Nyström M-Hilbert-Schmidt Independence Criterion*

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Quick Summary

- Faster estimation of Hilbert-Schmidt independence criterion (HSIC; $M=2$: [2], $M \geq 2$: [5, 6, 4], validness: [7]).
- Guarantee: same convergence rate as the quadratic time estimator.
- Existing accelerations: $M=2$, works efficiently in practice but without theoretical guarantees [8].
- Experiments on synthetic examples, dependency testing of media annotations, and causal discovery.

HSIC

- Given $X=(X_m)_{m=1}^M \sim \mathbb{P}$ on $\mathcal{X}=\times_{m=1}^M \mathcal{X}_m$, $\mathcal{X}_m$ is equipped with kernel k_m and feature map $\phi_{k_m}: \mathcal{X}_m \to \mathcal{H}_{k_m}$, HSIC takes the form

$$\mathrm{HSIC}_k(\mathbb{P}) = \left\| \mu_k(\mathbb{P}) - \mu_k\left(\otimes_{m=1}^M \mathbb{P}_m\right)\right\|_{\mathcal{H}_k}, \qquad k := \otimes_{m=1}^M k_m$$

with $\otimes_{m=1}^M \mathbb{P}_m$ the product of the marginal distributions $\mathbb{P}_m$, $m \in [M] := \{1,\ldots,M\}$, and $\mu_k(\mathbb{P}) = \mathbb{E}_{X\sim\mathbb{P}}[\phi_k(X)]$.

- Given an i.i.d. sample of M-tuples of size n

$$\hat{\mathbb{P}}_n := \left\{\left(x_1^1,\ldots,x_M^1\right),\ldots,\left(x_1^n,\ldots,x_M^n\right)\right\} \subset \mathcal{X}^n,$$

from $\mathbb{P}$, the V-statistic based estimator takes the form

$$\mathrm{HSIC}_k^2\left(\hat{\mathbb{P}}_n\right) := \frac{1}{n^2}\mathbf{1}_n^\top\left(\circ_{m\in[M]}\mathbf{K}_{k_m,n,n}\right)\mathbf{1}_n + \frac{1}{n^{2M}}\prod_{m\in[M]}\mathbf{1}_n^\top\mathbf{K}_{k_m,n,n}\mathbf{1}_n - \frac{2}{n^{M+1}}\mathbf{1}_n^\top\left(\circ_{m\in[M]}\mathbf{K}_{k_m,n,n}\mathbf{1}_n\right),$$

with Gram matrices

$$\mathbf{K}_{k_m,n,n} = \left[k_m\left(x_m^i, x_m^j\right)\right]_{i,j\in[n]} \in \mathbb{R}^{n\times n}, \tag{1}$$

and can be computed in $\mathcal{O}\left(n^2\right)$ time.

Proposed Nyström-based estimator

- Let $\tilde{\mathbb{P}}_{n'} = \left\{\left(\tilde{x}_1^1,\ldots,\tilde{x}_M^1\right),\ldots,\left(\tilde{x}_1^{n'},\ldots,\tilde{x}_M^{n'}\right)\right\}$ be a subsample of $\hat{\mathbb{P}}_n$.
- Our proposed Nyström-based estimator is given by

$$\mathrm{HSIC}_{k,\mathrm{N}}^2\left(\hat{\mathbb{P}}_n\right) = \boldsymbol{\alpha}_k^\top\left(\circ_{m\in[M]}\mathbf{K}_{k_m,n',n'}\right)\boldsymbol{\alpha}_k + \prod_{m\in[M]}\boldsymbol{\alpha}_{k_m}^\top\mathbf{K}_{k_m,n',n'}\boldsymbol{\alpha}_{k_m} - 2\boldsymbol{\alpha}_k^\top\left(\circ_{m\in[M]}\mathbf{K}_{k_m,n',n'}\boldsymbol{\alpha}_{k_m}\right),$$

$$\boldsymbol{\alpha}_{k_m} = \frac{1}{n}\left(\mathbf{K}_{k_m,n',n'}\right)^{-}\mathbf{K}_{k_m,n',n}\mathbf{1}_n,$$

$$\boldsymbol{\alpha}_k = \frac{1}{n}\left(\circ_{m\in[M]}\mathbf{K}_{k_m,n',n'}\right)^{-}\left(\circ_{m\in[M]}\mathbf{K}_{k_m,n',n}\right)\mathbf{1}_n,$$

where $\circ$ is the Hadamard product, $\mathbf{K}_{k_m,n',n'}$ is defined in (1), $\mathbf{K}_{k_m,n',n} = \left[k_m\left(\tilde{x}_m^i, x_m^j\right)\right]_{i\in[n'],j\in[n]} \in \mathbb{R}^{n'\times n}$, and $(\cdot)^-$ denotes pseudo-inverse.

- Runtime complexity of $\mathcal{O}\left(Mn'^3 + Mn'n\right)$, saving if $n' = o\left(n^{2/3}\right)$.
- Code: `https://github.com/FlopsKa/nystroem-mhsic/`.

Main Result

- For bounded kernels $(k_m)_{m=1}^M$ and the effective dimension $\mathcal{N}_X(\lambda) = \operatorname{tr}\left[\mu_{k\otimes k}(\mathbb{P})\left(\mu_{k\otimes k}(\mathbb{P})+\lambda I\right)^{-1}\right]$, it holds that

$$\left|\mathrm{HSIC}_k(\mathbb{P}) - \mathrm{HSIC}_{k,\mathrm{N}}\left(\hat{\mathbb{P}}_n\right)\right| = \mathcal{O}_P\left(n^{-1/2}\right),$$

assuming that the effective dimension either
  - decays polynomially:

$$\max_{m\in[M]}\left(\mathcal{N}_X(\lambda), \mathcal{N}_{X_m}(\lambda)\right) \leq c\lambda^{-\gamma}, \qquad n' = n^{1/(2-\gamma)}\log(n/\delta),$$

  for some $c>0$ and $\gamma \in (0,1]$ (computational savings if $\gamma < 1/2$), or
  - decays exponentially:

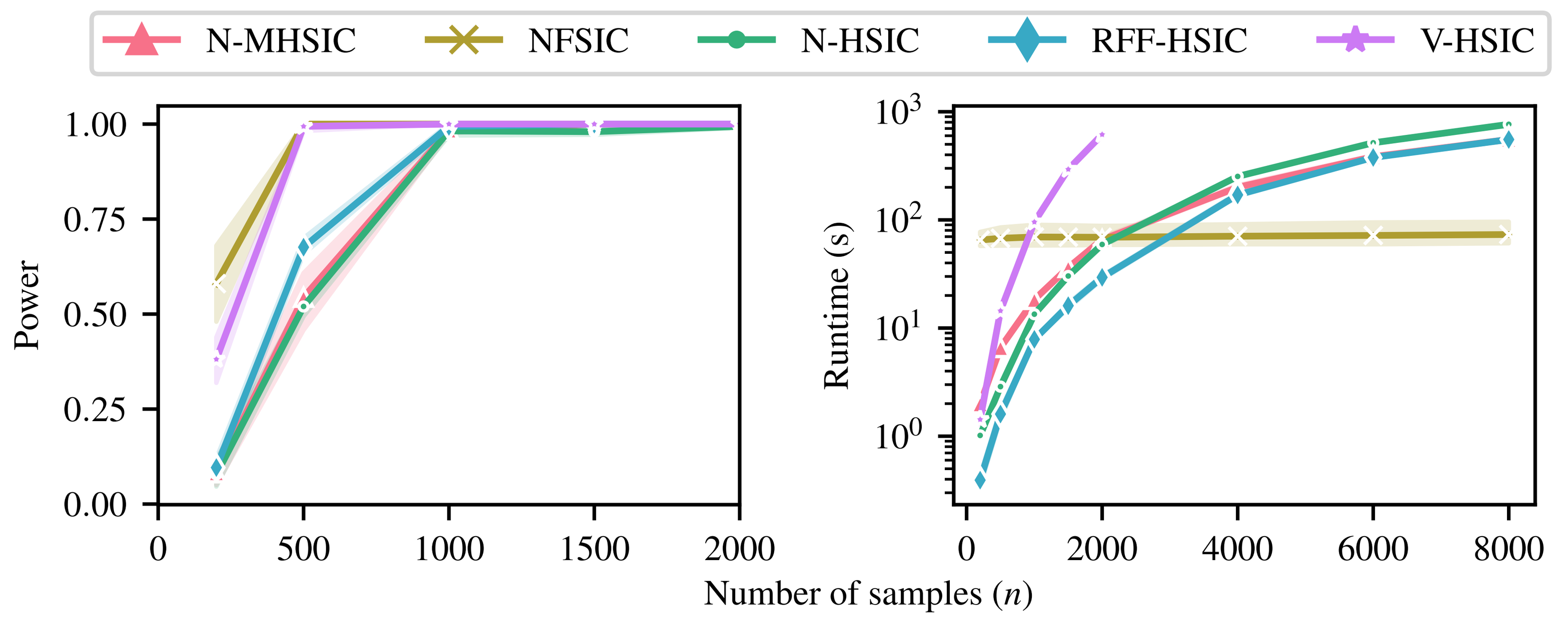
$$\max_{m\in[M]}\left(\mathcal{N}_X(\lambda), \mathcal{N}_{X_m}(\lambda)\right) \leq \log(1+c/\lambda)/\beta,$$

$$n' = \sqrt{n}\log\left(\sqrt{n}\max_{m\in[M]}\left(\frac{1}{\delta}, \frac{c}{6a_k^2}, \frac{c}{6a_{k_m}^2}\right)\right)$$

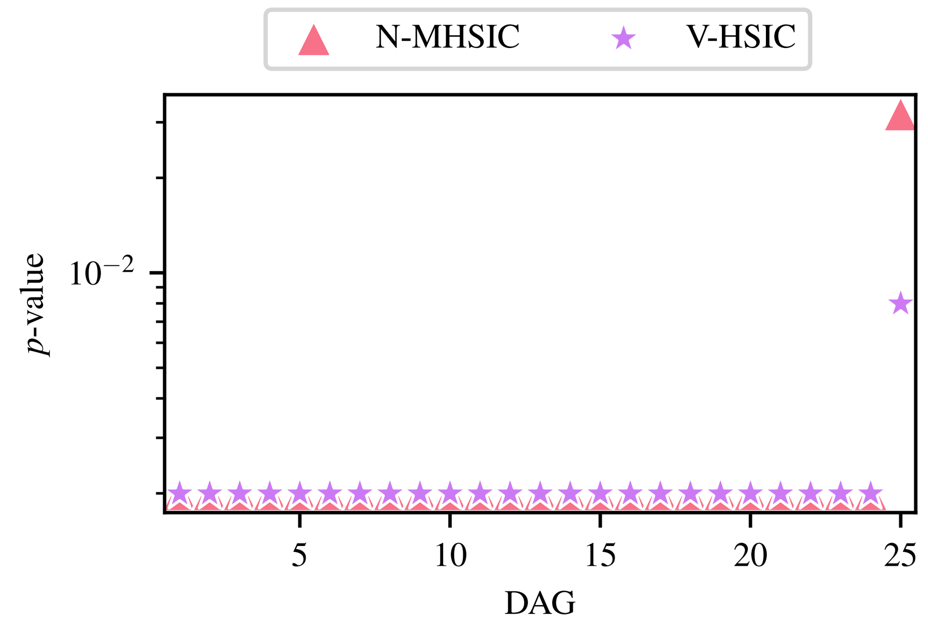
  for some $c>0$, $\beta>0$, a_k, a_{k_m} bounds on the kernels k, k_m ($m \in [M]$).
- The decay of the effective dimension can be linked to the decay of the eigenvalues of the covariance operator $\mu_{k\otimes k}(\mathbb{P})$ [1, Proposition 4, 5].

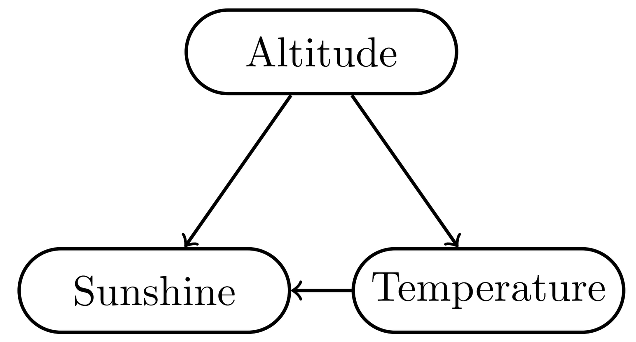
Example Applications

- Dependency estimation of media annotations ($M=2$).



- Weather causal discovery [3] ($M=3$).





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