Hypothesis Tests for Distributional Group Symmetry

with Applications to Particle Physics

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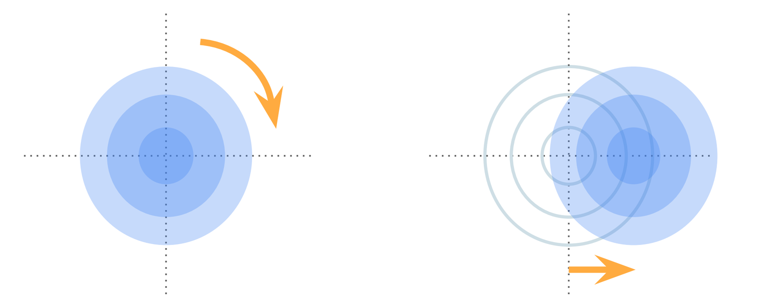
DOES A DATA DISTRIBUTION HAVE A GROUP SYMMETRY?

A distribution P is G**-invariant** if

$$P = g_* P \ , \ \forall g \in G$$

A conditional distribution $P_{Y|X}$ is G**-equivariant** if

$$P_{Y|X}(gx, B) = P_{Y|X}(x, g^{-1}B) \ , \ \forall g \in G \, , x \in \mathbf{X} \, , B \subseteq \mathbf{Y}$$



Given i.i.d. data $X_{1:n} = (X_1, \dots, X_n)$ from P, how do we check if P is G-symmetric?

Applications of a symmetry-checking tool

- Verifying model symmetry assumptions
- Checking if model has learned symmetry
- Discovering symmetries in science
- Testing model goodness-of-fit

Summary of main contributions

1. A general framework for testing (a) invariance of marginal/joint distributions and (b) equivariance of conditional distributions
2. A Monte Carlo algorithm for computing exact conditional p-values
3. Kernel-based test implementations

Extended work is found in [CBR23]

GROUP CHEATSHEET

GROUP

G = set of transformations with binary operator

1. associative
2. identity
3. inverse

HAAR MEASURE

λ = unique "uniform" distribution over

ACTION $= x \mapsto gx$

ORBIT

$O(x) = \{gx \in \mathbf{X} \colon g \in G\}$

REPRESENTATIVE

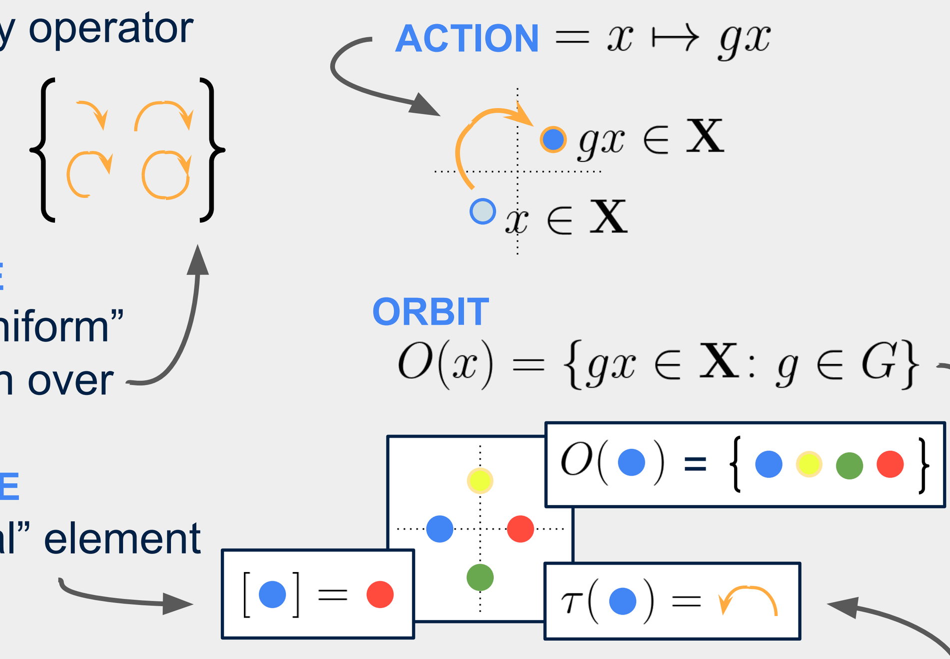
$[x]$ = "canonical" element of $O(x)$

ORBIT SELECTOR

$\gamma(x) = [x]$

REPRESENTATIVE INVERSION

$\tau(x) = g$ s.t. $\tau(x)\gamma(x) = x$



TESTING FOR INVARIANCE

Our idea: check invariance of P by testing distributional characterizations of invariance

Proposition 1 (simplified)

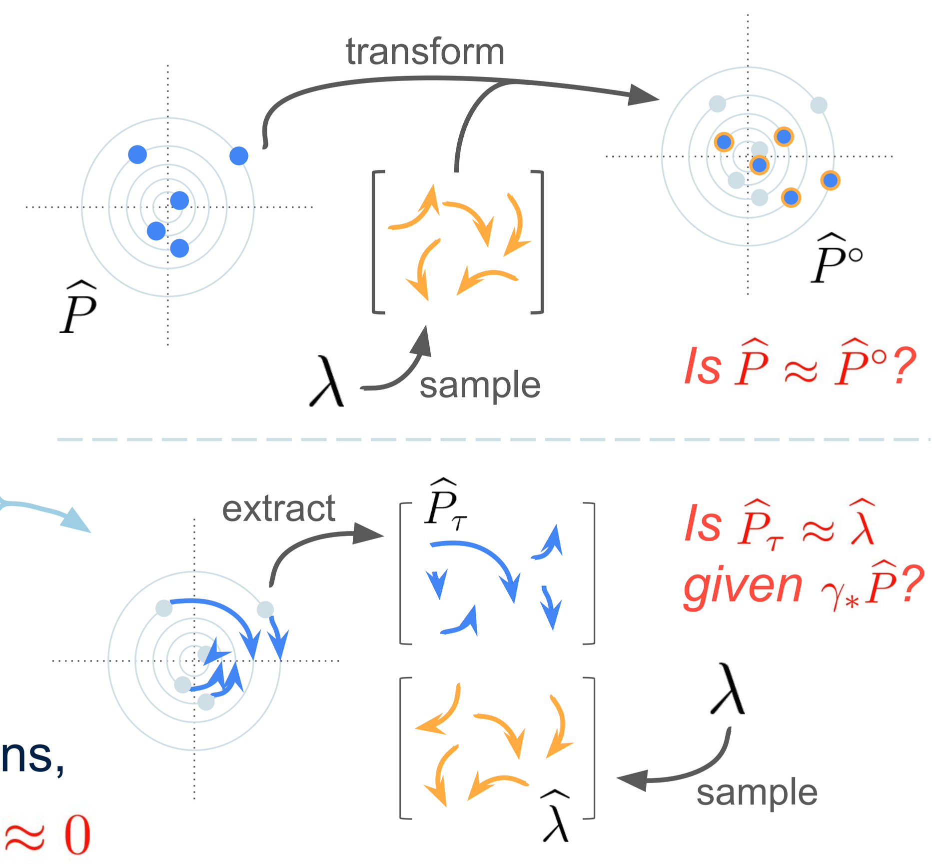
Assume G is compact. P is G-invariant iff

1. $P = P^\circ := \int_G g_* P \lambda(dg)$

   (P is invariant to *orbit-averaging*)

2. $P = \lambda \otimes \gamma_* P$

   (P factorizes into pushforward of Haar and distribution over orbit representatives)



Hypothesis testing for invariance

If P invariant $\implies$ for any metric D on distributions,

$$D(\widehat{P}, \widehat{P}^\circ) \approx 0 \quad \text{or} \quad D(\widehat{P}_\tau \otimes \gamma_* \widehat{P}, \widehat{\lambda} \otimes \gamma_* \widehat{P}) \approx 0$$

$\therefore$ If $D \gg 0 \implies P$ statistically unlikely to be invariant

Exact conditional Monte Carlo p-value

$\gamma(X)$ is sufficient for the class of G-invariant dist.'s

If P invariant $\implies$ cond. dist. of $X_{1:n}$ given $\gamma_* \widehat{P}$ known

$\implies$ can generate independent pseudosamples via transforms from λ

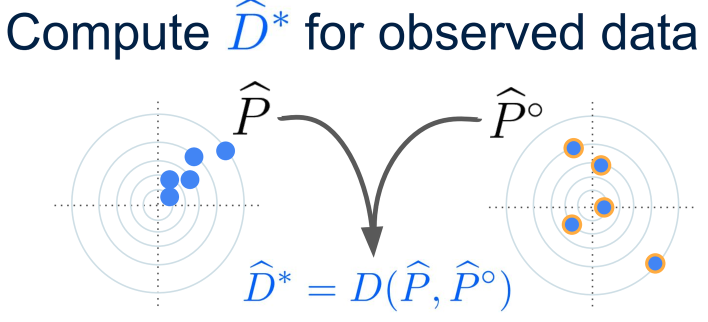
$\implies$ reject if p-value (Alg. 1) is less than α

Algorithm 1

(exact conditional MC p-value)

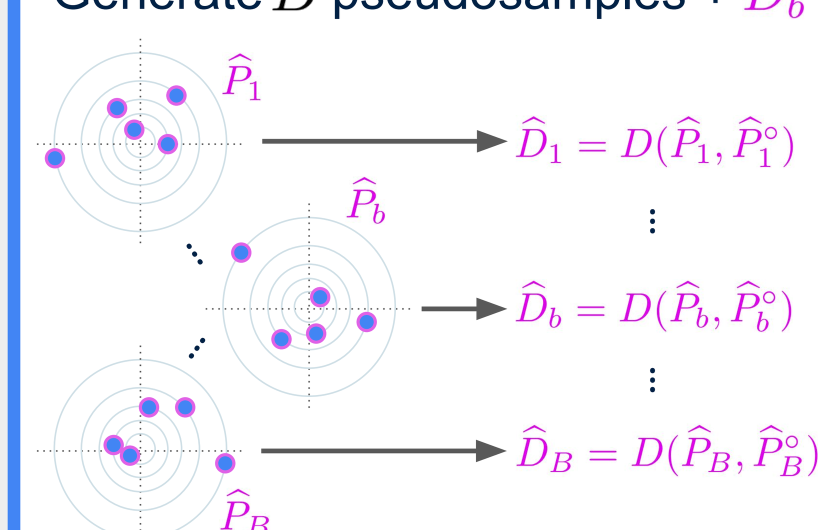
Step 1

Compute $\widehat{D}^*$ for observed data



Step 2

Generate B pseudosamples + $\widehat{D}_b$



Step 3

Compute p-value as

$$p_B = \frac{1 + \left|\{\widehat{D}_b \colon \widehat{D}_b \geq \widehat{D}^*\}\right|}{1 + B}$$

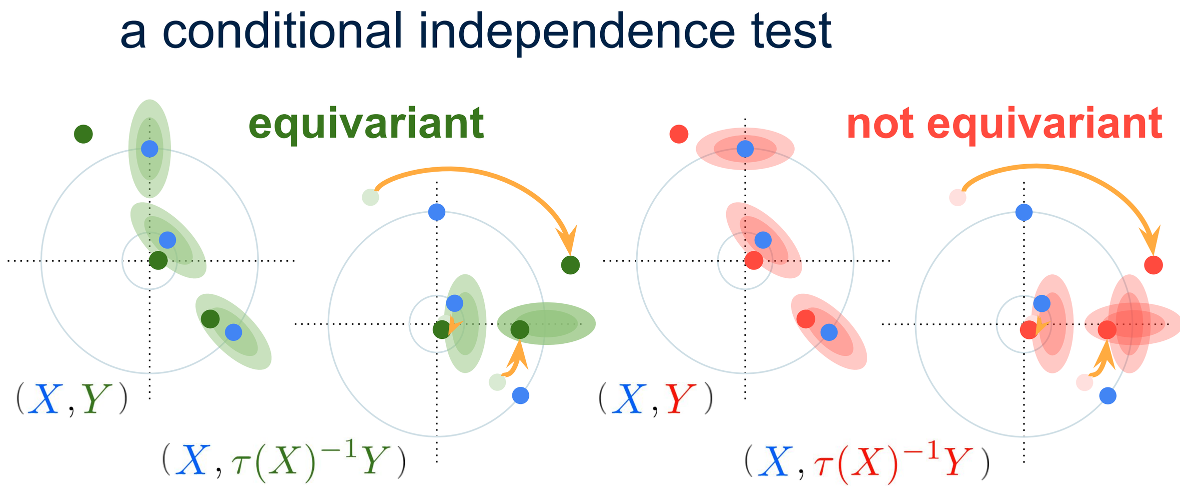
TESTING FOR EQUIVARIANCE

Theorem 2 (simplified): $P_{Y|X}$ is G-equivariant iff

$$X \perp\!\!\!\perp \tau(X)^{-1} Y \mid \gamma(X)$$

(only the orbit of X has info for $\tau(X)^{-1}Y$)

$\implies$ hypothesis testing for equivariance reduces to a conditional independence test



PARTICLE PHYSICS EXAMPLES

Experimental procedure

- In each simulation, sample n data points
- Calculate the proportion of rejections across $N = 1000$ simulations to estimate size/power

Tests for invariance

- 2sMMD (baseline): transform for 2nd sample and conduct kernel 2-sample test **[GBR+12]**
- MMD (Alg. 1): max. mean discrepancy metric
- CW **[FMR21]**: Cramér–Wold test for inv.

Test for equivariance

- KCI **[ZPJS11]**: kernel conditional indep. test

Large Hadron Collider dataset [KNS19]

Particle jets are produced when subatomic particles collide. By conservation of angular momentum, the distribution over 2D momenta of the two leading jet particles is invariant w.r.t. simultaneous 2D rotations.

Joint invariance

For $n = 100$, Tab. 1 shows the tests can identify symmetry w.r.t. simultaneous rotations, and reject symmetries w.r.t. (1) independent 2D rotations of the paired 2D momenta and (2) 4D rotations of the momenta as a 4D-vector.

$\alpha = 0.05$	simult. rotation	indep. rotation	4D rotation
2sMMD	0.035	0.967	0.983
MMD	0.038	1.000	1.000
CW	0.052	0.971	0.999

Table 1: rejection rate of tests

Equivariance

Joint rotation invariance can be seen as one momenta being rotationally-equivariant to rotations of the other.

For $n = 100$, KCI rejects equivariance at rate **0**, and rejects conditional invariance at rate **1**.

Top quark tagging [KPTR19]

Jet events can be classified as having decayed from a top quark or not. According to the Standard Model of physics, prediction of the top quark label based on the 2D momenta of the two leading jet particles should be conditionally invariant w.r.t. the Lorentz group $O(1,3)$.

For $n = 200$, KCI rejects conditional invariance w.r.t. the Lorentz group at rate **0.029**.

To verify KCI is meaningfully identifying symmetry, we simulate new labels conditionally on the energy of the 4-momentum of the particle. KCI rejects conditional invariance w.r.t. the Lorentz group at rate **0.781**.

[CBR23] K. Chiu and B. Bloem-Reddy. Non-parametric hypothesis tests for distributional group symmetry. *arXiv preprint arXiv:2307.15834*, 2023

[FMR21] R. Fraiman, L. Moreno, and T. Ransford. Application of the Cramér-Wold theorem to testing for invariance under group actions. *arXiv preprint arXiv:2109.01041*, 2021

[GBR+12] A. Gretton, K. M. Borgwardt, M. J. Rasch, B. Schölkopf, and A. Smola. A kernel two-sample test. *JMLR*, 13(1):723–773, 2012

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