Kernel Thinning and Stein Thinning

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Joint work with Raaz Dwivedi, Marina Riabiz, Wilson Ye Chen, Jon Cockayne, Pawel Swietach, Steven A. Niederer, Chris J. Oates, and Abhishek Shetty

Computational Cardiology: Developing multiscale *digital twins* of human hearts to non-invasively predict disease progression and therapy response [Niederer, Sacks, Girolami, and Willcox, 2021]

Single cell scale — Tissue scale — Organ scale

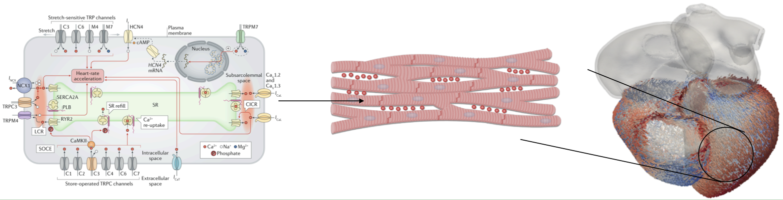


Figure credit: Marina Riabiz

Example (Heartbeats and arrhythmias)

- Whole-organ heartbeats are coordinated by calcium signaling in heart cells
- Dysregulation known to lead to life-threatening heart arrhythmias
- **Goal:** Model impact of calcium signaling dysregulation on heart function [Campos, Shiferaw, Prassl, Boyle, Vigmond, and Plank, 2015, Niederer, Lumens, and Trayanova, 2019, Colman, 2019]

Motivation: Computational Cardiology

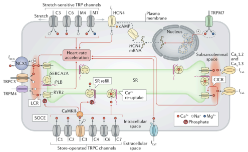
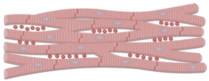
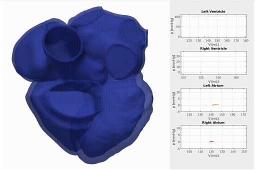
 →  → 

Figure credit: Augustin et al. 2020

Inferential Pipeline (Impact of calcium signaling dysregulation on heart function)

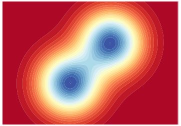
1. Estimate unknown calcium signaling model parameters from patient data
2. Capture uncertainty by sampling many likely parameter configurations
   - Run **Markov chain Monte Carlo (MCMC)** to (eventually) draw sample points from the posterior distribution $\mathbb{P}$ over unknown parameters
   - May require millions of sample points to adequately explore target distribution $\mathbb{P}$
3. Propagate uncertainty by simulating whole-heart model for each configuration
   - **Problem:** Each simulation requires 1000s of CPU hours!

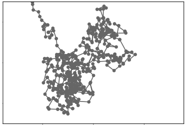
Questions: Can we accurately summarize $\mathbb{P}$ using many fewer points? How?

Distribution Compression

Goal: Accurately summarize a distribution $\mathbb{P}$ using a small number of points

Standard solutions





- **i.i.d. sampling** directly from $\mathbb{P}$
- **MCMC** with Markov chain converging to $\mathbb{P}$

Benefits: **Readily available** and **eventually high-quality**

- Provide asymptotically exact sample estimates $\mathbb{P}_n f = \frac{1}{n}\sum_{i=1}^n f(x_i)$ for intractable expectations $\mathbb{P}f = \mathbb{E}_{X\sim\mathbb{P}}[f(X)]$

Drawback: **Samples are too large!**

- Typical integration error $\mathbb{P}_n f - \mathbb{P}f = \Theta(n^{-1/2})$: need $n = 10000$ for 1% error
- Prohibitive for expensive downstream tasks and function evaluations

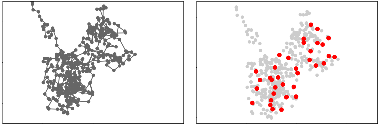
Idea: Directly compress the high-quality sample approximations $\mathbb{P}_n$

- Reduces general problem to approximating empirical distributions

Distribution Compression

Question: How do we effectively compress an empirical distribution $\mathbb{P}_n$?

Standard solutions



- **Uniform subsampling / i.i.d. sampling**
- **Standard thinning:** Keep every t-th point

Drawback: **Large loss in accuracy**, worst case integration error $= \Theta(\sqrt{t/n})$

- Compression from n to $\sqrt{n}$ points increases error from $\Theta(n^{-1/2})$ to $\Theta(n^{-1/4})$

Question: Can we do better?

Minimax lower bounds for worst-case integration error to $\mathbb{P}$

- $\Omega(n^{-1/2})$ for any compression procedure returning $\sqrt{n}$ points [Phillips and Tai, 2020]
- $\Omega(n^{-1/2})$ for any approximation based only on n i.i.d. points from $\mathbb{P}$

  [Tolstikhin, Sriperumbudur, and Muandet, 2017]

This talk: Introduce a more effective compression strategy – kernel thinning – that matches these lower bounds up to log factors

Problem Setup

Given:

- Input points $\mathcal{S}_{\text{in}} = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$ with empirical distribution $\mathbb{P}_n = \frac{1}{n}\sum_{i=1}^n \delta_{x_i}$
  - Pre-generated by any algorithm (i.i.d. sampling, MCMC, quadrature, kernel herding)
- Target output size s (e.g., $s = \sqrt{n}$ for heavy compression)

Goal: Return coreset $\mathcal{S}_{\text{out}} \subset \mathcal{S}_{\text{in}}$ with $|\mathcal{S}_{\text{out}}| = s$, $\mathbb{Q} = \frac{1}{s}\sum_{x \in \mathcal{S}_{\text{out}}} \delta_x$, and $o(s^{-1/2})$ (better-than-i.i.d.) worst-case integration error between $\mathbb{P}_n$ and $\mathbb{Q}$

Maximum Mean Discrepancies

Goal: Return coreset $\mathcal{S}_{\text{out}} \subset \mathcal{S}_{\text{in}}$ with $|\mathcal{S}_{\text{out}}| = s$, $\mathbb{Q} = \frac{1}{s}\sum_{x\in\mathcal{S}_{\text{out}}} \delta_x$, and $o(s^{-1/2})$ worst-case integration error between $\mathbb{P}_n$ and $\mathbb{Q}$

Quality measure: Maximum mean discrepancy (MMD) [Gretton, Borgwardt, Rasch, Schölkopf, and Smola, 2012]

$$\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n, \mathbb{Q}) = \sup_{\|f\|_{\mathbf{k}}\leq 1} |\mathbb{P}_n f - \mathbb{Q} f|$$

- Measures maximum discrepancy between input and coreset expectations over a class of real-valued test functions (unit ball of a reproducing kernel Hilbert space)
- Parameterized by a reproducing kernel $\mathbf{k}$: any symmetric ($\mathbf{k}(x,y) = \mathbf{k}(y,x)$) and positive semidefinite ($\sum_{i,l} c_i c_l \mathbf{k}(z_i, z_l) \geq 0, \forall z_i \in \mathbb{R}^d, c_i \in \mathbb{R}$) function
  - Gaussian: $\mathbf{k}(x,y) = e^{-\frac{1}{2}\|x-y\|_2^2}$, Inverse multiquadric: $\mathbf{k}(x,y) = \frac{1}{(1+\|x-y\|_2^2)^{1/2}}$
- Metrizes convergence in distribution for popular infinite-dimensional kernels (e.g., Gaussian, Matérn, B-spline, inverse multiquadric, sech, and Wendland)

Square-root Kernels

Definition (Square-root kernel)

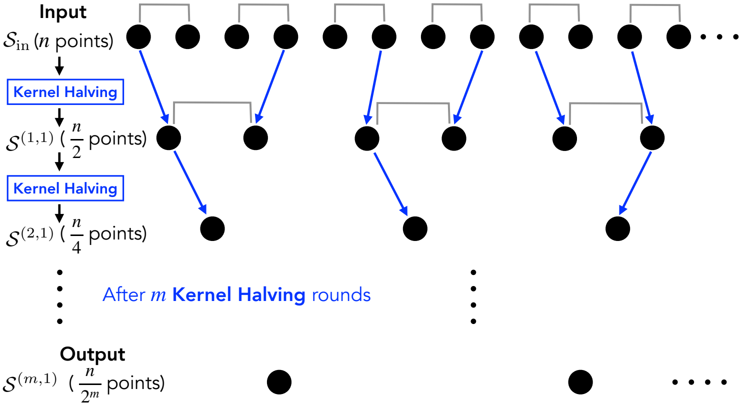
A reproducing kernel $\mathbf{k}_{\mathrm{rt}}$ is a *square-root kernel* for $\mathbf{k}$ if

$$\mathbf{k}(x,y) = \int_{\mathbb{R}^d} \mathbf{k}_{\mathrm{rt}}(x,z)\mathbf{k}_{\mathrm{rt}}(y,z)dz.$$

Name of kernel $\mathbf{k}(x,y)=\kappa(x-y)$	**Expression for** $\kappa(z)$	**Fourier transform** $\widehat{\kappa}(\omega)$	**Square-root kernel** $\mathbf{k}_{\mathrm{rt}}$
Gaussian(σ) : $\sigma > 0$	$\exp\left(-\frac{\\|z\\|_2^2}{2\sigma^2}\right)$	$\sigma^d \exp\left(-\frac{\sigma^2\\|\omega\\|_2^2}{2}\right)$	$\left(\frac{2}{\pi\sigma^2}\right)^{\frac{d}{4}}$ **Gaussian**$\left(\frac{\sigma}{\sqrt{2}}\right)$
Matérn(ν,γ) : $\nu > d, \gamma > 0$	$c_{\nu-\frac{d}{2}}(\gamma\\|z\\|_2)^{\nu-\frac{d}{2}}K_{\nu-\frac{d}{2}}(\gamma\\|z\\|_2)$	$\phi_{d,\nu,\gamma}\,(\gamma^2+\\|\omega\\|_2^2)^{-\nu}$	$A_{\nu,\gamma,d}$**Matérn**$(\frac{\nu}{2},\gamma)$
B-spline$(2\beta+1)$: $\beta \in 2\mathbb{N}+1$	$S_{2\beta+2,d}\prod_{j=1}^{d} \circledast^{2\beta+2}\mathbf{1}_{[-\frac{1}{2},\frac{1}{2}]}(z_j)$	$S'_{2\beta+2,d}\prod_{j=1}^{d}\frac{\sin^{2\beta+2}(\frac{\omega_j}{2})}{\omega_j^{2\beta+2}}$	$\widetilde{S}_{\beta,d}$**B-spline**(β)

- Exact square-root kernel not necessary: see Dwivedi and Mackey [2021] for convenient choices for inverse multiquadric, sech, Wendland, and all sufficiently smooth and integrable κ

1. **Initialization:** KT-SPLIT
   - Partitions input $\mathcal{S}_{\text{in}}$ into balanced candidate coresets, each of size s



   - Non-uniform randomness ensures $\mathbb{P}_n f - \mathbb{Q} f$ small for each f in the $\mathbf{k}_{\text{rt}}$ space

     $\Rightarrow$ **Theorem:** $\mathrm{MMD}_{\mathbf{k}} = \widetilde{\mathcal{O}}(s^{-1})$ vs. $\Omega(s^{-\frac{1}{2}})$ for i.i.d. sample [Dwivedi and Mackey, 2021]

Kernel Thinning [Dwivedi and Mackey, 2021]

1. **Initialization:** KT-SPLIT
   - Partitions input $\mathcal{S}_{\text{in}}$ into balanced candidate coresets, each of size s
   - Non-uniform randomness ensures $\mathbb{P}_n f - \mathbb{Q} f$ small for each f in the $\mathbf{k}_{\text{rt}}$ space

     $\Rightarrow$ **Theorem:** $\text{MMD}_{\mathbf{k}} = \widetilde{\mathcal{O}}(s^{-1})$ vs. $\Omega(s^{-\frac{1}{2}})$ for i.i.d. sample [Dwivedi and Mackey, 2021]
2. **Refinement:** KT-SWAP
   - Selects candidate coreset closest to $\mathcal{S}_{\text{in}}$ in terms of $\text{MMD}_{\mathbf{k}}$
   - Iteratively refines the coreset by replacing each coreset point in turn with the best alternative in $\mathcal{S}_{\text{in}}$, as measured by $\text{MMD}_{\mathbf{k}}$

Complexity

- Time: dominated by $\mathcal{O}(n^2)$ kernel evaluations
  - Reduces to $\mathcal{O}(n \log^3 n)$ for $s = \sqrt{n}$ using Compress++ of Shetty, Dwivedi, and Mackey [2022]
- Space: $\mathcal{O}(\min(nd, n^2))$
  - Reduces to $\mathcal{O}(\sqrt{n} d \log n)$ for $s = \sqrt{n}$ using Compress++

Related Work on MMD Coresets

Uniform distribution $\mathbb{P}$ on $[0,1]^d$: $\mathcal{O}(s^{-1}\log^d s)$ L^2 discrepancy MMD, s points

- Quasi-Monte Carlo [Hickernell, 1998, Novak and Wozniakowski, 2010], Online Haar strategy [Dwivedi, Feldheim, Gurel-Gurevich, and Ramdas, 2019]

Order $s^{-\frac{1}{2}}$ MMD coresets for general $\mathbb{P}$

- i.i.d. [Tolstikhin, Sriperumbudur, and Muandet, 2017], geometrically ergodic MCMC [Dwivedi and Mackey, 2021]
- Kernel herding [Chen, Welling, and Smola, 2010, Lacoste-Julien, Lindsten, and Bach, 2015], Stein points MCMC [Chen, Barp, Briol, Gorham, Girolami, Mackey, and Oates, 2019], Greedy sign selection [Karnin and Liberty, 2019]

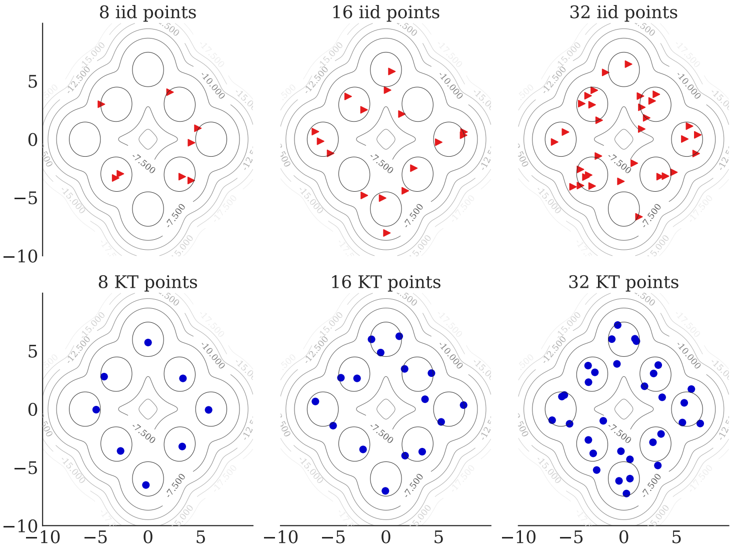
Finite-dimensional linear kernels on $\mathbb{R}^d$: $\mathcal{O}(\sqrt{d}s^{-1}\log^{2.5} s)$, s points

- Discrepancy construction [Harvey and Samadi, 2014]: does not cover infinite-dimensional $\mathbf{k}$

Unknown coreset quality

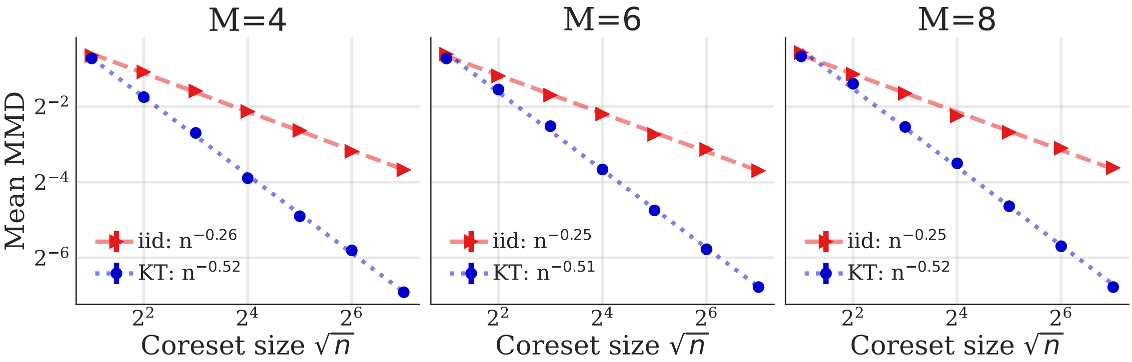
- Super-sampling with a reservoir [Paige, Sejdinovic, and Wood, 2016]: coreset quality not analyzed
- Support points [Mak and Joseph, 2018]
  - Optimal s coreset has $o(s^{-\frac{1}{2}})$ energy distance MMD but no construction given
  - Practical convex-concave procedures not analyzed or shown to be optimal

Kernel Thinning vs. i.i.d. Sampling: Mixture of Gaussians



- $\mathbb{P} = \frac{1}{M}\sum_{j=1}^{M}\mathcal{N}(\mu_j, \mathbf{I}_d)$
- $\mathbf{k}(x, y) = \exp(-\frac{1}{2\sigma^2}\|x - y\|_2^2)$ with $\sigma^2 = 2d$
- Even for small sample sizes, kernel thinning (KT) provides
  - Better stratification across components
  - Less clumping and fewer gaps within components

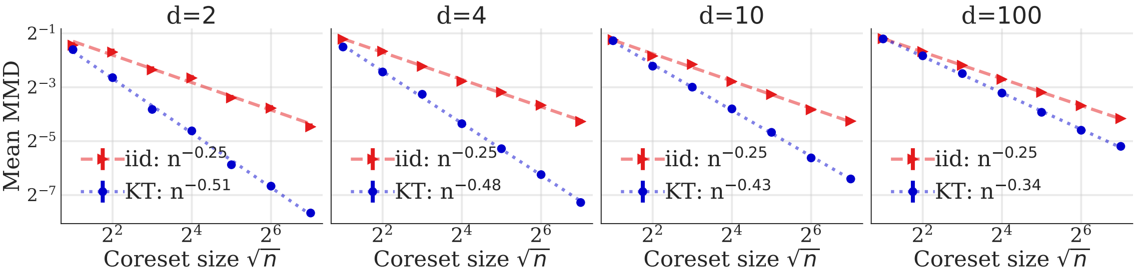
Kernel Thinning vs. i.i.d. Sampling: Mixture of Gaussians



Kernel thinning (KT) improves both rate of decay and order of magnitude of $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}, \mathbb{Q}_{KT})$

- $\mathbb{P} = \frac{1}{M}\sum_{j=1}^{M} \mathcal{N}(\mu_j, \mathbf{I}_d)$, $d = 2$
- $\mathbf{k}(x, y) = \exp(-\frac{1}{2\sigma^2}\|x - y\|_2^2)$ with $\sigma^2 = 2d$

Kernel Thinning vs. i.i.d. Sampling: Higher Dimensions



Kernel thinning (KT) improves both rate of decay and order of magnitude of $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}, \mathbb{Q}_{KT})$ even for high dimensions and small sample sizes

- $\mathbb{P} = \mathcal{N}(0, \mathbf{I}_d)$
- $\mathbf{k}(x, y) = \exp(-\frac{1}{2\sigma^2}\|x - y\|_2^2)$ with $\sigma^2 = 2d$

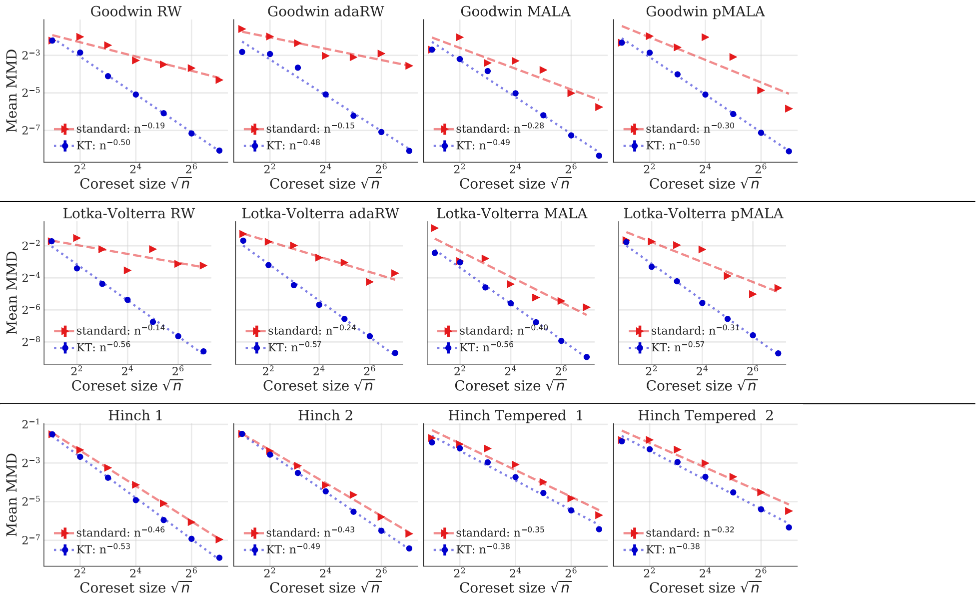
Kernel Thinning vs. Standard MCMC Thinning

Posterior inference for systems of ordinary differential equations (ODEs)

- $\mathbb{P}$ = posterior distribution of coupled ODE model parameters given observed data
- Goodwin model of oscillatory enzymatic control $(d = 4)$ [Goodwin, 1965]
- Lotka-Volterra model of oscillatory predator-prey evolution $(d = 4)$ [Lotka, 1925, Volterra, 1926]
- Hinch model of cardiac calcium signalling $(d = 38)$ [Hinch, Greenstein, Tanskanen, Xu, and Winslow, 2004]
  - Downstream goal: propagate model uncertainty through whole-heart simulation
  - Every sample point discarded via compression = 1000s of CPU hours saved

MCMC input points **[Riabiz, Chen, Cockayne, Swietach, Niederer, Mackey, and Oates, 2021]**

- Gaussian random walk (RW), adaptive RW (adaRW) [Haario, Saksman, and Tamminen, 1999]
  - 2 weeks of CPU time to generate each RW Hinch chain of length 4×10^6
- Metropolis-adjusted Langevin algorithm (MALA) [Roberts and Tweedie, 1996]
- Pre-conditioned MALA (pMALA) [Girolami and Calderhead, 2011]
- Discarded burn-in and standard thinned to form $\mathbb{P}_n$
- $\mathbf{k}(x, y) = \exp(-\frac{1}{2\sigma^2}\|x - y\|_2^2)$ with median heuristic σ^2 [Garreau, Jitkrittum, and Kanagawa, 2017]



KT improves rate of decay and magnitude of MMD, even when standard thinning is accurate

Something's Wrong

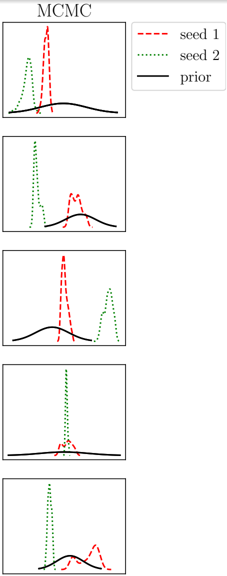
Problem: The Hinch Markov chains haven't mixed!

Solution: Use a more diffuse *tempered* posterior $\tilde{\mathbb{P}}$ for faster mixing

Problem: Tempering introduces a persistent bias

- MCMC points $\mathbb{P}_n$ will be summarizing the wrong distribution $\tilde{\mathbb{P}}$

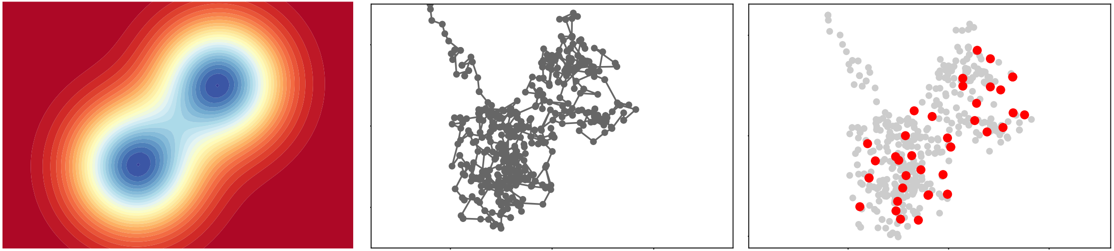
Question: Can we correct for such biases during compression?



Compression with Bias Correction

Question: Can we correct for distributional biases in $\mathbb{P}_n$ during compression?

- e.g., Biases due to off-target sampling, tempering, approximate MCMC, or burn-in



Difficulty: $\mathbb{P}_n$ alone is insufficient; need to measure distance to the true target $\mathbb{P}$

Measuring Distance to $\mathbb{P}$

Quality measure: Maximum mean discrepancy (MMD) [Gretton, Borgwardt, Rasch, Schölkopf, and Smola, 2012]

$$\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}, \mathbb{Q}) = \sup_{\|f\|_{\mathbf{k}} \leq 1} |\mathbb{P}f - \mathbb{Q}f| = \sqrt{(\mathbb{P} \times \mathbb{P})\mathbf{k} + (\mathbb{Q} \times \mathbb{Q})\mathbf{k} - 2(\mathbb{Q} \times \mathbb{P})\mathbf{k}}$$

Problem: Integration under $\mathbb{P}$ is typically intractable!

$\Rightarrow$ $\mathbb{P}\mathbf{k}$ and $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}, \mathbb{Q})$ cannot be computed in practice for most kernels

Idea: Only consider kernels $\mathbf{k}_{\mathbb{P}}$ with $\mathbb{P}\mathbf{k}_{\mathbb{P}}$ known *a priori* to be 0

- Then MMD computation only depends on $\mathbb{Q}$!

Kernel Stein Discrepancies

Idea: Consider $\mathrm{MMD}_{\mathbf{k}_{\mathbb{P}}}$ with $\mathbb{P}\mathbf{k}_{\mathbb{P}}$ known *a priori* to be 0

Kernel Stein discrepancy (KSD)

[Chwialkowski, Strathmann, and Gretton, 2016, Liu, Lee, and Jordan, 2016, Gorham and Mackey, 2017]

- $\mathbf{k}_{\mathbb{P}}(x, y) = \sum_{j=1}^{d} \frac{1}{p(x)p(y)} \nabla_{x_j} \nabla_{y_j} (p(x)\mathbf{k}(x, y)p(y))$ [Oates, Girolami, and Chopin, 2017]
  - $\mathbb{P}$ has differentiable Lebesgue density p
  - $\mathbf{k}$ is a bounded base kernel with bounded continuous derivatives
- $\mathbb{P}\mathbf{k}_{\mathbb{P}} = 0$ whenever $\nabla \log p$ is integrable [Gorham and Mackey, 2017]
- Depends on $\mathbb{P}$ through $\nabla \log p$: computable when normalization constant unknown

$\Rightarrow$ Kernel Stein discrepancy $\mathrm{MMD}_{\mathbf{k}_{\mathbb{P}}}(\mathbb{P}, \mathbb{Q})$ is computable!

Theorem (KSD controls convergence in distribution [Gorham and Mackey, 2017, Chen, Barp, Briol, Gorham, Girolami, Mackey, and Oates, 2019])

Consider the base kernel $\mathbf{k}(x, y) = (c^2 + \|\Gamma(x - y)\|_2^2)^{-1/2}$ for any $c > 0$ and positive definite Γ. If $\mathbb{P}$ has strongly log concave tails and Lipschitz $\nabla \log p$, then $\mathbb{Q}_s \Rightarrow \mathbb{P}$ whenever $\mathrm{MMD}_{\mathbf{k}_{\mathbb{P}}}(\mathbb{P}, \mathbb{Q}_s) \to 0$.

Stein Thinning

Idea: Greedily minimize KSD using points from $\mathcal{S}_{\text{in}} = \{x_1, \ldots, x_n\}$

[Riabiz, Chen, Cockayne, Swietach, Niederer, Mackey, and Oates, 2021]

- Choose initial approximation $\mathbb{Q}_1 = \delta_{y_1}$ with

$$y_1 \in \operatorname{argmin}_{y \in \mathcal{S}_{\text{in}}} \mathrm{MMD}_{\mathbf{k}_{\mathbb{P}}}(\mathbb{P}, \delta_y) = \operatorname{argmin}_{y \in \mathcal{S}_{\text{in}}} \mathbf{k}_{\mathbb{P}}(y, y)$$

- Iteratively construct $\mathbb{Q}_s = \frac{1}{s} \sum_{i=1}^{s} \delta_{y_i}$ with

$$\begin{aligned} y_s &\in \operatorname{argmin}_{y \in \mathcal{S}_{\text{in}}} \mathrm{MMD}_{\mathbf{k}_{\mathbb{P}}}(\mathbb{P}, \tfrac{s-1}{s}\mathbb{Q}_{s-1} + \tfrac{1}{s}\delta_y) \\ &= \operatorname{argmin}_{y \in \mathcal{S}_{\text{in}}} \mathbf{k}_{\mathbb{P}}(y, y) + 2\sum_{i=1}^{s-1} \mathbf{k}_{\mathbb{P}}(y_i, y) \end{aligned}$$

- Same point x_i can be selected multiple times
- Runtime $= \mathcal{O}(n \sum_{i=1}^{s} r_i)$ for $r_i \leq i$ the number of distinct points selected prior to round i (worst case $= \mathcal{O}(ns^2)$)

Stein Thinning Guarantees

Theorem (Stein thinning KSD guarantee [Riabiz, Chen, Cockayne, Swietach, Niederer, Mackey, and Oates, 2021]**)**

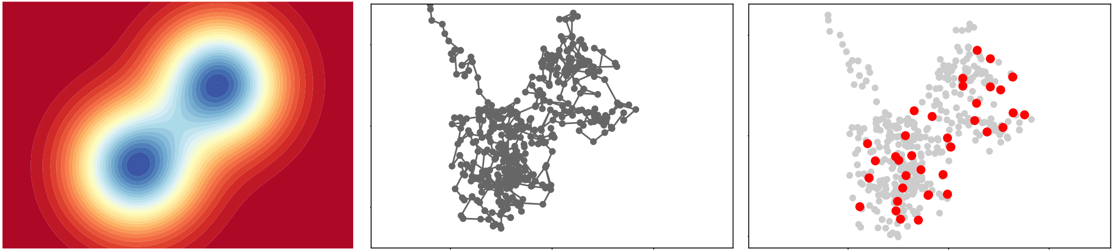
$$\mathrm{MMD}_{\mathbf{k}_{\mathbb{P}}}(\mathbb{P}, \mathbb{Q}_s)^2 \leq \inf_{w \in \Delta_{n-1}} \mathrm{MMD}_{\mathbf{k}_{\mathbb{P}}}(\mathbb{P}, \textstyle\sum_{i=1}^n w_i \delta_{x_i})^2 + \frac{(1+\log(s))}{s} \max_{x \in \mathcal{S}_{\text{in}}} \mathbf{k}_{\mathbb{P}}(x, x)$$

- *Expect* $\max_{x \in \mathcal{S}_{\text{in}}} \mathbf{k}_{\mathbb{P}}(x, x) = \mathcal{O}(\log(n))$ *for sub-Gaussian input and* $\mathbf{k}_{\mathbb{P}}(x, x) = \mathcal{O}(\|x\|_2^2)$

Takeaway: Stein thinning performs nearly as well as best simplex reweighting of $\mathcal{S}_{\text{in}}$

$\Rightarrow$ Nearly as well as Markov chain with burn-in removed!

$\Rightarrow$ Nearly as well as off-target sample after optimal importance sampling reweighting!



Stein Thinning Guarantees

Takeaway: Stein thinning performs nearly as well as best simplex reweighting of $\mathcal{S}_{\text{in}}$

$\Rightarrow$ Nearly as well as Markov chain with burn-in removed!

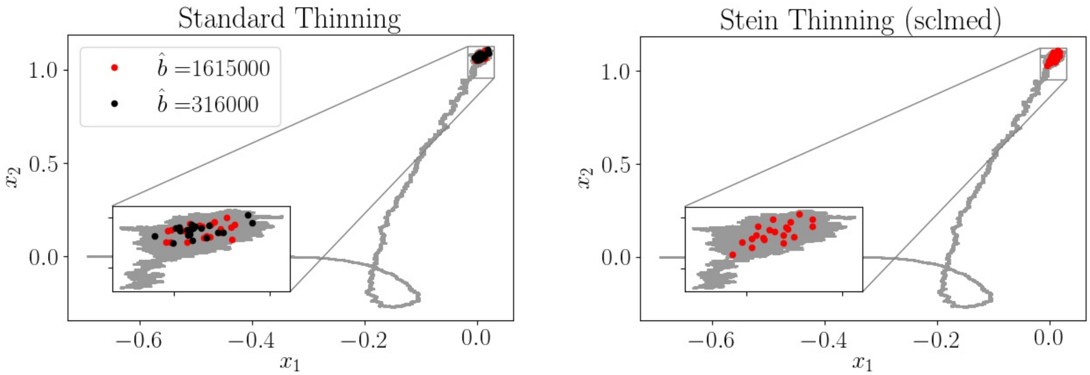
$\Rightarrow$ Neary as well as off-target sample after optimal importance sampling reweighting!

Theorem (Stein thinning corrects off-target sampling [Riabiz, Chen, Cockayne, Swietach, Niederer, Mackey, and Oates, 2021])

If $\mathcal{S}_{\text{in}}$ drawn $i.i.d.$ from $\tilde{\mathbb{P}}$, then, under mild conditions ($s \leq n$, $\log(n) = \mathcal{O}(s^{\beta/2})$ for some $\beta < 1$, and $\mathbb{E}[e^{\gamma \max\left(1, \frac{d\mathbb{P}}{d\tilde{\mathbb{P}}}(X_i)^2\right) \mathbf{k}_{\mathbb{P}}(X_i, X_i)}] < \infty$ for some $\gamma > 0$), $\text{MMD}_{\mathbf{k}_{\mathbb{P}}}(\mathbb{P}, \mathbb{Q}_s) \to 0$ almost surely as $s, n \to \infty$.

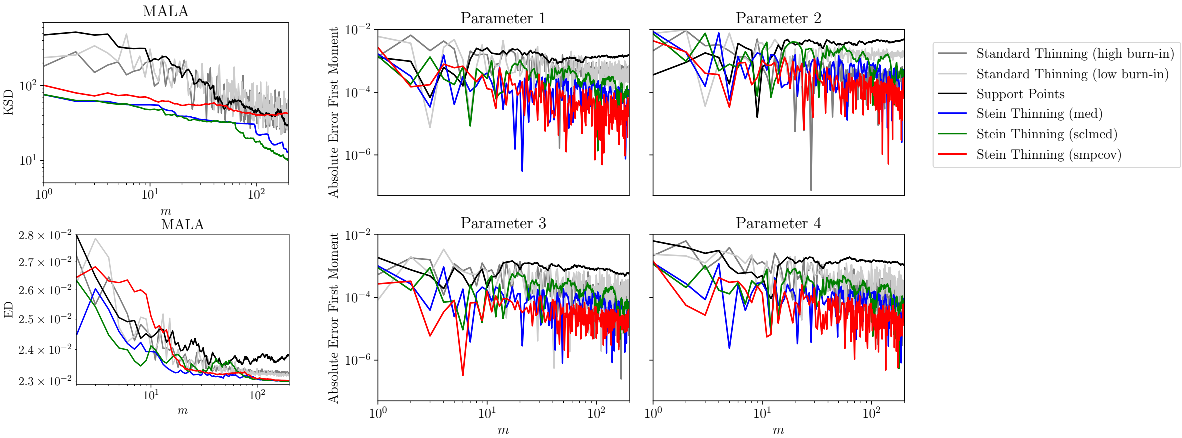
- Result extends to sufficiently ergodic Markov chains targeting $\tilde{\mathbb{P}}$

Goodwin model of oscillatory enzymatic control



- Projections on the first two coordinates of the `MALA` MCMC output
- First $s = 20$ points from Stein thinning vs. burn-in removal + standard thinning
- Substantial burn-in: $\hat{b}$ points out of 2×10^6 removed for standard thinning

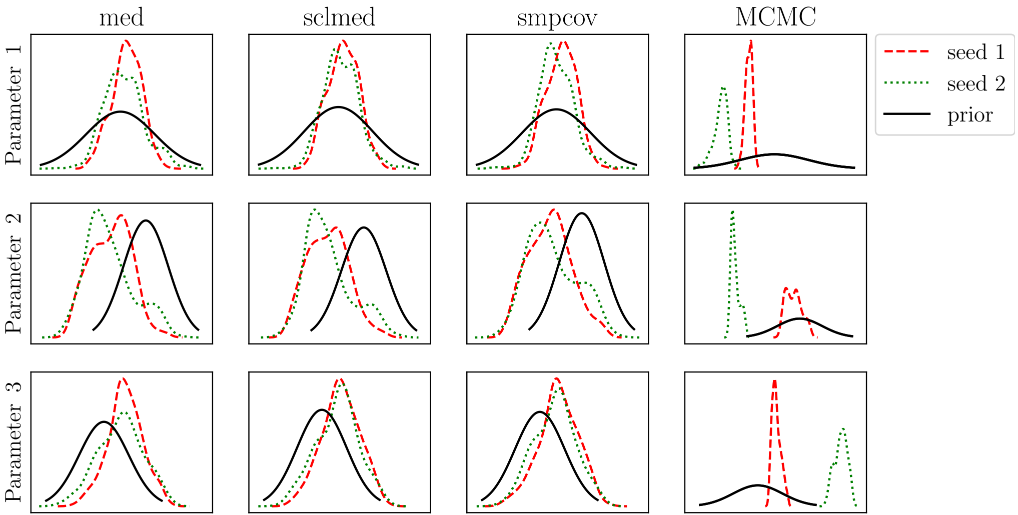
Goodwin model of oscillatory enzymatic control



Stein thinning outperforms standard thinning with high and low levels of burn-in removal in terms of KSD, energy distance (ED), and first moment estimation

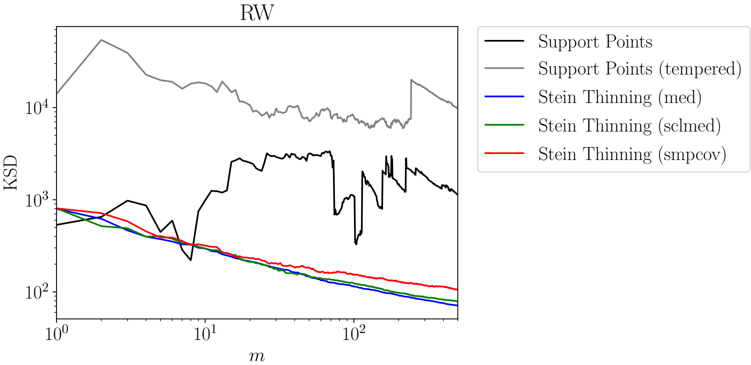
Stein Thinning in Action: Correcting for Tempering

Hinch model of cardiac calcium signalling: Tempering improves mixing



Stein Thinning in Action: Correcting for Tempering

Hinch model of cardiac calcium signalling



- Untempered support points compression yields poor summary due to poor mixing
- Tempered SP without bias correction is even worse (due to tempering bias)
- Tempering + Stein thinning bias correction improves approximation to $\mathbb{P}$

Conclusions

Summary

- New tools for summarizing a probability distribution more effectively than i.i.d. sampling or standard MCMC thinning
- Kernel thinning compresses an n point summary into a $\sqrt{n}$ point summary with better-than-i.i.d. approximation error
- Stein thinning simultaneously compresses and reduces biases due to off-target sampling, tempering, or burn-in
- Compress++ speeds up thinning algorithms without ruining their quality

Kernel Thinning and **Compress++**

Papers:
- arxiv.org/abs/2105.05842
- arxiv.org/abs/2110.01593
- arxiv.org/abs/2111.07941

Stein Thinning

Website: stein-thinning.org

Paper: arxiv.org/abs/2105.05842

Video: youtu.be/WwmTeLrNmOQ

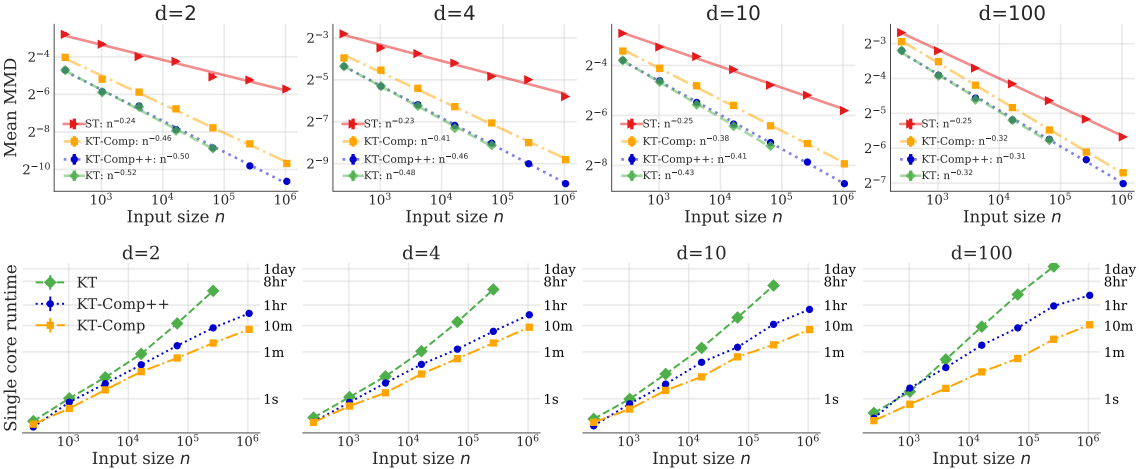
Package: github.com/microsoft/goodpoints

Generalized Kernel Thinning [Dwivedi and Mackey, 2022]

Question: Do you really need a square-root kernel?

1. KT-SPLIT with target kernel $\mathbf{k}$ yields
   - Similar or better MMD guarantees for analytic kernels (like Gaussian, IMQ, & sinc)
   - Dimension-free $\mathcal{O}(\frac{\sqrt{\log s}}{s})$ single-function integration error for any $\mathbf{k}$ and $\mathbb{P}$
2. KT-SPLIT with fractional power kernel $\mathbf{k}_\alpha$ yields
   - Improved MMD for kernels without $\mathbf{k}_{\mathrm{rt}}$ (like Laplace and non-smooth Matérn)
3. KT-SPLIT with $\mathbf{k} + \mathbf{k}_\alpha$ yields all of the above simultaneously!
   - We call this **kernel thinning+ (KT+)**

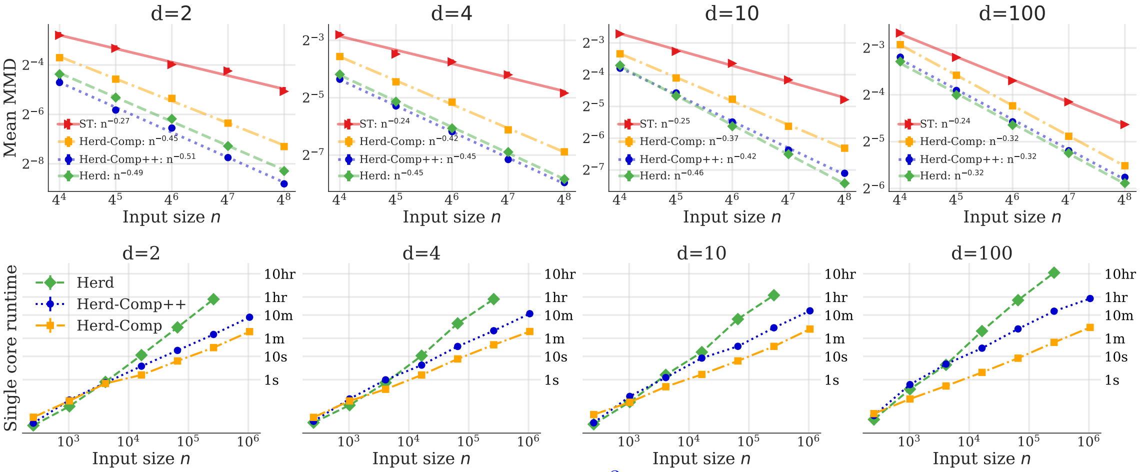
Question: Can we speed up thinning algorithms without ruining their quality?



Compress++ reduces n^2 runtime to $n \log^3 n$, applies to any thinning algorithm, and inflates error by at most a constant factor

Distribution Compression in Near-linear Time [Shetty, Dwivedi, and Mackey, 2022]

Question: Can we speed up thinning algorithms without ruining their quality?



Compress++ reduces n^2 runtime to $n \log^3 n$, applies to any thinning algorithm (e.g., kernel herding), and inflates error by at most a constant factor

Algorithm 1: COMPRESS: Given n points return thinned coreset of size $\sqrt{n}$

Input: halving algorithm HALVE, point sequence $\mathcal{S}_{\mathrm{in}}$ of size n

if $n = 1$ **then return** $\mathcal{S}_{\mathrm{in}}$

Partition $\mathcal{S}_{\mathrm{in}}$ into four arbitrary subsequences $\{\mathcal{S}_i\}_{i=1}^4$ each of size $n/4$

for $i = 1, 2, 3, 4$ **do**

  $\widetilde{\mathcal{S}}_i \leftarrow \textsc{Compress}(\mathcal{S}_i, \textsc{Halve}, \mathfrak{g})$ // return coresets of size $\sqrt{\frac{n}{4}}$

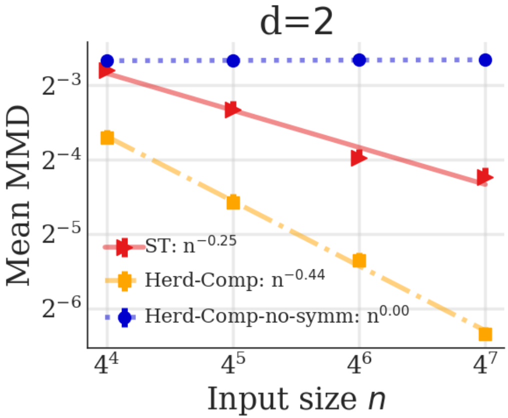
end

$\widetilde{\mathcal{S}} \leftarrow \textsc{Concatenate}(\widetilde{\mathcal{S}}_1, \widetilde{\mathcal{S}}_2, \widetilde{\mathcal{S}}_3, \widetilde{\mathcal{S}}_4)$ // coreset of size $2\sqrt{n}$

return $\textsc{Halve}(\widetilde{\mathcal{S}})$ // coreset of size $\sqrt{n}$

Error guarantees rely on unbiased halving ($\mathbb{E}[\mathbb{P}_{\textbf{Halve}}\mathbf{k} \mid \mathcal{S}_{\text{in}}] = \mathbb{P}_{in}\mathbf{k}$)

- Achieved for any halving algorithm by symmetrization: return either the outputted half or its complement with equal probability



Conclusions

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Future Directions

Many opportunities for future development

1. Unifying kernel thinning and Stein thinning
   - Can we simultaneously bias-correct $\mathbb{P}_n$ and, in the absence of bias, guarantee better-than-i.i.d. compression?
2. Value of swapping
   - KT-SWAP refinement stage typically leads to significant quality improvements over KT-SPLIT alone. Can we establish stronger guarantees for KT-SWAP?
3. Weighted compression
   - For applications that support weights, can we establish stronger guarantees for optimally weighted kernel and Stein thinning coresets?
4. Other metrics
   - For which other metrics is (significantly) better-than-i.i.d. compression achievable?

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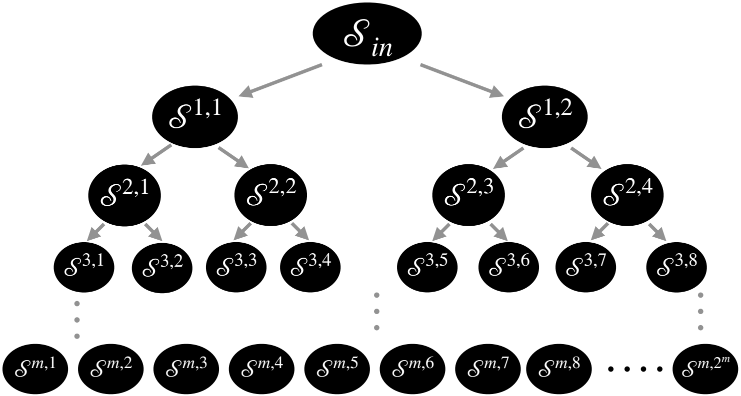
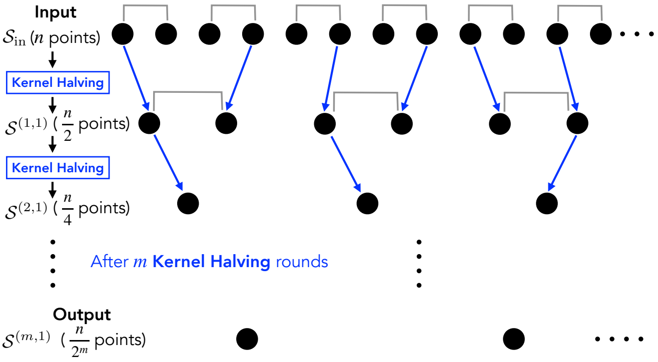
KT-SPLIT



KT-SPLIT partitions the input $\mathcal{S}_{\text{in}}$ recursively, first dividing the input sequence in half, then halving those halves into quarters, and so on

- Runs online: after i input points processed have output coresets of size $\frac{i}{2^m}$

KT-SPLIT



Each output coreset $\mathcal{S}^{(m,\ell)}$ is the result of repeated **kernel halving**

- On each halving round, remaining points are paired, and one point from each pair is selected using a new Hilbert space generalization of the self-balancing walk of Alweiss, Liu, and Sawhney [2020]
- Selection rule ensures that $\mathbb{P}_n\mathbf{k}_{\text{rt}} - \mathbb{Q}\mathbf{k}_{\text{rt}}$ remains small with high probability

Kernel Halving with a Self-Balancing Hilbert Walk

Algorithm: Self-balancing Hilbert Walk [Dwivedi and Mackey, 2021]

Input: sequence of functions $(f_i)_{i=1}^{n/2}$ in Hilbert space $\mathcal{H}$, threshold sequence $(\mathfrak{a}_i)_{i=1}^{n/2}$
$\psi_0 \leftarrow \mathbf{0} \in \mathcal{H}$
for $i = 1, 2, \ldots, n/2$ **do**
  $\alpha_i \leftarrow \langle \psi_{i-1}, f_i \rangle_{\mathcal{H}}$ // Compute Hilbert space inner product
  if $|\alpha_i| > \mathfrak{a}_i$:
    $\psi_i \leftarrow \psi_{i-1} - f_i \cdot \alpha_i / \mathfrak{a}_i$ // We choose $\mathfrak{a}_i$ to avoid this case with high probability
  else:
    $\eta_i \leftarrow 1$ with probability $\frac{1}{2}(1 - \alpha_i/\mathfrak{a}_i)$ and $\eta_i \leftarrow -1$ otherwise
    $\psi_i \leftarrow \psi_{i-1} + \eta_i f_i$
end
return $\psi_{n/2}$, sum of signed input functions // $\psi_{n/2} = \sum_{i=1}^{n/2} \eta_i f_i$ with high probability

1. **Kernel Halving:** If $f_i = \mathbf{k}_{\mathrm{rt}}(x_{2i-1}, \cdot) - \mathbf{k}_{\mathrm{rt}}(x_{2i}, \cdot)$, half of input points $\mathcal{S}_{\mathrm{out}}$ given sign 1
   $\Rightarrow \frac{1}{n}\psi_{n/2} = \mathbb{P}_n \mathbf{k}_{\mathrm{rt}} - \mathbb{Q}\mathbf{k}_{\mathrm{rt}}$ with $\mathbb{Q} = \frac{2}{n}\sum_{x \in \mathcal{S}_{\mathrm{out}}} \delta_x$
2. **Balance:** If $\mathcal{H} = \mathbf{k}_{\mathrm{rt}}$ RKHS, $\mathbb{P}_n \mathbf{k}_{\mathrm{rt}}(x) - \mathbb{Q}\mathbf{k}_{\mathrm{rt}}(x)$ is $\mathcal{O}(\sqrt{\log(n)}/n)$ sub-Gaussian, $\forall x$
   - In contrast, i.i.d. signs η_i give $\mathbb{P}_n \mathbf{k}_{\mathrm{rt}}(x) - \mathbb{Q}\mathbf{k}_{\mathrm{rt}}(x) = \Omega(1/\sqrt{n})$

Why the Square-root Kernel $\mathbf{k}_{\mathrm{rt}}$?

Theorem (L^∞ coresets for $(\mathbf{k}_{\mathrm{rt}}, \mathbb{P}_n)$ are MMD coresets for $(\mathbf{k}, \mathbb{P}_n)$ [Dwivedi and Mackey, 2021])

For any scalars $R, a, b \geq 0$ with $a + b = 1$, we have

$$\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n, \mathbb{Q}) \leq v_d R^{\frac{d}{2}} \cdot \|\mathbb{P}_n \mathbf{k}_{\mathrm{rt}} - \mathbb{Q}\mathbf{k}_{\mathrm{rt}}\|_\infty + 2\tau_{\mathbf{k}_{\mathrm{rt}}}(aR) + 2\|\mathbf{k}\|_\infty^{\frac{1}{2}} \cdot \max\{\tau_{\mathbb{P}_n}(bR), \tau_{\mathbb{Q}}(bR)\}$$

for $v_d \triangleq \pi^{d/4}/\Gamma(d/2+1)^{1/2}$.

- **L^∞ error:** $\|\mathbb{P}_n \mathbf{k}_{\mathrm{rt}} - \mathbb{Q}\mathbf{k}_{\mathrm{rt}}\|_\infty \triangleq \sup_{x\in\mathbb{R}^d} |\mathbb{P}_n \mathbf{k}_{\mathrm{rt}}(x) - \mathbb{Q}\mathbf{k}_{\mathrm{rt}}(x)|$
- **Tail decay of $(\mathbb{P}_n, \mathbb{Q}, \mathbf{k}_{\mathrm{rt}})$:** $\tau_{\mathbb{P}_n}(R) \triangleq \mathbb{P}_n(\|X\|_2 \geq R)$
- **Effective radius:** Want $\tau_{\mathbf{k}_{\mathrm{rt}}}(aR), \tau_{\mathbb{P}_n}(bR), \tau_{\mathbb{Q}}(bR) = \mathcal{O}(\frac{1}{\sqrt{n}})$
  - $R = \mathcal{O}(1)$ for compact support, $R = \mathcal{O}(\log(n))$ for sub-exponential decay
- When $(\mathbb{P}_n, \mathbb{Q}, \mathbf{k}_{\mathrm{rt}})$ are compactly supported, $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n, \mathbb{Q}) = \mathcal{O}(\|\mathbb{P}_n \mathbf{k}_{\mathrm{rt}} - \mathbb{Q}\mathbf{k}_{\mathrm{rt}}\|_\infty)$

L^∞ Coresets from Kernel Halving

Theorem (L^∞ guarantees for kernel halving [Dwivedi and Mackey, 2021])

With high probability,

1. **Kernel halving yields a 2-thinned L^∞ coreset $\mathbb{Q}_{\mathrm{KH}}^{(1)}$ satisying**
$$\|\mathbb{P}_n \mathbf{k}_{\mathrm{rt}} - \mathbb{Q}_{\mathrm{KH}}^{(1)} \mathbf{k}_{\mathrm{rt}}\|_\infty \leq \|\mathbf{k}_{\mathrm{rt}}\|_\infty \cdot \frac{2}{n} \mathfrak{M}_{\mathbf{k}_{\mathrm{rt}}}(\mathbb{P}_n)$$
2. **Repeated kernel halving yields a 2^m-thinned L^∞ coreset $\mathbb{Q}_{\mathrm{KH}}^{(m)}$ satisfying**
$$\|\mathbb{P}_n \mathbf{k}_{\mathrm{rt}} - \mathbb{Q}_{\mathrm{KH}}^{(m)} \mathbf{k}_{\mathrm{rt}}\|_\infty \leq \|\mathbf{k}_{\mathrm{rt}}\|_\infty \cdot \frac{2^m}{n} \mathfrak{M}_{\mathbf{k}_{\mathrm{rt}}}(\mathbb{P}_n)$$

- $\mathfrak{M}_{\mathbf{k}_{\mathrm{rt}}}(\mathbb{P}_n) = \mathcal{O}(\sqrt{\log n})$ for compactly supported $(\mathbb{P}, \mathbf{k}_{\mathrm{rt}})$ and $\mathcal{O}(\log n)$ in general
- With $m = \frac{1}{2}\log_2(n)$ rounds, yields $\sqrt{n}$ points with $\mathcal{O}(n^{-\frac{1}{2}} \log(n))$ L^∞ error
  - An equal-sized i.i.d. sample has $\Omega(n^{-\frac{1}{4}})$ L^∞ error
- **Near-optimal:** any procedure outputting $\sqrt{n}$ points must suffer $\Omega(n^{-\frac{1}{2}})$ L^∞ error for some $\mathbb{P}_n$ [Phillips and Tai, 2020, Thm. 3.1]

MMD Coresets from Kernel Thinning

Theorem (MMD guarantee for kernel thinning [Dwivedi and Mackey, 2021])

Kernel thinning returns a coreset $\mathbb{Q}_{KT}$ *with* $\sqrt{n}$ *points satisfying, with high probability,*

$$\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n,\mathbb{Q}_{KT}) = \begin{cases} \mathcal{O}\left(\sqrt{\frac{\log n}{n}}\right) & \text{for compact support } (\mathbb{P}, \mathbf{k}_{\mathrm{rt}}) \text{ (e.g., B-spline } \mathbf{k}) \\ \mathcal{O}\left(\frac{(\log n)^{\frac{d+2}{4}} \log\log n}{\sqrt{n}}\right) & \text{for sub-Gaussian } (\mathbb{P}, \mathbf{k}_{\mathrm{rt}}) \text{ (e.g., Gaussian } \mathbf{k}) \\ \mathcal{O}\left(\frac{(\log n)^{\frac{d+1}{2}} \log\log n}{\sqrt{n}}\right) & \text{for sub-exponential } (\mathbb{P}, \mathbf{k}_{\mathrm{rt}}) \text{ (e.g., Matérn } \mathbf{k}) \end{cases}$$

- An equal-sized i.i.d. sample has $\Omega(n^{-\frac{1}{4}})$ MMD
- Sub-exponential guarantees resemble the classical $\mathcal{O}(\frac{(\log n)^d}{\sqrt{n}})$ quasi-Monte Carlo error rates for uniform $\mathbb{P}$ on $[0,1]^d$ but apply to more general distributions on $\mathbb{R}^d$
- See the paper for non-asymptotic bounds with explicit constants and $\frac{n}{2^m}$ points

Related Work on L^∞ Coresets

L^∞ coresets for $\mathbb{P}_n$: $o(n^{-\frac{1}{4}})$ L^∞ error, $\sqrt{n}$ points

- Series of breakthroughs due to [Joshi, Kommaraji, Phillips, and Venkatasubramanian, 2011, Phillips, 2013, Phillips and Tai, 2018, 2020, Tai, 2020]

Best known L^∞ guarantees (for coreset of size $\sqrt{n}$)

- Phillips and Tai [2020]: $\mathcal{O}(\sqrt{d}n^{-\frac{1}{2}}\sqrt{\log n})$ error, $\Omega(n^4)$ time, $\Omega(n^2)$ space
- Tai [2020] (Gaussian $\mathbf{k}$): $\mathcal{O}(2^d n^{-\frac{1}{2}}\sqrt{\log(d \log n)})$ error, $\Omega(\max(d^{5d}, n^4))$ time
- Both are offline and require rebalancing after approximate halving steps
- This work: $\mathcal{O}(\sqrt{d}n^{-\frac{1}{2}}\log n)$ error, $\mathcal{O}(n^2)$ time, $\mathcal{O}(nd)$ space, online, exact halving
  - Sub-Gaussian $(\mathbf{k}_{\mathrm{rt}}, \mathbb{P})$: $\mathcal{O}(\sqrt{d}n^{-\frac{1}{2}}\sqrt{\log n \log\log n})$ error
  - Compact support $(\mathbf{k}_{\mathrm{rt}}, \mathbb{P})$: $\mathcal{O}(\sqrt{d}n^{-\frac{1}{2}}\sqrt{\log n})$ error