Advances in Distribution Compression

Lester Mackey

Microsoft Research New England

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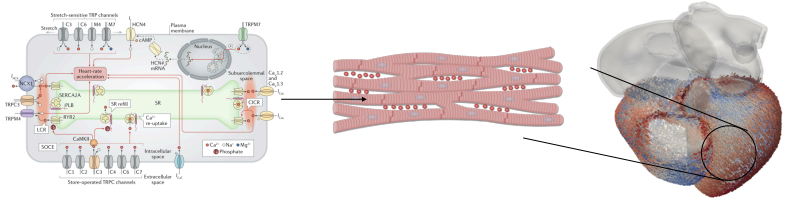
Joint work with Raaz Dwivedi, Marina Riabiz, Wilson Ye Chen, Jon Cockayne, Pawel Swietach, Steven A. Niederer, Chris J. Oates, Abhishek Shetty, and Carles Domingo-Enrich

Motivation: Computational Cardiology

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



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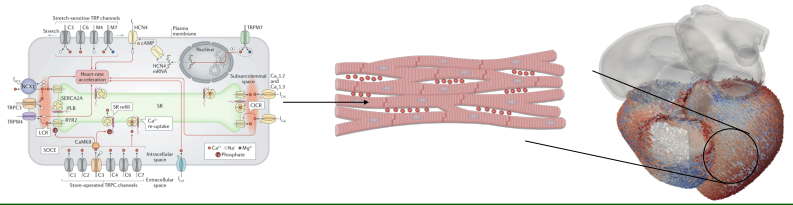

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Example (Heartbeats and arrhythmias)

- Whole-organ heartbeats are coordinated by calcium signaling in heart cells

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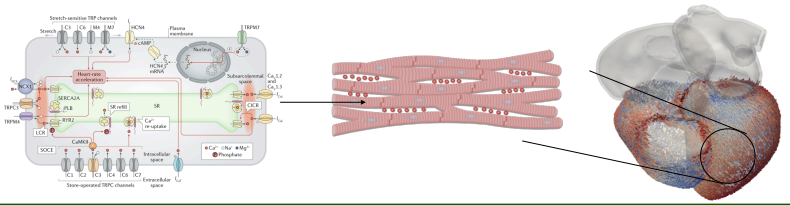

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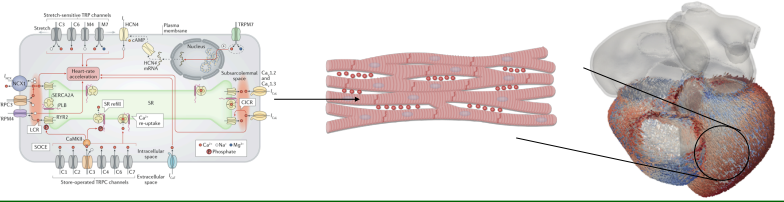

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Example (Heartbeats and arrhythmias)

- 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]

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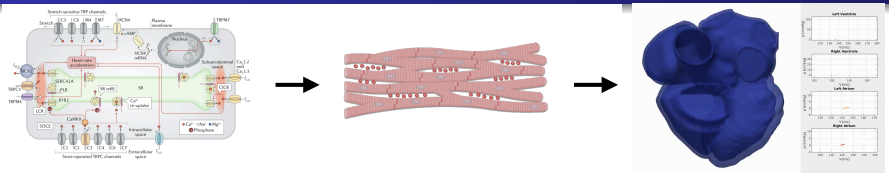

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Inferential Pipeline (Impact of calcium signaling dysregulation on heart function)

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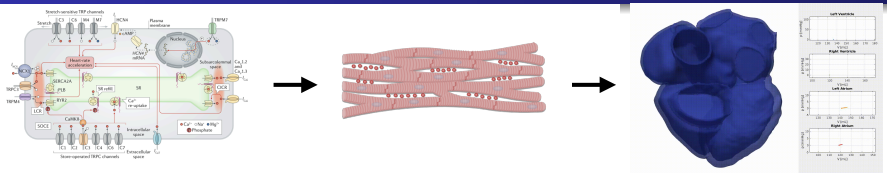

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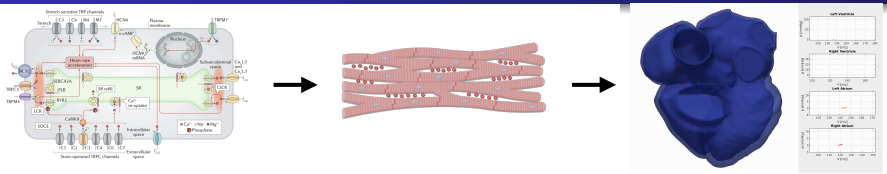

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2. Capture uncertainty by sampling many likely parameter configurations

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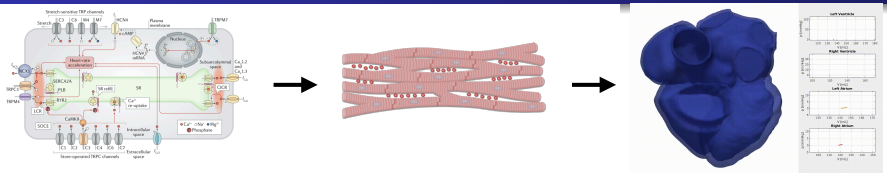

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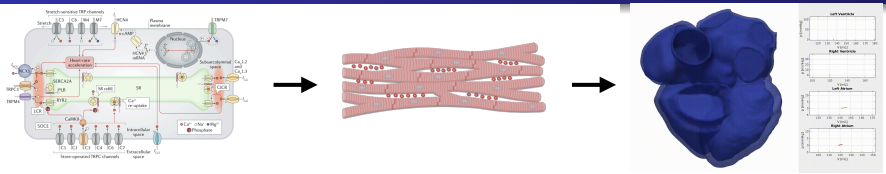

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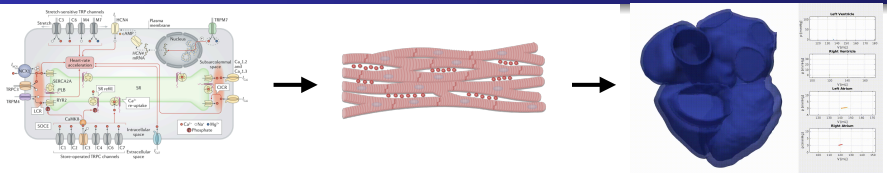

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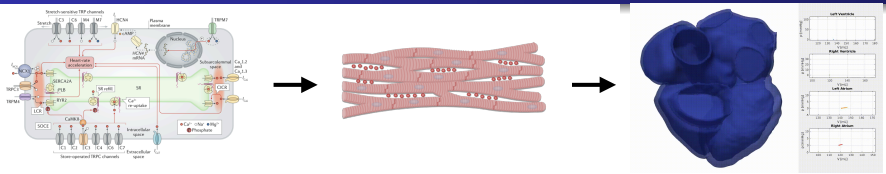

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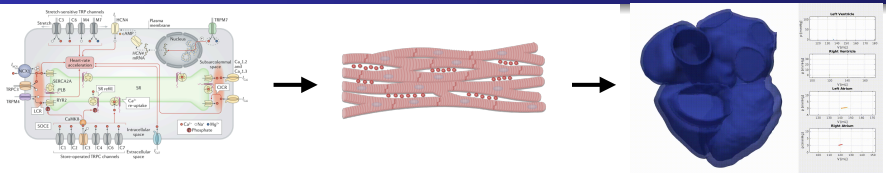

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Questions: Can we accurately summarize $\mathbb{P}$ using many fewer points? If so, how?

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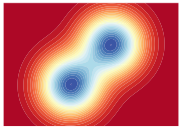

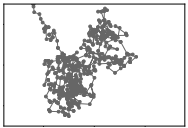

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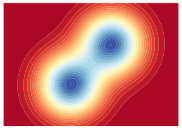

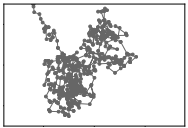

Benefits: **Readily available** and **eventually high-quality**

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

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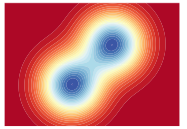

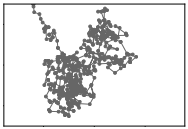

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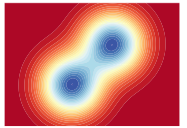

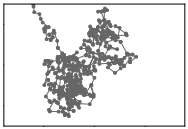

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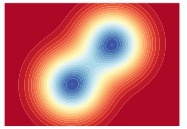

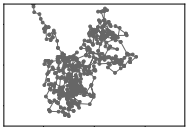

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Idea: Directly compress the high-quality sample approximations $\mathbb{P}_n$

- Reduces general problem to approximating empirical distributions

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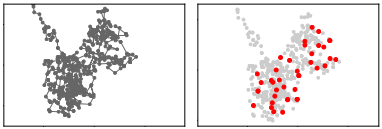

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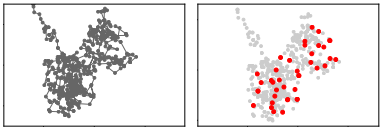

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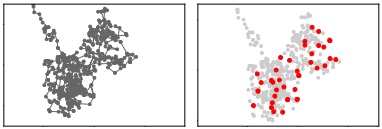

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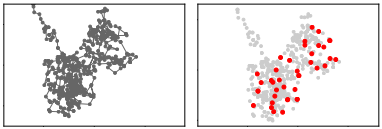

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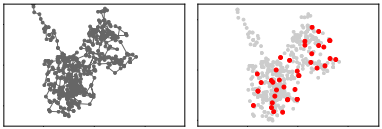

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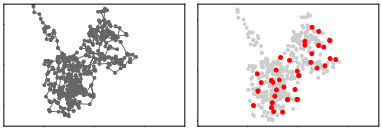

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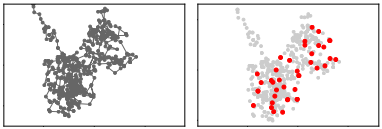

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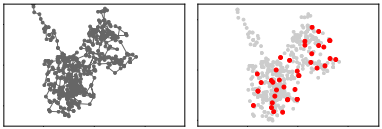

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This talk: Introduce a practical compression strategy – kernel thinning – that matches these lower bounds up to log factors, even for nonuniform and unbounded $\mathbb{P}$

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  - Pre-generated by any algorithm (i.i.d. sampling, MCMC, quadrature, kernel herding)

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

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

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- 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: $\mathbf{k}(x, y) = \frac{1}{(1+\|x-y\|_2^2)^{1/2}}$

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- 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)

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$\mathbf{k}(x, y) = \kappa(x-y)$	$\kappa(z)$	**Square-root** $\mathbf{k}_{\mathrm{rt}}$
Gaussian(σ)	$\exp\left(-\frac{\|z\|_2^2}{2\sigma^2}\right)$	**Gaussian**$\left(\frac{\sigma}{\sqrt{2}}\right)$
Matérn(ν, γ)	$(\gamma\|z\|_2)^{\nu-\frac{d}{2}} K_{\nu-\frac{d}{2}}(\gamma\|z\|_2)$	**Matérn**$(\frac{\nu}{2}, \gamma)$
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Theorem (L^∞ coresets for $\mathbf{k}_{\mathrm{rt}}$ are MMD coresets for $\mathbf{k}$ [Dwivedi and Mackey, 2024])

$$\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n, \mathbb{Q}) = \begin{cases} \mathcal{O}(\|\mathbb{P}_n\mathbf{k}_{\mathrm{rt}} - \mathbb{Q}\mathbf{k}_{\mathrm{rt}}\|_\infty) & \text{Compact support } \mathbf{k}_{\mathrm{rt}}, \mathbb{P}_n \\ \mathcal{O}(\|\mathbb{P}_n\mathbf{k}_{\mathrm{rt}} - \mathbb{Q}\mathbf{k}_{\mathrm{rt}}\|_\infty \log(\frac{1}{\|\mathbb{P}_n\mathbf{k}_{\mathrm{rt}} - \mathbb{Q}\mathbf{k}_{\mathrm{rt}}\|_\infty})^{\frac{d+1}{2}}) & \text{Subexponential } \mathbf{k}_{\mathrm{rt}}, \mathbb{P}_n \end{cases}$$

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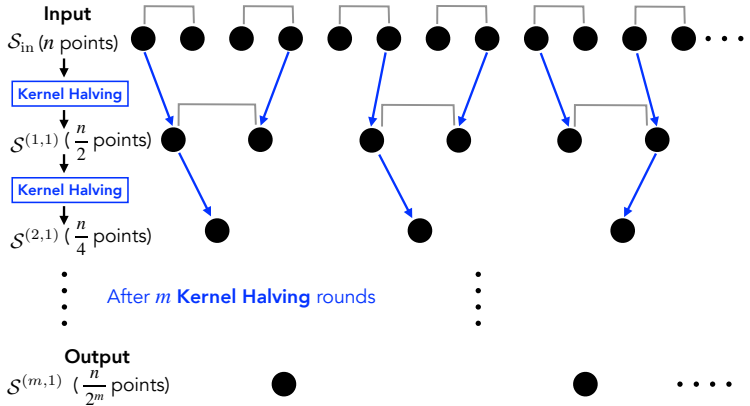

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- **Theorem:** $\|\mathbb{P}_n\mathbf{k}_{\text{rt}} - \mathbb{Q}\mathbf{k}_{\text{rt}}\|_\infty = \mathcal{O}(\frac{\sqrt{d}\log(n)}{n})$ with high probability [Dwivedi and Mackey, 2024]

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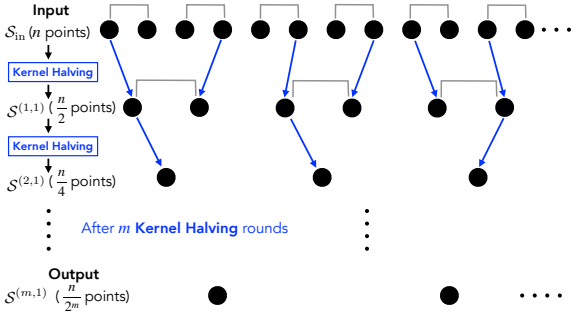

   - Non-uniform randomness ensures $\|\mathbb{P}_n \mathbf{k}_{\text{rt}} - \mathbb{Q}\mathbf{k}_{\text{rt}}\|_\infty$ small after each halving round

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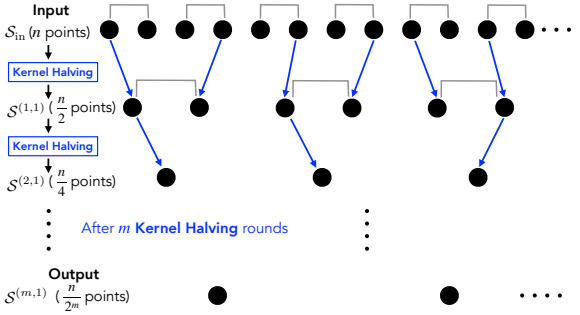

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     when $s = \sqrt{n}$ vs. $\Omega(n^{-\frac{1}{4}})$ for i.i.d. coreset [Dwivedi and Mackey, 2024]

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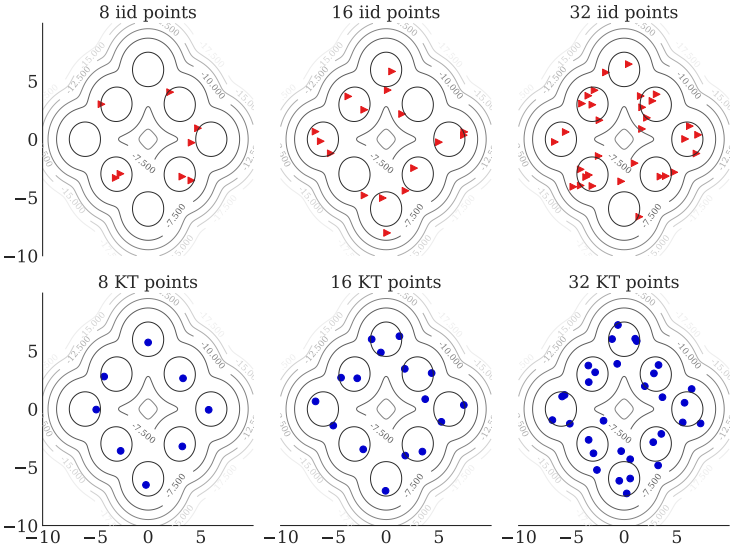
Complexity

- 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++

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

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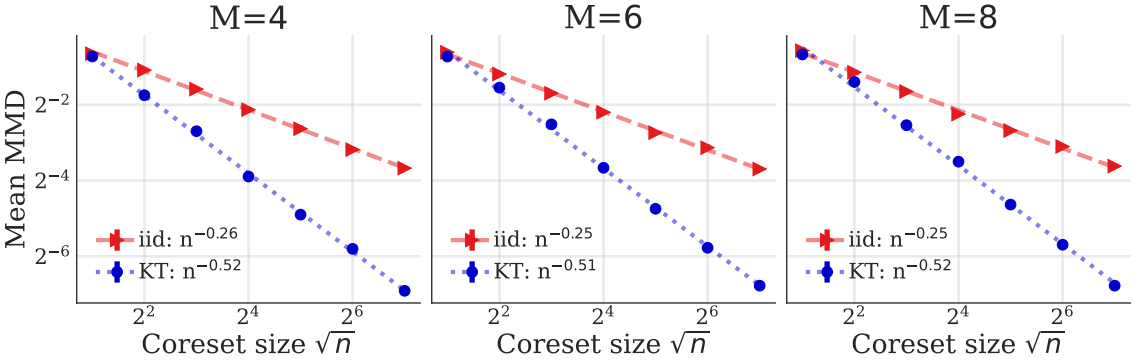

Kernel thinning (KT) improves both rate of decay and order of magnitude of $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}, \mathbb{Q}_{KT})$

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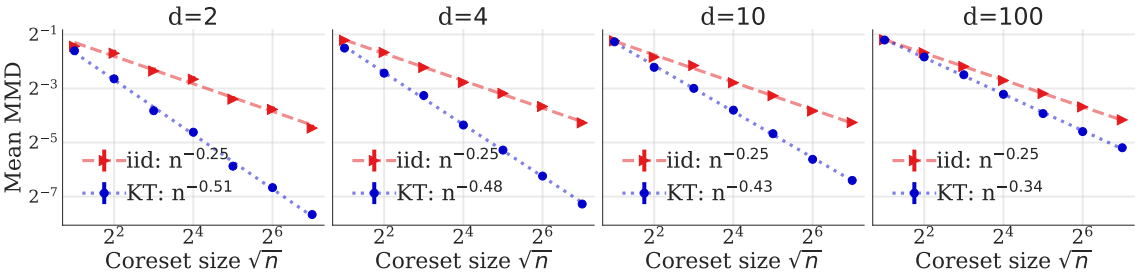
Kernel Thinning vs. i.i.d. Sampling: Higher Dimensions



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

- $\mathbb{P} = \mathcal{N}(0, \mathbf{I}_d)$
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Kernel Thinning vs. Standard MCMC Thinning

Posterior inference for systems of ordinary differential equations (ODEs)

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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
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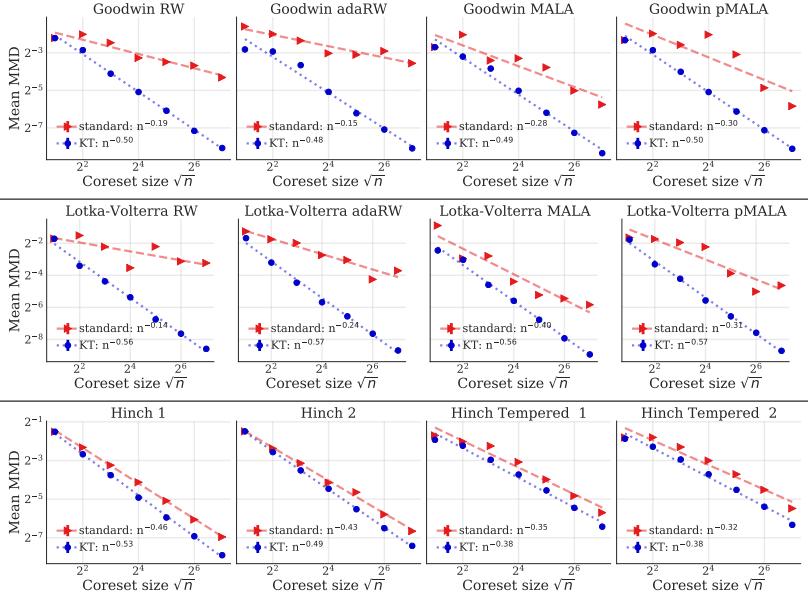
- Discarded burn-in and standard thinned to form $\mathbb{P}_n$
- $\mathbf{k}(x, y) = \exp(-\frac{1}{2\sigma^2}\|x - y\|_2^2)$ with median heuristic σ^2 [Garreau, Jitkrittum, and Kanagawa, 2017]



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

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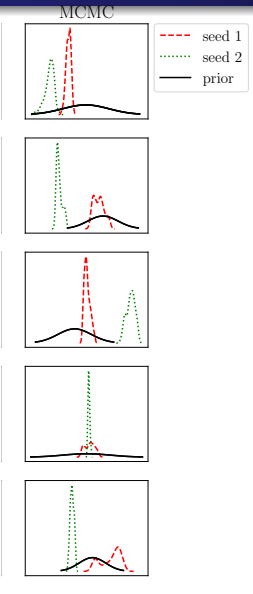
Problem: The Hinch Markov chains haven't mixed!



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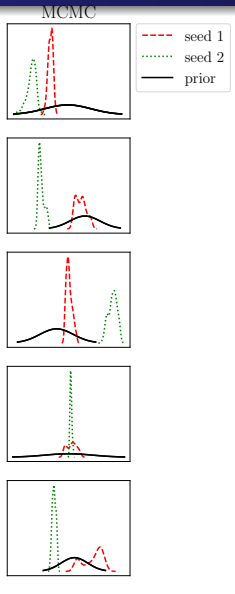

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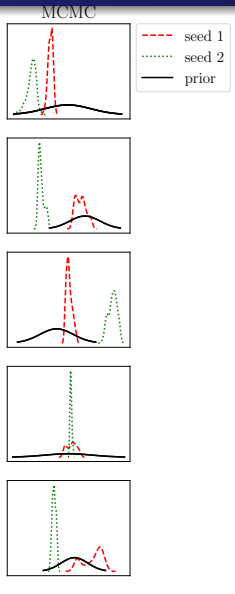

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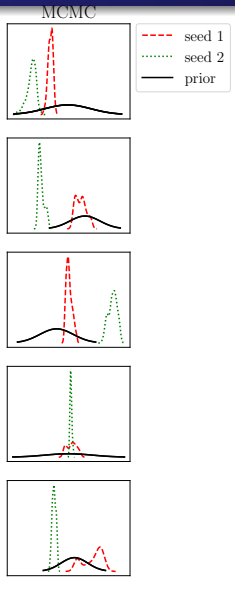
Question: Can we correct for such biases during compression?



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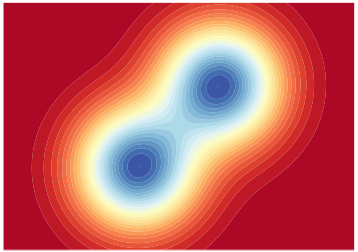

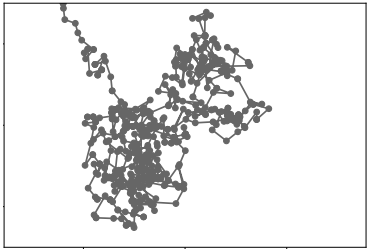

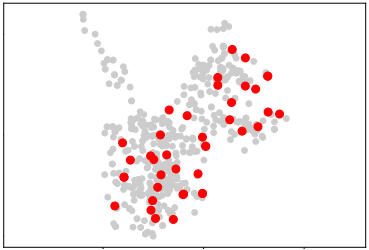

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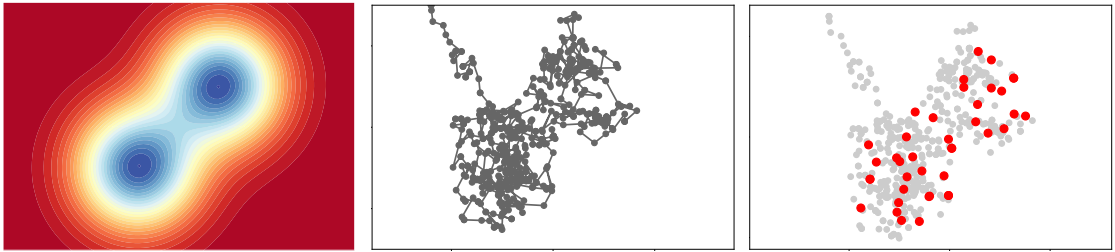

Difficulty: $\mathbb{P}_n$ alone is insufficient; need to measure distance to the true target $\mathbb{P}$

Measuring Distance to $\mathbb{P}$

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

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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 $\mathbb{Q}$!

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Kernel Stein discrepancy (KSD)

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- $\mathbf{k}_{\mathbb{P}}(x, y) = \sum_{j=1}^{d} \frac{1}{p(x)p(y)} \nabla_{x_j} \nabla_{y_j} (p(x)\mathbf{k}(x, y)p(y))$ [Oates, Girolami, and Chopin, 2017]
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Idea: Greedily minimize KSD using points from $\mathcal{S}_{\text{in}} = \{x_1, \ldots, x_n\}$

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- 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 $= \mathcal{O}(ns^2)$)

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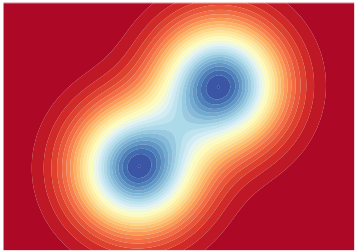

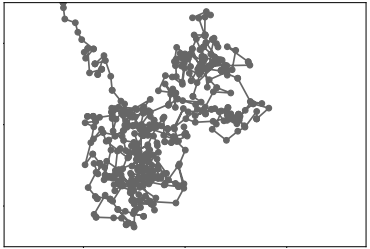

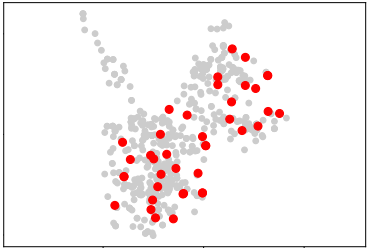

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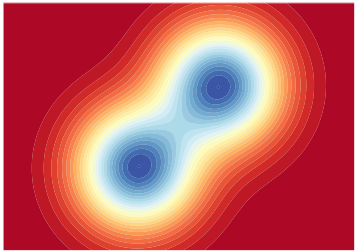
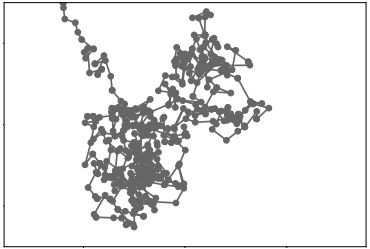
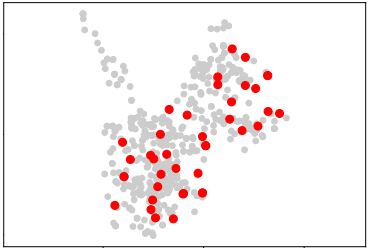
$\Rightarrow$ Nearly as well as off-target sample after optimal importance sampling reweighting!







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!

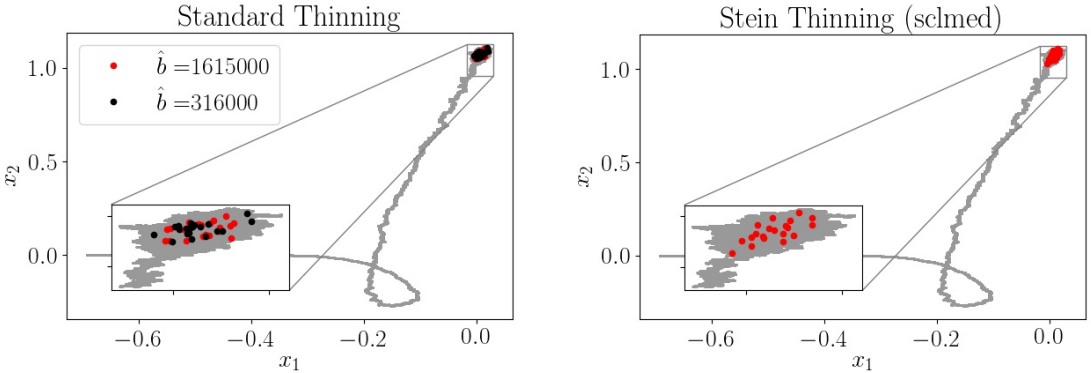
Theorem (Stein thinning corrects off-target sampling [Riabiz, Chen, Cockayne, Swietach, Niederer, Mackey, and Oates, 2021])

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 $\tilde{\mathbb{P}}$

Stein Thinning in Action: Correcting for Burn-in

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

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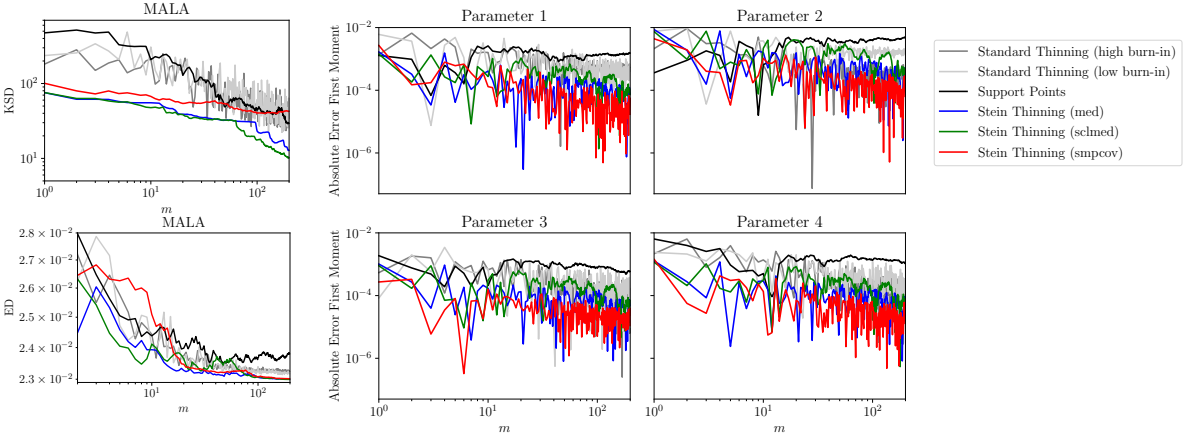
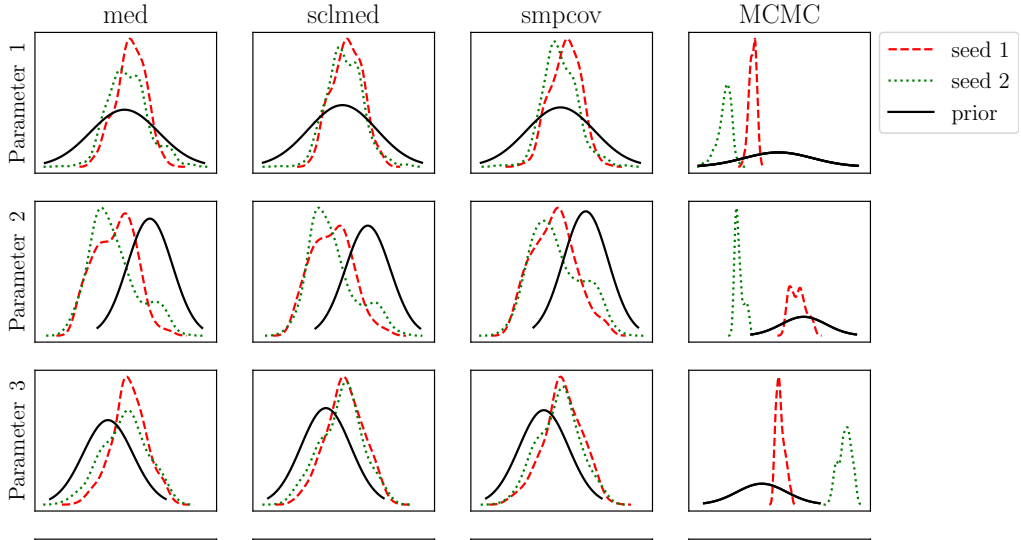


Stein thinning outperforms standard thinning with high and low levels of burn-in removal in terms of KSD, energy distance (ED), and first moment estimation

Stein Thinning in Action: Correcting for Tempering

Hinch model of cardiac calcium signalling: Tempering improves mixing



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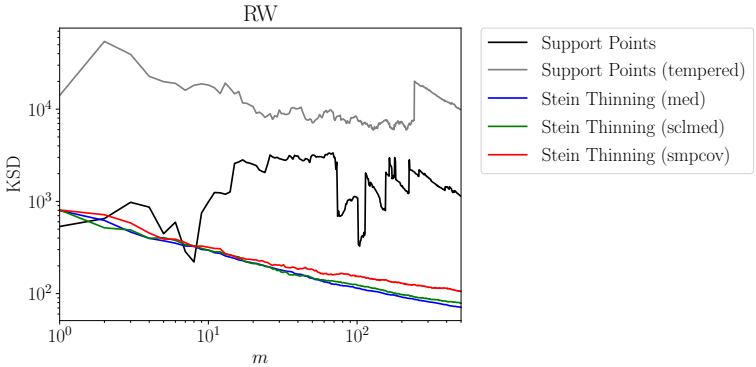

- Untempered support points compression yields poor summary due to poor mixing
- Tempered SP without bias correction is even worse (due to tempering bias)
- Tempering + Stein thinning bias correction improves approximation to $\mathbb{P}$

Conclusions

Summary

- New tools for summarizing a probability distribution more effectively than $\mathrm{i.i.d.}$ sampling or standard MCMC thinning
- Kernel thinning compresses an n point summary into a $\sqrt{n}$ point summary with better-than-$\mathrm{i.i.d.}$ 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

Package: github.com/microsoft/goodpoints

Stein Thinning

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   - 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+)**

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

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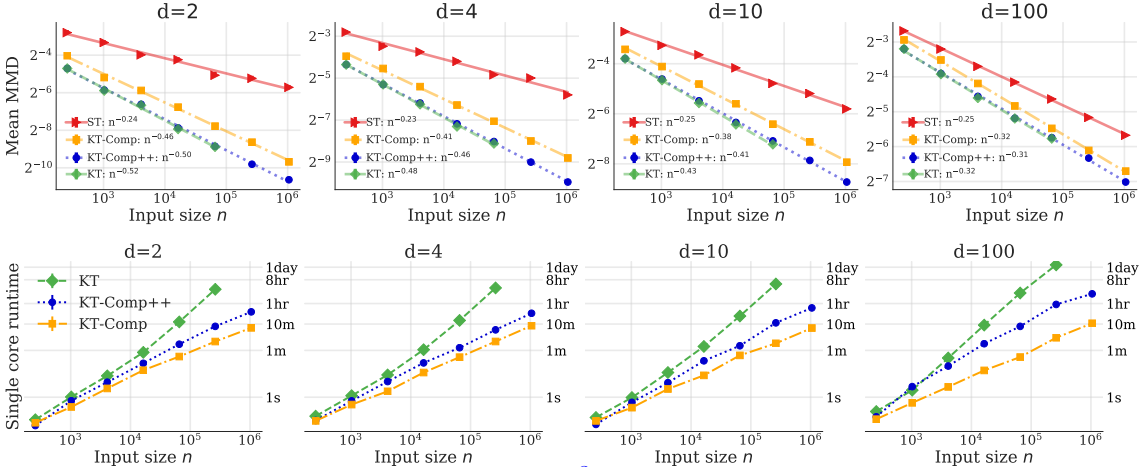

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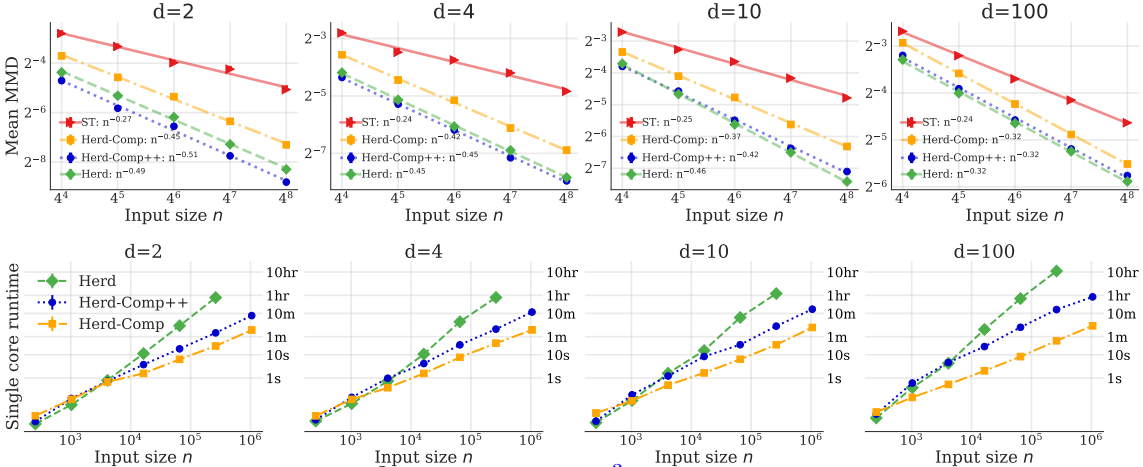

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Distribution Compression in Near-linear Time [Shetty, Dwivedi, and Mackey, 2022]

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

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

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

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

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

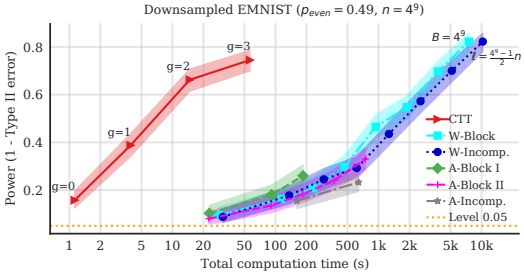
  $\widetilde{\mathcal{S}}_i \leftarrow \text{COMPRESS}(\mathcal{S}_i, \text{HALVE})$ // return coresets of size $\sqrt{\frac{n}{4}}$

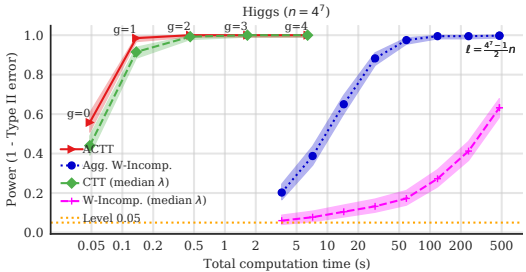
end

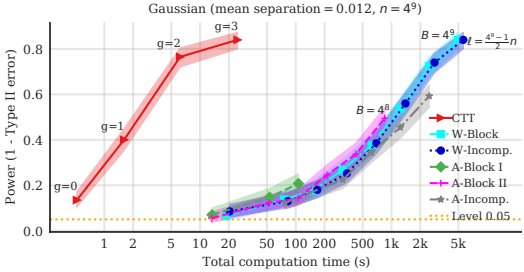
$\widetilde{\mathcal{S}} \leftarrow \text{CONCATENATE}(\widetilde{\mathcal{S}}_1, \widetilde{\mathcal{S}}_2, \widetilde{\mathcal{S}}_3, \widetilde{\mathcal{S}}_4)$ // coreset of size $2\sqrt{n}$

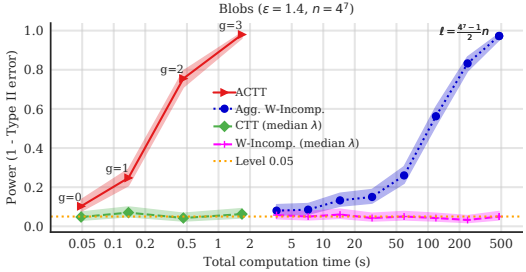
return $\text{HALVE}(\widetilde{\mathcal{S}})$ // coreset of size $\sqrt{n}$

Powerful Kernel Testing in Near-linear Time [Domingo-Enrich, Dwivedi, and Mackey, 2023]









Compress Then Test (▶ above) accelerates kernel two-sample testing with compression

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- Compress Then Test (CTT) accelerates kernel testing with compression

Kernel Thinning, **Compress++**, and **CTT**

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Future Directions

Many opportunities for future development

1. Unifying kernel thinning and Stein thinning
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4. Other metrics
   - For which other metrics is (significantly) better-than-i.i.d. compression achievable?

Related Work on MMD Coresets

Uniform distribution $\mathbb{P}$ on $[0,1]^d$: L^2 discrepancy MMD, s points

- Quasi-Monte Carlo [Chen, Skriganov, et al., 2002]: $\mathcal{O}(s^{-1}\log^{\frac{d-1}{2}} s)$
- Online Haar strategy [Dwivedi, Feldheim, Gurel-Gurevich, and Ramdas, 2019]: $\mathcal{O}(s^{-1}\log^{2d} s)$

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, 2024]
- 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

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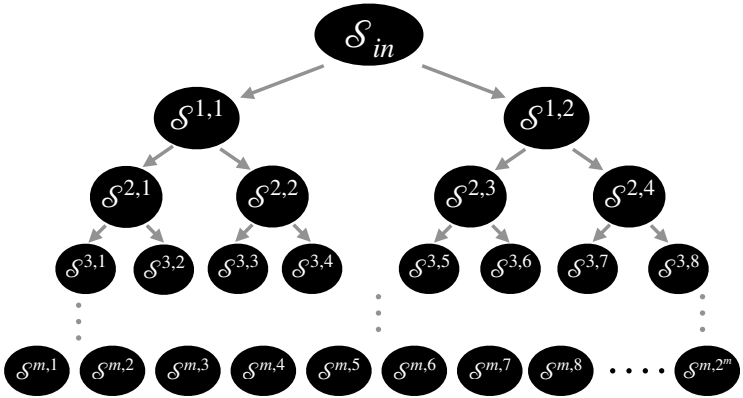
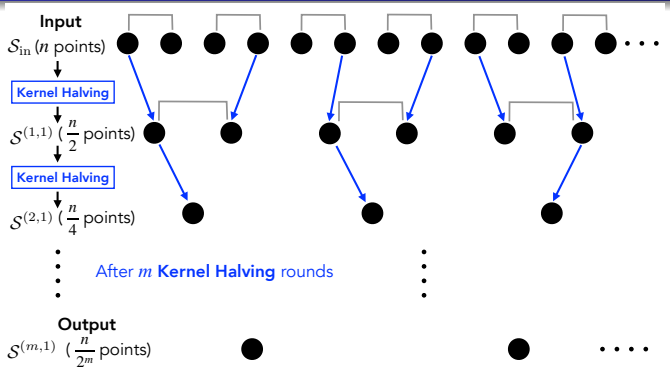
KT-SPLIT



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, 2024]

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, 2024])

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, 2024])

With high probability,

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

- $\mathfrak{M}_{\mathbf{k}_{\mathrm{rt}}}(\mathbb{P}_n) = \mathcal{O}(\sqrt{\log n})$ 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, 2024])

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

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

- An equal-sized i.i.d. sample has $\Omega(n^{-\frac{1}{4}})$ MMD
- Sub-exponential guarantees resemble the classical $\mathcal{O}\left(\frac{(\log n)^{\frac{d-1}{2}}}{\sqrt{n}}\right)$ 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

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

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