Aggregated Kernel Tests

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

a.schrab@ucl.ac.uk *antoninschrab.github.io*

Aggregated Kernel Tests

1. MMDAgg: MMD Aggregated Two-Sample Test
2. KSDAgg: KSD Aggregated Goodness-of-fit Test
3. AggInc: Efficient Aggregated Kernel Tests using Incomplete U-statistics

MMD Aggregated Two-Sample Test






Antonin Schrab † ‡ §

Ilmun Kim ∗

Mélisande Albert ⋆

Béatrice Laurent ⋆

Benjamin Guedj †§

Arthur Gretton ‡

† Centre for Artificial Intelligence, UCL

‡ Gatsby Computational Neuroscience Unit, UCL

§ Inria London Programme

∗ Department of Statistics & Data Science, Yonsei University

⋆ Institut de Mathématiques, Université de Toulouse

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 $\mathbb{R}^d$

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 $\mathbb{R}^d$

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

Two-sample problem

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

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

Type I error: controlled by α by design

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

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 $\mathbb{R}^d$

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

Type I error: controlled by α by design

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

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:** $\lambda \in (0, \infty)^d$

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:** $\lambda \in (0, \infty)^d$

Gaussian kernel: $K_i(u) = \frac{1}{\sqrt{\pi}} \exp\left(-u^2\right), u \in \mathbb{R}, i = 1, \ldots, d$

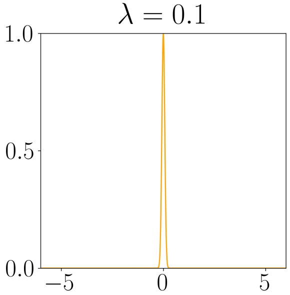
$$k_\lambda(x, y) := \frac{1}{\pi^{d/2} \lambda_1 \cdots \lambda_d} \exp\left(-\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{\lambda_i{}^2}\right)$$

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:** $\lambda \in (0, \infty)^d$

Gaussian kernel: $K_i(u) = \frac{1}{\sqrt{\pi}} \exp\left(-u^2\right), u \in \mathbb{R}, i = 1, \ldots, d$

$$k_{\lambda}(x, y) := \frac{1}{\pi^{d/2} \lambda_1 \cdots \lambda_d} \exp\left(-\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{{\lambda_i}^2}\right)$$

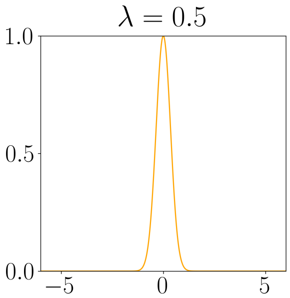


Kernels

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:** $\lambda \in (0,\infty)^d$

Gaussian kernel: $K_i(u) = \frac{1}{\sqrt{\pi}} \exp\left(-u^2\right), u \in \mathbb{R}, i = 1, \ldots, d$

$$k_\lambda(x,y) := \frac{1}{\pi^{d/2}\lambda_1 \cdots \lambda_d} \exp\left(-\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{{\lambda_i}^2}\right)$$

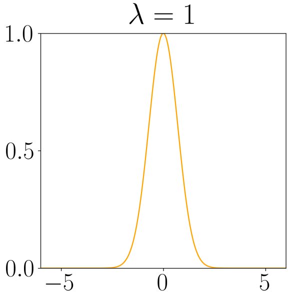


Kernels

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:** $\lambda \in (0, \infty)^d$

Gaussian kernel: $K_i(u) = \frac{1}{\sqrt{\pi}} \exp\left(-u^2\right), u \in \mathbb{R}, i = 1, \dots, d$

$$k_{\lambda}(x, y) := \frac{1}{\pi^{d/2} \lambda_1 \cdots \lambda_d} \exp\left(-\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{\lambda_i{}^2}\right)$$

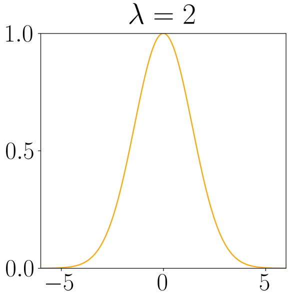


Kernels

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:** $\lambda \in (0,\infty)^d$

Gaussian kernel: $K_i(u) = \frac{1}{\sqrt{\pi}} \exp\left(-u^2\right), u \in \mathbb{R}, i = 1,\dots,d$

$$k_\lambda(x,y) := \frac{1}{\pi^{d/2}\lambda_1 \cdots \lambda_d} \exp\left(-\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{{\lambda_i}^2}\right)$$

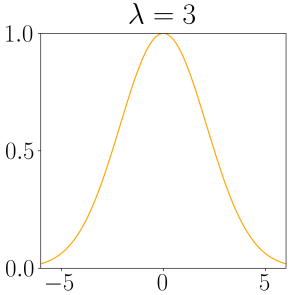


Kernels

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:** $\lambda \in (0, \infty)^d$

Gaussian kernel: $K_i(u) = \frac{1}{\sqrt{\pi}} \exp\left(-u^2\right), u \in \mathbb{R}, i = 1, \dots, d$

$$k_{\lambda}(x, y) := \frac{1}{\pi^{d/2} \lambda_1 \cdots \lambda_d} \exp\left(-\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{{\lambda_i}^2}\right)$$

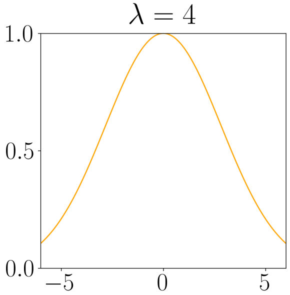


Kernels

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:** $\lambda \in (0,\infty)^d$

Gaussian kernel: $K_i(u) = \frac{1}{\sqrt{\pi}} \exp\left(-u^2\right), u \in \mathbb{R}, i = 1,\dots,d$

$$k_\lambda(x,y) := \frac{1}{\pi^{d/2}\lambda_1 \cdots \lambda_d} \exp\left(-\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{{\lambda_i}^2}\right)$$

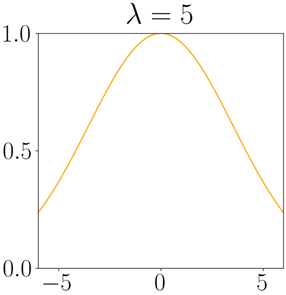


Kernels

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:** $\lambda \in (0, \infty)^d$

Gaussian kernel: $K_i(u) = \frac{1}{\sqrt{\pi}} \exp\left(-u^2\right), u \in \mathbb{R}, i = 1, \dots, d$

$$k_\lambda(x, y) := \frac{1}{\pi^{d/2} \lambda_1 \cdots \lambda_d} \exp\left(-\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{{\lambda_i}^2}\right)$$



Two-sample test using the Maximum Mean Discrepancy

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:** $\lambda \in (0, \infty)^d$

Two-sample test using the Maximum Mean Discrepancy

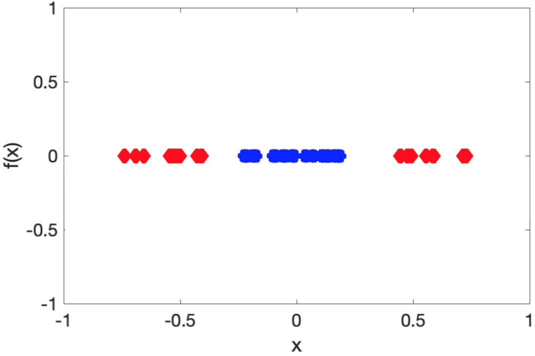
Kernel: $k_\lambda(x, y) := \prod_{i=1}^{d} \frac{1}{\lambda_i} K_i\left(\frac{x_i - y_i}{\lambda_i}\right)$ **Bandwidth:** $\lambda \in (0, \infty)^d$

$$\mathrm{MMD}_\lambda(p, q) := \sup_{f \in \mathcal{H}_\lambda : \|f\|_{\mathcal{H}_\lambda} \le 1} \left| \mathbb{E}_{X \sim p}[f(X)] - \mathbb{E}_{Y \sim q}[f(Y)] \right|$$

Two-sample test using the Maximum Mean Discrepancy

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:** $\lambda \in (0,\infty)^d$

$$\mathrm{MMD}_\lambda(p,q) := \sup_{f\in\mathcal{H}_\lambda : \|f\|_{\mathcal{H}_\lambda}\le 1} \left|\mathbb{E}_{X\sim p}[f(X)] - \mathbb{E}_{Y\sim q}[f(Y)]\right|$$

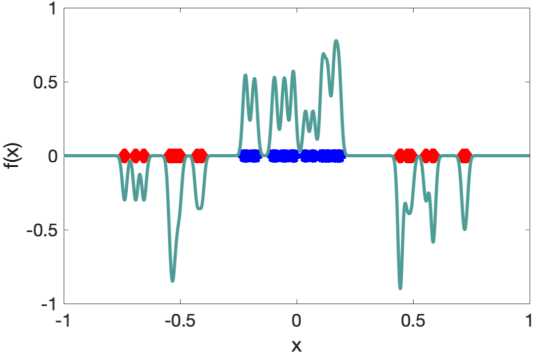


$p \neq q$

Two-sample test using the Maximum Mean Discrepancy

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:** $\lambda \in (0, \infty)^d$

$$\mathrm{MMD}_\lambda(p, q) := \sup_{f \in \mathcal{H}_\lambda : \|f\|_{\mathcal{H}_\lambda} \leq 1} \left| \mathbb{E}_{X \sim p}[f(X)] - \mathbb{E}_{Y \sim q}[f(Y)] \right|$$



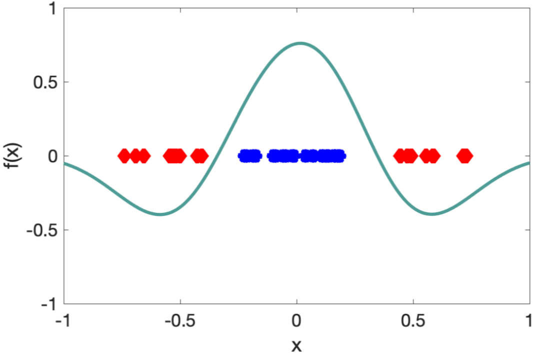
$p \neq q$

bandwidth λ: too small

Two-sample test using the Maximum Mean Discrepancy

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:** $\lambda \in (0, \infty)^d$

$$\mathrm{MMD}_\lambda(p, q) := \sup_{f \in \mathcal{H}_\lambda : \|f\|_{\mathcal{H}_\lambda} \leq 1} \left| \mathbb{E}_{X \sim p}[f(X)] - \mathbb{E}_{Y \sim q}[f(Y)] \right|$$



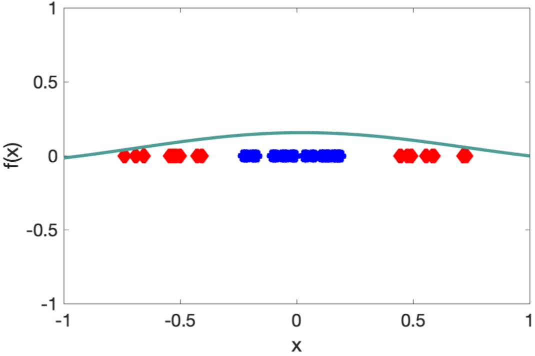
$p \neq q$

bandwidth λ: well-calibrated

Two-sample test using the Maximum Mean Discrepancy

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:** $\lambda \in (0, \infty)^d$

$$\mathrm{MMD}_\lambda(p, q) := \sup_{f \in \mathcal{H}_\lambda : \|f\|_{\mathcal{H}_\lambda} \le 1} \left| \mathbb{E}_{X \sim p}[f(X)] - \mathbb{E}_{Y \sim q}[f(Y)] \right|$$



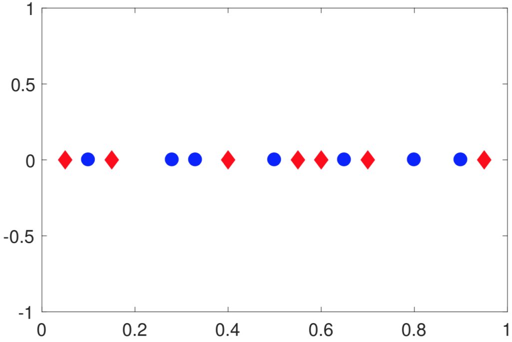
$p \neq q$

bandwidth λ: too large

Two-sample test using the Maximum Mean Discrepancy

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:** $\lambda \in (0,\infty)^d$

$$\mathrm{MMD}_\lambda(p,q) := \sup_{f \in \mathcal{H}_\lambda : \|f\|_{\mathcal{H}_\lambda} \le 1} \left| \mathbb{E}_{X\sim p}[f(X)] - \mathbb{E}_{Y\sim q}[f(Y)] \right|$$

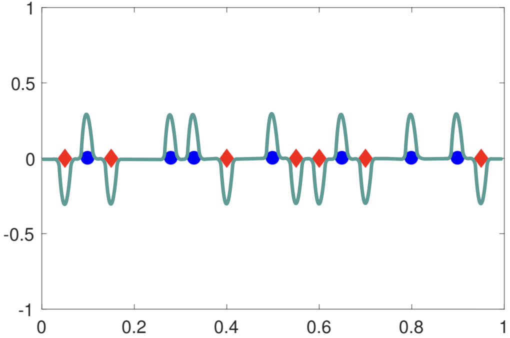


$p = q$

Two-sample test using the Maximum Mean Discrepancy

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:** $\lambda \in (0, \infty)^d$

$$\mathrm{MMD}_\lambda(p, q) := \sup_{f \in \mathcal{H}_\lambda : \|f\|_{\mathcal{H}_\lambda} \leq 1} \left| \mathbb{E}_{X\sim p}[f(X)] - \mathbb{E}_{Y\sim q}[f(Y)] \right|$$



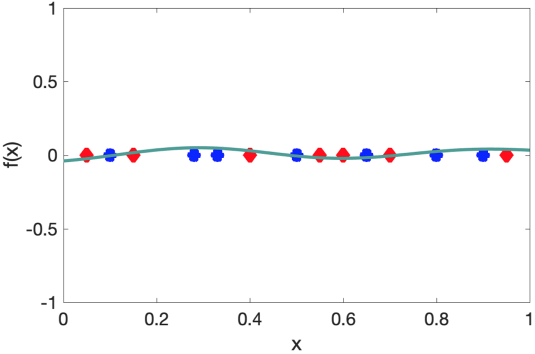
$p = q$

bandwidth λ**:** too small

Two-sample test using the Maximum Mean Discrepancy

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:** $\lambda \in (0, \infty)^d$

$$\mathrm{MMD}_\lambda(p, q) := \sup_{f \in \mathcal{H}_\lambda : \|f\|_{\mathcal{H}_\lambda} \leq 1} \left| \mathbb{E}_{X \sim p}[f(X)] - \mathbb{E}_{Y \sim q}[f(Y)] \right|$$



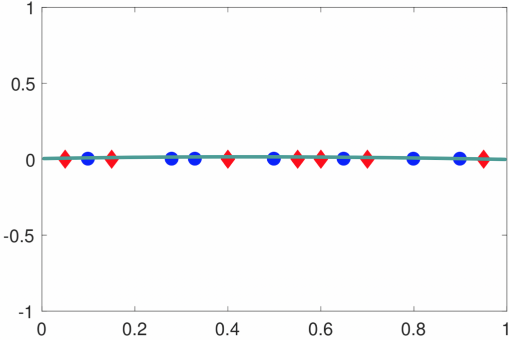
$p = q$

bandwidth λ: well-calibrated

Two-sample test using the Maximum Mean Discrepancy

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:** $\lambda \in (0,\infty)^d$

$$\mathrm{MMD}_\lambda(p,q) := \sup_{f \in \mathcal{H}_\lambda : \|f\|_{\mathcal{H}_\lambda} \leq 1} \left| \mathbb{E}_{X\sim p}[f(X)] - \mathbb{E}_{Y\sim q}[f(Y)] \right|$$



$p = q$

bandwidth λ: too large

Bandwidth intuition

- **Small sample sizes**: only global differences are detectable
  - **Small bandwidth**: wrongly detects artificial local differences under $\mathcal{H}_0$
  - **Large bandwidth**: well-suited to detect global differences under $\mathcal{H}_a$

Bandwidth intuition

- **Small sample sizes**: only global differences are detectable
  - **Small bandwidth**: wrongly detects artificial local differences under $\mathcal{H}_0$
  - **Large bandwidth**: well-suited to detect global differences under $\mathcal{H}_a$
- **Large sample sizes**: local differences are detectable
  - **Small bandwidth**: well-suited to detect local differences under $\mathcal{H}_a$
  - **Large bandwidth**: fails to detect local differences under $\mathcal{H}_a$

Bandwidth intuition

- **Small sample sizes**: only global differences are detectable
  - **Small bandwidth**: wrongly detects artificial local differences under $\mathcal{H}_0$
  - **Large bandwidth**: well-suited to detect global differences under $\mathcal{H}_a$
- **Large sample sizes**: local differences are detectable
  - **Small bandwidth**: well-suited to detect local differences under $\mathcal{H}_a$
  - **Large bandwidth**: fails to detect local differences under $\mathcal{H}_a$

$\Longrightarrow$ **Bandwidths** should decrease as the **sample sizes** increase

Bandwidth intuition

- **Small sample sizes**: only global differences are detectable
  - **Small bandwidth**: wrongly detects artificial local differences under $\mathcal{H}_0$
  - **Large bandwidth**: well-suited to detect global differences under $\mathcal{H}_a$
- **Large sample sizes**: local differences are detectable
  - **Small bandwidth**: well-suited to detect local differences under $\mathcal{H}_a$
  - **Large bandwidth**: fails to detect local differences under $\mathcal{H}_a$

$\Longrightarrow$ **Bandwidths** should decrease as the **sample sizes** increase

- Choice of **bandwidth** is **crucial** for test power!

Bandwidth intuition

- **Small sample sizes**: only global differences are detectable
  - **Small bandwidth**: wrongly detects artificial local differences under $\mathcal{H}_0$
  - **Large bandwidth**: well-suited to detect global differences under $\mathcal{H}_a$
- **Large sample sizes**: local differences are detectable
  - **Small bandwidth**: well-suited to detect local differences under $\mathcal{H}_a$
  - **Large bandwidth**: fails to detect local differences under $\mathcal{H}_a$

$\Longrightarrow$ **Bandwidths** should decrease as the **sample sizes** increase

- Choice of **bandwidth** is **crucial** for test power!
- **Bandwidth** selection methods: **median heuristic** & **data splitting**

Bandwidth intuition

- **Small sample sizes**: only global differences are detectable
  - **Small bandwidth**: wrongly detects artificial local differences under $\mathcal{H}_0$
  - **Large bandwidth**: well-suited to detect global differences under $\mathcal{H}_a$
- **Large sample sizes**: local differences are detectable
  - **Small bandwidth**: well-suited to detect local differences under $\mathcal{H}_a$
  - **Large bandwidth**: fails to detect local differences under $\mathcal{H}_a$

$\Longrightarrow$ **Bandwidths** should decrease as the **sample sizes** increase

- Choice of **bandwidth** is **crucial** for test power!
- **Bandwidth** selection methods: **median heuristic** & **data splitting**
- **Our method:** aggregate multiple tests with different **bandwidths**

Maximum Mean Discrepancy estimator

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

Maximum Mean Discrepancy estimator

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

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

MMD test for a fixed bandwidth λ

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

MMD test for a fixed bandwidth λ

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

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 $\mathcal{H}_0$-simulated test statistics

MMD test for a fixed bandwidth λ

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

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 $\mathcal{H}_0$-simulated test statistics

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

MMD test for a fixed bandwidth λ

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

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 $\mathcal{H}_0$-simulated test statistics

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

Wild bootstrap: case $m = n$, $\epsilon_1, \dots, \epsilon_n \overset{\text{iid}}{\sim} \mathrm{Unif}\{-1, 1\}$ (Rademacher)

$$\frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} \epsilon_i \epsilon_j \Big(k_\lambda(X_i, X_j) - k_\lambda(X_i, Y_j) - k_\lambda(Y_i, X_j) + k_\lambda(Y_i, Y_j) \Big)$$

MMD test for a fixed bandwidth λ

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

Quantile: $\widehat{q}^\lambda_{1-\alpha}$ is the $\lceil (B+1)(1-\alpha) \rceil$-th largest value of $\widehat{\mathrm{MMD}}^2_\lambda(\mathbb{X}_m, \mathbb{Y}_n)$ and B $\mathcal{H}_0$-simulated test statistics

Permutations: $\widehat{\mathrm{MMD}}^2_\lambda(\mathbb{X}^\sigma_m, \mathbb{Y}^\sigma_n)$ where $(\mathbb{X}^\sigma_m, \mathbb{Y}^\sigma_n) = \sigma(\mathbb{X}_m \cup \mathbb{Y}_n)$

Wild bootstrap: case $m = n$, $\epsilon_1, \ldots, \epsilon_n \overset{\text{iid}}{\sim} \text{Unif}\{-1, 1\}$ (Rademacher)

$$\frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} \epsilon_i \epsilon_j \left(k_\lambda(X_i, X_j) - k_\lambda(X_i, Y_j) - k_\lambda(Y_i, X_j) + k_\lambda(Y_i, Y_j) \right)$$

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

MMD test for a fixed bandwidth λ

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

Quantile: $\widehat{q}^{\lambda}_{1-\alpha}$ is the $\lceil (B+1)(1-\alpha) \rceil$-th largest value of $\widehat{\mathrm{MMD}}^2_\lambda(\mathbb{X}_m, \mathbb{Y}_n)$ and B $\mathcal{H}_0$-simulated test statistics

Permutations: $\widehat{\mathrm{MMD}}^2_\lambda(\mathbb{X}^\sigma_m, \mathbb{Y}^\sigma_n)$ where $(\mathbb{X}^\sigma_m, \mathbb{Y}^\sigma_n) = \sigma(\mathbb{X}_m \cup \mathbb{Y}_n)$

Wild bootstrap: case $m = n$, $\epsilon_1, \dots, \epsilon_n \overset{\text{iid}}{\sim} \mathrm{Unif}\{-1, 1\}$ (Rademacher)

$$\frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} \epsilon_i \epsilon_j \Big(k_\lambda(X_i, X_j) - k_\lambda(X_i, Y_j) - k_\lambda(Y_i, X_j) + k_\lambda(Y_i, Y_j) \Big)$$

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

Time complexity: $\mathcal{O}\Big(B\,(m+n)^2 \Big)$

MMDAgg for a collection of bandwidths Λ

MMDAgg for a collection of bandwidths Λ

Bonferroni multiple testing: non-asymptotic level α

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

MMDAgg for a collection of bandwidths Λ

Bonferroni multiple testing: non-asymptotic level α

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

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

MMDAgg for a collection of bandwidths Λ

Bonferroni multiple testing: non-asymptotic level α

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

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

MMDAgg: non-asymptotic level α

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

MMDAgg for a collection of bandwidths Λ

Bonferroni multiple testing: non-asymptotic level α

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

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

MMDAgg: non-asymptotic level α

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

- positive weights $(w_\lambda)_{\lambda\in\Lambda}$ satisfying $\sum_{\lambda\in\Lambda} w_\lambda \leq 1$

MMDAgg for a collection of bandwidths Λ

Bonferroni multiple testing: non-asymptotic level α

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

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

MMDAgg: non-asymptotic level α

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

- positive weights $(w_\lambda)_{\lambda\in\Lambda}$ satisfying $\sum_{\lambda\in\Lambda} w_\lambda \le 1$
- correction u_α defined as

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

MMDAgg for a collection of bandwidths Λ

Bonferroni multiple testing: non-asymptotic level α

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

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

MMDAgg: non-asymptotic level α

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

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

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

- more powerful than Bonferroni correction as $u_\alpha \geq \alpha$

MMDAgg for a collection of bandwidths Λ

Bonferroni multiple testing: non-asymptotic level α

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

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

MMDAgg: non-asymptotic level α

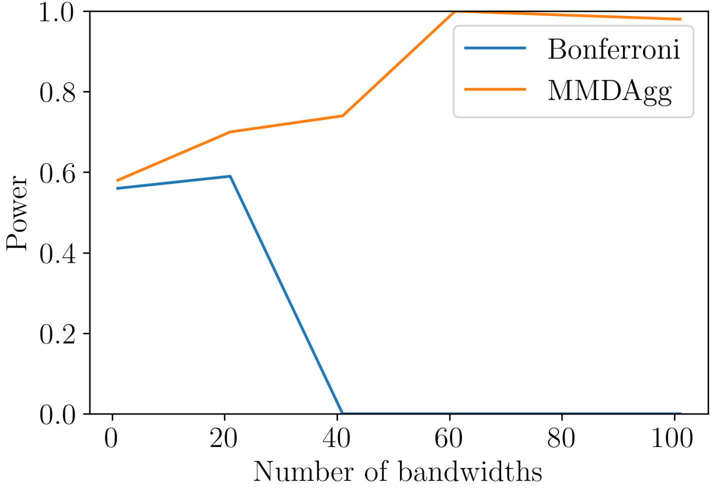
$$\Delta_\alpha^\Lambda(\mathbb{X}_m, \mathbb{Y}_n) := \mathbb{1}\left(\widehat{\mathrm{MMD}}_\lambda^2(\mathbb{X}_m, \mathbb{Y}_n) > \widehat{q}_{1-u_\alpha w_\lambda}^\lambda \text{ for some } \lambda \in \Lambda\right)$$

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

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

- more powerful than Bonferroni correction as $u_\alpha \geq \alpha$
- time complexity $\mathcal{O}\left(|\Lambda|\,(B_1 + B_2)\,(m+n)^2\right)$

Multiple testing correction comparison



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

$$\Lambda(-i, i), \quad i \in \{0, 10, 20, 30, 40, 50\}$$

Sobolev balls

Regularity/smoothness assumption: $p - q \in \mathcal{S}_d^s(R)$

Sobolev balls

Regularity/smoothness assumption: $p - q \in \mathcal{S}_d^s(R)$

Sobolev balls:

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

- radius $R > 0$
- dimension d
- smoothness parameter $s > 0$ (unknown)
- Fourier transform $\widehat{f}(\xi) := \int_{\mathbb{R}^d} f(x) e^{-ix^\top \xi} \mathrm{d}x$

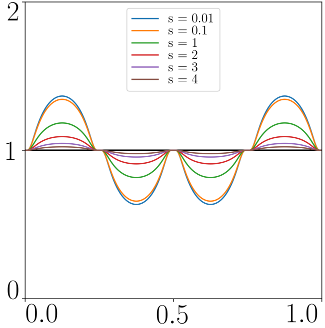
Sobolev balls

Regularity/smoothness assumption: $p - q \in \mathcal{S}_d^s(R)$

Sobolev balls:

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

- radius $R > 0$
- dimension d
- smoothness parameter $s > 0$ (unknown)
- Fourier transform $\widehat{f}(\xi) := \int_{\mathbb{R}^d} f(x) e^{-ix^\top \xi} \mathrm{d}x$



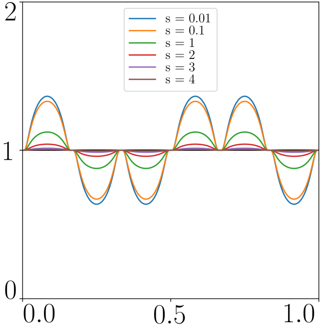
Sobolev balls

Regularity/smoothness assumption: $p - q \in \mathcal{S}_d^s(R)$

Sobolev balls:

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

- radius $R > 0$
- dimension d
- smoothness parameter $s > 0$ (unknown)
- Fourier transform $\widehat{f}(\xi) := \int_{\mathbb{R}^d} f(x) e^{-ix^\top \xi} \mathrm{d}x$



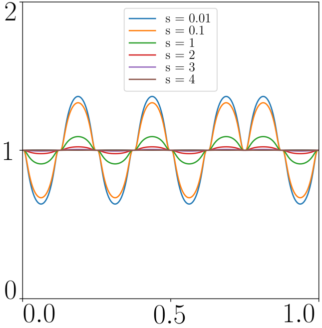
Sobolev balls

Regularity/smoothness assumption: $p - q \in \mathcal{S}_d^s(R)$

Sobolev balls:

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

- radius $R > 0$
- dimension d
- smoothness parameter $s > 0$ (unknown)
- Fourier transform $\widehat{f}(\xi) := \int_{\mathbb{R}^d} f(x) e^{-ix^\top \xi} \mathrm{d}x$



Minimax adaptivity over Sobolev balls

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: $(m+n)^{-2s/(4s+d)}$

Adaptive over $\{\mathcal{S}_d^s(R) : s > 0, R > 0\}$

MMDAgg Experiment

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

MMDAgg Experiment

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

$$\mathcal{P} := \{0, \dots, 9\} \quad \mathcal{Q}_2 := \mathcal{P} \setminus \{8, 6\} \quad \mathcal{Q}_4 := \mathcal{P} \setminus \{8, 6, 4, 2\}$$

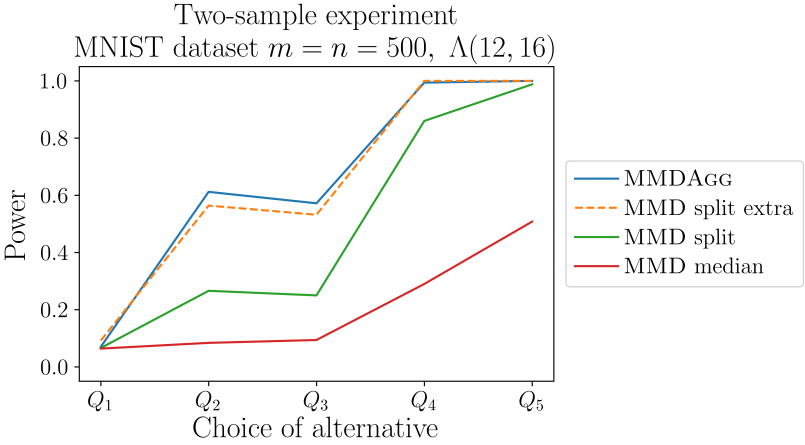
$$\mathcal{Q}_1 := \mathcal{P} \setminus \{8\} \quad \mathcal{Q}_3 := \mathcal{P} \setminus \{8, 6, 4\} \quad \mathcal{Q}_5 := \mathcal{P} \setminus \{8, 6, 4, 2, 0\}$$

MMDAgg Experiment

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

$$\mathcal{P} := \{0, \dots, 9\} \quad \mathcal{Q}_2 := \mathcal{P} \setminus \{8, 6\} \quad \mathcal{Q}_4 := \mathcal{P} \setminus \{8, 6, 4, 2\}$$

$$\mathcal{Q}_1 := \mathcal{P} \setminus \{8\} \quad \mathcal{Q}_3 := \mathcal{P} \setminus \{8, 6, 4\} \quad \mathcal{Q}_5 := \mathcal{P} \setminus \{8, 6, 4, 2, 0\}$$



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

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 $\mathbb{R}^d$

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

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 $\mathbb{R}^d$

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

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

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

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 $\mathbb{R}^d$

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

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

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

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

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 $\mathbb{R}^d$

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

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

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

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

KSD: $\mathrm{KSD}^2_{p,\lambda}(q) := \mathrm{MMD}^2_{h_{p,\lambda}}(p,q) = \mathbb{E}_{q,q}[h_{p,\lambda}(Z,Z')]$

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 $\mathbb{R}^d$

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

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

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

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

KSD: $\mathrm{KSD}^2_{p,\lambda}(q) := \mathrm{MMD}^2_{h_{p,\lambda}}(p, q) = \mathbb{E}_{q,q}[h_{p,\lambda}(Z, Z')]$

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

KSDAgg: KSD Aggregated test

Wild bootstrap: asymptotic level α

$$\frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} \epsilon_i \epsilon_j h_{p,\lambda}(Z_i, Z_j) \qquad \text{where} \qquad \epsilon_i \sim \text{Unif}\{-1, 1\}$$

KSDAgg: KSD Aggregated test

Wild bootstrap: asymptotic level α

$$\frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} \epsilon_i \epsilon_j h_{p,\lambda}(Z_i, Z_j) \qquad \text{where} \qquad \epsilon_i \sim \text{Unif}\{-1, 1\}$$

Parametric bootstrap: non-asymptotic level α

$$\frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h_{p,\lambda}(\widetilde{Z}_i, \widetilde{Z}_j) \qquad \text{where} \qquad \widetilde{Z}_i \overset{\text{iid}}{\sim} p$$

KSDAgg: KSD Aggregated test

Wild bootstrap: asymptotic level α

$$\frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} \epsilon_i \epsilon_j h_{p,\lambda}(Z_i, Z_j) \qquad \text{where} \qquad \epsilon_i \sim \text{Unif}\{-1, 1\}$$

Parametric bootstrap: non-asymptotic level α

$$\frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h_{p,\lambda}(\widetilde{Z}_i, \widetilde{Z}_j) \qquad \text{where} \qquad \widetilde{Z}_i \overset{\text{iid}}{\sim} p$$

KSDAgg:

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

Wild bootstrap: asymptotic level α

$$\frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} \epsilon_i \epsilon_j h_{p,\lambda}(Z_i, Z_j) \qquad \text{where} \qquad \epsilon_i \sim \text{Unif}\{-1, 1\}$$

Parametric bootstrap: non-asymptotic level α

$$\frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h_{p,\lambda}(\widetilde{Z}_i, \widetilde{Z}_j) \qquad \text{where} \qquad \widetilde{Z}_i \overset{\text{iid}}{\sim} p$$

KSDAgg:

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

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

KSDAgg Experiment

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

model: Normalizing Flow density

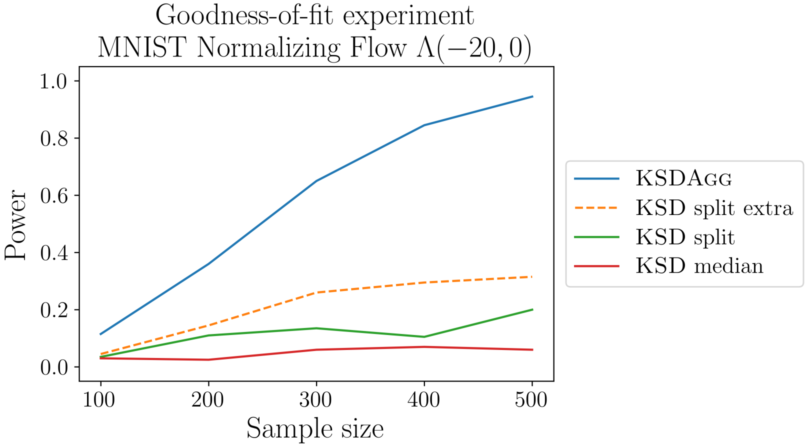
samples: true MNIST digits

KSDAgg Experiment

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

model: Normalizing Flow density

samples: true MNIST digits



What about HSICAgg?

Independence problem:

Given paired samples $\big((X_1, Y_1), \dots, (X_n, Y_n)\big)$ 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?

What about HSICAgg?

Independence problem:

Given paired samples $\big((X_1, Y_1), \dots, (X_n, Y_n)\big)$ 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?

Hilbert-Schmidt Independence Criterion:

$$\mathrm{HSIC}_{k,\ell}(r) := \mathrm{MMD}_\kappa(p \otimes q, r)$$
$$\kappa\big((X, Y), (X', Y')\big) := k(X, X')\ell(Y, Y')$$

What about HSICAgg?

Independence problem:

Given paired samples $\big((X_1, Y_1), \dots, (X_n, Y_n)\big)$ 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?

Hilbert-Schmidt Independence Criterion:

$$\mathrm{HSIC}_{k,\ell}(r) \coloneqq \mathrm{MMD}_\kappa(p \otimes q, r)$$
$$\kappa\big((X, Y), (X', Y')\big) \coloneqq k(X, X')\ell(Y, Y')$$

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.

AggInc: MMDAggInc, KSDAggInc & HSICAggInc

Efficient Aggregated Kernel Tests using Incomplete U-statistics


Antonin Schrab †‡§


Ilmun Kim ∗


Benjamin Guedj †§


Arthur Gretton ‡

† Centre for Artificial Intelligence, UCL
‡ Gatsby Computational Neuroscience Unit, UCL
§ Inria London Programme
∗ Department of Statistics & Data Science, Yonsei University

AggInc

- **Complete U-statistic:**

$$\frac{1}{N(N-1)} \sum_{1 \le i \ne j \le N} h(Z_i, Z_j)$$

AggInc

- **Complete U-statistic:**

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

- **Quadratic-time MMDAgg, KSDAgg & HSICAgg:**

$$\mathcal{O}\Big(|\Lambda| \left(B_1 + B_2\right) N^2\Big)$$

AggInc

- **Complete U-statistic:**

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

- **Quadratic-time MMDAgg, KSDAgg & HSICAgg:**

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

- **Incomplete U-statistic:**

$$\frac{1}{|\mathcal{D}|} \sum_{(i,j) \in \mathcal{D}} h(Z_i, Z_j) \qquad \mathcal{D} \subseteq \Big\{(i,j) : 1 \leq i \neq j \leq N\Big\}$$

AggInc

- **Complete U-statistic:**

$$\frac{1}{N(N-1)} \sum_{1 \le i \ne j \le N} h(Z_i, Z_j)$$

- **Quadratic-time MMDAgg, KSDAgg & HSICAgg:**

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

- **Incomplete U-statistic:**

$$\frac{1}{|\mathcal{D}|} \sum_{(i,j) \in \mathcal{D}} h(Z_i, Z_j) \qquad \mathcal{D} \subseteq \Big\{(i,j) : 1 \le i \ne j \le N\Big\}$$

- **Efficient MMDAggInc, KSDAggInc & HSICAggInc:**

$$\mathcal{O}\Big(|\Lambda|\,(B_1 + B_2)\,|\mathcal{D}|\Big)$$

AggInc

- **Complete U-statistic:**

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

- **Quadratic-time MMDAgg, KSDAgg & HSICAgg:**

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

- **Incomplete U-statistic:**

$$\frac{1}{|\mathcal{D}|} \sum_{(i,j) \in \mathcal{D}} h(Z_i, Z_j) \qquad \mathcal{D} \subseteq \Big\{(i,j) : 1 \leq i \neq j \leq N\Big\}$$

- **Efficient MMDAggInc, KSDAggInc & HSICAggInc:**

$$\mathcal{O}\Big(|\Lambda|\,(B_1 + B_2)\,|\mathcal{D}|\Big)$$

- **Linear-time** if $|\mathcal{D}| = cN$

AggInc: uniform separation rates

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

AggInc: uniform separation rates

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

MMDAgg & HSICAgg rates: $\left(\frac{N}{\ln(\ln(N))}\right)^{-2s/(4s+d)}$

AggInc: uniform separation rates

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

MMDAgg & HSICAgg rates: $\left(\dfrac{N}{\ln(\ln(N))}\right)^{-2s/(4s+d)}$

MMDAggInc & HSICAggInc rates: $\left(\dfrac{|\mathcal{D}|/N}{\ln(\ln(|\mathcal{D}|/N))}\right)^{-2s/(4s+d)}$

AggInc: uniform separation rates

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

MMDAgg & HSICAgg rates: $\left(\dfrac{N}{\ln(\ln(N))}\right)^{-2s/(4s+d)}$

MMDAggInc & HSICAggInc rates: $\left(\dfrac{|\mathcal{D}|/N}{\ln(\ln(|\mathcal{D}|/N))}\right)^{-2s/(4s+d)}$

- $|\mathcal{D}| \asymp N^2$: recover the **Agg** rate

AggInc: uniform separation rates

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

MMDAgg & HSICAgg rates: $\left(\dfrac{N}{\ln(\ln(N))}\right)^{-2s/(4s+d)}$

MMDAggInc & HSICAggInc rates: $\left(\dfrac{|\mathcal{D}|/N}{\ln(\ln(|\mathcal{D}|/N))}\right)^{-2s/(4s+d)}$

- $|\mathcal{D}| \asymp N^2$: recover the **Agg** rate

- $N \lesssim |\mathcal{D}| \lesssim N^2$: cost $|\mathcal{D}|/N^2$ incurred in the **Agg** rate

Trade-off: computational efficiency / rate of convergence

AggInc: uniform separation rates

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

MMDAgg & HSICAgg rates: $\left(\dfrac{N}{\ln(\ln(N))}\right)^{-2s/(4s+d)}$

MMDAggInc & HSICAggInc rates: $\left(\dfrac{|\mathcal{D}|/N}{\ln(\ln(|\mathcal{D}|/N))}\right)^{-2s/(4s+d)}$

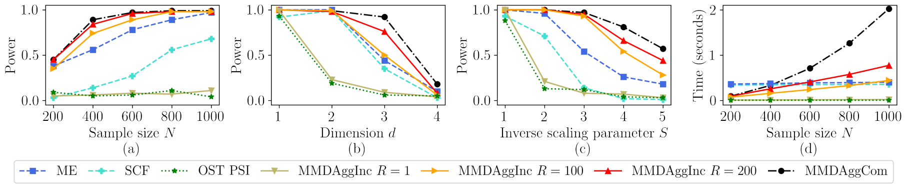
- $|\mathcal{D}| \asymp N^2$: recover the **Agg** rate

- $N \lesssim |\mathcal{D}| \lesssim N^2$: cost $|\mathcal{D}|/N^2$ incurred in the **Agg** rate
Trade-off: computational efficiency / rate of convergence

- $|\mathcal{D}| \lesssim N$: no guarantee that the **AggInc** rate converges to 0

MMDAggInc: experiments

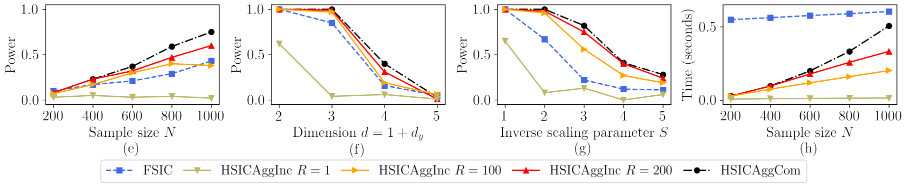
Perturbed uniform densities



ME (Mean Embeddings) & SCF (Smooth Characteristic Functions): Jitkrittum, W., Szabó, Z., Chwialkowski, K. P., and Gretton, A. **Interpretable distribution features with maximum testing power**. In NeurIPS 2016.

OST PSI (One-sided Test Post Selection Inference): Kübler, J. M., Jitkrittum, W., Schölkopf, B., and Muandet, K. **Learning kernel tests without data splitting**. NeurIPS 2020.

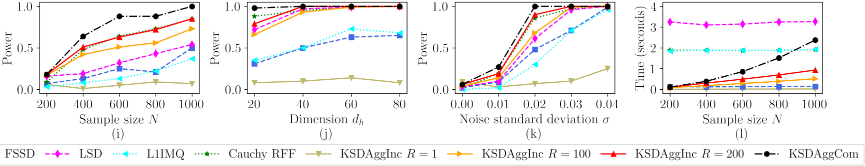
Perturbed uniform densities



FSIC (Finite Set Independence Criterion): Jitkrittum, W., Szabó, Z., and Gretton, A. **An adaptive test of independence with analytic kernel embeddings**. In ICML 2017.

KSDAggInc: experiments

Gaussian-Bernoulli Restricted Boltzmann Machine



FSSD (Finite Set Stein Discrepancy): Jitkrittum, W., Xu, W., Szabó, Z., Fukumizu, K., and Gretton, A. **A linear-time kernel goodness-of-fit test**. In NeurIPS 2017.

LSD (Learned Stein Discrepancy): Grathwohl, W., Wang, K.-C., Jacobsen, J.-H., Duvenaud, D., and Zemel, R. **Learning the Stein discrepancy for training and evaluating energy-based models without sampling**. In ICML 2020.

L1 IMQ & Cauchy RFF (Random Fourier Features): Huggins, J. and Mackey, L. **Random feature Stein discrepancies**. In NeurIPS 2018.

Thank you for your attention!
Any Questions?

SCAN ME — MMDAgg

SCAN ME — KSDAgg

SCAN ME — AggInc

SCAN ME — Code