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

University College London
Centre for Artificial Intelligence
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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

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Given independent samples

- $\mathbb{X}_m := (X_1, \dots, X_m)$ where $X_i \overset{\text{iid}}{\sim} p$ in $\mathbb{R}^d$
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Statistical hypothesis testing:

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

What is a 'good' test Δ?

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

Sobolev balls

Sobolev balls:

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

- radius $R > 0$
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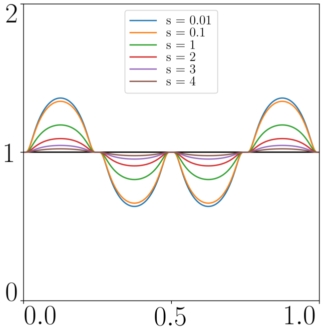

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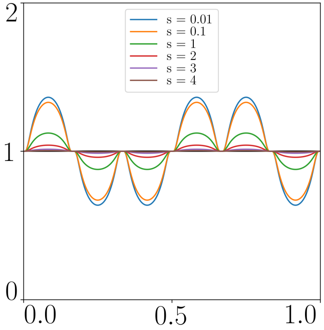

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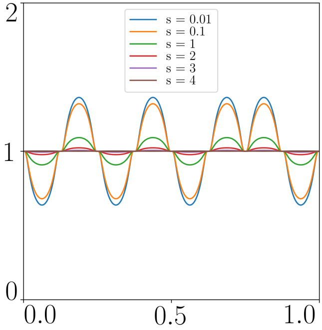

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Reproducing Kernel Hilbert Space (RKHS): inner product space of real-valued functions $\mathcal{H}_k$ satisfying:

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

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

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

Gaussian kernel

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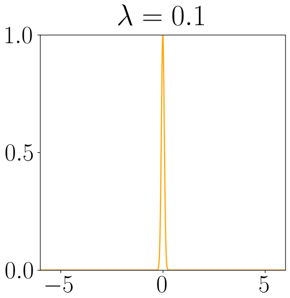

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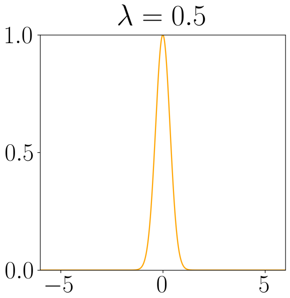

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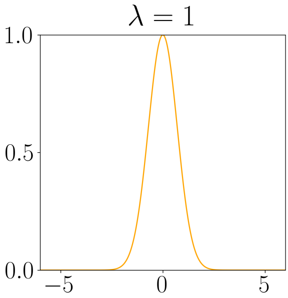

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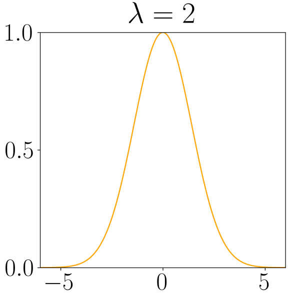

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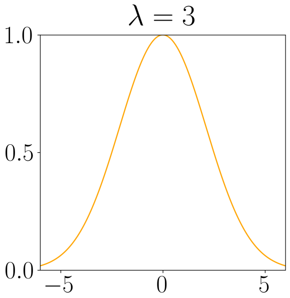

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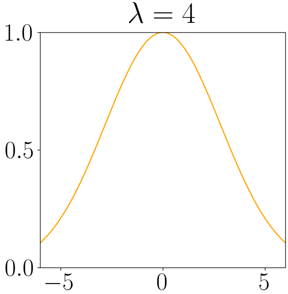

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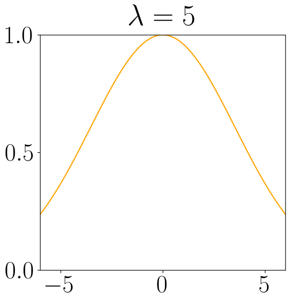

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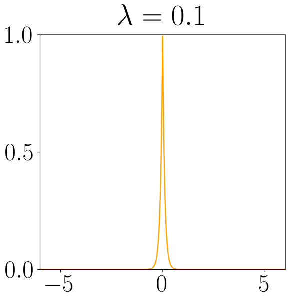

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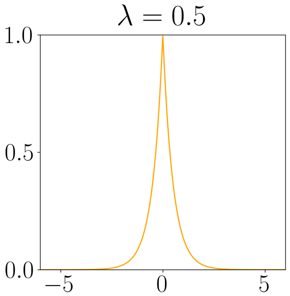

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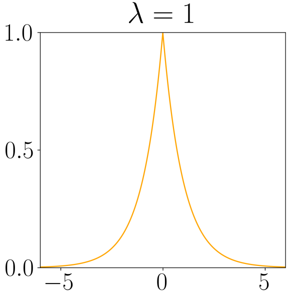

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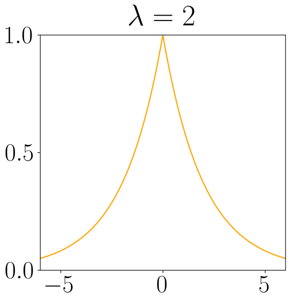

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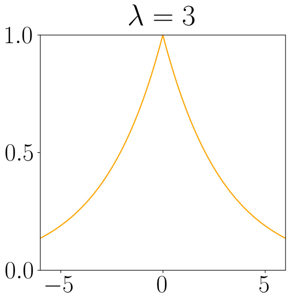

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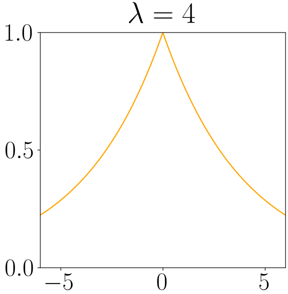

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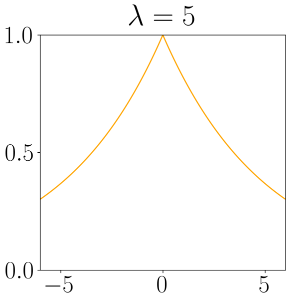

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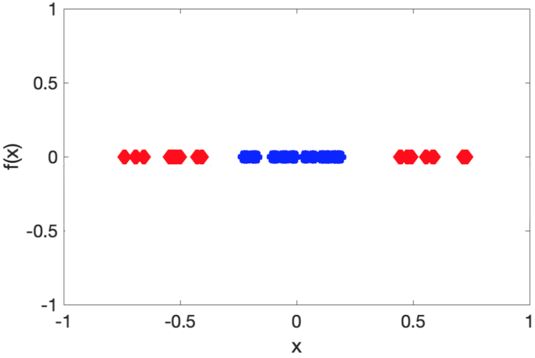

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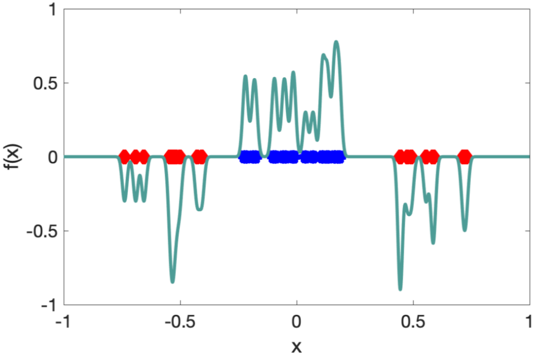

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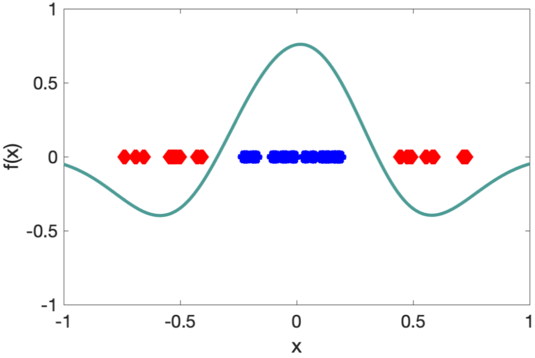

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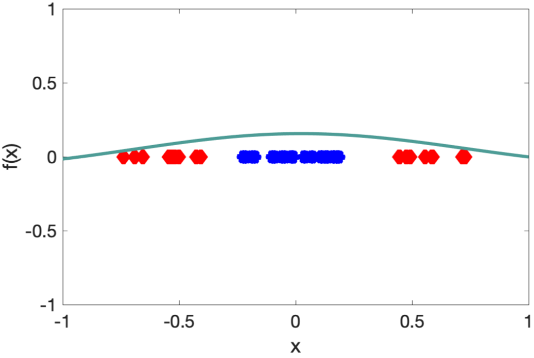

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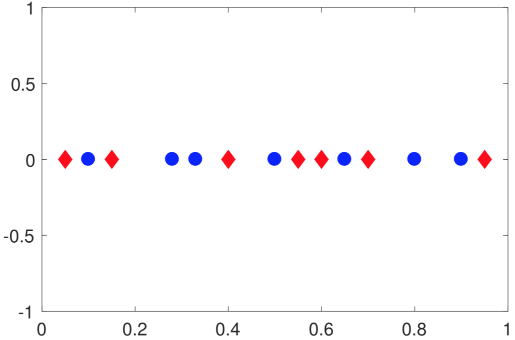

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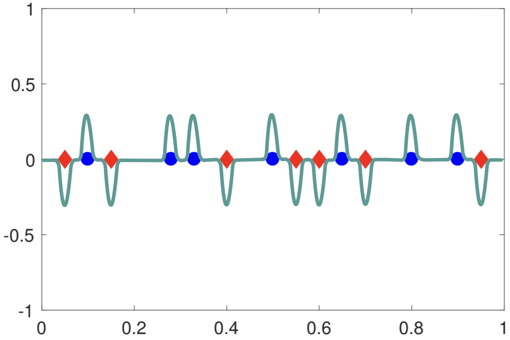

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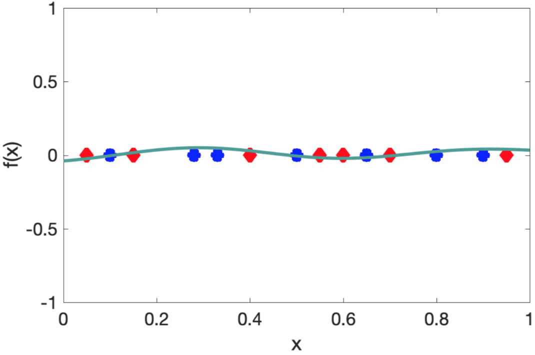

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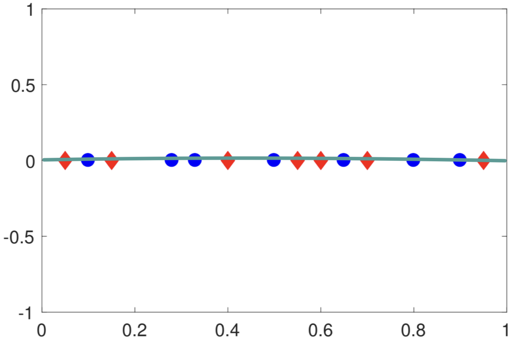

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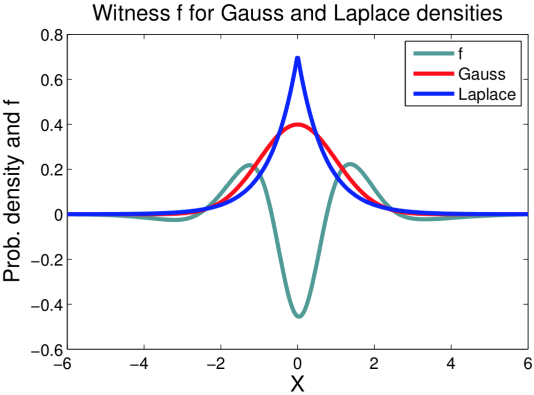

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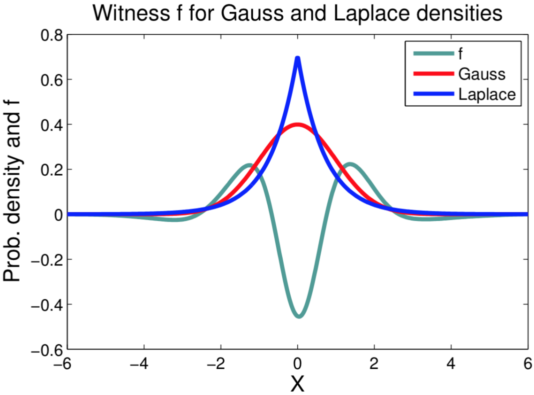

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Characteristic kernel: property on the kernel which ensures that

$$\mathrm{MMD}_\lambda(p,q) = 0 \quad \Longleftrightarrow \quad p = q$$

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

$\implies$ non-asymptotic power guarantees

MMD single test using permutations

Maximum Mean Discrepancy: $\mathrm{MMD}^2_\lambda(p, q)$ 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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Quantile: $\widehat{q}^{\,\lambda}_{1-\alpha}$ is the $\lceil(B+1)(1-\alpha)\rceil$-th largest value of the B permuted test statistics together with the original test statistic

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Single test: well-calibrated non-asymptotic level α

$$\Delta^\lambda_\alpha(\mathbb{X}_m,\mathbb{Y}_n) \coloneqq \mathbb{1}\left(\widehat{\mathrm{MMD}}^2_\lambda(\mathbb{X}_m,\mathbb{Y}_n) > \widehat{q}^{\,\lambda}_{1-\alpha}\right)$$

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Assumption: equal sample sizes $m = n$

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$$\Delta^\lambda_\alpha(\mathbb{X}_n, \mathbb{Y}_n) := \mathbb{1}\left(\widehat{\mathrm{MMD}}^2_\lambda(\mathbb{X}_n, \mathbb{Y}_n) > \widehat{q}^{\lambda}_{1-\alpha} \right)$$

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

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

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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$\Longrightarrow$ 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)

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

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

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

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

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

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

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For each $\lambda \in \Lambda$:

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- compute B_2 simulated MMD test statistics
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MMDAgg time complexity:

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

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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$\Longrightarrow$ 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 $\Lambda = \left\{\lambda^{(j)}\right\}_{1\leq j\leq N}$

- **(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

Weighting strategies

- **median bandwidth:** $(\lambda_{med})_i \coloneqq \mathrm{median}\{|z_i - z'_i| : z, z' \in \mathbb{X}_m \cup \mathbb{Y}_n, z \neq z'\}$
- **finite collection Λ of bandwidths:** for $\ell_-, \ell_+ \in \mathbb{N}$ with $N = 1 + \ell_- + \ell_+$

$$\Lambda(\ell_-, \ell_+) \coloneqq \left\{2^\ell \lambda_{med} \in (0,\infty)^d : \ell \in \{\ell_-, \dots, \ell_+\}\right\} = \left\{\lambda^{(j)} : j = 1, \dots, N\right\}$$

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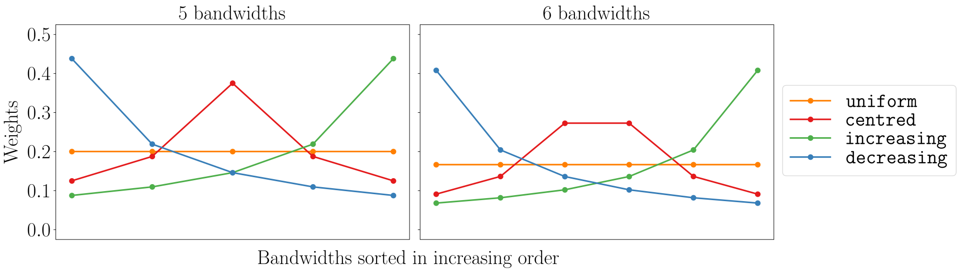
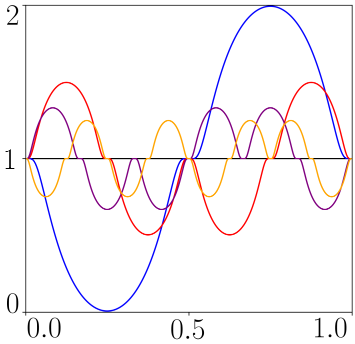
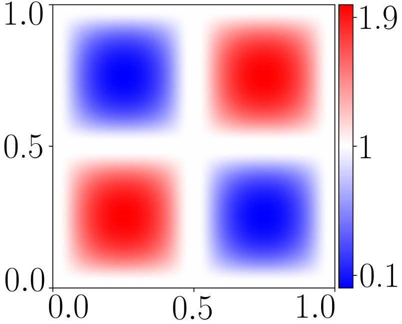
- **uniform weights:** $w_{\lambda^{(j)}} \coloneqq 1 \ / \ N$
- **increasing weights:** $w_{\lambda^{(j)}} \coloneqq C \ / \ (N + 1 - j)$
- **decreasing weights:** $w_{\lambda^{(j)}} \coloneqq C \ / \ j$
- **centred weights:** $w_{\lambda^{(j)}} \coloneqq C \ / \ \left(\left| \frac{N+1}{2} - j \right|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



MMDAgg experiment: perturbed uniform distribution

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





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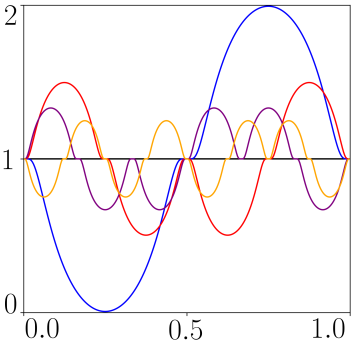

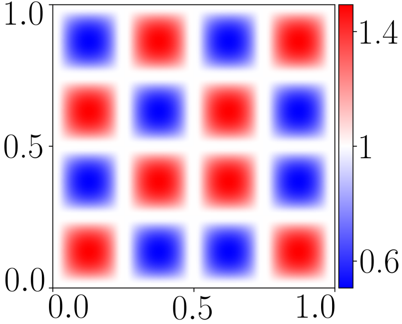

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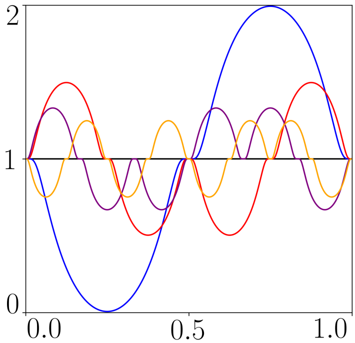

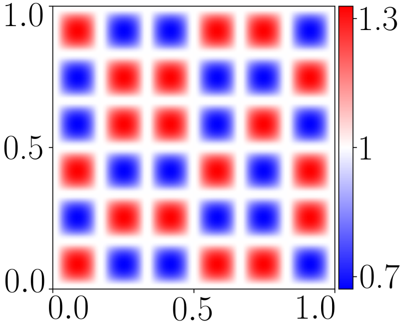

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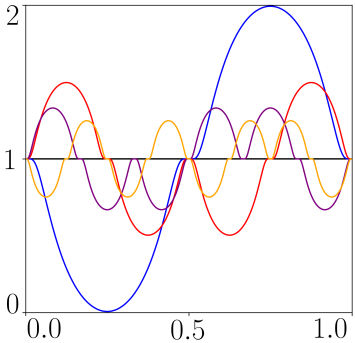
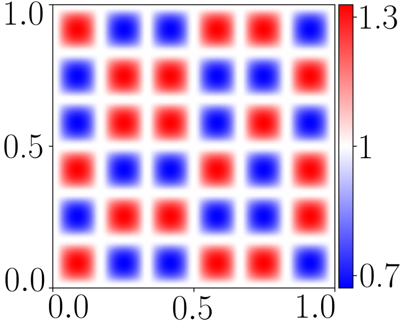
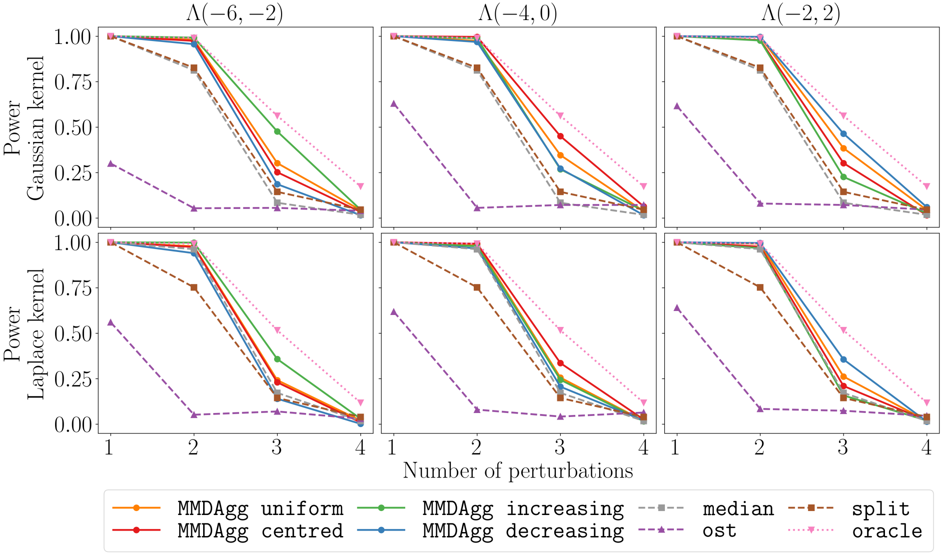




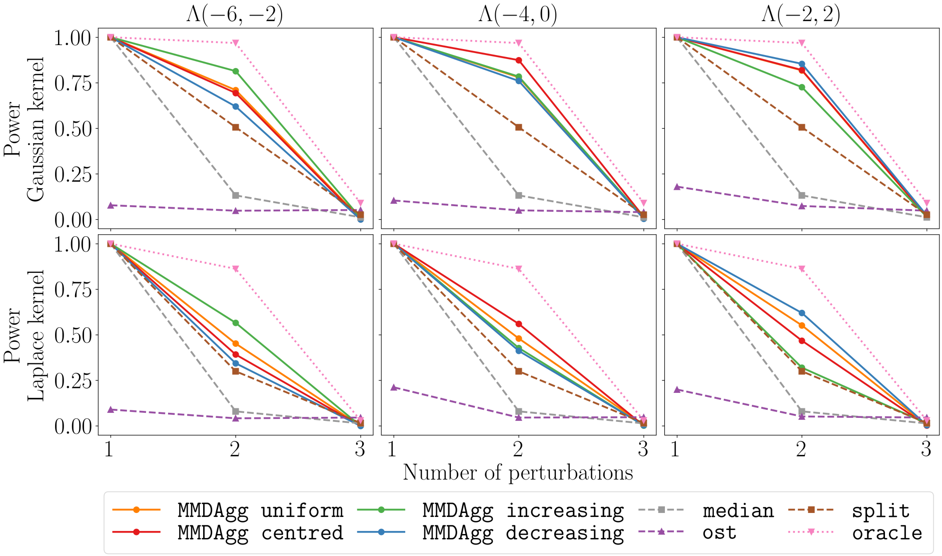
Perturbed uniform densities: used in the proof of lower bound on uniform separation rate over Sobolev balls $(m+n)^{-2s/(4s+d)}$ (**minimax rate**)

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



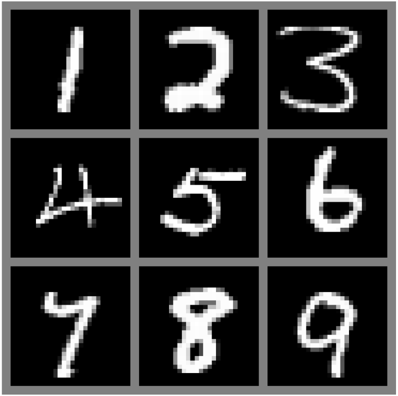
`ost`: Kübler et al. **Learning kernel tests without data splitting**. *NeurIPS*, 2020.

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

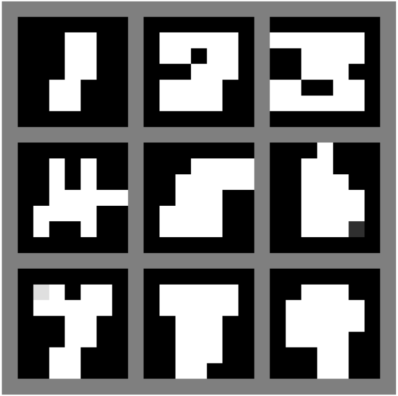
$\mathcal{Q}_3$: 0, 1, 2, 3, 5, 7, 9

$\mathcal{Q}_4$: 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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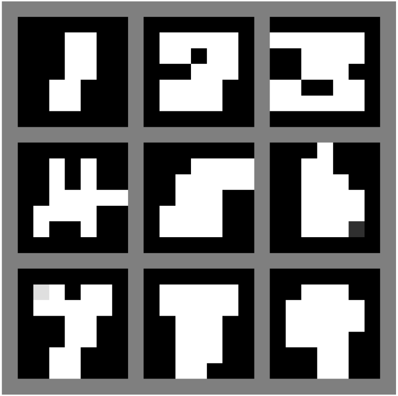

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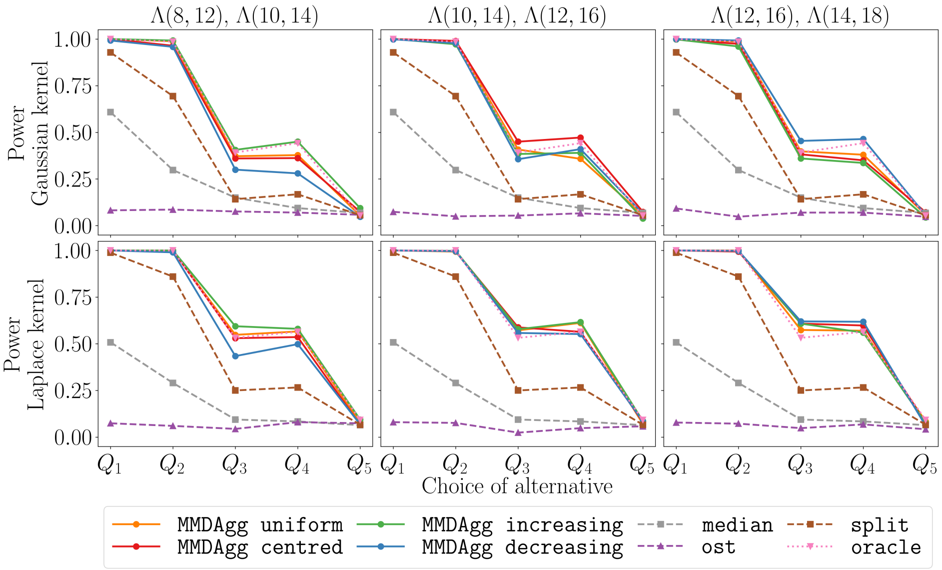
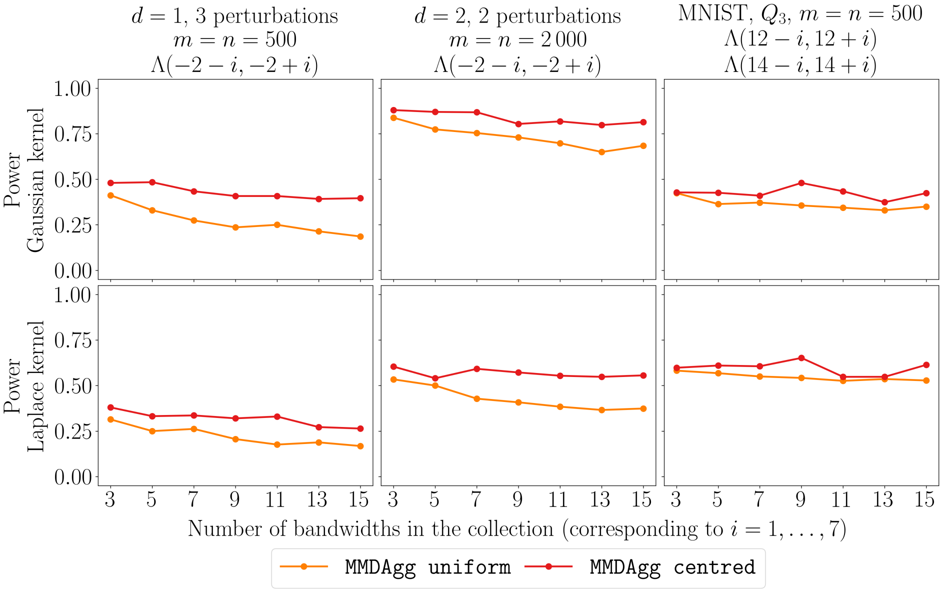
Images: dimension 49

Problem: inherently lower-dimensional

MMDAgg experiment: MNIST (m=n=500)



MMDAgg experiment: collections of bandwidths



MMDAgg: conclusion

MMDAgg test:

- aggregate MMD tests with different kernel bandwidths (or kernels)
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MMDAgg theoretical results:

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

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- wide range of kernels

MMDAgg experimental results:

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

MMDAgg: paper & code

MMDAgg paper

SCAN ME

MMDAgg code

SCAN ME

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

Goodness-of-fit problem

Given • a model probability density p on $\mathbb{R}^d$ (or score function $\nabla \log p(z)$)

• samples $\mathbb{Z}_n := (Z_1, \ldots, Z_n)$ where $Z_i \overset{\text{iid}}{\sim} q$ in $\mathbb{R}^d$

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

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Stein kernel:

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

Goodness-of-fit problem

Given • a model probability density p on $\mathbb{R}^d$ (or score function $\nabla \log p(z)$)

• samples $\mathbb{Z}_n := (Z_1, \dots, Z_n)$ where $Z_i \overset{\text{iid}}{\sim} q$ in $\mathbb{R}^d$

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

Stein kernel: not translation invariant

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Goodness-of-fit problem

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Quadratic-time estimator:

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

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 $\Delta^{\Lambda}_{\alpha,p}$: reject null hypothesis $\mathcal{H}_0 : p = q$ if

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

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

KSDAgg: uniform separation rate

Integral transform: $(\kappa \diamond f)(y) \coloneqq \int_{\mathbb{R}^d} \kappa(x, y) f(x) \, \mathrm{d}x$

Kernel assumption: $A_\lambda \coloneqq \mathbb{E}_{q,q}[h_{p,\lambda}(Z, Z')^2] < \infty$

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Theorem

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

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

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

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Stein kernel is **not** translation invariant:

$\Longrightarrow$ cannot work in Fourier domain using Plancherel's Theorem

$\Longrightarrow$ cannot obtain uniform separation rate over Sobolev balls

KSDAgg: 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
   - Uniform separation rate
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Gaussian-Bernoulli Restricted Boltzmann Machine GBRBM

Graphical model:
- binary hidden variable $h \in \{-1, 1\}^{40}$
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initialisation: $b \sim \mathcal{N}(0, I_{50}), \;\; c \sim \mathcal{N}(0, I_{40}), \;\; B \sim \mathrm{Unif}\,\{-1, 1\}^{50\times 40}$

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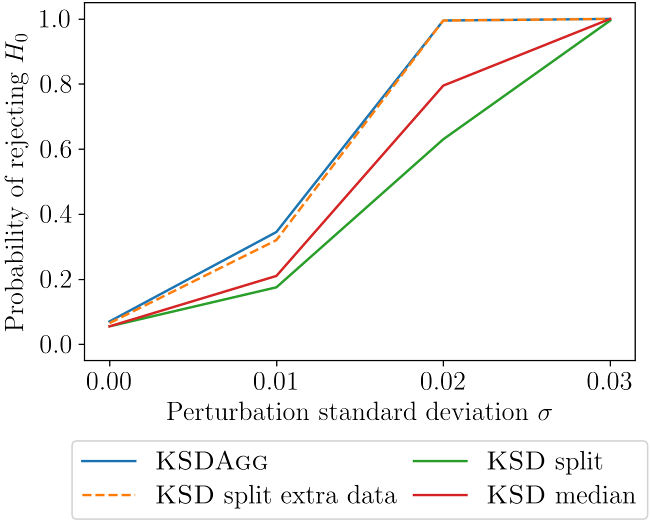
Experiment: model p and 1000 samples obtained using a Gibbs sampler for the GBRBM with Gaussian noise $\mathcal{N}(0, \sigma)$ injected into each entry of B

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 $28^2 = 784$

MNIST

NF

NF

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

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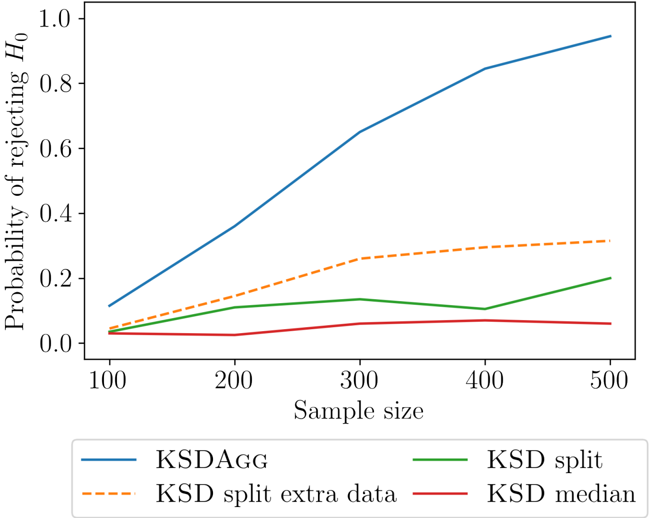

KSDAgg: conclusion

KSDAgg test:

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- wide range of kernels

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KSDAgg experimental results:

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

KSDAgg: paper & code

KSDAgg paper

SCAN ME

KSDAgg code

SCAN ME

What about HSICAgg?

Independence problem:

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

- joint probability density r
- marginal probability densities p and q

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

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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]

[1]Institut de Mathématiques de Toulouse ; UMR5219, Université de Toulouse ; CNRS, INSA, F-31077 Toulouse, France.
[2]CEA, DEN, DER, F-13108 Saint-Paul-lez-Durance, France.

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Thank you for your attention!
Any questions?

MMDAgg

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