

# Ch 13. Conditional Independence Testing

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# Conditional Independence Testing: Overview

## Problem Setting

Given i.i.d. samples  $(X_i, Y_i, W_i)_{i \in [n]}$ , test the null hypothesis:

$$H_0 : X \perp\!\!\!\perp Y \mid W$$

where  $W$  is a **confounder** variable.

- Is the feature  $X$  associated with response  $Y$  after accounting for  $W$ ?
- Related to **variable selection** in high-dimensional regression
  - Testing  $H_{0,j} : X_j \perp\!\!\!\perp Y \mid X_{-j}$  for feature selection

# Marginal vs. Conditional Independence

## Marginal Independence

$$H_0 : X \perp\!\!\!\perp Y$$

- No conditioning on any variable
- Does not account for confounding effects of  $W$
- **Easy** to test via permutation tests

# Marginal vs. Conditional Independence

## Conditional Independence

$$H_0 : X \perp\!\!\!\perp Y \mid W$$

- Must account for the confounder  $W$
- **Easy** when  $W$  is discrete (local permutation test)
- **Hard** (impossible) when  $W$  is continuous (hardness result)

# Q&A: Why is Chapter 13 in This Book?

## Question

Chapter 13 does not seem directly related to conformal prediction. Why is it included in this book?

## Answer

- This chapter demonstrates the broader applications of **permutation tests** and **exchangeability**
- The book's core techniques extend beyond conformal prediction:
  - Chapter 2's permutation test framework
  - Chapter 4's test-conditional coverage hardness results
  - Chapter 11-12's binning approaches
- Emphasizes the **unifying theme** of “distribution-free inference” and shows how exchangeability-based arguments apply to hypothesis testing

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# Setup: Marginal Independence Testing

## Problem Setting

- Data:  $(X_1, Y_1), \dots, (X_n, Y_n) \stackrel{\text{i.i.d.}}{\sim} P$
- Null hypothesis:  $H_0 : X \perp\!\!\!\perp Y$
- Equivalently:  $P \in \mathcal{P}_{X \perp\!\!\!\perp Y}$  (product distributions)

## Test Statistic

Any function  $T : (\mathcal{X} \times \mathcal{Y})^n \rightarrow \mathbb{R}$  measuring evidence against  $H_0$ .

**Example (real-valued data):**

$$T((X_1, Y_1), \dots, (X_n, Y_n)) = |\text{Corr}((X_1, \dots, X_n), (Y_1, \dots, Y_n))|$$

# Permutation Test for Marginal Independence

## Key Insight

Under  $H_0 : X \perp\!\!\!\perp Y$ , permuting  $X_i$ 's while fixing  $Y_i$ 's doesn't change the distribution!

$$(X_\sigma, \mathbf{Y}) \stackrel{d}{=} (\mathbf{X}, \mathbf{Y}) \quad \text{for all } \sigma \in \mathcal{S}_n$$

## Notation

- $\mathbf{X} = (X_1, \dots, X_n)$ ,  $\mathbf{Y} = (Y_1, \dots, Y_n)$
- $X_\sigma = (X_{\sigma(1)}, \dots, X_{\sigma(n)})$  for  $\sigma \in \mathcal{S}_n$

# Theorem 13.1: Validity of the Permutation Test

## Theorem 13.1

Fix any test statistic  $T : (\mathcal{X} \times \mathcal{Y})^n \rightarrow \mathbb{R}$ . Define the test:

$$\psi(\mathbf{X}, \mathbf{Y}) = \mathbb{1}\left\{\frac{1}{n!} \sum_{\sigma \in \mathcal{S}_n} \mathbb{1}\{T(X_\sigma, \mathbf{Y}) \geq T(\mathbf{X}, \mathbf{Y})\} \leq \alpha\right\}$$

Then  $\psi$  is a **valid test** of  $H_{X \perp\!\!\!\perp Y}$ :

$$\mathbb{P}_P(\psi(\mathbf{X}, \mathbf{Y}) = 1) \leq \alpha \quad \text{for all } P \in \mathcal{P}_{X \perp\!\!\!\perp Y}$$

## Proof Idea

- Under  $H_0$ :  $P = P_X \times P_Y$
- Conditioning on  $\mathbf{Y}$ :  $X_1, \dots, X_n$  remain i.i.d.  $\sim P_X$
- Apply Theorem 2.4 (permutation test validity from Chapter 2)

# Q&A: Alternative Test Statistics

## Question

What are some alternative test statistics  $T$  that can be used instead of the absolute Pearson correlation for testing marginal/conditional independence?

## Answer: Alternative Test Statistics

- 1 **Spearman's rank correlation:**  $|\text{Corr}(\text{rank}(X), \text{rank}(Y))|$ 
  - Robust to outliers, captures monotonic relationships
- 2 **Distance correlation** (Székely et al., 2007)
  - Detects nonlinear dependencies, equals zero iff independent
- 3 **HSIC** (Hilbert-Schmidt Independence Criterion)
  - Kernel-based measure of dependence
- 4 **Mutual information estimators**
  - Information-theoretic measure of dependence

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# Local Permutation Test: Motivation

## Key Idea

When  $W$  is discrete, group data points by their  $W$  value:

- Within each group (same  $W = w$ ):  $X$  and  $Y$  are **independent**
- Permute  $X$  values **only within groups**
- This preserves the null distribution!

## Intuition

- Think of  $W$  as defining “subpopulations”
- Under  $H_0 : X \perp\!\!\!\perp Y \mid W$ , within each subpopulation  $X$  and  $Y$  are independent
- Same logic as marginal independence test, applied locally

# Local Permutation Test: Definition

## Allowed Permutations

Define the set of permutations that **preserve  $W$  values**:

$$\mathcal{S}_n(\mathbf{W}) = \{\sigma \in \mathcal{S}_n : W_{\sigma(i)} = W_i \text{ for all } i \in [n]\}$$

## Test Definition (Equation 13.4)

$$\begin{aligned} \psi(\mathbf{X}, \mathbf{Y}, \mathbf{W}) \\ = \mathbb{1}\left\{ \frac{1}{|\mathcal{S}_n(\mathbf{W})|} \sum_{\sigma \in \mathcal{S}_n(\mathbf{W})} \mathbb{1}\{T(X_\sigma, \mathbf{Y}, \mathbf{W}) \geq T(\mathbf{X}, \mathbf{Y}, \mathbf{W})\} \leq \alpha \right\} \end{aligned}$$

- Only permute  $X$  values among data points with *same*  $W$  value
- This is called a “**local**” permutation test

# Theorem 13.2: Validity of Local Permutation Test

## Theorem 13.2

Fix any test statistic  $T : (\mathcal{X} \times \mathcal{Y} \times \mathcal{W})^n \rightarrow \mathbb{R}$ . Let  $(X_i, Y_i, W_i)_{i \in [n]} \stackrel{\text{i.i.d.}}{\sim} P$ . Then  $\psi$  is a **valid test** of  $H_{X \perp\!\!\!\perp Y|W}$ :

$$\mathbb{P}_P(\psi(\mathbf{X}, \mathbf{Y}, \mathbf{W}) = 1) \leq \alpha \quad \text{for all } P \in \mathcal{P}_{X \perp\!\!\!\perp Y|W}$$

## Key Points

- **Distribution-free:** No assumptions on  $P$  (beyond conditional independence)
- **Test statistic-free:** Works for any choice of  $T$
- Proof uses same techniques as Chapter 2 (permutation test validity)



# Proof Sketch: Theorem 13.2

## 1 Conditional on $\mathbf{W}$ and $\mathbf{Y}$

Under  $H_0 : X \perp\!\!\!\perp Y \mid W$ , conditioning on  $(\mathbf{W}, \mathbf{Y})$ :

$X_1, \dots, X_n$  are independent (but not identically distributed)

with  $X_i \sim P_{X|W}(\cdot | W_i)$ .

## 2 Exchangeability Within Groups

For any  $\sigma \in \mathcal{S}_n(\mathbf{W})$ : since  $W_{\sigma(i)} = W_i$ ,

$$(X_\sigma, \mathbf{Y}) \mid \mathbf{W} \stackrel{d}{=} (\mathbf{X}, \mathbf{Y}) \mid \mathbf{W}$$

## 3 Apply Permutation Test Logic

Average over permutations  $\sigma \in \mathcal{S}_n(\mathbf{W})$  to get valid p-value.

# When is the Local Permutation Test Powerful?

## Factor 1: Number of “Clashes”

- **Clashes:** pairs  $i \neq j$  with  $W_i = W_j$
- Many clashes  $\Rightarrow$  rich set of permutations  $\Rightarrow$  potential for power
- No clashes (all  $W_i$  unique)  $\Rightarrow |\mathcal{S}_n(\mathbf{W})| = 1 \Rightarrow$  **no power**

## Factor 2: Choice of Test Statistic $T$

- $T$  must discriminate between null and alternative
- Standard considerations for hypothesis testing

## Critical Observation

If  $W$  is **continuous**, all  $W_i$ 's are distinct a.s.  $\Rightarrow$  **No power!**

# Q&A: How is the Confounder $W$ Determined?

## Question

How is the confounder  $W$  typically determined in practice? It seems like finding an appropriate  $W$  would be important, and trivial confounders might also exist.

## Answer

- This chapter **assumes  $W$  is given** — identifying  $W$  is a separate problem
- In practice,  $W$  selection is crucial:
  - **Domain knowledge:** Prior understanding of causal relationships
  - **Variable selection:** In high-dimensional settings,  $W = X_{-j}$  (all other variables)
  - **Causal discovery:** Learn DAG structure to identify confounders
- Wrong  $W$  choice  $\Rightarrow$  spurious association or missed association

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# The Problem with Continuous $W$

## Continuous Confounder Challenge

When  $W$  has a **nonatomic** (continuous) distribution:

- $\mathbb{P}(W_i = W_j) = 0$  for  $i \neq j$
- No two data points share the same  $W$  value
- Local permutation test has no power

## Question

Can we design *any* valid test with nontrivial power for continuous  $W$ ?

## Answer: NO!

Theorem 13.3 shows this is **impossible** in a distribution-free setting.

# Theorem 13.3: Hardness Result

## Theorem 13.3

If the test  $\psi$  has Type I error bounded by  $\alpha$  for any distribution:

$$\mathbb{P}_P(\psi(\mathbf{X}, \mathbf{Y}, \mathbf{W}) = 1) \leq \alpha \quad \text{for all } P \in \mathcal{P}_{X \perp\!\!\!\perp Y|W}$$

Then the **power** of the test is not better than random for any  $P$  with  $P_W$  nonatomic:

$$\mathbb{P}_P(\psi(\mathbf{X}, \mathbf{Y}, \mathbf{W}) = 1) \leq \alpha \quad \text{for all } P \text{ with } P_W \text{ nonatomic}$$

## Interpretation

For continuous  $W$ : **any** valid test has power  $\leq \alpha$  (no better than random guessing!)

# Proof Sketch: Theorem 13.3

## Key Technique: Sample-Resample (Lemma 4.15)

Same technique as hardness results in Chapters 4, 11, 12!

- 1 Fix arbitrary sequence  $(X^{(i)}, Y^{(i)}, W^{(i)})_{i \in [M]}$  with distinct  $W^{(i)}$
- 2 Empirical distribution  $\hat{P}_M = \frac{1}{M} \sum_{i=1}^M \delta_{(X^{(i)}, Y^{(i)}, W^{(i)})}$
- 3 Under  $\hat{P}_M$ :  $X, Y$  are deterministic functions of  $W$
- 4  $\Rightarrow$  Trivially  $X \perp\!\!\!\perp Y \mid W$  under  $\hat{P}_M$ !
- 5 Valid test must have  $\mathbb{P}_{\hat{P}_M}(\psi = 1) \leq \alpha$
- 6 By Lemma 4.15: this extends to any  $P$  with nonatomic  $P_W$

# Connection to Previous Hardness Results

## Recurring Theme in the Book

**Discrete case:** Distribution-free inference is possible (Chapter 4.3, 11.3, 13.2)

**Continuous case:** Distribution-free inference faces fundamental limits (Chapter 4.4, 11.4, 13.3)

## Same Proof Technique

- Chapter 4: Test-conditional coverage
- Chapter 11: Distribution-free regression
- Chapter 12: ECE calibration
- Chapter 13: Conditional independence testing

All use the **sample-resample lemma** (Lemma 4.15)!



# Q&A: Alternative Approaches Without Permutation Tests

## Question

Are there methods to test conditional independence without using permutation tests?

## Answer: Alternative Approaches (from Bibliographic Notes)

- 1 **Conditional Chatterjee's correlation** (Azadkia & Chatterjee, 2021)
  - Asymptotically valid, no smoothness assumptions needed
- 2 **Model-X framework** (Candès et al., 2018)
  - Assumes knowledge of  $P_{X|W}$
  - Resample  $X$  under the null using known conditional distribution

# Q&A: Alternative Approaches Without Permutation Tests

## Question

Are there methods to test conditional independence without using permutation tests?

## Answer: Alternative Approaches (from Bibliographic Notes)

- 3 **Knockoff filter** (Barber & Candès, 2015)
  - Uses “pairwise exchangeability” for FDR control
- 4 **Generalized Covariance Measure** (Shah & Peters, 2020)
  - Uses residuals from regression of  $X$  on  $W$  and  $Y$  on  $W$

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# Escaping the Hardness Result

## The Dilemma

- Distribution-free: Valid for *all*  $P \in \mathcal{P}_{X \perp\!\!\!\perp Y|W}$
- But: No power for continuous  $W$ !

## Solution: Restrict the Null Hypothesis

- Add a **smoothness assumption** on the conditional distribution
- Control Type I error against a *smaller* class of nulls
- Allows nontrivial power while maintaining (approximate) validity

# Smoothness Assumption

## Lipschitz Condition (Equation 13.7)

Assume the map  $w \mapsto P_{X|W}(\cdot|w)$  is  $L$ -Lipschitz w.r.t. Hellinger distance:

$$d_H(P_{X|W}(\cdot|w), P_{X|W}(\cdot|w')) \leq L\|w - w'\|$$

for all  $w, w' \in \mathcal{W}$ .

# Smoothness Assumption

## Hellinger Distance

For distributions  $P_1, P_2$  with densities  $f_1, f_2$ :

$$d_H(P_1, P_2) = \left( \frac{1}{2} \int_{\mathcal{X}} \left( \sqrt{f_1(x)} - \sqrt{f_2(x)} \right)^2 d\mu(x) \right)^{1/2}$$

## Restricted Null

$$\mathcal{P}_{X \perp\!\!\!\perp Y|W}^L = \{P \in \mathcal{P}_{X \perp\!\!\!\perp Y|W} : (13.7) \text{ holds with constant } L\}$$

# Binned Local Permutation Test

## Key Idea

- Partition  $\mathcal{W}$  into bins:  $\mathcal{W} = \cup_k \mathcal{W}_k$
- Bin diameter bounded:  $\max_k \sup_{w, w' \in \mathcal{W}_k} \|w - w'\| \leq h$

## Allowed Permutations

$$\mathcal{S}_n^{\text{bin}}(\mathbf{W}) = \{\sigma \in \mathcal{S}_n : W_{\sigma(i)} \text{ and } W_i \text{ are in the same bin for all } i\}$$

## Test Definition (Equation 13.8)

$$\psi(\mathbf{X}, \mathbf{Y}, \mathbf{W})$$

$$:= \mathbb{1}\left\{ \frac{1}{|\mathcal{S}_n^{\text{bin}}(\mathbf{W})|} \sum_{\sigma \in \mathcal{S}_n^{\text{bin}}(\mathbf{W})} \mathbb{1}\{T(X_\sigma, \mathbf{Y}, \mathbf{W}) \geq T(\mathbf{X}, \mathbf{Y}, \mathbf{W})\} \leq \alpha \right\}$$

# Theorem 13.4: Validity of Binned Test

## Theorem 13.4

Fix any  $T : (\mathcal{X} \times \mathcal{Y} \times \mathcal{W})^n \rightarrow \mathbb{R}$ . Let  $(X_i, Y_i, W_i)_{i \in [n]} \stackrel{\text{i.i.d.}}{\sim} P$ .  
 For any partition with  $\max_k \sup_{w, w' \in \mathcal{W}_k} \|w - w'\| \leq h$ :

$$\mathbb{P}_P(\psi(\mathbf{X}, \mathbf{Y}, \mathbf{W}) = 1) \leq \alpha + Lh\sqrt{2n} \quad \text{for all } P \in \mathcal{P}_{X \perp\!\!\!\perp Y|W}^L$$

- Type I error:  $\alpha + Lh\sqrt{2n}$  (not exactly  $\alpha$ )
- Choose bin size  $h = o(n^{-1/2}) \Rightarrow$  nearly valid test
- Trade-off: smaller  $h$  = more valid, but fewer permutations = less power



# Proof Sketch: Theorem 13.4

## 1 Construct Auxiliary Distribution $\tilde{P}$

- Express  $P$  as mixture:  $P = \sum_k \pi_k \cdot P^{(k)}$  where  $\pi_k = \mathbb{P}(W \in \mathcal{W}_k)$
- Define  $\tilde{P} = \sum_k \pi_k \cdot (P_X^{(k)} \times P_{(Y,W)}^{(k)})$
- Under  $\tilde{P}$ :  $X \perp\!\!\!\perp (Y, W) \mid K$  where  $K = k(W)$  (bin index)

## 2 $\tilde{P}$ Satisfies Conditional Independence

- By construction:  $X \perp\!\!\!\perp (Y, W) \mid K$  under  $\tilde{P}$
- Local permutation test with discrete confounder  $K$  is **exactly valid**
- $\Rightarrow \mathbb{P}_{\tilde{P}}(\psi = 1) \leq \alpha$

# Proof Sketch: Theorem 13.4

## 3 Bound Distance Between $P$ and $\tilde{P}$

Using smoothness assumption and Hellinger distance properties:

$$d_H(P_{X|W}(\cdot|w), P_X^{(k)}) \leq Lh \quad \text{for all } w \in \mathcal{W}_k$$

This gives:

$$d_H^2(P, \tilde{P}) \leq (Lh)^2$$

## 4 Extend to $n$ Samples

- Subadditivity of squared Hellinger distance:

$$d_H^2(P^n, \tilde{P}^n) \leq n(Lh)^2$$

- Total variation bound:

$$d_{TV}(P^n, \tilde{P}^n) \leq \sqrt{2}d_H(P^n, \tilde{P}^n) \leq Lh\sqrt{2n}$$

Therefore:

$$\mathbb{P}_P(\psi = 1) \leq \mathbb{P}_{\tilde{P}}(\psi = 1) + Lh\sqrt{2n} \leq \alpha + Lh\sqrt{2n}$$

# Q&A: Hellinger Distance Convexity

## Question

In the proof of Theorem 13.4, it mentions that  $d_H(\cdot, \cdot)$  is convex in each argument. I believe  $d_H^2(\cdot, \cdot)$  is convex, but  $d_H(\cdot, \cdot)$  itself is not. Is my understanding correct?

## Answer

- $d_H^2(P, Q)$  is **convex** in each argument (jointly convex)
- $d_H(P, Q)$  is generally **not convex**
- What the proof actually uses (Equation 13.9):

$$d_H(P_{X|W}(\cdot|w), P_X^{(k)}) \leq Lh$$

- This follows from  $P_X^{(k)}$  being a convex combination, using  $d_H^2$  convexity and Jensen's inequality
- The proof logic is correct;  $d_H^2$  convexity is the key property

# Q&A: Kernel Blurring for Continuous $W$ ?

## Question

The local permutation test faces issues when  $W$  is continuous, similar to Chapter 11. Can kernel-based blurring techniques from Chapter 11 be applied here?

## Answer

- Chapter 11's blurring: Smooths the target  $Y$  to avoid hardness
- Chapter 13's binning: Discretizes  $W$  to enable testing

# Q&A: Kernel Blurring for Continuous $W$ ?

## Question

The local permutation test faces issues when  $W$  is continuous, similar to Chapter 11. Can kernel-based blurring techniques from Chapter 11 be applied here?

## Answer

- **Kernel-based approaches are possible:**
  - Weighted permutations among data points with similar  $W$  values
  - Kernel  $K(w, w')$  determines permutation probabilities
  - See: Sen et al. (2017), Kim et al. (2022)
- Key trade-off: More permutations  $\Leftrightarrow$  larger approximation error
- Both binning and kernel methods aim to approximate discrete case

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# Connections to Other Chapters

Topic	Discrete	Continuous
Test-conditional coverage (Ch 4)	Possible	Hard
Distribution-free regression (Ch 11)	Possible	Hard
ECE calibration (Ch 12)	Estimable	Not estimable
Conditional indep. testing (Ch 13)	Valid test	No power

## Unifying Theme

- **Discrete setting:** Repeated observations enable inference
- **Continuous setting:** Fundamental impossibility results
- **Smoothness assumptions:** Bridge between the two
- **Binning:** Convert continuous to approximately discrete

Thank you!



# References I

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