Near-Optimal Compression In Near-Linear Time

Raaz Dwivedi, Lester Mackey, Abhishek Shetty

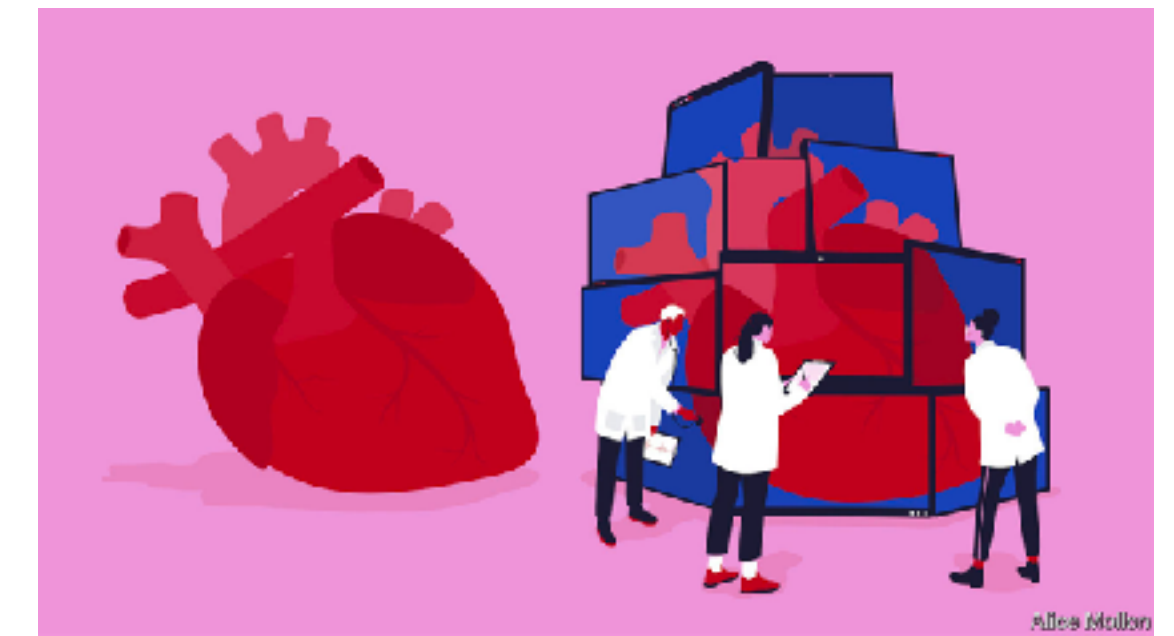raaz@mit.edu

Kernel Methods for Numerical Integration,
SIAM Conference on Uncertainty Quantification
Apr 13, 2022

Computational cardiology

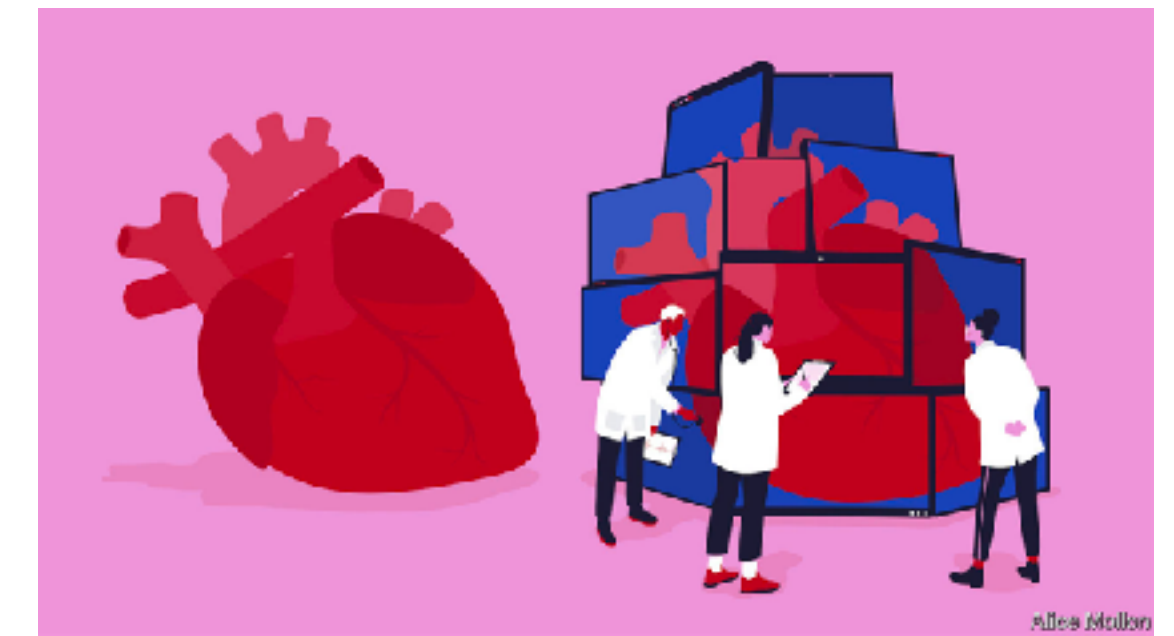Modeling **digital twin heart** to predict therapy response in a *non-invasive way* requires single-cell modeling.
A common methodology:

- Estimate single cell model using Bayesian set-up: Use millions of Markov chain Monte Carlo (MCMC) points to approximate posterior $\mathbb{P}^\star$

- Propagate uncertainty at heart-level by passing these points to the whole-heart simulator

$$\mathbb{P}^\star f \triangleq \int f(x) d\mathbb{P}^\star(x) \approx \frac{1}{n} \sum_{i=1}^{n} f(x_i) \triangleq \mathbb{P}_n f$$

$x_i =$ MCMC sample for single cell model parameters
$f =$ heart simulator

Niederer et al., 2011; Augustin et al., 2016; Strocchi et al., 2020

Computational cardiology

Modeling **digital twin heart** to predict therapy response in a *non-invasive way* requires single-cell modeling.
A common methodology:

- Estimate single cell model using Bayesian set-up: Use millions of Markov chain Monte Carlo (MCMC) points to approximate posterior $\mathbb{P}^\star$

- Propagate uncertainty at heart-level by passing these points to the whole-heart simulator

Niederer et al., 2011; Augustin et al., 2016; Strocchi et al., 2020

$$\mathbb{P}^\star f \triangleq \int f(x) d\mathbb{P}^\star(x) \approx \frac{1}{n} \sum_{i=1}^{n} f(x_i) \triangleq \mathbb{P}_n f$$

x_i = MCMC sample for single cell model parameters
f = heart simulator

1 Million MCMC samples ~ 2 weeks
Single evaluation of f ~ 5 weeks

Can <u>NOT</u> use all million samples….!

Goal: Represent $\mathbb{P}^\star$ using a <u>few</u> high quality points $(x_i)_{i=1}^n$

Common solutions: I.I.D. sampling, and MCMC sampling exhibit a <u>slow root-n</u> Monte Carlo rate $\left| \mathbb{P}^\star f - \mathbb{P}_n f \right| = \Theta(n^{-1/2})$, e.g., ~$10^6$ points for 0.1% error

- Prohibitive for computationally expensive f

Goal: Represent $\mathbb{P}^\star$ using a few high quality points $(x_i)_{i=1}^n$

Common solutions: I.I.D. sampling, and MCMC sampling exhibit a <u>slow root-n</u> Monte Carlo rate $\left| \mathbb{P}^\star f - \mathbb{P}_n f \right| = \Theta(n^{-1/2})$, e.g., ~$10^6$ points for 0.1% error

- Prohibitive for computationally expensive f

Data compression: Approximate $\mathbb{P}^\star$ by compressing given n points

- Uniform thinning, or standard thinning—-choose every t−th point

Goal: Represent $\mathbb{P}^\star$ using a few high quality points $(x_i)_{i=1}^n$

Common solutions: I.I.D. sampling, and MCMC sampling exhibit a slow root-n Monte Carlo rate $\left|\mathbb{P}^\star f - \mathbb{P}_n f\right| = \Theta(n^{-1/2})$, e.g., ~$10^6$ points for 0.1% error

- Prohibitive for computationally expensive f

Data compression: Approximate $\mathbb{P}^\star$ by compressing given n points

- Uniform thinning, or standard thinning—-choose every t—th point

- Accuracy degrades with such thinning—$\Theta(\sqrt{t/n})$ worst-case error—same as the Monte Carlo rate with n/t points; e.g., $n^{-1/4}$ rate with $\sqrt{n}$ points

Goal: Represent $\mathbb{P}^\star$ using a <u>few</u> high quality points $(x_i)_{i=1}^n$

Common solutions: I.I.D. sampling, and MCMC sampling exhibit a <u>slow root-n</u> Monte Carlo rate $\left| \mathbb{P}^\star f - \mathbb{P}_n f \right| = \Theta(n^{-1/2})$, e.g., ~$10^6$ points for 0.1% error

- Prohibitive for computationally expensive f

Data compression: Approximate $\mathbb{P}^\star$ by compressing given n points

- Uniform thinning, or standard thinning–-choose every $t-$th point

- Accuracy degrades with such thinning–$\Theta(\sqrt{t/n})$ worst-case error–same as the Monte Carlo rate with n/t points; e.g., $n^{-1/4}$ rate with $\sqrt{n}$ points

Can we do better?

Minimax lower bounds

There exists some $\mathbb{P}^{\star}$ such that the worst-case integration error

- Is $\Omega(n^{-1/2})$ for **any compression scheme** returning $\sqrt{n}$ points
  [Philips and Tai, 2020]

Minimax lower bounds

There exists some $\mathbb{P}^\star$ such that the worst-case integration error

- Is $\Omega(n^{-1/2})$ for **any compression scheme** returning $\sqrt{n}$ points
  [Philips and Tai, 2020]

- Is $\Omega(n^{-1/2})$ for **any approximation** based on n i.i.d. points
  [Tolstikhin, Sriperumbudur, and Muandet, 2017]

This talk: Kernel thinning-Compress++

- **KT-Compress++**: A practical strategy based on two new algorithms to provide near-optimal compression in near-linear time

    - **Kernel thinning (KT)**: Provides near-optimal compression

    - **Compress++**: Provides significantly reduced runtime for generic thinning algorithms with minimal worsening of error

This talk: Kernel thinning-Compress++

- **KT-Compress++**: A practical strategy based on two new algorithms to provide near-optimal compression in near-linear time

  - **Kernel thinning (KT)**: Provides near-optimal compression

  - **Compress++**: Provides significantly reduced runtime for generic thinning algorithms with minimal worsening of error

- Overall, KT-Compress++ a solution for finding
  - better than Monte Carlo points
  - high quality coresets
  - good prototypes

Problem set-up

- **Input**:

  Points $(x_i)_{i=1}^n$ with empirical distribution $\mathbb{P}_{in} \triangleq \dfrac{1}{n} \sum\limits_{i=1}^{n} \delta_{x_i}$

  Target output size s ($s = \sqrt{n}$ for heavy compression)

- **Goal:**

  Return a subset of input points with size s, empirical distribution $\mathbb{P}_{out}$
  with error rate $o(s^{-1/2})$, i.e., better than Monte Carlo rate

Reproducing kernel Hilbert space (RKHS)

- RKHS of $\mathbf{k}$ is given by $\mathbb{H}_{\mathbf{k}} \triangleq \overline{\mathrm{span}}\{\mathbf{k}(x, \cdot), x \in \mathcal{X}\}$

- $\mathbb{H}_{\mathbf{k}}$ is dense in the space of continuous functions for universal $\mathbf{k}$ like

$$\text{Gaussian } \mathbf{k}(x, y) = \exp\left(-\frac{1}{2}\|x - y\|^2\right); \text{IMQ } \mathbf{k}(x, y) = \frac{1}{(1 + \|x - y\|^2)^{1/2}}$$
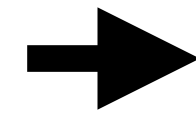
$\mathbf{k} : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ is a reproducing kernel if the matrix $\mathbf{K} = (\mathbf{k}(x_i, x_j))_{i,j=1}^n$
is a symmetric positive definite matrix for any n and any $(x_1, \ldots, x_n)$
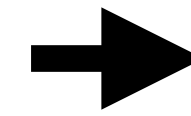
Kernel Thinning

$$x_1, x_2, \ldots, x_n$$

kernel $\mathbf{k}$

$$\mathbb{P}_{in} \triangleq \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$$

➡️

Kernel Thinning (KT)
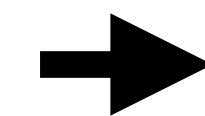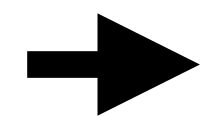
➡️

Non-uniform sub-sample of size s

$$y_1, \ldots, y_s$$

$$\mathbb{P}_{KT} \triangleq \frac{1}{s} \sum_{i=1}^{s} \delta_{y_i}$$

Kernel Thinning: A two-staged procedure

$$x_1, x_2, \ldots, x_n$$

kernel $\mathbf{k}$

$$\mathbb{P}_{in} \triangleq \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$$

➡️

Kernel Thinning (KT)

➡️

Non-uniform sub-sample of size s

$$y_1, \ldots, y_s$$

$$\mathbb{P}_{KT} \triangleq \frac{1}{s} \sum_{i=1}^{s} \delta_{y_i}$$

- **Stage 1:** $m = \dfrac{1}{2} \log_2(n/s)$ recursive rounds of **non-uniform splitting** the parent coreset in two equal-sized children coresets

$\mathcal{S}_{in}$

$\mathcal{S}^{1,1}$ $\mathcal{S}^{1,2}$

$\mathcal{S}^{2,1}$ $\mathcal{S}^{2,2}$ $\mathcal{S}^{2,3}$ $\mathcal{S}^{2,4}$

$\mathcal{S}^{3,1}$ $\mathcal{S}^{3,2}$ $\mathcal{S}^{3,3}$ $\mathcal{S}^{3,4}$ $\mathcal{S}^{3,5}$ $\mathcal{S}^{3,6}$ $\mathcal{S}^{3,7}$ $\mathcal{S}^{3,8}$

$\mathcal{S}^{m,1}$ $\mathcal{S}^{m,2}$ $\mathcal{S}^{m,3}$ $\mathcal{S}^{m,4}$ $\mathcal{S}^{m,5}$ $\mathcal{S}^{m,6}$ $\mathcal{S}^{m,7}$ $\mathcal{S}^{m,8}$ $\ldots$ $\mathcal{S}^{m,2^m}$

15

Kernel Thinning: A two-staged procedure

$$x_1, x_2, \ldots, x_n$$

kernel $\mathbf{k}$

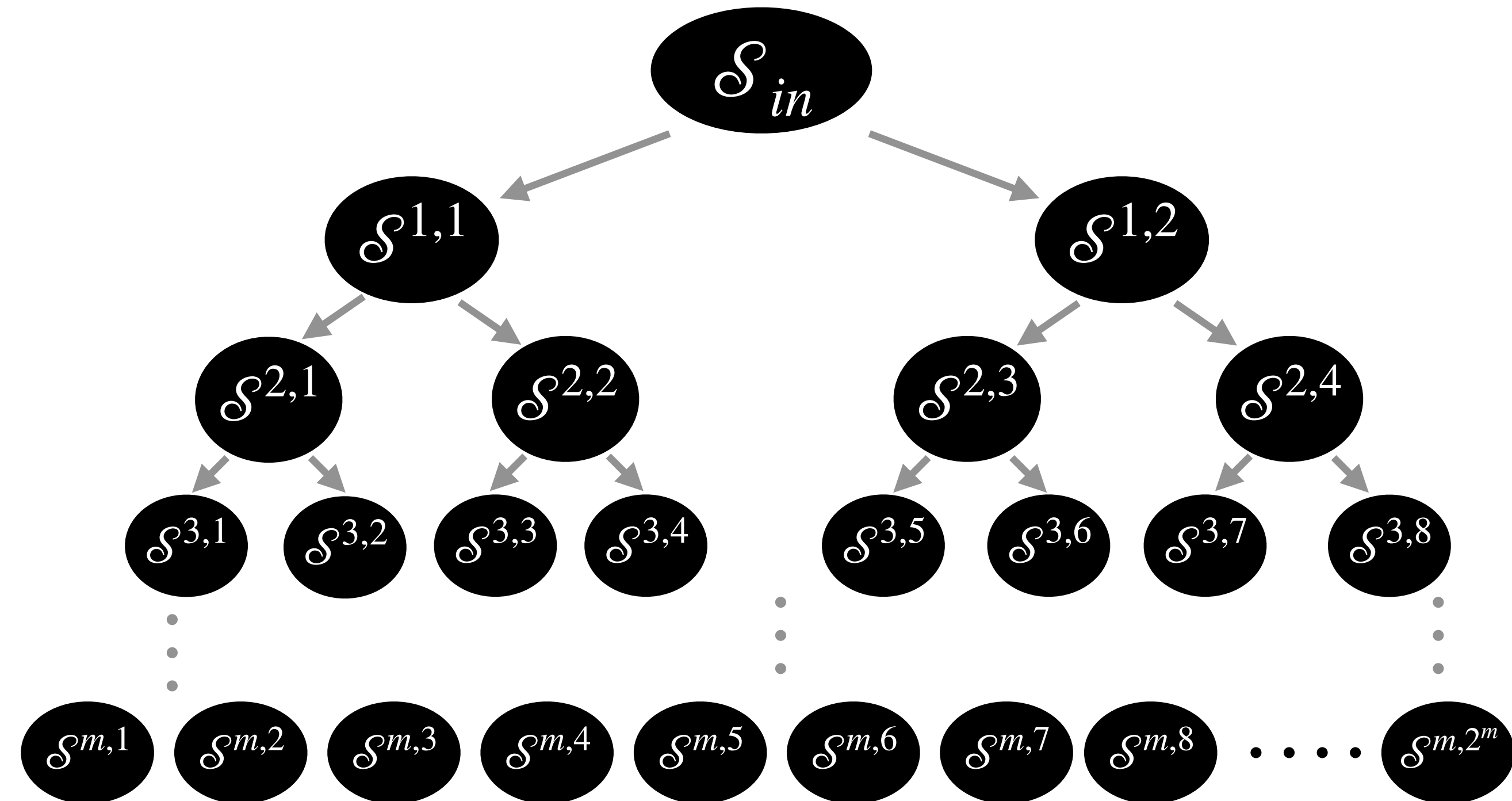$$\mathbb{P}_{in} \triangleq \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$$

$\rightarrow$

Kernel Thinning (KT)

$\rightarrow$
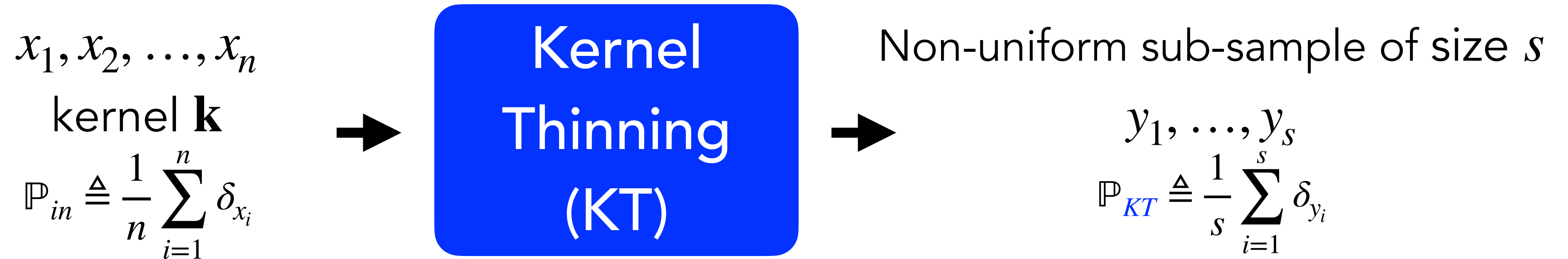
Non-uniform sub-sample of size s

$$y_1, \ldots, y_s$$

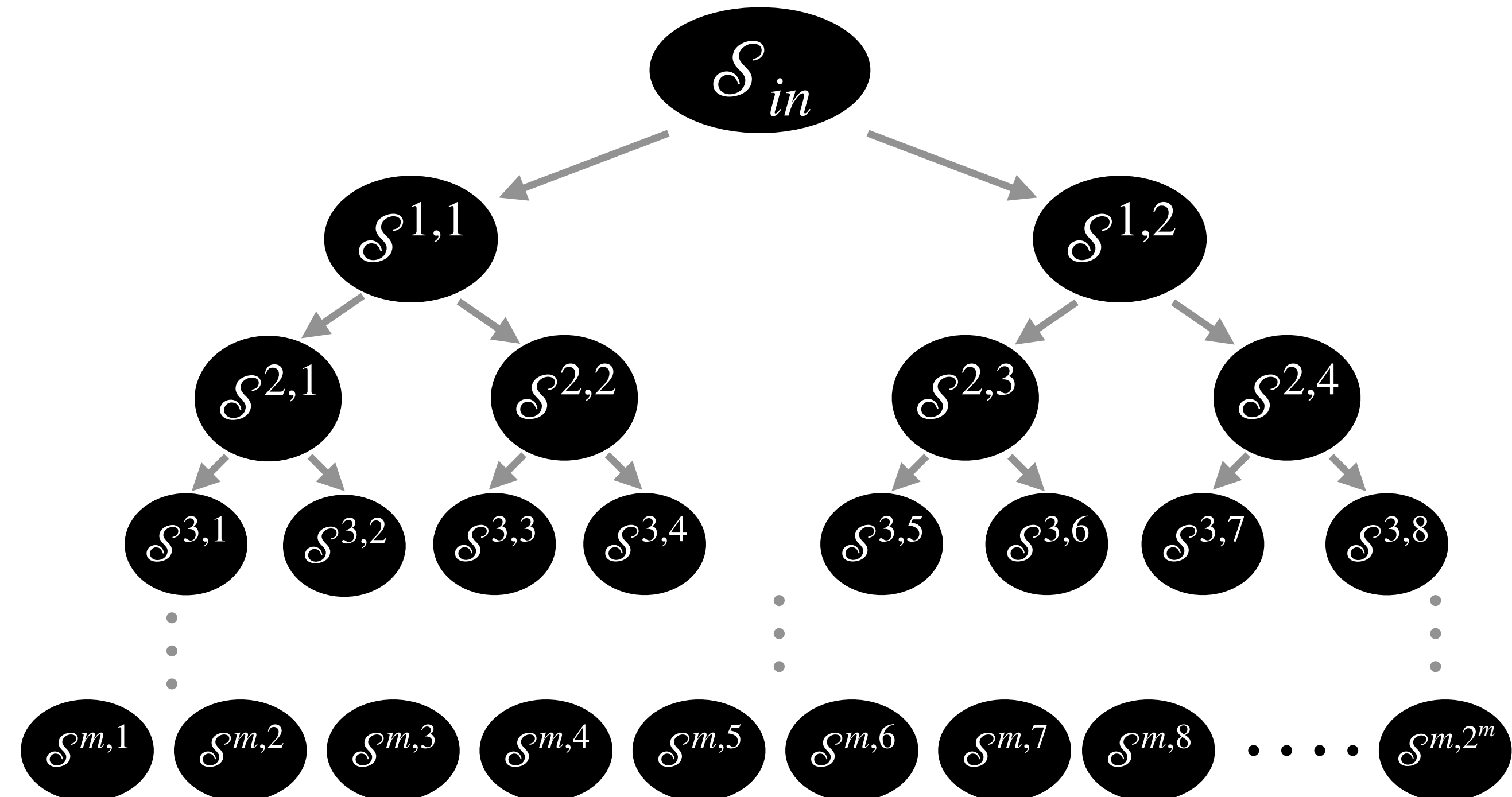$$\mathbb{P}_{KT} \triangleq \frac{1}{s} \sum_{i=1}^{s} \delta_{y_i}$$

- **Stage 1:** $m = \dfrac{1}{2} \log_2(n/s)$ recursive rounds of **non-uniform splitting** the parent coreset in two equal-sized children coresets

- **Stage 2:** Point-by-point **refinement** of the best child coreset

Kernel Thinning: Better than Monte Carlo rate for $\mathbb{P}_{in}$

With n input points, s output points, with high probability over the randomness in KT, **for any fixed** $g \in \mathbb{H}_{\mathbf{k}}$ we have

$$|\mathbb{P}_{in}g - \mathbb{P}_{KT}g| \lesssim \frac{1}{s} \cdot \|g\|_{\mathbf{k}}\sqrt{\|\mathbf{k}\|_\infty \left(\log s + \log\log(n/s)\right)} \ll \mathcal{O}\left(\frac{1}{\sqrt{s}}\right)$$

Monte Carlo rate
(standard thinning rate)

for any kernel on any space!

Kernel Thinning: Better than Monte Carlo rate for $\mathbb{P}_{in}$

With n input points, $\sqrt{n}$ output points, with high probability over the randomness in KT, **for any fixed** $g \in \mathbb{H}_{\mathbf{k}}$ we have

$$|\mathbb{P}_{in}g - \mathbb{P}_{KT}g| \lesssim \frac{1}{\sqrt{n}} \cdot \|g\|_{\mathbf{k}}\sqrt{\|\mathbf{k}\|_{\infty}\log n} \ll \mathcal{O}\left(\frac{1}{n^{1/4}}\right)$$

Monte Carlo rate
(standard thinning rate)

for any kernel on any space!

18

Kernel Thinning: Better than Monte Carlo rate for $\mathbb{P}_{in}$

With n input points, $\sqrt{n}$ output points, with high probability over the randomness in KT, **for any fixed** $g \in \mathbb{H}_{\mathbf{k}}$ we have

$$|\mathbb{P}_{in} g - \mathbb{P}_{KT} g| \lesssim \frac{1}{\sqrt{n}} \cdot \|g\|_{\mathbf{k}} \sqrt{\|\mathbf{k}\|_{\infty} \log n} \ll \mathcal{O}\left(\frac{1}{n^{1/4}}\right)$$

Monte Carlo rate
(standard thinning rate)

$$\text{If } |\mathbb{P}^{\star} g - \mathbb{P}_{in} g| = \mathcal{O}\left(\sqrt{\frac{\log n}{n}}\right) \text{ then } |\mathbb{P}^{\star} g - \mathbb{P}_{KT} g| = \mathcal{O}\left(\sqrt{\frac{\log n}{n}}\right)$$

19

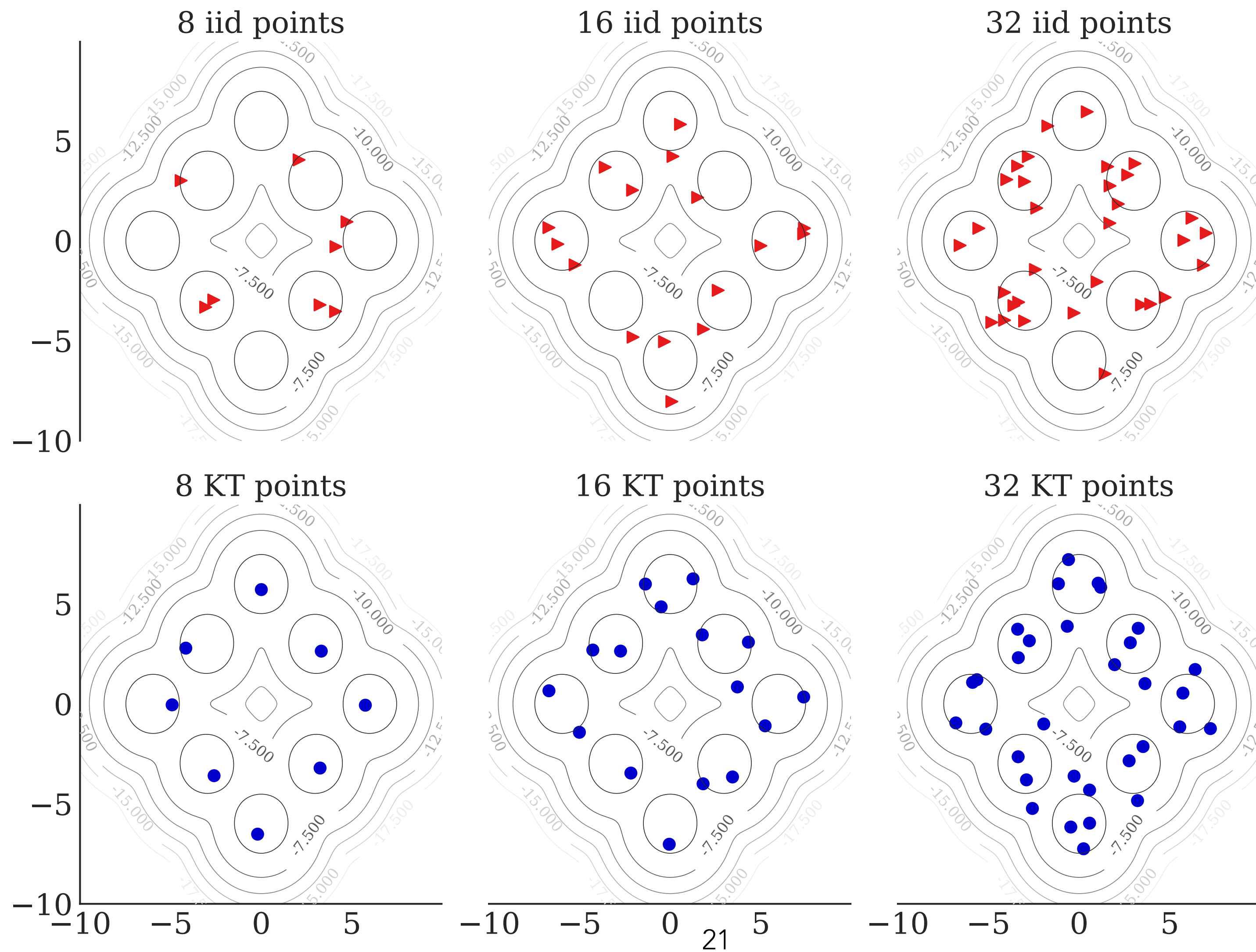# Monte Carlo input + KT $\Rightarrow$ Better than Monte Carlo output for $\mathbb{P}^\star$

With n input points, $\sqrt{n}$ output points, with high probability over the randomness in KT, **for any fixed** $g \in \mathbb{H}_\mathbf{k}$ we have

$$|\mathbb{P}_{in}g - \mathbb{P}_{KT}g| \lesssim \frac{1}{\sqrt{n}} \cdot \|g\|_\mathbf{k}\sqrt{\|\mathbf{k}\|_\infty \log n} \ll \mathcal{O}\left(\frac{1}{n^{1/4}}\right)$$

Monte Carlo rate
(standard thinning rate)

$$\text{If } |\mathbb{P}^\star g - \mathbb{P}_{in}g| = \mathcal{O}\left(\sqrt{\frac{\log n}{n}}\right) \text{ then } |\mathbb{P}^\star g - \mathbb{P}_{KT}g| = \mathcal{O}\left(\sqrt{\frac{\log n}{n}}\right)$$

- This is the Monte Carlo rate for input!
- Easily satisfied for input from iid sampling, MCMC, quadrature methods …

Intuition: KT finds ``diverse and representative'' points

Worst-case error

- For points in $\mathbb{R}^d$, **the worst-case error**—-Maximum Mean Discrepancy (MMD) error–in the reproducing kernel Hilbert space (RKHS) satisfies

$$\sup_{\|g\|_{\mathbf{k}} \leq 1} |\mathbb{P}_{in}g - \mathbb{P}_{KT}g|$$

Worst-case error: $\widetilde{O}(n^{-1/2})$ with $\sqrt{n}$ points for decaying $\mathbf{k}$

- For points in $\mathbb{R}^d$, **the worst-case error**—-Maximum Mean Discrepancy (MMD) error—in the reproducing kernel Hilbert space (RKHS) satisfies

$$\sup_{\|g\|_{\mathbf{k}} \leq 1} |\mathbb{P}_{in} g - \mathbb{P}_{KT} g| \lesssim_d \begin{cases} n^{-1/2}\sqrt{\log n} & \text{(Compactly supported; e.g., B-spline } \mathbf{k}) \\ n^{-1/2}\sqrt{\log^{d/2+1} n \log\log n} & \text{(Sub-Gaussian tails; e.g., Gaussian } \mathbf{k}) \\ n^{-1/2}\sqrt{\log^{d+1} n \log\log n} & \text{(Sub-exponential tails; e.g., Matern } \mathbf{k}) \end{cases}$$

Assuming similar tails for $\mathbf{P}_{in}$

- For output size s, the MMD error is $\widetilde{O}(1/s)$

Monte Carlo input + KT $\Rightarrow$ Better than Monte Carlo output for $\mathbb{P}^\star$

- For points in $\mathbb{R}^d$, **the worst-case error**—-Maximum Mean Discrepancy (MMD) error—in the reproducing kernel Hilbert space (RKHS) satisfies

$$\sup_{\|g\|_{\mathbf{k}}\leq 1} |\mathbb{P}^\star g - \mathbb{P}_{KT} g| \lesssim_d \begin{cases} n^{-1/2}\sqrt{\log n} & \text{(Compactly supported; e.g., B-spline } \mathbf{k}) \\ n^{-1/2}\sqrt{\log^{d/2+1} n \log\log n} & \text{(Sub-Gaussian tails; e.g., Gaussian } \mathbf{k}) \\ n^{-1/2}\sqrt{\log^{d+1} n \log\log n} & \text{(Sub-exponential tails; e.g., Matern } \mathbf{k}) \end{cases}$$

Assuming similar tails for $\mathbf{P}_{in}$

whenever $\sup_{\|g\|_{\mathbf{k}}\leq 1} |\mathbb{P}^\star g - \mathbb{P}_{in} g| \lesssim n^{-1/2}$ —-holds for iid / fast mixing MCMC input

24

Comparison with related work

- finding good approximations to $\mathbb{P}^{\star}$ by thinning, reweighting or directly

Related work: $\sqrt{n}$ points with $\mathcal{O}(n^{-1/4})$ MMD

- **Known guarantees *no better* than Monte Carlo rate**:

  Standard thinning iid points [Tolstikhin-Sriperumbudur-Muandet, 2017]

  Standard thinning geometrically ergodic MCMC [Dwivedi-Mackey 2021]

  Kernel herding for infinite-dimensional kernels [Chen-Welling-Smola 2010, Lacoste-Julien-Lindsten-Bach 2015]

  Stein Points MCMC [Chen-Barp-Briol-Gorham-Girolami-Mackey-Oates, 2019]

  Greedy sign selection [Karnin-Liberty 2019]

- ***Unknown* guarantees**:

  Support points [Mak-Joseph 2018]

  Supersampling from a reservoir [Paige-Sejdinovic-Wood, 2016]:

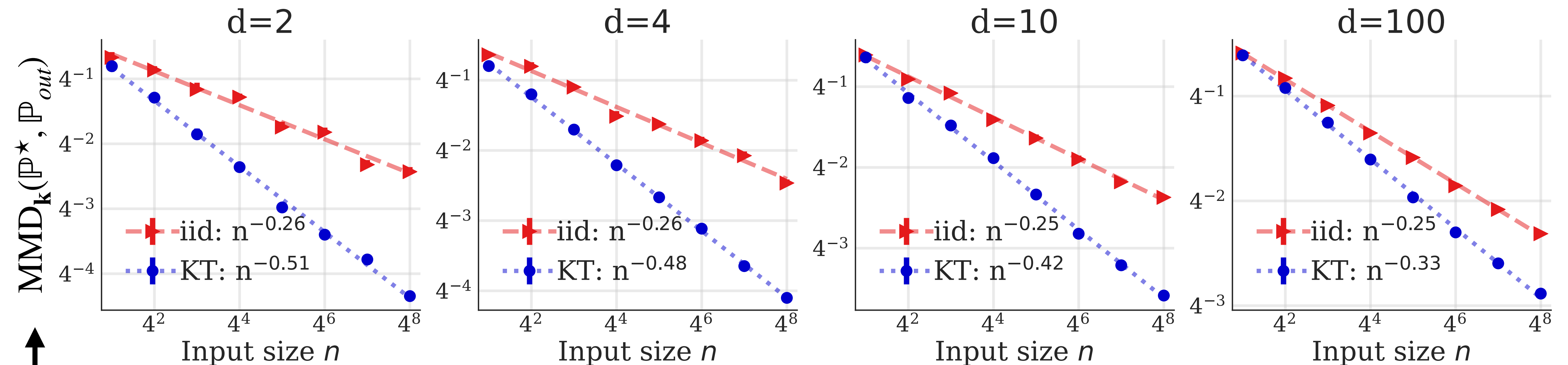# Related work: $\sqrt{n}$ points with $o(n^{-1/4})$ MMD

- **Finite-dimensional linear kernels:** Discrepancy construction [Harvey and Samadi, 2014]

- **Uniform $\mathbb{P}^\star$ on $[0,1]^d$:**
  Quasi Monte Carlo [Hickernell 1998, Novak-Wozniakowski 2010] ,
  Haar thinning [Dwivedi-Feldheim-Gurel-Gurevich-Ramdas 2019]

- **$\mathbb{P}^\star$ with *bounded* support with known $\mathbb{P}^\star k$:**
  Bayesian quadrature [O'Hagan 1991]
  Bayes' Sard cubtature [Karvonen et al. 2018]
  Determinantal point processes [Belhadji et al. 2020]

- **(k, $\mathbb{P}^\star$) with *known/bounded* eigenfunctions:**
  Determinantal point process kernel quadrature [Belhadji et al. 2019]
  Black-box importance sampling [Liu et al. 2018]

Kernel thinning advantages

1. $\sqrt{n}$ points with $O(\sqrt{\log n/n})$ integration-error for any fixed function in the RKHS for any kernel on any space (iid sampling gives $\Omega(n^{-1/4})$ error)

2. $\sqrt{n}$ points with $\widetilde{O}(n^{-1/2})$-worst-case/MMD error for decaying kernels

3. Valid for **non-uniform** target distributions with **unbounded support**

4. Valid for **infinite-dimensional** smooth/decaying kernels

5. Valid for **generic input points** including iid/MCMC/quadrature etc with mild conditions

6. Requires **only kernel evaluations** to implement

7. **Matches MMD lower bounds** up to log factors

8. **Matches L^∞-error lower bounds** up to log factors

KT vs iid: Gaussian $\mathbb{P}^\star$ in $\mathbb{R}^d$
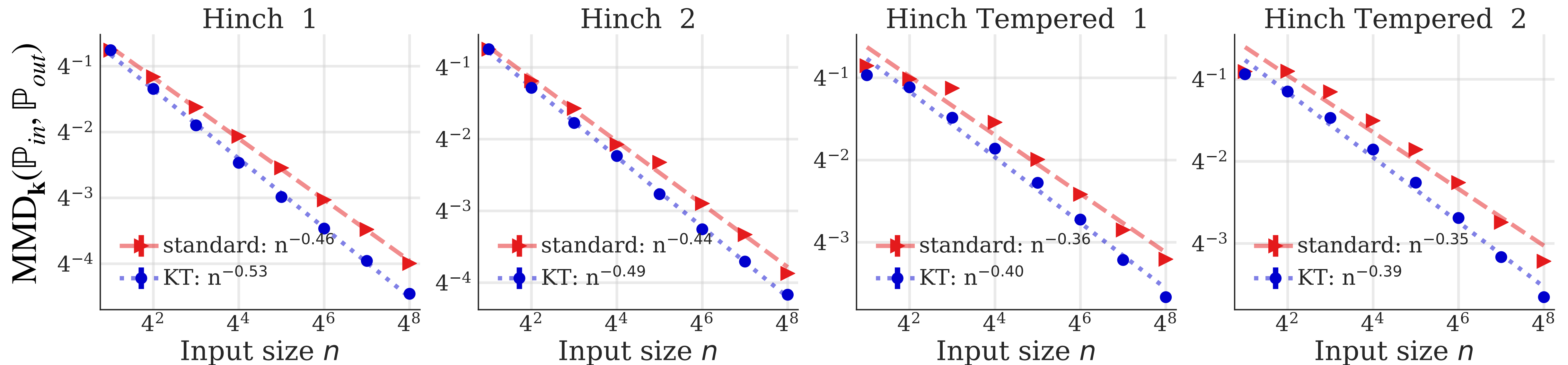
(Gaussian kernel with $\sigma^2 = 2d$)

In practice, significant gains even in dimension $d = 100$

(Worst-case error in the unit
ball of Gaussian RKHS)
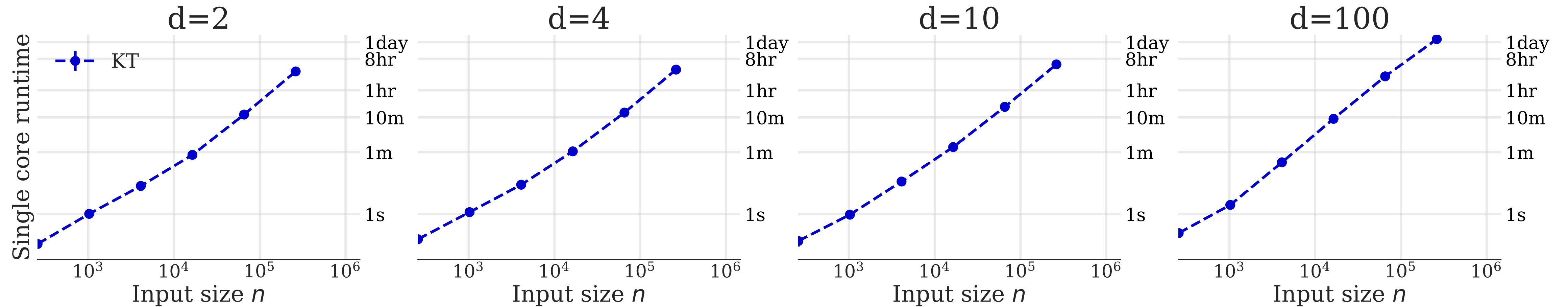
KT on MCMC samples from computational cardiology

In this setting with $d = 38$, standard thinning is already good (the chain is mixing slowly), but KT provides further improvement! Each point saves 1000s of CPU hours!!

*MCMC samples taken from Riabiz-Chen-Cockayne-Swietach-Niederer-Mackey-Oates, 2021
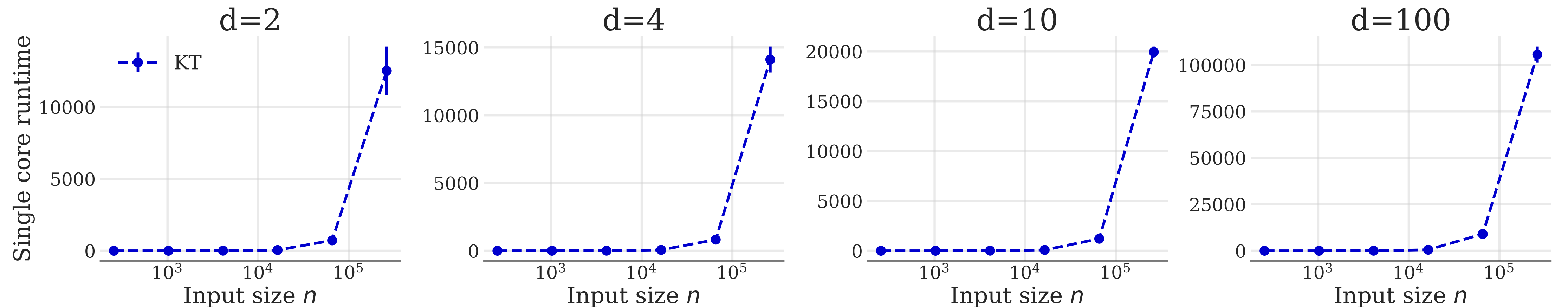
KT drawback: n^2 runtime with n input points

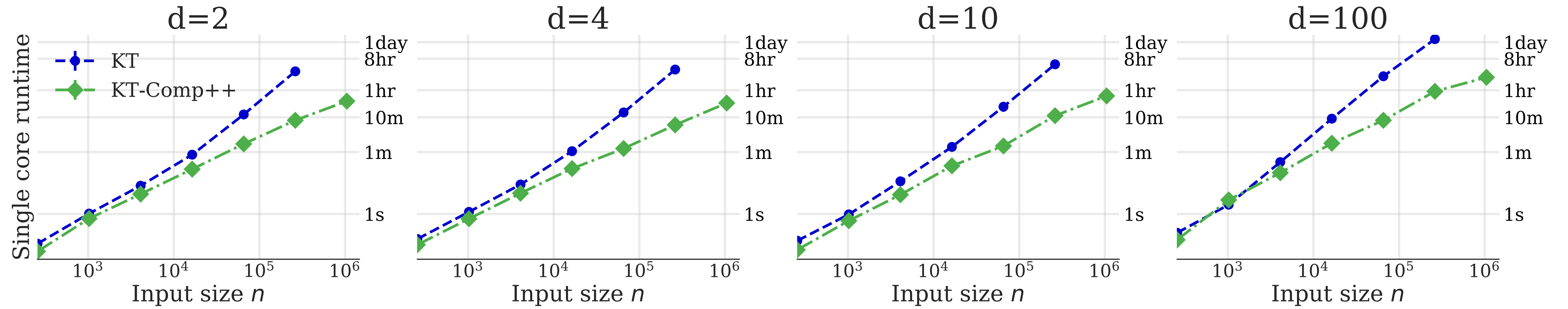Y-axis = **Runtime in log-scale** (Runtime dominated by kernel evaluations)

Y-axis = **Runtime in linear scale** (seconds)

Compress++: Reducing runtime

Compress++: Reducing runtime with minimal loss in accuracy!!

Compress++: A recursive strategy to reduce runtime for **generic thinning** algorithms

Thinning algorithm with n^2 runtime and sub-Gaussian error $e(n)$ $\longrightarrow$ Compress++ $\longrightarrow$ $\sqrt{n}$-thinning algorithm with $n\log^3 n$ runtime and sub-Gaussian error $4e(n)$

Compress($\mathcal{S}$, $\mathfrak{g}$, ALG):

- If size($\mathcal{S}$) == 1, **Return** $\mathcal{S}$

- Else:

    (i) Call Compress separately on 4 equal splits of $\mathcal{S}$

    (ii) Concatenate the 4 outputs from step (i)

    (iii) **Return** Halved output of step (ii) using ALG

Summary:

KT-Compress++ provides near-optimal compression in near-linear time

n points ➡️ **Standard Thinning** ➡️ $\sqrt{n}$ points with $\dfrac{1}{n^{1/4}}$ error (Monte Carlo rate)

n points ➡️ **Kernel Thinning (KT)** ➡️ $\sqrt{n}$ points with $\widetilde{O}\left(\dfrac{1}{\sqrt{n}}\right)$ error in n^2 time

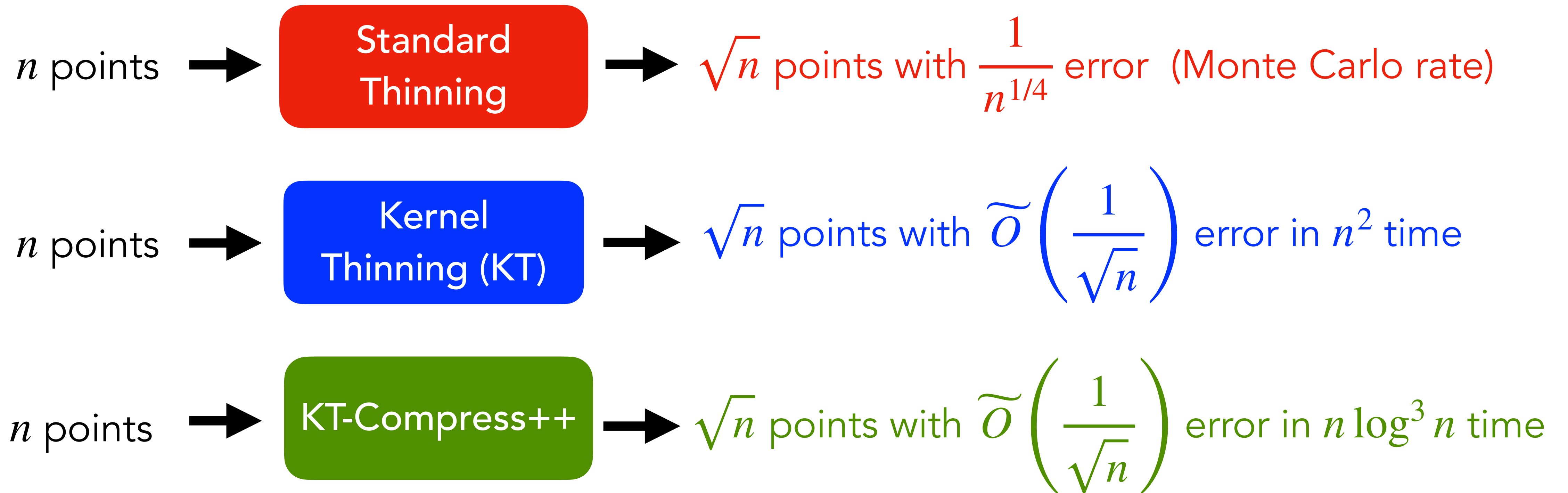n points ➡️ **KT-Compress++** ➡️ $\sqrt{n}$ points with $\widetilde{O}\left(\dfrac{1}{\sqrt{n}}\right)$ error in $n\log^3 n$ time

🐍 python™ **pip install goodpoints**

arXiv.org https://arxiv.org/abs/2105.05842   [Kernel Thinning, COLT 2021]
https://arxiv.org/abs/2110.01593   [Generalized Kernel Thinning, ICLR 2022]
https://arxiv.org/pdf/2111.07941.pdf [Distribution Compression In Near-linear Time, ICLR 2022]

Additional slides

Details of kernel thinning

KT: A two-staged algorithm

- **Input**: Kernel $\mathbf{k}$, input points $\mathscr{S}_{in}$ of size n, thinning factor m

- **KT-Split**:

  - Split $\mathscr{S}_{in}$ into 2^m balanced candidate coresets each of size $\dfrac{n}{2^m}$

  - When $m = \dfrac{1}{2}\log_2 n$, we have $\sqrt{n}$ coresets each of size $\sqrt{n}$

- **KT-Swap**:

  - Pick the best candidate coreset that minimized $\mathbf{MMD_k}$ to input

  - Iteratively refine each point in the selected coreset by swapping with the best alternative $\mathscr{S}_{in}$ if it improves the MMD error

Computation: $\mathcal{O}(n^2)$ kernel evaluations
Storage: $n\min(n, d)$

KT-Split

- Repeated rounds of splitting the parent coreset in two equal-sized children coresets

- Runs online, after seeing t input points, the bottom nodes have $t/2^m$ points

KT-Split

- One path on the tree is obtained by repeated **kernel halving**

- At each halving round, remaining points are paired, and one point is selected **non-uniformly** from each pair using a **new Hilbert space generalization of the self-balancing walk** of [Alweiss-Liu-Sawhney 2020]

Input

$\mathcal{S}_{\text{in}}$ (n points)

$\downarrow$

Kernel Halving

$\downarrow$

$\mathcal{S}^{(1,1)}$ ($\dfrac{n}{2}$ points)

$\downarrow$

Kernel Halving

$\downarrow$

$\mathcal{S}^{(2,1)}$ ($\dfrac{n}{4}$ points)

m **Kernel Halving** rounds

Output

$\mathcal{S}^{(m,1)}$ ($\dfrac{n}{2^m}$ points)

40

Algorithm 2: Self-balancing Hilbert Walk

Input: sequence of functions $(f_i)_{i=1}^n$ in Hilbert space $\mathcal{H}$, threshold sequence $(\mathfrak{a}_i)_{i=1}^n$

$\psi_0 \leftarrow 0 \in \mathcal{H}$

for $i = 1, 2, \ldots, n$ **do**

    $\alpha_i \leftarrow \langle \psi_{i-1}, f_i \rangle_{\mathcal{H}}$ // Compute Hilbert space inner product

    if $|\alpha_i| > \mathfrak{a}_i$**:**

        $\psi_i \leftarrow \psi_{i-1} - f_i \cdot \alpha_i / \mathfrak{a}_i$

    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 ψ_n, combination of signed input functions

Algorithm 2: Self-balancing Hilbert Walk

Input: sequence of functions $(f_i)_{i=1}^n$ in Hilbert space $\mathcal{H}$, threshold sequence $(\mathfrak{a}_i)_{i=1}^n$

$\psi_0 \leftarrow 0 \in \mathcal{H}$

for $i = 1, 2, \ldots, n$ **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 $\mathfrak{a}_i$ such that this step **does not occur** 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 ψ_n, combination of signed input functions

Algorithm 2: Self-balancing Hilbert Walk

Input: sequence of functions $(f_i)_{i=1}^n$ in Hilbert space $\mathcal{H}$, threshold sequence $(\mathfrak{a}_i)_{i=1}^n$

$\psi_0 \leftarrow \mathbf{0} \in \mathcal{H}$

for $i = 1, 2, \ldots, n$ **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 $\mathfrak{a}_i$ such that this step **does not occur** 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 ψ_n, combination of signed input functions

- Exact **Kernel halving**: When $f_i = \mathbf{k}(x_{2i}, \cdot) - \mathbf{k}(x_{2i-1}, \cdot)$, exactly half of input points ($\mathcal{S}_{out}$) given -1 sign after $n/2$ steps

$$\frac{1}{n}\psi = \frac{1}{n}\sum_{x \in S_{in}} \mathbf{k}(x, \cdot) - \frac{2}{n}\sum_{x \in S_{out}} \mathbf{k}(x, \cdot) = \mathbb{P}_{in}\mathbf{k} - \mathbb{P}_{out}\mathbf{k}$$

43

Algorithm 2: Self-balancing Hilbert Walk

Input: sequence of functions $(f_i)_{i=1}^n$ in Hilbert space $\mathcal{H}$, threshold sequence $(\mathfrak{a}_i)_{i=1}^n$

$\psi_0 \leftarrow \mathbf{0} \in \mathcal{H}$

for $i = 1, 2, \ldots, n$ **do**

    $\alpha_i \leftarrow \langle \psi_{i-1}, f_i \rangle_{\mathcal{H}}$ // Compute Hilbert space inner product

    if $|\alpha_i| > \mathfrak{a}_i$:

        $\psi_i \leftarrow \psi_{i-1} - f_i \cdot \alpha_i / \mathfrak{a}_i$

    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 ψ_n, combination of signed input functions

- **Balance**: If $\mathbf{k}$ is a reproducing kernel, for all $g \in \mathbb{H}_{\mathbf{k}}$,

$$\langle \psi_n, g \rangle_{\mathbf{k}} = \mathbb{P}_{in} g - \mathbb{P}_{out} g \text{ is } \mathcal{O}(n^{-1} \cdot \sqrt{\log n} \cdot \|g\|_{\mathbf{k}})\text{-sub-Gaussian}$$

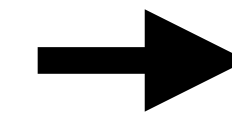If η_i were chosen i.i.d., the sub-Gaussian parameter is $\Omega(n^{-1/2})$

Details of Compress++

Compress++: A simple two-stage algorithm

n points, parameter $\mathfrak{g}$,
halving algorithm HALVE $\quad\blacktriangleright\quad$ **Compress** $\quad\blacktriangleright\quad$ $2^g\sqrt{n}$ points

For example:

HALVE = Kernel thinning by a factor of 2

THIN = Kernel thinning by a factor of $2^{\mathfrak{g}}$
(other algorithms can be used too!)

$2^{\mathfrak{g}}$ thinning
algorithm THIN

$\sqrt{n}$ points

46

Compress++: A simple two-stage algorithm

n points, parameter $\mathfrak{g}$, halving algorithm HALVE $\longrightarrow$ **Compress** $\longrightarrow$ $2^g\sqrt{n}$ points

$\downarrow$

$2^{\mathfrak{g}}$ thinning algorithm THIN

$\downarrow$

$\sqrt{n}$ points

Compress($\mathcal{S}$, $\mathfrak{g}$, ALG):

- If size($\mathcal{S}$) == $4^{\mathfrak{g}}$, **Return** $\mathcal{S}$

- Else:

    (i) Call Compress separately on 4 equal splits of $\mathcal{S}$

    (ii) Concatenate the 4 outputs from step (i)

    (iii) **Return** Halved output of step (ii) using ALG

Compress++: Informal guarantee

Under some mild conditions, with $\mathfrak{g} = \log\log n + 1$, we have

- **Sub-Gaussian error inflation by at most 4:**
  If $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n, \mathbb{P}_{HALVE}) \sim e_1(n)$ and $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n, \mathbb{P}_{THIN}) \sim e_2(n)$ then
  $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n, \mathbb{P}_{Compress++}) \sim 4 \max(e_1(n), e_2(n))$

$$\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_{in}, \mathbb{P}_{out}) = \sup_{\|g\|_{\mathbf{k}} \leq 1} |\mathbb{P}_{in}g - \mathbb{P}_{out}g|$$

Compress++: Informal guarantee

Under some mild conditions, with $\mathfrak{g} = \log\log n + 1$, we have

- **Sub-Gaussian error inflation by at most 4:**
  If $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n, \mathbb{P}_{HALVE}) \sim e_1(n)$ and $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n, \mathbb{P}_{THIN}) \sim e_2(n)$ then
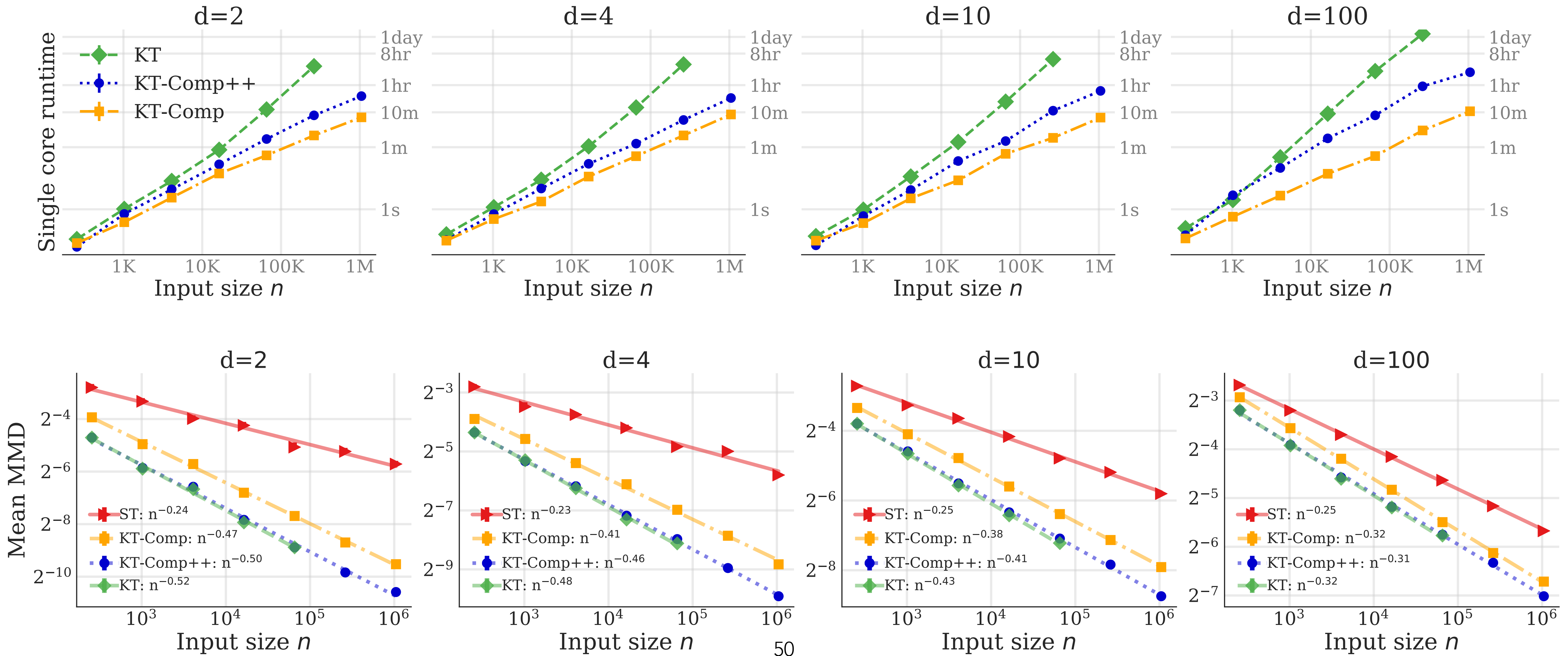 $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P}_n, \mathbb{P}_{Compress++}) \sim 4\max(e_1(n), e_2(n))$

- **Quadratic reduction in runtime**:
  If runtime of HALVE and THIN with n points is $\mathcal{O}(n^{\tau})$ then the runtime of
  Compress++ with n points is $\mathcal{O}(n^{\tau/2})$ if $\tau > 2$ and $\mathcal{O}(n\log^3 n)$ if $\tau = 2$.
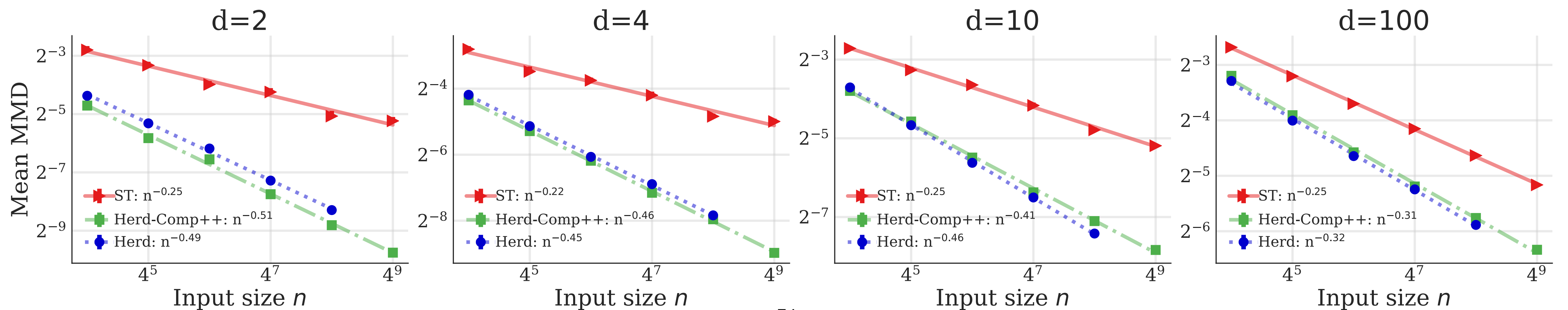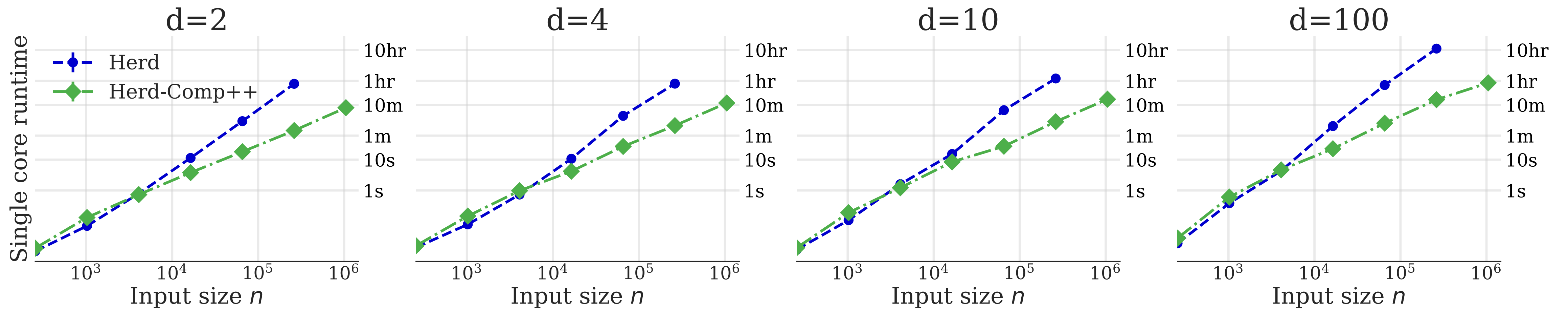
KT vs Compress ($\mathfrak{g} = 0$) vs Compress++ ($\mathfrak{g} = 4$)

The input algorithms Halve and Thin to Compress++ are derived from KT

50

Results for Compress++ with kernel herding (Herd)

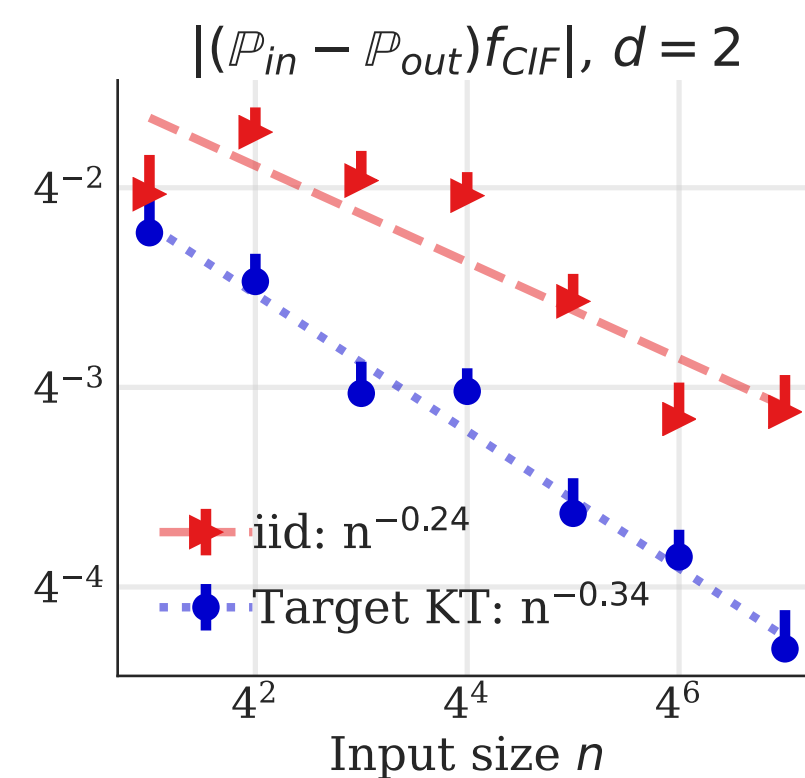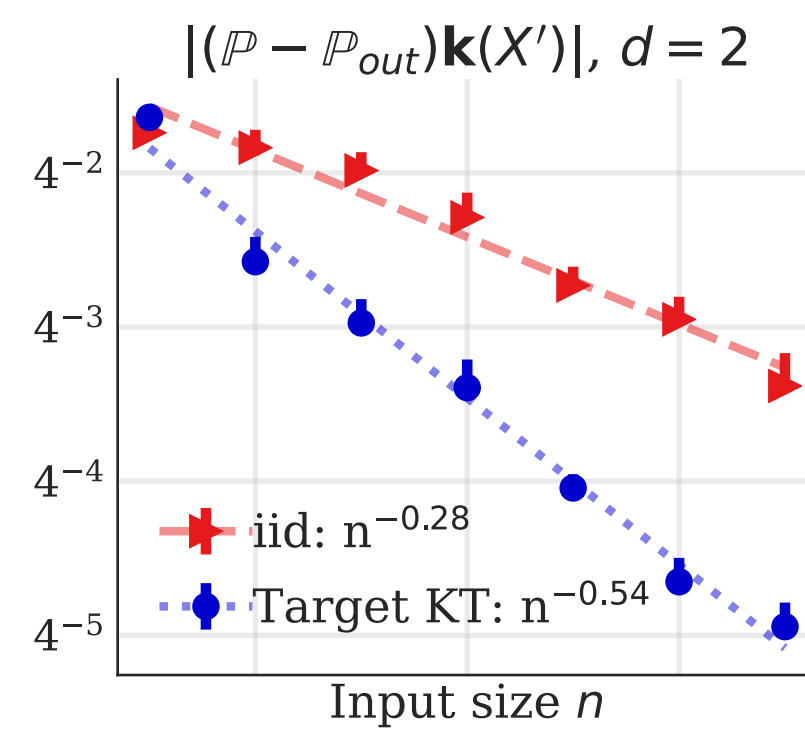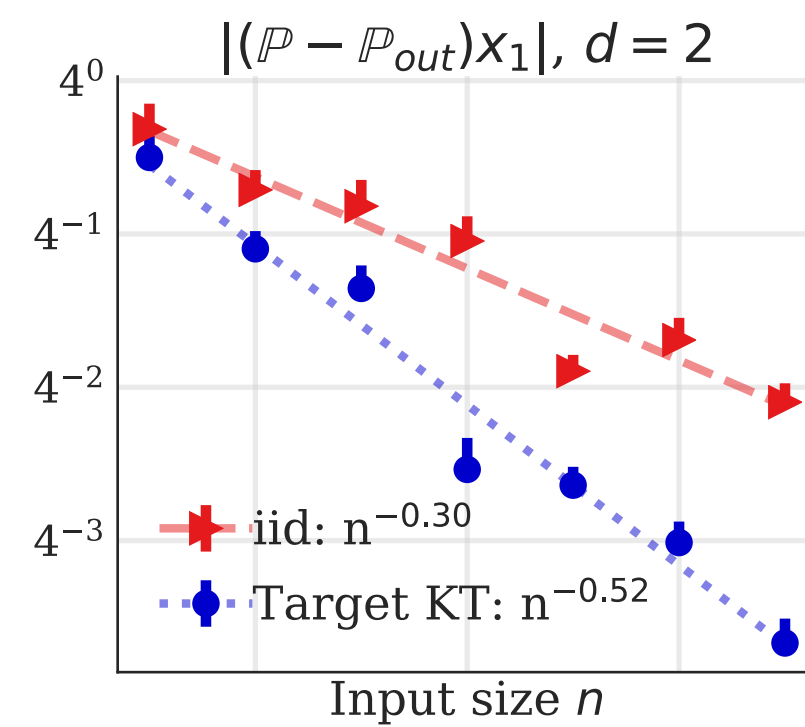Results for Compress++ with kernel herding (Herd)

Lower bounds

Lower bounds

- For smooth kernels, there exists a target $\mathbb{P}$, such that a coreset of size $\sqrt{n}$ suffers an MMD error of $\min(\sqrt{\dfrac{d}{n}}, n^{-1/4})$. [Philips and Tai 2020]

- For characteristic kernels, there exists a target $\mathbb{P}$, such that any estimator based on n i.i.d. input points must suffer at least $n^{-1/2}$ MMD error. [Tolstikhin et al. 2017]

Both bounds apply to Gaussian and Matérn kernels
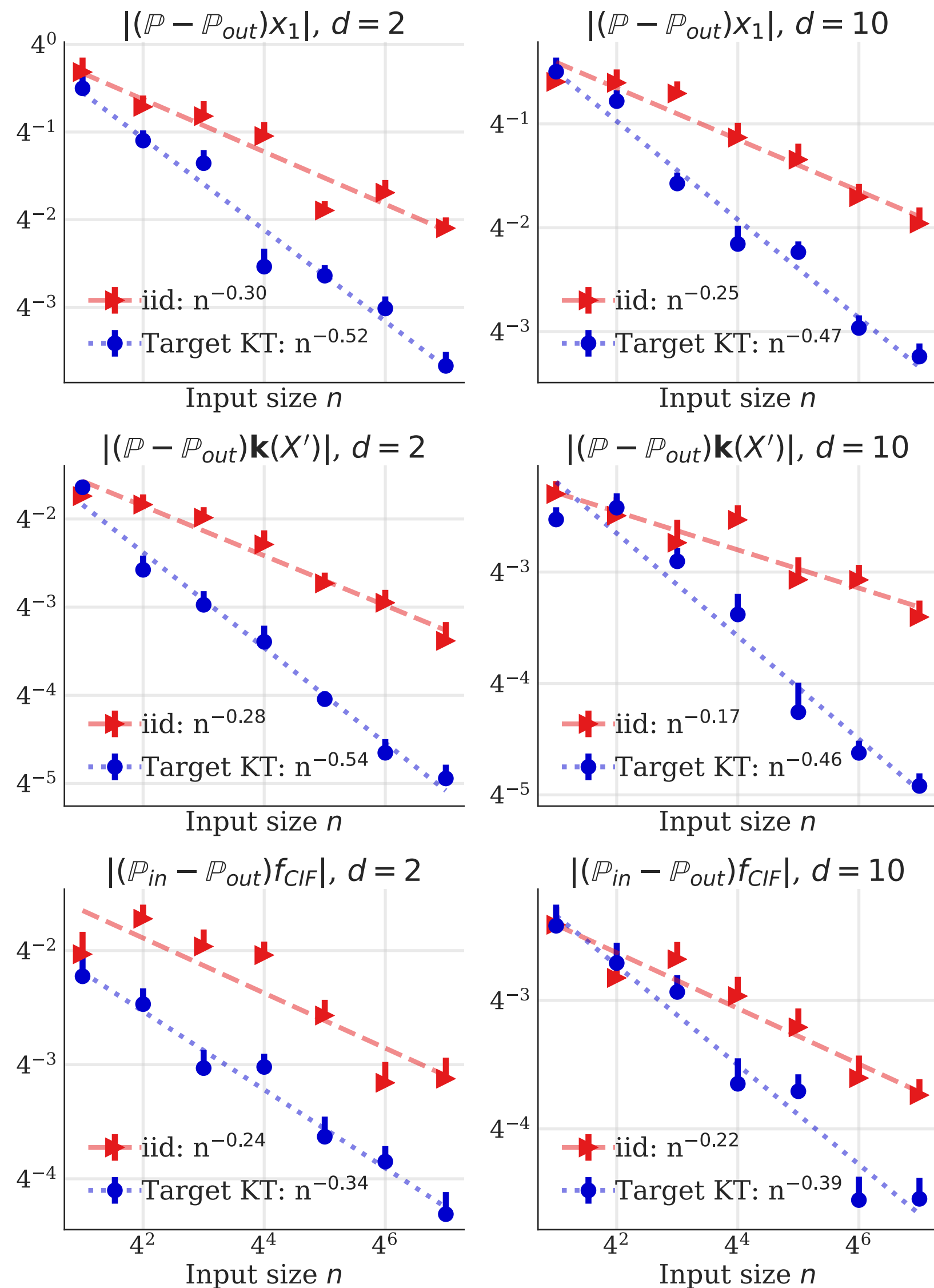
Single function +
Additional MCMC Experiments

Better error for functions inside and outside of RKHS

(Gaussian $\mathbf{k}$ with $\sigma^2 = 2d$ and standard Gaussian $\mathbb{P}^\star$)

$|(\mathbb{P} - \mathbb{P}_{out})x_1|$, $d = 2$

iid: $n^{-0.30}$
Target KT: $n^{-0.52}$

Input size n

$|(\mathbb{P} - \mathbb{P}_{out})\mathbf{k}(X')|$, $d = 2$

iid: $n^{-0.28}$
Target KT: $n^{-0.54}$

Input size n

$|(\mathbb{P}_{in} - \mathbb{P}_{out})f_{CIF}|$, $d = 2$

iid: $n^{-0.24}$
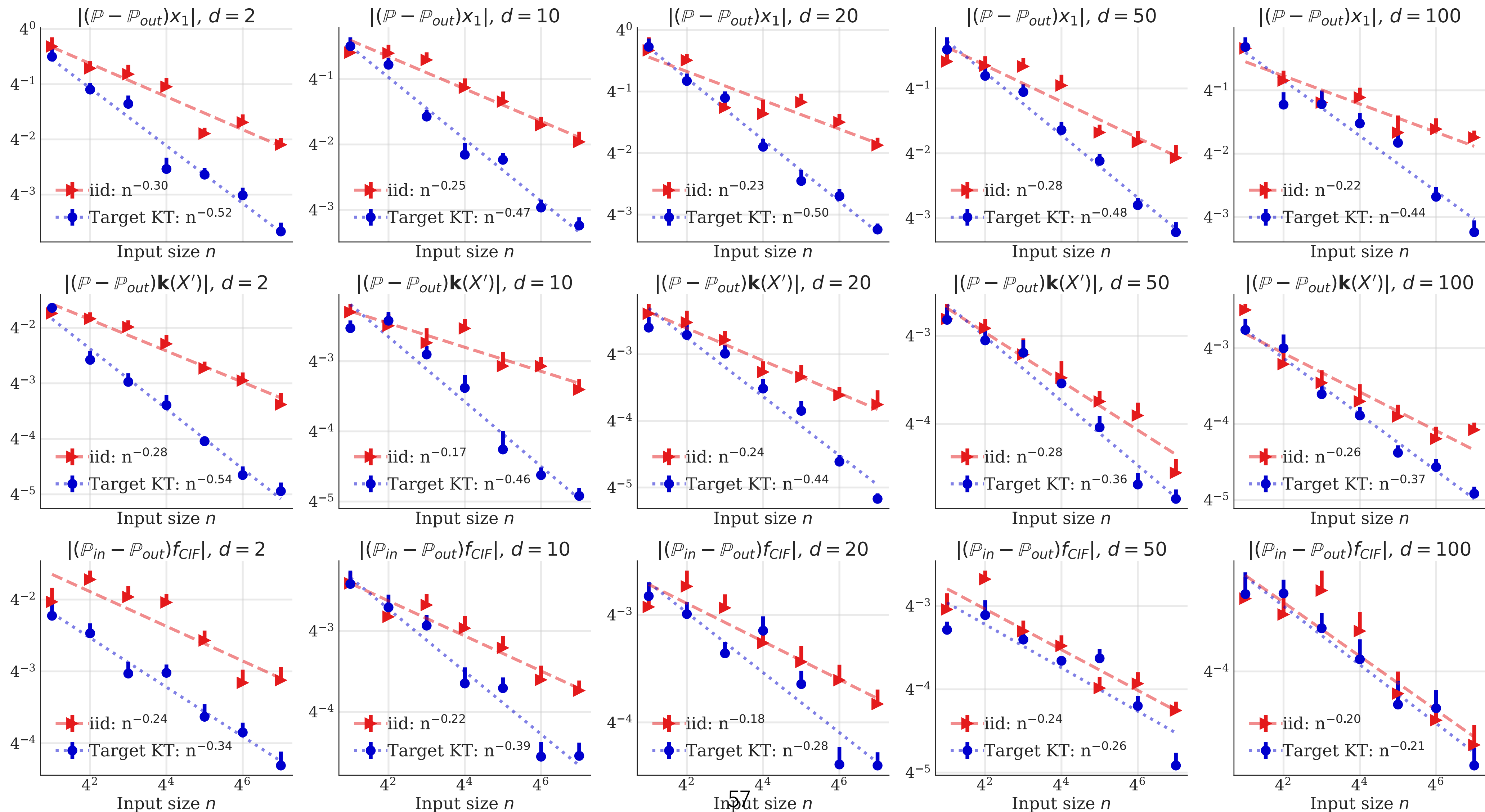Target KT: $n^{-0.34}$

Input size n

Better error for functions inside and outside of RKHS

(Gaussian $\mathbf{k}$ with $\sigma^2 = 2d$ and standard Gaussian $\mathbb{P}^\star$)

Better error for functions inside and outside of RKHS

(Gaussian $\mathbf{k}$ with $\sigma^2 = 2d$ and standard Gaussian $\mathbb{P}^{\star}$)

MCMC experiments: Differential equation models

Dimension $d = 4$

1. Lotka-Volterra model
   oscillatory enzymatic control, [1925, 1926]
2. Goodwin model
   oscillatory predator-prey evolution, [1965]

X

1. Posterior

X

1. Random walk (RW)
   [Metropolis et al. 1953, Hastings 1970]
2. Adaptive random walk (adaRW)
   [Haario et al. 1999]
3. Metropolis adjusted Langevin algorithm (MALA) [Roberts et al. 1996]
4. Preconditioned-MALA (pMALA)
   [Girolami et al. 2011]

Dimension $d = 38$

3. Hinch calcium signal model
   [Hinch-Greenstein-Tanskanen-Xu-Winslow, 2004]

X

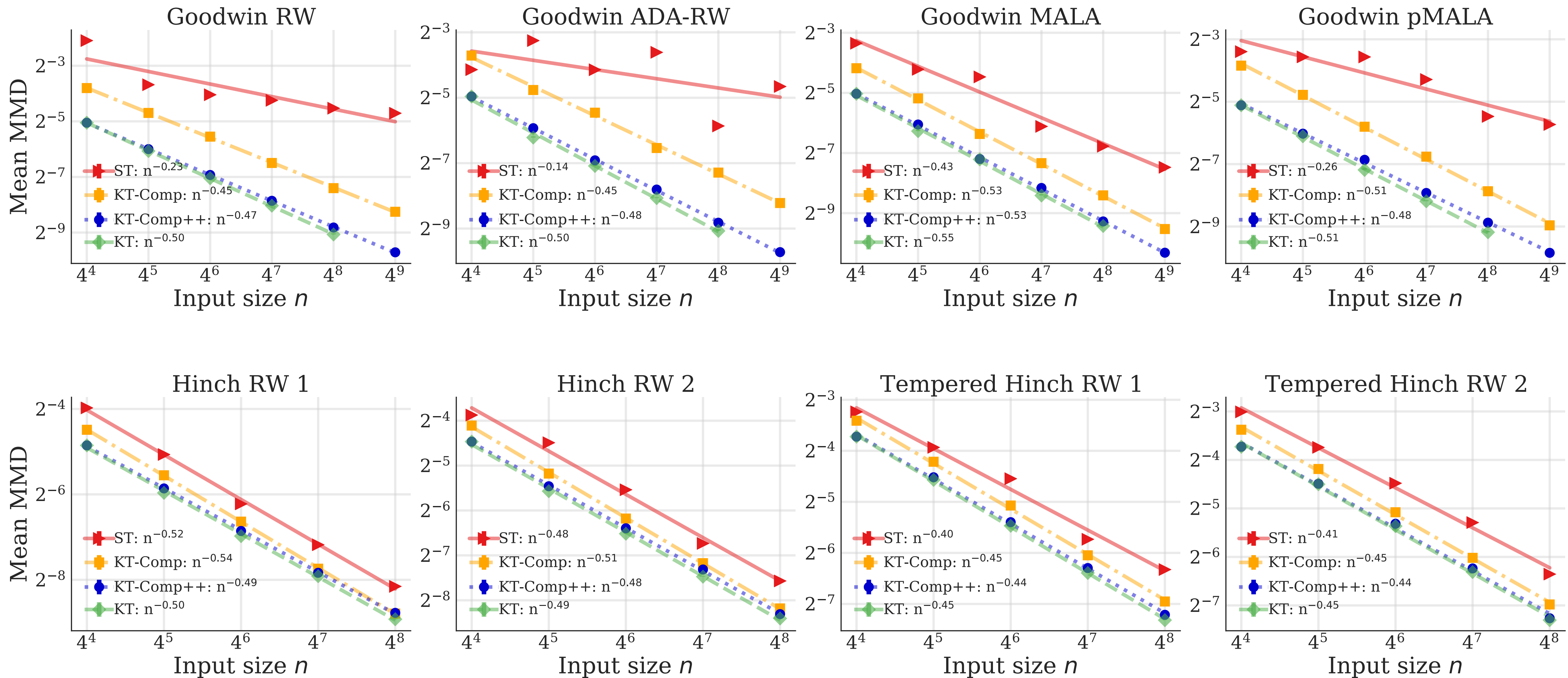1. Posterior
2. Tempered posterior

X

1. Random walk (RW) - run 1
2. Random walk (RW) - run 2

For KT, we use Gaussian kernel, and chose its bandwidth via median heuristic [Garreau et al. 2017]

MCMC samples taken from Riabiz-Chen-Cockayne-Swietach-Niederer-Mackey-Oates, 2021

Results for MCMC experiments

Details for KT result

Target KT MMD rates: $\sqrt{n}$ points with $\widetilde{O}(n^{-1/2})$ error

- More generally

$$\widetilde{O}\left(\frac{1}{\sqrt{n}}\right) \text{ error rate for analytic kernels}$$

$$\widetilde{O}\left(\frac{n^{d/2m}}{\sqrt{n}}\right) \text{ for } m\text{-times differentiable kernels}$$
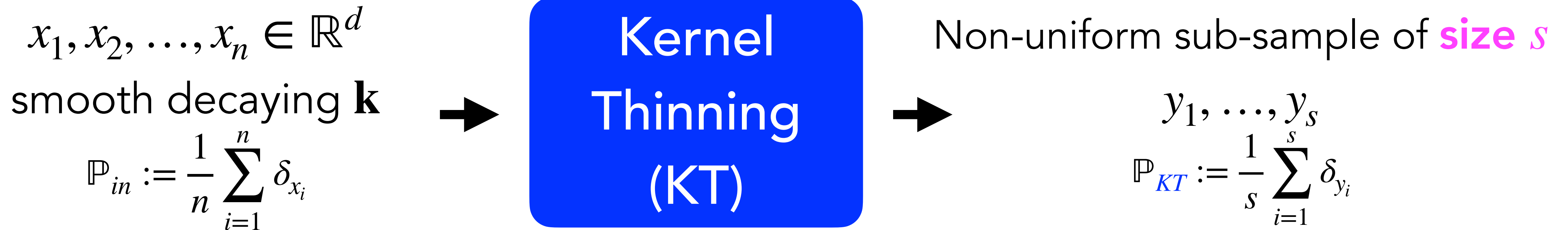
- We state explicit constants with dependence on kernel hyper-parameters in the paper

Generalized kernel thinning

	Root KT	Target KT	KT+ [Best of both worlds]
KT-Split kernel	$\mathbf{k}_{rt}$	$\mathbf{k}$	$\mathbf{k} + \mathbf{k}_{\alpha-rt}$
Single-function error	Same as MMD error	$\sqrt{\dfrac{\log n}{n}}$ **For arbitrary k on arbitrary domain**	$\sqrt{\dfrac{\log n}{n}}$
MMD error	See <u>slide</u>	$\sqrt{\dfrac{\log^{ad+b} n}{n}}$ Analytic $\mathbf{k}$ $\sqrt{\dfrac{n^{d/m}}{n}}$ m-times differentiable $\mathbf{k}$	Min(Target KT Error, α-Root KT)

$\mathbf{k}(x, y) = \int \mathbf{k}_{rt}(x, z) \mathbf{k}_{rt}(z, y) dz$ & $\mathbf{k}_{\alpha-rt} =_{62} \widehat{(\widehat{\mathbf{k}})^{\alpha}}$ where ˆ denotes Fourier transform

Target KT or KT+: Better than Monte Carlo rate

$x_1, x_2, \ldots, x_n \in \mathbb{R}^d$

smooth decaying $\mathbf{k}$

$$\mathbb{P}_{in} := \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$$

➡️

Kernel Thinning (KT)

➡️

Non-uniform sub-sample of **size** s

$$y_1, \ldots, y_s$$

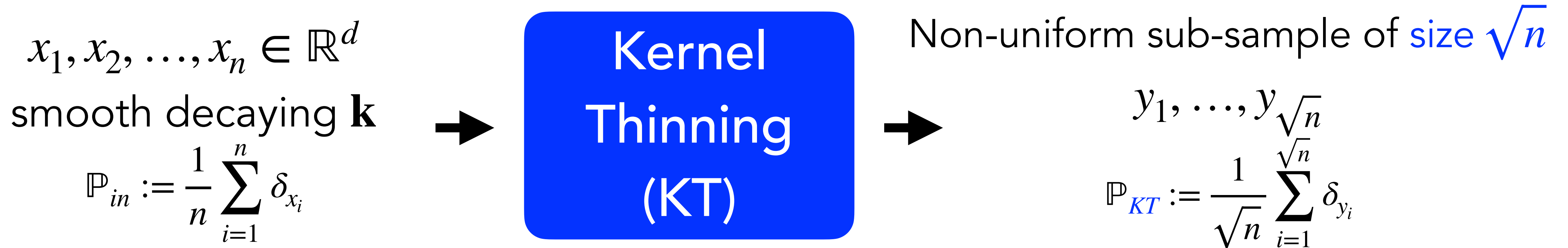$$\mathbb{P}_{KT} := \frac{1}{s} \sum_{i=1}^{s} \delta_{y_i}$$

For any fixed $g \in \mathbb{H}_{\mathbf{k}}$, with probability $1 - \delta$ over the randomness in KT, we have

$$|\mathbb{P}_{in} g - \mathbb{P}_{KT} g| \leq \frac{1}{s} \cdot \|g\|_{\mathbf{k}} \sqrt{\frac{8}{3} \|\mathbf{k}\|_\infty \log\left(\frac{4}{\delta}\right) \log\left(\frac{6s \log(n/s)}{\delta}\right)}$$

Much faster than the Monte Carlo rate for standard/uniform thinning $\mathcal{O}\left(\frac{1}{\sqrt{s}}\right)$

Target KT or KT+: Better than Monte Carlo rate

$x_1, x_2, \ldots, x_n \in \mathbb{R}^d$

smooth decaying $\mathbf{k}$

$\mathbb{P}_{in} := \dfrac{1}{n} \sum\limits_{i=1}^{n} \delta_{x_i}$

$\longrightarrow$

Kernel Thinning (KT)

$\longrightarrow$

Non-uniform sub-sample of size $\sqrt{n}$

$y_1, \ldots, y_{\sqrt{n}}$

$\mathbb{P}_{KT} := \dfrac{1}{\sqrt{n}} \sum\limits_{i=1}^{\sqrt{n}} \delta_{y_i}$

For any fixed $g \in \mathbb{H}_{\mathbf{k}}$, with probability $1 - \delta$ over the randomness in KT, we have

$$|\mathbb{P}_{in}g - \mathbb{P}_{KT}g| \leq \frac{1}{\sqrt{n}} \cdot \|g\|_{\mathbf{k}} \sqrt{\frac{8}{3} \|\mathbf{k}\|_\infty \log\left(\frac{4}{\delta}\right) \log\left(\frac{6\sqrt{n}\log\sqrt{n}}{\delta}\right)}$$

Much faster than the Monte Carlo rate for standard/uniform thinning $\mathcal{O}\left(\dfrac{1}{n^{1/4}}\right)$

Properties of MMD

- Maximum mean discrepancy (MMD) = worst-case integration discrepancy between two distributions over a class of real-valued test functions

$$\text{MMD}_{\mathbf{k}}(\mathbb{P}_{in}, \mathbb{P}_{out}) = \sup_{\|g\|_{\mathbf{k}} \leq 1} |\mathbb{P}_{in}g - \mathbb{P}_{out}g|$$

[Gretton-Borgwardt-Rasch-Schölkopf-Smola, 2012]

- **MMD metrizes convergence in distribution** for popular infinite-dimensional kernels like Gaussian, Matern, IMQ, B-spline

[Simon-Gabriel-Barp-Schölkopf-Mackey, 2020]