Variable Selection for Kernel Two-Sample Tests

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Question: How to Compare Two Samples

- **Given**: Samples from unknown distributions P and Q in $\mathbb{R}^D$.
- **Goal**:
  - Do P and Q differ?
  - Select d variables maximally distinguishing differences between P and Q!

$\sim P$

$\sim Q$

Maximum Mean Discrepancy (MMD)

- A kernel function $K(\cdot,\cdot)$ is called a positive semi-definite kernel if

$$\sum_{i,j} c_i c_j K(x_i, x_j) \geq 0, \quad \forall x_i, x_j.$$

- A positive semi-definite kernel K induces a unique RKHS $\mathcal{H}_K$.
- MMD statistic:

$$\mathrm{MMD}(\mu,\nu;K) \triangleq \sup_{f\in\mathcal{H}_K, \|f\|_{\mathcal{H}_K}\leq 1} \left\{ \mathbb{E}_\mu[f] - \mathbb{E}_\nu[f] \right\}$$

- Squared MMD statistic:

$$\mathrm{MMD}(\mu,\nu;K)^2 = \mathbb{E}_{x,x'\sim\mu}[K(x,x')] + \mathbb{E}_{y,y'\sim\nu}[K(y,y')] - \mathbb{E}_{x\sim\mu,y\sim\nu}[K(x,y)].$$

- Empirical MMD estimator:

$$S^2(\mathbf{x}^n,\mathbf{y}^m;K) = \frac{1}{n^2}\sum_{i,j\in[n]} K_{i,j}^{x,x} + \frac{1}{m^2}\sum_{i,j\in[m]} K_{i,j}^{y,y} - \frac{2}{mn}\sum_{i\in[n],j\in[m]} K_{i,j}^{x,y}.$$

MMD Variable Selection

- Pick the optimal variable selection z to maximize MMD:

$$\max_{z\in\mathcal{Z}} \quad S^2(\mathbf{x}^n,\mathbf{y}^m;K_z)$$

where $\quad z\in\mathcal{Z} := \{z\in\mathbb{R}^D : \|z\|_2 = 1, \|z\|_0 = d\}.$

Statistical Performance Guarantees

Define the sample size $N = n \wedge m$ and

$$\hat{z} = \arg\max_{z\in\mathcal{Z}} S^2(\mathbf{x}^n,\mathbf{y}^m;K_z),$$

- Under null hypothesis $H_0: \mu=\nu$, with high probability,

$$S^2(\mathbf{x}^n,\mathbf{y}^m;K_{\hat{z}}) \lesssim \frac{D}{N}\left[\log\frac{D}{N} + \log\frac{1}{\eta}\right].$$

- Under mild assumptions regarding μ and ν under H_1, it holds that

$$S(\mathbf{x}^n,\mathbf{y}^m;K_{\hat{z}}) \geq \Delta - O(1/\sqrt{N}),$$

where $\Delta > 0$ is a sufficiently large number.

- Example: Linear Kernel MMD. For $K_z(x,y) = \sum_{k\in[D]} z[k]x[k]y[k]$,

$$\max_{z\in\mathcal{Z}} \ a^{\mathrm{T}} z, \qquad a[k] = \left(\frac{1}{n}\sum_{i\in[n]} x_i[k] - \frac{1}{m}\sum_{j\in[m]} y_j[k]\right)^2.$$

Advantages: closed-form solution available!
Concerns: Only first-order moment condition is used!

$$\mathrm{MMD}^2(\mu,\nu;K_z) = \sum_{k\in[D]} z[k]\left(\overline{x}[k] - \overline{y}[k]\right)^2, \quad \overline{x} = \mathbb{E}[\mu], \overline{y} = \mathbb{E}[\nu].$$

Quadratic Kernel MMD

- For $K_z(x,y) = \left(\sum_{k\in[D]} z[k]x[k]y[k] + c\right)^2$, reduces to MIQP:

$$\max_{z\in\mathbb{R}^D} \left\{ S^2(\mathbf{x}^n,\mathbf{y}^m;K_z) = z^{\mathrm{T}}Az + z^{\mathrm{T}}t : \ \|z\|_2 = 1, \|z\|_0 = d \right\}.$$

When $t=0$, standard **sparse PCA** formulation (Li and Xie, 2020).

- Combinatorial formulation:

$$\max_{\substack{S\subseteq[D]:\ |S|\leq d,\\ z\in\mathbb{R}^D}} \left\{ z^{\mathrm{T}}Az + z^{\mathrm{T}}t : \ \|z\|_2 = 1, z[k]=0, \forall k\notin S \right\}.$$

For fixed set S, it reduces to the **trust-region subproblem** (TRS) that is efficiently solvable.

Mixed-integer SDP reformulation

The Q-MMD optimization is equivalent to

$$\begin{aligned} \max_{Z\in\mathbb{S}^+_{D+1}, q\in\mathcal{Q}} \quad & \langle \tilde{A}, Z\rangle \\ \text{s.t.} \quad & Z_{i,i} \leq q[i], \quad i\in[D], \\ & Z_{0,0} = 1, \mathrm{Tr}(Z) = 2, \end{aligned}$$

where the set $\mathcal{Q} = \{q\in\{0,1\}^D : \ \sum_{k\in[D]} q_i = d\},$. It further admits two valid inequalities:

$$\begin{aligned} \sum_{j\in[D]} |Z_{i,j}| &\leq \sqrt{d}q[i], \quad \forall i\in[D] \\ |Z_{i,j}| &\leq M_{i,j}q[i], \quad \forall i,j\in[D] \end{aligned}$$

where $M_{i,j} = 1$ for $i=j$ and otherwise $M_{i,j} = 1/2$.

– Exact algorithm: cutting-plane algorithm;
– Approximation algorithm: convex relaxation of MISDP.

Performance Guarantees of Convex Relaxation

$$\mathrm{optval(MISDP)} \leq \mathrm{optval(SDP)} \leq \|t\|_2 + \min\left\{ D/d\cdot\mathrm{optval(MISDP)}, d\cdot\mathrm{optval(MISDP)} - \min_k |t[k]| \right\}.$$

- Population quadratic MMD statistic:

$$\mathrm{MMD}(\mu,\nu;K_z)^2 = z^{\mathrm{T}}\mathcal{A}(\mu,\nu)z + z^{\mathrm{T}}\mathcal{T}(\mu,\nu),$$

where $\mathcal{A}(\mu,\nu)$ is a $\mathbb{R}^{D\times D}$-valued mapping such that

$$(\mathcal{A}(\mu,\nu))_{k_1,k_2} = \left(\mathbb{E}_{x\sim\mu}[x[k_1]x[k_2]] - \mathbb{E}_{y\sim\nu}[y[k_1]y[k_2]]\right)^2$$

and $\mathcal{T}(\mu,\nu)$ is a $\mathbb{R}^D$-valued mapping such that

$$\mathcal{T}(\mu,\nu)[k] = 2c\left(\mathbb{E}_{x\sim\mu}[x[k]] - \mathbb{E}_{y\sim\nu}[y[k]]\right)^2.$$

Only first- and second-order moment conditions are used for Q-MMD variable selection!

Gaussian Kernel MMD

- Define $Z := zz^{\mathrm{T}} \in \mathbb{S}^+_D$ and $M_{x,y} := \frac{1}{2\gamma}(x-y)(x-y)^{\mathrm{T}} \in \mathbb{S}^+_D$.
- Consider Gaussian kernel

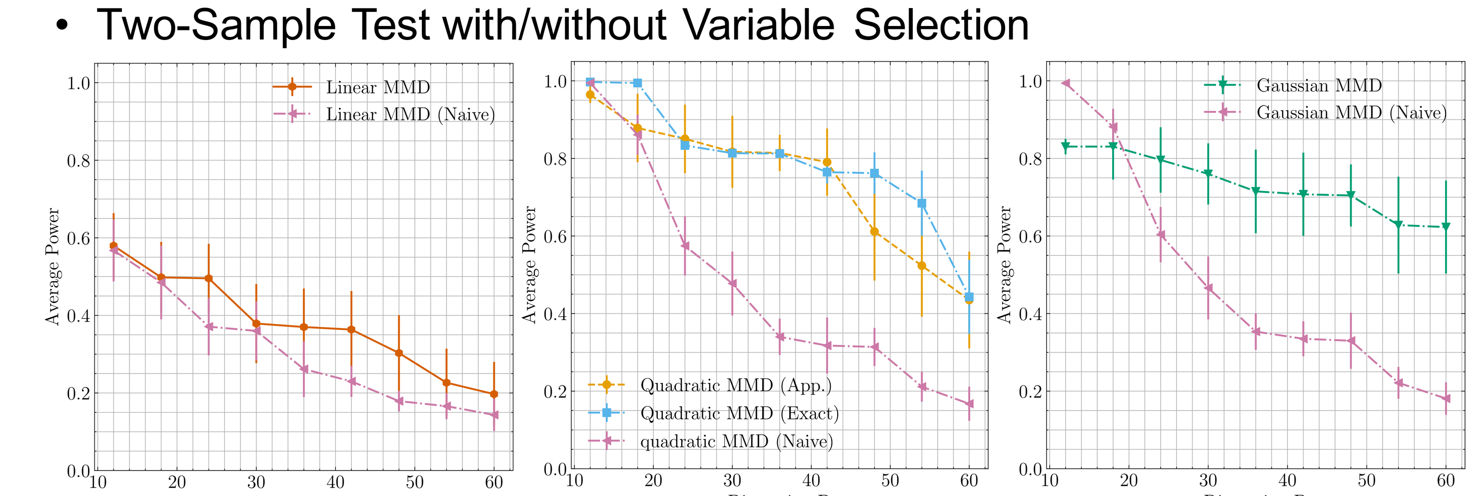
$$K_z(x,y) = \exp\left[-\frac{\left(\sum_{k\in[D]} z[k](x[k]-y[k])\right)^2}{2\gamma} \right] = \exp\left(-\frac{\langle Z, M_{x,y}\rangle}{2\gamma} \right)$$

- Rank and ℓ_0-norm constraint optimization:

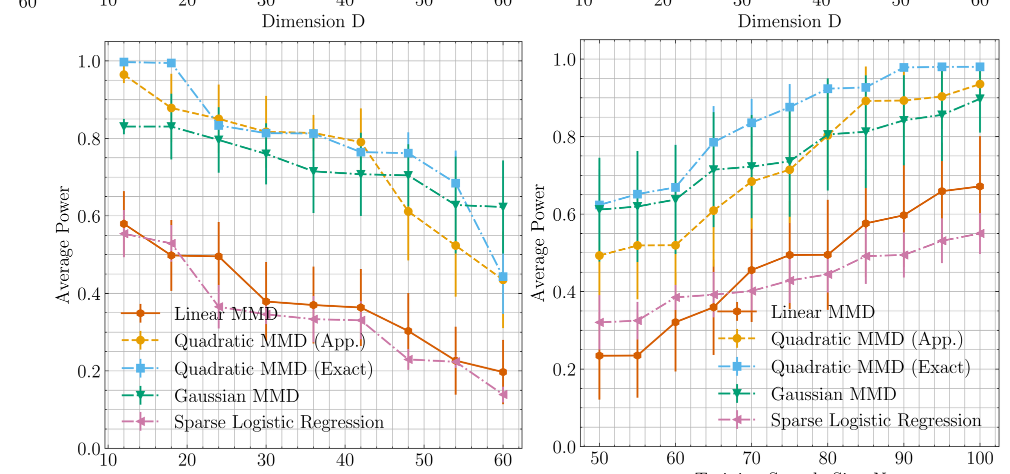
$$\begin{aligned} \min_{Z\in\mathbb{S}^+_D:\mathrm{Tr}(Z)=1} \quad & \frac{2\sum e^{-\langle Z, M_{x_i,y_j}\rangle}}{mn} - \frac{\sum e^{-\langle Z, M_{x_i,x_j}\rangle}}{n^2} - \frac{\sum e^{-\langle Z, M_{y_i,y_j}\rangle}}{m^2} \\ \text{s.t.} \quad & \|Z\|_0 \leq d^2, \mathrm{rank}(Z) = 1, \end{aligned}$$

Numerical Study

- Two-Sample Test with/without Variable Selection



- Two-Sample Test with Synthetic Dataset



- Two-Sample Test with Large-Scale Dataset
- $D = 500$, $d^* = 20$
- Non-discovery proportion : $\frac{|I^*\setminus I|}{|I^*|}$
- False-discovery proportion : $\frac{|I\setminus I^*|}{|I|}$