

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 : *Theorem 13.1*

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) : *Theorem 13.2*
- **Hard** (impossible) when W is continuous (hardness result) : *Theorem 13.3*

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)

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!

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

- $\mathbf{X} = (X_1, \dots, X_n)$, $\mathbf{Y} = (Y_1, \dots, Y_n)$
- $X_\sigma = (X_{\sigma(1)}, \dots, X_{\sigma(n)})$ 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:

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

Then ψ 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. $\sim P_X \Rightarrow$ Checking X_i 's exchangeability.

Recall: Permutation test for exchangeability

Recall: Theorem 2.4

For any function $T : \mathcal{Z}^n \rightarrow \mathbb{R}$, the p-value p defined as:

$$p := \frac{\sum_{\sigma \in S_n} \mathbf{1}\{T(\mathbf{X}_\sigma) \geq T(\mathbf{X})\}}{n!}$$

satisfies $\mathbb{E}_P[p \leq \tau] \leq \tau$ for all $\tau \in [0, 1]$ and $P \in \mathcal{P}_{\text{exch}}$.

Plug-in $T \leftarrow T(\mathbf{X}, \mathbf{Y})$ into Theorem 2.4, concluded the proof.

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

By Theorem 2.4, we can use any test statistic T to construct a valid permutation test. Here are some examples:

- 1 **Spearman's rank correlation** [3]: $|\text{Corr}(\text{rank}(X), \text{rank}(Y))|$
 - rank is similar to order statistics' index
 - Robust to outliers, captures monotonic relationships

Q&A: Alternative Test Statistics

Answer: Alternative Test Statistics

2 Distance correlation [4]

- Using distance covariance
- $\mathcal{V}^2(X, Y) := \|f_{X,Y}(t, s) - f_X(t)f_Y(s)\|^2$
- Detects nonlinear dependencies, equals zero iff independent

3 HSIC (Hilbert-Schmidt Independence Criterion) [2]

- $HSIC(p_{xy}, \mathcal{F}, \mathcal{G}) := \|C_{xy}\|_{HS}^2 = \mathbb{E}_{x,x',y,y'}[k(x, x') I(y, y')] + \mathbb{E}_{x,x'}[k(x, x')] \mathbb{E}_{y,y'}[I(y, y')] - 2\mathbb{E}_{x,y}[\mathbb{E}_{x'}[k(x, x')] \mathbb{E}_{y'}[I(y, y')]]$
- RKHS-based 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 $H_0 : X \perp\!\!\!\perp Y | W$, within each subpopulation X and Y are independent
- Same logic as marginal independence test, applied locally

Local Permutation Test: Permutation

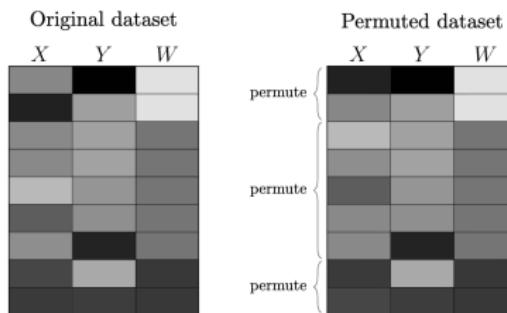


Figure 1: Visualization of a dataset with a discrete confounder along with a local permutation of the covariate [1]

Allowed Permutations

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

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

Local Permutation Test: Definition

Test Definition (Equation 13.4)

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

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

- 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 ψ is a **valid test** of $H_{X \perp\!\!\!\perp Y|W}$:

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

- **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)

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) $\Rightarrow |S_n(\mathbf{W})| = 1 \Rightarrow$ **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!**

Proof Sketch: Theorem 13.2

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

Under $H_0 : X \perp\!\!\!\perp Y | W$, 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 $W_{\sigma(i)} = W_i$,

$$(X_\sigma, \mathbf{Y}) | \mathbf{W} \stackrel{d}{=} (\mathbf{X}, \mathbf{Y}) | \mathbf{W} \cdots \quad (13.6)$$

Proof Sketch: Theorem 13.2

3 Using quantile technique

We can check that $\mathcal{S}_n(\mathbf{w}) = \{\sigma \circ \sigma' : \sigma' \in \mathcal{S}_n(\mathbf{w})\}$ for any $\sigma \in \mathcal{S}_n(\mathbf{w})$. So,

$$\hat{q}(\mathbf{x}_\sigma, \mathbf{y}, \mathbf{w}) = \text{Quantile}(T((\mathbf{x}_\sigma)_{\sigma'}, \mathbf{y}, \mathbf{w})_{\sigma' \in \mathcal{S}_n(\mathbf{w})}; 1-\alpha) = \hat{q}(\mathbf{x}, \mathbf{y}, \mathbf{w})$$

Therefore,

$$\begin{aligned} & \frac{1}{|\mathcal{S}_n(\mathbf{w})|} \sum_{\sigma \in \mathcal{S}_n(\mathbf{w})} \mathbf{1}\{\psi(x_\sigma, y, \mathbf{w}) = 1\} \\ &= \frac{1}{|\mathcal{S}_n(\mathbf{w})|} \sum_{\sigma \in \mathcal{S}_n(\mathbf{w})} \mathbf{1}\{T(x_\sigma, y, \mathbf{w}) > \hat{q}(x, y, \mathbf{w})\} \\ &= \frac{1}{|\mathcal{S}_n(\mathbf{w})|} \sum_{\sigma \in \mathcal{S}_n(\mathbf{w})} \mathbf{1}\left\{T(x_\sigma, y, \mathbf{w}) > \text{Quantile}((T(x_{\sigma'}, y, \mathbf{w}))_{\sigma' \in \mathcal{S}_n(\mathbf{w})}; 1 - \alpha)\right\} \\ &\leq \alpha \end{aligned}$$

Proof Sketch: Theorem 13.2

4 (13.6) implies that

$$\mathbb{P}_P(\psi(\mathbf{X}, \mathbf{Y}, \mathbf{W}) = 1 \mid \mathbf{W}) = \mathbb{P}_P(\psi(\mathbf{X}_\sigma, \mathbf{Y}, \mathbf{W}) = 1 \mid \mathbf{W})$$

holds for each $\sigma \in \mathcal{S}_n(\mathbf{W})$. Taking an average over $\sigma \in \mathcal{S}_n(\mathbf{W})$,

$$\begin{aligned} & \mathbb{P}_P(\psi(\mathbf{X}, \mathbf{Y}, \mathbf{W}) = 1 \mid \mathbf{W}) \\ &= \frac{1}{|\mathcal{S}_n(\mathbf{W})|} \sum_{\sigma \in \mathcal{S}_n(\mathbf{W})} \mathbb{P}_P(\psi(X_\sigma, \mathbf{Y}, \mathbf{W}) = 1 \mid \mathbf{W}) \\ &= \mathbb{E}_{\mathbb{P}} \left[\frac{1}{|\mathcal{S}_n(\mathbf{W})|} \sum_{\sigma \in \mathcal{S}_n(\mathbf{W})} \mathbf{1}\{\psi(X_\sigma, \mathbf{Y}, \mathbf{W}) = 1\} \mid \mathbf{W} \right] \leq \alpha \end{aligned}$$

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The Problem with Continuous W

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

$$\mathbb{P}(W_i = W_j) = 0 \text{ for } i \neq j$$

- No two data points share the same W value
- Local permutation test has no power

Theorem 13.3: Hardness Result

Theorem 13.3

If the test ψ has Type I error bounded by α 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 α)
- 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} : $X \perp\!\!\!\perp (Y, W) | K$ where $K = k(W)$ (bin index)

2 \tilde{P} Satisfies Conditional Independence

- By construction: $X \perp\!\!\!\perp (Y, W) | K$ 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:

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

This gives:

$$d_{\text{H}}^2(P, \tilde{P}) \leq (Lh)^2$$

4 Extend to n Samples

- Subadditivity of squared Hellinger distance:

$$d_{\text{H}}^2(P^n, \tilde{P}^n) \leq n(Lh)^2$$

- Total variation bound:

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

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!

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