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MMD Aggregated Two-Sample Test KSD Aggregated Goodness-of-fit Test

University College London
Centre for Artificial Intelligence
Gatsby Computational Neuroscience Unit
Inria London Programme

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Overview

1 MMDAgg: MMD Aggregated Two-Sample Test

- Two-sample problem
- MMD single test
- MMD aggregated test
- Experiments

2 KSDAgg: KSD Aggregated Goodness-of-fit Test

- Goodness-of-fit problem & KSD tests
- Uniform separation rate
- Experiments

MMD Aggregated Two-Sample Test



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Two-sample problem

Two-sample problem:

Given independent samples

- $\mathbb{X}_m := (\textcolor{blue}{X}_1, \dots, \textcolor{blue}{X}_m)$ where $X_i \stackrel{\text{iid}}{\sim} p$ in \mathbb{R}^d
- $\mathbb{Y}_n := (\textcolor{red}{Y}_1, \dots, \textcolor{red}{Y}_n)$ where $Y_i \stackrel{\text{iid}}{\sim} q$ in \mathbb{R}^d

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Statistical hypothesis testing:

$$\begin{array}{lll} \mathcal{H}_0: p = q & \text{against} & \mathcal{H}_a: p \neq q \\ \Delta(\mathbb{X}_m, \mathbb{Y}_n) = 1 & \iff & \text{reject } \mathcal{H}_0 \\ \Delta(\mathbb{X}_m, \mathbb{Y}_n) = 0 & \iff & \text{fail to reject } \mathcal{H}_0 \end{array}$$

What is a ‘good’ test Δ ?

By design: probability of type I error is α -controlled

$$\mathbb{P}_{\textcolor{blue}{p} \times \textcolor{blue}{p}}(\Delta(\mathbb{X}_{\textcolor{blue}{m}}, \mathbb{Y}_{\textcolor{blue}{n}}) = 1) \leq \alpha$$

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Uniform separation rate: What is the smallest value of $\|\mathbf{p} - \mathbf{q}\|_2$ which always ensures that Δ β -controls (\star) for any \mathbf{p} and \mathbf{q} satisfying $\mathbf{p} - \mathbf{q} \in \mathcal{C}$?

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$$\mathbb{P}_{p \times p}(\Delta(\mathbb{X}_m, \mathbb{Y}_n) = 1) \leq \alpha$$

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$$\mathbb{P}_{p \times q}(\Delta(\mathbb{X}_m, \mathbb{Y}_n) = 0) \leq \beta \quad (\star)$$

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Question: Which class of functions \mathcal{C} to use?

Sobolev balls

Sobolev balls:

$$\mathcal{S}_d^s(R) := \left\{ f \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d) : \int_{\mathbb{R}^d} \|\xi\|_2^{2s} |\widehat{f}(\xi)|^2 d\xi \leq (2\pi)^d R^2 \right\}$$

- radius $R > 0$
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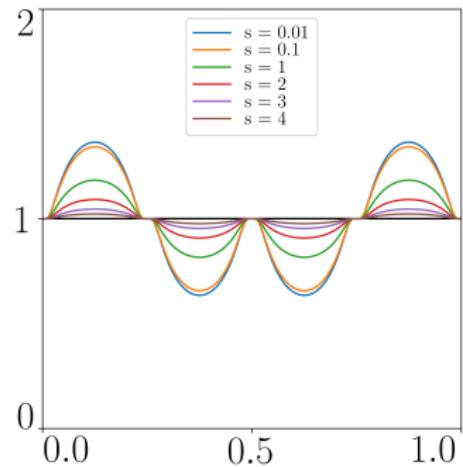
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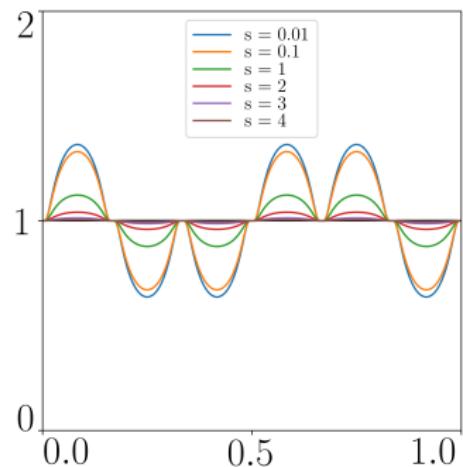
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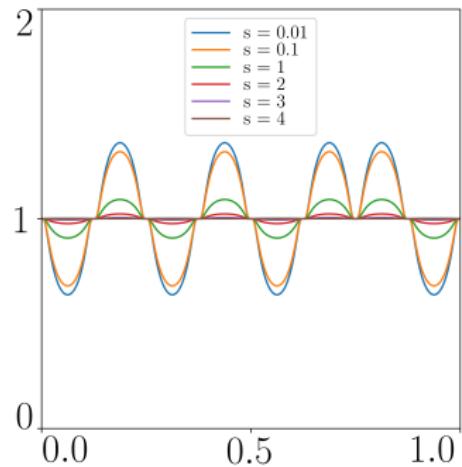
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Kernel: positive definite function $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$

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Reproducing Kernel Hilbert Space (RKHS): inner product space of real-valued functions \mathcal{H}_k satisfying:

- $k(\cdot, x) \in \mathcal{H}_k$
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Translation-invariant kernel: $k(x, y) := \prod_{i=1}^d K_i(x_i - y_i)$

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Bandwidth: $\lambda = (\lambda_1, \dots, \lambda_d) \in (0, \infty)^d$ giving the kernel

$$k_\lambda(x, y) := \prod_{i=1}^d \frac{1}{\lambda_i} K_i\left(\frac{x_i - y_i}{\lambda_i}\right)$$

Gaussian kernel

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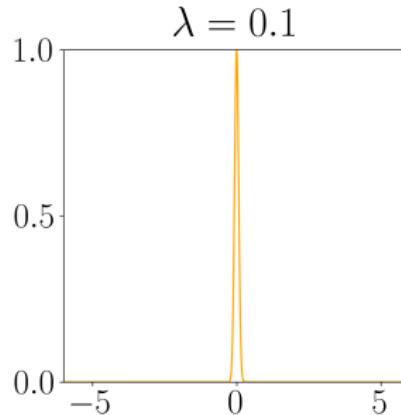
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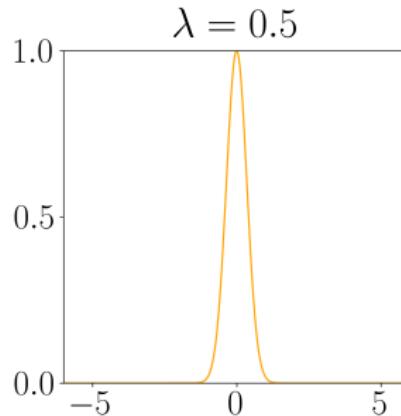


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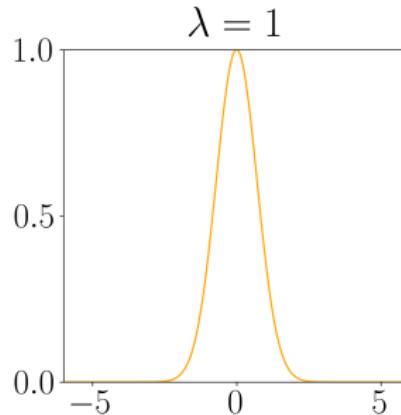


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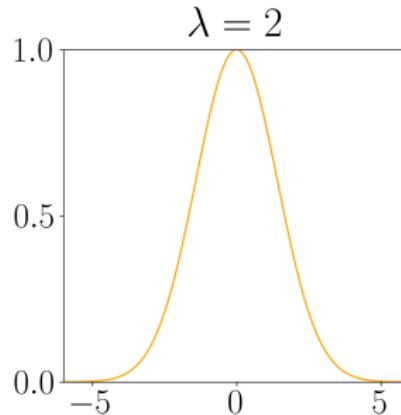


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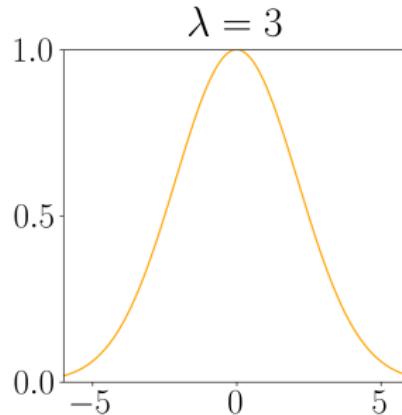


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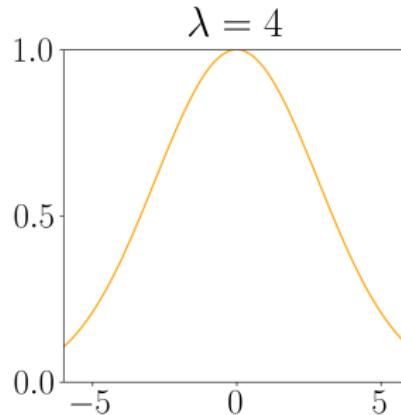


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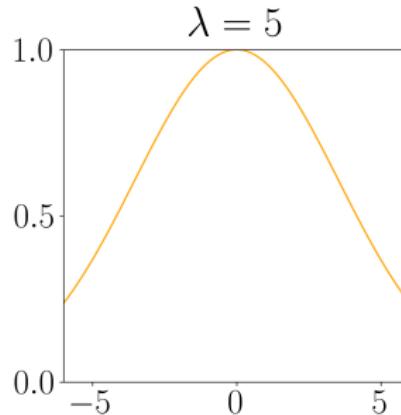


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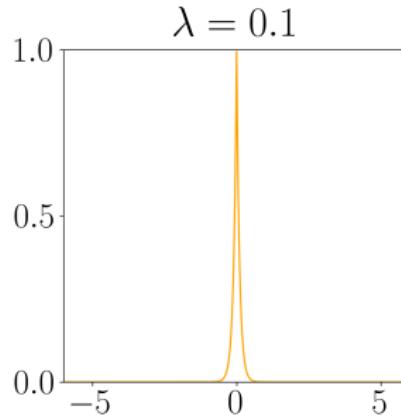
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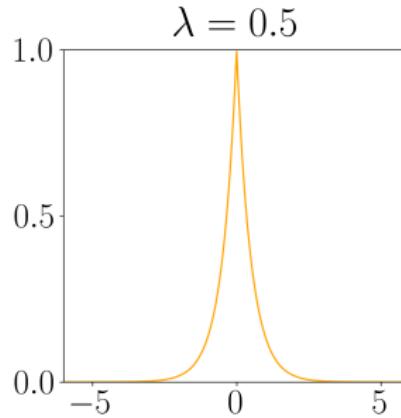


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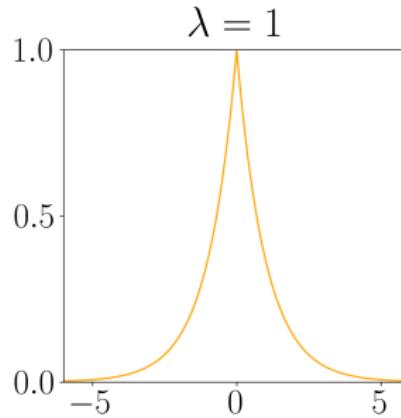


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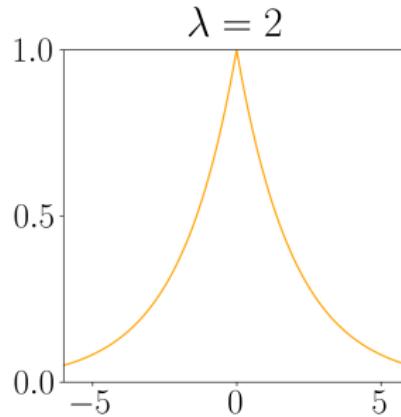


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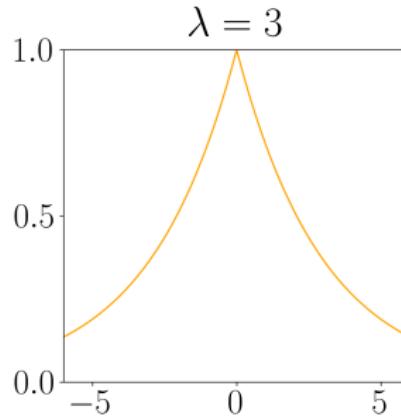


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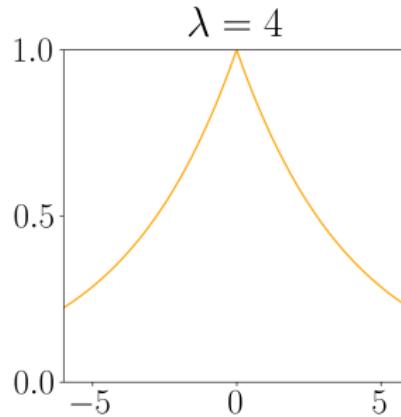


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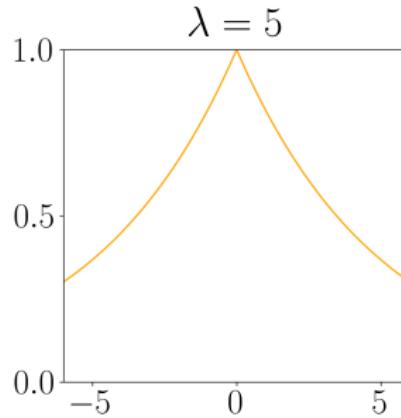


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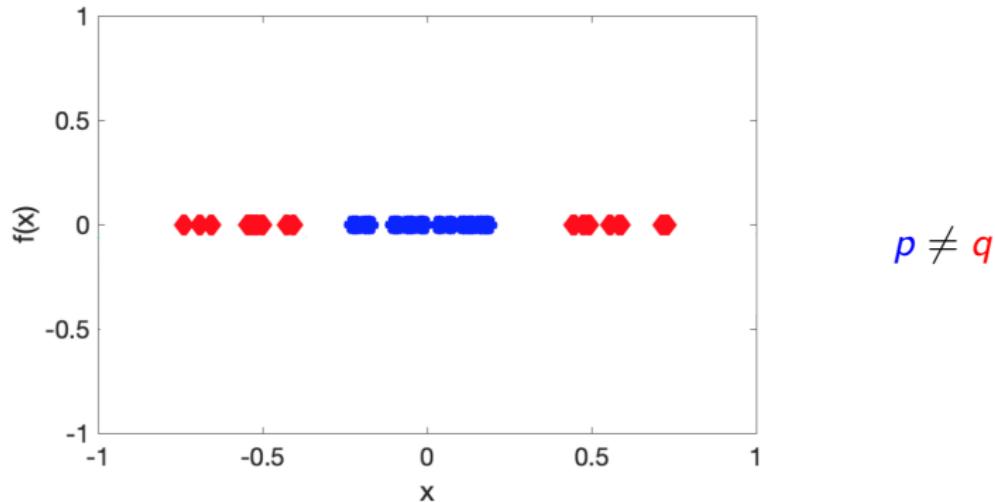
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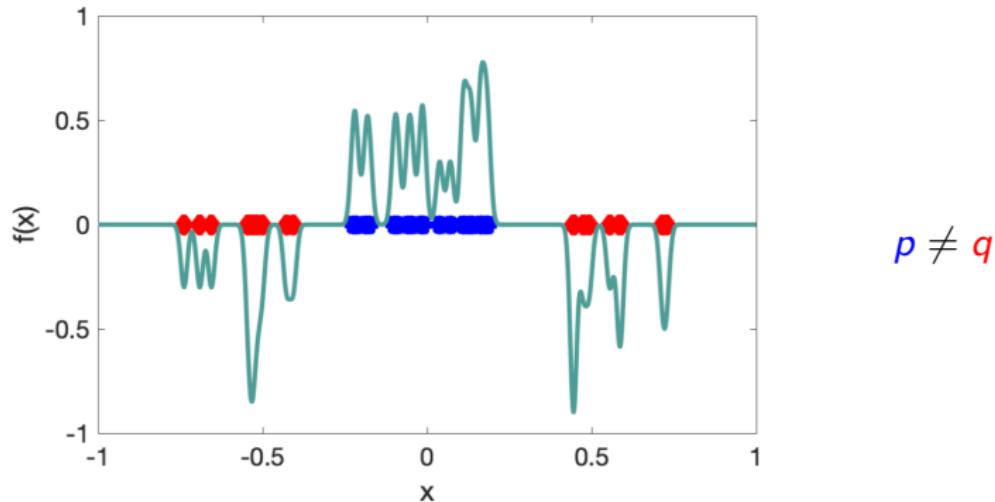
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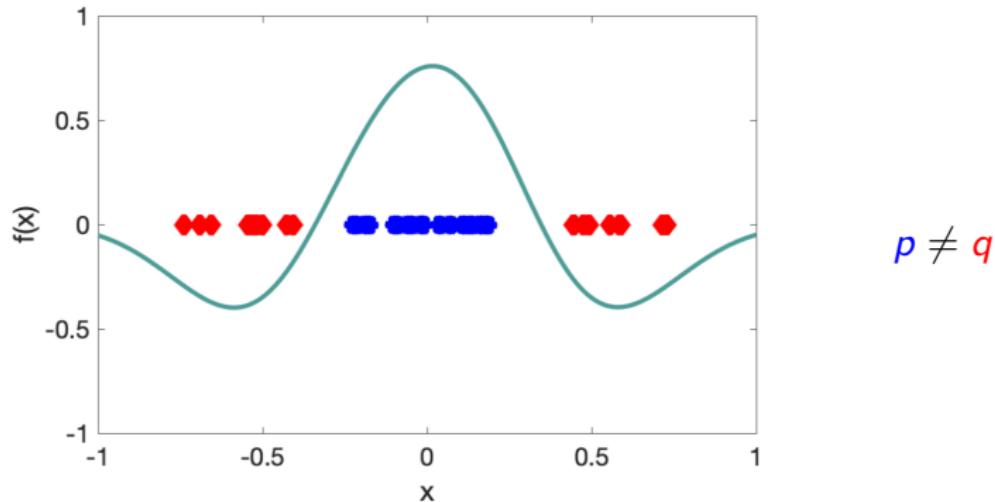


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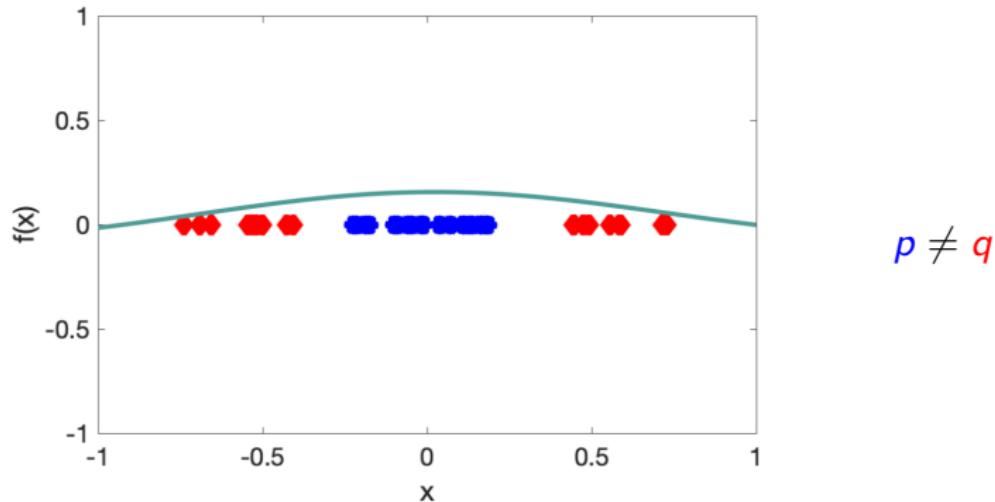


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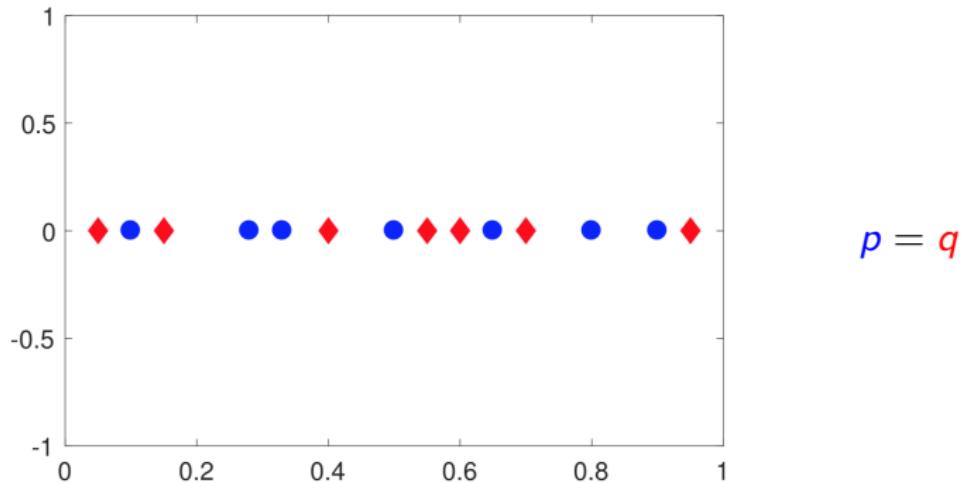


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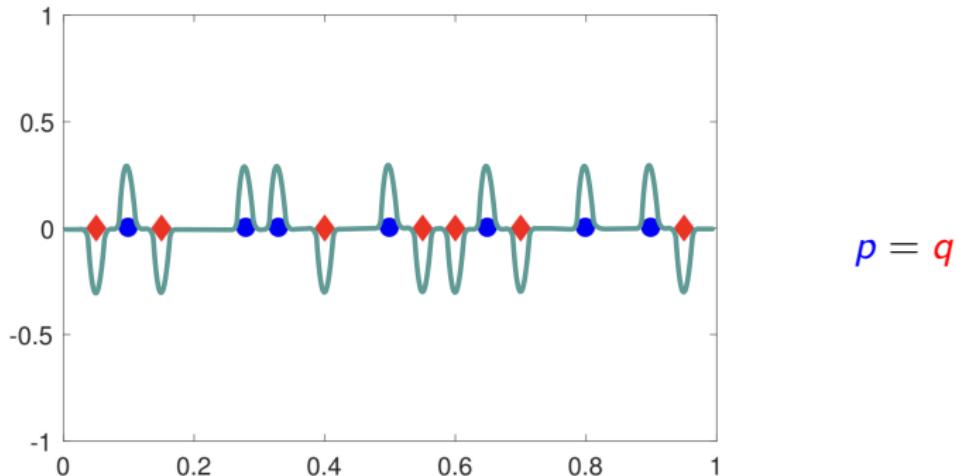
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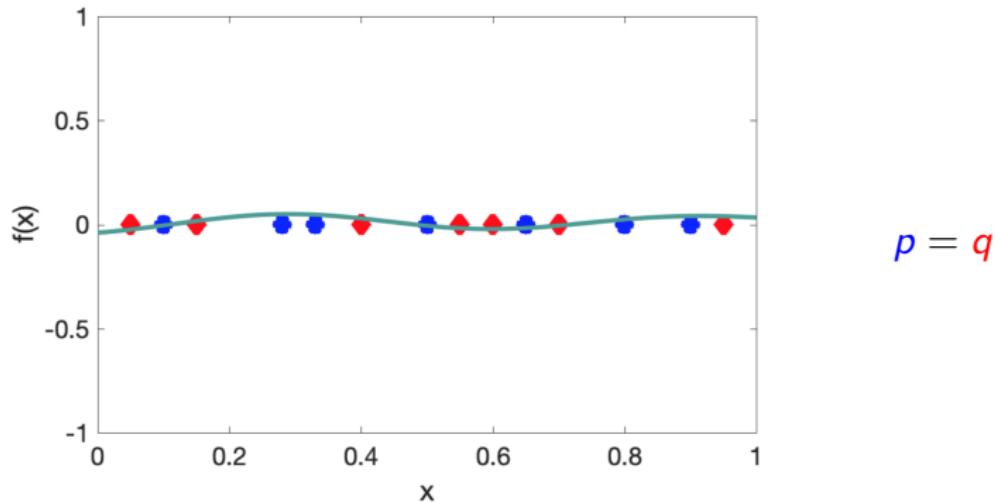


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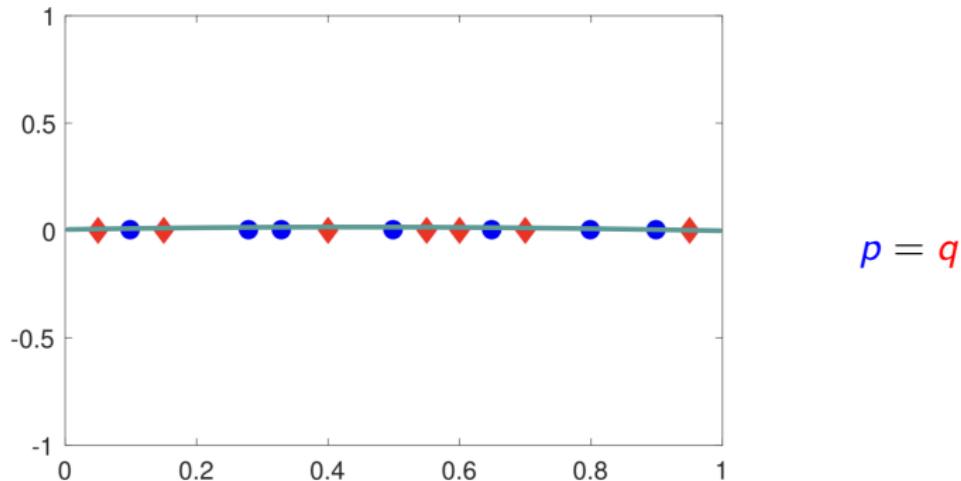


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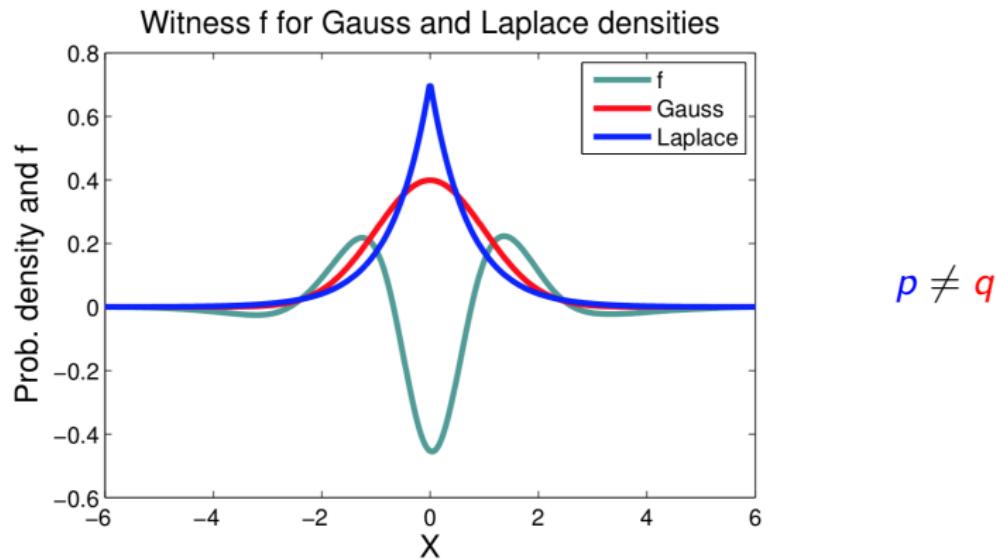


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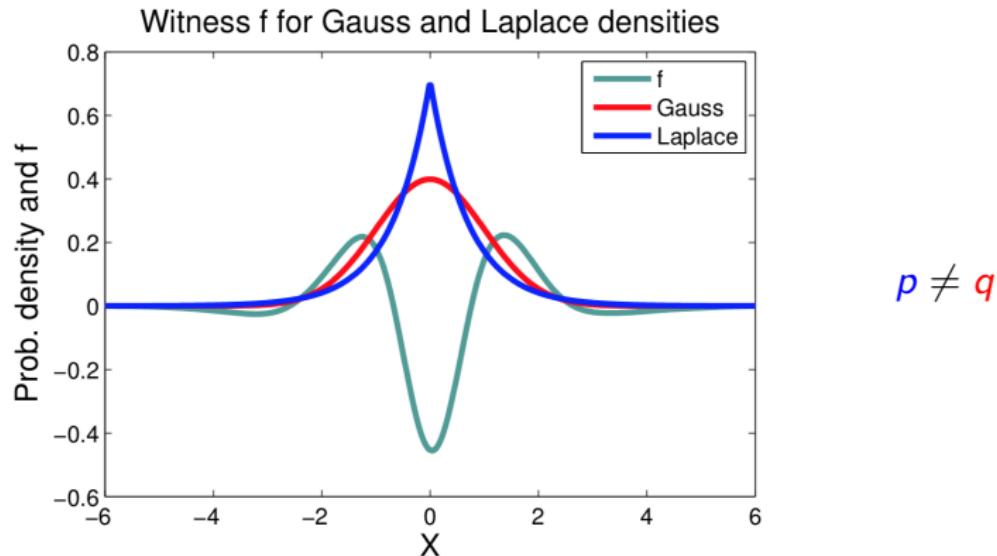
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Characteristic kernel: property on the kernel which ensures that

$$\text{MMD}_{\lambda}(p, q) = 0 \iff p = q$$

Fukumizu et al. Kernel measures of conditional dependence. *NeurIPS*, 2008.

Bandwidth intuition

- **Small sample sizes:** only global differences are detectable
 - **Small bandwidth:** wrongly detects artificial local differences under \mathcal{H}_0
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Bandwidths should decrease as the **sample sizes** increase

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Our paper: propose new method which

- aggregates multiple tests with different bandwidths

- avoids using arbitrary heuristics or data splitting

⇒ non-asymptotic power guarantees

MMD single test using permutations

Maximum Mean Discrepancy: $\text{MMD}_{\lambda}^2(p, q)$ is equal to

$$\mathbb{E}_{X, X' \sim p}[k_{\lambda}(X, X')] - 2 \mathbb{E}_{X \sim p, Y \sim q}[k_{\lambda}(X, Y)] + \mathbb{E}_{Y, Y' \sim q}[k_{\lambda}(Y, Y')]$$

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Assumption: equal sample sizes $m = n$

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MMD single test: uniform separation rate

Minimax rate over Sobolev balls: $(m + n)^{-2s/(4s+d)}$

Theorem

For $\alpha \in (0, e^{-1})$, $s > 0$, $R > 0$, $B \in \mathbb{N}$ large enough, using either permutations or a wild bootstrap, the test $\Delta_\alpha^{\lambda^*}$ with

$$\lambda_i^* = (m + n)^{-2/(4s+d)}, i = 1, \dots, d$$

is optimal in the minimax sense over the Sobolev ball $\mathcal{S}_d^s(R)$

$$\rho\left(\Delta_\alpha^{\lambda^*}, \mathcal{S}_d^s(R), \beta\right) \leq C(d, s, R, \alpha, \beta) (m + n)^{-2s/(4s+d)}.$$

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For $\alpha \in (0, e^{-1})$, $s > 0$, $R > 0$, $B \in \mathbb{N}$ large enough, using either permutations or a wild bootstrap, the test $\Delta_\alpha^{\lambda^*}$ with

$$\lambda_i^* = (m + n)^{-2/(4s+d)}, i = 1, \dots, d$$

is optimal in the minimax sense over the Sobolev ball $\mathcal{S}_d^s(R)$

$$\rho\left(\Delta_\alpha^{\lambda^*}, \mathcal{S}_d^s(R), \beta\right) \leq C(d, s, R, \alpha, \beta) (m + n)^{-2s/(4s+d)}.$$

⇒ single test $\Delta_\alpha^{\lambda^*}$ is **optimal** but **not adaptive** over Sobolev balls:

- **optimal:** uniform separation rate of $\Delta_\alpha^{\lambda^*}$ achieves the minimax rate
- **not adaptive:** λ^* depends on the unknown smoothness parameter s of $\mathcal{S}_d^s(R)$ (i.e. cannot be implemented)

MMDAgg: MMD aggregated test

1 MMDAgg: MMD Aggregated Two-Sample Test

- Two-sample problem
- MMD single test
- **MMD aggregated test**
- Experiments

2 KSDAgg: KSD Aggregated Goodness-of-fit Test

- Goodness-of-fit problem & KSD tests
- Uniform separation rate
- Experiments

MMDAgg: MMD Aggregated test

Single test: Δ_α^λ for some bandwidth λ

Reject null hypothesis $\mathcal{H}_0 : p = q$ if

$$\widehat{\text{MMD}}_\lambda^2(\mathbb{X}_m, \mathbb{Y}_n) > \widehat{q}_{1-\alpha}^\lambda$$

MMDAgg: MMD Aggregated test

Aggregated test MMDAgg: Δ_α^Λ for some finite collection of bandwidths Λ

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How to ensure calibrated non-asymptotic level α for MMDAgg?

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How to ensure calibrated non-asymptotic level α for MMDAgg?

Introduce:

- positive weights $(w_\lambda)_{\lambda \in \Lambda}$ satisfying $\sum_{\lambda \in \Lambda} w_\lambda \leq 1$ (chosen by the user)
- correction u_α defined as

$$u_\alpha = \sup \left\{ u > 0 : \mathbb{P}_{p \times p} \left(\max_{\lambda \in \Lambda} \left(\widehat{\text{MMD}}_\lambda^2(\mathbb{X}_m, \mathbb{Y}_n) - \widehat{q}_{1-u w_\lambda}^\lambda \right) > 0 \right) \leq \alpha \right\}$$

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Aggregated test MMDAgg: Δ_α^Λ for some finite collection of bandwidths Λ

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The supremum can be estimated using the bisection method.

The probability can be estimated using a Monte-Carlo approximation.

MMDAgg: time complexity

$$\Delta_\alpha^\Lambda(\mathbb{X}_m, \mathbb{Y}_n) := \mathbb{1} \left(\widehat{\text{MMD}}_\lambda^2(\mathbb{X}_m, \mathbb{Y}_n) > \widehat{q}_{1-u_\alpha w_\lambda}^\lambda \text{ for some } \lambda \in \Lambda \right)$$

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- compute original MMD test statistic $\widehat{\text{MMD}}_\lambda^2(\mathbb{X}_m, \mathbb{Y}_n)$

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 - used to estimate the quantile $\widehat{q}_{1-u w_\lambda}^\lambda$

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MMDAgg time complexity:

$$\mathcal{O}(|\Lambda| (B_1 + B_2)(m + n)^2)$$

MMDAgg: uniform separation rate

Minimax rate over Sobolev balls: $(m + n)^{-2s/(4s+d)}$

Theorem

For $\alpha \in (0, e^{-1})$, $s > 0$, $R > 0$, $B_1, B_2, B_3 \in \mathbb{N}$ large enough, using either permutations or a wild bootstrap, the aggregated MMDAgg test $\Delta_\alpha^{\Lambda^*}$ with

$$\Lambda^* := \left\{ 2^{-\ell} \mathbb{1}_d : \ell \in \left\{ 1, \dots, \left\lceil \frac{2}{d} \log_2 \left(\frac{m+n}{\ln(\ln(m+n))} \right) \right\rceil \right\} \right\}$$

and $w_{\Lambda^*} := \frac{6}{\pi^2 \ell^2}$, is (almost) **optimal** and **adaptive** over the Sobolev balls $\{\mathcal{S}_d^s(R) : s > 0, R > 0\}$

$$\rho \left(\Delta_\alpha^{\Lambda^*}, \mathcal{S}_d^s(R), \beta \right) \leq C(d, s, R, \alpha, \beta) \left(\frac{m+n}{\ln(\ln(m+n))} \right)^{-2s/(4s+d)}.$$

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⇒ price to pay for **adaptivity** over $\{\mathcal{S}_d^s(R) : s > 0, R > 0\}$ is a $\ln(\ln(m+n))$ term in the **optimal** minimax rate

MMDAgg: summary of theoretical results

Minimax rate over Sobolev balls: $(m + n)^{-2s/(4s+d)}$

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Single test: Δ_α^{λ} for a kernel bandwidth λ

- **optimal:** uniform separation rate of $\Delta_\alpha^{\lambda^*}$ is $(m + n)^{-2s/(4s+d)}$
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- **not adaptive:** λ^* depends on unknown parameter s of $\mathcal{S}_d^s(R)$

MMDAgg test: Δ_α^Λ for a collection of kernel bandwidths $\Lambda = \{\lambda^{(j)}\}_{1 \leq j \leq N}$

- **(almost) optimal:** uniform separation rate of $\Delta_\alpha^{\Lambda^*}$ is

$$\left(\frac{m + n}{\ln(\ln(m + n))} \right)^{-2s/(4s+d)}$$

- **adaptive:** Λ^* is independent of unknown parameters s and R of $\mathcal{S}_d^s(R)$

MMDAgg: Experiments

1 MMDAgg: MMD Aggregated Two-Sample Test

- Two-sample problem
- MMD single test
- MMD aggregated test
- Experiments

2 KSDAgg: KSD Aggregated Goodness-of-fit Test

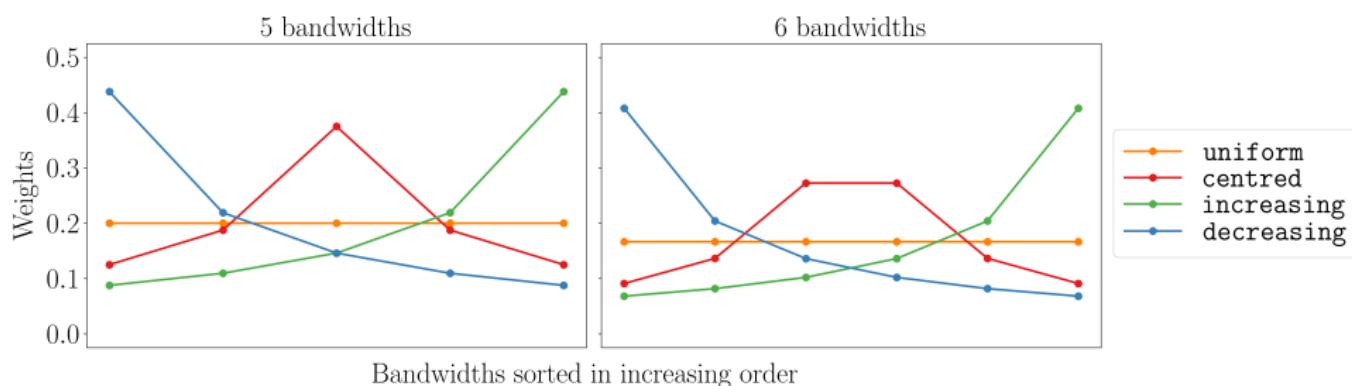
- Goodness-of-fit problem & KSD tests
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- Experiments

Weighting strategies

- **median bandwidth:** $(\lambda_{med})_i := \text{median}\{|z_i - z'_i| : z, z' \in \mathbb{X}_m \cup \mathbb{Y}_n, z \neq z'\}$
- **finite collection Λ of bandwidths:** for $\ell_-, \ell_+ \in \mathbb{N}$ with $N = 1 + \ell_- + \ell_+$
 $\Lambda(\ell_-, \ell_+) := \left\{ 2^\ell \lambda_{med} \in (0, \infty)^d : \ell \in \{\ell_-, \dots, \ell_+\} \right\} = \left\{ \lambda^{(j)} : j = 1, \dots, N \right\}$

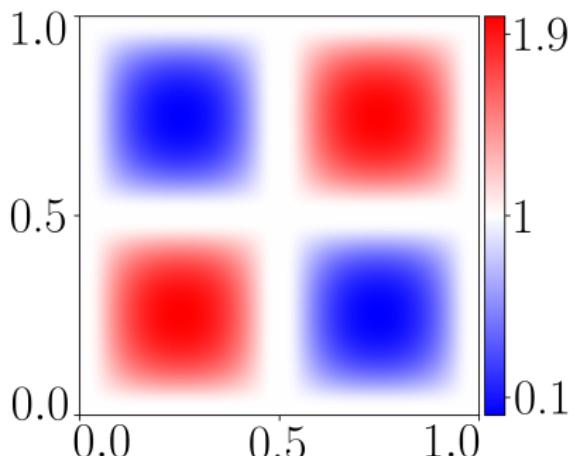
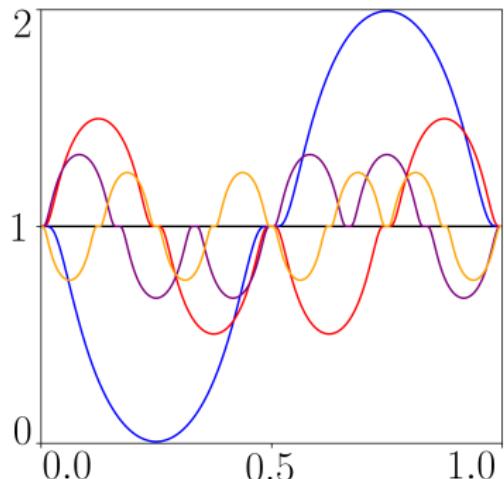
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- **uniform weights:** $w_{\lambda^{(j)}} := 1 / N$
- **increasing weights:** $w_{\lambda^{(j)}} := C / (N + 1 - j)$
- **decreasing weights:** $w_{\lambda^{(j)}} := C / j$
- **centred weights:** $w_{\lambda^{(j)}} := C / (|\frac{N+1}{2} - j| + 1)$ or $C / (|\frac{N+1}{2} - j| + \frac{1}{2})$



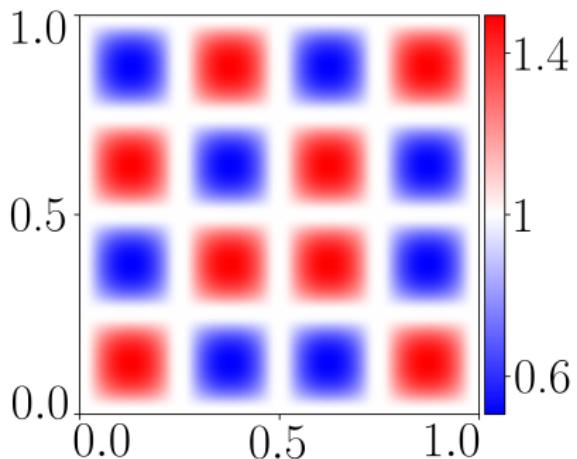
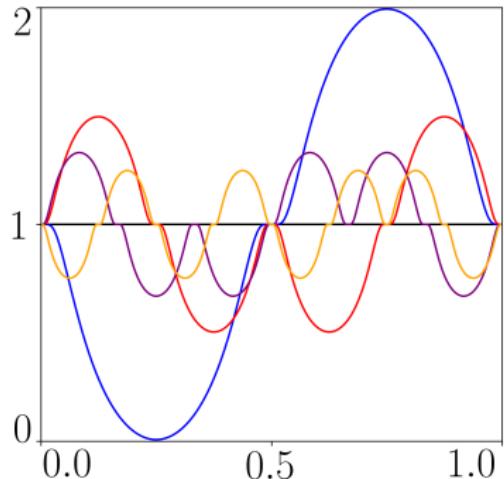
MMDAgg experiment: perturbed uniform distribution

Perturbed uniform densities: belong to Sobolev ball $\mathcal{S}_d^s(R)$



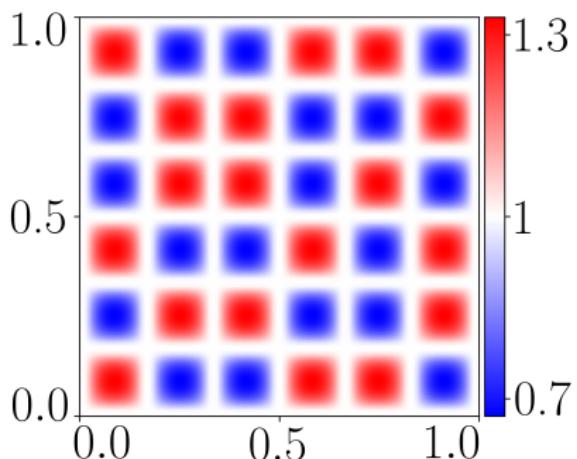
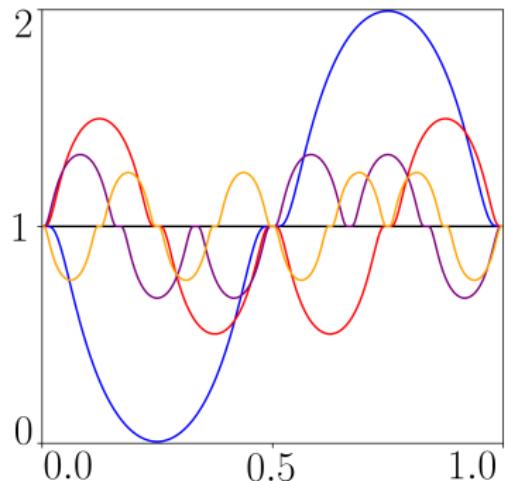
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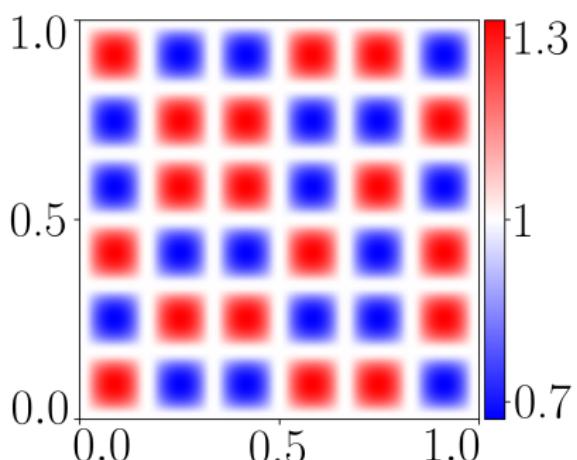
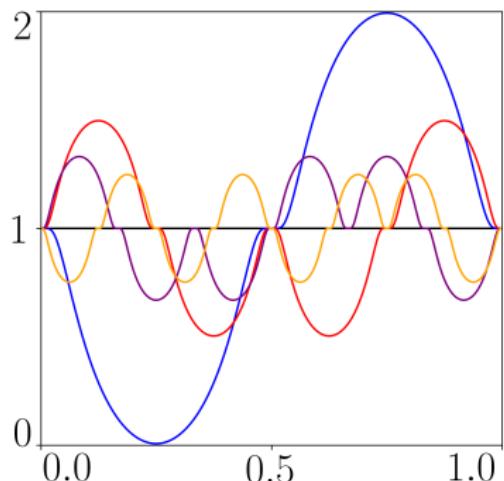
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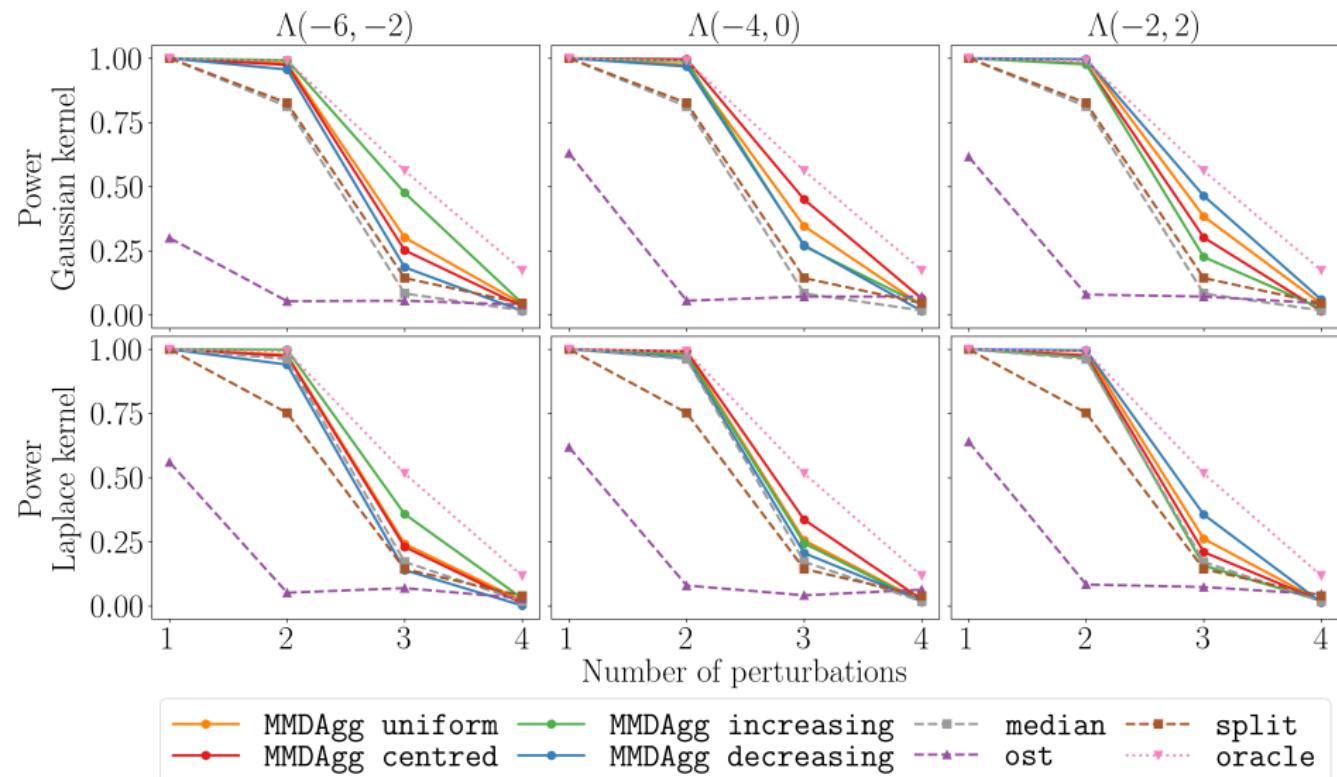
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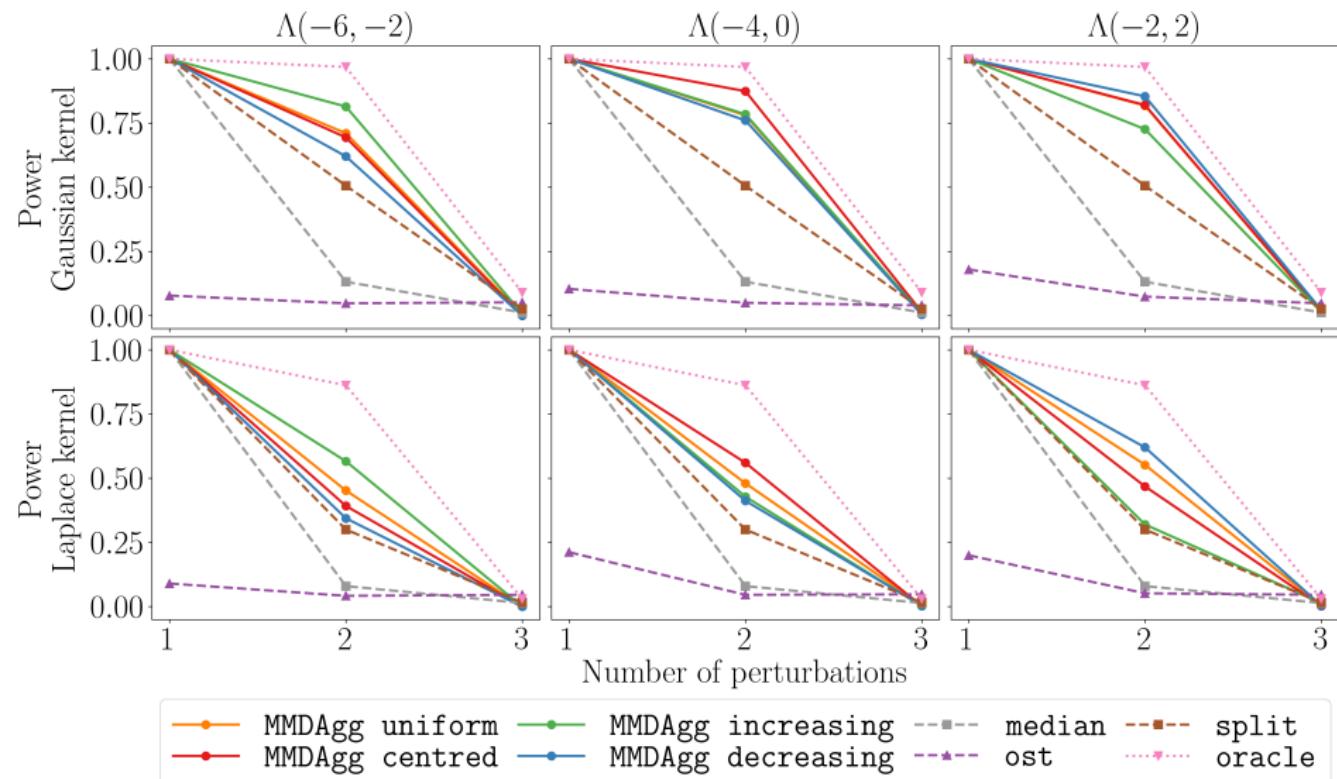
Perturbed uniform densities: used in the proof of lower bound on uniform separation rate over Sobolev balls $(m+n)^{-2s/(4s+d)}$ (**minimax rate**)

MMDAgg experiment: perturbed uniform 1d ($m=n=500$)



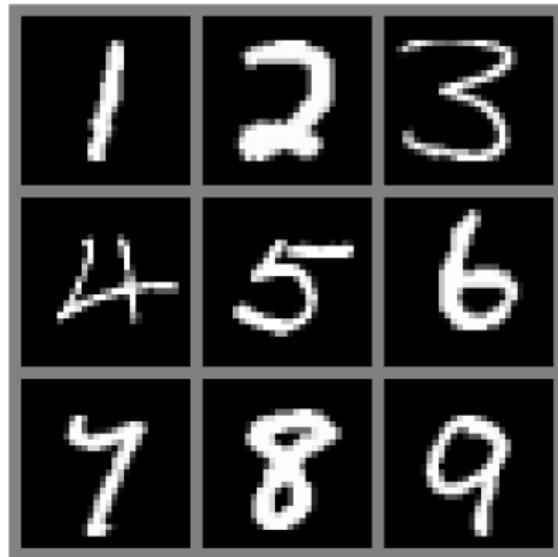
ost: Kübler et al. Learning kernel tests without data splitting. NeurIPS, 2020.

MMDAgg experiment: perturbed uniform 2d ($m=n=2000$)



MMDAgg experiment: MNIST

MNIST digits:



$\mathcal{P} : 0, 1, 2, 3, 4, 5, 6, 7, 8, 9$

$\mathcal{Q}_1 : 1, 3, 5, 7, 9$

$\mathcal{Q}_2 : 0, 1, 3, 5, 7, 9$

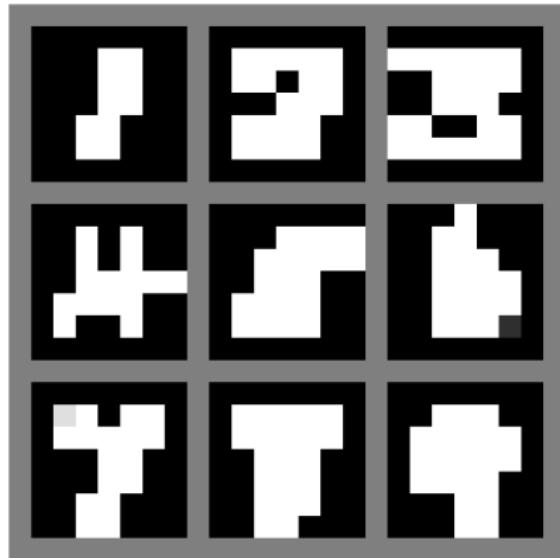
$\mathcal{Q}_3 : 0, 1, 2, 3, 5, 7, 9$

$\mathcal{Q}_4 : 0, 1, 2, 3, 4, 5, 7, 9$

$\mathcal{Q}_5 : 0, 1, 2, 3, 4, 5, 6, 7, 9$

MMDAgg experiment: MNIST

MNIST digits: images down-sampled to 7×7 resolution



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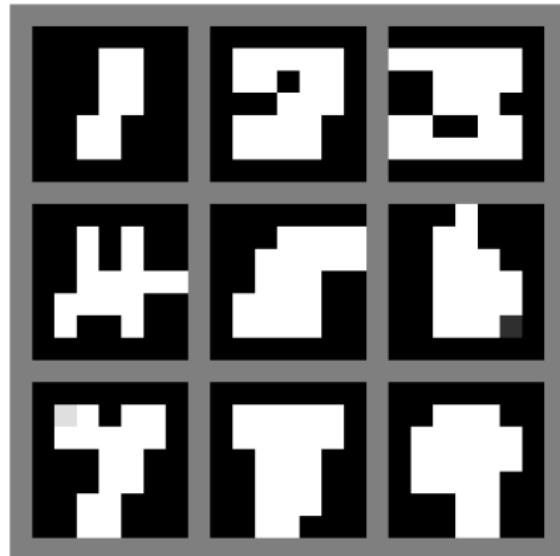
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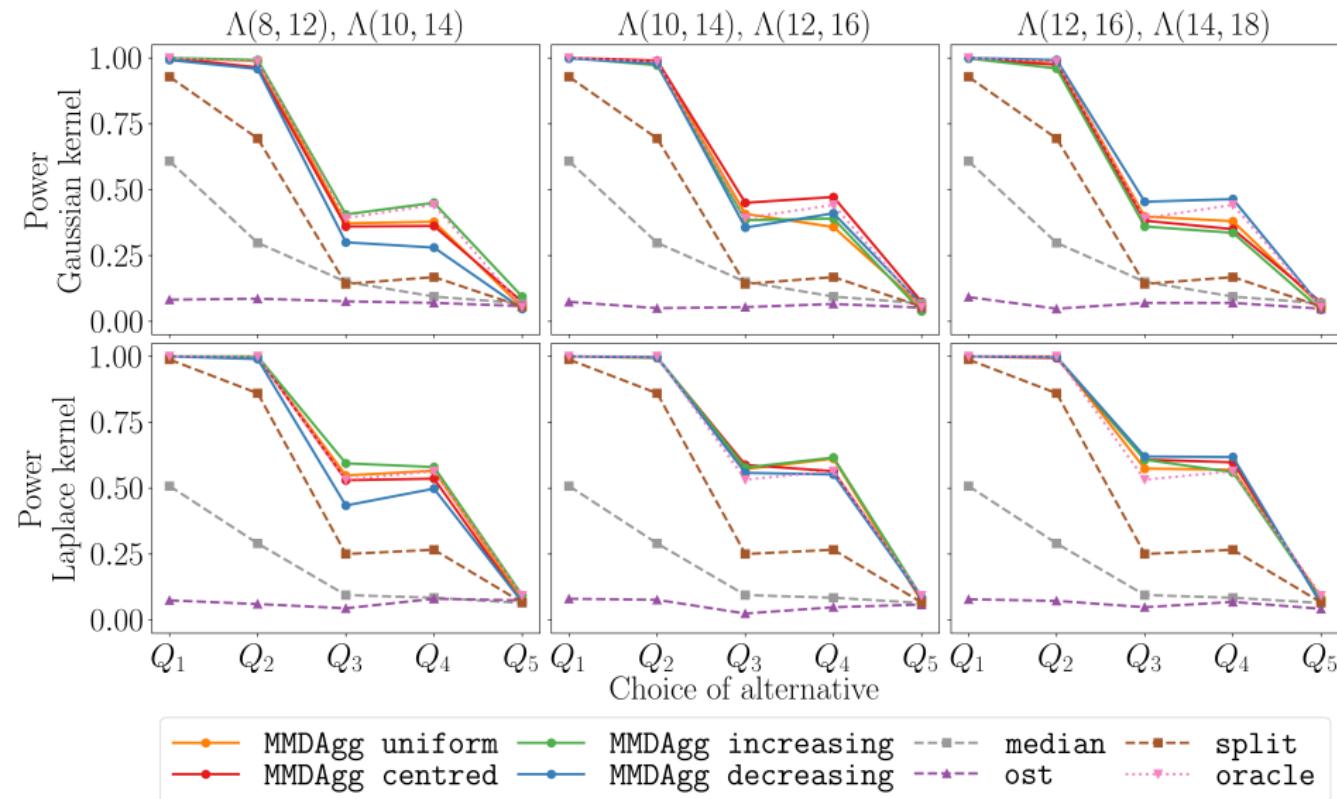
$$\mathcal{Q}_4 : 0, 1, 2, 3, 4, 5, 7, 9$$

$$\mathcal{Q}_5 : 0, 1, 2, 3, 4, 5, 6, 7, 9$$

Images: dimension 49

Problem: inherently lower-dimensional

MMDAgg experiment: MNIST ($m=n=500$)

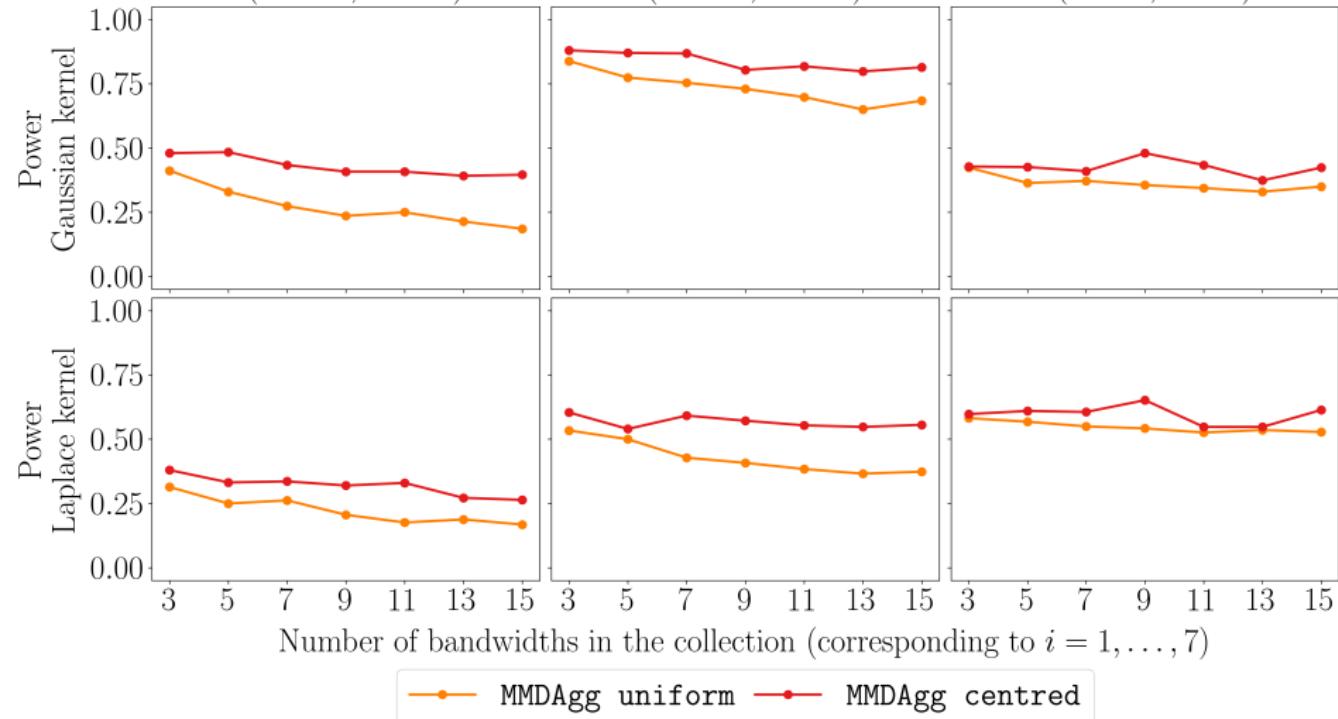


MMDAgg experiment: collections of bandwidths

$d = 1, 3$ perturbations
 $m = n = 500$
 $\Lambda(-2 - i, -2 + i)$

$d = 2, 2$ perturbations
 $m = n = 2000$
 $\Lambda(-2 - i, -2 + i)$

MNIST, Q_3 , $m = n = 500$
 $\Lambda(12 - i, 12 + i)$
 $\Lambda(14 - i, 14 + i)$



MMDAgg: conclusion

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MMDAgg theoretical results:

- optimal in the minimax sense (up to $\log(\log(m + n))$ term)
- adaptive test over Sobolev balls $\{S_d^s(R) : s > 0, R > 0\}$
- quantile estimation: wild bootstrap or permutations
- wide range of kernels

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MMDAgg experimental results:

- outperforms state-of-the-art MMD adaptive tests

MMDAgg paper



MMDAgg code



KSD Aggregated Goodness-of-fit Test



Antonin
Schrab

†‡§



Benjamin
Guedj

†§



Arthur
Gretton

‡

† Centre for Artificial Intelligence, UCL

‡ Gatsby Computational Neuroscience Unit, UCL

§ Inria London Programme

KSDAgg: Goodness-of-fit problem & KSD tests

1 MMDAgg: MMD Aggregated Two-Sample Test

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2 KSDAgg: KSD Aggregated Goodness-of-fit Test

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- Uniform separation rate
- Experiments

Goodness-of-fit problem

Given

- a model probability density p on \mathbb{R}^d (or score function $\nabla \log p(z)$)
- samples $Z_n := (Z_1, \dots, Z_n)$ where $Z_i \stackrel{\text{iid}}{\sim} q$ in \mathbb{R}^d

can we decide whether or not $p \neq q$ holds?

Goodness-of-fit problem

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Stein kernel:

$$h_{p,\lambda}(x, y) := \left(\nabla \log p(x)^\top \nabla \log p(y) \right) k_\lambda(x, y) + \nabla \log p(y)^\top \nabla_1 k_\lambda(x, y) \\ + \nabla \log p(x)^\top \nabla_2 k_\lambda(x, y) + \sum_{i=1}^d \frac{\partial}{\partial x_i \partial y_i} k_\lambda(x, y)$$

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Stein kernel: not translation invariant

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Stein identity: $\mathbb{E}_{Z \sim p}[h_{p,\lambda}(Z, \cdot)] = 0$

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Quadratic-time estimator:

$$\widehat{\text{KSD}}_{p,\lambda}^2(\mathbb{Z}_n) := \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h_{p,\lambda}(Z_i, Z_j)$$

Chwialkowski et al. A kernel test of goodness of fit. In ICML, 2016.

Liu et al. A kernelized Stein discrepancy for goodness-of-fit tests. In ICML, 2016.

KSDAgg: KSD Aggregated test

Wild bootstrap: well-calibrated asymptotic level α

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Aggregated test KSDAgg $\Delta_{\alpha,p}^\Lambda$: reject null hypothesis $\mathcal{H}_0 : p = q$ if

$$\widehat{\text{KSD}}_{p,\lambda}^2(Z_n) > \hat{q}_{1-u_\alpha w_\lambda}^\lambda \quad \text{for some } \lambda \in \Lambda$$

- weights $\sum_{\lambda \in \Lambda} w_\lambda \leq 1$
- level correction u_α

KSDAgg: Uniform separation rate

1 MMDAgg: MMD Aggregated Two-Sample Test

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- MMD single test
- MMD aggregated test
- Experiments

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For $\alpha \in (0, e^{-1})$, $\beta \in (0, 1)$, $B_1, B_2, B_3 \in \mathbb{N}$ large enough, using either a wild bootstrap or a parametric bootstrap, the condition

$$\|p - q\|_2^2 \geq \min_{\lambda \in \Lambda} \left(\|(\textcolor{blue}{p} - \textcolor{red}{q}) - h_{p,\lambda} \diamond (\textcolor{blue}{p} - \textcolor{red}{q})\|_2^2 + C \log\left(\frac{1}{\alpha w_\lambda}\right) \frac{\sqrt{A_\lambda}}{\beta n} \right)$$

guarantees β -control over the probability of type II error of KSDAgg

$$\mathbb{P}_{\textcolor{red}{q}}\left(\Delta_{\alpha, \textcolor{blue}{p}}^{\textcolor{orange}{\Lambda}}(\mathbb{Z}_n) = 0\right) \leq \beta.$$

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Stein kernel is **not** translation invariant:

- ⇒ cannot work in Fourier domain using Plancherel's Theorem
- ⇒ cannot obtain uniform separation rate over Sobolev balls

KSDAgg: Experiments

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Gaussian-Bernoulli Restricted Boltzmann Machine GBRBM

- Graphical model:**
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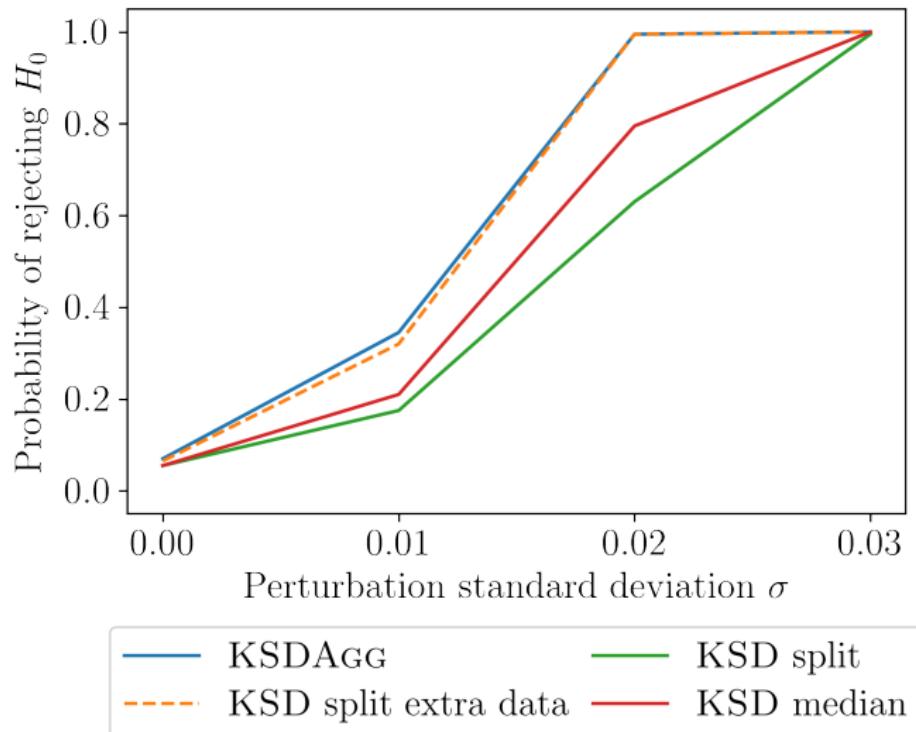
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Experiment: model p and **1000 samples** obtained using a Gibbs sampler for the GBRBM with Gaussian noise $\mathcal{N}(0, \sigma)$ injected into each entry of B

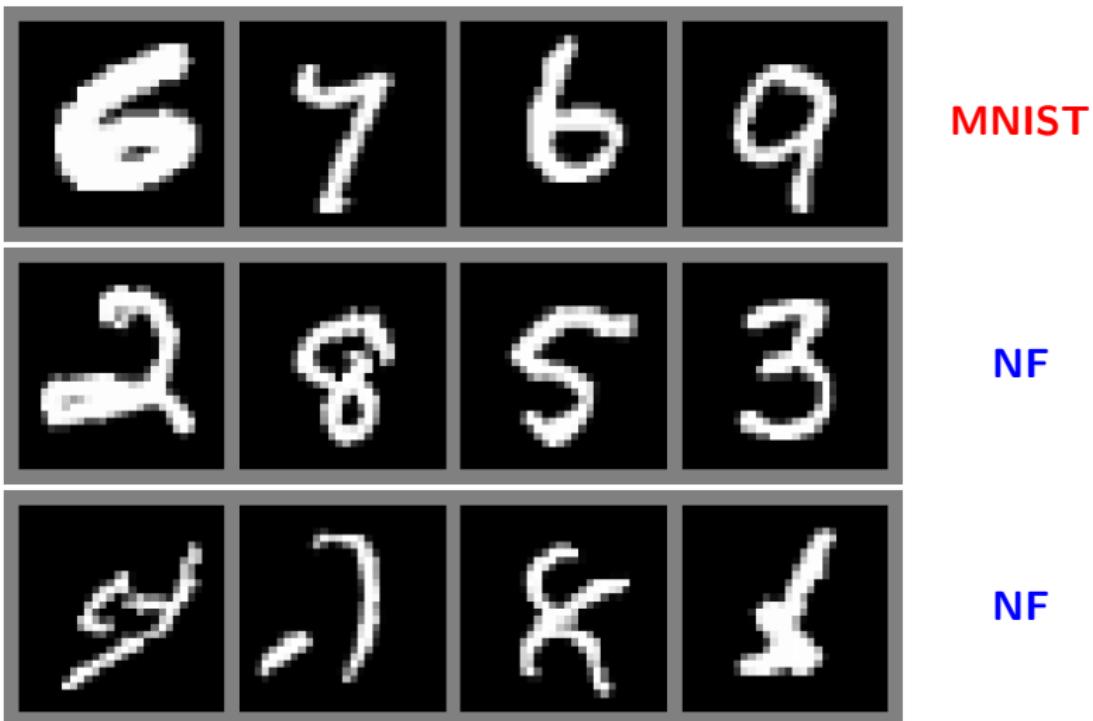
KSDAgg experiment: GBRBM $\Lambda(-20, 0)$



KSDAgg experiment: MNIST Normalizing Flow $\Lambda(-20, 0)$

Model: Normalizing Flow (generative model) with probability density p

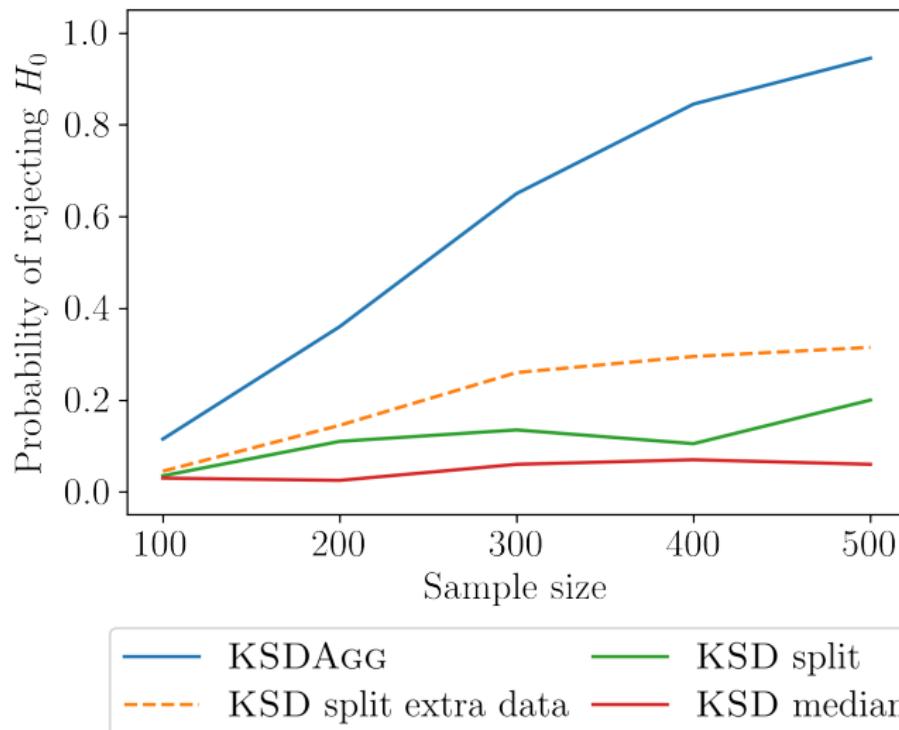
Samples: true MNIST samples in dimension $28^2 = 784$



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KSDAgg paper



KSDAgg code



What about HSICAgg?

Independence problem:

Given paired samples $((X_1, Y_1), \dots, (X_n, Y_n))$ in $\mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$ with

- joint probability density r
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Hilbert-Schmidt Independence Criterion:

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ADAPTIVE TEST OF INDEPENDENCE BASED ON HSIC MEASURES.

Mélisande Albert^{*,1}, Béatrice Laurent^{†,1}, Amandine Marrel^{‡,2}, and Anouar Meynaoui^{§,1,2}

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Toulouse, France.

²CEA, DEN, DER, F-13108 Saint-Paul-lez-Durance, France.

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Thank you for your attention!

Any questions?

MMDAgg



paper

KSDAgg



paper



code



code