# Compress Then Test: Powerful Kernel Testing in Near-linear Time




Carles Domingo-Enrich[1] Raaz Dwivedi[2,3] Lester Mackey[4]

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github.com/microsoft/goodpoints


## Kernel two-sample testing

- $\mathbb{X}_n = (X_i)_{1\le i\le n}$ i.i.d. sample of $\mathbb{P}$, $\mathbb{Y}_n = (Y_i)_{1\le i\le n}$ i.i.d. sample of $\mathbb{Q}$.
- Null hypothesis: $\mathscr{H}_0 : \mathbb{P} = \mathbb{Q}$
- Non-parametric form via kernel maximum mean discrepancy (MMD)

$$\mathscr{H}_0 : \mathrm{MMD}^2_{\mathbf{k}}(\mathbb{P},\mathbb{Q}) \triangleq \mathbb{E}_{X,X'\sim\mathbb{P}}\mathbf{k}(X,X') + \mathbb{E}_{Y,Y'\sim\mathbb{P}}\mathbf{k}(Y,Y') - 2\mathbb{E}_{X\sim\mathbb{P},Y\sim\mathbb{Q}}\mathbf{k}(X,Y) = 0$$

with Test statistic: $\Delta(\mathbb{X}_n,\mathbb{Y}_n) = \begin{cases} 0 & \text{if } \mathrm{MMD}^2_{\mathbf{k}}(\mathbb{X}_n,\mathbb{Y}_n) < t_\alpha \text{ (accept } \mathscr{H}_0) \\ 1 & \text{if } \mathrm{MMD}^2_{\mathbf{k}}(\mathbb{X}_n,\mathbb{Y}_n) \ge t_\alpha \text{ (reject } \mathscr{H}_0) \end{cases}$

## Prior MMD strategies are slow

- Computing MMD takes $O(n^2)$ time

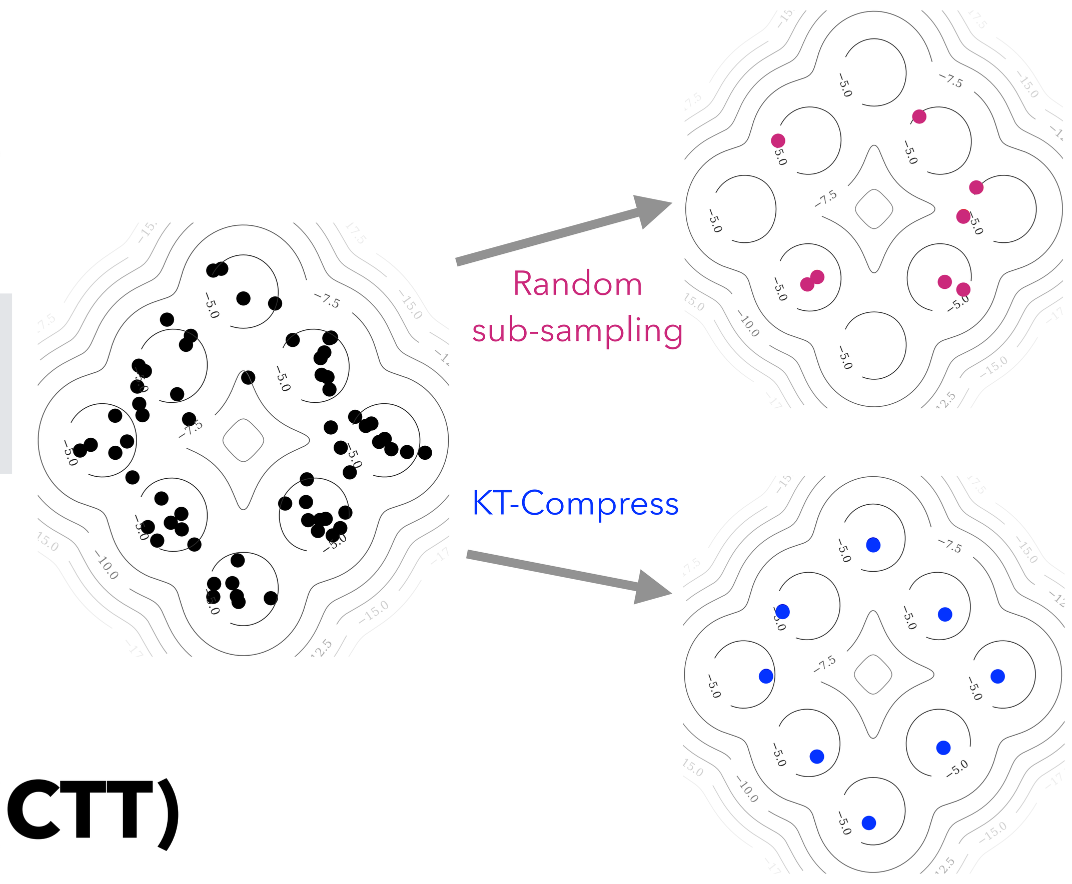
$$\mathrm{MMD}^2_{\mathbf{k}}(\mathbb{X}_n,\mathbb{Y}_n) = \frac{\sum_{i,i'=1}^n \mathbf{k}(X_i,X_{i'})}{n^2} + \frac{\sum_{j,j'=1}^n \mathbf{k}(Y_j,Y_{j'})}{n^2} - \frac{2\sum_{i=1}^n\sum_{j=1}^n \mathbf{k}(X_i,Y_j)}{n^2}$$

- Can we speed up the test while
  - A. respecting Type I error: reject null rarely when $\mathbb{P} = \mathbb{Q}$, and
  - B. keeping our test powerful: reject null often when $\mathbb{P} \neq \mathbb{Q}$?
- Prior speedup strategies sacrifice power!

## Speed up testing by compressing

- Compress $\mathbb{X}_n$ to $\hat{\mathbb{X}}_m$ of size $m = \sqrt{n}$ with small $\mathrm{MMD}^2_{\mathbf{k}}(\mathbb{X}_n,\hat{\mathbb{X}}_m)$

| | Random subsampling | KT-Compress (Shetty et al., 2023) |
|---|---|---|
| $\mathrm{MMD}_{\mathbf{k}}(\mathbb{X}_n,\hat{\mathbb{X}}_m)$ | $O(n^{-1/4})$ | $\tilde{O}(n^{-1/2})$ |
| Time | $O(n^{1/2})$ | $\tilde{O}(n)$ |




## Compress Then Test (CTT)

1. Run KT-Compress to get $\mathbb{X}_n \to \hat{\mathbb{X}}_m$ & $\mathbb{Y}_n \to \hat{\mathbb{Y}}_m$ with $m = 2^{\mathfrak{g}}\sqrt{n}$
2. Use $\mathrm{MMD}^2_{\mathbf{k}}(\hat{\mathbb{X}}_m,\hat{\mathbb{Y}}_m)$ instead of $\mathrm{MMD}^2_{\mathbf{k}}(\mathbb{X}_n,\mathbb{Y}_n)$
3. Compute threshold $t_\alpha$ via *cheap permutations*: Group data into $s \ll \sqrt{n}$ bins, sample $\mathscr{B}$ permutations of $[s]$, and permute the $s$ bins

**CTT runtime:** $\tilde{O}(n) + O(s^2B)$ if $\mathfrak{g} = \log\log n$

**Original test runtime:** $O(n^2B)$

# Compress (the Data and) Then Test

1. Turns quadratic time tests to near-linear time tests
2. Provides up to 200x speed-up (1 hour → 20 sec)
3. Maintains level *and* power provably
4. Works with kernel approximations (Low-rank CTT)
5. Applies for kernel selection (Aggregated CTT)

## CTT guarantees

**A. Exact Type 1 error:**

If $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P},\mathbb{Q}) = 0$, then $\Pr[\Delta(\mathbb{X}_n,\mathbb{Y}_n) = 1] = \alpha$

**B. Power:**

If $\mathrm{MMD}_{\mathbf{k}}(\mathbb{P},\mathbb{Q}) \ge$ Separation$(\beta)$, then $\Pr[\Delta(\mathbb{X}_n,\mathbb{Y}_n) = 1] \ge 1-\beta$

| Test name | MMD separation | Runtime |
|---|---|---|
| CTT (ours, Thm. 1) | $\frac{R_{\mathbf{k},\mathbf{k}}(\mathbb{P},n,\delta,\mathfrak{g})}{2^{\mathfrak{g}}\sqrt{n}} + n^{-\frac{1}{2}}$ | $4^{\mathfrak{g}} n\log n$ |
| Complete MMD (Gretton et al., 2012a) | $n^{-\frac{1}{2}}$ | $n^2$ |
| Block MMD (Zaremba et al., 2013) | $(Bn)^{-\frac{1}{4}}$ | $Bn$ |
| Incomplete MMD (Yamada et al., 2019) | $\ell^{-\frac{1}{4}}$ | $\ell$ |

| Tails of $\mathbb{P}$ on $\mathbb{R}^d$ | Choice of $\mathbf{k}'$ | $R_{\mathbf{k},\mathbf{k}}(\mathbb{P},n,\delta,\mathfrak{g})$ |
|---|---|---|
| Compact | Compact $\mathbf{k}_{\mathrm{rt}}$ | $(\log\frac{n}{\delta})^2$ |
| Subexp | Analytic $\mathbf{k}$ | $(\log\frac{n}{\delta})^{\frac{3d+5}{2}}$ |
| Subexp | Subexp $\mathbf{k}_{\mathrm{rt}}$ | $c_{m,\delta}(\log\frac{n}{\delta})^{\frac{d+5}{2}}$ |
| $\rho$-Heavy-tail | $\rho$-Heavy-tail $\mathbf{k}_{\mathrm{rt}}$ | $(\frac{n}{\delta})^{\frac{d}{2\rho}}(\log\frac{n}{\delta})^{\frac{d+5}{2}}$ |

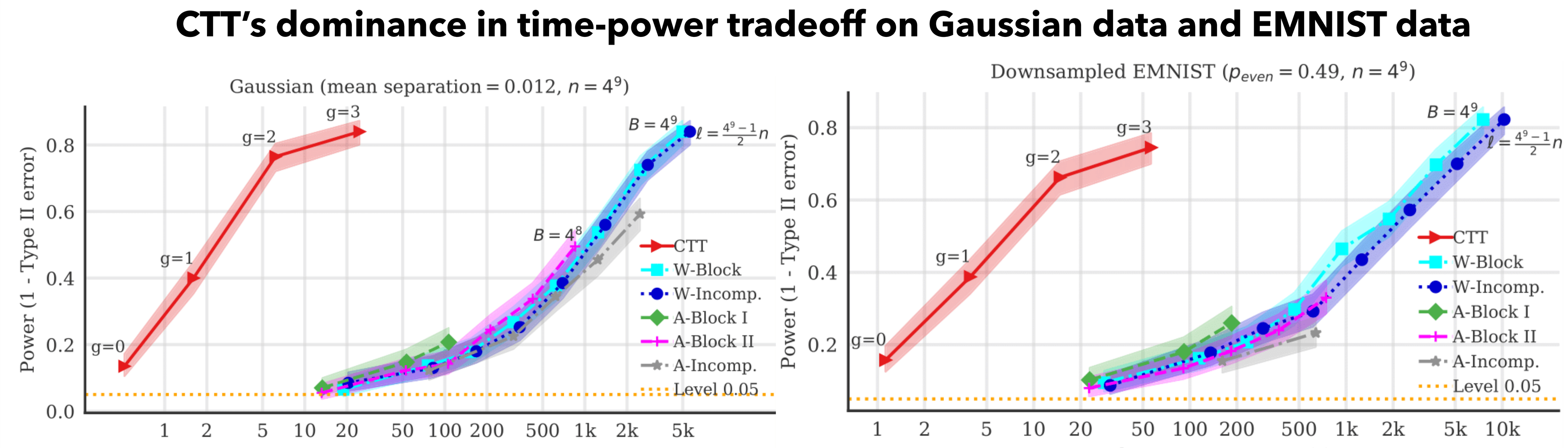
$B$ = Number of blocks used in Block MMD test

$\ell$ = Number of ordered index pairs in Incomplete MMD test

$\delta$ = Failure probability for CTT guarantees

$\mathbf{k}'$ = auxiliary kernel used by KT-Compress & $\mathbf{k}(x,y) = \int \mathbf{k}_{\mathrm{rt}}(x,z)\mathbf{k}_{\mathrm{rt}}(z,y)dz$

**CTT's dominance in time-power tradeoff on Gaussian and EMNIST data**

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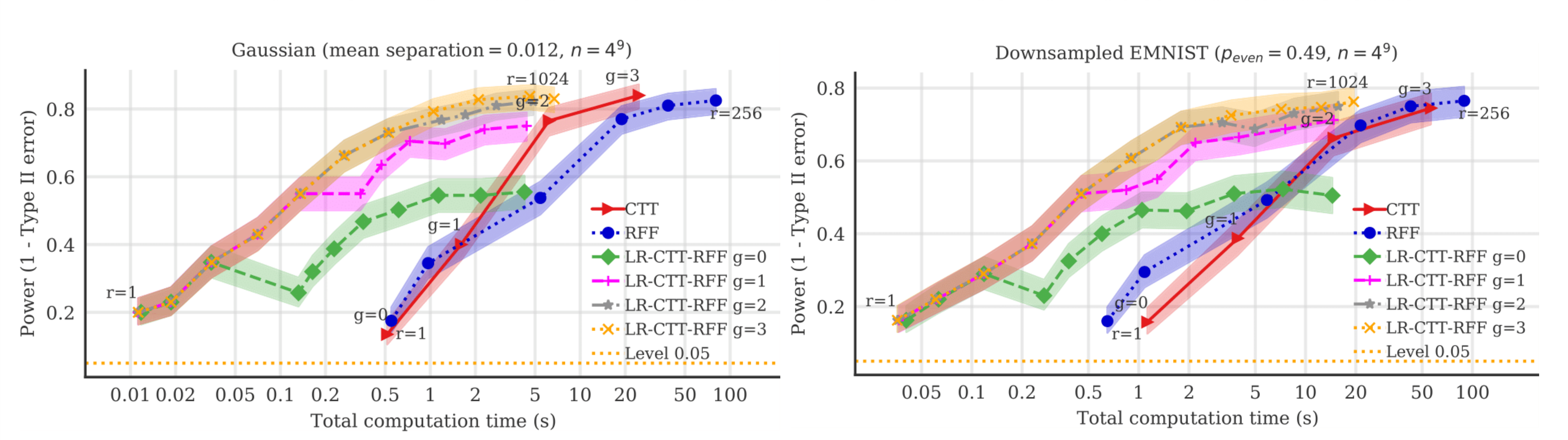


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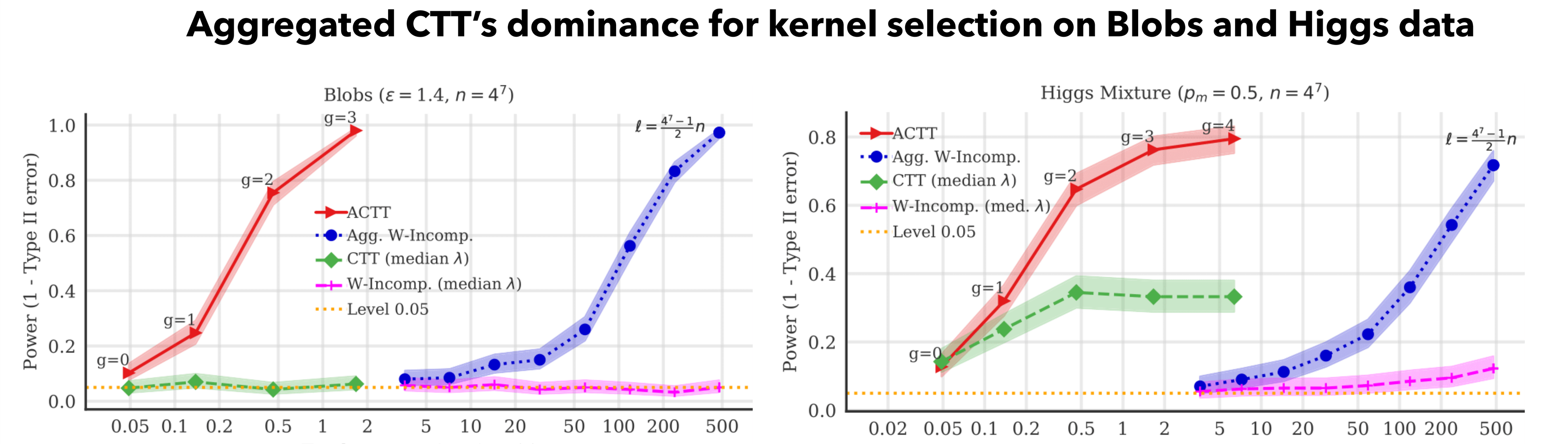

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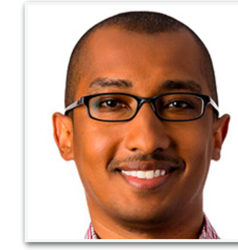
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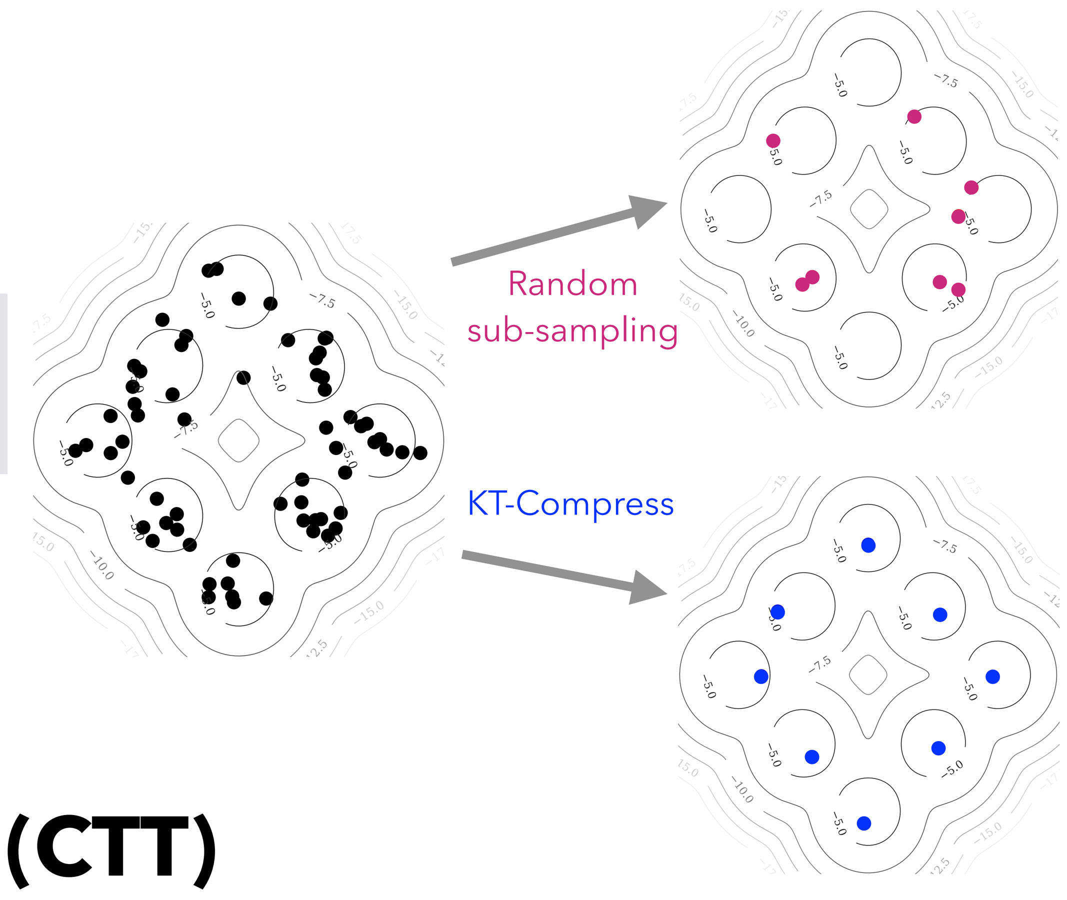
| Time | $O(m)$ | $\tilde{O}(m^2)$ |

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**Total runtime**: $\tilde{O}(4^{\mathfrak{g}}n) = \tilde{O}(n)$ if $\mathfrak{g} = \log\log n$

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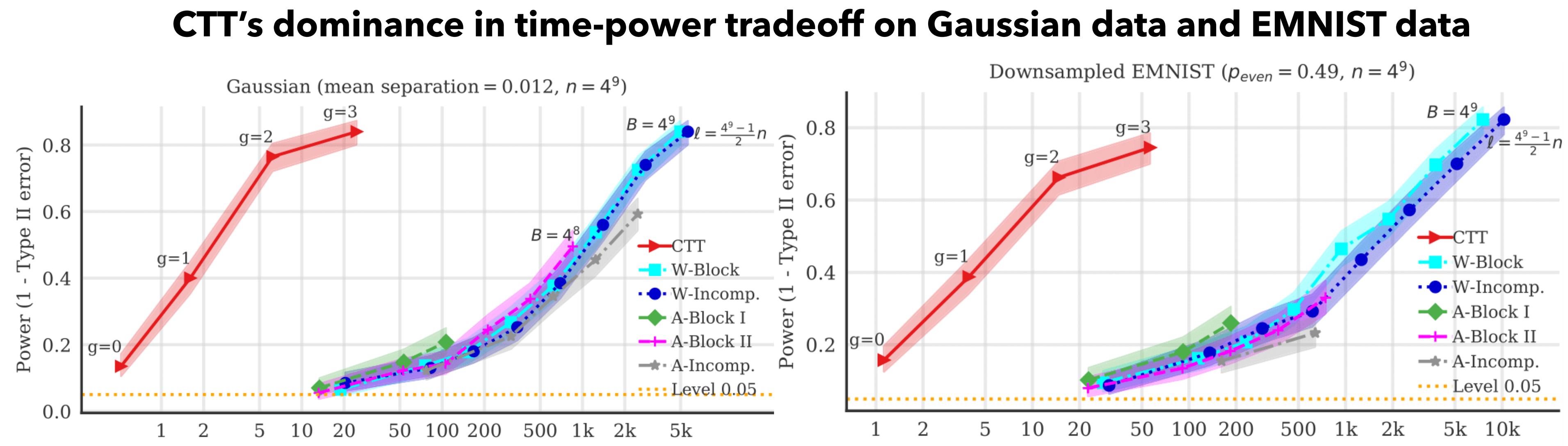


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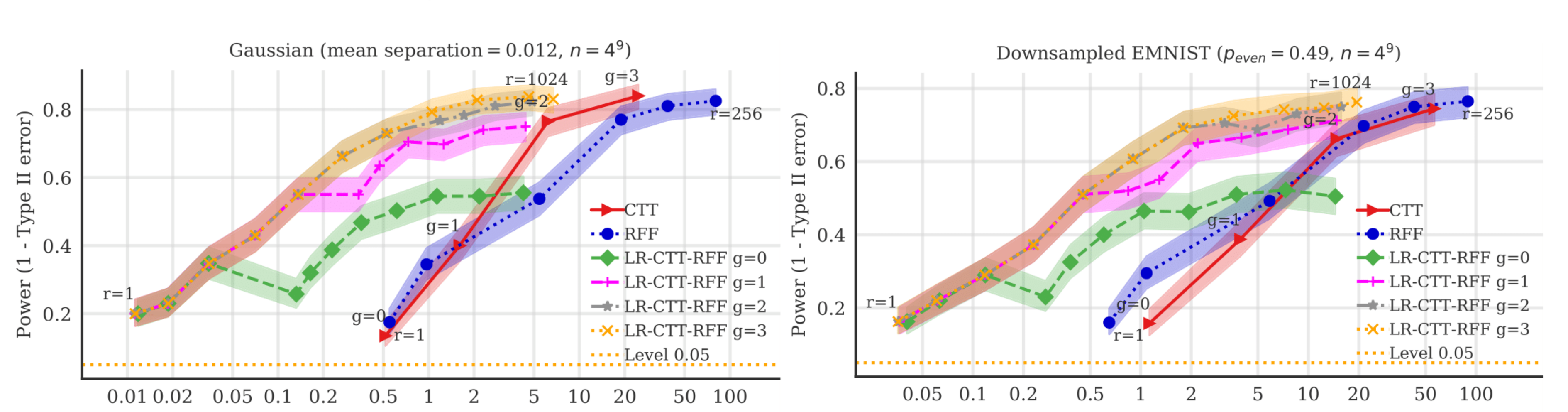


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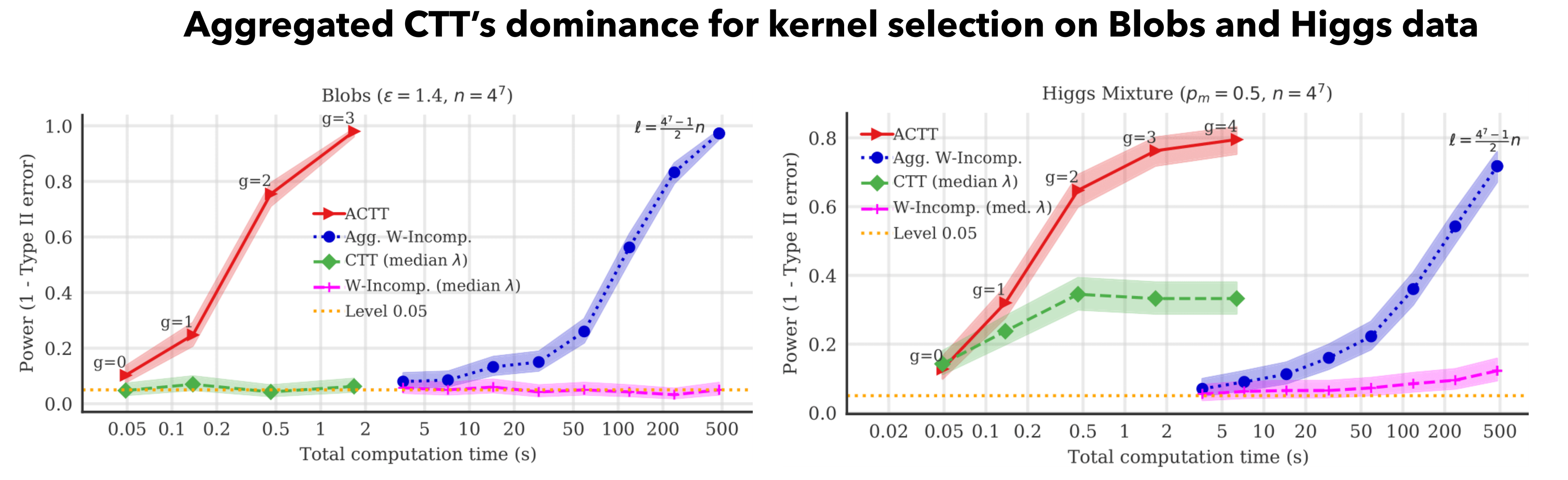


1. Compress $\mathbb{X}_m, \mathbb{Y}_m$ to $\hat{\mathbb{X}}_m, \hat{\mathbb{Y}}_m$ each of size $2^{\mathfrak{g}}\sqrt{m}$ using KT-Compress: $\tilde{O}(4^{\mathfrak{g}}m)$ time
2. Use $\mathrm{MMD}_{\mathbf{k}}^2(\hat{\mathbb{X}}_m, \hat{\mathbb{Y}}_m)$ as the test statistic: $\tilde{O}(4^{\mathfrak{g}}m)$ time

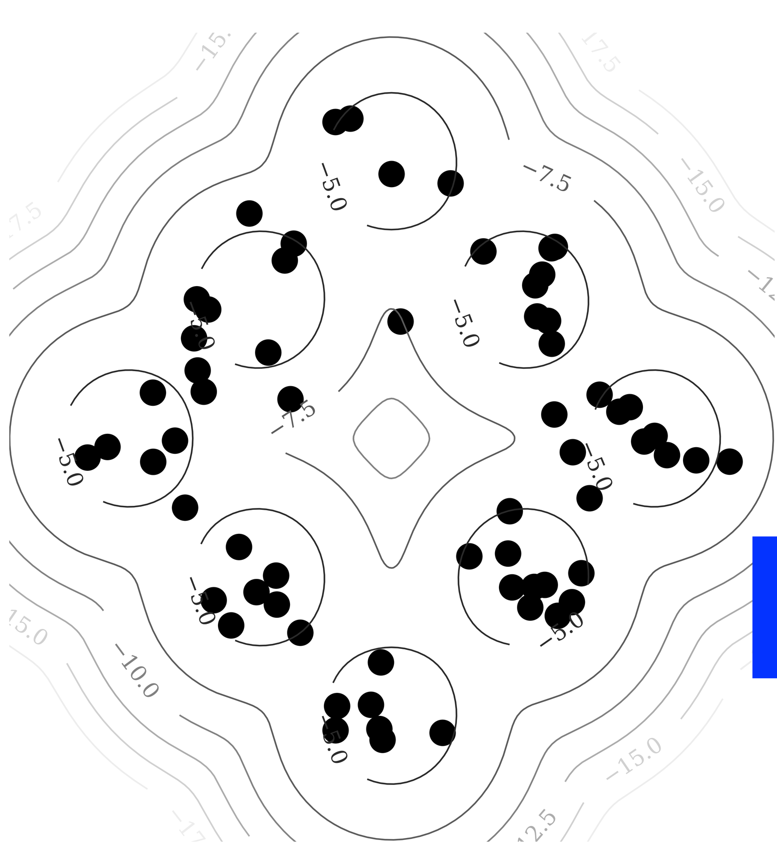
Total runtime: $\tilde{O}(m)$ if $\mathfrak{g} = \log\log m$

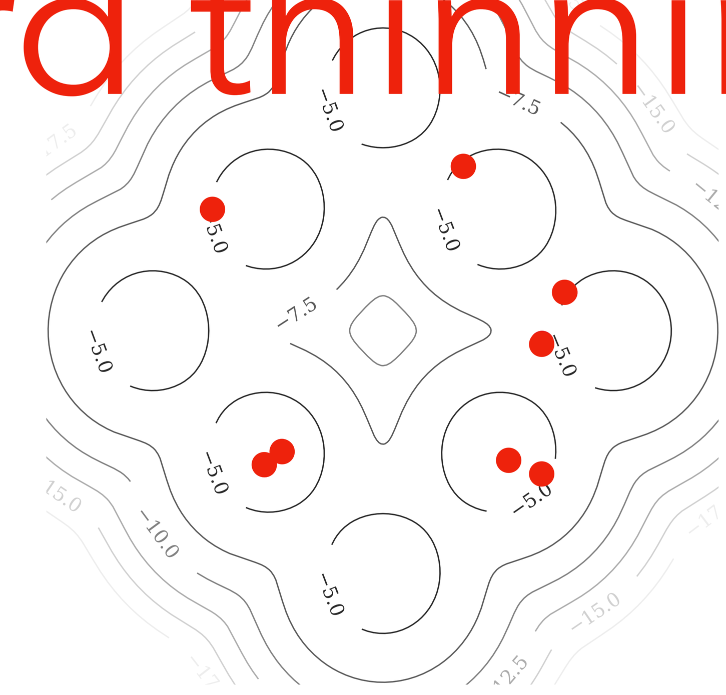
# Visual comparison on $\mathbb{P}^\star = 8$

iid input points

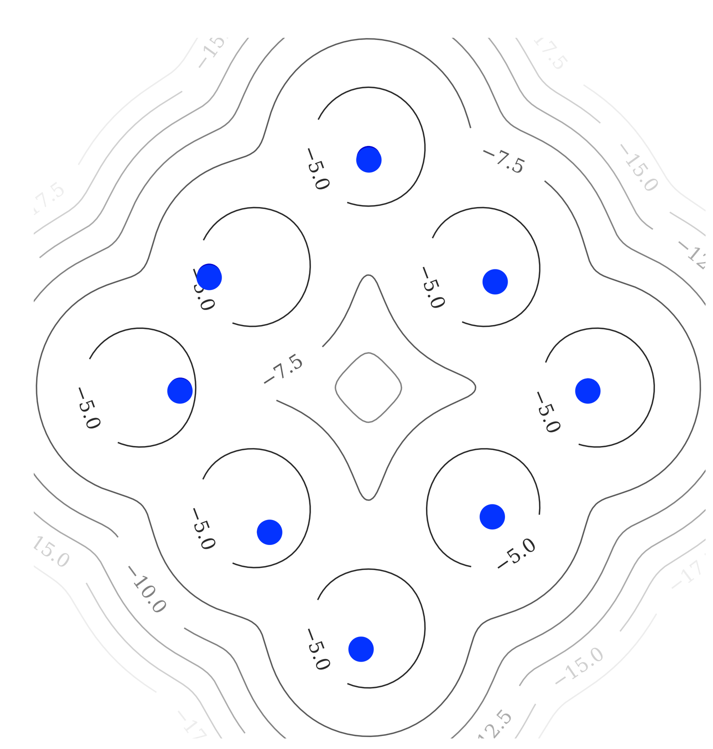
8 output points

Standard thinning





Kernel thinning



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