Are these datasets the same?
Learning kernels for efficient and fair two-sample tests

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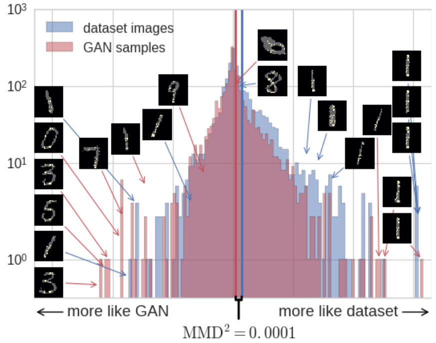
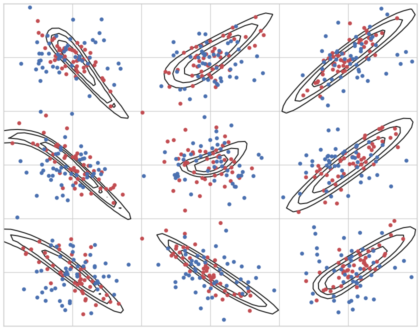
University of British Columbia (UBC) / Alberta Machine Intelligence Institute (Amii)

[ICLR-17]



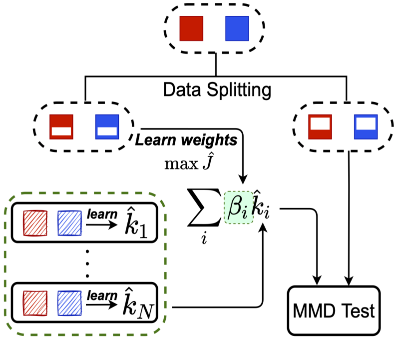
Hsiao-Yu (Fish) Tung
Heiko Strathmann
Soumyajit De
Aaditya Ramdas
Alex Smola
Arthur Gretton

[ICML-20]



Feng Liu
Wenkai Xu
Jie Lu
Guangquan Zhang
Arthur Gretton

[NeurIPS-21]



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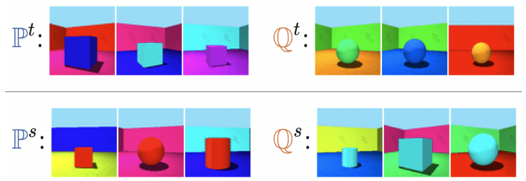
new!



Namrata Deka

TrustML - 15 Feb 2022

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  - Deploy it on some distribution $\mathbb{Q}$, might be sort of like $\mathbb{P}$
    - and probably changes over time…

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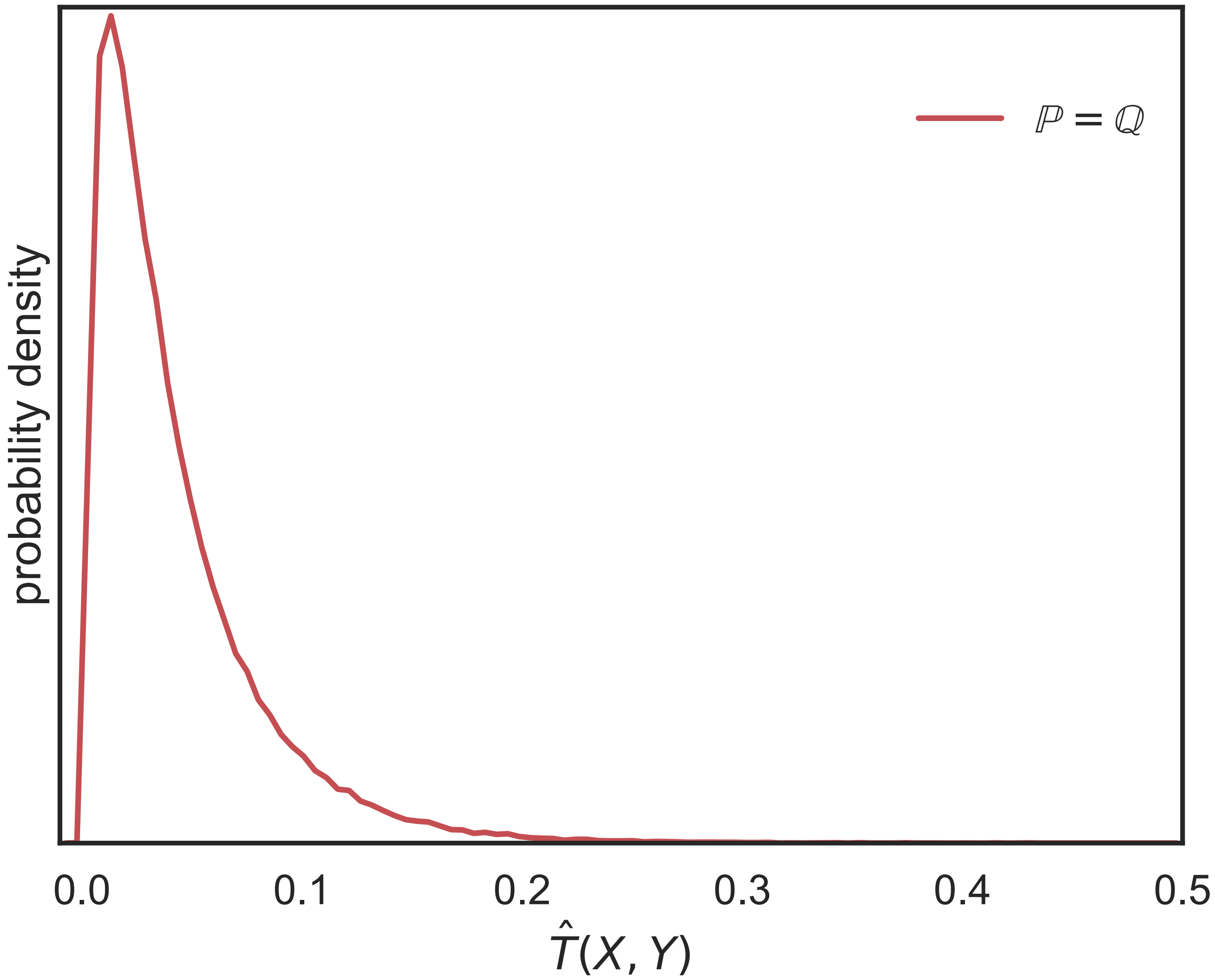
- Reject H_0 if test statistic $\hat{T}(X, Y) > c_\alpha$

What's a hypothesis test again?



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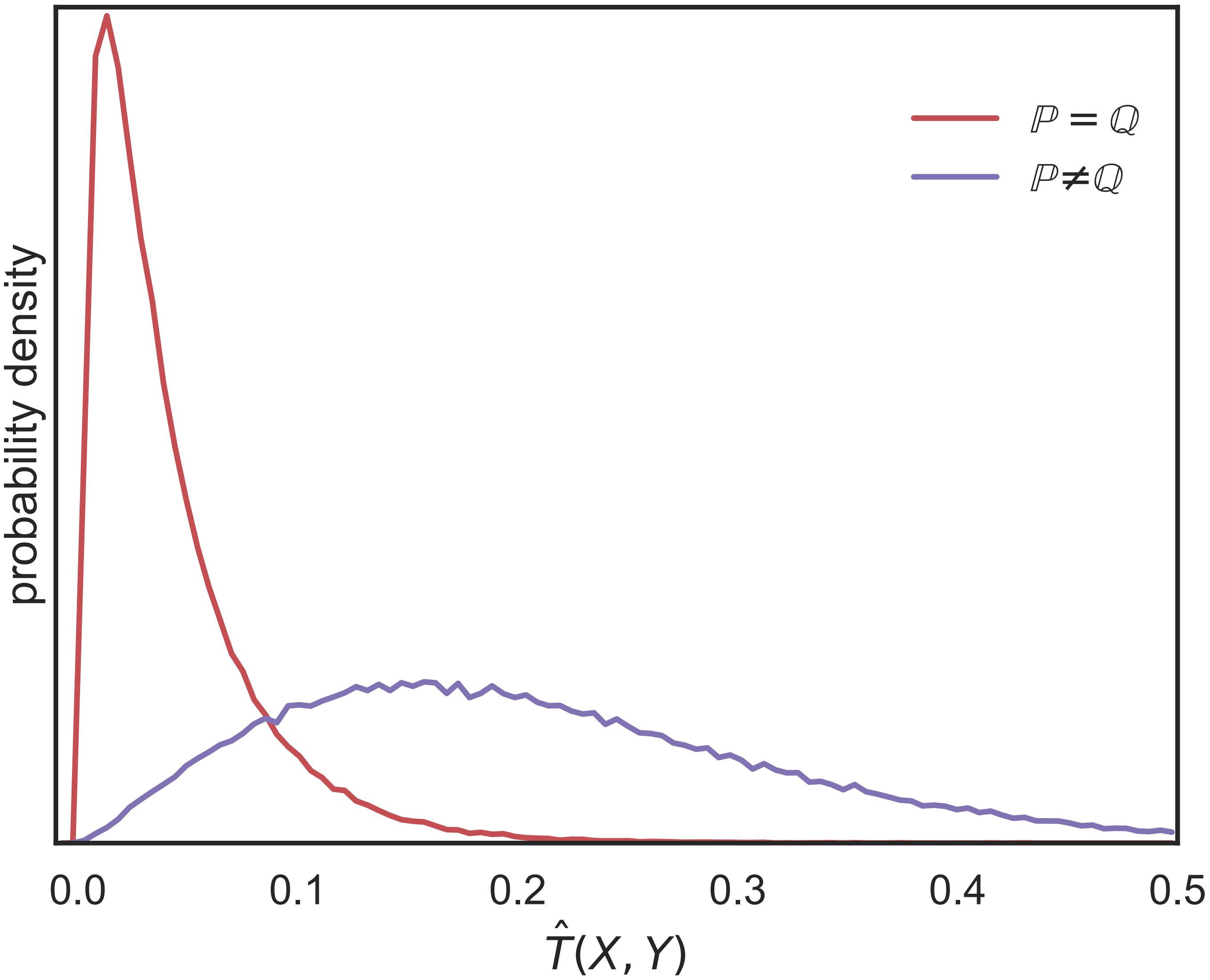

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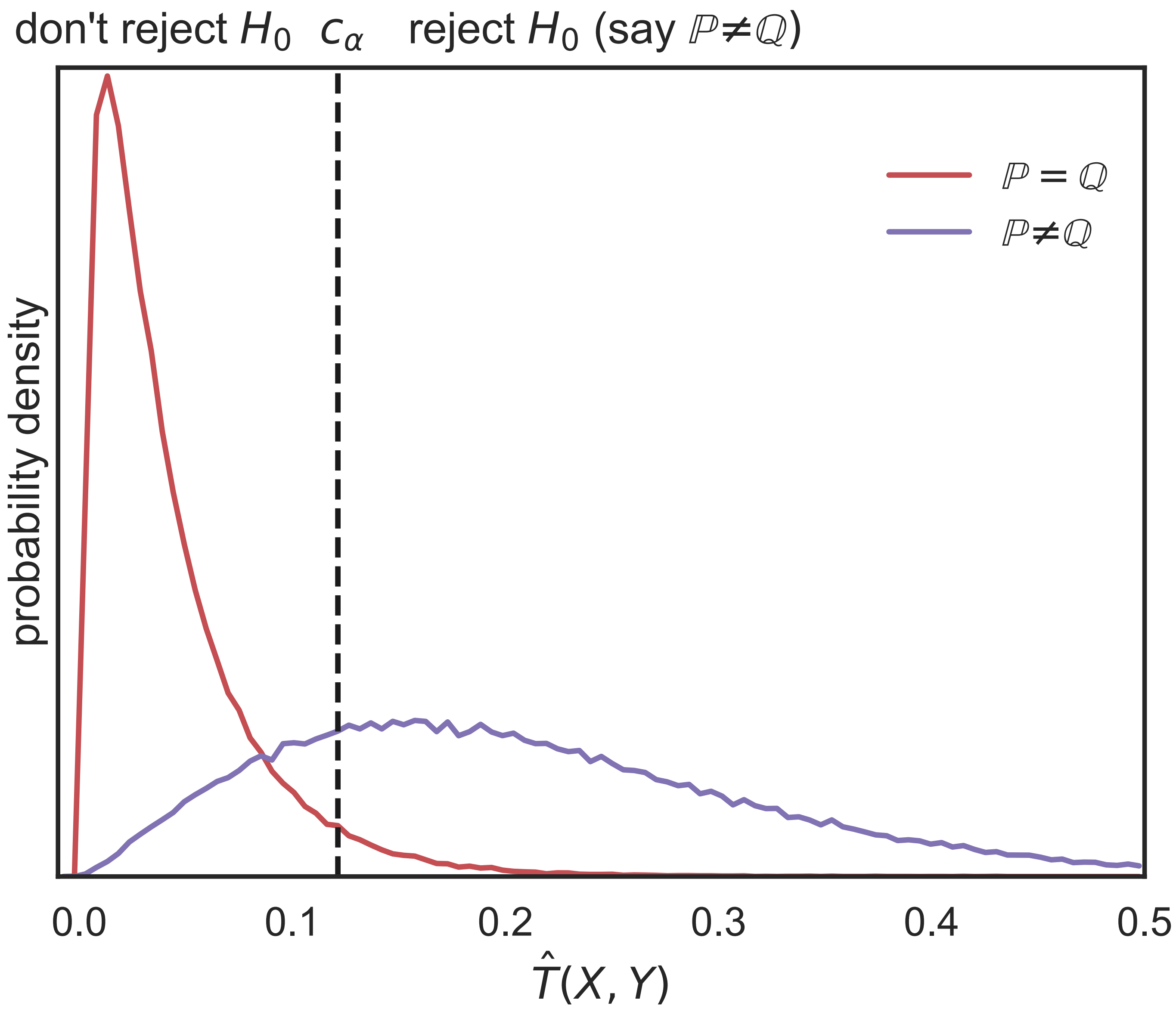

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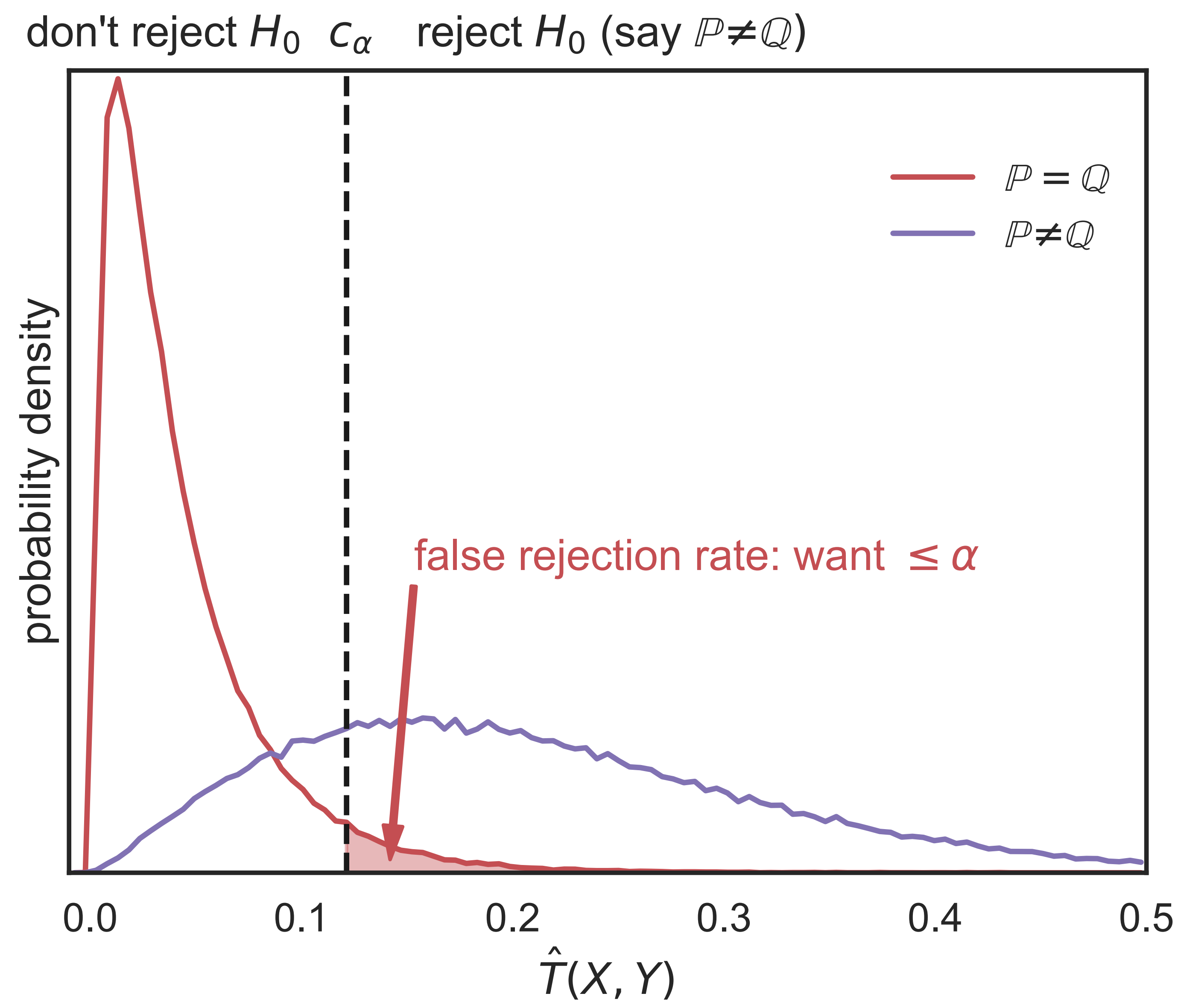

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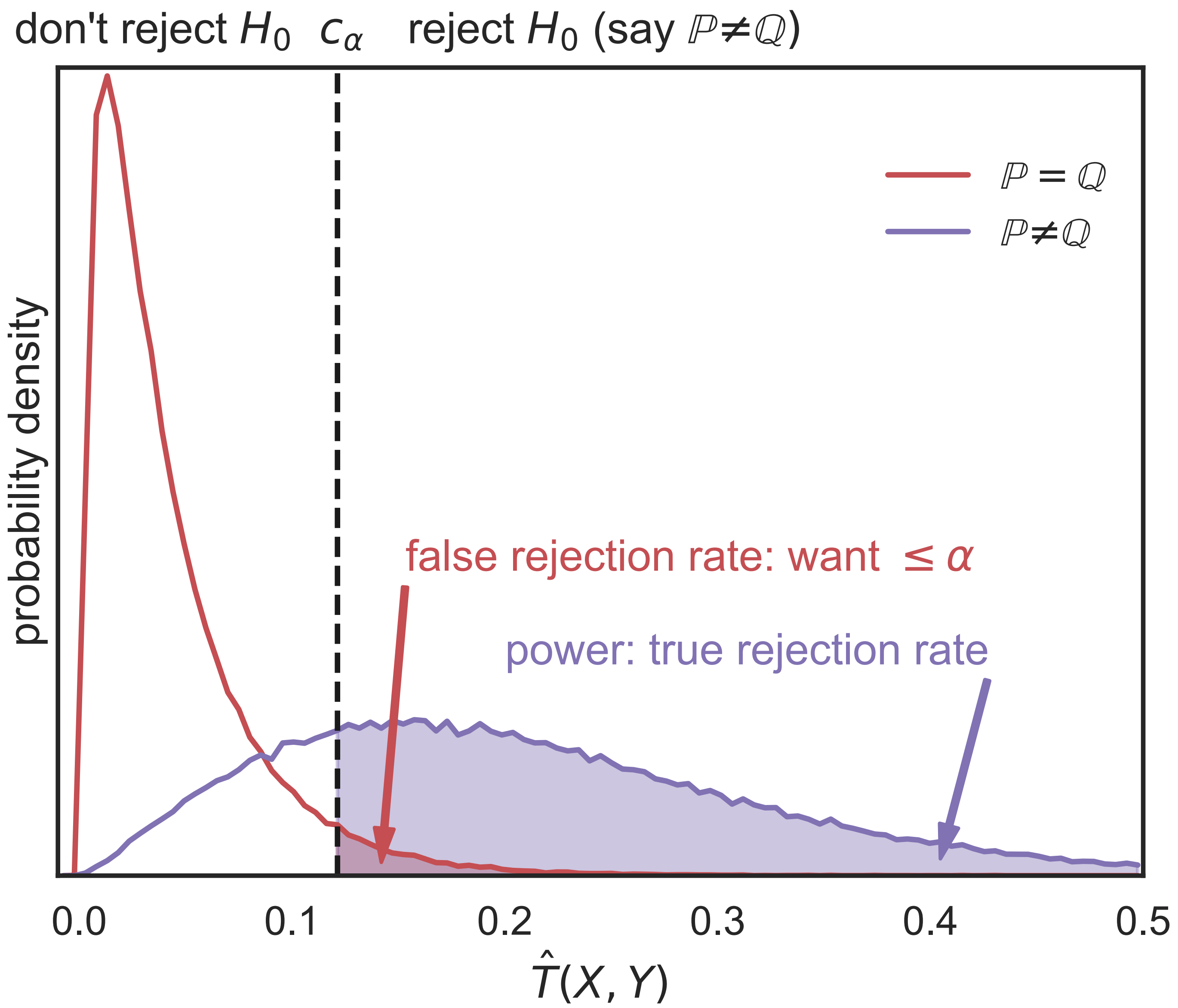

Permutation testing to find c_α

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

$X_1 \quad X_2 \quad X_3 \quad X_4 \quad X_5 \qquad Y_1 \quad Y_2 \quad Y_3 \quad Y_4 \quad Y_5$

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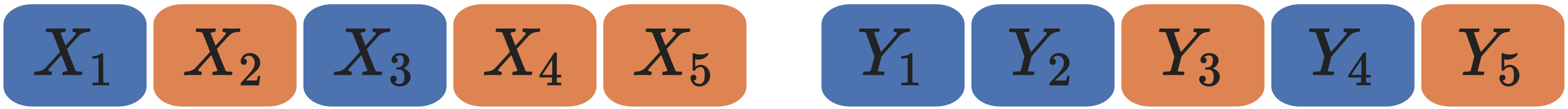

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This is a *kernel-based* distance between distributions

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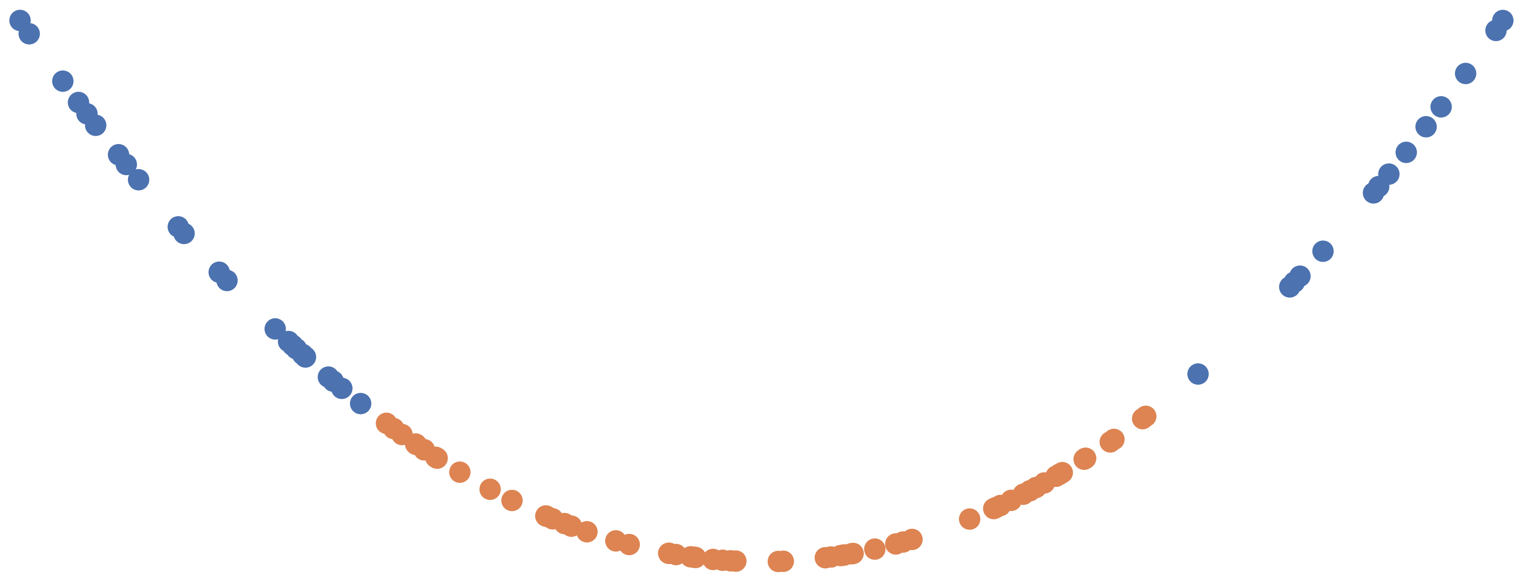

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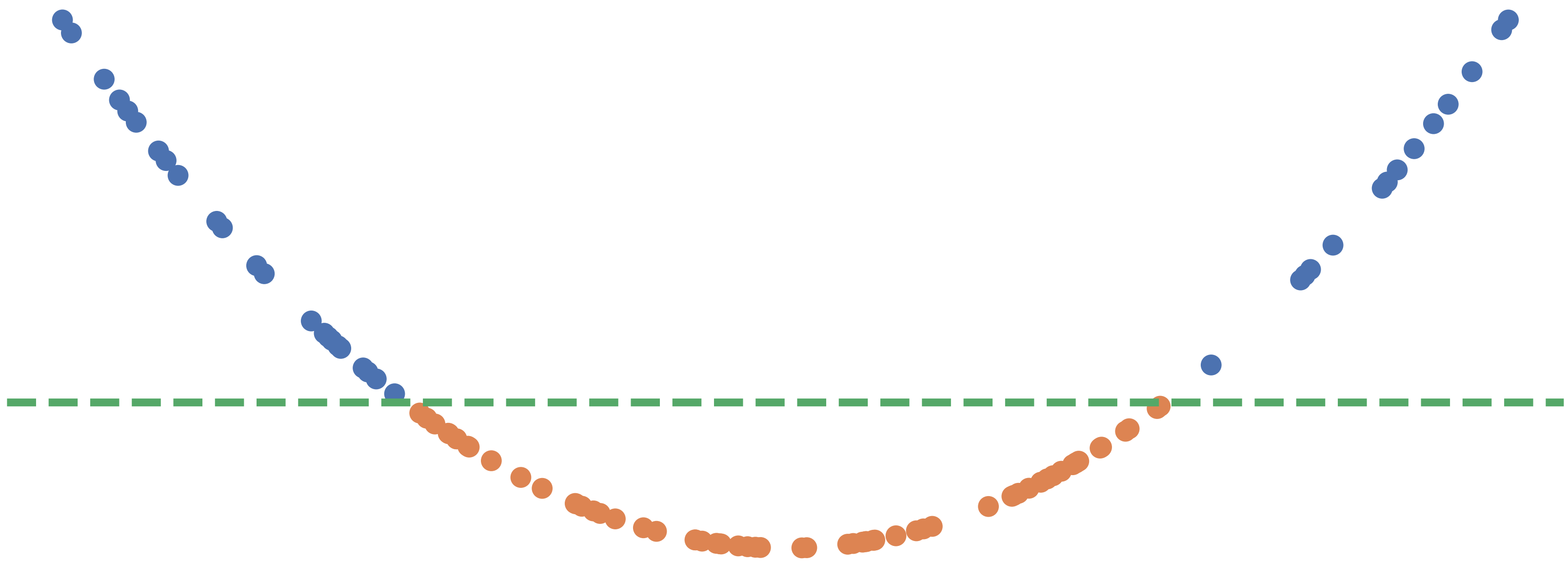

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- $\|f\|_\mathcal{H} = \sqrt{\alpha^\mathsf{T} K \alpha}$ gives kernel notion of smoothness

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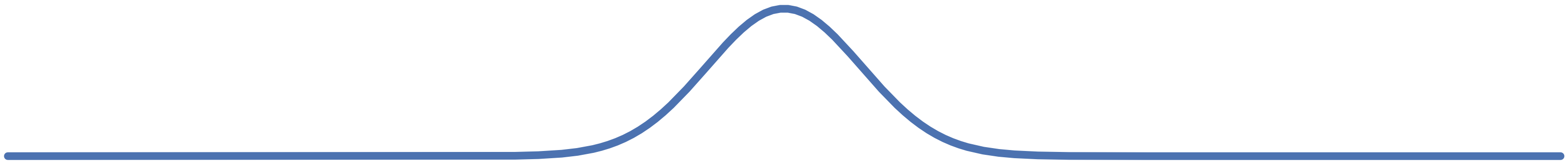

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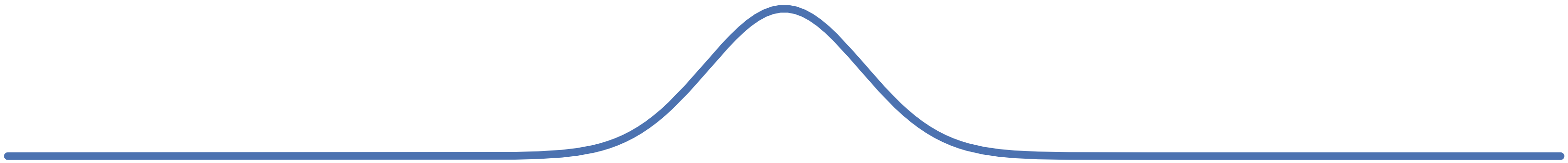

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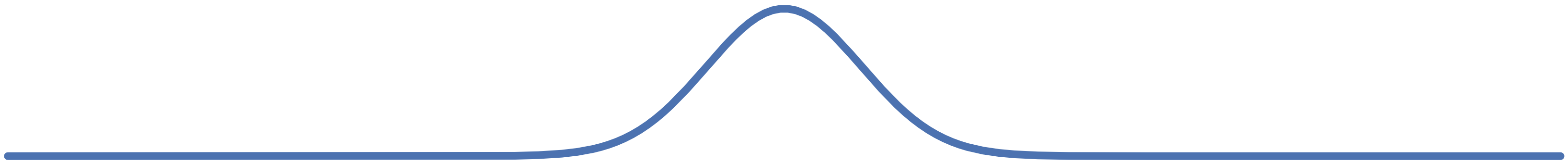

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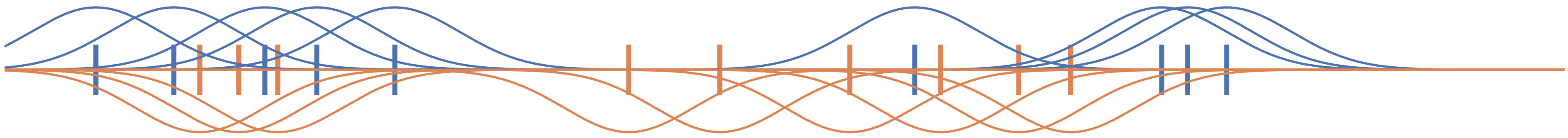

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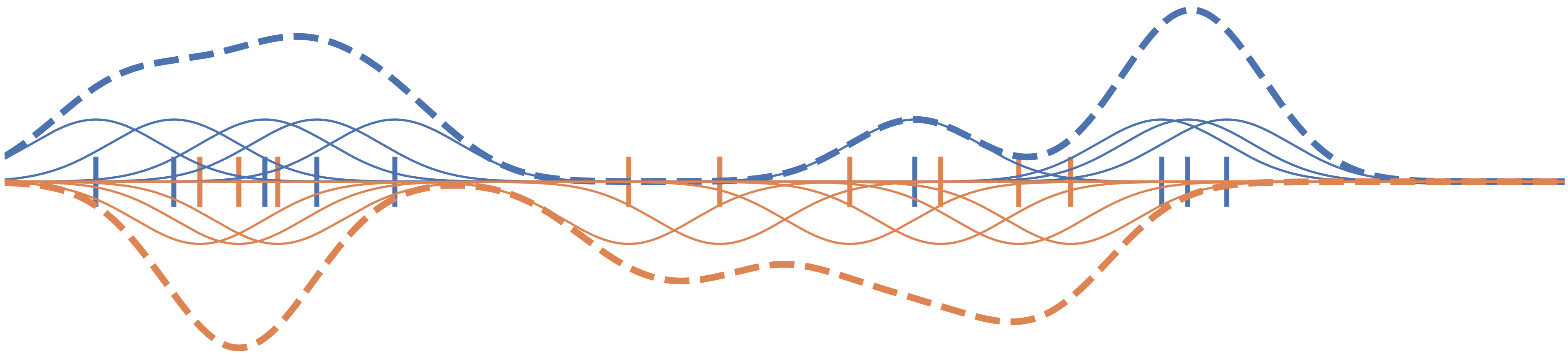

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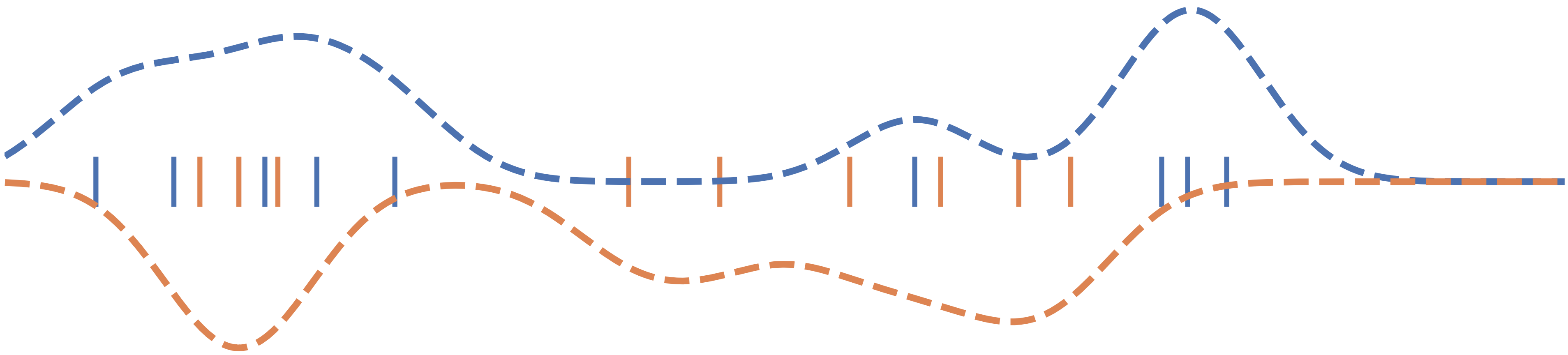

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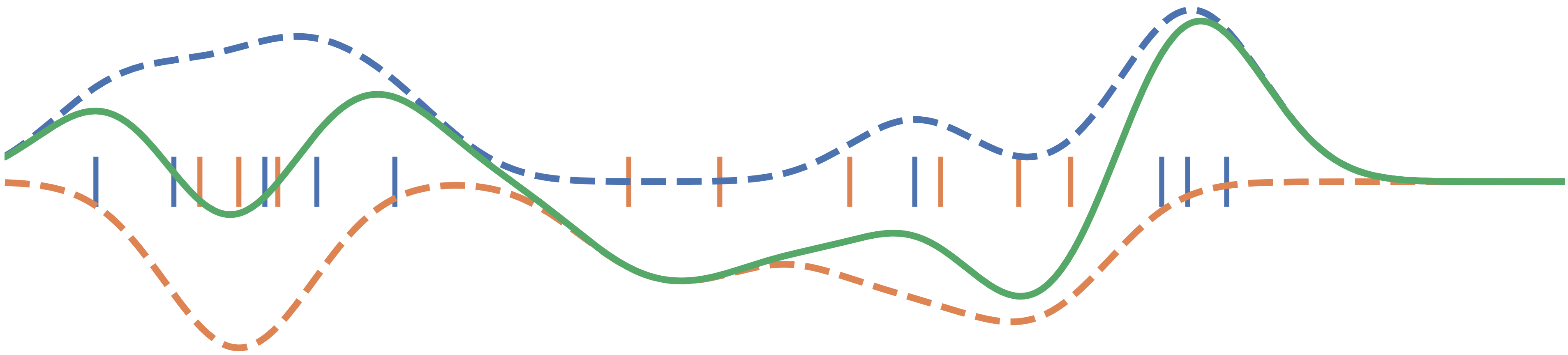

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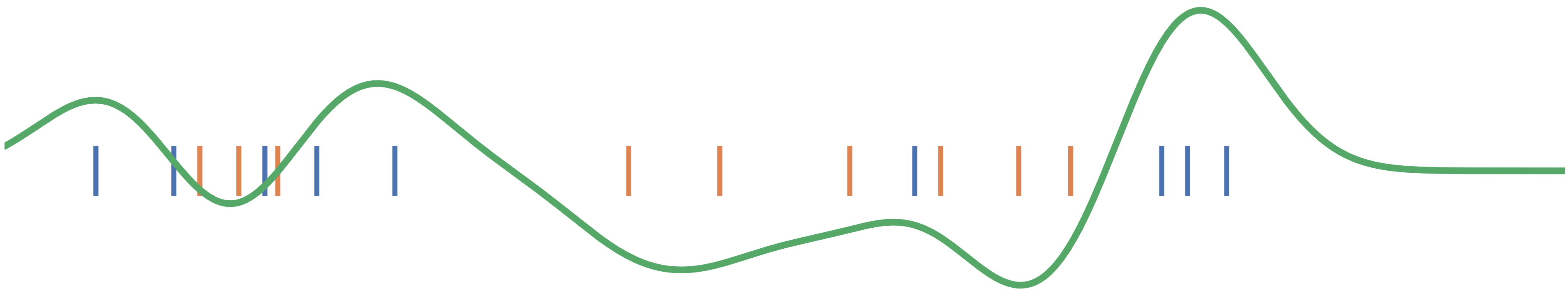

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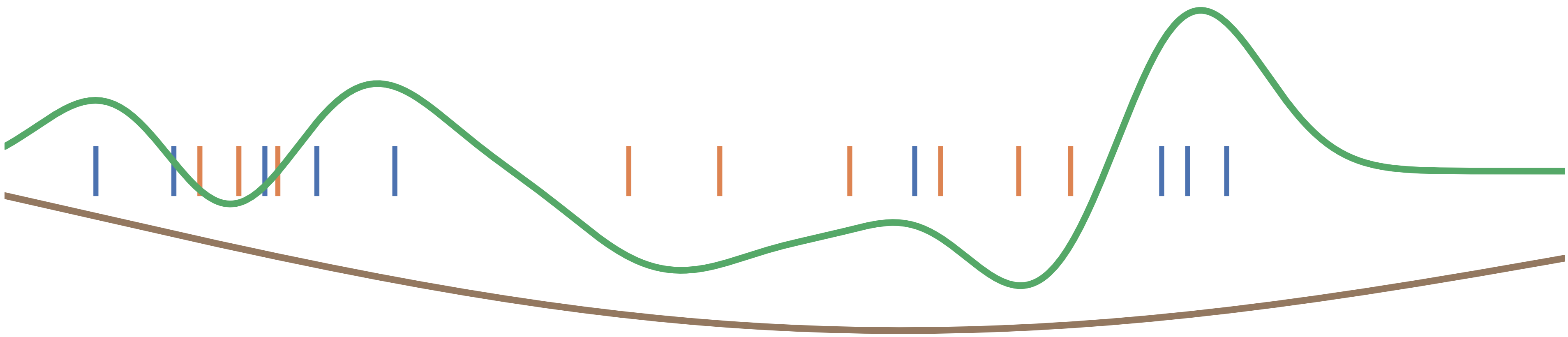

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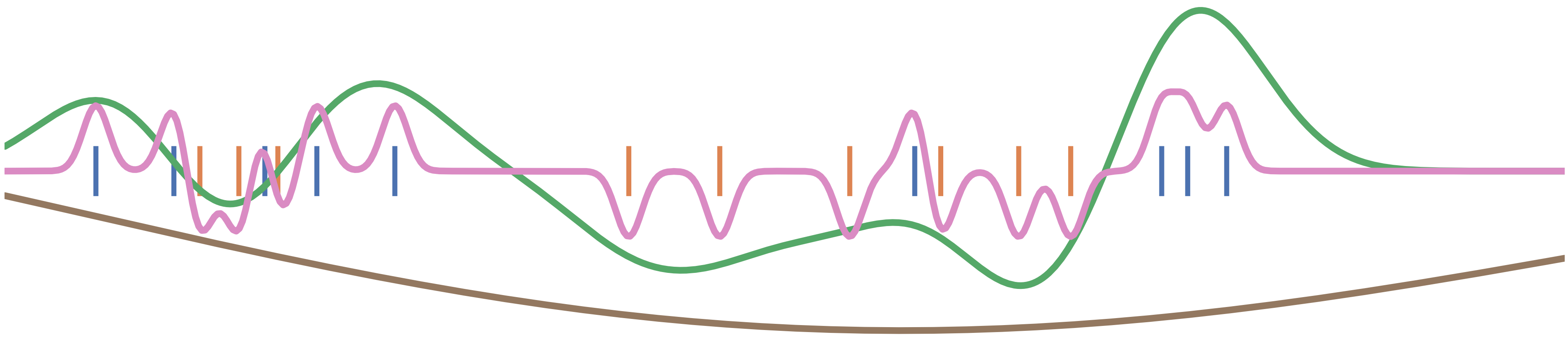

Maximum Mean Discrepancy (MMD)

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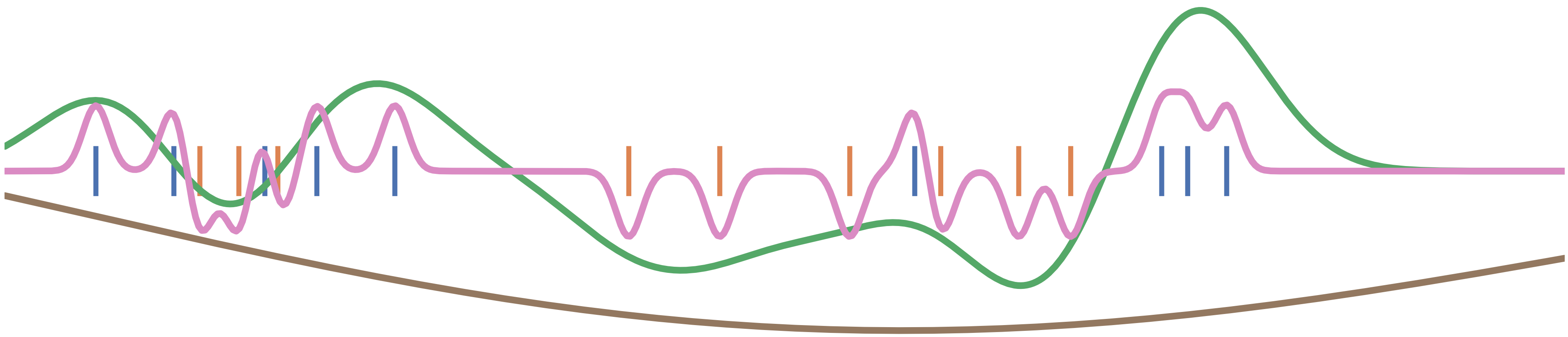

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$$\mathrm{MMD}_k^2(\mathbb{P}, \mathbb{Q}) = \mathop{\mathbb{E}}_{X, X' \sim \mathbb{P}}[k(X, X')] + \mathop{\mathbb{E}}_{Y, Y' \sim \mathbb{Q}}[k(Y, Y')] - 2 \mathop{\mathbb{E}}_{\substack{X \sim \mathbb{P} \\ Y \sim \mathbb{Q}}}[k(X, Y)]$$

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K_{XX}

	1.0	0.2	0.6
	0.2	1.0	0.5
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1.0	0.8	0.7
0.8	1.0	0.6
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K_{XY}

0.3	0.1	0.2
0.2	0.3	0.3
0.2	0.1	0.4

MMD as feature matching

$$\mathrm{MMD}_k(\mathbb{P}, \mathbb{Q}) = \left\| \mathop{\mathbb{E}}_{X \sim \mathbb{P}}[\varphi(X)] - \mathop{\mathbb{E}}_{Y \sim \mathbb{Q}}[\varphi(Y)] \right\|_{\mathcal{H}}$$

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- Many kernels: **infinite-dimensional** $\mathcal{H}$

MMD-based tests

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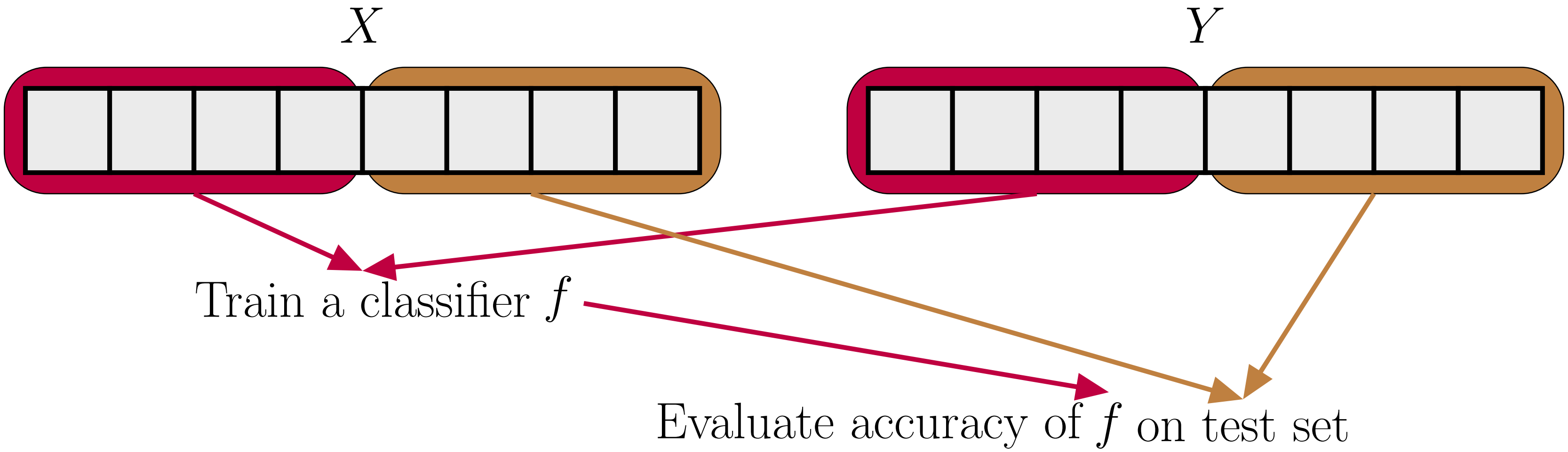
- Need enormous n if kernel is bad for problem

Classifier two-sample tests



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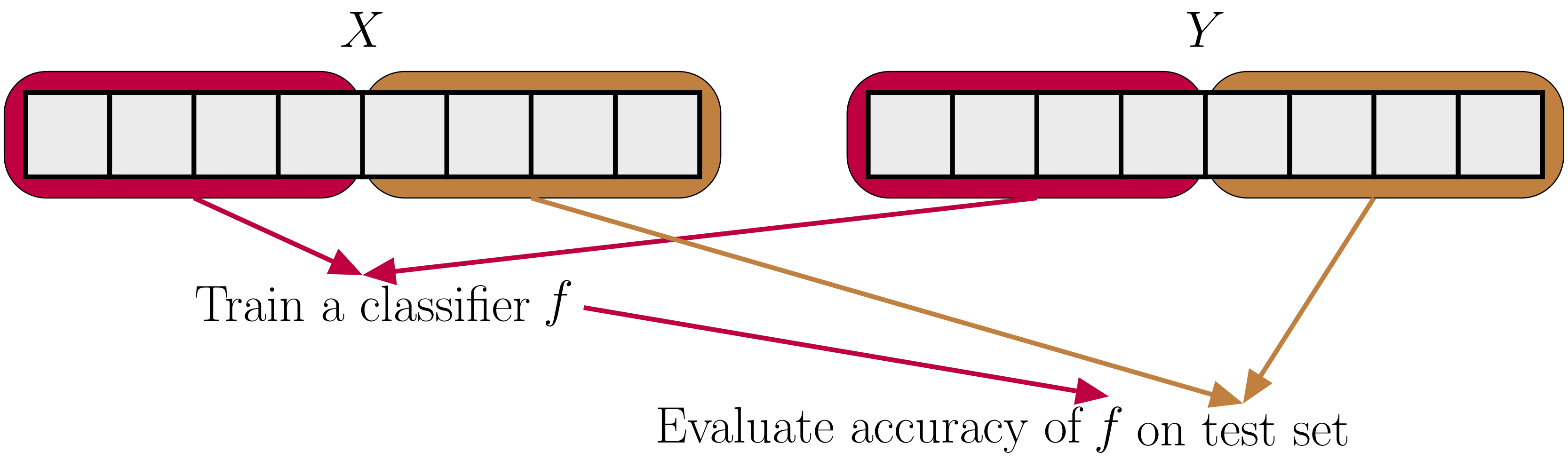

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  - Same idea as NNGP approximation
- Generalize to a **deep kernel**:

$$k_\psi(x,y) = \kappa\left(\phi_\psi(x), \phi_\psi(y)\right)$$

Normal deep learning $\subset$ deep kernels

- Take $k_\psi(x, y) = \frac{1}{4} f_\psi(x) f_\psi(y)$
- Final function in $\mathcal{H}_\psi$ will be $a f_\psi(x)$

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- Take $k_\psi(x, y) = \frac{1}{4} f_\psi(x) f_\psi(y) + 1$
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On Calibration of Modern Neural Networks

Chuan Guo [*1] **Geoff Pleiss** [*1] **Yu Sun** [*1] **Kilian Q. Weinberger** [1]

So what?

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[Submitted on 30 Nov 2020]

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- We know theoretically deep learning can learn some things faster than any kernel method [see Malach+ ICML-21 + refs]
- But deep kernel learning ≠ traditional kernel models
  - exactly like how usual deep learning ≠ linear models

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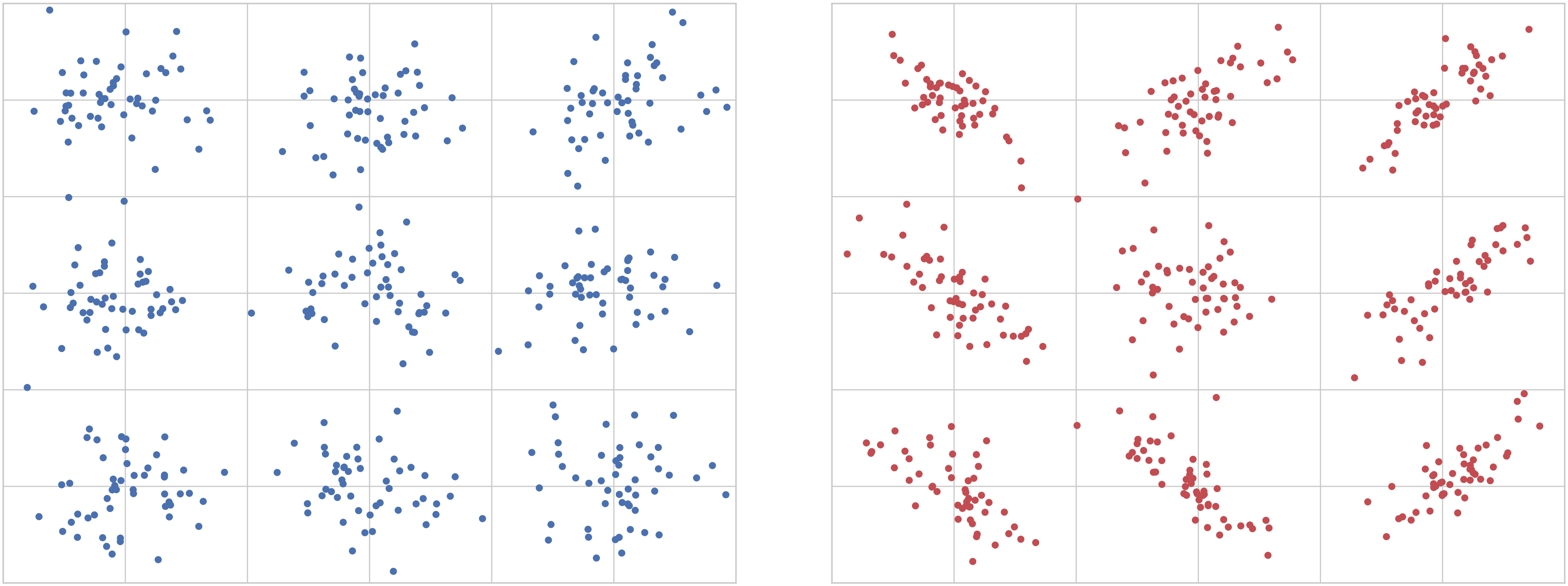
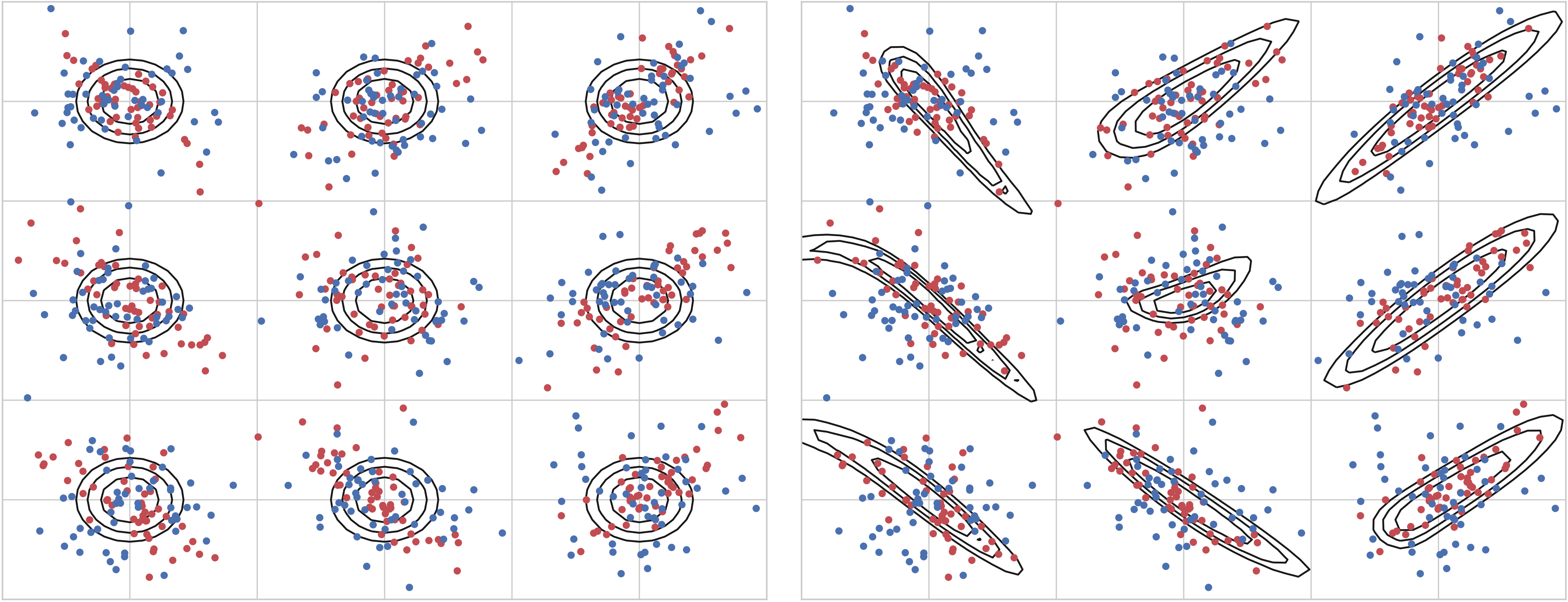
- Can show uniform $\mathcal{O}_P(n^{-\frac{1}{3}})$ convergence of estimator

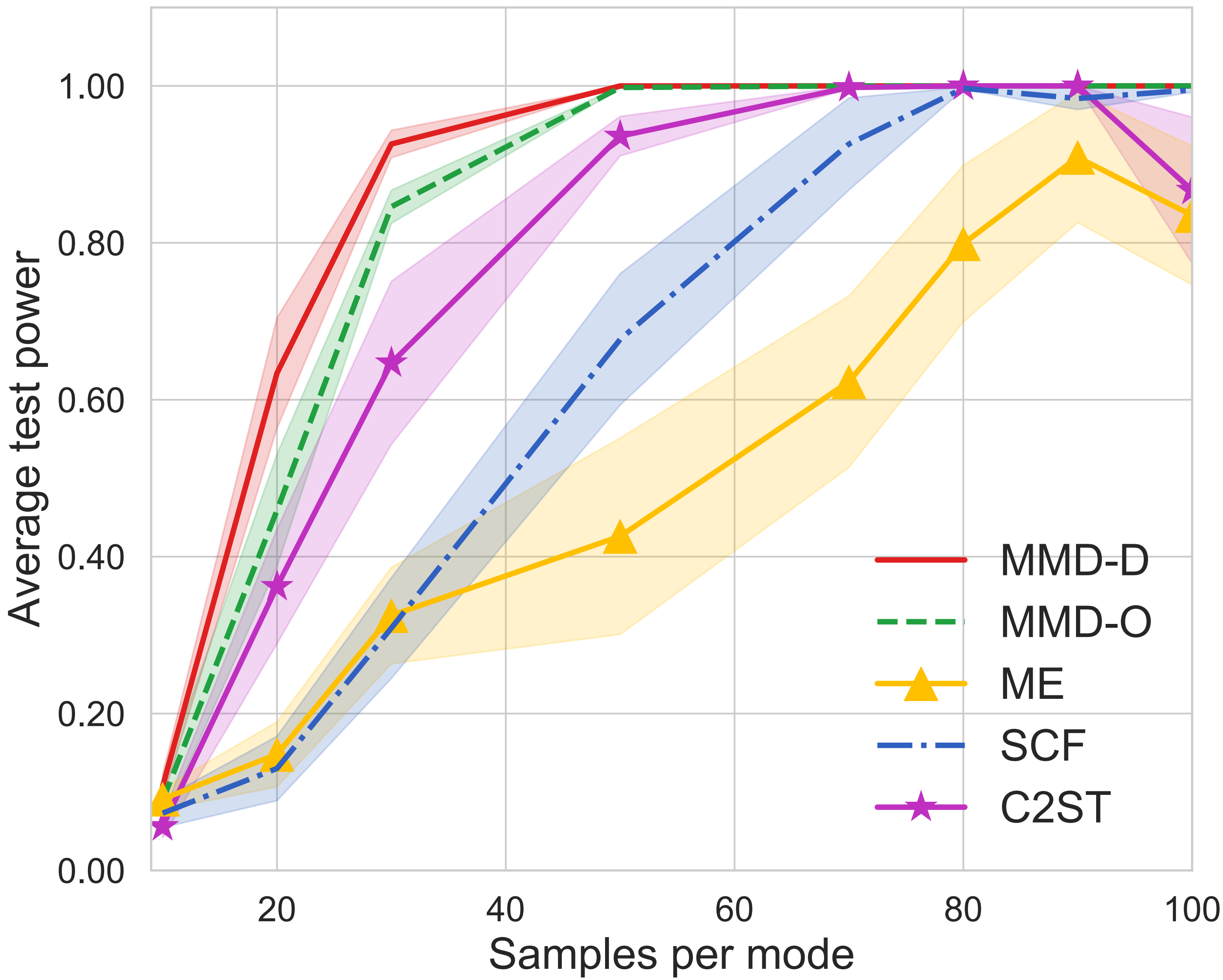
Blobs dataset



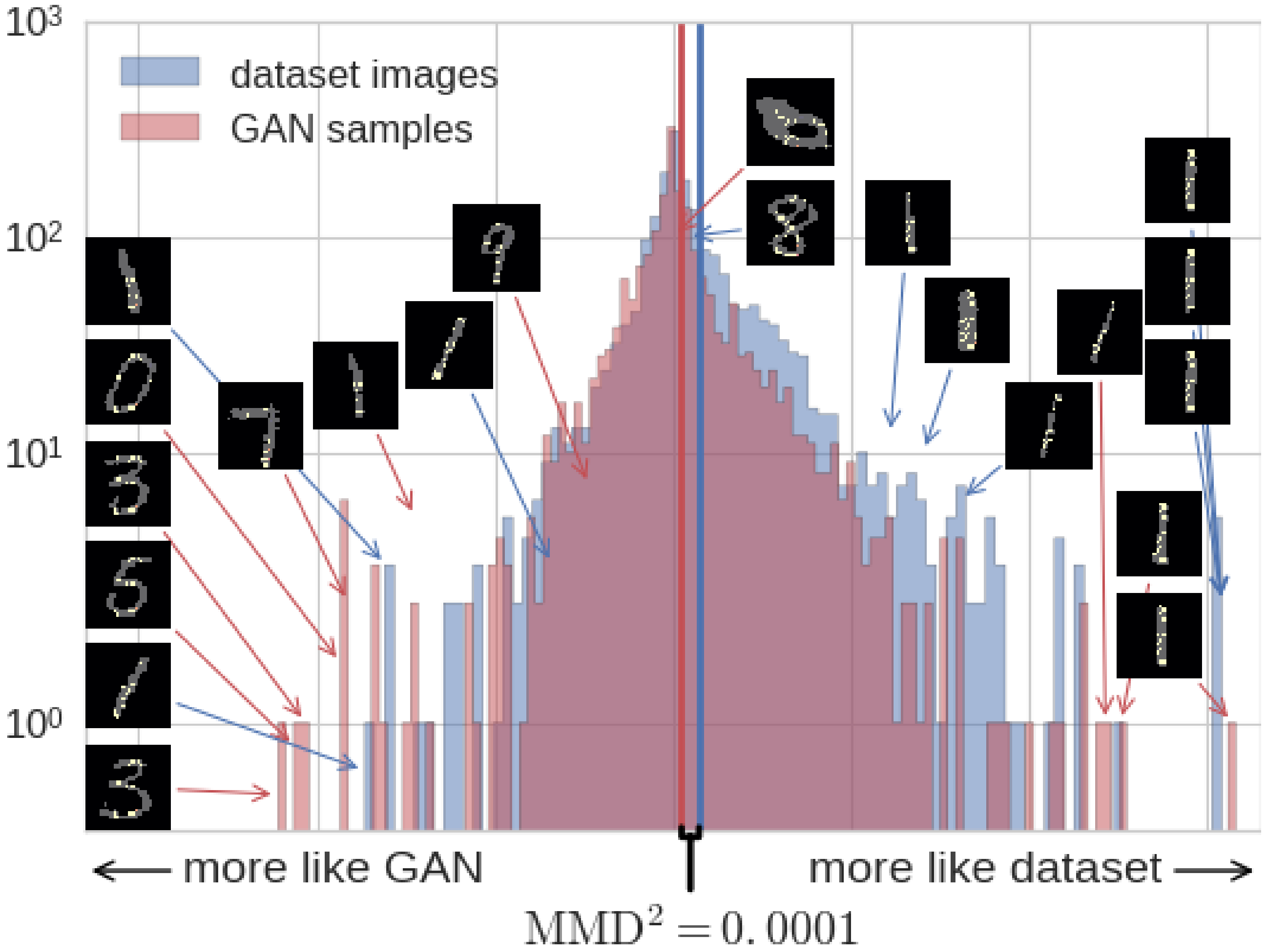
Blobs kernels



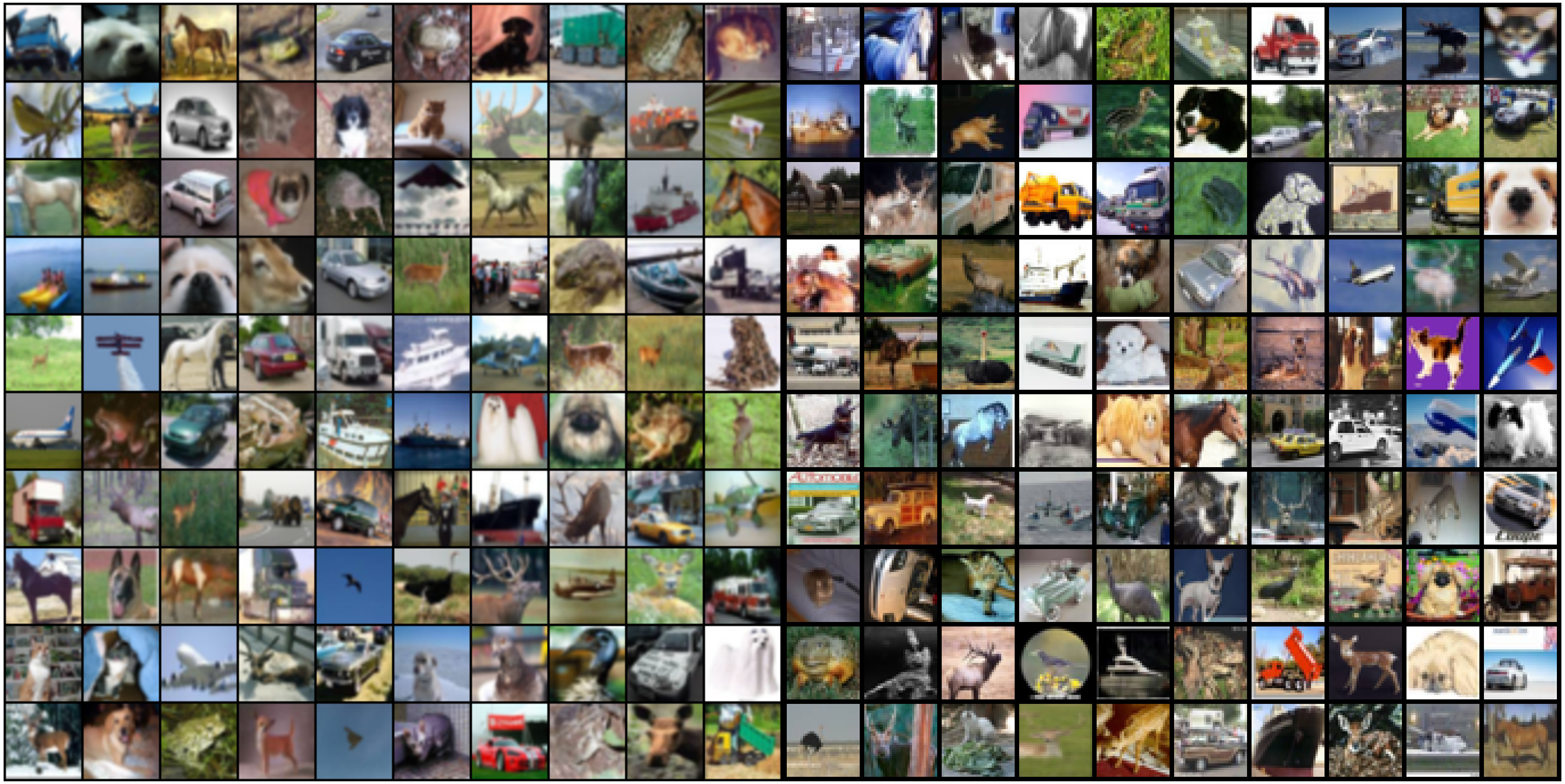
Blobs results



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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- 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

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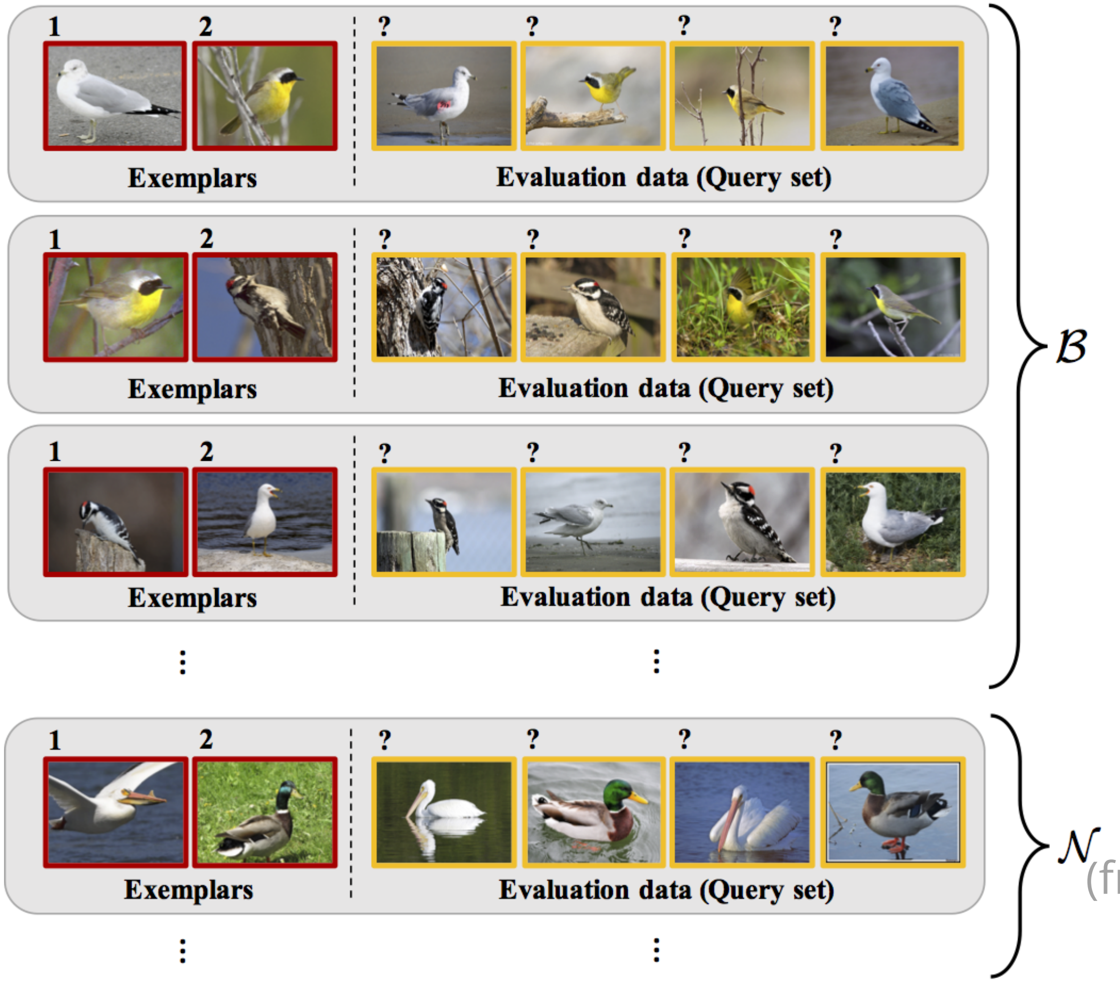
- Similar setup to meta-learning:



(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?

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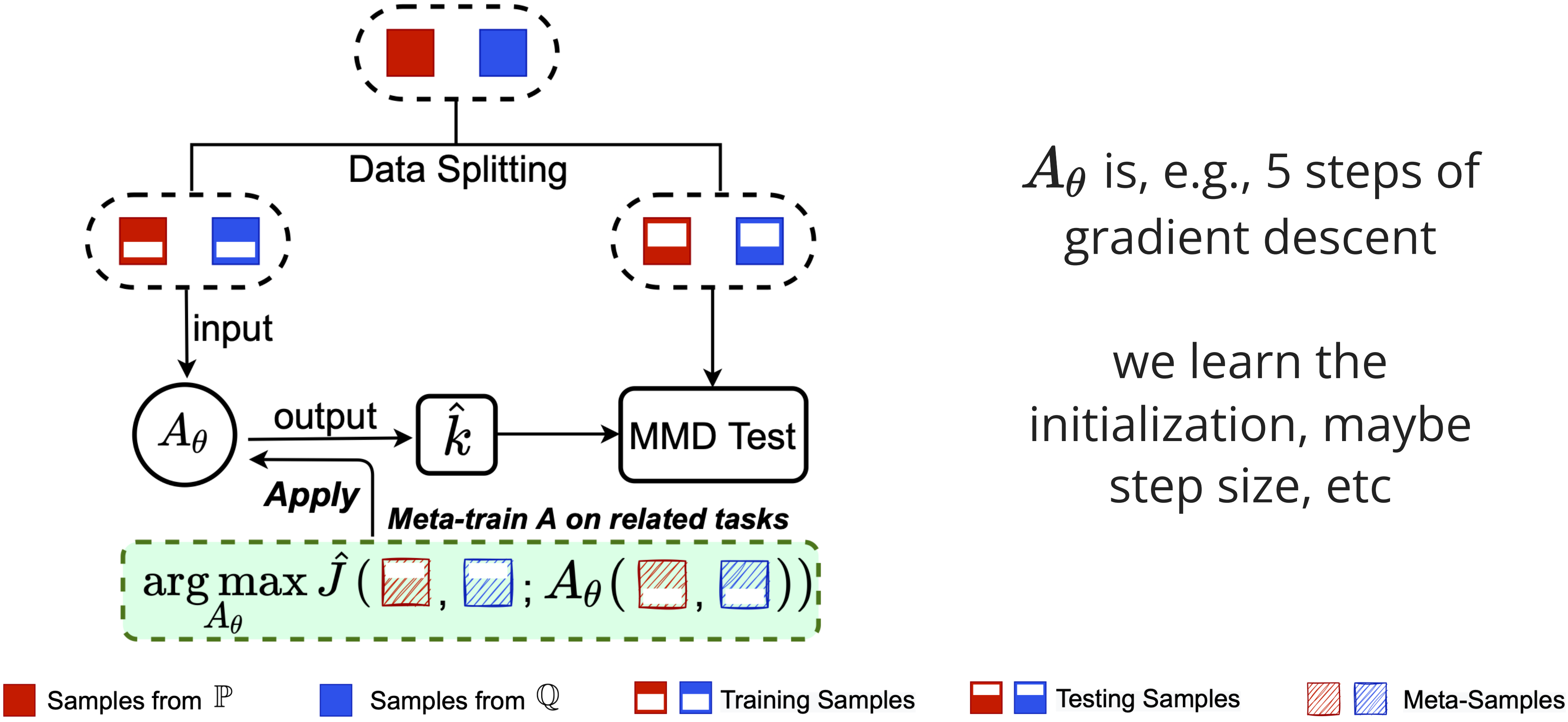
- CIFAR-10 has 60,000 images, but CIFAR-10.1 only has 2,031
- Where do we get related data from?
- One option: set up tasks to distinguish classes of CIFAR-10 (airplane vs automobile, airplane vs bird, ...)

One approach (MAML-like)



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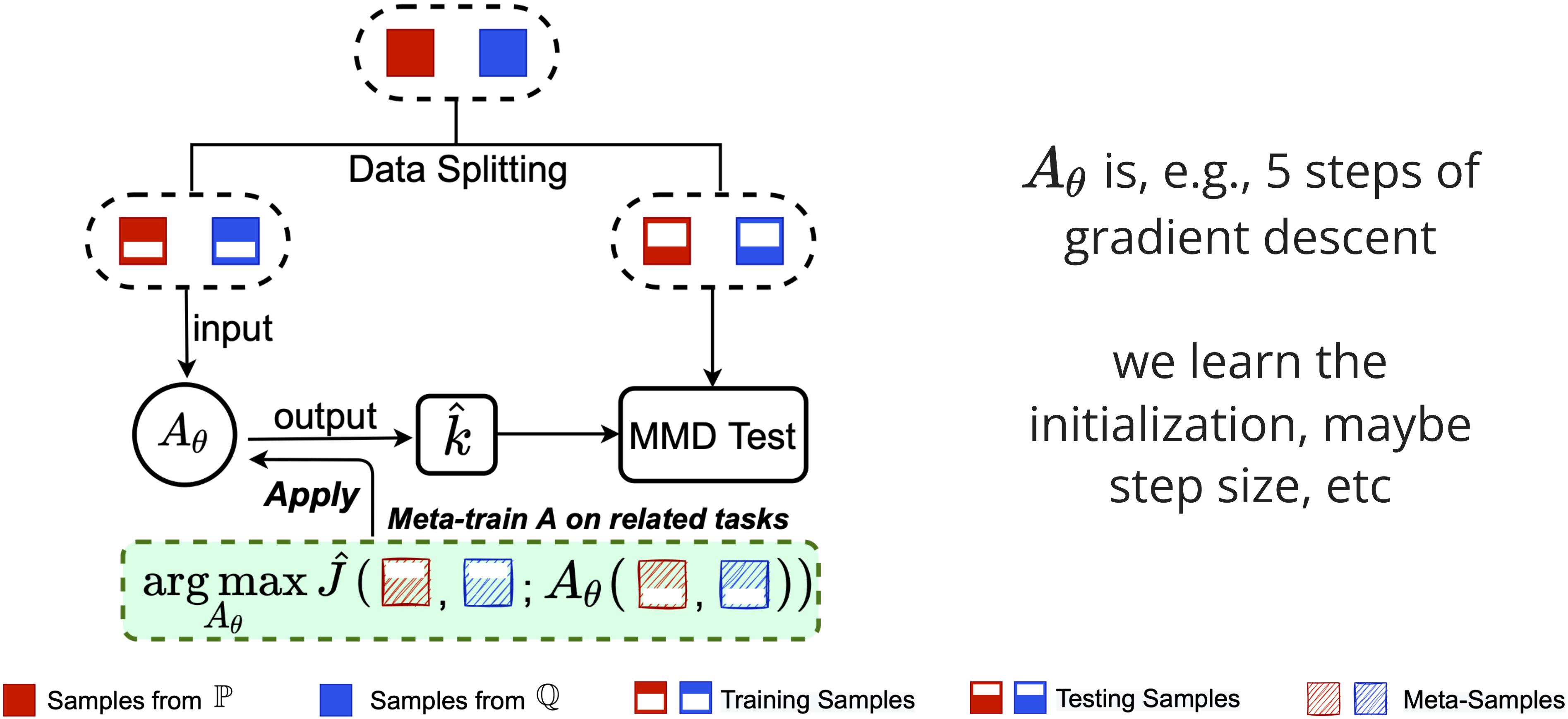

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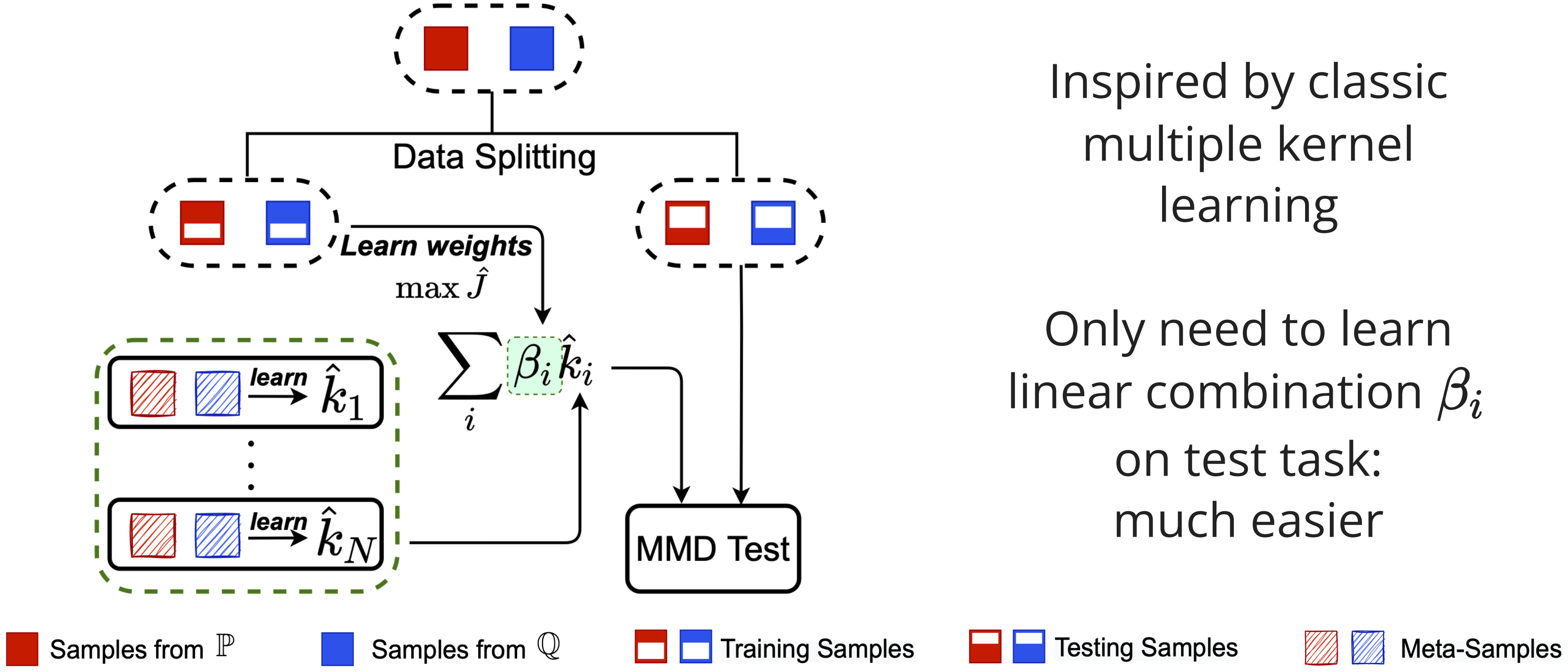
This works, but not as well as we'd hoped...
Initialization might work okay on everything, not really adapt

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

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- But multiplier is *much* better:
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Theoretical analysis for Meta-MKL

- 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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- Also useful for **fair representation learning**
  - e.g. can distinguish “creditworthy” vs not, can't distinguish by race

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Choose k with $\min_k \rho_k^s - \rho_k^t$

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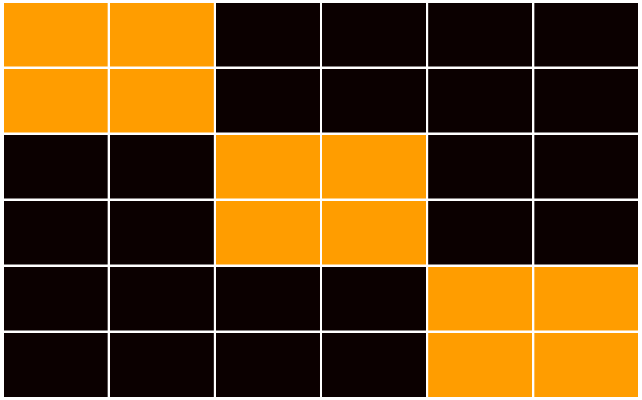
  - Can estimate c_α inside the optimization
  - Better, but tends to “stall out” in minimizing ρ_k^s

Block estimator [Zaremba+ NeurIPS-13]

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



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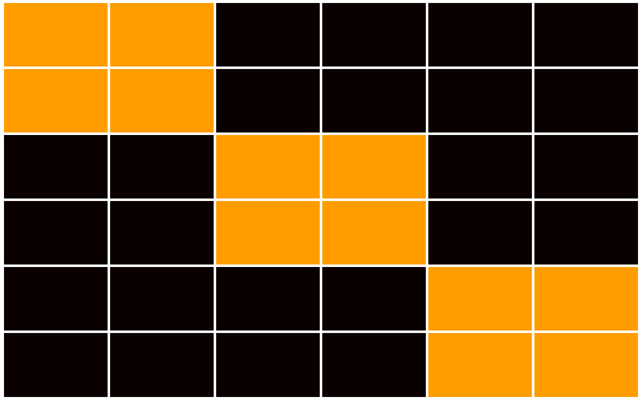

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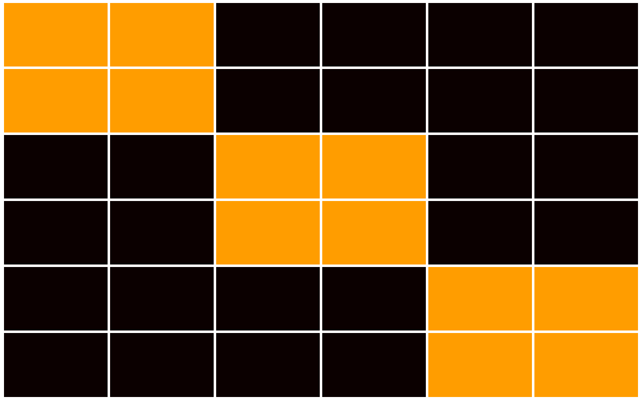

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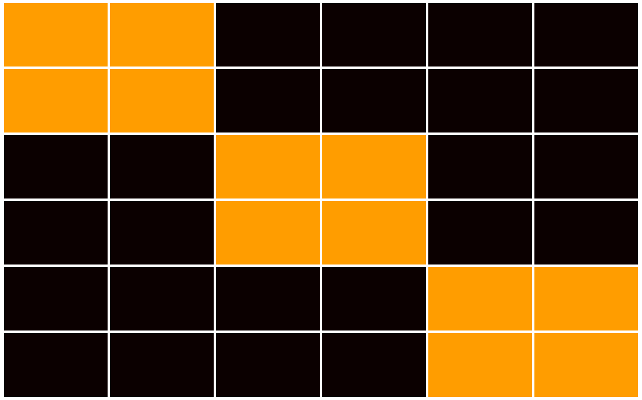

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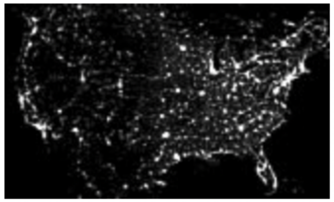
  - κ could be deep itself, with adversarial optimization
  - For now, just Gaussians with different lengthscales

Adult

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
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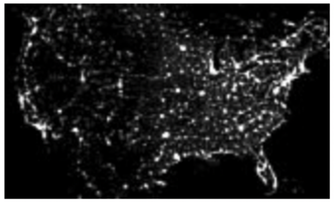

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Shapes3D

$\mathbb{P}^t$:

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ci-ratio	Method	Pr(target)↑	Pr(sensitive)↓	Pr(sensitive) fine-tuned↓
$(0.1, 0.1)$	Laftr	0.2500	0.6100	1.000 ($\sigma = 0.111$)
	Cfair	0.2500	0.6071	**0.8929** ($\sigma = 0.087$)
	Ffvae	0.1785	0.6428	1.000 ($\sigma = 0.0695$)
	Ours	**1.000**	**0.2500**	0.9642 ($\sigma = 0.007$)
$(0.33, 0.66)$	Laftr	0.285	0.607	1.000 ($\sigma = 0.237$)
	Cfair	0.2857	0.6071	1.000 ($\sigma = 0.234$)
	Ffvae	0.9642	1.000	1.000 ($\sigma = 0.075$)
	Ours	1.000	**0.5614**	**0.6842** ($\sigma = 0.005$)

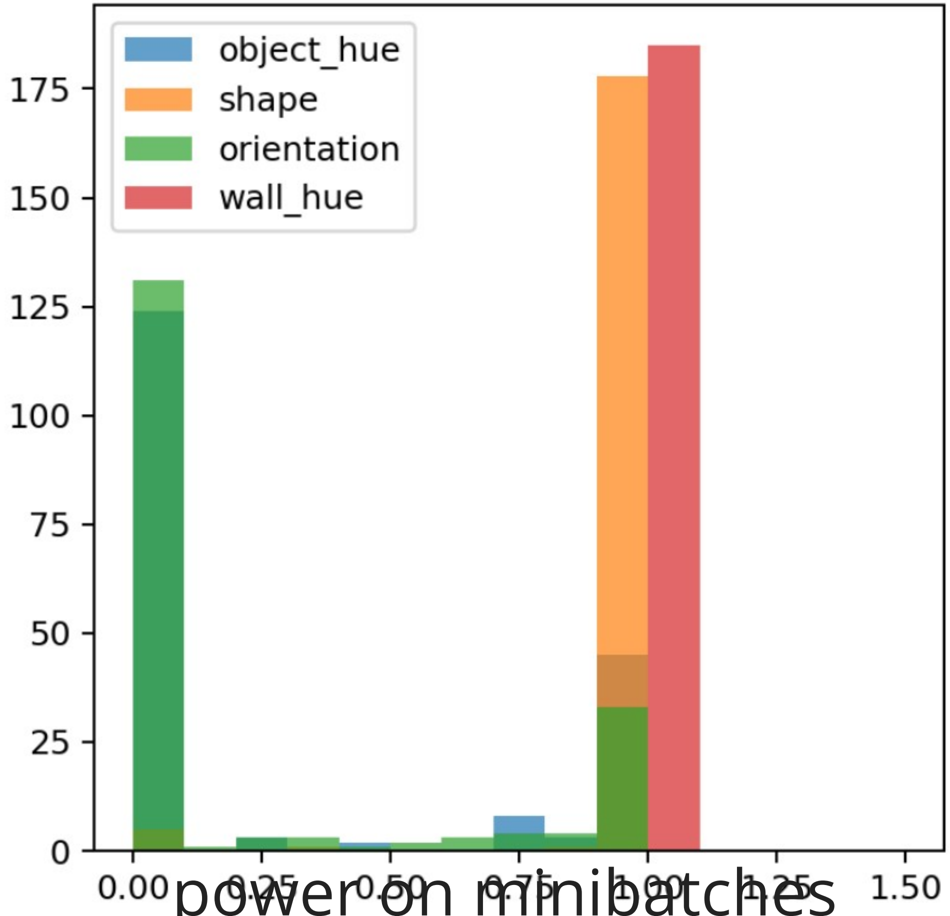
(a) **Adult dataset:** Our method outperforms all others even when additional layers are trained to maximize the sensitive power (albeit with smaller bandwidths in the under-represented scenario).

ci-ratio	Method	Pr(target)↑	Pr(sensitive)↓	Pr(sensitive) fine-tuned↓
$(0.1, 0.1)$	Laftr	1.000	1.000	1.000 ($\sigma = 0.001$)
	Cfair	1.000	1.000	1.000 ($\sigma = 0.003$)
	Ffvae	0.9574	0.9787	1.000 ($\sigma = 0.1002$)
	Ours	**1.000**	**0.0744**	**0.9625** ($\sigma = 0.0205$)
$(0.9, 0.1)$	Laftr	1.000	1.000	1.000 ($\sigma = 0.006$)
	Cfair	1.000	1.000	1.000 ($\sigma = 0.005$)
	Ffvae	**0.8723**	**0.8723**	1.000 ($\sigma = 0.092$)
	Ours	0.1383	1.000	1.000 ($\sigma = 0.006$)

(b) **3DShapes dataset:** Our method is able to outperform others in the under-represented case, but the highly correlated scenario of **ci-ratio**=(0.9,0.1) is a failure case.

Multiple targets / sensitive attributes

$$\max_k \frac{1}{|\mathcal{T}|} \sum_{t \in \mathcal{T}} \rho_k^t - \frac{1}{|\mathcal{S}|} \sum_{s \in \mathcal{S}} \rho_k^s$$



power on minibatches

Remaining challenges

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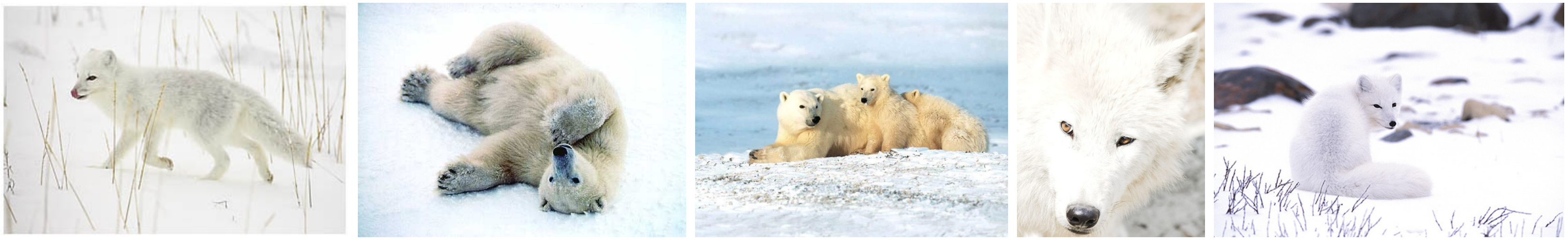

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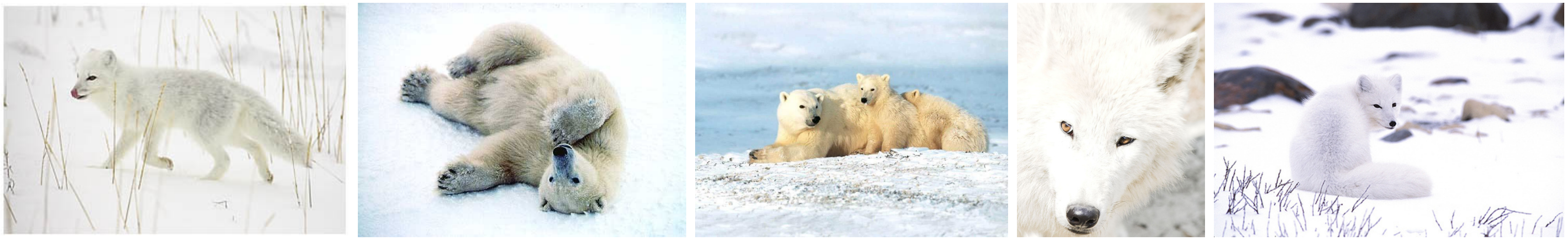

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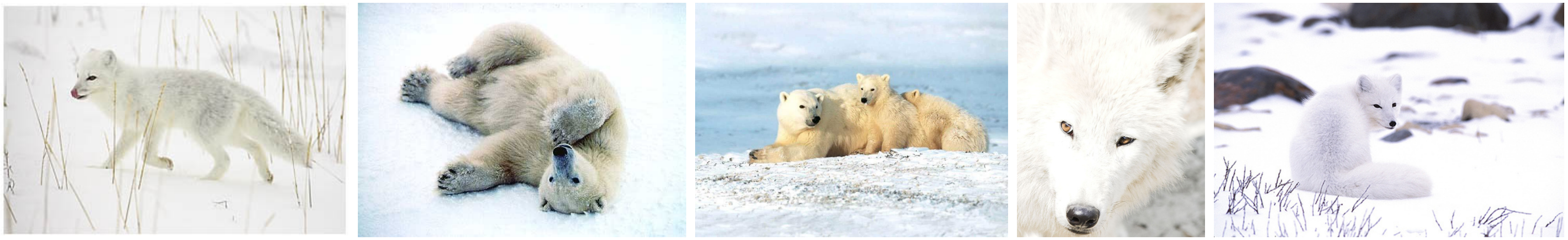

- Avoid the need for data splitting (selective inference)
  - Kübler+ NeurIPS-20 gave one method, but very limited

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"