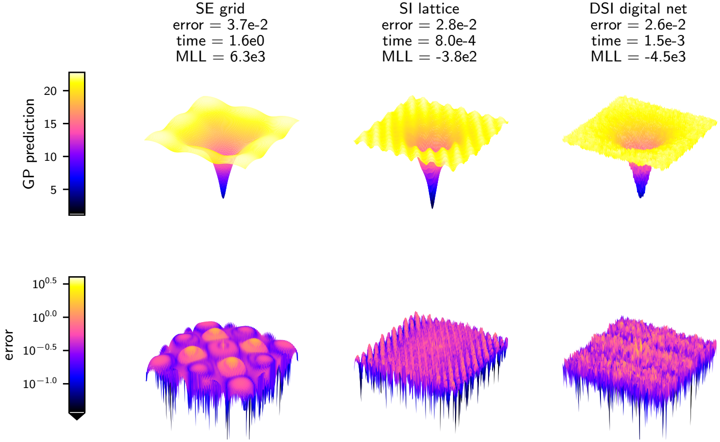

Figure: GP modeling of the 2-dimensional Ackley function with $n = 4096$ points.

Scientific Machine Learning (sciML) for Solving PDEs

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Advantages

- Easy setup of solvers, with just a few lines of code specifying the PDE
- Flexible parameterizations, from a zoo of neural architectures or GP kernels
- Scalable training, enabled by GPU acceleration libraries such as `PyTorch` [90]
- Rapid inference, thanks to fast and parallelizable evaluation of sciML models; especially evident in operator learning of PDEs with random coefficients [8, 62]

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Use of low-discrepancy points in sciML

- Collocation points for training sciML models, especially neural architectures [76, 12, 59]
- Solving PDEs with fast GPs, often with random coefficients [54, 55, 114]
- As space filling designs, may be useful when pairing with Sobolev inequalities [27, 26]

Popular SciML Models

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Neural network architectures for physics informed ML [57] and operators learning [61]

1. Physics Informed Neural Networks (PINNs), for PDEs with deterministic coefficients [93]
2. Deep Operator Networks (DeepONets), for PDEs with random coefficients [77]
3. Fourier Neural Operators (FNOs), for resolution-invariant operator learning [73]

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Gaussian process (GP) models, with strong theoretical backing and convergence guarantees [87]

1. GPs methods for PDEs, with deterministic coefficients which optimize function and derivatives observations to match governing equations and minimize RKHS norm [14, 15]
2. GP operator learning, often via vector-valued GPs with resolution-invariance [56, 80, 5]
3. Hybrid GP and neural network operator learning, often using GPs with neural prior means to leverage the theoretical backing of GPs and flexibility of neural architectures [79, 86, 88]

Modeling Radiative Transfer with a SciML DeepONet Neural Architecture

The DeepONet accelerates inference while honoring PDE constraints and overcoming the ray effect

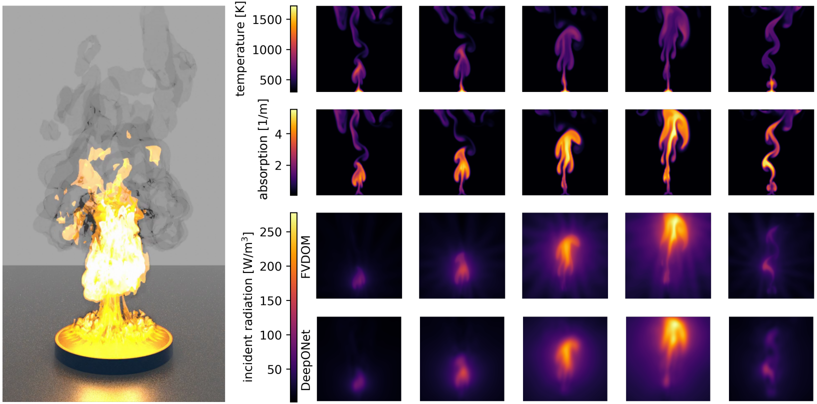

Figure: Predicted incident radiation from unknown temperature and absorption coefficients in a pool fire compared to reference finite volume discrete-ordinate method (FVDOM).

My Papers: Collaborations Across Academia, National Labs, and Industry

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- [116]: Fast Gaussian Process Regression for High-Dimensional Functions with Derivative Information.
  During my 2025 DOE SCGSR Program fellowship at Sandia National Laboratories.
  Collaboration with Pieterjan M Robbe and Fred J Hickernell.
  Published in the First International Conference on Probabilistic Numerics, PMLR.
- [48]: Quasi-Monte Carlo Methods: What, Why, and How?
  Collaboration with Fred J Hickernell and Nathan Kirk.
  Published in the Monte Carlo and Quasi-Monte Carlo Methods 2024 Proceedings.
- [110]: On Bounding and Approximating Functions of Multiple Expectations Using Quasi-Monte Carlo.
  Collaboration with Jagadeeswaran Rathinavel.
  Published in the Monte Carlo and Quasi-Monte Carlo Methods 2022 Proceedings.

My Papers: Collaborations Across Academia, National Labs, and Industry

- [16]: Challenges in Developing Great Quasi-Monte Carlo Software.
  Collaboration with Sou-Cheng T Choi, Yuhan Ding, Fred J Hickernell, and Jagadeeswaran Rathinavel.
  Published in the Monte Carlo and Quasi-Monte Carlo Methods 2022 Proceedings.
- [17]: Quasi-Monte Carlo Software.
  Collaboration with Sou-Cheng T Choi, Fred J Hickernell, Jagadeeswaran Rathinavel, and Michael J McCourt.
  Published in the Monte Carlo and Quasi-Monte Carlo Methods 2020 Proceedings.
- [111]: (Quasi-)Monte Carlo Importance Sampling with QMCPy.
  Collaboration with Fred J Hickernell, Sou-Cheng T Choi, Michael J McCourt, and Jagadeeswaran Rathinavel.
  Published in the 2021 IIT Undergraduate Research Journal.

My Papers: Collaborations Across Academia, National Labs, and Industry

- [113]: A Neural Surrogate Solver for Radiation Transfer.
  During my 2024 Scientific Machine Learning Researcher appointment at FM.
  Collaboration with Xiaoyi Lu and Yi Wang.
  Published through the NeurIPS 2024 Workshop on Data-Driven and Differentiable Simulations, Surrogates, and Solvers.
- [112]: SigOpt Mulch: An Intelligent System for AutoML of Gradient Boosted Trees.
  During my 2021 Machine Learning Engineer appointment at SigOpt (acquired by Intel).
  Collaboration with Michael McCourt, Xinran Zhu, Eric Hans Lee, and Bolong Cheng.
  Published in a 2023 Knowledge-Based Systems Journal.
- [114]: Computationally Efficient and Error Aware Surrogate Construction for Numerical Solutions of Subsurface Flow Through Porous Media.
  During my 2023 Graduate Internship appointment at Los Alamos National Laboratory.
  Collaboration with Aleksandra Pachalieva, Daniel O'Malley, James M Hyman, Fred J Hickernell, and Nicolas W Hengartner.
  Published in a 2024 Advances in Water Resources Journal.

My Papers: Collaborations Across Academia, National Labs, and Industry

- [39]: GalCEM. I. An Open-Source Detailed Isotopic Chemical Evolution Code and
  [40]: GalCEM: GALactic Chemical Evolution Model.
  Collaboration with Eda Gjergo, Anthony Ruth, Emanuele Spitoni, Francesca Matteucci, Xilong Fan, Jinning Liang, Marco Limongi, Yuta Yamazaki, Motohiko Kusakabe, and Toshitaka Kajino.
  Published in the 2023 Astrophysical Journal Supplement Series and Astrophysics Source Code Library respectively.
- [108]: QMCPy: A Python Software for Randomized Low-Discrepancy Sequences, Quasi-Monte Carlo, and Fast Kernel Methods.
  Submitted to ACM TOMS (Transactions on Mathematical Software).
- [109]: Credible Intervals for Probability of Failure with Gaussian Processes.
  During my 2022 Givens Associate Internship appointment at Argonne National Laboratories.
  Collaboration with Vishwas Rao.
  Currently, an unpublished preprint.

My Papers: Collaborations Across Academia, National Labs, and Industry

- [50]: Empirical Bernstein and Betting Confidence Intervals for Randomized Quasi-Monte Carlo.
  Collaboration with Art Owen, Aadit Jain, and Fred Hickernell.
  Currently, an unpublished preprint.
- [2], Operator Learning at Machine Precision
  During my 2025 DOE SCGSR fellowship at Sandia National Laboratories.
  Collaboration with Houman Owhadi, Aras Bacho, Xianjin Yang, Théo Bourdais, Edoardo Calvello, Matthieu Darcy, Alex Hsu, and Bamdad Hosseini.
  Currently, an unpublished preprint.
- [115], Fast Bayesian Multilevel Quasi-Monte Carlo
  Developed during my 2025 DOE SCGSR fellowship at Sandia National Laboratories.
  Collaboration with Pieterjan M Robbe and Fred J Hickernell.
  Currently, an unpublished preprint.

My Contributions: Novel Algorithms, Implementations, and Applications

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1. Developed `QMCPy` (`https://qmcsoftware.github.io/QMCSoftware/`) [17, 16, 48, 108, 110], a unified open-source Python library for Quasi-Monte Carlo algorithms
2. Built `LDData` (`https://github.com/QMCSoftware/LDData`), which stores lattice generating vectors, digital net generating matrices, and quality low-discrepancy point sets in standardized formats with an interface in `QMCPy`
3. Implemented into `QMCPy` the first interface to certain randomized low-discrepancy sequences, including lattices, higher-order digital nets, higher-order digital net scrambling with either linear matrix scrambling (LMS) or nested uniform scrambling (NUS), and Halton scrambling with either LMS or NUS [108]
4. Developed vectorized Quasi-Monte Carlo stopping criterion to estimate and quantify error for functions of multiple integrals [110], and provided an implementation in `QMCPy`
5. Derived new digitally-shift-invariant (DSI) kernels whose RKHSs contain smooth functions [108] including a new order 4 smoothness kernel whose form has not appeared elsewhere in the literature

My Contributions: Novel Algorithms, Implementations, and Applications

6. Implemented into `QMCPy` the first Python interface to fast kernel method utilities [108] including shift-invariant (SI) and digitally-shift-invariant (DSI) kernels of varying smoothness as well as the fast Fourier transform in bit-reversed order (FFTBR), the inverse FFTBR (IFFTBR), and the fast Walsh–Hadamard transform (FWHT)
7. Developed `FastGPs` (`https://alegresor.github.io/fastgps/`) [116], an open-source Python library for fast Gaussian process regression algorithms pairing low-discrepancy points with (digitally)-shift-invariant kernels
8. Derived and analyzed novel fast multitask GPs and fast derivative-informed GP [116] with an available implementation in the `FastGPs` package
9. Developed numerous applications of Quasi-Monte Carlo, fast Gaussian process regression, and/or scientific machine learning [109, 114, 113, 2, 115, 112, 39, 40] with collaborators from academia, national labs, and industry

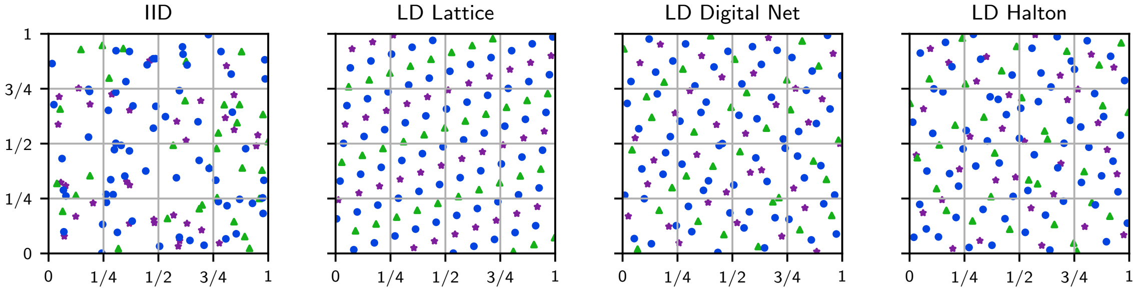
Quasi-Monte Carlo Formulation

QMC is an efficient algorithm for high-dimensional numerical integration

$$\mu = \int_{\mathcal{T}} g(\boldsymbol{t})\lambda(\mathrm{d}\boldsymbol{t}) = \int_{[0,1]^d} f(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \approx \frac{1}{n}\sum_{i=0}^{n-1} f(\boldsymbol{x}_i), \qquad \boldsymbol{x}_0,\dots,\boldsymbol{x}_{n-1} \in [0,1]^d$$

Classic Monte Carlo has error like $\mathcal{O}(1/\sqrt{n})$ using IID points $(\boldsymbol{x}_i)_{i=0}^{n-1}$

QMC has errors like $\mathcal{O}(1/n)$ using low discrepancy (LD) points with greater uniformity



Adaptive QMC for High-Dimensional Asian Option Pricing

Automatically choose sample size n to meet a user specified error tolerance

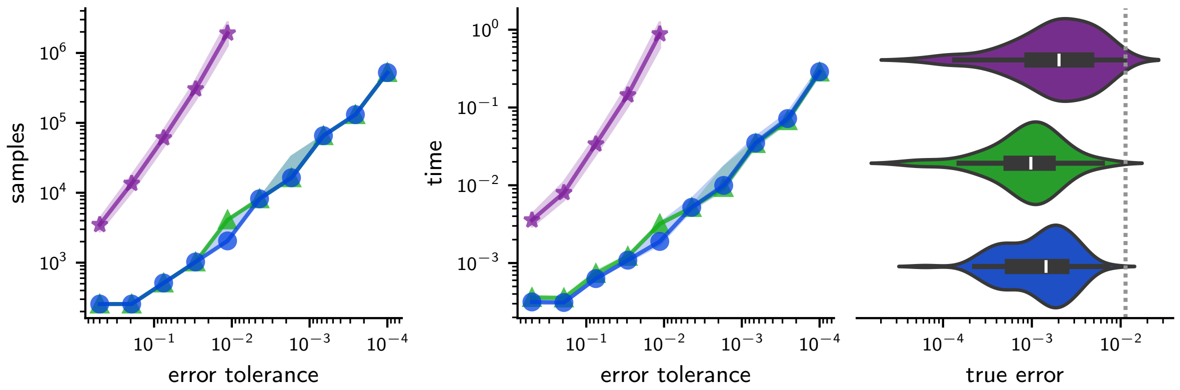


Figure: IID MC vs QMC digital net vs QMC lattice.

QMCPy Software

`pip install qmcpy` or visit qmcsoftware.github.io/QMCSoftware/ [17, 16, 48, 110]

A Python software unifying QMC tools from across the literature

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- Randomized low-discrepancy sequences
  - Lattices: random shifts
  - Digital nets: random digital shifts, LMS, Owen scrambling (NUS), higher-order nets
  - Halton points: digital shifts, permutation scrambles, NUS

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- Diverse use cases: financial options, parameterized PDEs, sensitivity indices, ...

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- Diverse use cases: financial options, parameterized PDEs, sensitivity indices, ...
- Adaptive stopping criteria: choosing n to meet user-specified error tolerance ε
  - IID Monte Carlo with guaranteed confidence intervals [46]
  - QMC with replications, see [71] or [85, Chapter 17]
  - QMC via decay tracking of Fourier or Walsh coefficients [47]
  - QMC via Bayesian cubature using fast Gaussian processes [95]
  - Multilevel IID Monte Carlo [37, 100, 102] and Multilevel QMC [38, 101]
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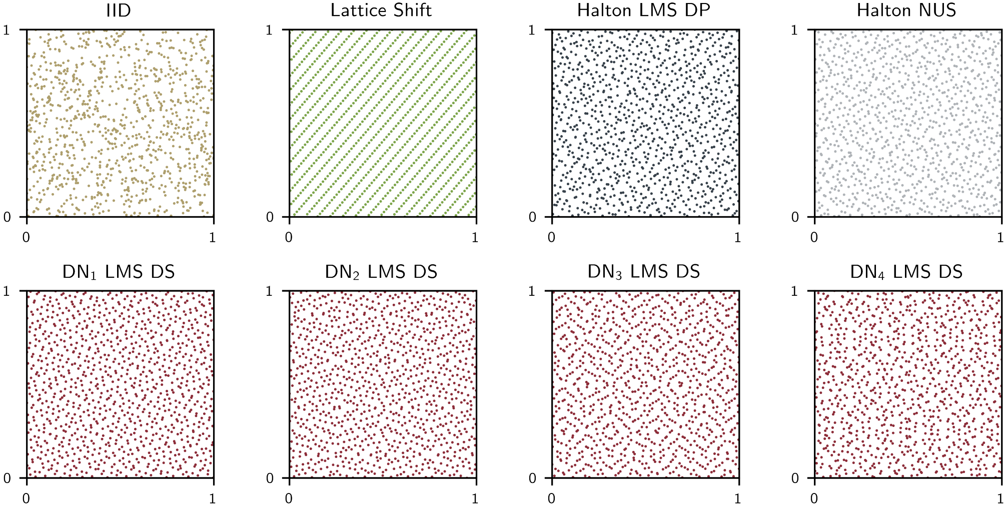
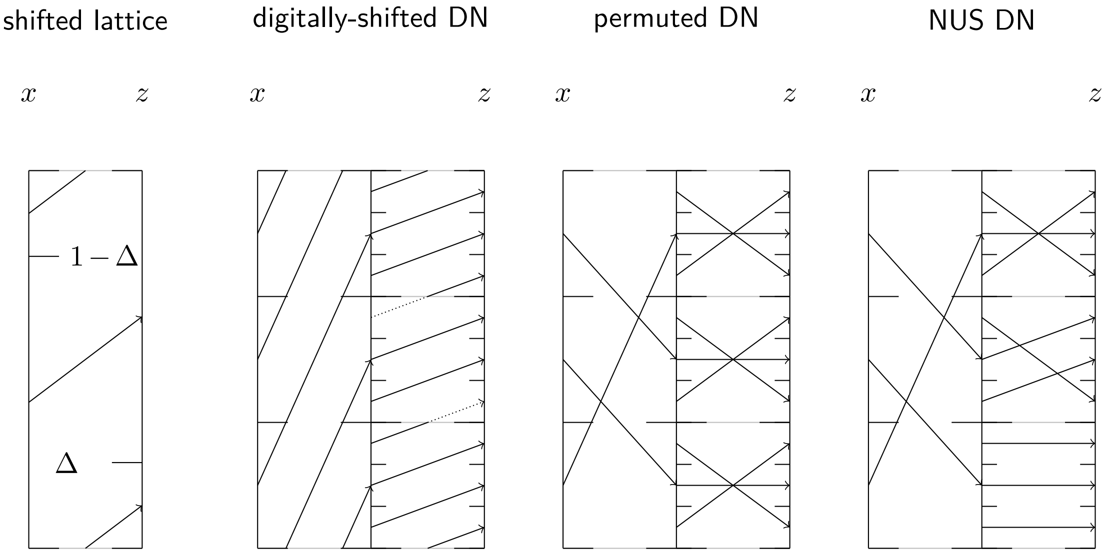
  - Vectorized IID Monte Carlo and QMC algorithms for functions of multiple integrands [110]
- Special kernels and fast transforms: used for fast Gaussian process regression

IID and Low-Discrepancy Points

Including higher-order α digital nets (DN_α) and higher-order scramblings

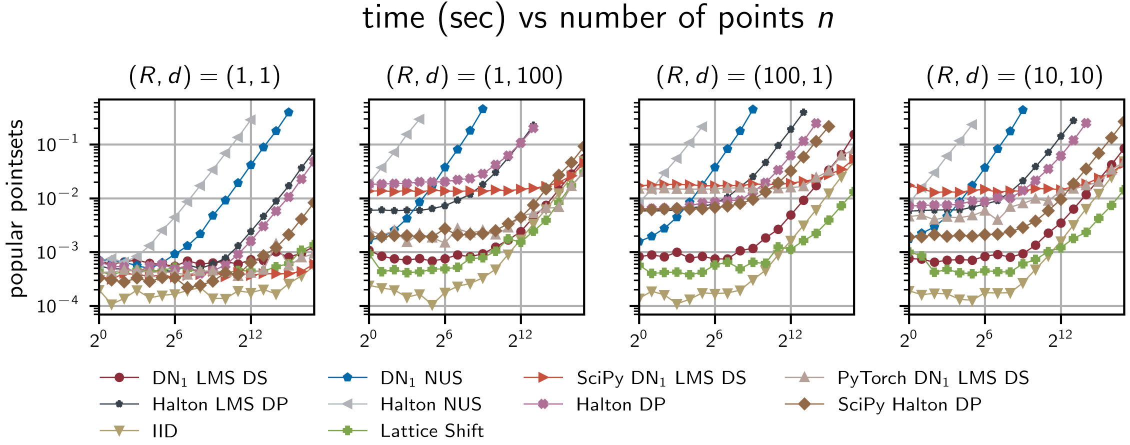


Randomizations of Low-Discrepancy (LD) Point Sets



Speed of Generating IID and Low-Discrepancy (LD) Points

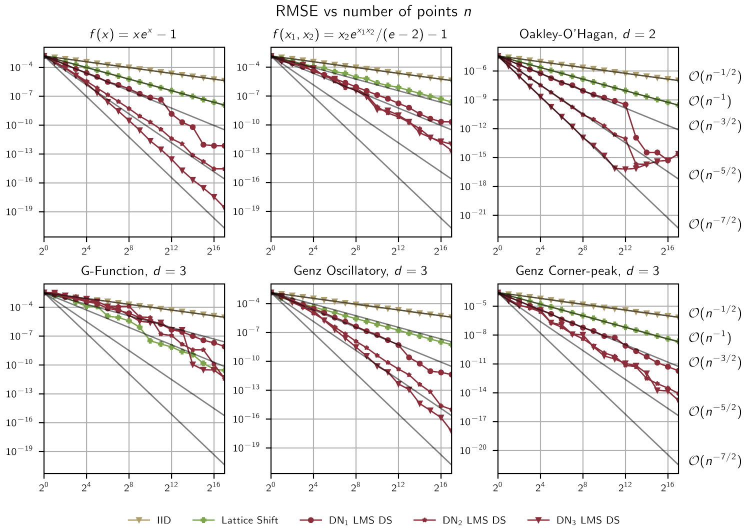
Randomized LD points are as fast to generate as IID points



R randomizations of n points in d dimensions

Root Mean Squared Error (RMSE) of Randomized QMC

Higher-order digital nets achieve higher-order convergence for low-dimensional functions



Automatic Single-Level Stopping Criteria for Asian Option Pricing

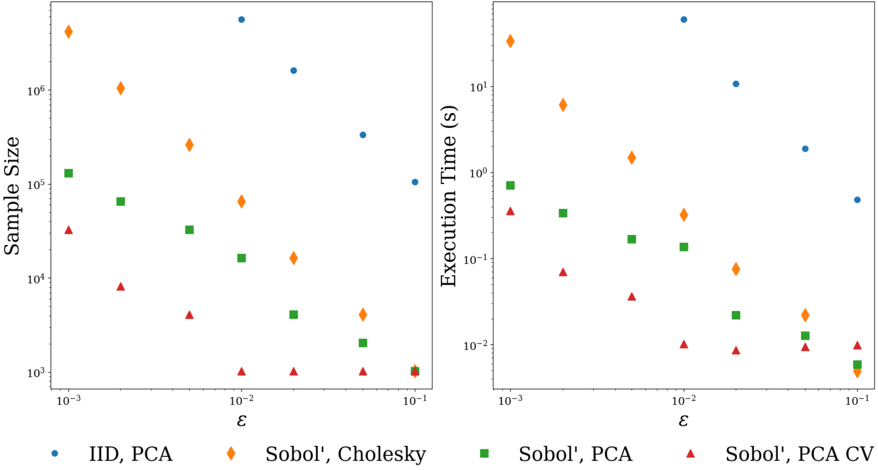


Figure: Using the principal component analysis (PCA) decomposition of the Brownian motion provides substantial savings compared to the Cholesky decomposition. Control variates provide additional savings.

Comparison of Automatic Stopping Criteria in QMCPy

QMCPy Class	Point Sets	Guaranteed	Vectorized	Multilevel	References
CubMCCLT	IID				[46]
CubMCCLTVec	IID		✓		[46]
CubMCG	IID	✓			[46]
CubQMCRepStudentT	LD		✓		[71]
CubQMCNetG	DigitalNetB2	✓	✓		[45]
CubQMCLatticeG	Lattice	✓	✓		[52]
CubQMCBayesNetG	DigitalNetB2	✓	✓		[97]
CubQMCBayesLatticeG	Lattice	✓	✓		[96]
CubMLMC	IID			✓	[37]
CubMLMCCont	IID			✓	[19]
CubMLQMC	LD			✓	[38]
CubMLQMCCont	LD			✓	[99]

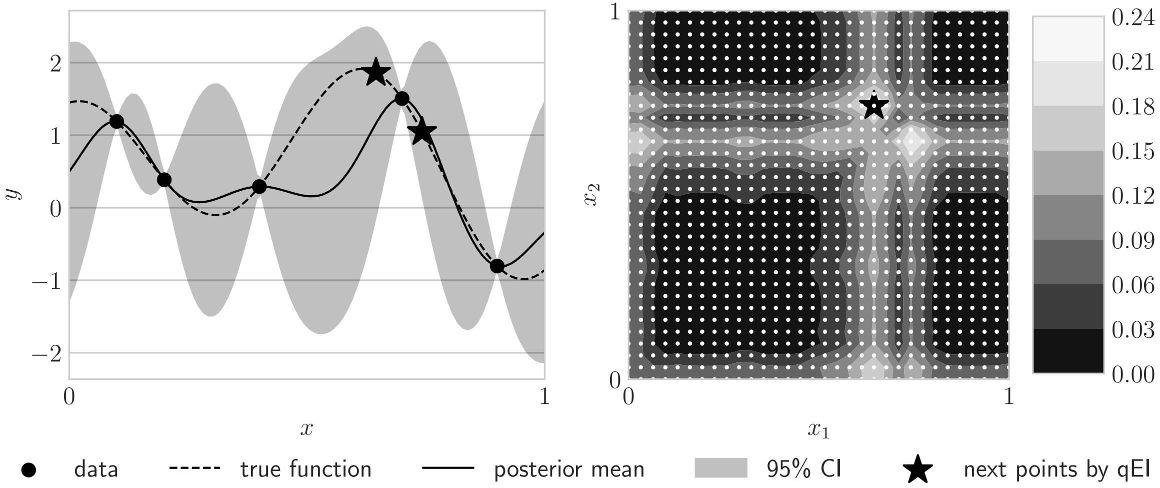
New (Q)MC Stopping Criteria for Functions of Multiple Expectations

Vectorized (Q)MC algorithms propagate bounds using interval arithmetic [110]

$s = C(\boldsymbol{\mu})$	$s^- = C^-(\boldsymbol{\mu}^-, \boldsymbol{\mu}^+)$	$s^+ = C^+(\boldsymbol{\mu}^-, \boldsymbol{\mu}^+)$
$\mu_1 + \mu_2$	$\mu_1^- + \mu_2^-$	$\mu_1^+ + \mu_2^+$
$\mu_1 - \mu_2$	$\mu_1^- - \mu_2^+$	$\mu_1^+ - \mu_2^-$
$\mu_1 \cdot \mu_2$	$\min(\mu_1^-\mu_2^-, \mu_1^-\mu_2^+, \mu_1^+\mu_2^-, \mu_1^+\mu_2^+)$	$\max(\mu_1^-\mu_2^-, \mu_1^-\mu_2^+, \mu_1^+\mu_2^-, \mu_1^+\mu_2^+)$
μ_1 / μ_2	$\begin{cases} -\infty, & 0 \in [\mu_2^-, \mu_2^+] \\ \min\left(\frac{\mu_1^-}{\mu_2^-}, \frac{\mu_1^+}{\mu_2^-}, \frac{\mu_1^-}{\mu_2^+}, \frac{\mu_1^+}{\mu_2^+}\right), & 0 \notin [\mu_2^-, \mu_2^+] \end{cases}$	$\begin{cases} \infty, & 0 \in [\mu_2^-, \mu_2^+] \\ \max\left(\frac{\mu_1^-}{\mu_2^-}, \frac{\mu_1^+}{\mu_2^-}, \frac{\mu_1^-}{\mu_2^+}, \frac{\mu_1^+}{\mu_2^+}\right), & 0 \notin [\mu_2^-, \mu_2^+] \end{cases}$
$\min(\mu_1, \mu_2)$	$\min(\mu_1^-, \mu_2^-)$	$\min(\mu_1^+, \mu_2^+)$
$\max(\mu_1, \mu_2)$	$\max(\mu_1^-, \mu_2^-)$	$\max(\mu_1^+, \mu_2^+)$

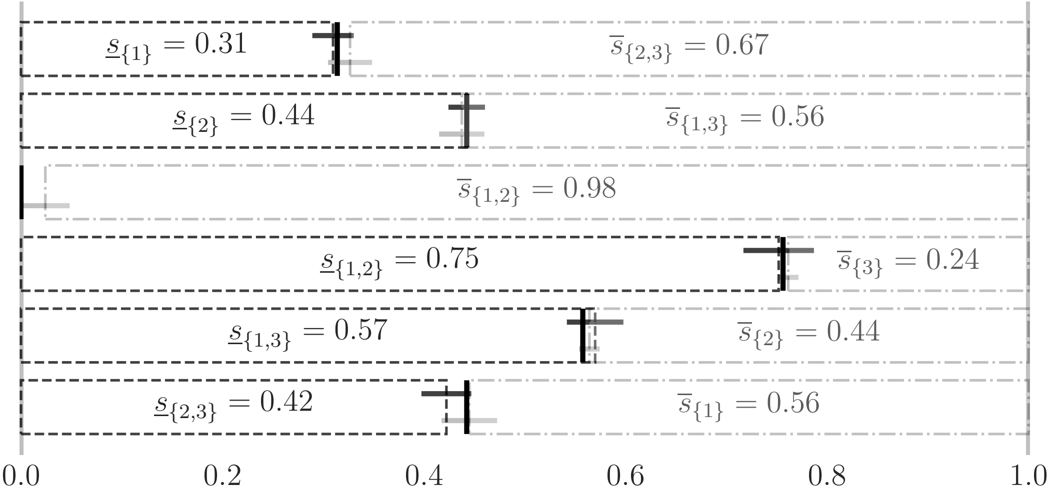
Bayesian Optimization with a Vectorized Acquisition Function

The utility of sampling at each grid point on the right is an expectation to be approximated with QMC



Approximating Sensitivity for the Ishigami function

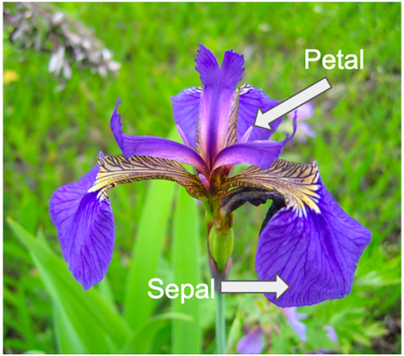
Each sensitivity index may be written as a ratio involving three expectations



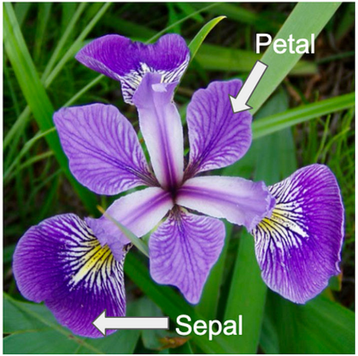
Iris Species Classification by Attributes

Which iris flower attributes are most important to determining its species (setosa, versicolor, or virginica)?

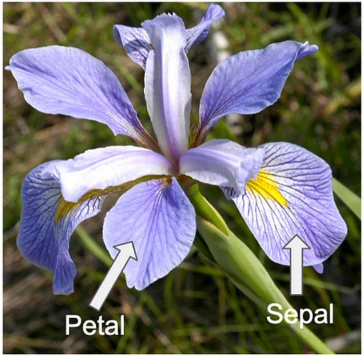
Iris setosa



Iris versicolor



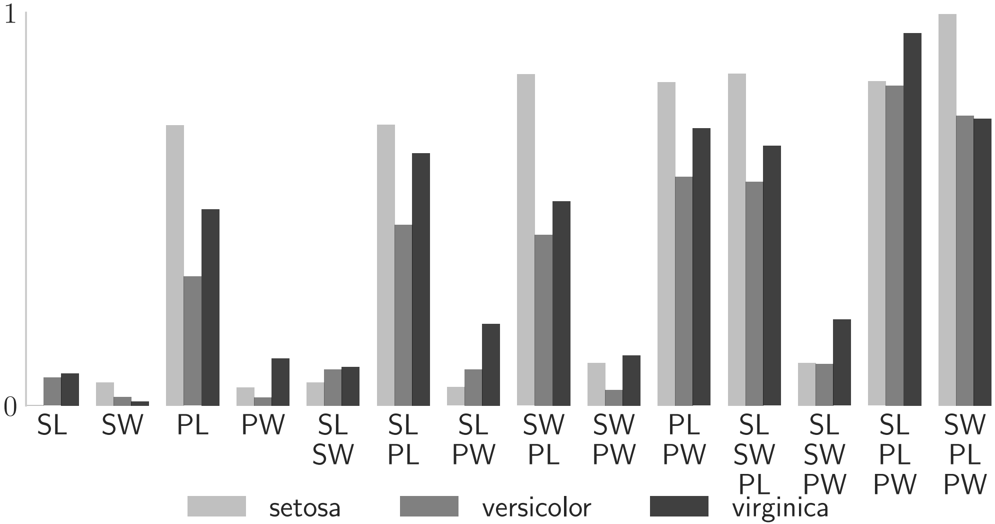
Iris virginica



Available attributes: petal length (PL), petal width (PW), sepal length (SL), sepal width (SW)

Sensitivity Indices for a Neural Network

Quantify the importance of subsets of inputs to classifying Iris species



Gaussian Processes Formulation

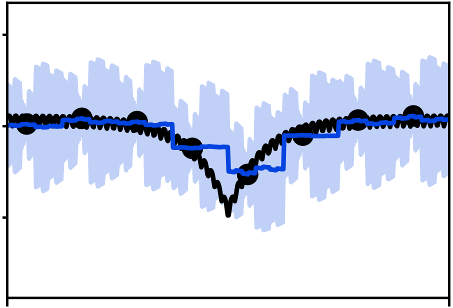
Flexible interpolation models with built-in UQ [94, 31]

$f \sim \mathrm{GP}(0,K)$ with posterior mean and covariance

$$\mathbb{E}[f(\boldsymbol{x})|\boldsymbol{f}] = \boldsymbol{K}(\boldsymbol{x})\mathsf{K}^{-1}\boldsymbol{f}$$

$$\mathbb{V}[f(\boldsymbol{x})|\boldsymbol{f}] = K(\boldsymbol{x},\boldsymbol{x}) - \boldsymbol{K}(\boldsymbol{x})^T\mathsf{K}^{-1}\boldsymbol{K}(\boldsymbol{x})$$

- SPD $K:[0,1]^d \times [0,1]^d \to \mathbb{R}$
- Sampling locations $\mathsf{X} = \{\boldsymbol{x}_i\}_{i=0}^{n-1}$
- Sample values $\boldsymbol{f} = \{f(\boldsymbol{x}_i)\}_{i=0}^{n-1}$
- Kernel vector $\boldsymbol{K}(\boldsymbol{x}) = \{K(\boldsymbol{x},\boldsymbol{x}_i)\}_{i=0}^{n-1}$
- Gram matrix $\mathsf{K} = \{K(\boldsymbol{x}_i,\boldsymbol{x}_{i'})\}_{i,i'=0}^{n-1}$



Typically requires $\mathcal{O}(n^2)$ storage and $\mathcal{O}(n^3+n^2d)$ computations

Fast GPs Pairing LD Points with Special Kernels

Fast GPs Pairing LD Points with Special Kernels

1. **LD Lattices + Shift-Invariant (SI) Kernels**
   - Give circulant Gram matrices $\mathsf{K} = \{K(\boldsymbol{x}_i, \boldsymbol{x}_{i'})\}_{i,i'=0}^{n-1}$

   $\therefore$ Eigendecomp $\mathsf{K} = \mathsf{V}\Lambda\overline{\mathsf{V}}$ where $\overline{\mathsf{V}}$ is the DFT matrix $\to$ FFT in $\mathcal{O}(n \log n)$

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2. **LD Digital Nets + Digitally-Shift-Invariant (DSI) Kernels**
   - Give Recursive Symmetric Block Toeplitz (RSBT) Gram matrices K

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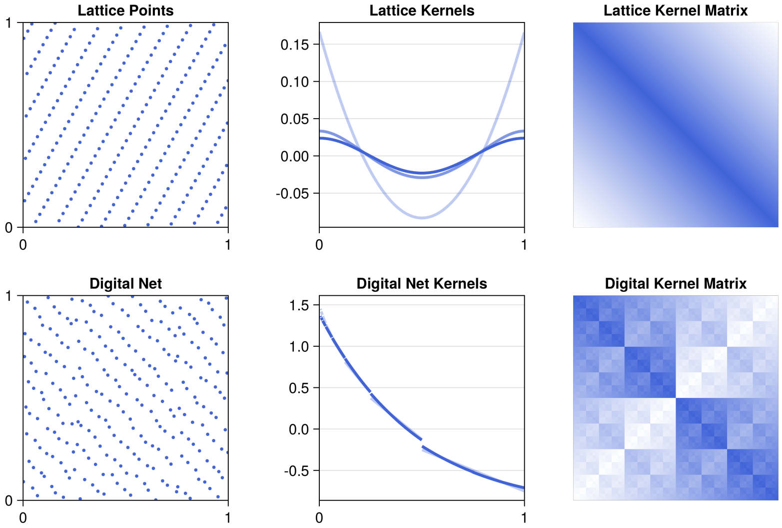
Let $\boldsymbol{v}_1 = \mathbf{1}/\sqrt{n}$ and $\boldsymbol{k}_1$ be the first columns of $\overline{\boldsymbol{V}}$ and K respectively:

$$\boldsymbol{\lambda} := \Lambda \mathbf{1} = \sqrt{n}\Lambda\overline{\boldsymbol{v}}_1 = \sqrt{n}\overline{\mathsf{V}}\mathsf{V}\Lambda\overline{\boldsymbol{v}}_1 = \sqrt{n}\overline{\mathsf{V}}\boldsymbol{k}_1$$

- $\mathsf{K}\boldsymbol{a}$, $\mathsf{K}^{-1}\boldsymbol{a}$, and $|\mathsf{K}|$ can all be computed in $\mathcal{O}(n \log n + nd)$ computations
- Only requires evaluating and storing the first column of K

Lattices + SI K = Circulant K and Digital Nets + DSI K = RSBT K



Standard GPs vs Fast GPs using LD points and (D)SI Kernels

Comparison of methods and requirements for both storage and computations

$\{\boldsymbol{x}_i\}_{i=0}^{n-1}$ points	K structure	factor K method	K storage	form K cost
any	general SPD	Cholesky	$\mathcal{O}(n^2)$	$\mathcal{O}(n^2 d)$
rank-1 lattice	SPD SI	(I)FFTBR	$\mathcal{O}(n)$	$\mathcal{O}(nd)$
base 2 digital net	SPD DSI	FWHT	$\mathcal{O}(n)$	$\mathcal{O}(nd)$

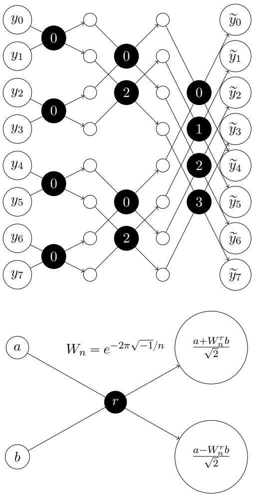
$\{\boldsymbol{x}_i\}_{i=0}^{n-1}$	factor K cost	K$\boldsymbol{y}$ cost	K$^{-1}\boldsymbol{y}$ cost	|K| cost
any	$\mathcal{O}(n^3)$	$\mathcal{O}(n^2)$	$\mathcal{O}(n^2)$	$\mathcal{O}(n^2)$
rank-1 lattice	$\mathcal{O}(n\log n)$	$\mathcal{O}(n\log n)$	$\mathcal{O}(n\log n)$	$\mathcal{O}(n\log n)$
base 2 digital net	$\mathcal{O}(n\log n)$	$\mathcal{O}(n\log n)$	$\mathcal{O}(n\log n)$	$\mathcal{O}(n\log n)$

Table: When evaluating (forming) K, we assume the cost of evaluating the kernel is $\mathcal{O}(d)$. Factorization of the SPD Gram matrix K is the cost of computing the eigendecomposition or Cholesky decomposition. The costs of matrix-vector multiplication K$\boldsymbol{y}$, solving a linear system K$^{-1}\boldsymbol{y}$ (when K is symmetric positive definite), and computing the determinant $|$K$|$ are the costs after performing the decomposition.

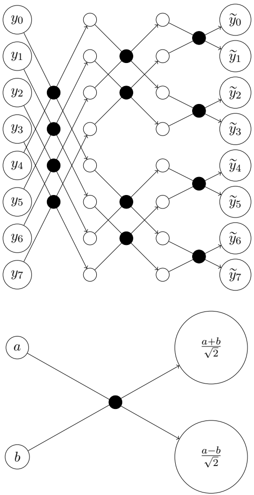
Fast Transforms for Decomposing Fast GP Gram Matrices

Fast Fourier Transform with bit-reversal (FFTBR) and the Fast Walsh–Hadamard Transform (FWHT)

FFTBR



FWHT



Product Kernels that are Shift-Invariant (SI) and Periodic

Product kernel

$$K(\boldsymbol{x},\boldsymbol{x}') = \gamma \prod_{j=1}^d \left(1+\eta_j K_{\alpha_j}(x_j,x_j')\right) \qquad \forall \boldsymbol{x},\boldsymbol{x}' \in [0,1)^d.$$

For smoothness parameters $\boldsymbol{\alpha} \in \mathbb{R}^d_{>1/2}$, our univariate SI kernels take the form

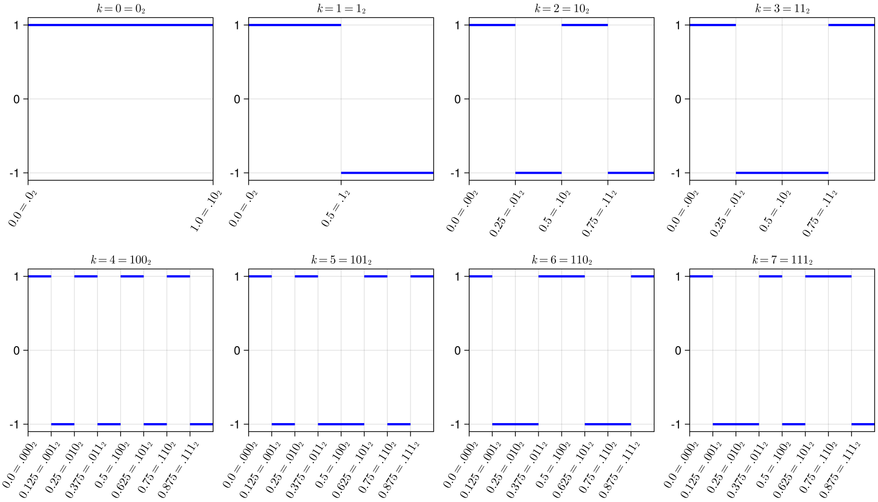
$$K_\alpha(x,x') = \frac{(-1)^{\alpha+1}(2\pi)^{2\alpha}}{(2\alpha)!} B_{2\alpha}((x-x') \mod 1)$$

with B_p is the p^{th} Bernoulli polynomial. May be written in terms of a decaying Fourier series. The inner product of the univariate SI kernel's RKHS is

$$\langle f,g\rangle_{K_\alpha} \propto \int_0^1 f^{(\alpha)}(x) g^{(\alpha)}(x) \mathrm{d}x.$$

Orthonormal Walsh Function Basis for L_2

Digitally-shift-invariant kernels are written in terms of Walsh Functions wal_k for $k \in \mathbb{N}_0$



New Higher-Order Digitally-Shift-Invariant Product Kernels in Base $b=2$

DSI kernels are *not* periodic, but they are discontinuous; yet their RKHSs contain smooth functions

For $x,x' \in [0,1)$, let $\beta(x) := -\lfloor \log_2(x) \rfloor$ and for $\nu \in \mathbb{N}$ let $t_\nu(x) = 2^{-\nu\beta(x)}$.
Write $x \oplus x' := \sum_{k \in \mathbb{N}} ((\mathsf{x}_k + \mathsf{x}'_k) \mod 2) 2^{-k}$, the XOR of $x = \sum_{k\in\mathbb{N}} \mathsf{x}_k 2^{-k}$ and $x' = \sum_{k\in\mathbb{N}} \mathsf{x}'_k 2^{-k}$.

$$K_\alpha(x,x') := \ddot{K}_{\alpha,0,0}(x \oplus x', 0)$$

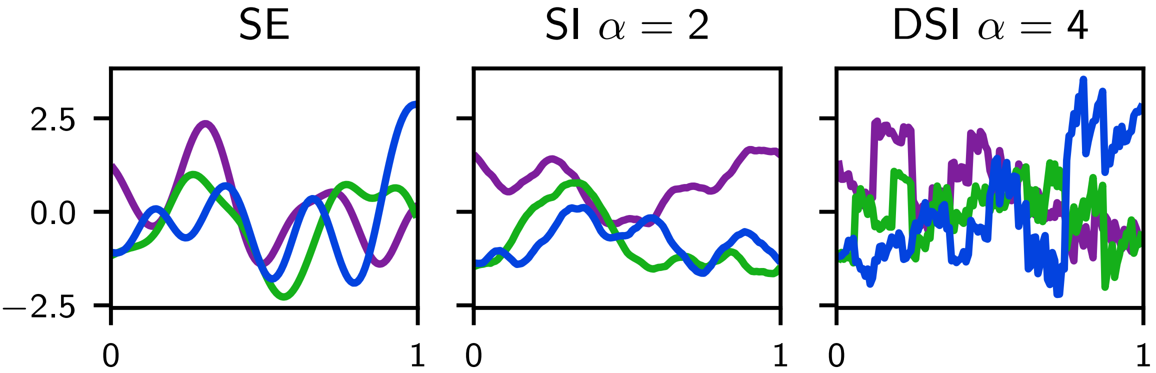
$$\ddot{K}_{\alpha,0,0}(x,0) = \begin{cases} -1 + -\beta(x)x + \frac{5}{2}\left[1 - t_1(x)\right], & \alpha = 2 \\ -1 + \beta(x)x^2 - 5\left[1-t_1(x)\right]x + \frac{43}{18}\left[1-t_2(x)\right], & \alpha = 3 \\ -1 - \frac{2}{3}\beta(x)x^3 + 5\left[1-t_1(x)\right]x^2 - \frac{43}{9}\left[1-t_2(x)\right]x & \\ \quad + \frac{701}{294}\left[1-t_3(x)\right] + \beta(x)\left[\frac{1}{48}\sum_{a=0}^\infty \frac{\mathrm{wal}_{2^a}(x)}{2^{3a}} - \frac{1}{42}\right], & \alpha = 4 \end{cases}.$$

For any $\alpha \in \mathbb{N}_{>2}$, one may compute $\ddot{K}_{\alpha,0,0}(x,x')$ using the algorithm in [4, Theorem 2].
The RKHSs of these kernels contain smooth functions. Specifically, $H(Q_\alpha) \subseteq H(K_\alpha)$ where

$$\langle f,g \rangle_{Q_\alpha} = \sum_{l=1}^{\alpha-1} \int_0^1 f^{(l)}(x)\mathrm{d}x \int_0^1 g^{(l)}(x)\mathrm{d}x + \int_0^1 f^{(\alpha)}(x) g^{(\alpha)}(x)\mathrm{d}x.$$

Prior Draws from GPs with Different Kernels

Squared exponential (SE) kernel, the $\alpha = 2$ SI kernel, and the $\alpha = 4$ DSI kernel



FastGPs Software

`pip install fastgps` or visit alegresor.github.io/fastgps/ [116]

A scalable Python software for fast GPs regression requiring only $\mathcal{O}(n \log n)$ computations

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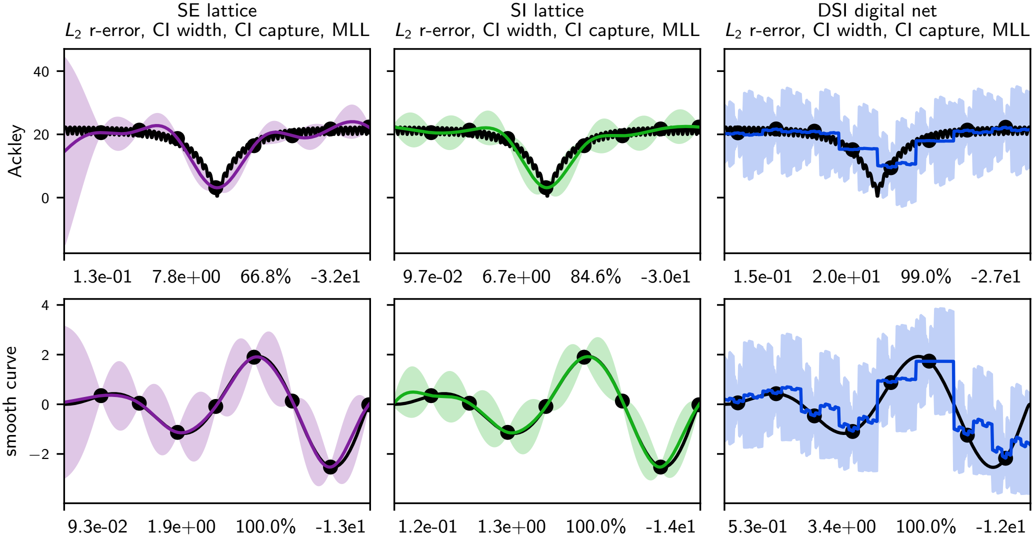
A scalable Python software for fast GPs regression requiring only $\mathcal{O}(n \log n)$ computations

1. Kernel hyperparameter optimization of marginal log likelihood (MLL) or generalized cross validation (GCV) loss
2. Fast Bayesian cubature for uncertainty quantification in Quasi-Monte Carlo
3. Fast multitask GPs with support for different sample sizes for each task; potentially useful for multi-fidelity simulations and Multilevel Monte Carlo
4. Batched GPs for simultaneously modeling vector-output simulations
5. GPU support enabled by the `PyTorch` stack
6. Flexible LD sequences and SI/DSI kernels with various LD randomizations and kernels of higher-order smoothness using the implementation in `QMCPy`
7. Fast Derivative Informed GPs for simulations coupled with automatic differentiation
8. Efficient variance projections for non-greedy Bayesian optimization in multilevel methods

Fast GPR Examples in One Dimension [117], $n = 8$



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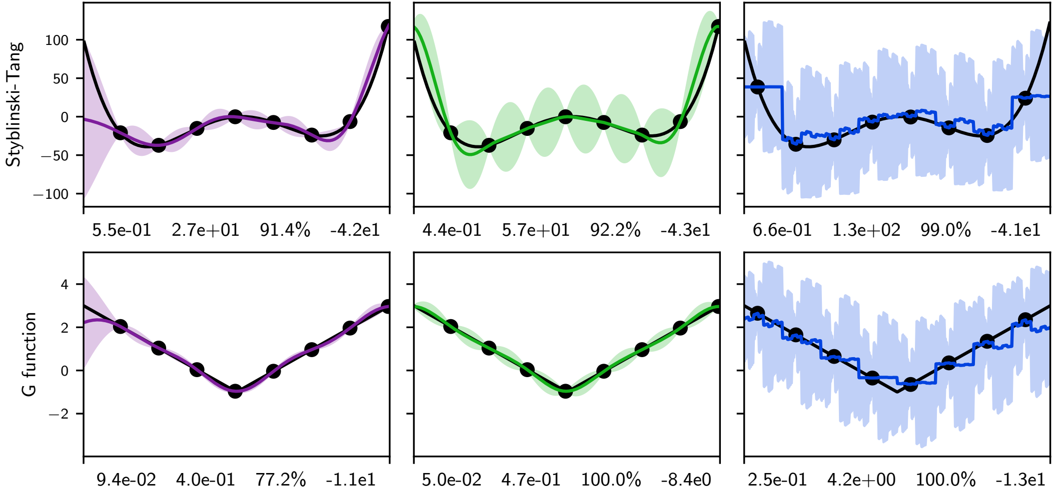
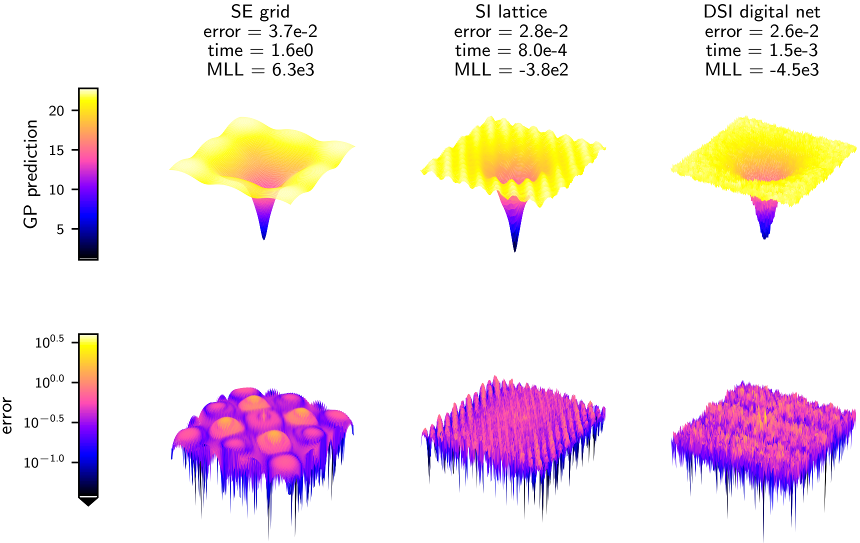


Fast GPR for the Ackley Function in Two Dimensions [117], $n = 4096$



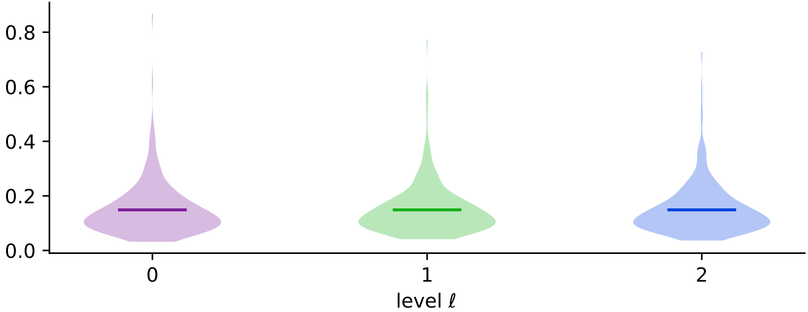
Multilevel (Multitask) Modeling

Given a multilevel simulation

$$f : \{1,\dots,L\} \times [0,1]^d \to \mathbb{R},$$

we want to model $f(L,\cdot)$, the true (maximum-fidelity) simulation.

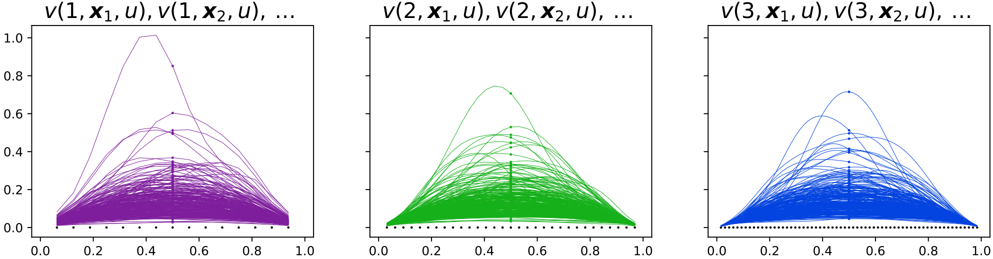
- $f(\ell,\boldsymbol{x})$ simulates at level $\ell \in \{1,\dots,L\}$ and with parameters $\boldsymbol{x} \in [0,1]^d$
- Cost C_ℓ typically greater on higher levels
- $f(1,\cdot), f(2,\cdot),\dots,f(L,\cdot)$ are typically highly correlated



Numerical Solutions of PDEs with Random Coefficients

$$f(\ell, \boldsymbol{x}) = \mathcal{F}(v(\ell, \boldsymbol{x}, \cdot))$$

- $v : \{1, \dots, L\} \times [0,1]^d \times \Omega$ is the numerical solution to the PDE
- $\boldsymbol{x}$ represent random coefficients, e.g. coefficients in a Karhunen–Loève expansion
- ℓ controls the fidelity of the numerical solver e.g. the mesh width is $2^{-\ell}$
- $\mathcal{F}$ is a (possibly non-linear) functional of the PDE solution, e.g.,
  - $\mathcal{F}(v(\ell, \boldsymbol{x}, \cdot)) = \mathbb{E}[v(\ell, \boldsymbol{x}, \boldsymbol{U})]$ where $\boldsymbol{U} \sim \mathcal{U}(\Omega)$, or
  - $\mathcal{F}(v(\ell, \boldsymbol{x}, \cdot)) = v(\ell, \boldsymbol{x}, u)$ for some $u \in \Omega$, e.g., $u = 1/2$ shown below



Fast Bayesian Multilevel Quasi-Monte Carlo Without Replications [115]

$$\mathbb{E}[f(L,\boldsymbol{X})] = \sum_{\ell=1}^{L} \mathbb{E}[\underbrace{f(\ell,\boldsymbol{X}) - f(\ell-1,\boldsymbol{X})}_{\Delta_\ell(\boldsymbol{X})}], \quad \boldsymbol{X} \sim \mathcal{U}[0,1]^d, \qquad f(0,\cdot) = 0$$

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MLMC $\mathbb{E}[\Delta_\ell(\boldsymbol{X})] \approx \frac{1}{n_\ell} \sum_{i=0}^{n_\ell-1} \Delta_\ell(\boldsymbol{x}_i^\ell)$ for IID $\boldsymbol{x}_0^\ell, \dots, \boldsymbol{x}_{n_\ell-1}^\ell \sim \mathcal{U}[0,1]^d$

- $n_\ell \propto \sqrt{\mathbb{V}[\Delta_\ell(\boldsymbol{X})]/C_\ell}$ chosen to optimally minimize error [37]

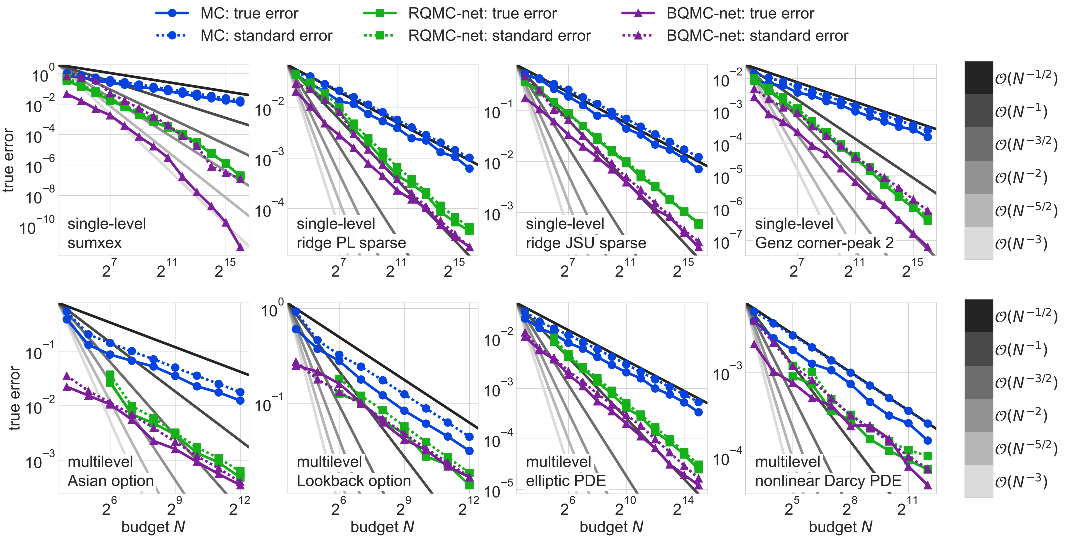
RMLQMC with replications $\mathbb{E}[\Delta_\ell(\boldsymbol{X})] \approx \frac{1}{R} \sum_{r=1}^{R} \frac{1}{n_\ell} \sum_{i=0}^{n_\ell-1} \Delta_\ell(\boldsymbol{x}_{ri}^\ell)$ [38]

- IID randomizations of low-discrepancy point $\{\boldsymbol{x}_{1i}^\ell\}_{i=0}^{n_\ell-1}, \dots, \{\boldsymbol{x}_{Ri}^\ell\}_{i=0}^{n_\ell-1}$.
- n_ℓ greedily doubled on level where $\mathbb{V}[\Delta_\ell(\boldsymbol{X})]/(n_\ell C_\ell)$ the largest
- Variance approximated by sample variance across R sub-means

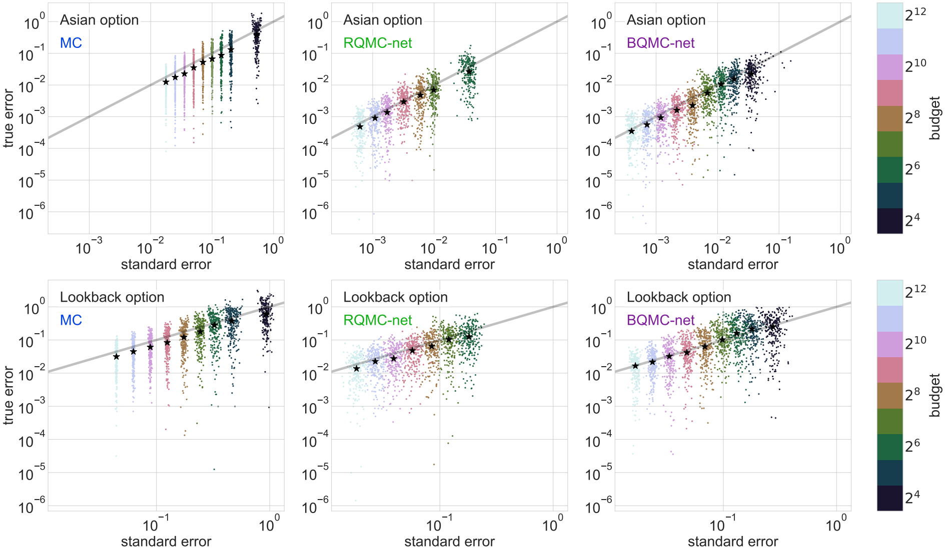
New BMLQMC Bayesian MLQMC without replications $\mathbb{E}[\Delta_\ell(\boldsymbol{X})] \approx \frac{1}{n_\ell} \sum_{i=0}^{n_\ell-1} \Delta_\ell(\boldsymbol{x}_i^\ell)$

- $\{\boldsymbol{x}_i^\ell\}_{i=0}^{n_\ell-1}$ a single randomized low-discrepancy point set
- n_ℓ greedily doubled on level with maximum variance reduction for the cost
- Variance taken to be posterior variance with $\Delta_\ell \sim \mathrm{GP}(\tau, K_\ell)$ (independent GPs)

Convergence with Increasing Budgets: LD Digital Nets



Multilevel Error Estimate Accuracy: LD Digital Nets



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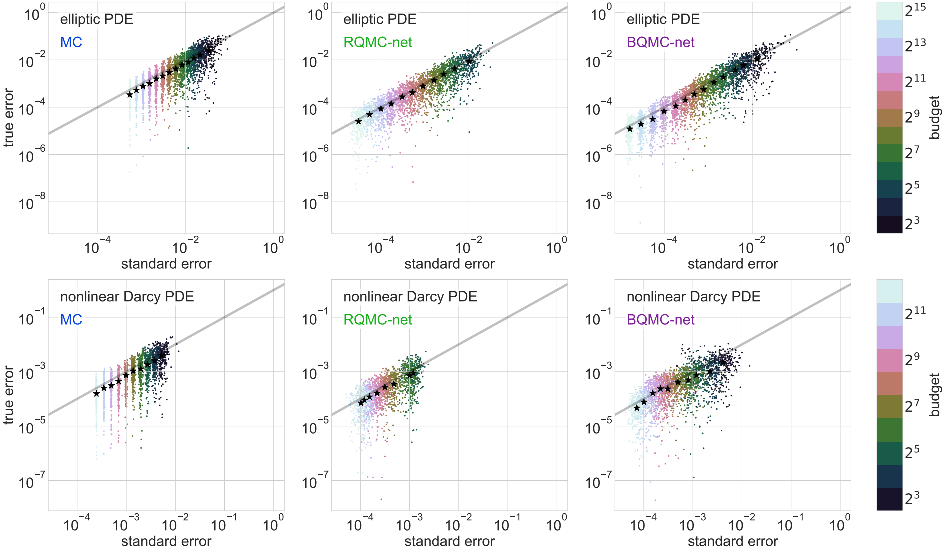
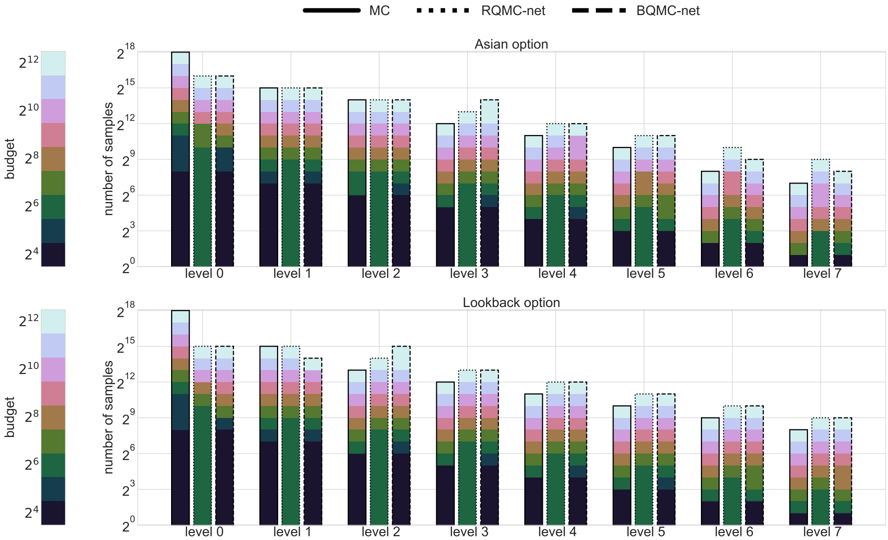


Multilevel Sample Allocation: LD Digital Nets



Multitask Gaussian Processes

$$f(\ell,\boldsymbol{x}) \sim \mathrm{GP}(0,K)$$

$N = n_1 + \cdots + n_L$ sampling locations $\mathcal{D} = \mathcal{D}_1 \cup \cdots \cup \mathcal{D}_L$ where $\mathcal{D}_\ell = \left\{\left(\ell,\boldsymbol{x}_i^\ell\right)\right\}_{i=0}^{n_\ell-1}$. Posterior mean and covariance

$$\mathbb{E}[f(\ell,\boldsymbol{x})] = \boldsymbol{K}^T(\ell,\boldsymbol{x})\mathsf{K}^{-1}\boldsymbol{f}$$
$$\mathbb{V}[f(\ell,\boldsymbol{x})] = K((\ell,\boldsymbol{x}),(\ell,\boldsymbol{x})) - \boldsymbol{K}^T(\ell',\boldsymbol{x}')\mathsf{K}^{-1}\boldsymbol{K}(\ell,\boldsymbol{x})$$

- $\boldsymbol{K}(\ell,\boldsymbol{x}) = K(\mathcal{D},(\ell,\boldsymbol{x}))$ and $\boldsymbol{f} = f(\mathcal{D})$ are length N vectors
- $\mathsf{K} = K(\mathcal{D},\mathcal{D}^T)$ is the $N \times N$ Gram matrix

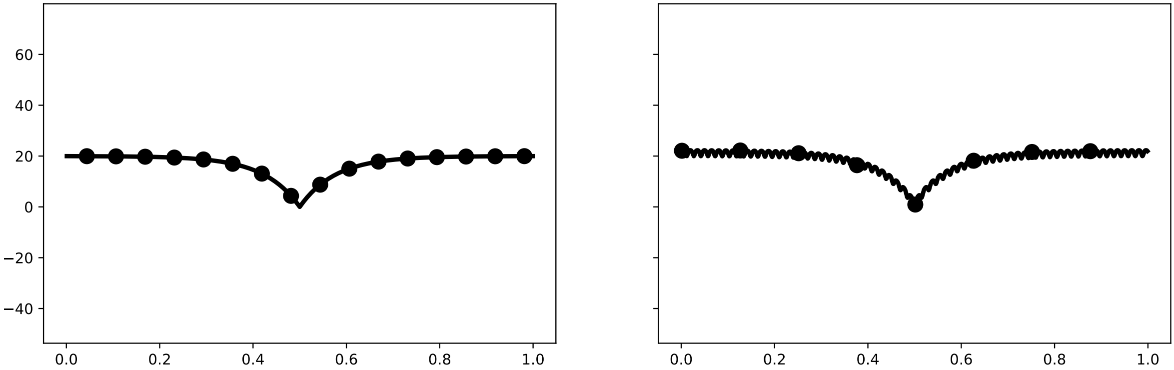
Kernel K depends on hyperparameters $\boldsymbol{\theta}$ e.g. global scale, lengthscale, etc.
Hyperparameters $\boldsymbol{\theta}$ often chosen to minimize negative marginal log likelihood (NMLL)

$$\mathrm{NMLL} \propto \boldsymbol{f}^T\mathsf{K}^{-1}\boldsymbol{f} + \log|\mathsf{K}| + \log(2\pi)N$$

$\therefore$ Multitask GPs require computing $\mathsf{K}^{-1}\boldsymbol{f}$ and $\log|\mathsf{K}|$ $\implies$ standard cost $\mathcal{O}(N^3)$

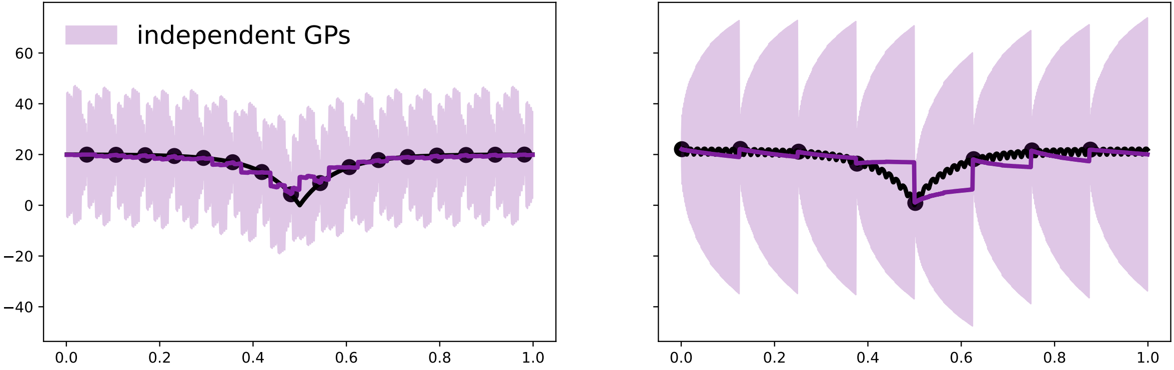
Independent GPs vs a Multitask GP (MTGP)

Low Fidelity Left, High Fidelity Right



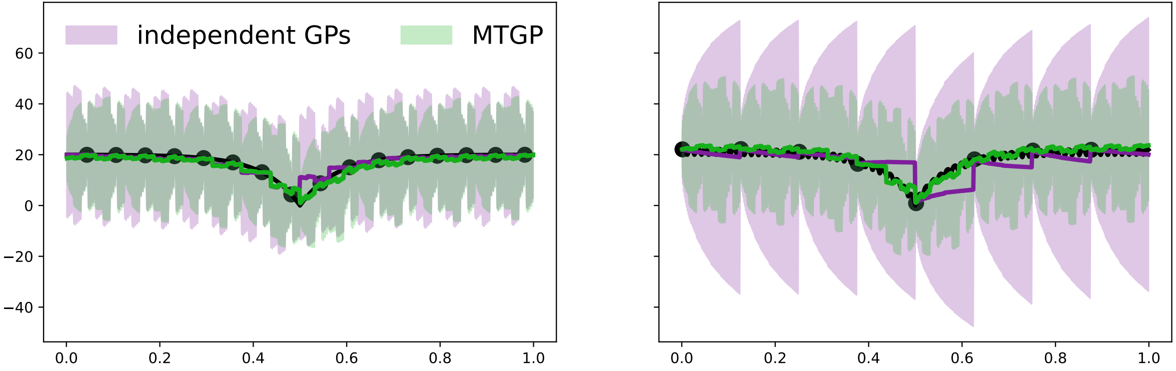
Independent GPs vs a Multitask GP (MTGP)

Low Fidelity Left, High Fidelity Right



Independent GPs vs a Multitask GP (MTGP)

Low Fidelity Left, High Fidelity Right



Product Kernels for Multitask GPs

Common to assume

$$K((\ell,\boldsymbol{x}),(\ell',\boldsymbol{x}')) = R(\ell,\ell')Q(\boldsymbol{x},\boldsymbol{x}')$$

- $R : \{1,\dots,L\} \times \{1,\dots,L\} \to \mathbb{R}$ an SPD kernel over levels e.g.

$$\mathsf{R} = \{R(\ell,\ell')\}_{\ell,\ell'=1}^L = \mathsf{B}\mathsf{B}^T + \mathrm{diag}(\boldsymbol{\nu}), \quad \boldsymbol{\nu} \in \mathbb{R}_+^L, \quad \mathsf{B} \in \mathbb{R}^{L\times r}, \quad \text{rank } r \leqslant L$$

- $Q : [0,1]^d \times [0,1]^d \to \mathbb{R}$ an SPD kernel over parameters

$$\mathsf{K} = \begin{pmatrix} \mathsf{K}_{11} & \cdots & \mathsf{K}_{1L} \\ \vdots & \ddots & \vdots \\ \overline{\mathsf{K}_{1L}} & \cdots & \mathsf{K}_{LL} \end{pmatrix} = \begin{pmatrix} R_{11}\mathsf{Q}_{11} & \cdots & R_{1L}\mathsf{Q}_{1L} \\ \vdots & \ddots & \vdots \\ \overline{R_{1L}\mathsf{Q}_{1L}} & \cdots & R_{LL}\mathsf{Q}_{LL} \end{pmatrix}$$

- $R_{\ell\ell'} = R(\ell,\ell')$ is a scalar
- $\mathsf{Q}_{\ell\ell'} = Q(\mathcal{D}_\ell, \mathcal{D}_{\ell'}^T)$ is an $n_\ell \times N_{\ell'}$ Gram matrix

New Fast Multitask GPs

$$\mathsf{K} = \begin{pmatrix} R_{11}\mathsf{Q}_{11} & \cdots & R_{1L}\mathsf{Q}_{1L} \\ \vdots & \ddots & \vdots \\ \overline{R_{1L}\mathsf{Q}_{1L}} & \cdots & R_{LL}\mathsf{Q}_{LL} \end{pmatrix}$$

Idea: Force "nice" structure in $\mathsf{Q}_{\ell\ell'}$ through special pairings of $\mathsf{X}_\ell = \{\boldsymbol{x}_i^\ell\}_{i=1}^{n_\ell}$ and Q

1. X_ℓ a lattice and Q a shift-invariant (SI) kernel $\implies$ $\mathsf{Q}_{\ell\ell'}$ block circulant
2. X_ℓ a (base 2) digital net and Q a digitally-SI (DSI) kernel $\implies$ $\mathsf{Q}_{\ell\ell}$ block RSBT

Technicalities

- Lattices and digital nets require sample sizes $n_\ell = 2^{m_\ell}$
- Lattices $\mathsf{X}_1,\dots,\mathsf{X}_L$: same generating vector, possibly different random shifts
- Circulant matrices diagonalizable by FFT
- Digital nets $\mathsf{X}_1,\dots,\mathsf{X}_L$: same generating matrices, possibly different digital shifts
- RSBT matrices diagonalizable by FWHT

Fast Multitask GPs Continued

$$\mathsf{K}_{\ell\ell'} = R_{\ell\ell'}\mathsf{Q}_{\ell\ell'} = \mathsf{V}_{m_\ell}\Sigma_{\ell\ell'}\overline{\mathsf{V}_{m_{\ell'}}}$$

- $\overline{\mathsf{V}_m}$ a $2^m \times 2^m$ *fast transform matrix*
  1. Lattice X_ℓ with SI Q makes $\overline{\mathsf{V}_{m_\ell}}$ the Fast Fourier Transform
  2. Digital Net X_ℓ with DSI Q makes $\overline{\mathsf{V}_{m_\ell}}$ the Fast Walsh Hadamard Transform
- $\mathsf{V}_m\boldsymbol{a}$ and $\overline{\mathsf{V}_m}\boldsymbol{a}$ both cost only $\mathcal{O}(m2^m)$ to compute
- The first column of $\overline{\mathsf{V}_m}$ is $\mathbf{1}_m/\sqrt{2^m}$
- $\Sigma_{\ell\ell'}$ a diagonal block matrix characterized by

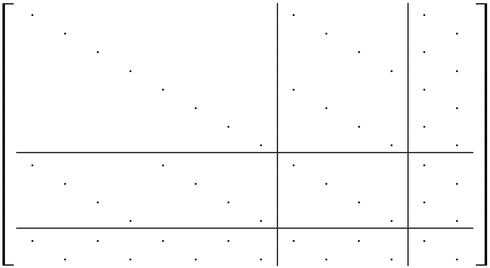
$$\boldsymbol{\sigma}_{\ell\ell'} = \Sigma_{\ell\ell'}\mathbf{1}_{m_{\ell'}} = \sqrt{2^{m_{\ell'}}}\,\overline{\mathsf{V}_{m_\ell}}\boldsymbol{k}_{\ell\ell',1}$$

where $\boldsymbol{k}_{\ell\ell',1}$ is the first column of $\mathsf{K}_{\ell\ell'}$, and we assume $m_\ell \geqslant m_{\ell'}$

Fast Multitask GPs Gram Matrix Structure

$$\mathsf{K} = \begin{pmatrix} \mathsf{V}_{m_1} & & \\ & \ddots & \\ & & \mathsf{V}_{m_L} \end{pmatrix} \begin{pmatrix} \Sigma_{11} & \cdots & \Sigma_{1L} \\ \vdots & \ddots & \vdots \\ \overline{\Sigma_{1L}} & \cdots & \Sigma_{LL} \end{pmatrix} \begin{pmatrix} \overline{\mathsf{V}_{m_1}} & & \\ & \ddots & \\ & & \overline{\mathsf{V}_{m_L}} \end{pmatrix} =: \mathsf{V}\Sigma\overline{\mathsf{V}}$$

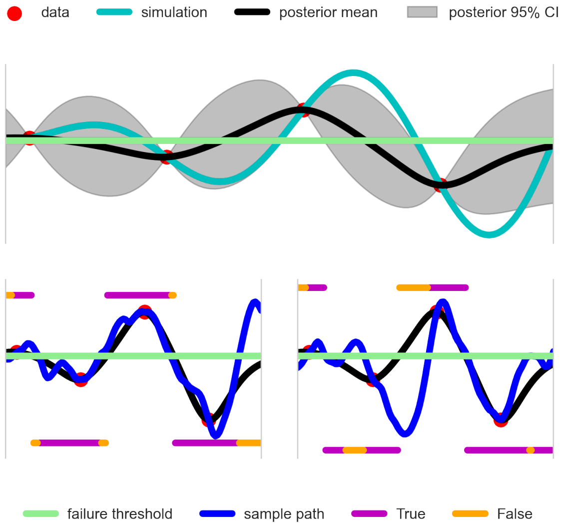
For example, if $n_1 = 8$, $n_2 = 4$, and $n_3 = 2$ then Σ has the following structure

$\Sigma =$ 

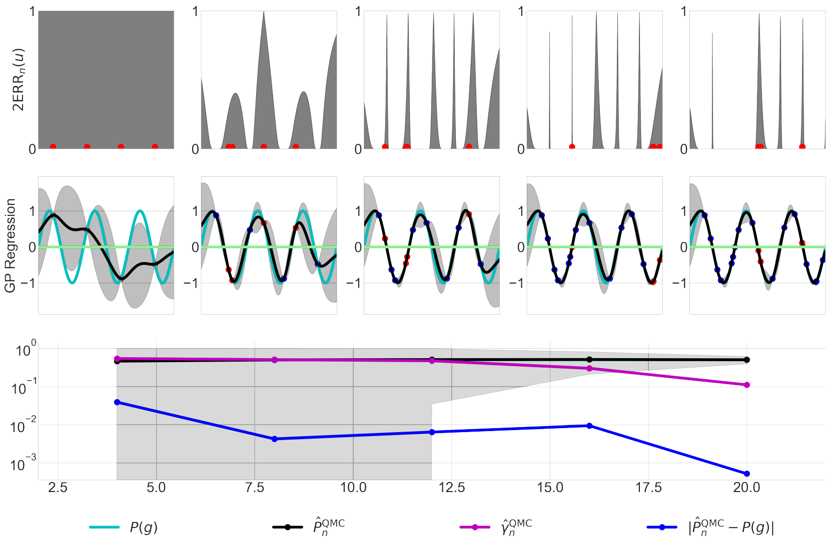
Thesis contains algorithm for efficiently computing $\Sigma^{-1}\widehat{f}$ and $\log\lvert\Sigma\rvert$ with cost & storage analysis

New Gaussian Processes for Reliability Analysis [109]

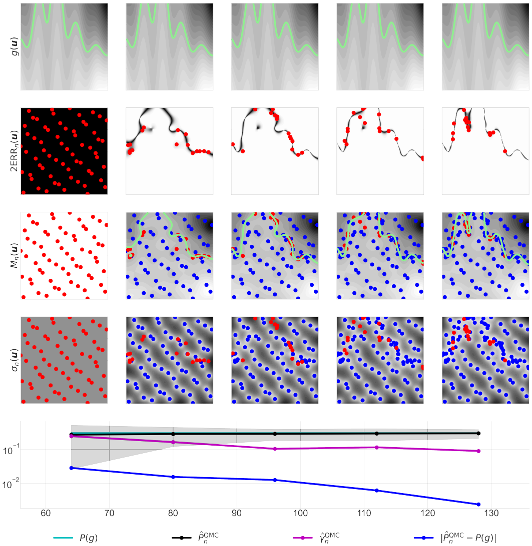
Guaranteed credible intervals for probability of failure estimation with GPs



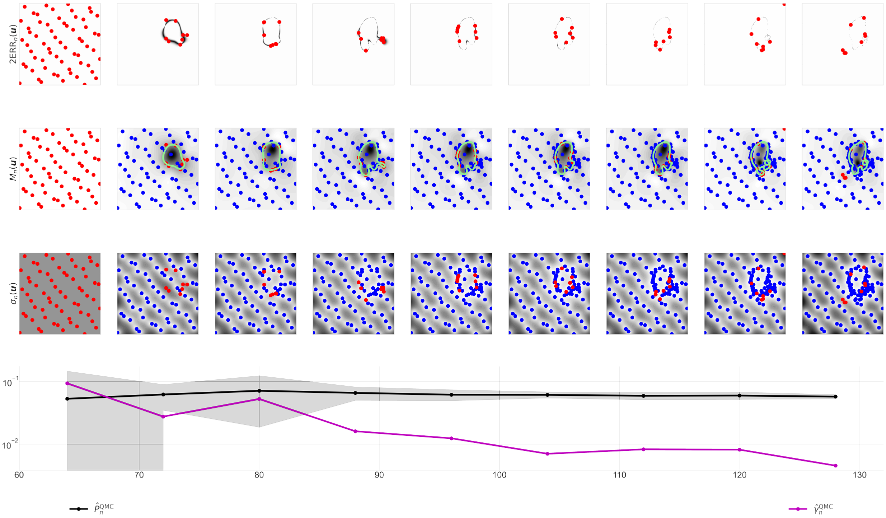
Sine Function in $d = 1$ Dimension



Multimodal Function in $d = 2$ Dimensions

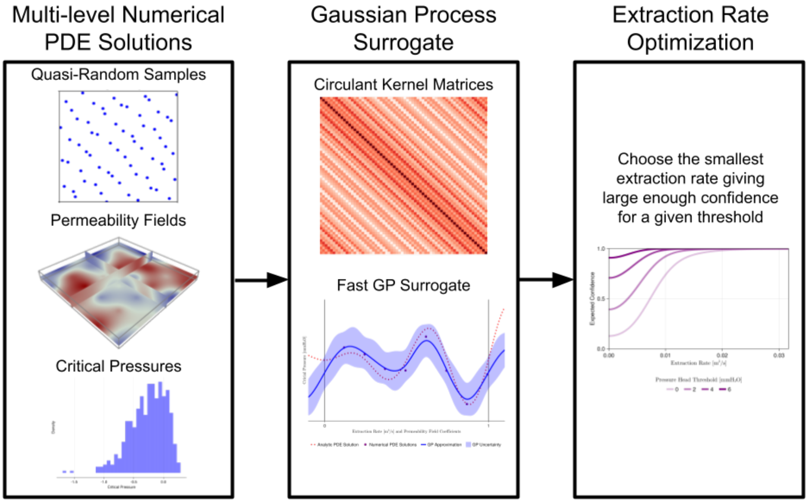


Tsunami Model from UM-Bridge [104] in $d=2$ Dimensions

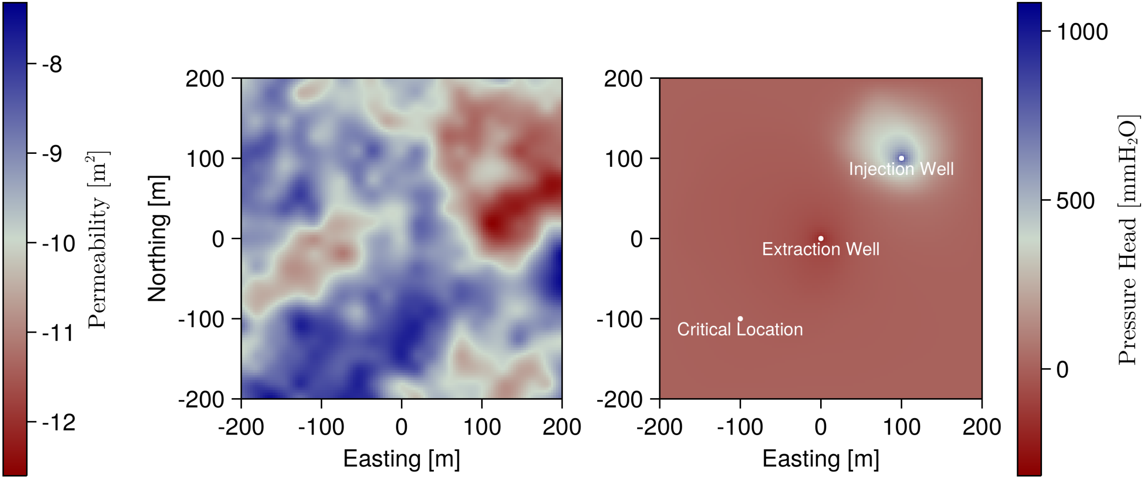


New Fast Gaussian Processes (GPs) for the Darcy Equation [114]

Error-aware multilevel GPs for modeling subsurface flow through porous media

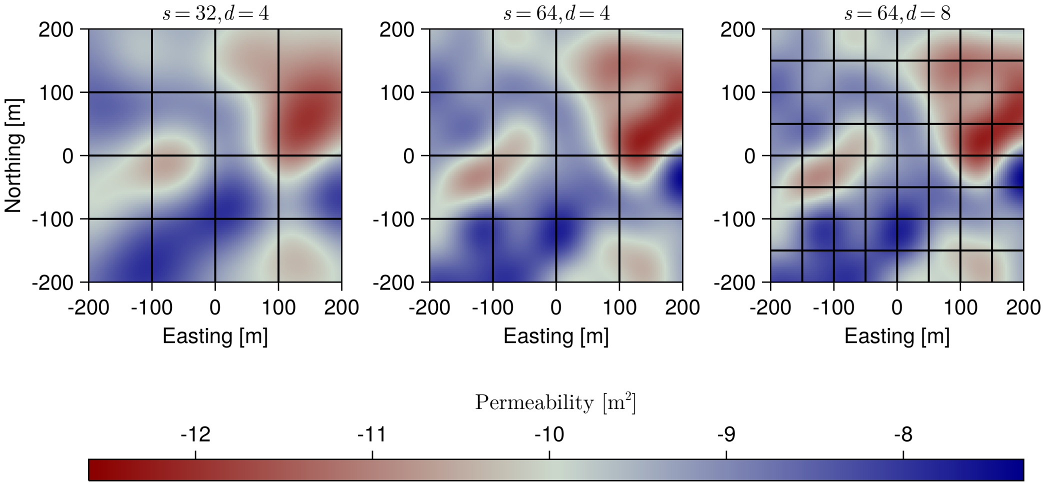


Permeability Field and Pressure Field from Darcy's Equation



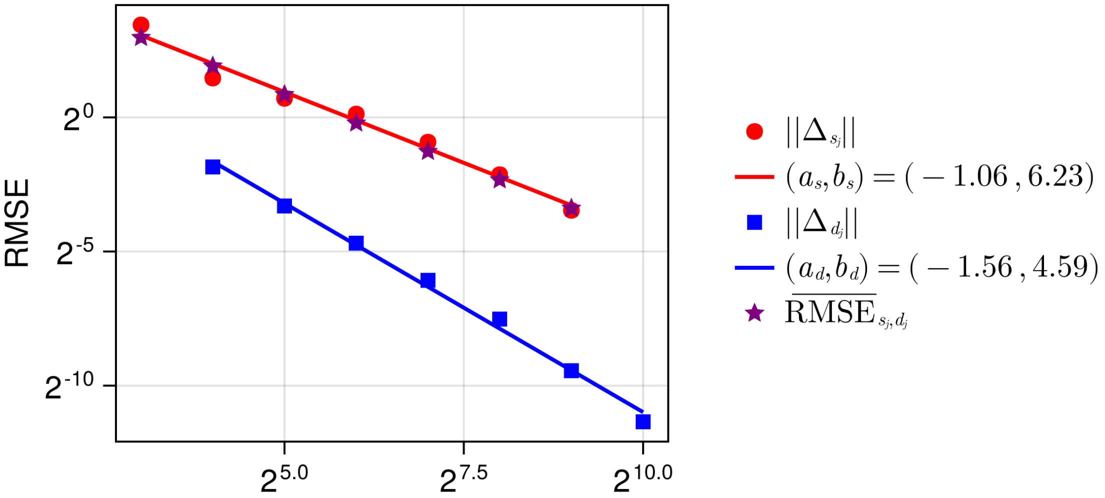
Multi-Resolution Permeability Field Decomposition

Discretized in both the number of KL terms s and the number of mesh points d



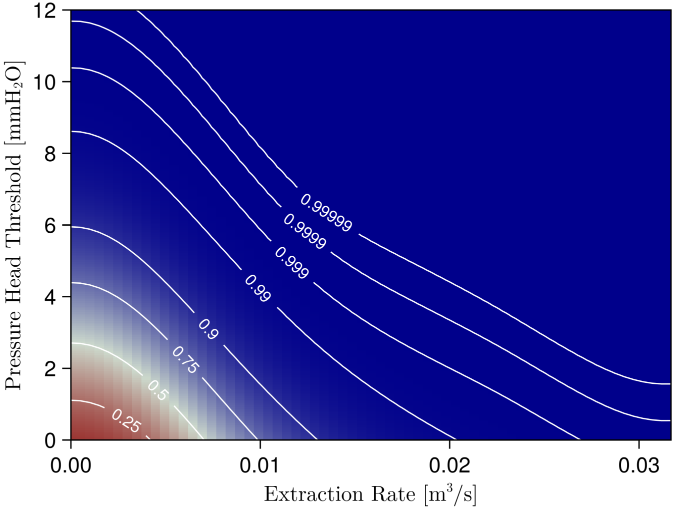
Tracking Convergence of Both Discretization Errors

Two-dimensional subsurface left and three-dimensional subsurface right



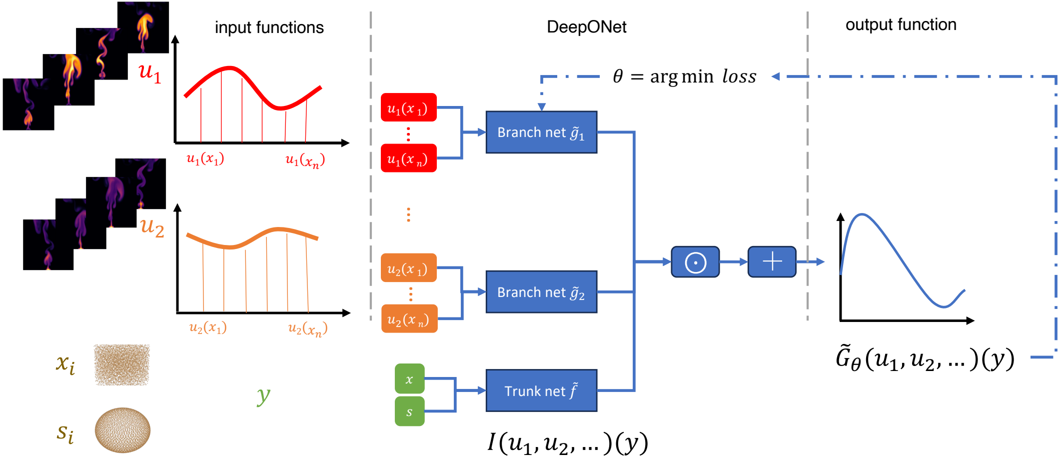
Confidence Pressure Remains Below Critical Threshold

Two-dimensional subsurface left and three-dimensional subsurface right



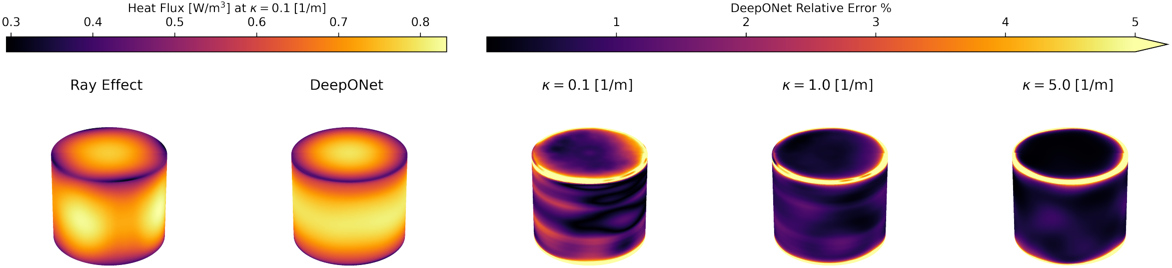
New Neural Radiative Transfer [113]

Using Deep Operator Network scientific machine learning models to accelerate radiative transfer simulations



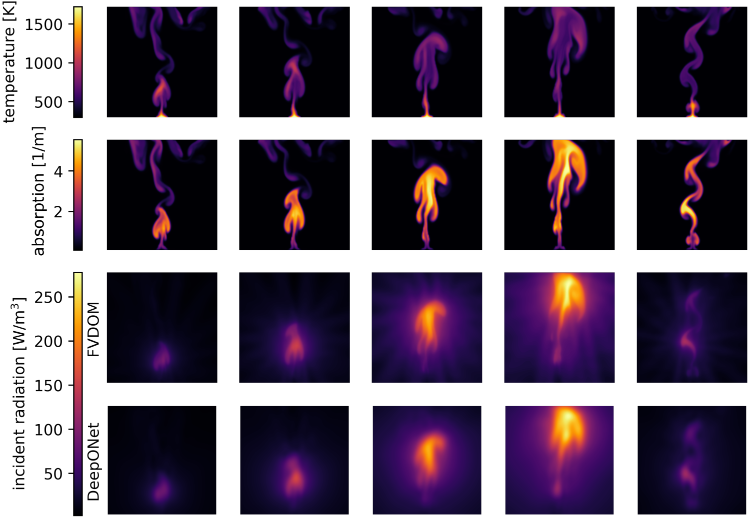
Modeling Gray Gas in a Cylinder

DeepONets honor radiative transfer physics and overcome the ray effect in traditional numerical PDE solvers



Modeling a Two-Dimensional Pool Fire

Compared against reference finite volume discrete-ordinate method (FVDOM) in `FireFOAM`



New SciML for Exact Recovery of Nonlinear PDEs [2]

Learning the approximate Hessian operator enables sciML to converge to machine precision

Newton–Kantorovich solution trajectories of PDE solutions $\{v_n(c)\}_{n=0}^S$ for random coefficients c

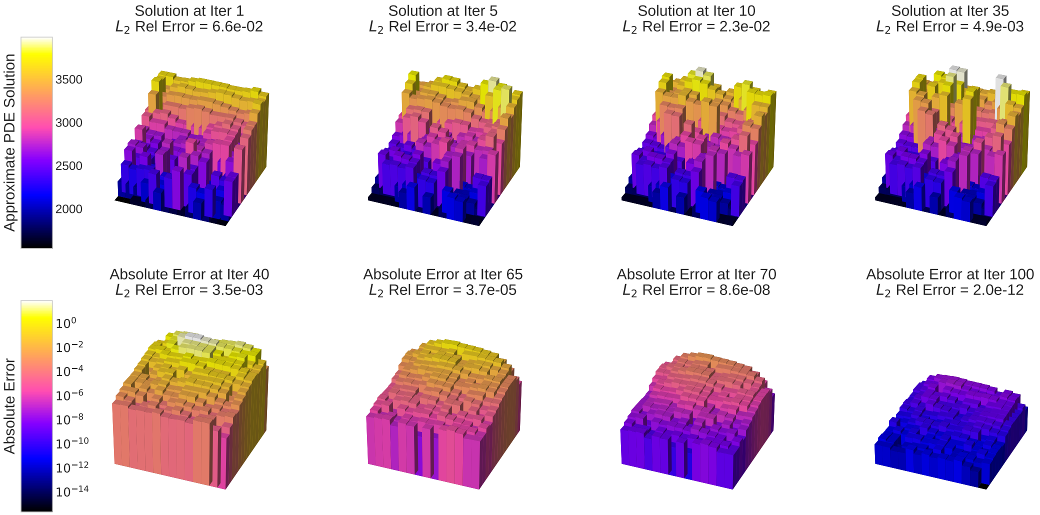
$$v_{n+1}(c) = v_n(c) - \alpha H^{-1}(v,c,\lambda)\frac{\partial F^T}{\partial v}(v,c)F(v,c)$$

$$H(v,c,\lambda) = L(v,c,\lambda)L^T(v,c,\lambda) = \frac{\partial F^T}{\partial v}(v,c)\frac{\partial F}{\partial v}(v,c) + \lambda \mathsf{I}$$

	Existing sciML Methods	Novel CHONKNORIS Method
Learn to predict	a function (operator learning)	an operator (learning to learn)
Learned Map	$c \mapsto v_S$	$(v,c,\lambda) \mapsto L(v,c,\lambda)$
Input $\mapsto$ Output Sizes	$\mathcal{O}(N) \mapsto \mathcal{O}(N)$	$\mathcal{O}(N) \mapsto \mathcal{O}(N^2)$
Achievable Errors	$\approx \mathcal{O}(10^{-2})$ or $\mathcal{O}(10^{-3})$	machine precision $\mathcal{O}(10^{-16})$

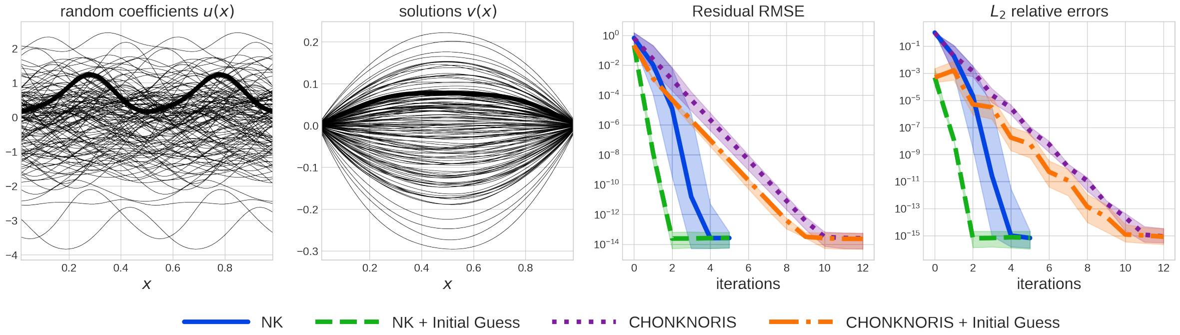
Newton–Kantorovich (NK) Iteration for Seismic Imaging

Finds subsurface velocity from a surface acoustic signal [120, 21]



Nonlinear Elliptic PDE

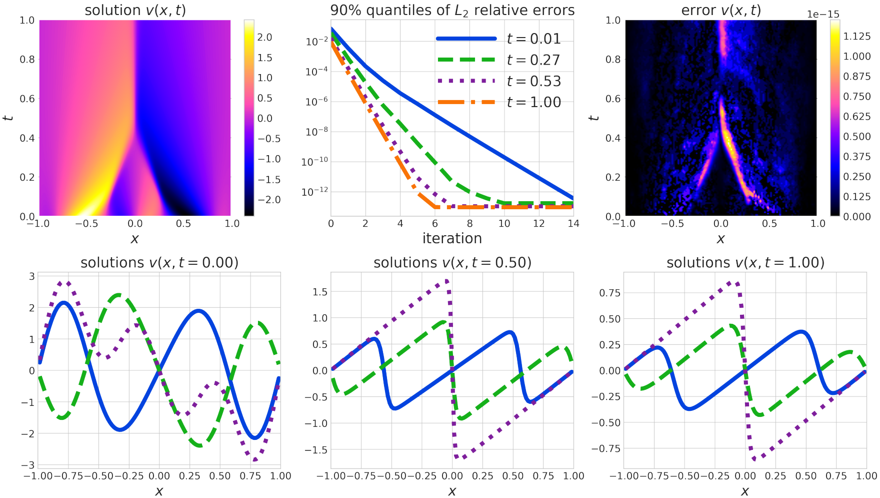
CHONKNORIS achieves machine precision recovery in 12 iterations



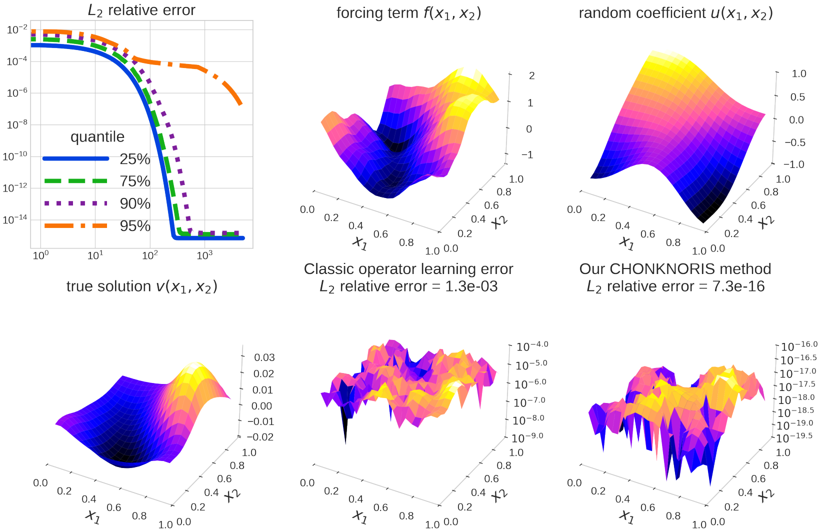
- CHONKNORIS requires more iterations but avoids cubic inversion cost in NK method
- Initial guess from existing sciML method can accelerate convergence

Burgers' Equation with Shocks via Implicit Time Stepping

CHONKNORIS (at each time step) recovers solutions f to within 10^{-16} error

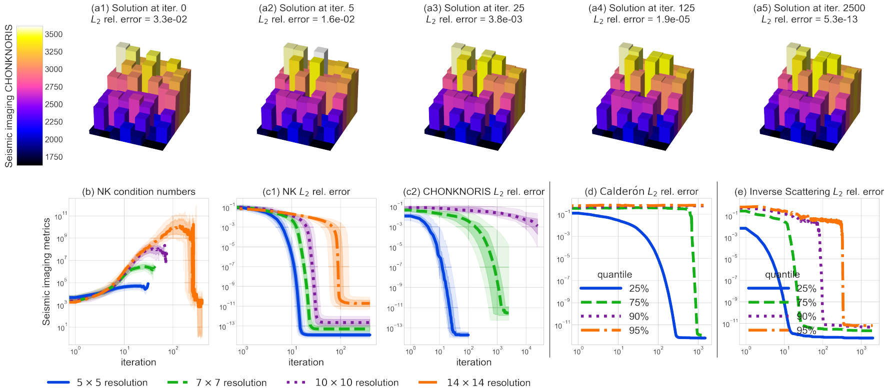


Darcy Flow in Two Dimensions



Inverse Problems

CHONKNORIS can exactly recover rough solutions at low resolutions



CHONKNORIS struggles to predict the ill conditioned matrices from

- fine discretizations
- rough coefficients
- near convergence perturbations

Summary

`pip install qmcpy`: qmcsoftware.github.io/QMCSoftware/ for Quasi-Monte Carlo

- Low-discrepancy sequences with randomizations
- Automatic transforms, to rewrite problem into $f : [0,1]^d \to \mathbb{R}$ with uniform stochasticity
- Diverse use cases, including financial options, parameterized PDEs, sensitivity indices, ...
- Adaptive stopping criteria, and vectorized algorithms for functions of multiple expectations
- (Digitally)-shift-invariant kernels, of varying smoothness

`pip install fastgps`: alegresor.github.io/fastgps/ for fast Gaussian process

- Single task and multitask fast GPs as well as baseline standard GPs
- Kernel hyperparameter optimization via MLL or GCV losses
- Fast Bayesian cubature, including for multitask GPs
- Efficient batched GPs with GPU support

Applications of QMC, fast GPs, sciML, and more

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