Aggregated Kernel Tests

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MMD Aggregated Two-Sample Test






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Two-sample problem

- samples $\mathbb{X}_m := (X_1, \ldots, X_m)$, $X_i \overset{\text{iid}}{\sim} p$ in $\mathbb{R}^d$
- samples $\mathbb{Y}_n := (Y_1, \ldots, Y_n)$, $Y_i \overset{\text{iid}}{\sim} q$ in $\mathbb{R}^d$

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$$\mathcal{H}_0 \colon p = q \quad \text{against} \quad \mathcal{H}_a \colon p \neq q$$

$$\Delta(\mathbb{X}_m, \mathbb{Y}_n) = 1 \iff \text{reject } \mathcal{H}_0$$

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Type I error: controlled by α by design

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

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

Type II error: find a condition on $\|p - q\|_2$ to control by β

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

Kernels

Kernel: $k_\lambda(x, y) := \prod_{i=1}^{d} \frac{1}{\lambda_i} K_i\left(\frac{x_i - y_i}{\lambda_i}\right)$ **Bandwidth:** $\lambda \in (0, \infty)^d$

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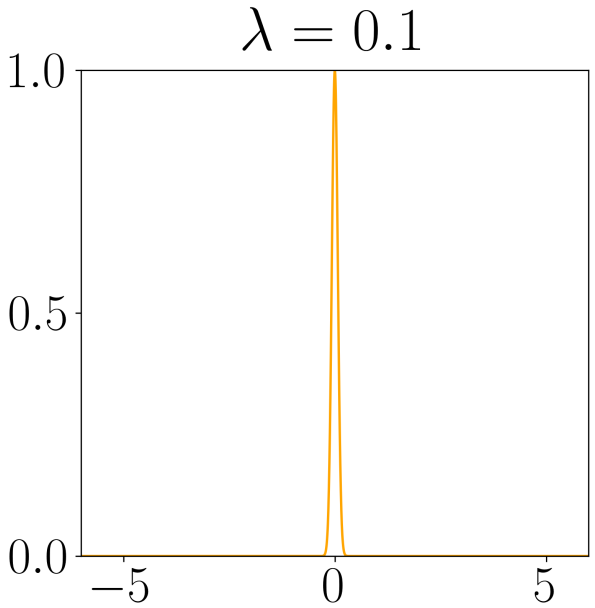

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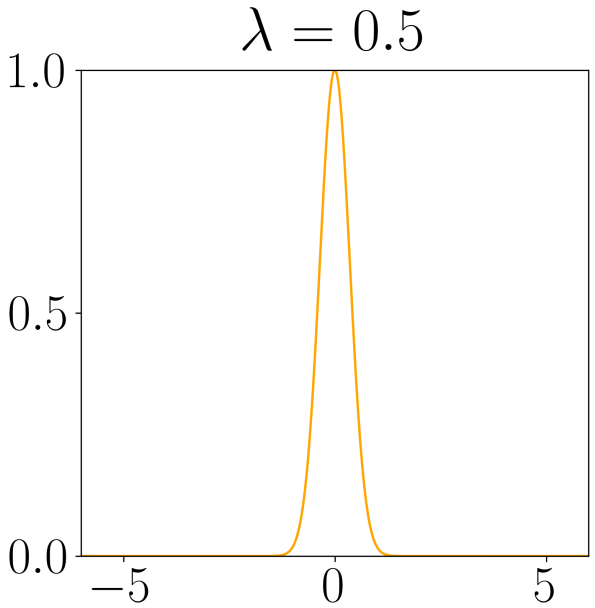

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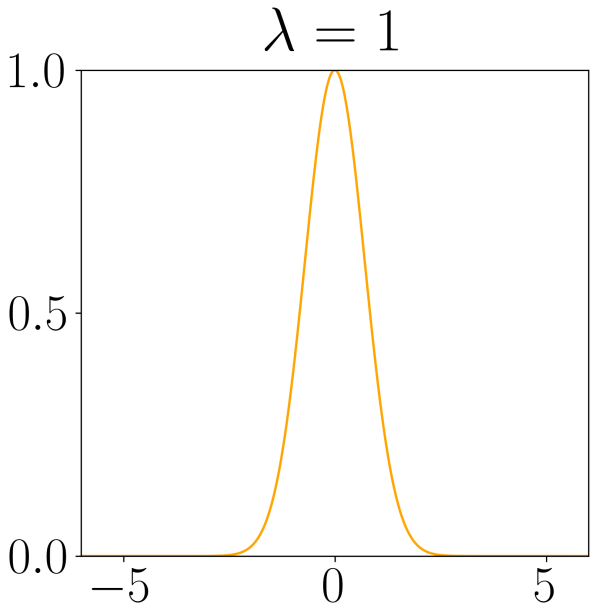

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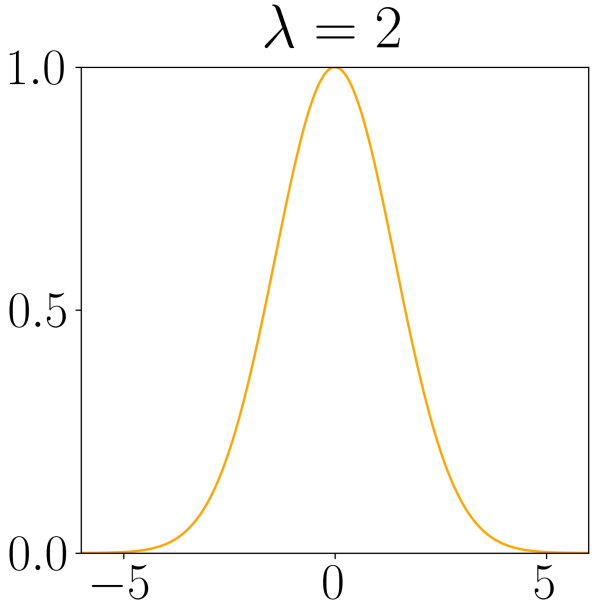

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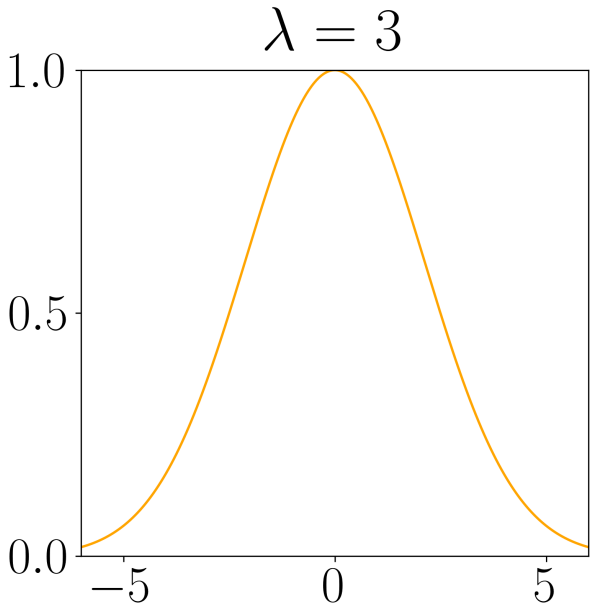

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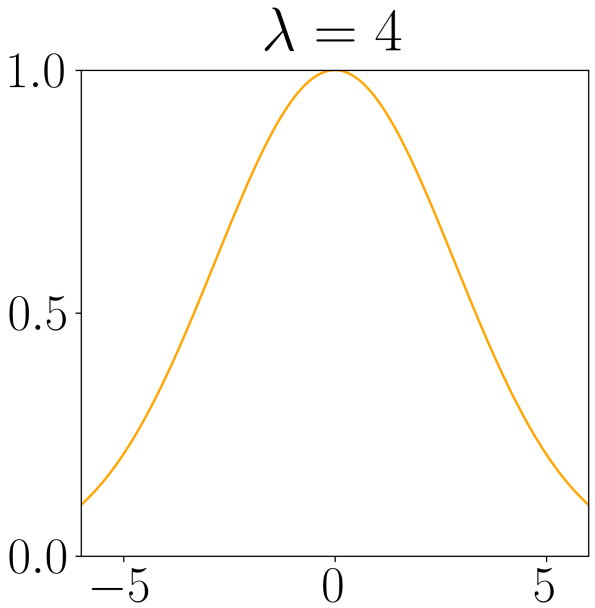

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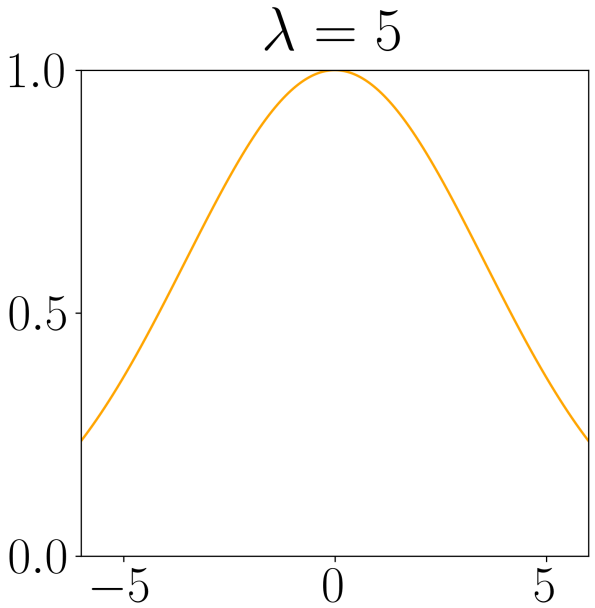

Two-sample test using the Maximum Mean Discrepancy

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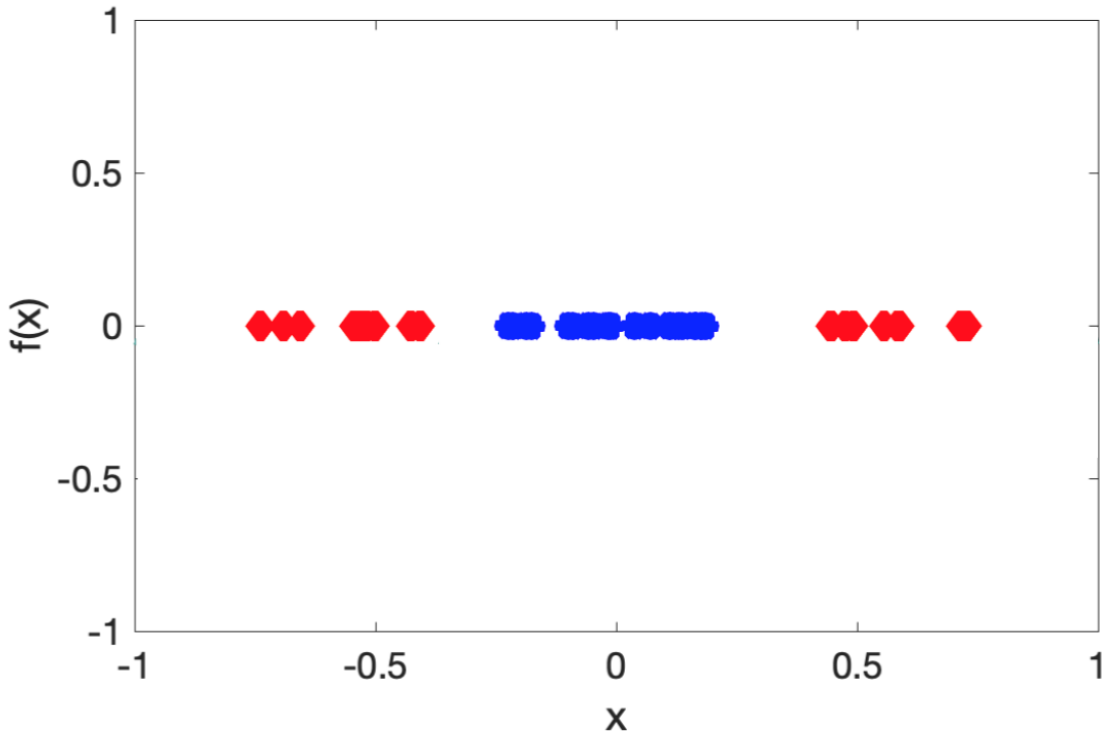

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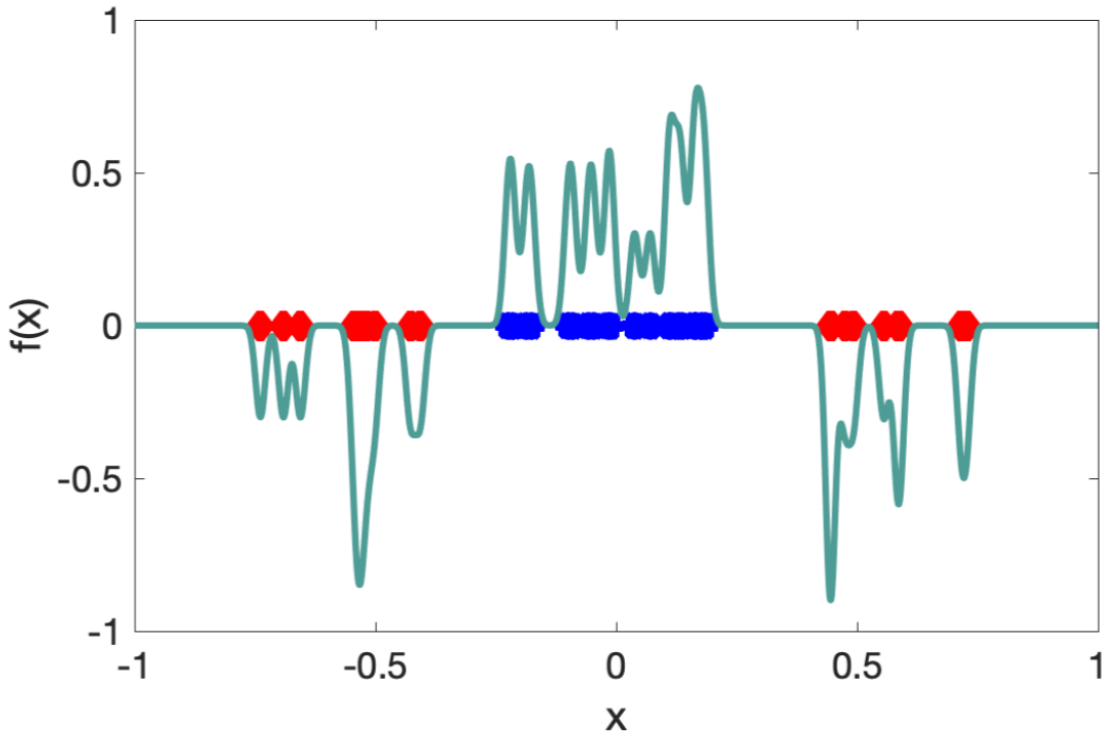

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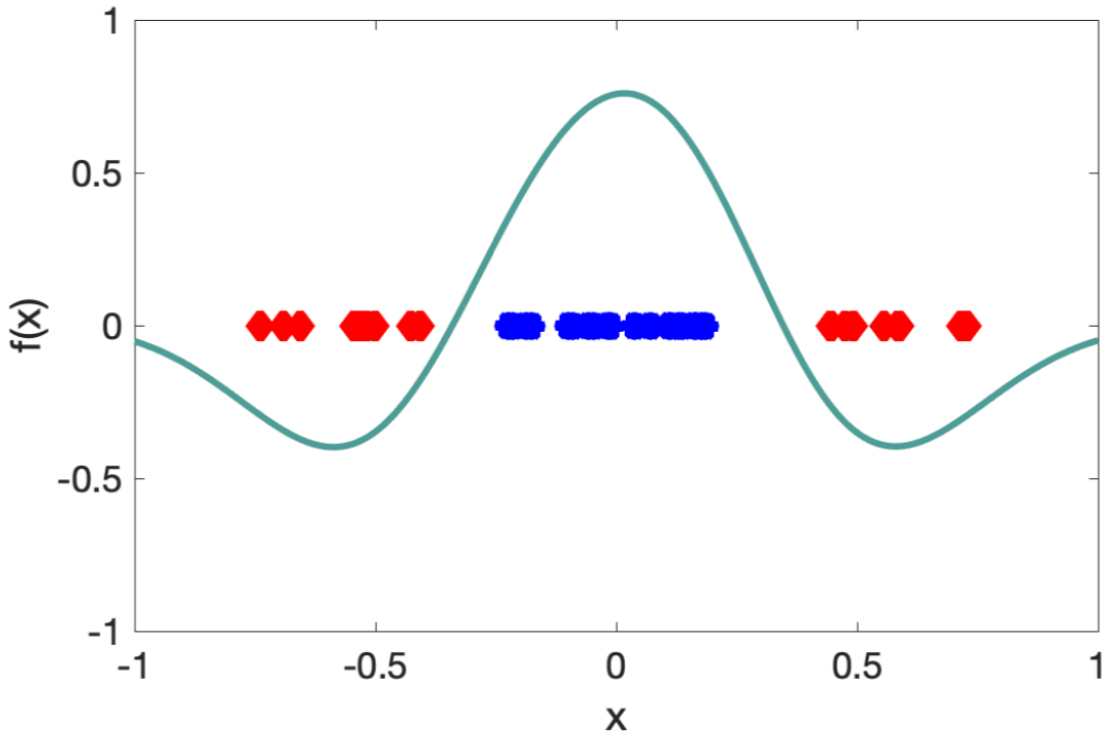

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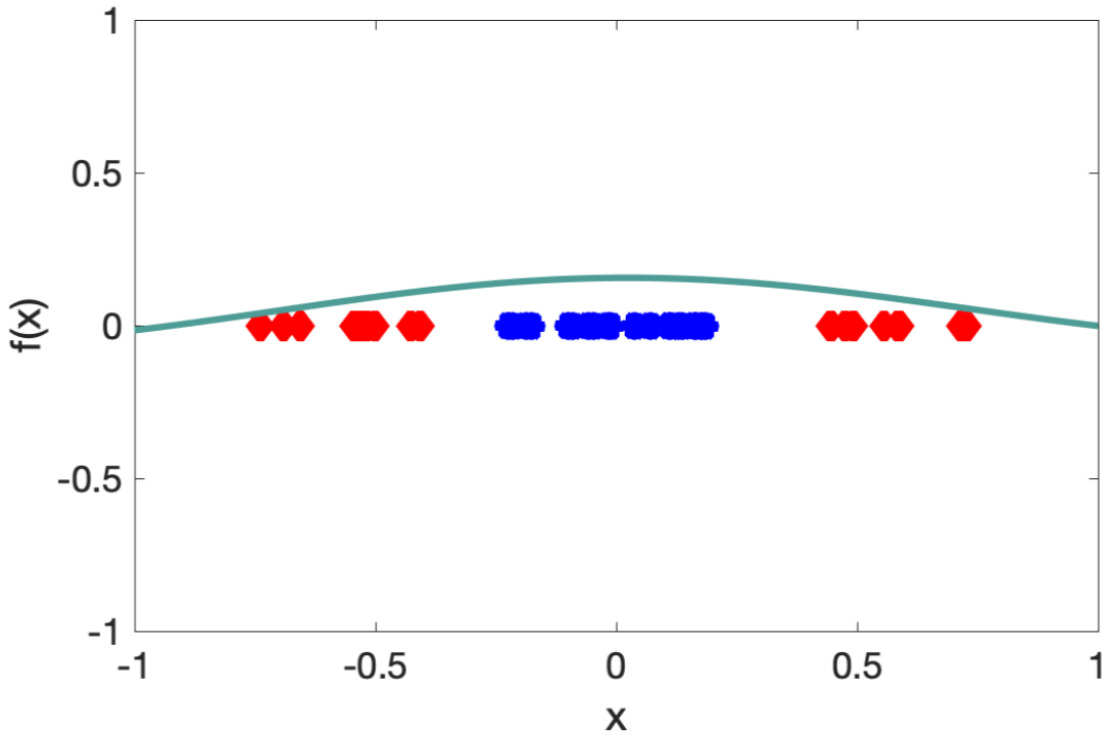

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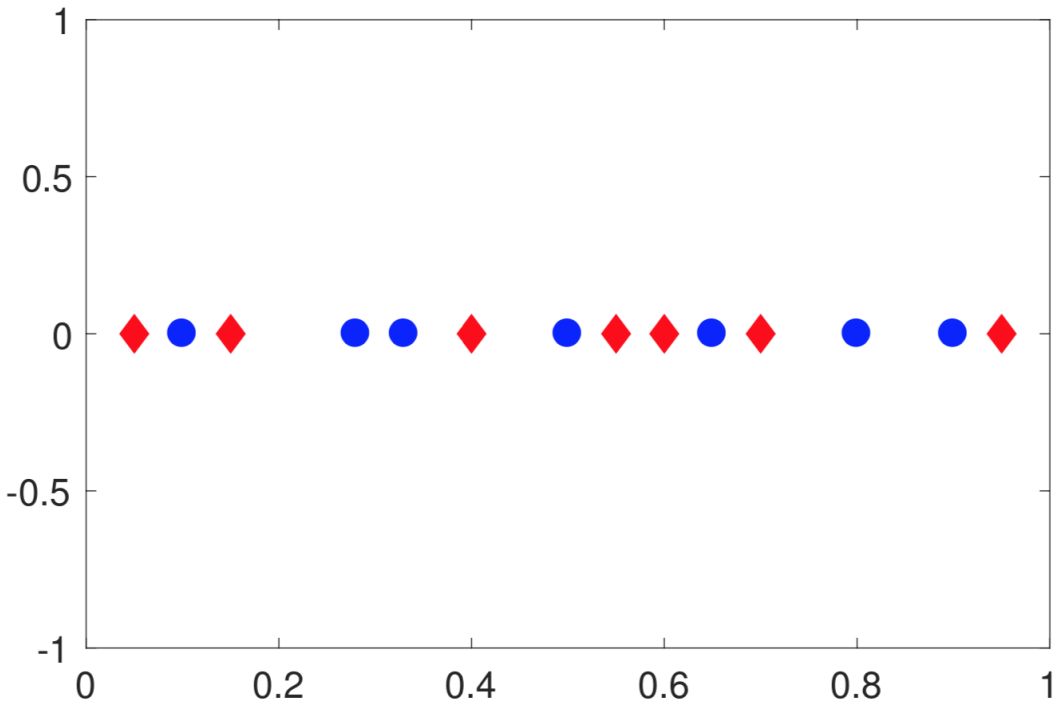

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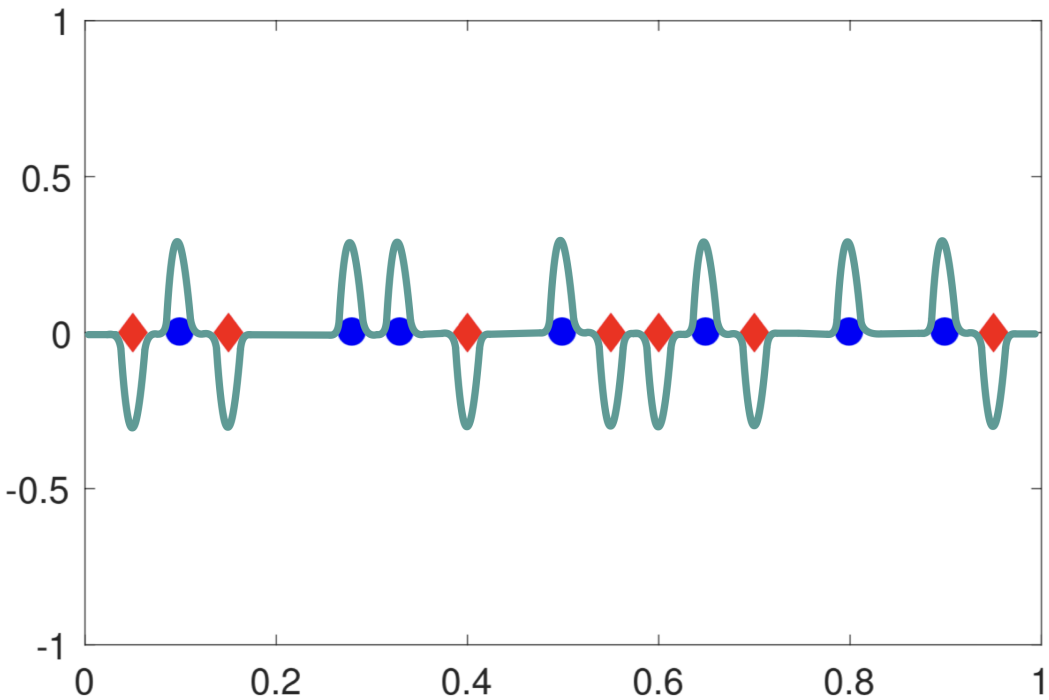

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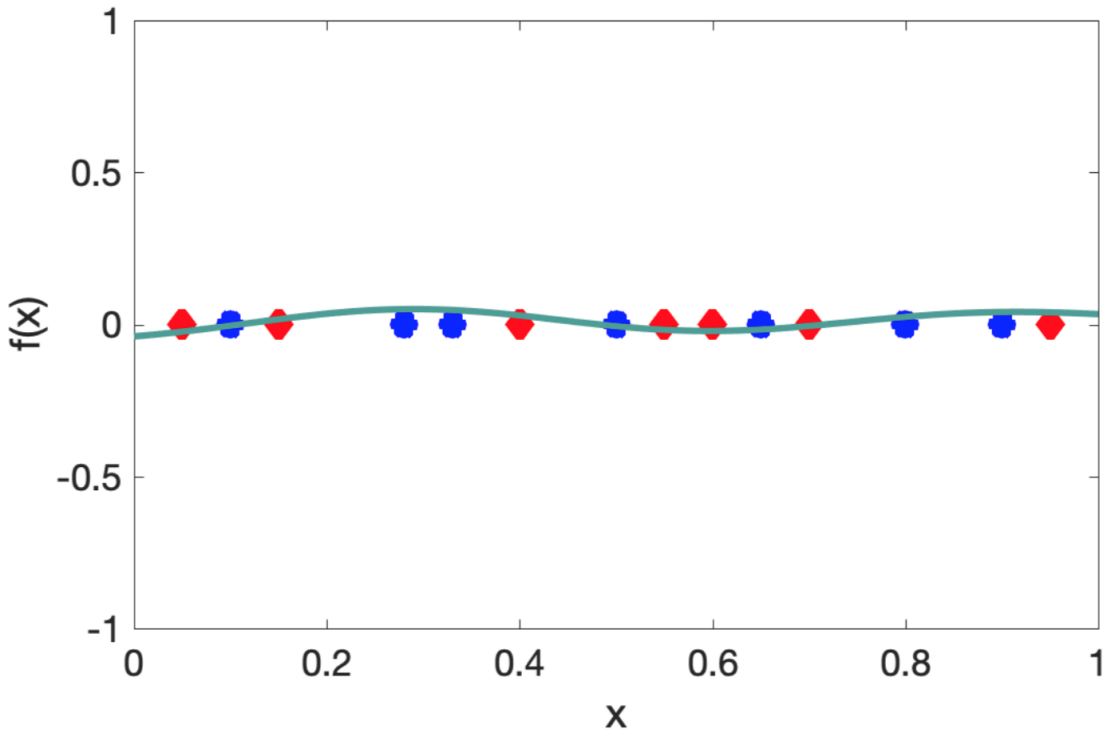

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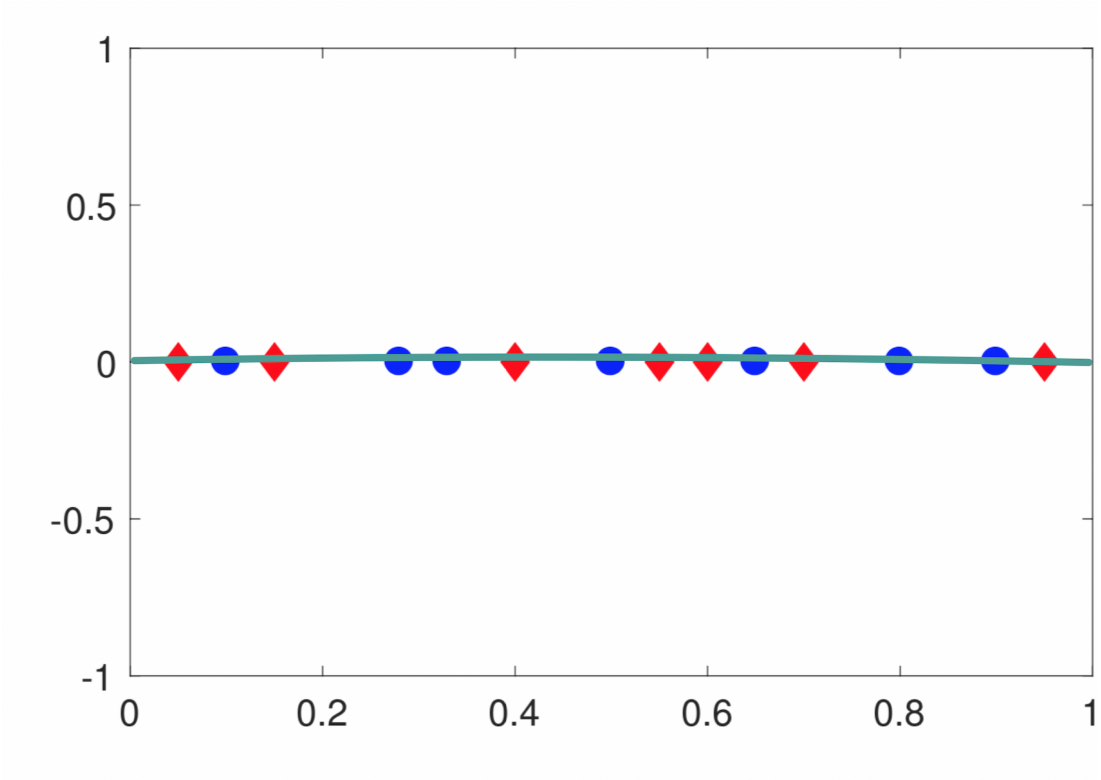

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Bandwidth intuition

- **Small sample sizes**: only global differences are detectable
  - **Small bandwidth**: wrongly detects artificial local differences under $\mathcal{H}_0$
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- **Our method:** aggregate multiple tests with different **bandwidths**

Maximum Mean Discrepancy estimator

$$\begin{aligned}\mathrm{MMD}^2_\lambda(p, q) \;:=\; & \mathbb{E}_{p,p}[k_\lambda(X, X')] \\ & - 2\,\mathbb{E}_{p,q}[k_\lambda(X, Y)] \\ & + \mathbb{E}_{q,q}[k_\lambda(Y, Y')]\end{aligned}$$

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$$\begin{aligned}\widehat{\mathrm{MMD}}^2_\lambda(\mathbb{X}_m, \mathbb{Y}_n) &:= \frac{1}{m(m-1)} \sum_{1 \le i \ne i' \le m} k_\lambda(X_i, X_{i'}) \\ &\quad - \frac{2}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} k_\lambda(X_i, Y_j) \\ &\quad + \frac{1}{n(n-1)} \sum_{1 \le j \ne j' \le n} k_\lambda(Y_j, Y_{j'})\end{aligned}$$

MMD test for a fixed bandwidth λ

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

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Quantile: $\widehat{q}_{1-\alpha}^\lambda$ is the $\lceil (B+1)(1-\alpha) \rceil$-th largest value of $\widehat{\mathrm{MMD}}_\lambda^2(\mathbb{X}_m, \mathbb{Y}_n)$ and B permuted test statistics

$$\widehat{\mathrm{MMD}}_\lambda^2(\mathbb{X}_m^\sigma, \mathbb{Y}_n^\sigma) \quad \text{where} \quad (\mathbb{X}_m^\sigma, \mathbb{Y}_n^\sigma) = \sigma(\mathbb{X}_m \cup \mathbb{Y}_n)$$

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$$\widehat{\mathrm{MMD}}_\lambda^2(\mathbb{X}_m^\sigma, \mathbb{Y}_n^\sigma) \quad \text{where} \quad (\mathbb{X}_m^\sigma, \mathbb{Y}_n^\sigma) = \sigma(\mathbb{X}_m \cup \mathbb{Y}_n)$$

Non-asymptotic level α

MMD test for a fixed bandwidth λ

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Non-asymptotic level α

Time complexity:

$$\mathcal{O}\left(B\,(m+n)^2\right)$$

MMDAgg for a collection of bandwidths Λ

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

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Non-asymptotic level α

Time complexity:

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

Minimax adaptivity over Sobolev balls

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

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Theorem

$$\Lambda^* := \left\{ 2^{-\ell} \mathbb{1}_d : \ell \in \left\{ 1, \dots, \left\lceil \frac{2}{d} \log_2 \left(\frac{m+n}{\ln(\ln(m+n))} \right) \right\rceil \right\} \right\}, \quad w_\lambda := \frac{6}{\pi^2 \ell^2}$$

Assuming $p - q \in \mathcal{S}_d^s(R)$, *the condition*

$$\|p - q\|_2 \geq C \left(\frac{m+n}{\ln(\ln(m+n))} \right)^{-2s/(4s+d)}$$

guarantees control over the probability of type II error of MMDAgg

$$\mathbb{P}_{p \times q} \left(\Delta_\alpha^{\Lambda^*}(\mathbb{X}_m, \mathbb{Y}_n) = 0 \right) \leq \beta.$$

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

MMDAgg Experiment

$$\Lambda(\ell_-, \ell_+) := \left\{ 2^{\ell} \lambda_{med} : \ell \in \{\ell_-, \ldots, \ell_+\} \right\} \qquad w_\lambda := 1 / |\Lambda|$$

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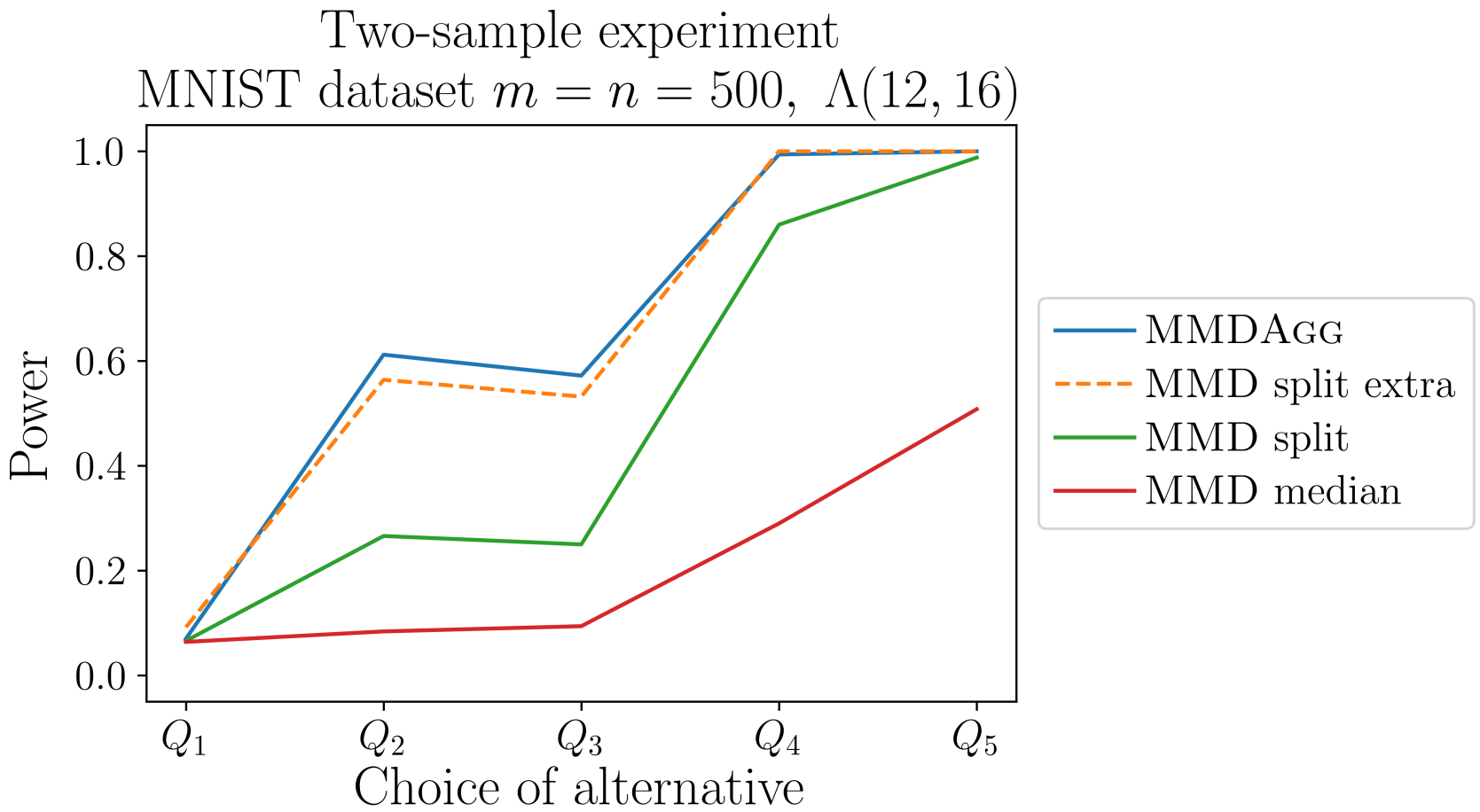

KSD Aggregated Goodness-of-fit Test

Antonin Schrab
† ‡ §

Benjamin Guedj
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‡

† Centre for Artificial Intelligence, UCL
‡ Gatsby Computational Neuroscience Unit, UCL
§ Inria London Programme

Goodness-of-fit problem & Kernel Stein Discrepancy

- model with probability density p or score function $\nabla \log p(z)$ on $\mathbb{R}^d$
- samples $\mathbb{Z}_n := (Z_1, \ldots, Z_n)$, $Z_i \overset{\text{iid}}{\sim} q$ in $\mathbb{R}^d$

$$\mathcal{H}_0 \colon p = q \qquad \text{against} \qquad \mathcal{H}_a \colon p \neq q$$

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Stein kernel: $h_{p,\lambda}(x, y)$ defined as

$$\left(\nabla \log p(x)^\top \nabla \log p(y)\right) k_\lambda(x, y) + \nabla \log p(y)^\top \nabla_1 k_\lambda(x, y)$$
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$\Lambda(\ell_-, \ell_+) := \left\{2^\ell \lambda_{med} : \ell \in \{\ell_-, \ldots, \ell_+\}\right\}$ $\qquad$ $w_\lambda := 1 / |\Lambda|$

model: Normalizing Flow density

samples: true MNIST digits

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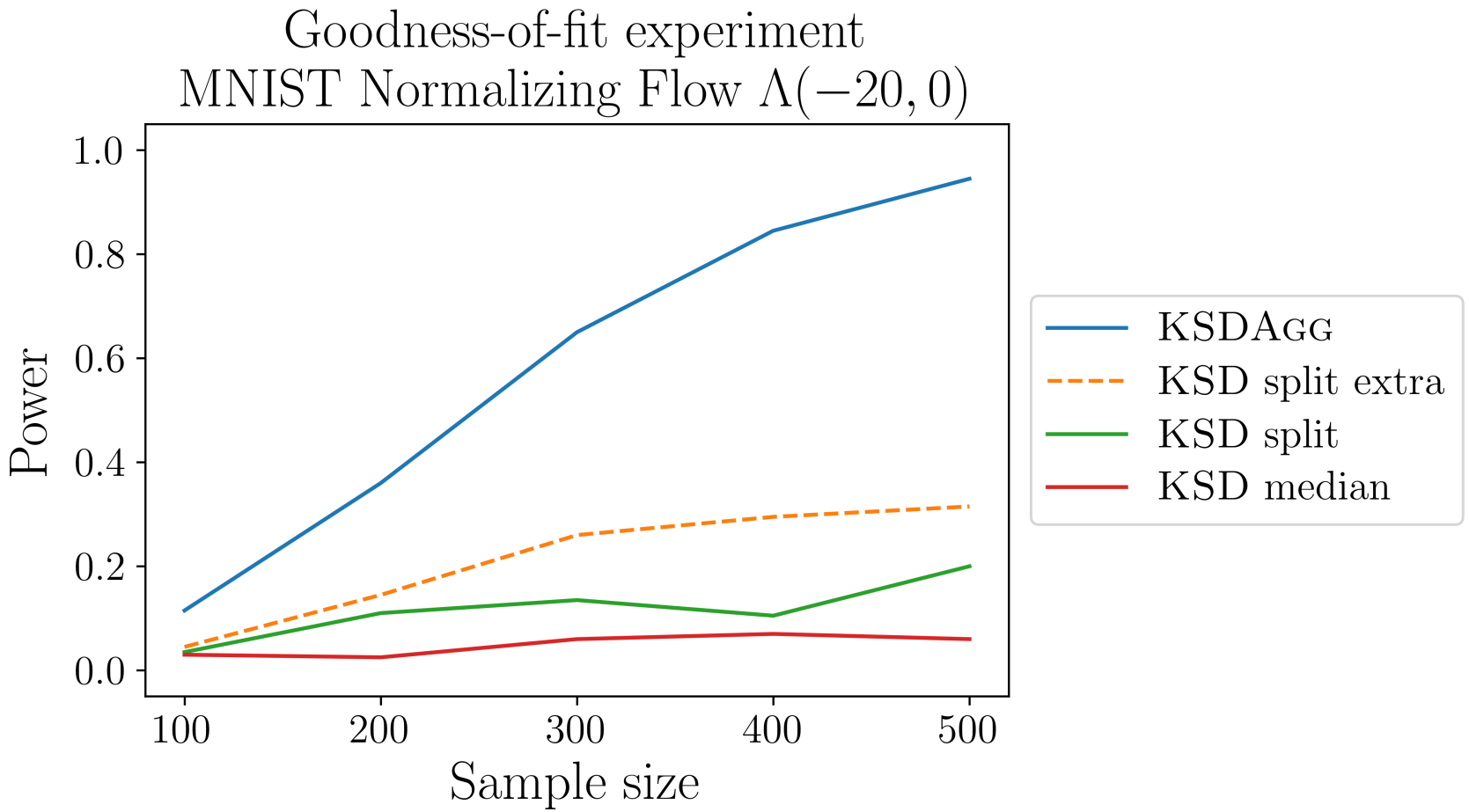

What about HSICAgg?

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

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- 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.

Efficient Aggregated Kernel Tests using Incomplete U-statistics




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AggInc

- **Complete U-statistic:**

$$\sum_{1 \leq i \neq j \leq N} h(Z_i, Z_j)$$

AggInc

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- retain **high power** & **outperform** state-of-the-art linear-time tests

Thank you for your attention!

MMDAgg

paper

code

KSDAgg

paper

code

AggInc: coming out soon!