Are these datasets the same?
Two-sample testing for data scientists

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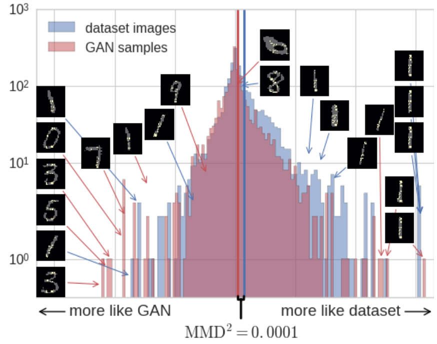
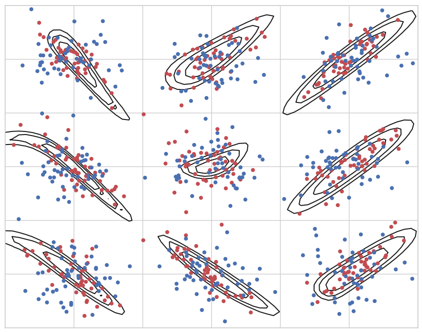
[ICLR-17]



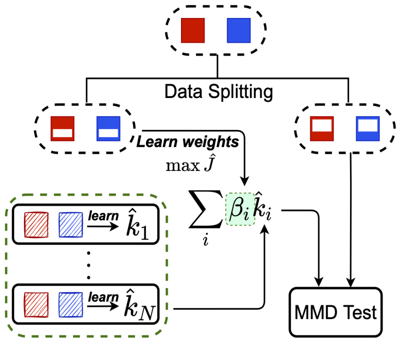
Hsiao-Yu (Fish) Tung
Heiko Strathmann
Soumyajit De
Aaditya Ramdas
Alex Smola
Arthur Gretton

[ICML-20]



Feng Liu
Wenkai Xu
Jie Lu
Guangquan Zhang
Arthur Gretton

[NeurIPS-21]



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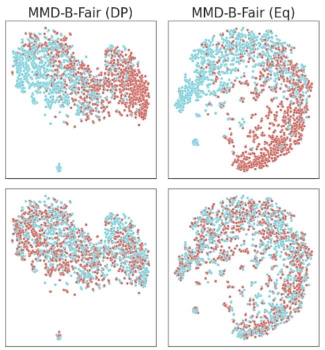
[AISTATS-23]



Namrata Deka

Pacific Conference on Artificial Intelligence – April 2, 2023

Data drift

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  - Train on i.i.d. samples from some distribution, $X_i \sim \mathbb{P}$
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- Given samples from two unknown distributions

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- Independence testing: is $P(X, Y) = P(X)P(Y)$?

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- Reject null hypothesis H_0 if test statistic $\hat{T}(X, Y) > c_\alpha$

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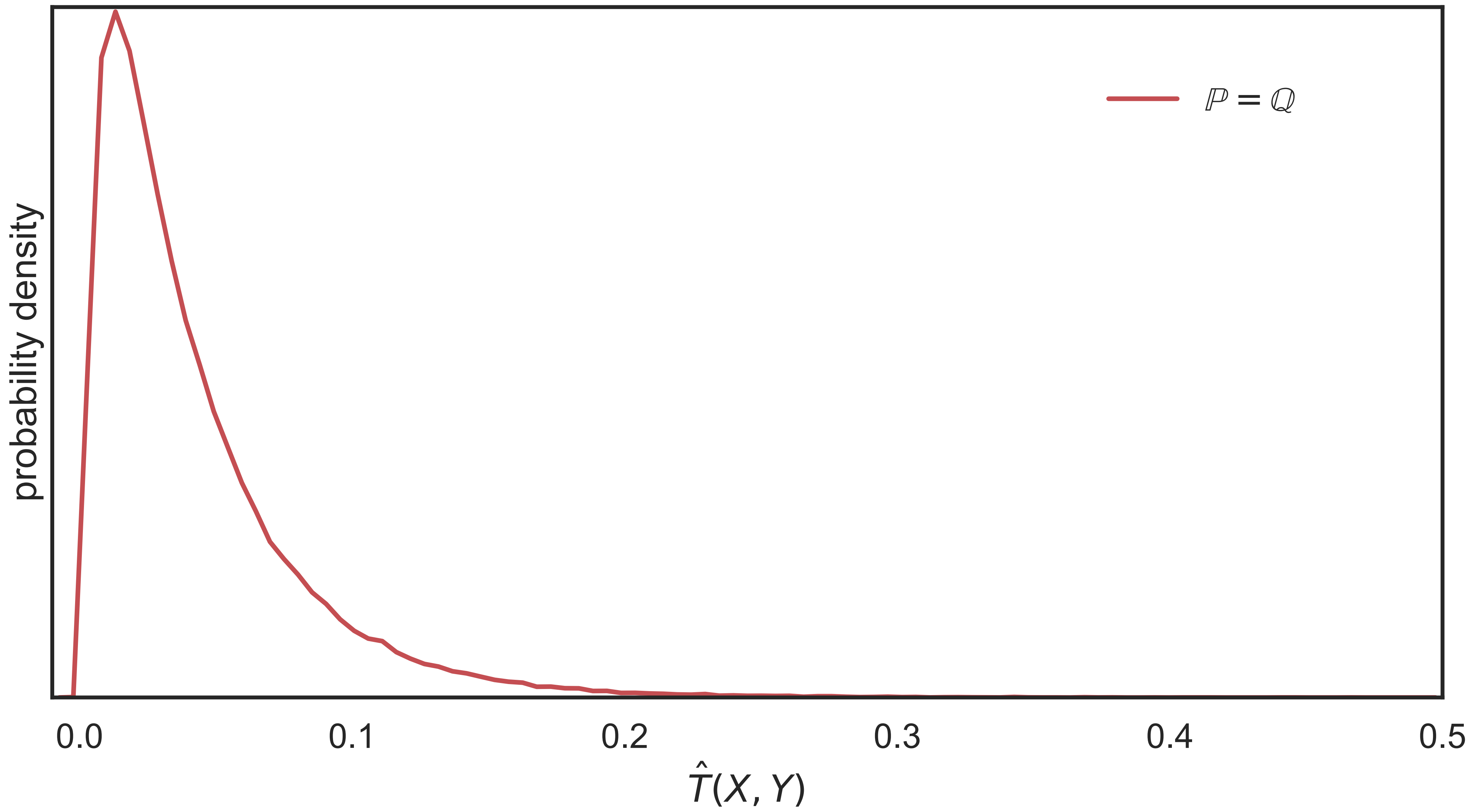

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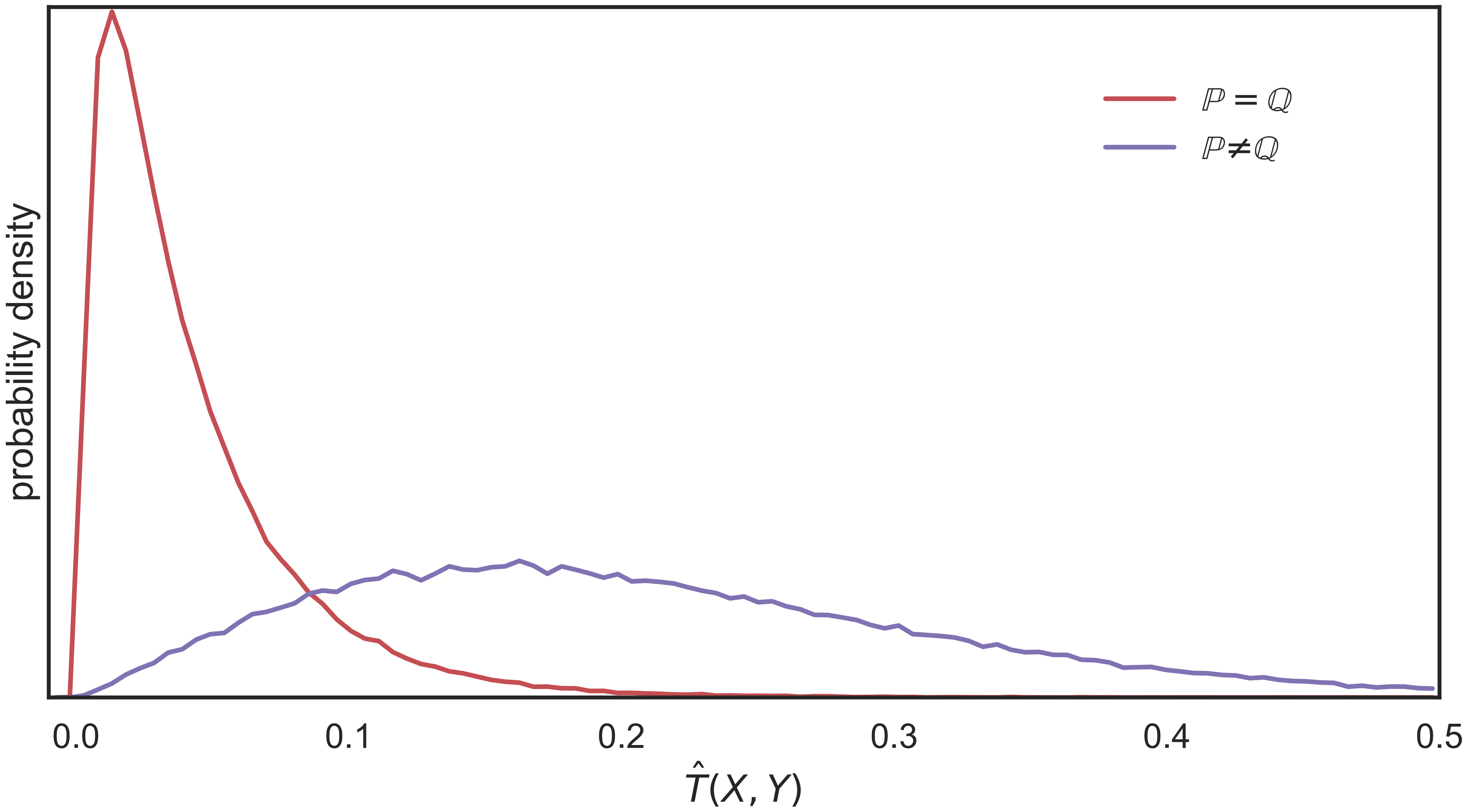

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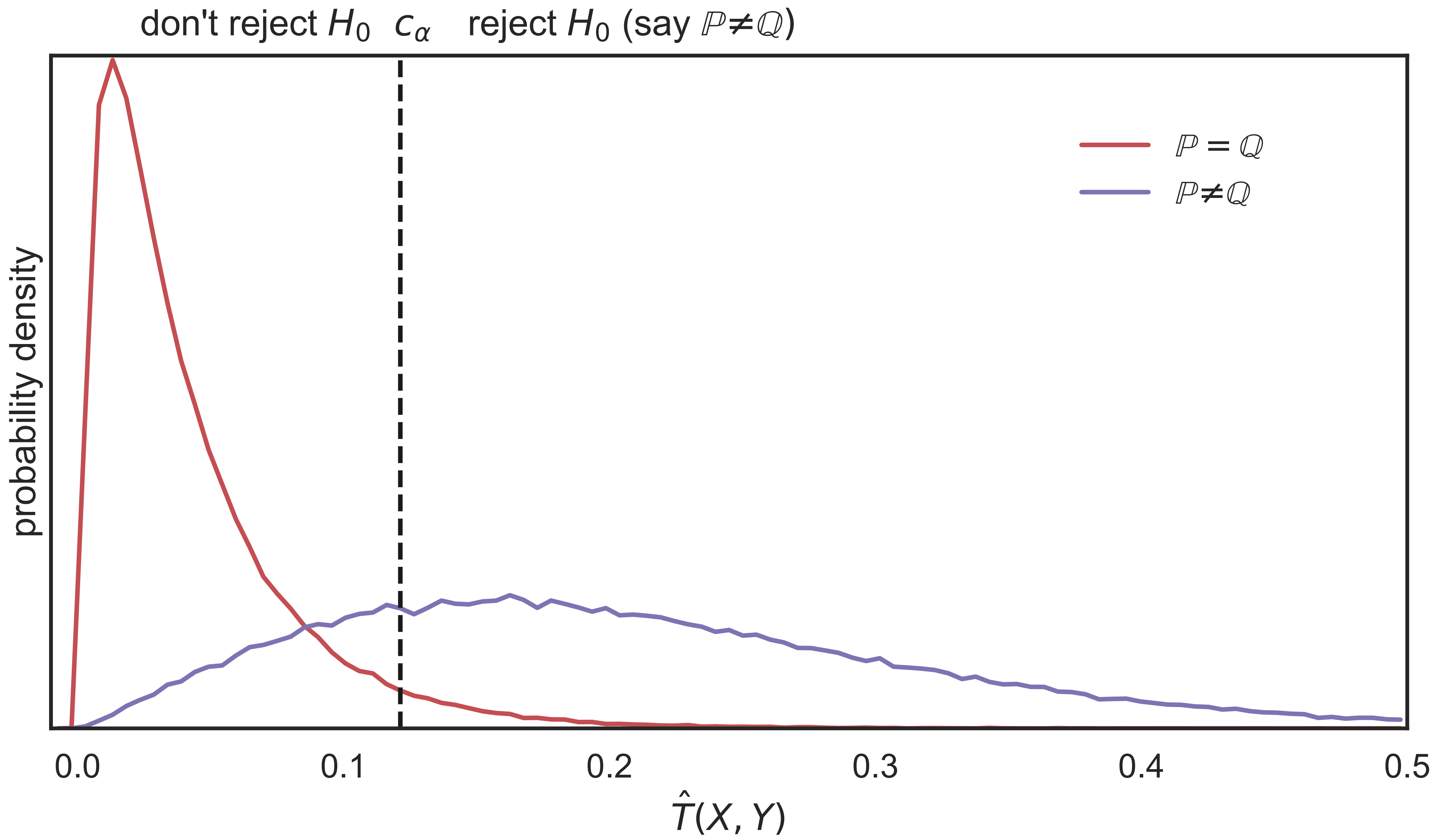

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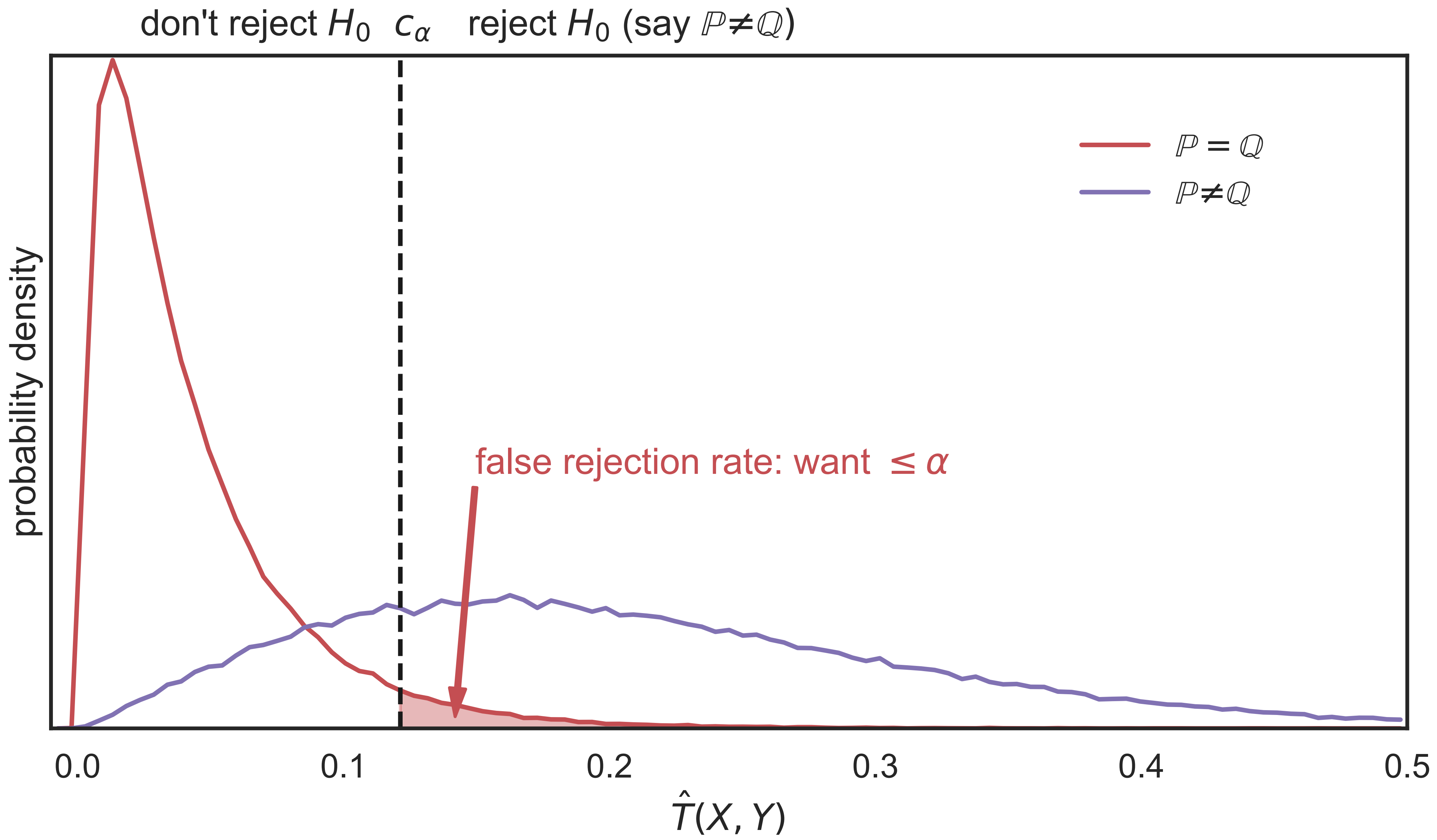

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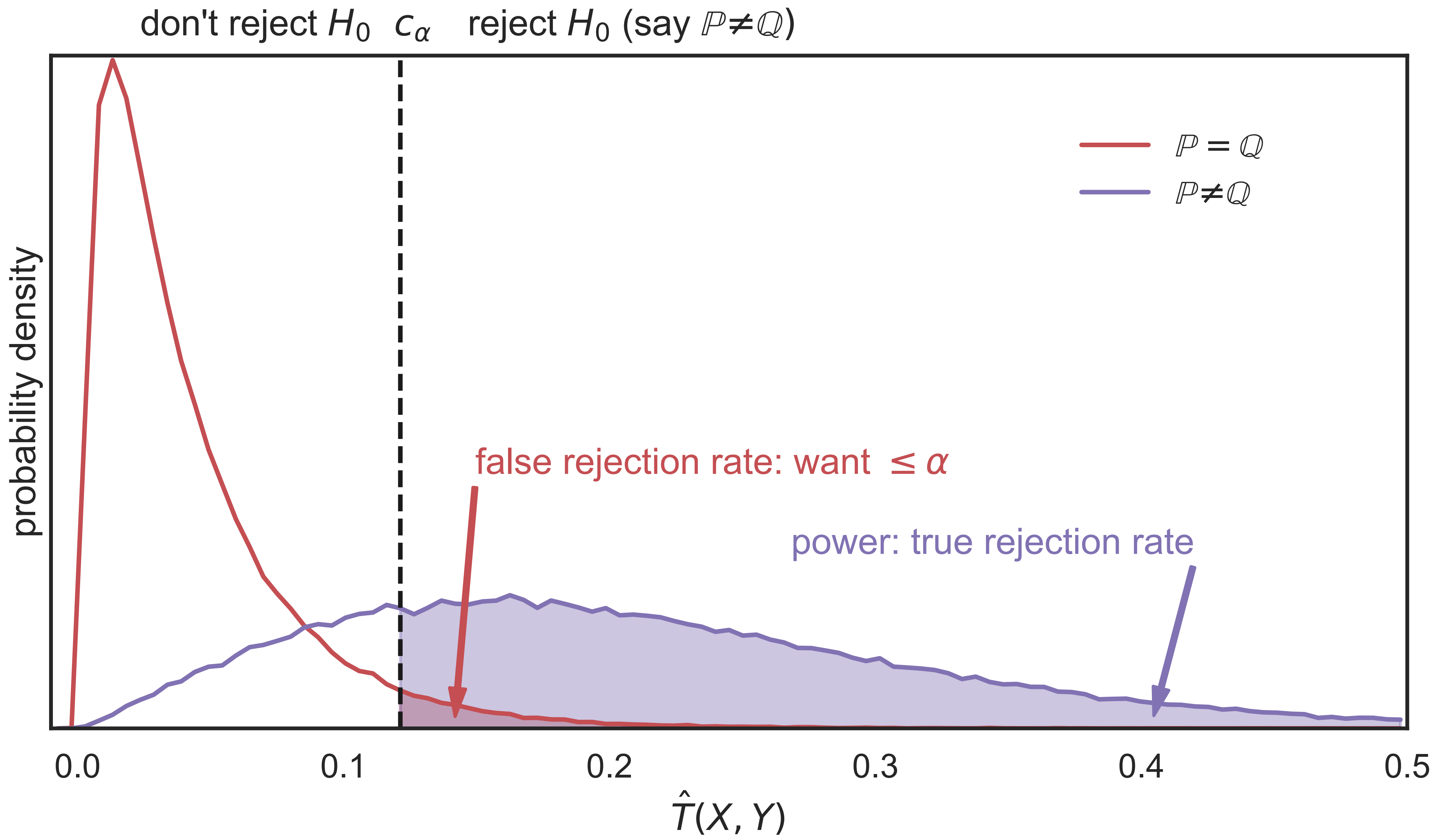

Permutation testing to find c_α

Need $\Pr_{H_0}\left(\hat{T}(X, Y) > c_\alpha\right) \le \alpha$

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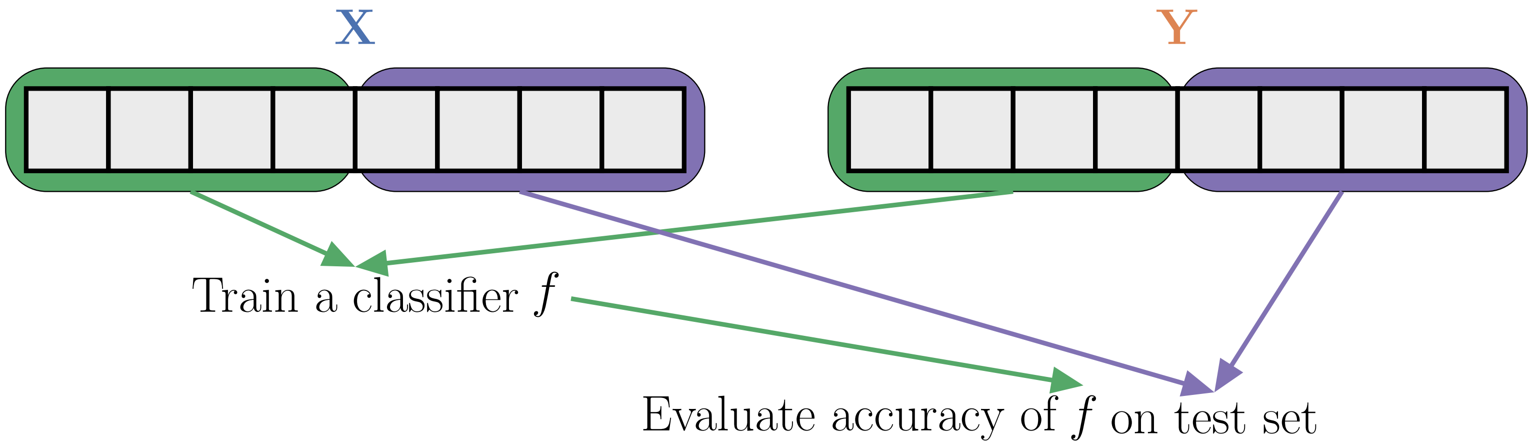
Classifier two-sample tests

- We need a $\hat{T}(X, Y)$ that's large if $\mathbb{P} \neq \mathbb{Q}$, small if $\mathbb{P} = \mathbb{Q}$



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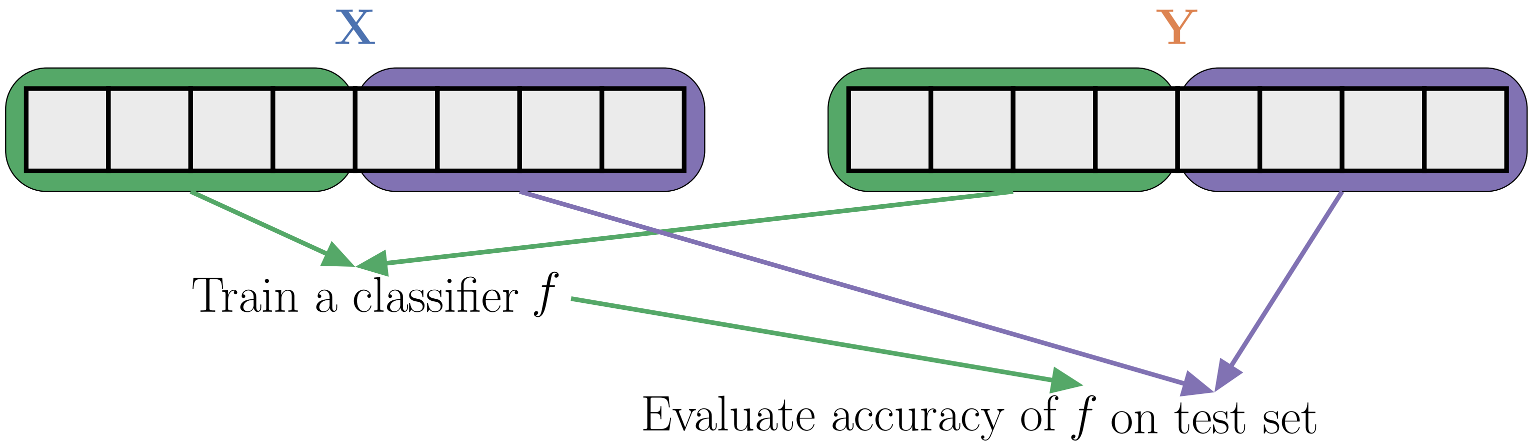

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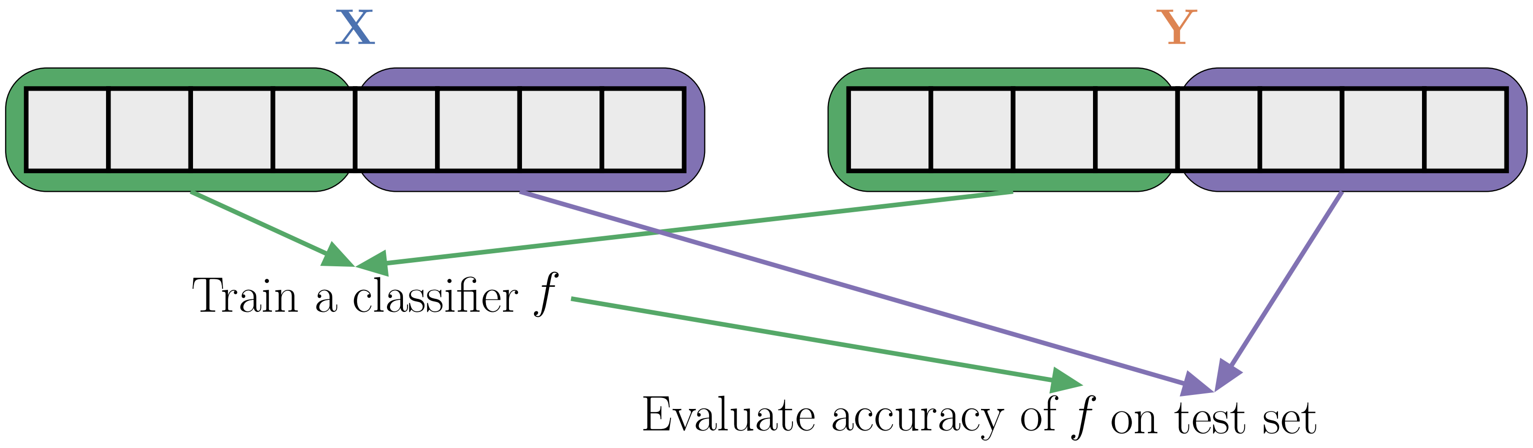

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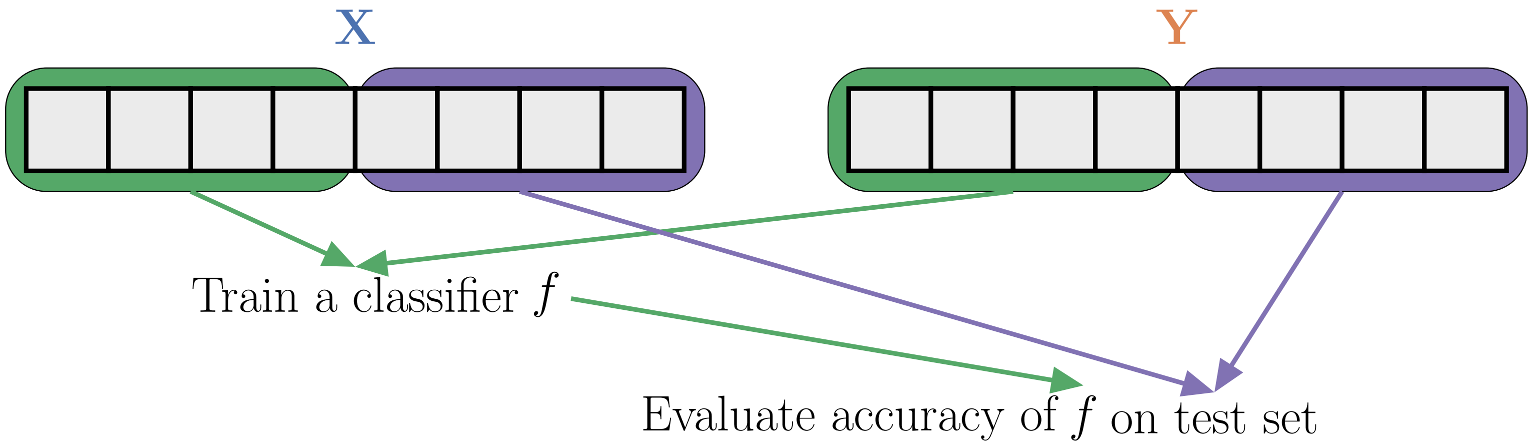

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  - If $\mathbb{P} = \mathbb{Q}$, $\hat{T} \to$ normal distribution (but permuting on test set is better)

A more general framework

- C2ST-L: $\hat{T}(X, Y) = \operatorname*{mean}_{x \in X_{test}}[f(x)] - \operatorname*{mean}_{y \in Y_{test}}[f(y)]$
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- What if we use more general *features* of the data?

$$\hat{T}(X, Y) = \left\| \operatorname*{mean}_{x \in X_{test}}[\varphi(x)] - \operatorname*{mean}_{y \in Y_{test}}[\varphi(y)] \right\|$$

Difference between mean embeddings

$$\hat{T}(X, Y)^2 = \left\| \underset{x \in X_{test}}{\text{mean}}[\varphi(x)] - \underset{y \in Y_{test}}{\text{mean}}[\varphi(y)] \right\|^2$$

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	1.0	0.2	0.6
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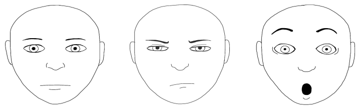

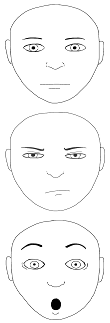

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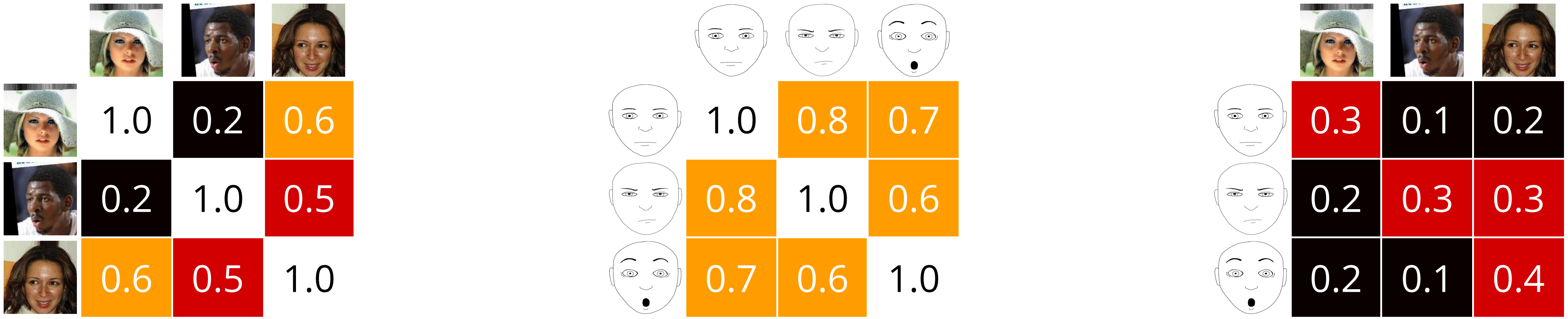

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K_{XY}

	0.3	0.1	0.2
	0.2	0.3	0.3
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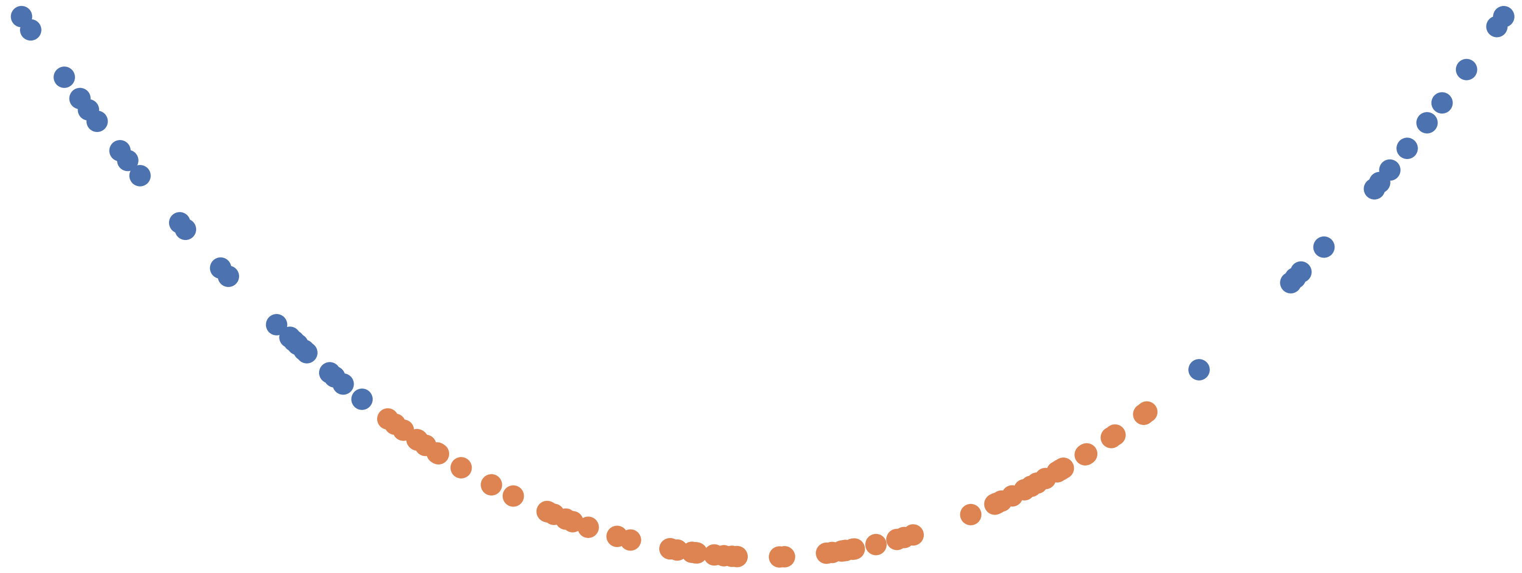

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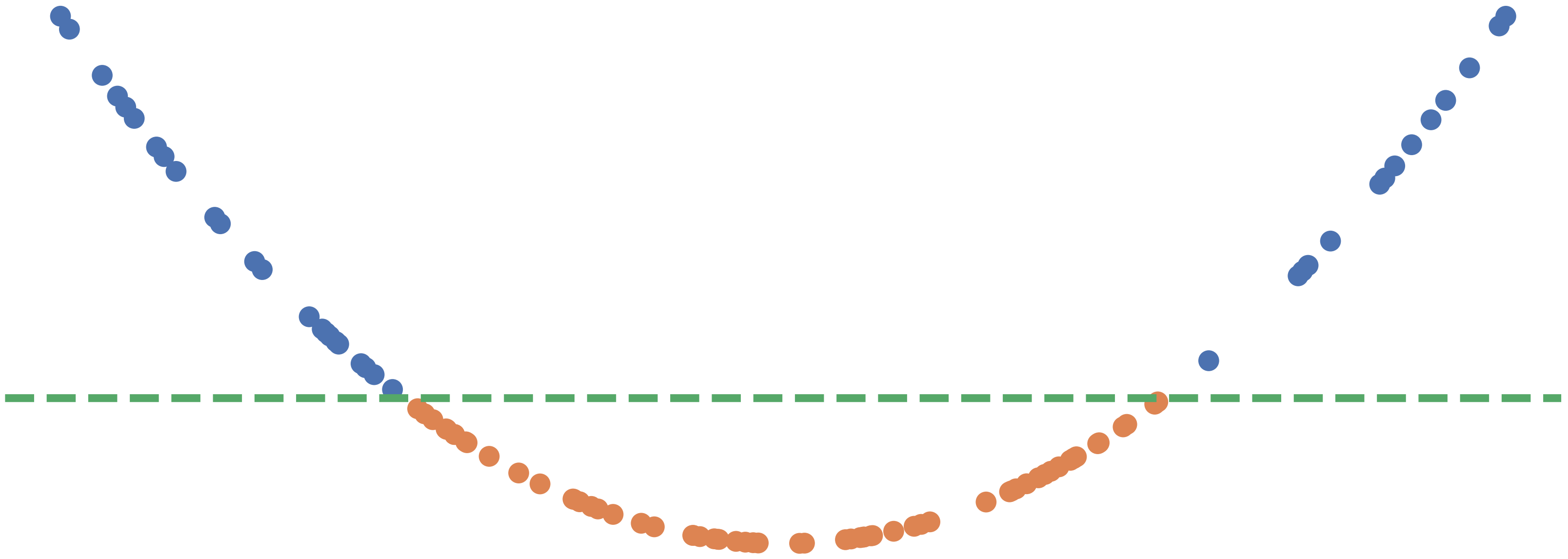

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- Example: Gaussian RBF

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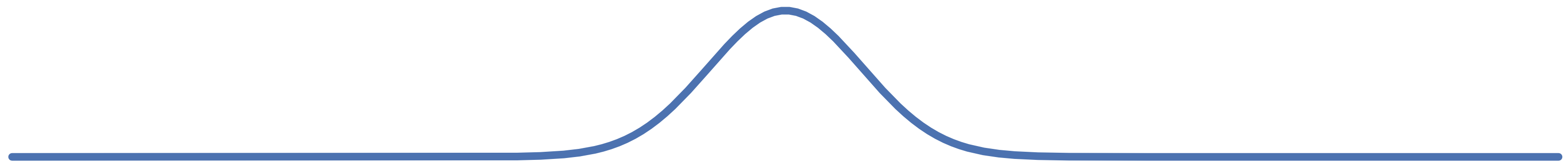

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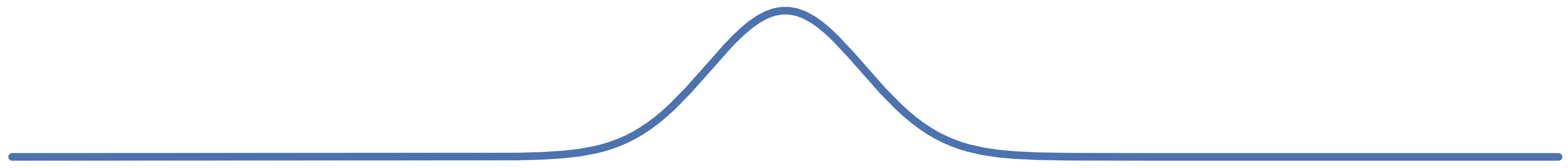

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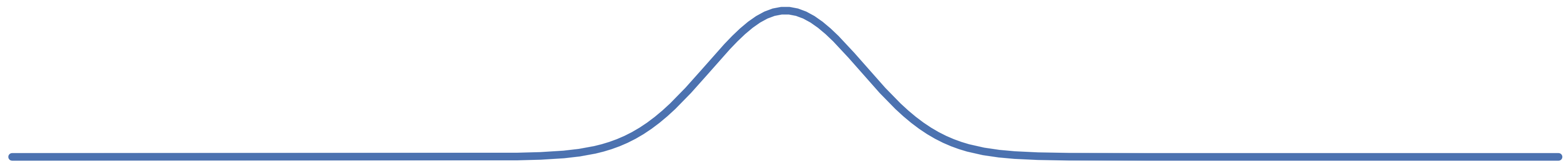

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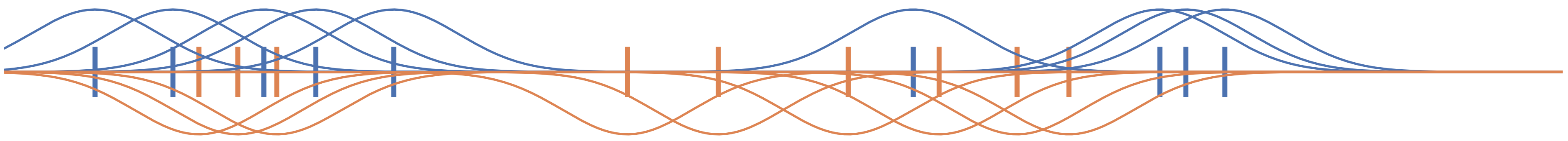

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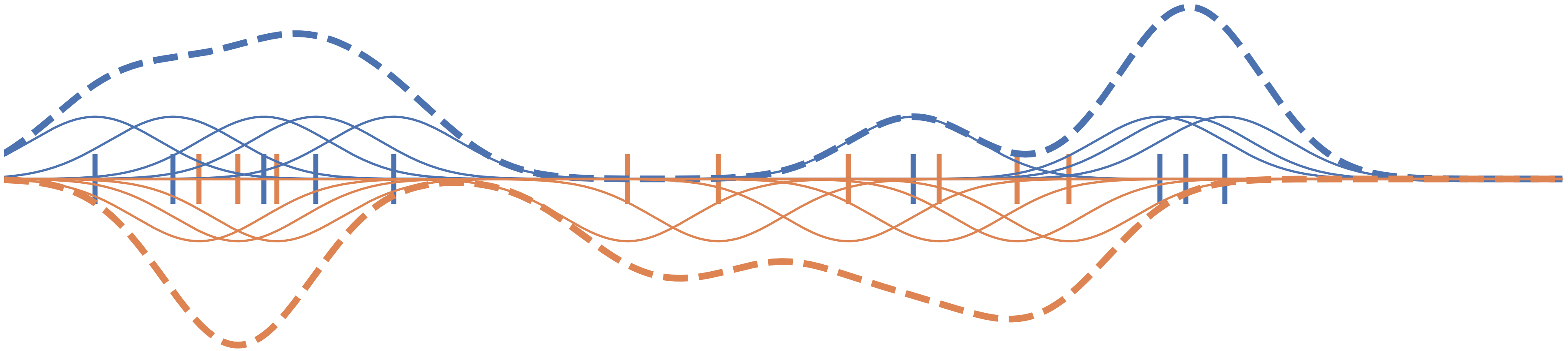

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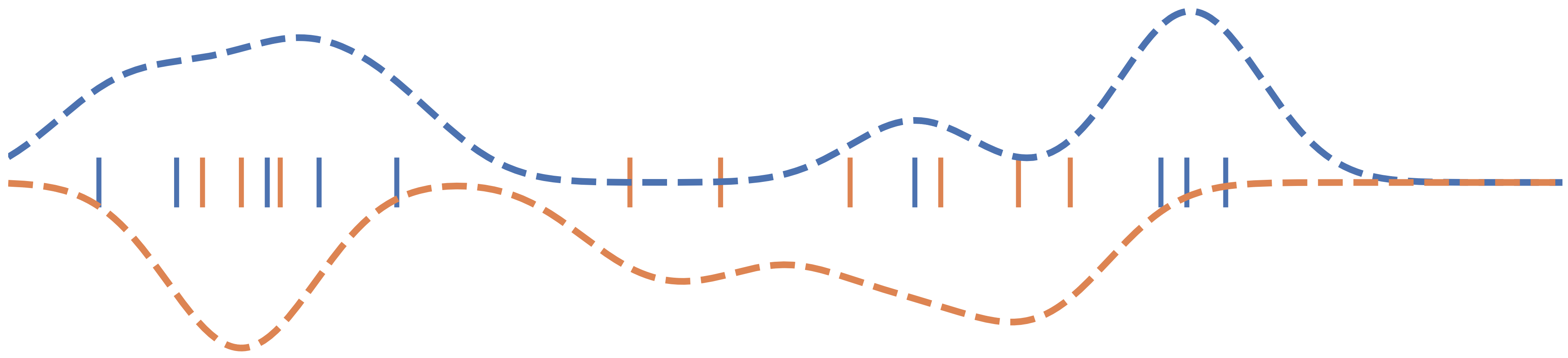

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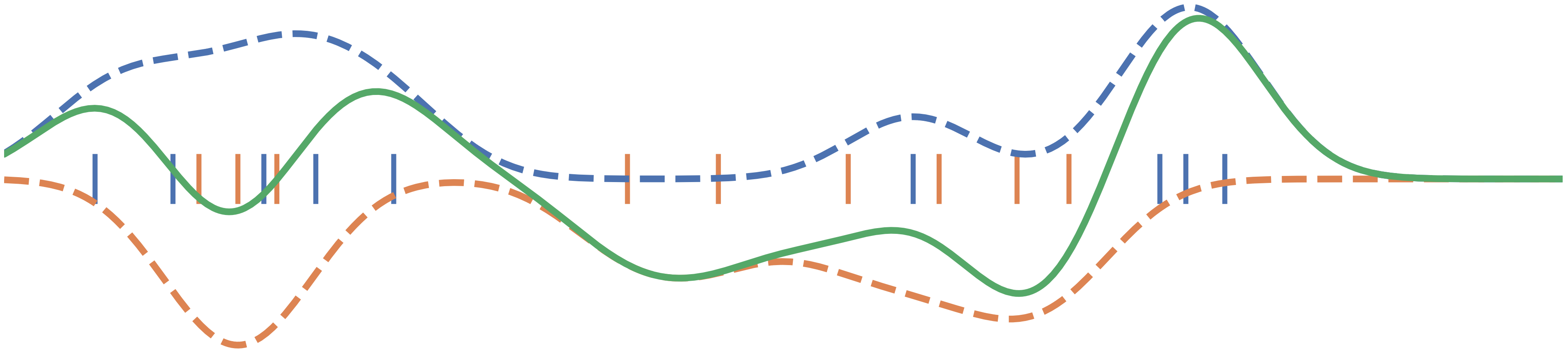

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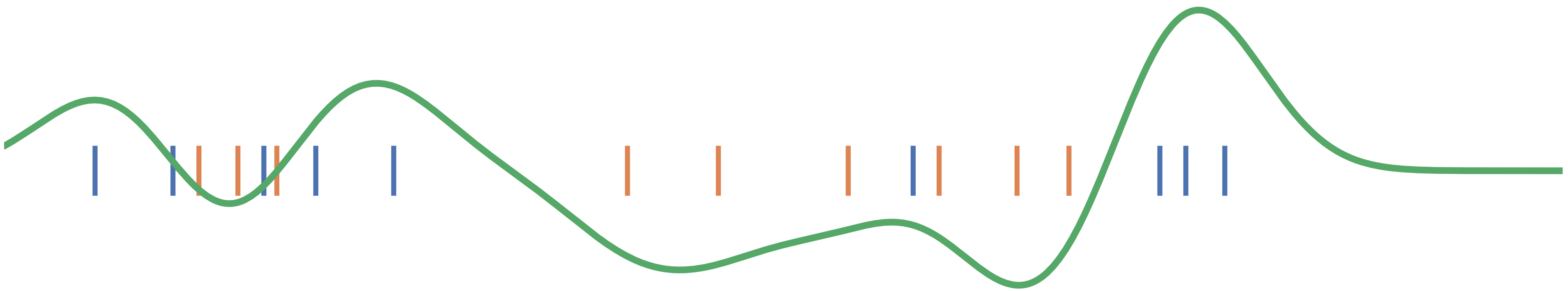

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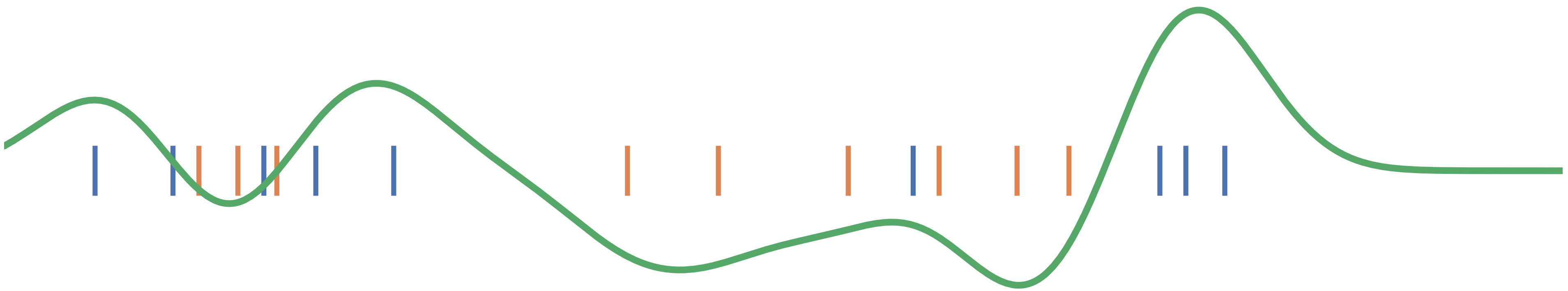

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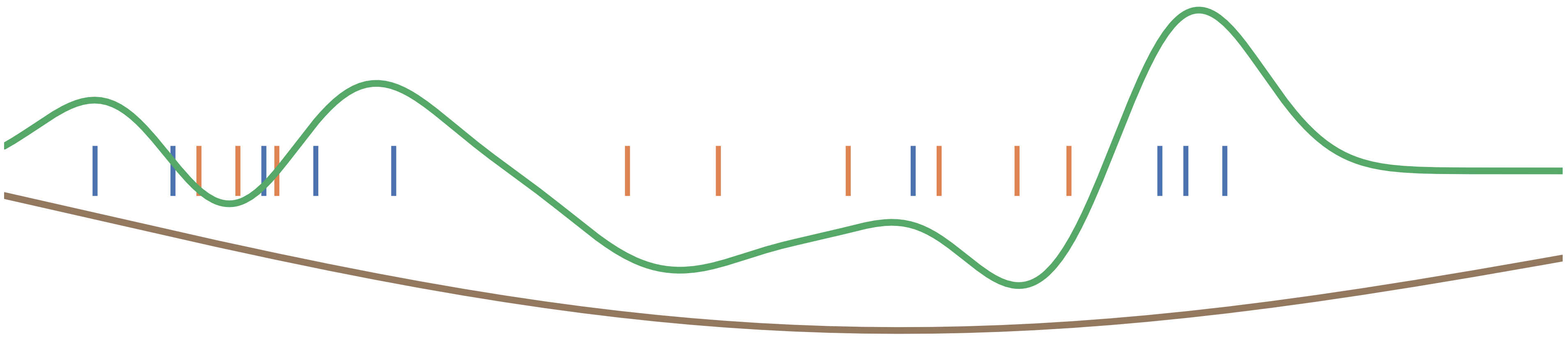

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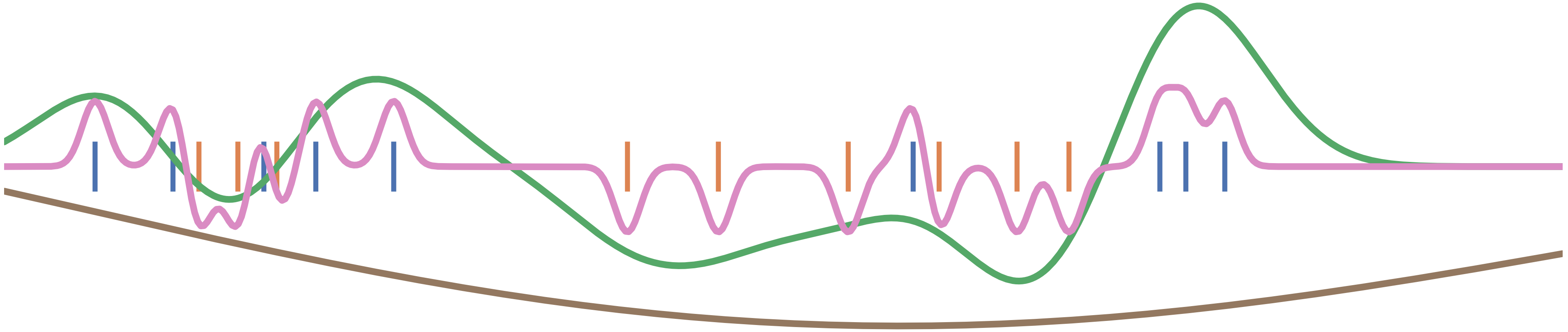

MMD-based tests

- If k is *characteristic*, $\mathrm{MMD}(\mathbb{P}, \mathbb{Q}) = 0$ iff $\mathbb{P} = \mathbb{Q}$
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- Need enormous n if the kernel is bad for this problem!

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  - $\kappa(u, v) = u \cdot v$ gives MMD as $\|\mathbb{E}\,\phi(x) - \mathbb{E}\,\phi(y)\|$

Optimizing power of MMD tests

- Asymptotics of $\widehat{\mathrm{MMD}}^2$ give us immediately that

$$\Pr_{H_1}\left(n\widehat{\mathrm{MMD}}^2 > c_\alpha\right) \approx \Phi\left(\frac{\sqrt{n}\,\mathrm{MMD}^2}{\sigma_{H_1}} - \frac{c_\alpha}{\sqrt{n}\sigma_{H_1}}\right)$$

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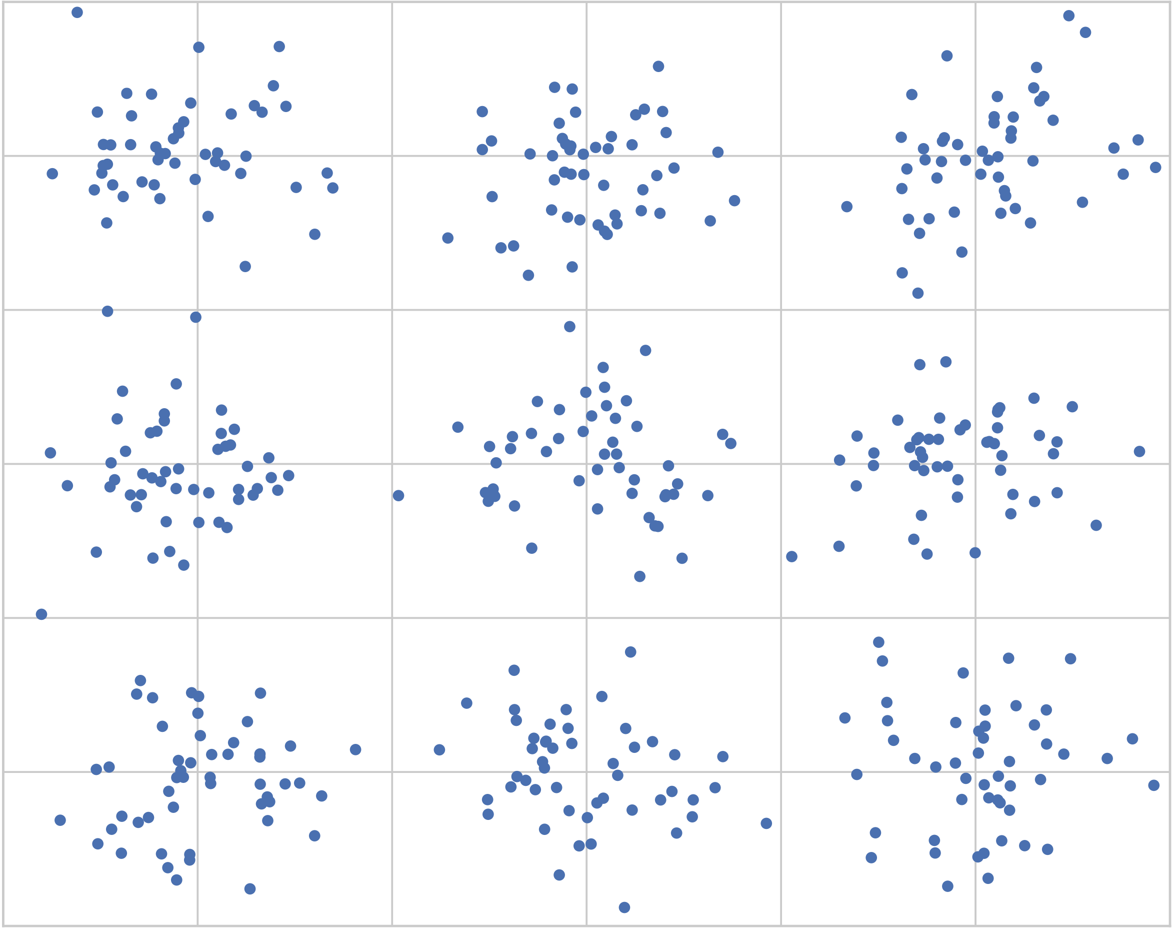
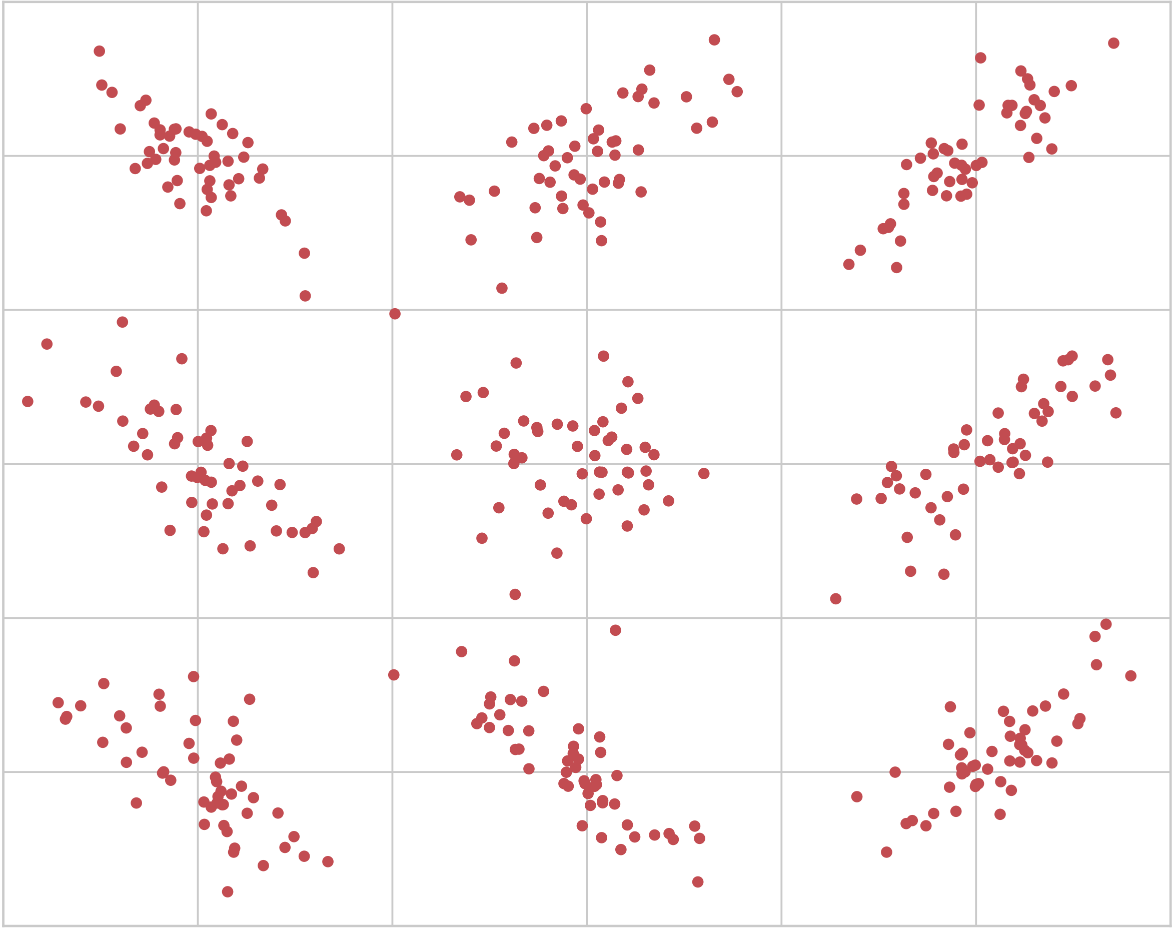
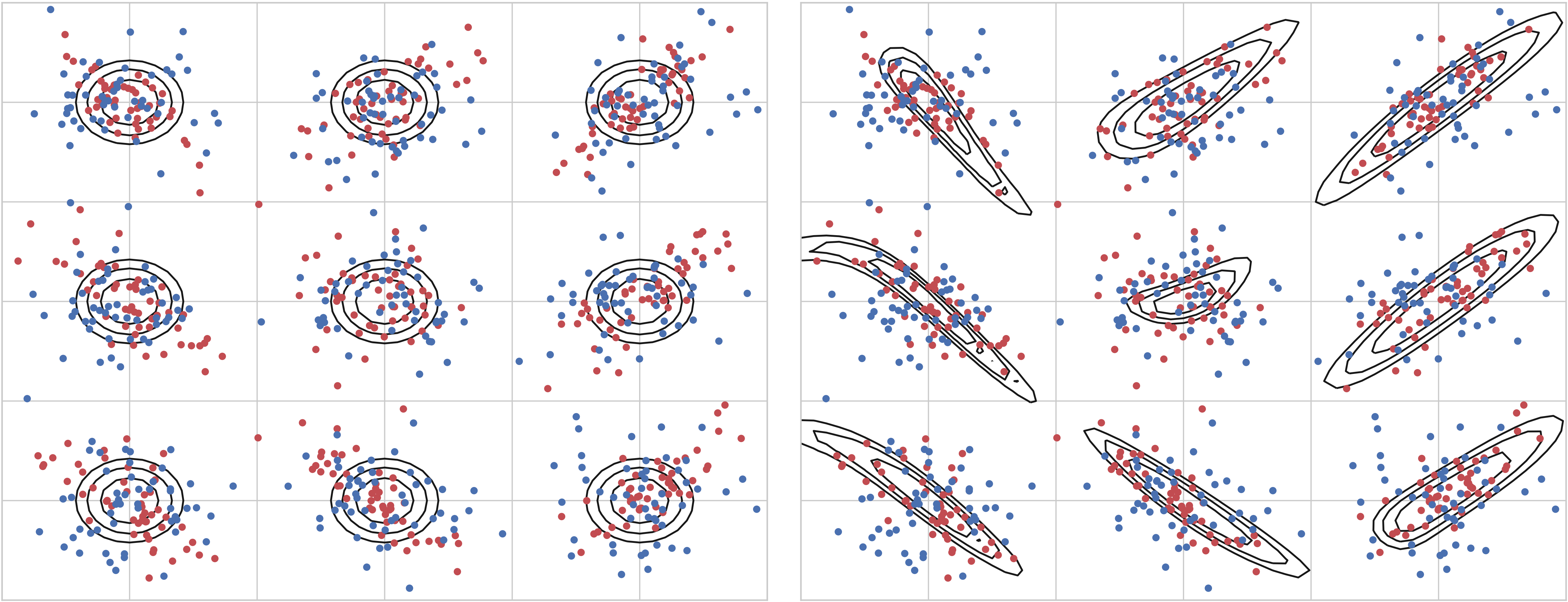
- Can show uniform $\mathcal{O}_P(n^{-\frac{1}{3}})$ convergence of estimator

Blobs dataset

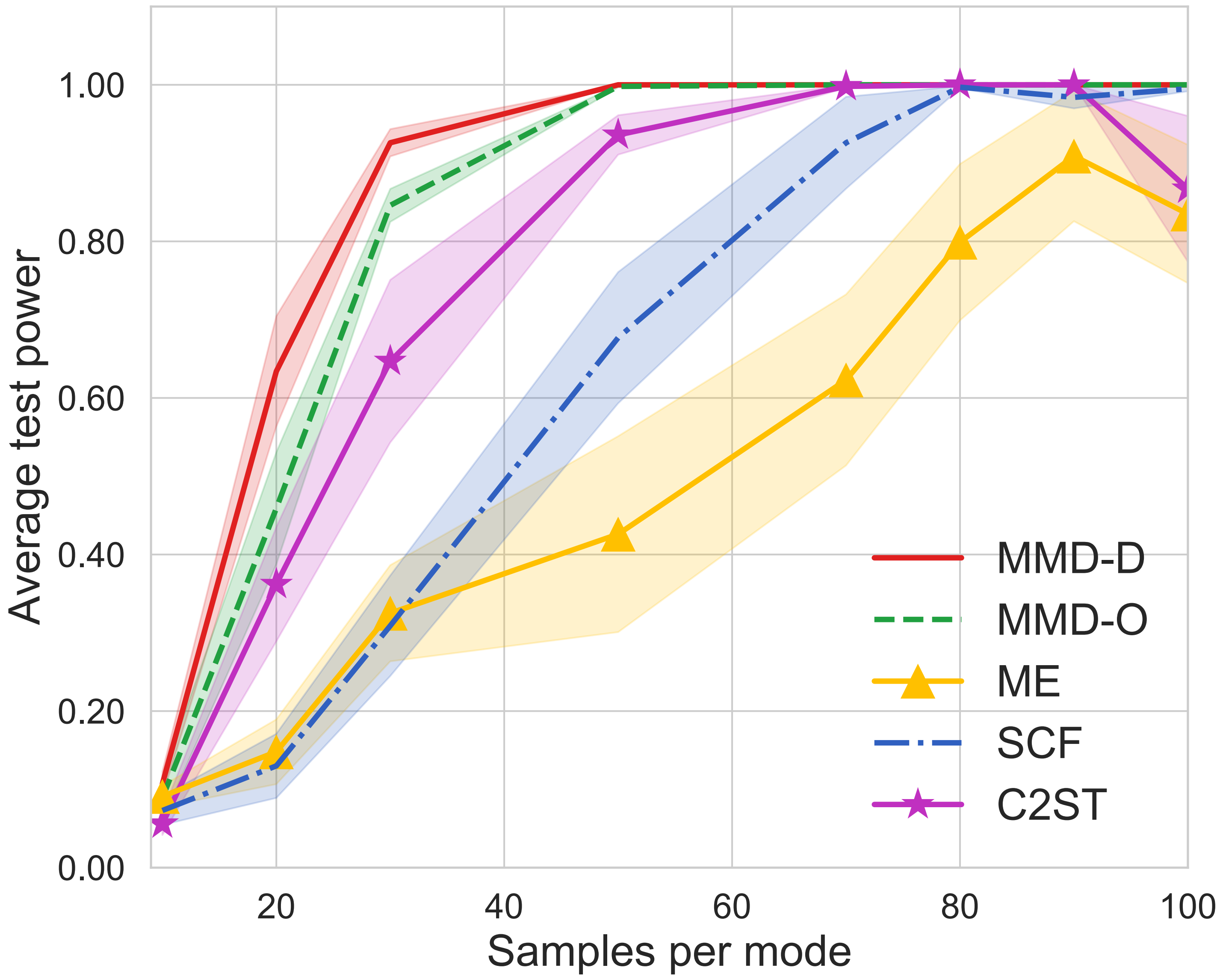




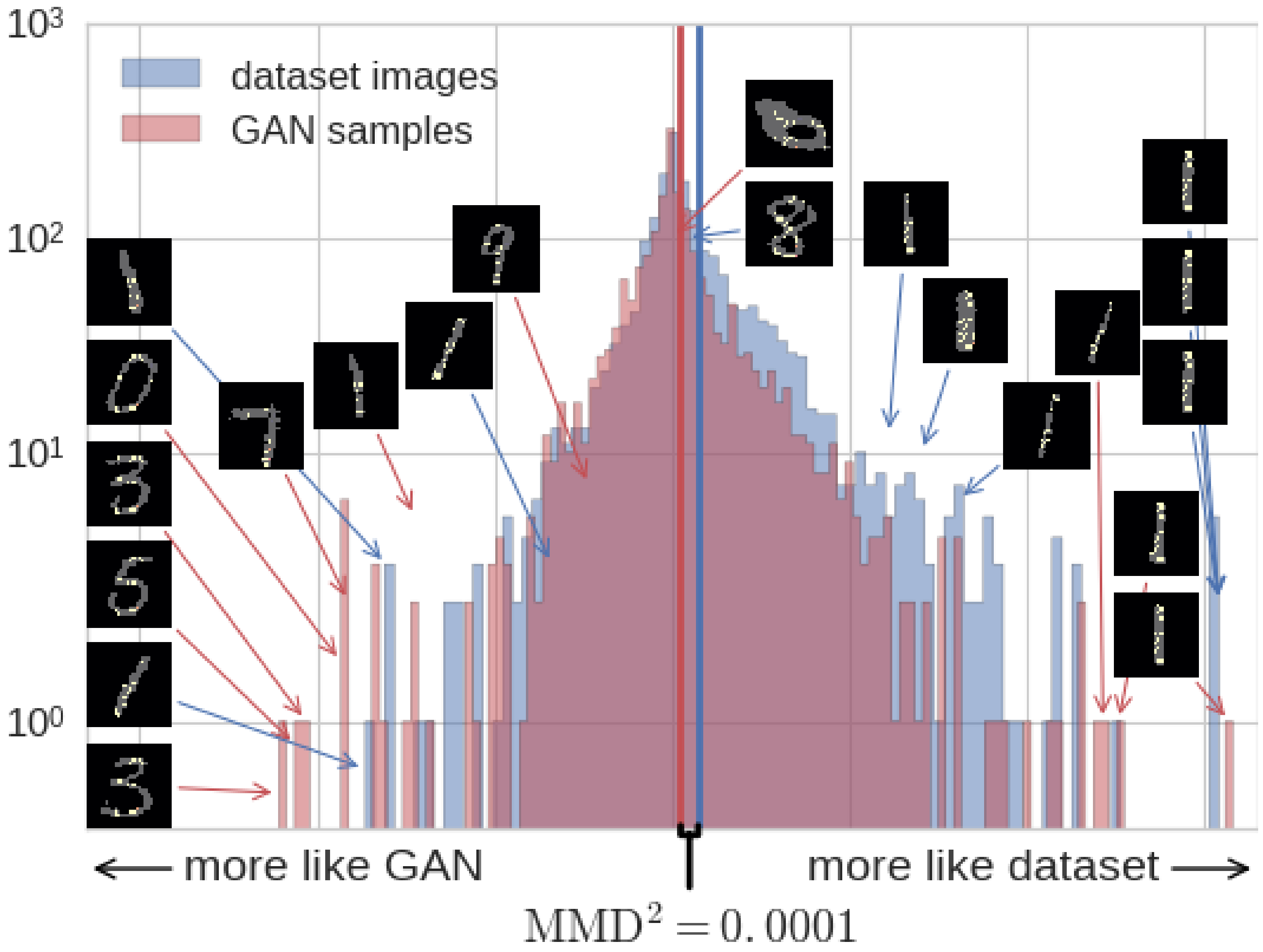
Blobs kernels



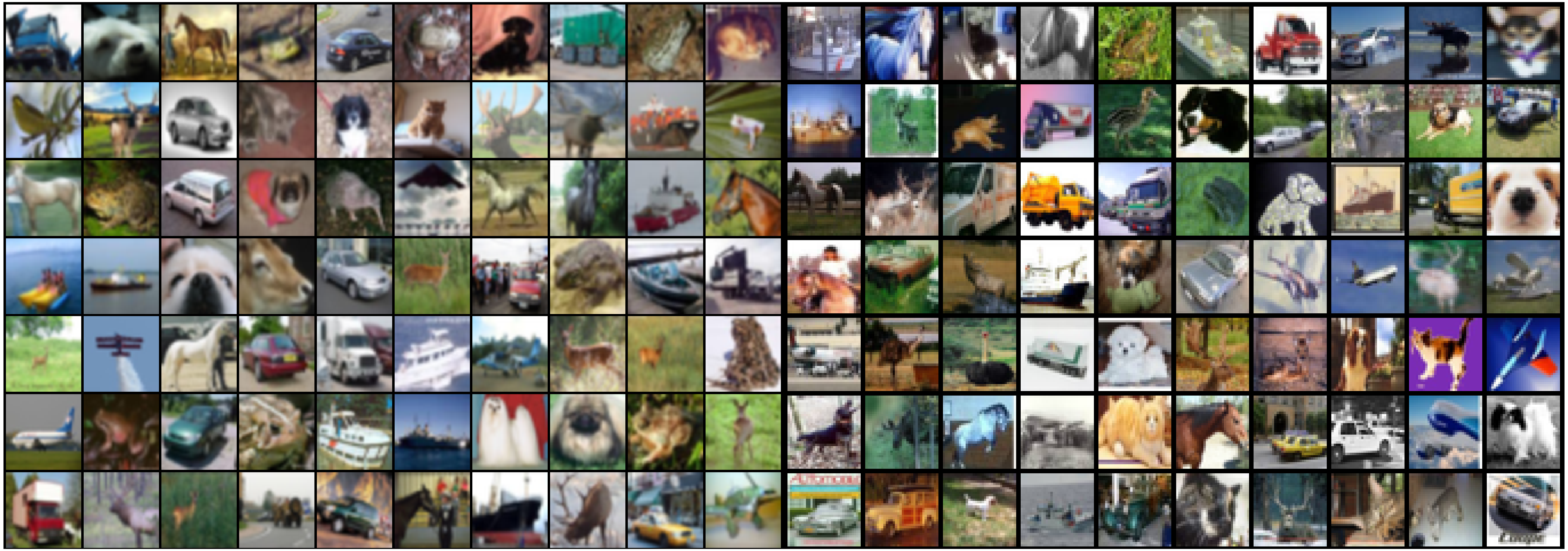
Blobs results



Investigating a GAN on MNIST



CIFAR-10 vs CIFAR-10.1



Train on 1 000, test on 1 031, repeat 10 times. Rejection rates:

ME	SCF	C2ST	MMD-O	MMD-D
0.588	0.171	0.452	0.316	**0.744**

Ablation vs classifier-based tests

	Cross-entropy			Max power		
Dataset	**Sign**	**Lin**	**Ours**	**Sign**	**Lin**	**Ours**
Blobs	0.84	0.94	0.90	–	0.95	0.99
High-d Gauss. mix.	0.47	0.59	0.29	–	0.64	0.66
Higgs	0.26	0.40	0.35	–	0.30	0.40
MNIST vs GAN	0.65	0.71	0.80	–	0.94	1.00

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- Need enough data to pick a good kernel
- Also need enough test data to actually detect the difference
- Best split depends on best kernel's quality / how hard to find
  - Don't know that ahead of time; can't try more than one

Meta-testing

- One idea: what if we have *related* problems?

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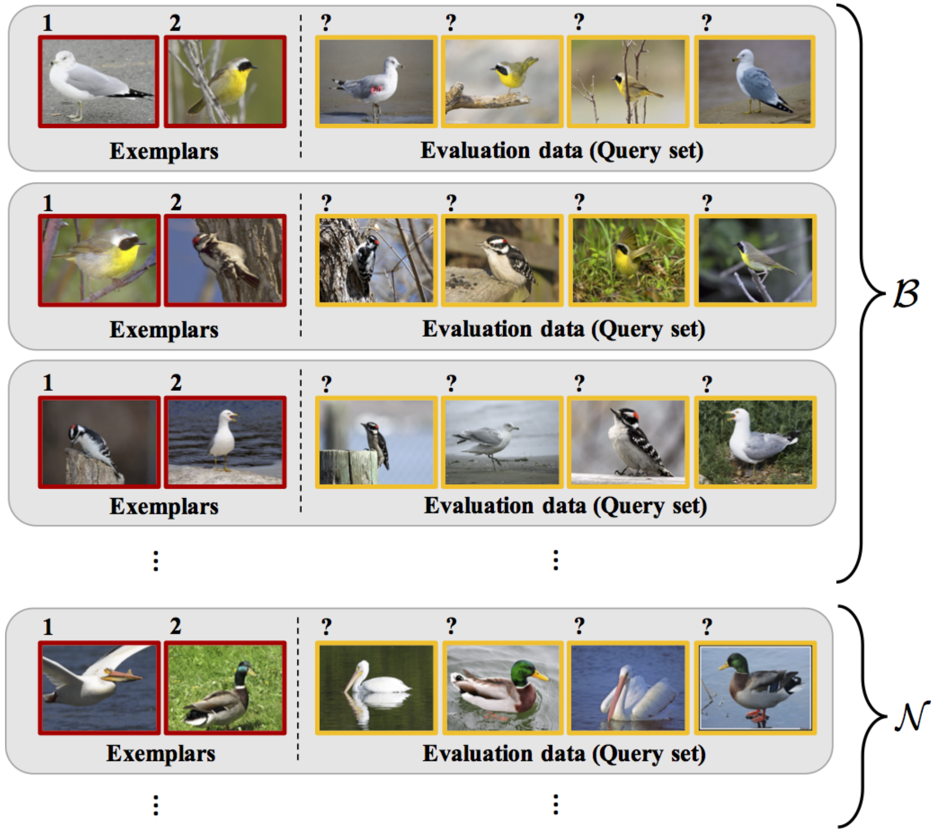
- Similar setup to meta-learning:



(from Wei+ 2018)

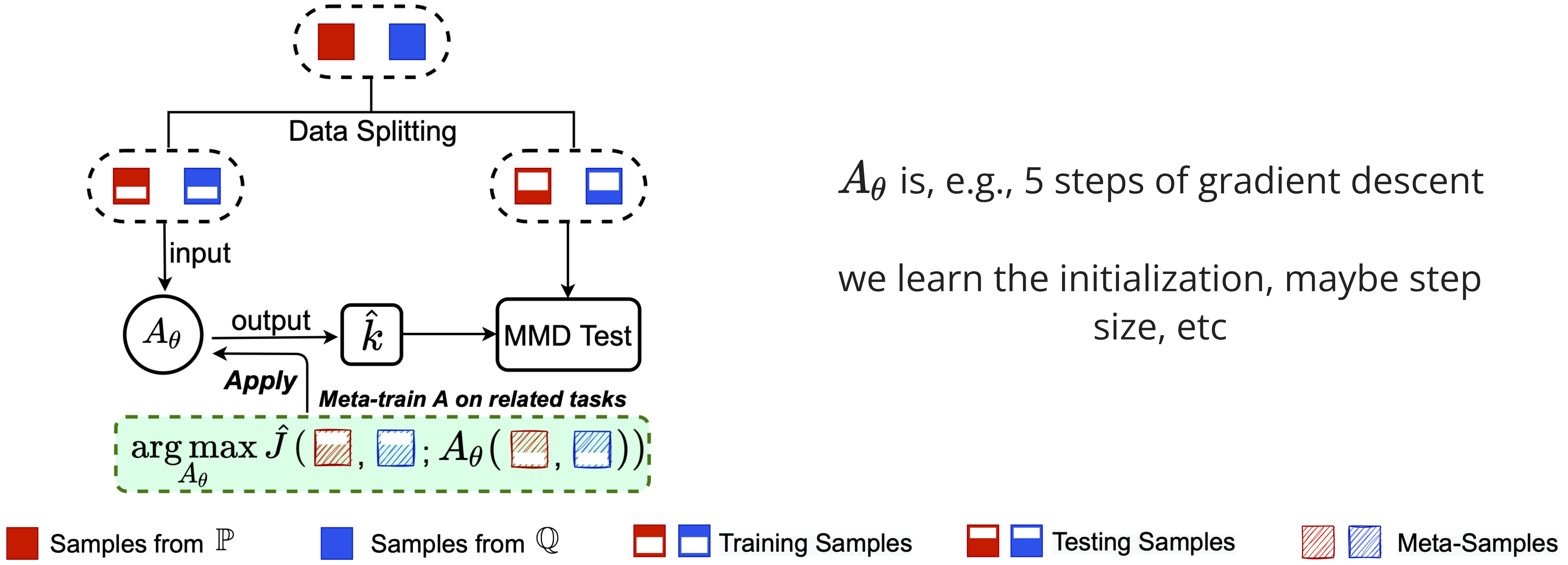
Meta-testing for CIFAR-10 vs CIFAR-10.1

- CIFAR-10 has 60,000 images, but CIFAR-10.1 only has 2,031
- Where do we get related data from?

Meta-testing for CIFAR-10 vs CIFAR-10.1

- CIFAR-10 has 60,000 images, but CIFAR-10.1 only has 2,031
- Where do we get related data from?
- One option: set up tasks to distinguish classes of CIFAR-10
  - airplane vs automobile, airplane vs bird, ...

One approach (MAML-like)



A_θ is, e.g., 5 steps of gradient descent

we learn the initialization, maybe step size, etc

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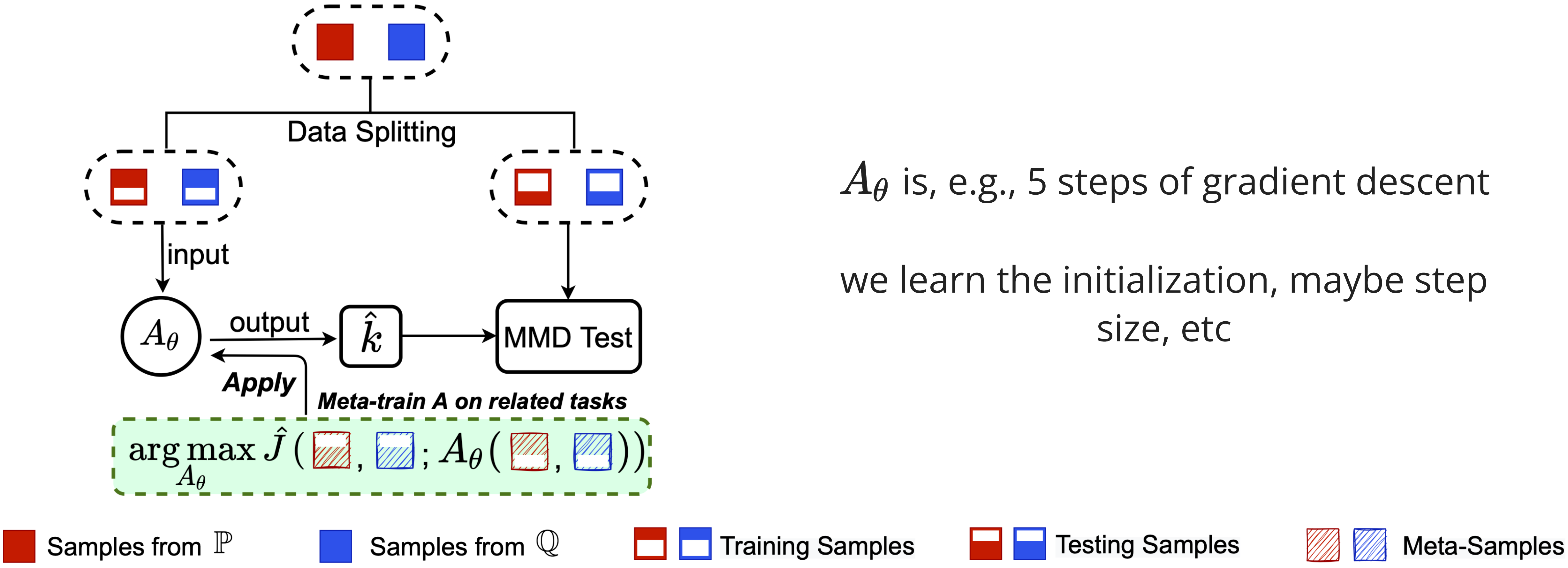

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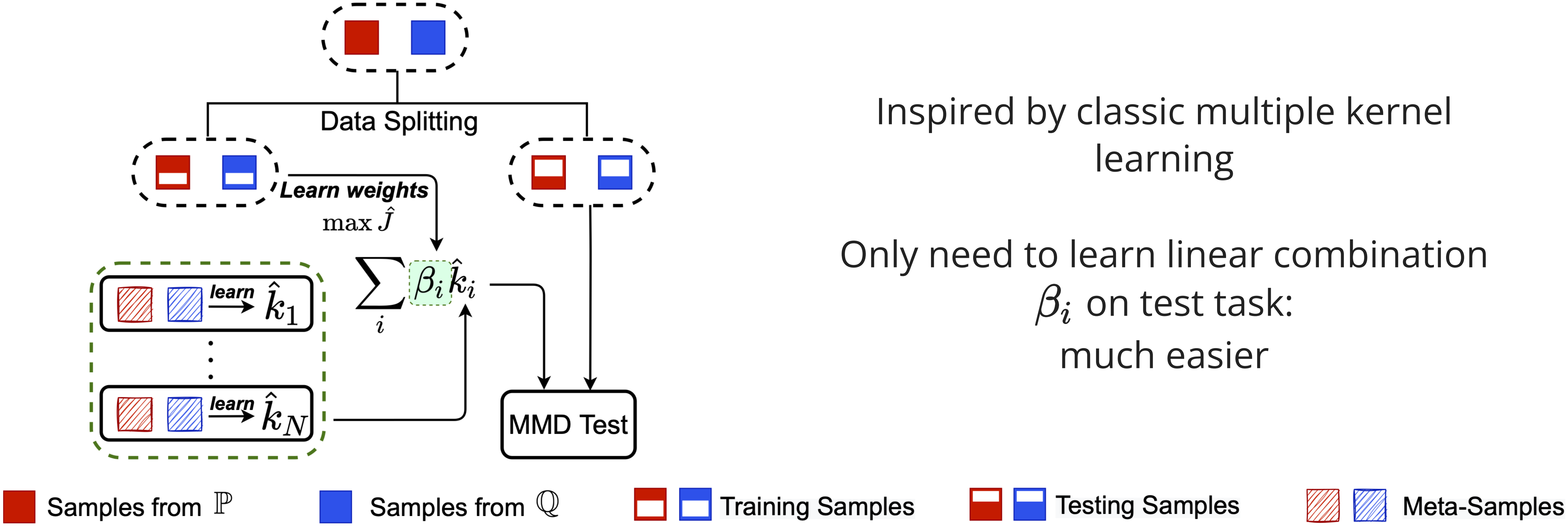
This works, but not as well as we'd hoped...
Initialization might work okay on everything, not really adapt

Another approach: Meta-MKL



Inspired by classic multiple kernel learning

Only need to learn linear combination β_i on test task: much easier

Theoretical analysis for Meta-MKL

- Same big-O dependence on test task size 😐
- But multiplier is *much* better:
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- Same big-O dependence on test task size 😐
- But multiplier is *much* better:
  based on number of meta-training tasks, not on network size
- Coarse analysis: assumes one meta-tasks is “related” enough
  - We compete with picking the single best related kernel
  - Haven't analyzed meaningfully combining related kernels (yet!)

Results on CIFAR-10.1

Methods	$m_{tr} = 100$			$m_{tr} = 200$		
	$m_{te} = 200$	$m_{te} = 500$	$m_{te} = 900$	$m_{te} = 200$	$m_{te} = 500$	$m_{te} = 900$
ME	$0.084_{\pm 0.009}$	$0.096_{\pm 0.016}$	$0.160_{\pm 0.035}$	$0.104_{\pm 0.013}$	$0.202_{\pm 0.020}$	$0.326_{\pm 0.039}$
SCF	$0.047_{\pm 0.013}$	$0.037_{\pm 0.011}$	$0.047_{\pm 0.015}$	$0.026_{\pm 0.009}$	$0.018_{\pm 0.006}$	$0.026_{\pm 0.012}$
C2ST-S	$0.059_{\pm 0.009}$	$0.062_{\pm 0.007}$	$0.059_{\pm 0.007}$	$0.052_{\pm 0.011}$	$0.054_{\pm 0.011}$	$0.057_{\pm 0.008}$
C2ST-L	$0.064_{\pm 0.009}$	$0.064_{\pm 0.006}$	$0.063_{\pm 0.007}$	$0.075_{\pm 0.014}$	$0.066_{\pm 0.011}$	$0.067_{\pm 0.008}$
MMD-O	$0.091_{\pm 0.011}$	$0.141_{\pm 0.009}$	$0.279_{\pm 0.018}$	$0.084_{\pm 0.007}$	$0.160_{\pm 0.011}$	$0.319_{\pm 0.020}$
MMD-D	$0.104_{\pm 0.007}$	$0.222_{\pm 0.020}$	$0.418_{\pm 0.046}$	$0.117_{\pm 0.013}$	$0.226_{\pm 0.021}$	$0.444_{\pm 0.037}$
AGT-KL	$0.170_{\pm 0.032}$	$0.457_{\pm 0.052}$	$0.765_{\pm 0.045}$	$0.152_{\pm 0.023}$	$0.463_{\pm 0.060}$	$0.778_{\pm 0.050}$
Meta-KL	$0.245_{\pm 0.010}$	$0.671_{\pm 0.026}$	$0.959_{\pm 0.013}$	$0.226_{\pm 0.015}$	$0.668_{\pm 0.032}$	$0.972_{\pm 0.006}$
Meta-MKL	$\mathbf{0.277}_{\pm 0.016}$	$\mathbf{0.728}_{\pm 0.020}$	$\mathbf{0.973}_{\pm 0.008}$	$\mathbf{0.255}_{\pm 0.020}$	$\mathbf{0.724}_{\pm 0.026}$	$\mathbf{0.993}_{\pm 0.003}$

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  - e.g. can distinguish “creditworthy” vs not, but **can't** distinguish by race

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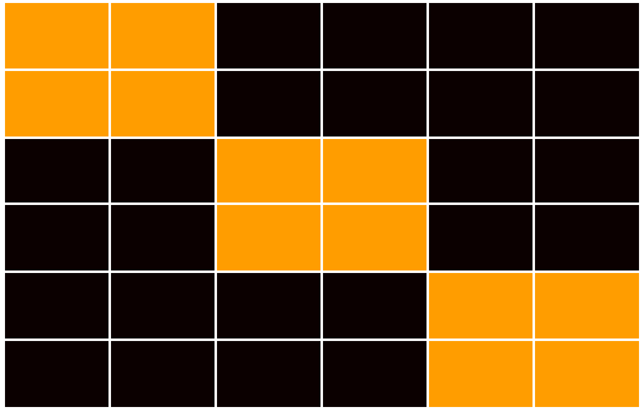
  - Better, but tends to “stall out” in minimizing ρ_k^s

Block estimator [Zaremba+ NeurIPS-13]

- Use previous $\widehat{\mathrm{MMD}}$ on b blocks, each of size B



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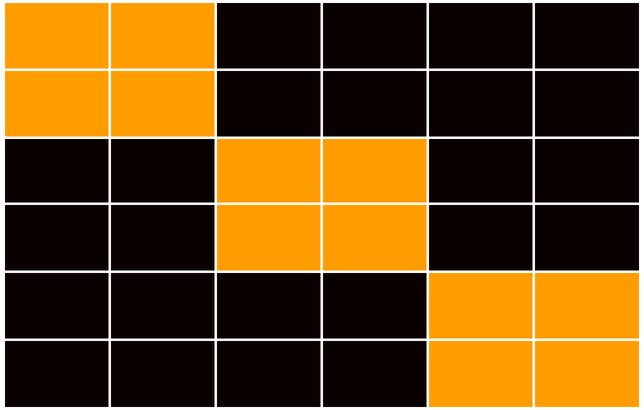

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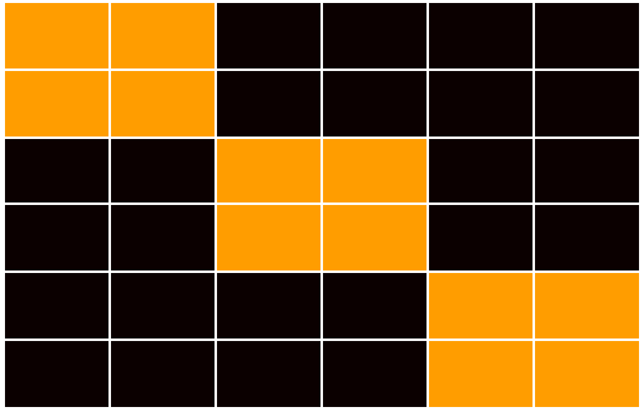

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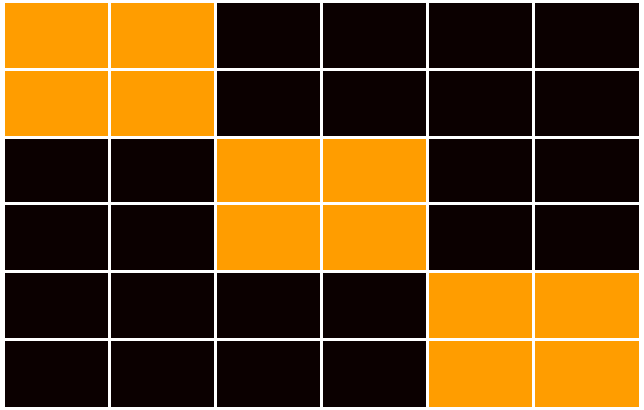

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  - For now, just Gaussians with different lengthscales

Adult Data Set

Download: Data Folder, Data Set Description

Abstract: Predict whether income exceeds $50K/yr based on census data. Also known as "Census Income" dataset.

Data Set Characteristics:	Multivariate	**Number of Instances:**	48842	**Area:**	Social
Attribute Characteristics:	Categorical, Integer	**Number of Attributes:**	14	**Date Donated**	1996-05-01
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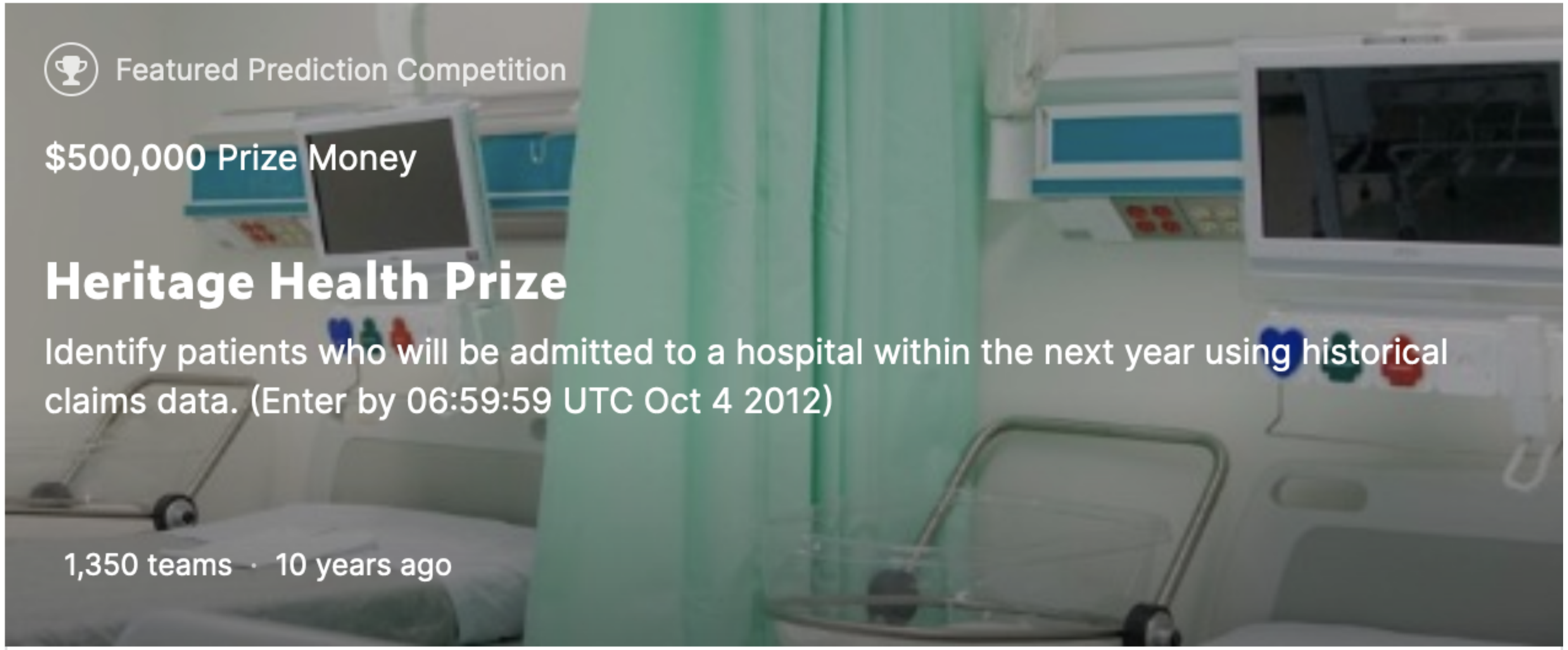

Learned representations

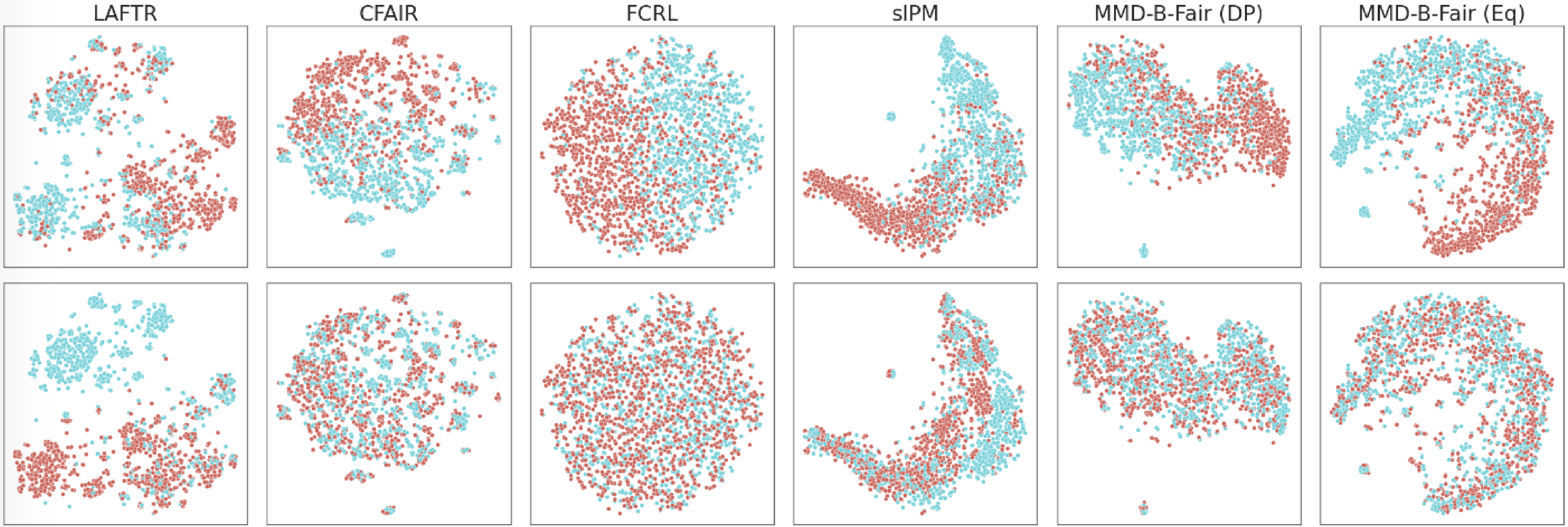

Figure 4: t-SNE visualizations of Adult representations, colored by target attribute (top) and sensitive attribute (bottom).

Quality of transfer learning

Transfer Label		LAFTR	CFAIR	FCRL	sIPM	MMD-B-Fair (DP)	MMD-B-Fair (Eq)
MSC2a3	acc	57.2	62.5	58.0	**72.8**	71.3	70.3
	DP	52.3	65.1	**99.2**	69.3	72.2	84.5
	Eq	57.4	70.1	**98.0**	69.9	71.8	86.6
METAB3	acc	**72.9**	72.2	53.9	72.4	70.7	69.4
	DP	52.3	65.1	**97.7**	54.5	65.6	82.1
	Eq	61.3	77.1	**97.6**	63.4	74.6	92.1
ARTHSPHIN	acc	66.4	65.9	59.3	**70.6**	67.5	67.8
	DP	52.3	65.1	**98.0**	74.6	83.0	87.7
	Eq	54.9	70.1	**98.1**	76.7	84.9	90.0
NEUMENT	acc	64.4	61.9	60.1	**68.0**	67.1	67.3
	DP	52.3	65.1	**99.1**	72.9	86.8	94.5
	Eq	54.9	69.7	**97.5**	73.2	86.7	95.4
MISCHRT	acc	71.0	67.3	69.3	**73.5**	73.0	72.5
	DP	52.3	65.1	**98.6**	85.0	87.2	96.4
	Eq	59.4	79.0	**98.2**	88.5	88.6	97.5

Table 1: Using Heritage Health representations to predict various downstream tasks. **Red** marks the best result per row, blue second-best, and green third-best.

- Check if your data is different than it used to be!
- Pretty good method: train a classifier, check how accurate
- More powerful: use an optimized kernel method

A good takeaway

Combining a deep architecture with a kernel machine that takes the higher-level learned representation as input can be quite powerful.

— Y. Bengio & Y. LeCun (2007), "Scaling Learning Algorithms towards AI"