

Nonparametric Independence Tests: Space Partitioning and Kernel Approaches

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- Statistical tests of **independence**
 - ▶ Multivariate
 - ▶ Nonparametric
- Two **kinds of tests**:
 - ▶ Strongly consistent, distribution-free
 - ▶ Asymptotically α -level
- Three **test statistics**:
 - ▶ L_1 distance
 - ▶ Log-likelihood
 - ▶ Kernel dependence measure (HSIC)

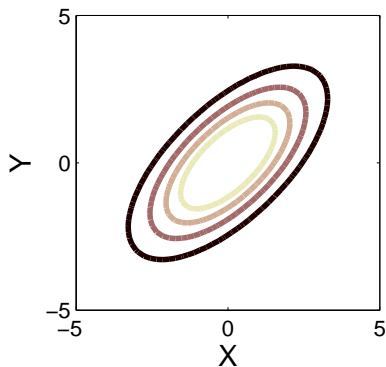
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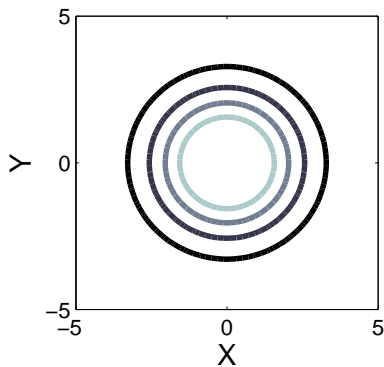
Problem overview

- Given distribution P_r , test $\mathcal{H}_0 : P_r = P_{r_x} P_{r_y}$
- Continuous valued, multivariate:** $\mathcal{X} := \mathbb{R}^d$ and $\mathcal{Y} := \mathbb{R}^{d'}$

Dependent P_{XY}



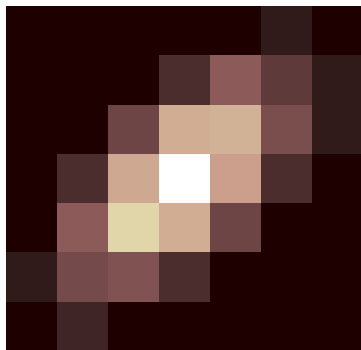
Independent $P_{XY} = P_X P_Y$



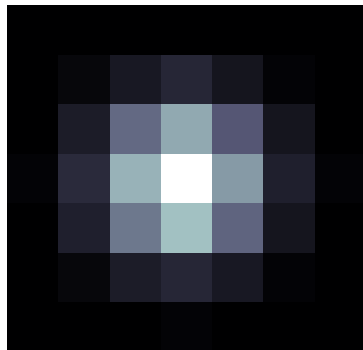
Problem overview

- **Finite i.i.d. sample** $(X_1, Y_1), \dots, (X_n, Y_n)$ from \Pr
- Partition space \mathcal{X} into m_n bins, space \mathcal{Y} into m'_n bins

Discretized empirical P_{XY}



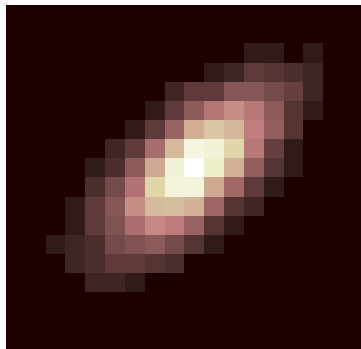
Discretized empirical $P_X P_Y$



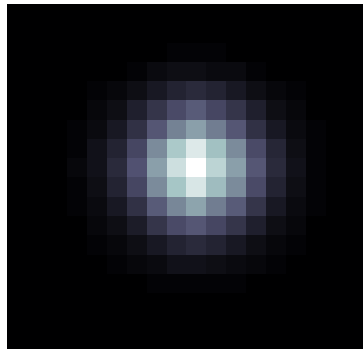
Problem overview

- **Finite i.i.d. sample** $(X_1, Y_1), \dots, (X_n, Y_n)$ from \Pr
- **Refine partition** m_n, m'_n for increasing n

Discretized empirical P_{XY}



Discretized empirical $P_X P_Y$



- Space partition

- ▶ $\mathcal{P}_n = \{A_{n,1}, \dots, A_{n,m_n}\}$ of $\mathcal{X} = \mathbb{R}^d$
- ▶ $\mathcal{Q}_n = \{B_{n,1}, \dots, B_{n,m'_n}\}$ of $\mathcal{Y} = \mathbb{R}^{d'}$,

- Empirical measures

- ▶ $\nu_n(A \times B) = n^{-1} \#\{i : (X_i, Y_i) \in A \times B, i = 1, \dots, n\}$
- ▶ $\mu_{n,1}(A) = n^{-1} \#\{i : X_i \in A, i = 1, \dots, n\}$
- ▶ $\mu_{n,2}(B) = n^{-1} \#\{i : Y_i \in B, i = 1, \dots, n\}$

- Test statistic:

$$L_n(\nu_n, \mu_{n,1} \times \mu_{n,2}) = \sum_{A \in \mathcal{P}_n} \sum_{B \in \mathcal{Q}_n} |\nu_n(A \times B) - \mu_{n,1}(A) \cdot \mu_{n,2}(B)|.$$

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L_1 : Distribution-free strong consistent test

- **Test:** reject \mathcal{H}_0 when

$$L_n(\nu_n, \mu_{n,1} \times \mu_{n,2}) > c_1 \sqrt{\frac{m_n m'_n}{n}}, \quad \text{where } c_1 > \sqrt{2 \ln 2}.$$

- ▶ **Distribution-free**
- ▶ **Strongly consistent:** after random sample size, test makes a.s. no error

- **Conditions**

- ▶ $\lim_{n \rightarrow \infty} m_n m'_n / n = 0$,
- ▶ $\lim_{n \rightarrow \infty} m_n / \ln n = \infty$, $\lim_{n \rightarrow \infty} m'_n / \ln n = \infty$,
- ▶ \mathcal{P}_n and \mathcal{Q}_n cells shrink:

$$\lim_{n \rightarrow \infty} \max_{A \in \mathcal{P}_n, A \cap S \neq \emptyset} \text{diam}(A) = 0$$

S any sphere centred at origin

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Type I error:

- Start with goodness of fit

$$L_n(\mu_{n,1}, \mu_1) = \sum_{A \in \mathcal{P}_n} |\mu_{n,1}(A) - \mu_1(A)|.$$

- Associated bound Beirlant et al. (2001), Biau and Györfi (2005)

$$\Pr\{L_n(\mu_{n,1}, \mu_1) > \varepsilon\} \leq 2^{m_n} e^{-n\varepsilon^2/2} \quad \text{for all } 0 < \varepsilon$$

- Then decompose:

$$\begin{aligned} L_n(\nu_n, \mu_{n,1} \times \mu_{n,2}) &\leq \sum_{A \in \mathcal{P}_n} \sum_{B \in \mathcal{Q}_n} |\nu_n(A \times B) - \nu(A \times B)| \\ &+ \underbrace{\sum_{A \in \mathcal{P}_n} \sum_{B \in \mathcal{Q}_n} |\nu(A \times B) - \mu_1(A) \cdot \mu_2(B)|}_{=0 \text{ under } \mathcal{H}_0} + \underbrace{\sum_{A \in \mathcal{P}_n} \sum_{B \in \mathcal{Q}_n} |\mu_1(A) \cdot \mu_2(B) - \mu_{n,1}(A) \cdot \mu_{n,2}(B)|}_{\leq L_n(\mu_{n,1}, \mu_1) + L_n(\mu_{n,2}, \mu_2)}. \end{aligned}$$

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- Decompose

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$$\sum_{A \in \mathcal{P}_n} \sum_{B \in \mathcal{Q}_n} |\nu(A \times B) - \mu_1(A) \cdot \mu_2(B)| \rightarrow 2 \sup_C |\nu(C) - \mu_1 \times \mu_2(C)| > 0$$

- ▶ C Borel subset of $\mathbb{R}^d \times \mathbb{R}^{d'}$; see Barron et al. (1992)

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- **Additional conditions:**

$$\lim_{n \rightarrow \infty} \max_{A \in \mathcal{P}_n} \mu_1(A) = 0, \quad \lim_{n \rightarrow \infty} \max_{B \in \mathcal{Q}_n} \mu_2(B) = 0,$$

- **Asymptotic distribution:** Under \mathcal{H}_0 ,

$$\sqrt{n} (L_n(\nu_n, \mu_{n,1} \times \mu_{n,2}) - C_n) / \sigma \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1), \quad \sigma^2 = 1 - 2/\pi.$$

- ▶ Upper bound: $C_n \leq \sqrt{2m_n m'_n / (\pi n)}$

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$$L_n(\nu_n, \mu_{n,1} \times \mu_{n,2}) > \sqrt{2m_n m'_n / (\pi n)} + \sigma / \sqrt{n} \Phi^{-1}(1 - \alpha)$$

- ▶ Φ denotes standard normal distribution.

- **Properties of test:**

- ▶ **Not** distribution-free (nonatomic)

- ▶ α level: probability of Type I error asymptotically $\leq \alpha$

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Proof: sketch only

- **Problem:** samples in each bin **not independent**
- Define the **poisson random variable** $N_n \sim \text{Poisson}(n)$.
- Define the **poisson variables**:

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and

$$n\mu_{N_n,2}(B) = \#\{i : Y_i \in B, i = 1, \dots, N_n\}$$

- New **Poissonized statistic**:

$$\tilde{L}_n(\nu_n, \mu_{n,1} \times \mu_{n,2}) = \sum_{A \in \mathcal{P}_n} \sum_{B \in \mathcal{Q}_n} |\nu_{N_n}(A \times B) - \mu_{N_n,1}(A) \cdot \mu_{N_n,2}(B)|.$$

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Proof sketch (continued, part 1)

- If poissonized statistic converges...

$$\left(\sqrt{n} \left[\tilde{L}_n - \mathbf{E}(\tilde{L}_n) \right], \frac{N_n - n}{\sqrt{n}} \right) \xrightarrow{\mathcal{D}} \mathcal{N} \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma^2 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

- ...then test statistic converges:

$$\frac{\sqrt{n}}{\sigma} (L_n(\nu_n, \mu_{n,1} \times \mu_{n,2}) - \mathbf{E}(\tilde{L}_n)) \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1)$$

- (proof by comparing characteristic functions) Beirlant et al. (1994)

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Proof sketch (continued, part 2)

- **Convergence for Poisson** e.g. Jacod and Protter(2004, p. 170)

$$\frac{1}{\sqrt{n}}(Z_n - n) \xrightarrow{\mathcal{D}} Z \quad \text{as } n \rightarrow \infty$$

- where $Z \sim \mathcal{N}(0, 1)$. Likewise

$$\nu_{N_n}(A \times B) - \mu_{N_n,1}(A)\mu_{N_n,2}(B) \stackrel{\mathcal{D}}{\approx} Z \sqrt{\frac{\mu_1(A)\mu_2(B)}{n}}$$

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- Require earlier conditions on m_n, m'_n , and n
- Test: reject \mathcal{H}_0 when

$$l_n(\nu_n, \mu_{n,1} \times \mu_{n,2}) \geq m_n m'_n n^{-1} (2 \log(n + m_n m'_n) + 1).$$

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- **Distribution-free, strongly consistent**
- **Asymptotically α -level test:** reject \mathcal{H}_0 when

$$nl_n(\nu_n, \mu_{n,1} \times \mu_{n,2}) > m_n m'_n + \sqrt{2m_n m'_n} \Phi^{-1}(1 - \alpha)$$

Proof sketch (strong consistent)

- Under \mathcal{H}_0

$$I_n(\nu_n, \nu) - I_n(\nu_n, \mu_{n,1} \times \mu_{n,2}) = I_n(\mu_{n,1}, \mu_1) + I_n(\mu_{n,2}, \mu_2) \geq 0.$$

- Relevant **large deviation bound** Kallenberg(1985), Quine and Robinson (1985)

$$\Pr\{I_n(\nu_n, \nu)/2 > \epsilon\} = e^{-n(\epsilon+o(1))}.$$

- Under \mathcal{H}_1 , **Pinsker**:

$$L_n^2(\nu_n, \mu_{n,1} \times \mu_{n,2}) \leq I_n(\nu_n, \mu_{n,1} \times \mu_{n,2}).$$

- Assume $k(x, \cdot) = k(\|x - \cdot\|)$
- Kernel test statistic:

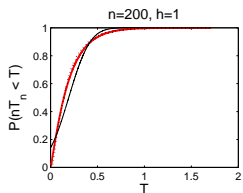
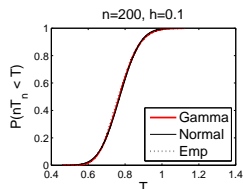
$$T_n := \frac{1}{n^2} \text{tr}(KHK'H)$$

- ▶ $K_{i,j} = k(x_i, x_j)$, centering $H = I - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^\top$
- ▶ $K'_{i,j} = k(y_i, y_j)$
- **Decreasing bandwidth:** L^2 distance between densities
- **Fixed bandwidth:** Smoothed distance between characteristic functions
Feuerverger (1993) **OR** difference between distribution embeddings to RKHS
Berlinet and Thomas-Agnan (2003), Gretton et al. (2008)

Asymptotic α -level tests

- Asymptotic distribution under \mathcal{H}_0 :
- Gaussian** using first two moments (**decreasing bandwidth**) Hall (1984), Cotterill and Csörgő (1985)
- Two parameter Gamma** using first two moments (**fixed bandwidth**) Feuerverger (1993), Gretton (2008)

$$nT_n \sim \frac{x^{\alpha-1} e^{-x/\beta}}{\beta^\alpha \Gamma(\alpha)}$$
$$\alpha = \frac{(\mathbf{E}(T_n))^2}{\text{var}(T_n)}, \quad \beta = \frac{n\text{var}(T_n)}{\mathbf{E}(T_n)}.$$

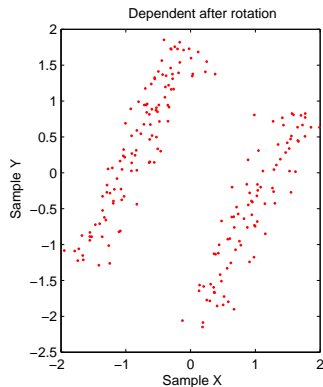
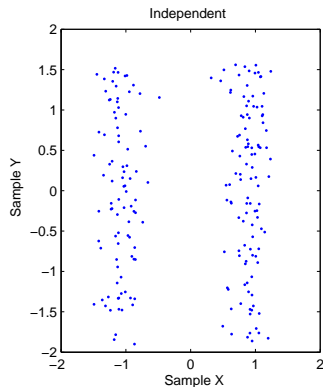


- Threshold NOT distribution-free:** moments under \mathcal{H}_0 computed using sample

Experimental results

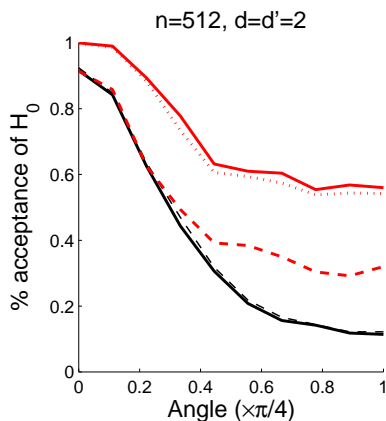
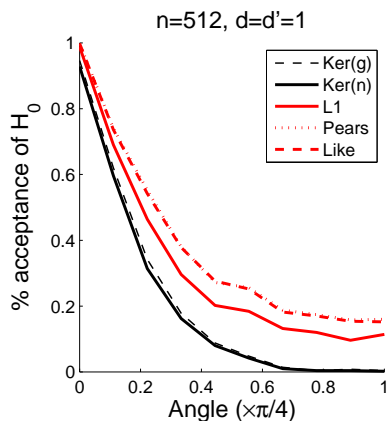
- Experimental setup:

- ▶ Independent sample $(X_1, Y_1), \dots, (X_n, Y_n)$
- ▶ Rotate sample to create dependence
- ▶ Embed randomly in \mathbb{R}^d , remaining subspace Gaussian noise



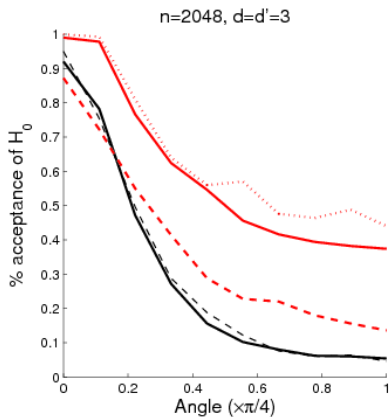
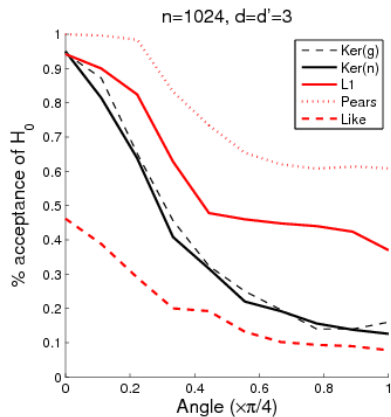
Experimental results

- Comparison of asymptotically α -level tests
- Given distribution \Pr , test $\mathcal{H}_0 : \Pr = \Pr_x \Pr_y$
- Continuous valued, multivariate: $\mathcal{X} := \mathbb{R}^d$ and $\mathcal{Y} := \mathbb{R}^{d'}$



Experimental results

- Higher dimensions: $d = d' = 3$



- Multi-dimensional nonparametric independence tests
 - ▶ Strongly consistent, distribution-free
 - ▶ Asymptotically α -level
- Test statistics
 - ▶ L_1 distance
 - ▶ Log likelihood
 - ▶ Kernel dependence measure (HSIC)
- In experiments:
- Kernel tests have better performance, but...
- ...threshold estimated from sample
- Further work:
 - ▶ Distribution-free threshold for kernel α -level test
 - ▶ Consistent null distribution estimate for kernel α -level test
 - ▶ Proof of χ^2 test conjecture