Variable Selection for Kernel Two-Sample Tests

Jie Wang, Santanu S. Dey, Yao Xie

Georgia Tech ISyE H. Milton Stewart School of Industrial and Systems Engineering

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Question: How to Compare Two Samples

- **Given**: Samples from unknown distributions P and Q in $\mathbb{R}^D$.

 $\sim P$
- Does P and Q differ?

 $\sim Q$
- Select d variables that maximally distinguish differences between P and Q

Maximum Mean Discrepancy (MMD)

- Kernel function $K(\cdot,\cdot)$ is positive semi-definite (PSD) if

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

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

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

- 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:

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

MMD Variable Selection

- Pick the optimal variable selection z to maximize MMD:

$$\max_{z\in\mathcal{Z}} \; S^2(\mathbf{x}^n, \mathbf{y}^m; K_z)$$
$$\text{where} \quad z\in\mathcal{Z} := \{z\in\mathbb{R}^D : \|z\|_2 = 1, \|z\|_0 = d\}.$$

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.

- 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!
Only mean condition is used: $\overline{x} = \mathbb{E}[\mu], \overline{y} = \mathbb{E}[\nu]$,

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

Quadratic Kernel MMD

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

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

- 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 **trust-region subproblem**.

Mixed-integer SDP reformulation

The Q-MMD optimization is equivalent to

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

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

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

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

– **Exact algorithm:** cutting-plane algorithm;

– **Approximation algorithm:**

(I) Return the best over all d-sparse truncation of columns of A and all basis vectors:

$$V_{(\mathrm{I})} \geq \mathrm{optval}(\mathrm{MIQP})/\sqrt{d} - 2\|t\|_{(d+1)}.$$

(II) Solve the problem by dropping ℓ_0-norm constraint and return its d-sparse truncation:

$$V_{(\mathrm{II})} \geq d/D \cdot \mathrm{optval}(\mathrm{MIQP}) - d/D \cdot \|t\|_2 - \left(1 + \sqrt{d/D}\right)\cdot\|t\|_{(d)}.$$

- 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

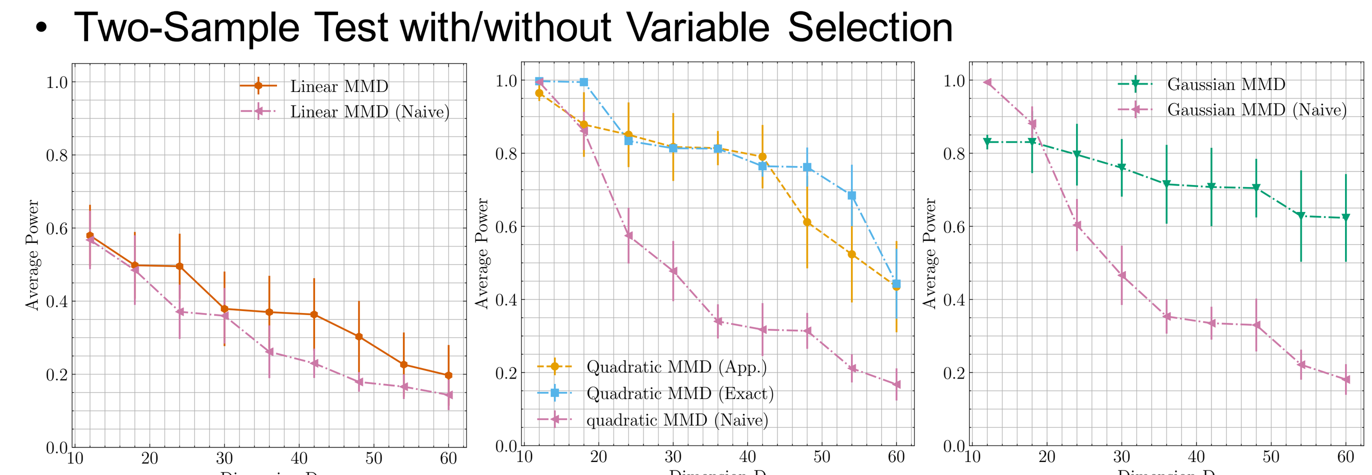
$$(\mathcal{A}(\mu,\nu))_{k_1,k_2} = (\mathbb{E}_{x\sim\mu}[x[k_1]x[k_2]] - \mathbb{E}_{y\sim\nu}[y[k_1]y[k_2]])^2$$

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

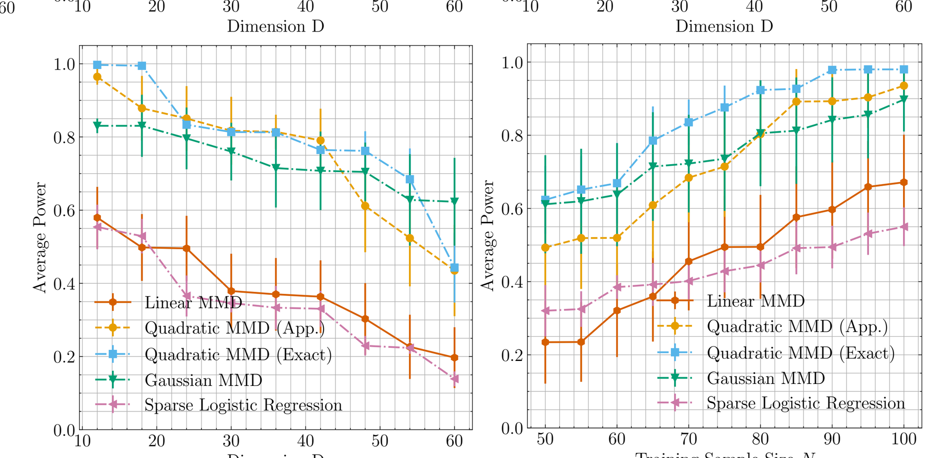
$$\mathcal{T}(\mu,\nu)[k] = 2c\left(\mathbb{E}_{x\sim\mu}[x[k]] - \mathbb{E}_{y\sim\nu}[y[k]]\right)^2.$$

Only 1st and 2nd-order moment conditions are used.

- 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 : $\frac{|I\setminus I^*|}{|I|}$