Robust Signal Detection using a Classifier Decorrelated through Optimal Transport (CDOT)

Purvasha Chakravarti

Department of Statistical Science University College London p.chakravarti@ucl.ac.uk

Joint work with Mikael Kuusela and Larry Wasserman, Carnegie Mellon University

ML4Jets 2022 Nov 3, 2022

GOAL: supervised signal detection when signal is known

- Model-dependent search: Search for NP signals when the signal model is known.
- Supervised classifier: Use a supervised classifier trained on MC simulations to perform cuts on the data.
- Decorrelation via Optimal Transport: Use Optimal Transport to make the classifier cuts independent of the protected variables (resonant features), e.g. the invariant mass.
- Test combining multiple cuts: Fit the BG distribution of the protected variable jointly for the different cuts.
- Robust to background misspecification: Check whether the procedure is robust to background misspecification.

Data

Two sources of data are at hand:

• Background + signal (Monte Carlo) sample - labelled observations

Background:
$$\mathcal{B}$$
Signal: \mathcal{S}

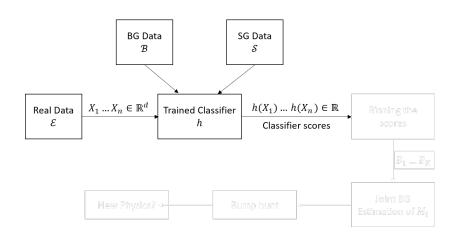
Used to train the classifier

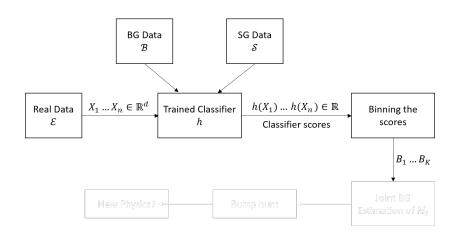
 Real experimental sample (Background + possible signal) - unlabelled observations

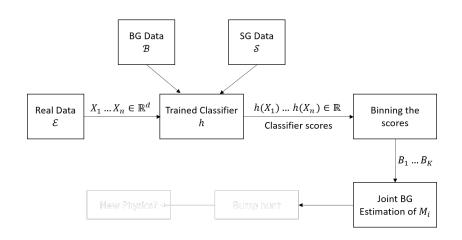
Experimental:
$$\mathcal{E} = \{X_1, \dots, X_n\}$$

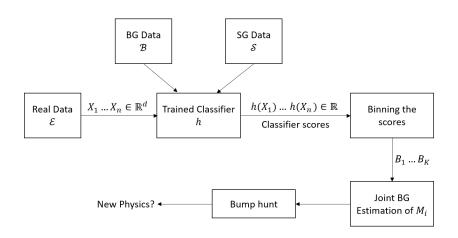
Protected Variable: M_1, \dots, M_n

Use \mathcal{E} to perform cuts and $M_i's$ to perform signal detection using bump hunting.









Problem with BG estimation: sculpting

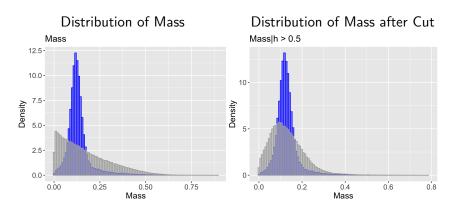
When we cut on the classifier scores the distribution of M_i 's changes!

Problem with BG estimation: sculpting

When we cut on the classifier scores the distribution of $M'_i s$ changes!

Example: Protected variable: Mass, Cut: Classfier output h > 0.5.

Grey: BG, Blue: SG



Idea behind decorrelation

Idea: Can the protected variable have the same background distribution after cuts as before cuts?

Idea behind decorrelation

Idea: Can the protected variable have the same background distribution after cuts as before cuts?

Need to make classifier output independent (not just *decorrelated*) of the protected variable for background data. (DisCo Fever [Kasieczka, Shih (2001.05310)], MoDe [Kitouni et al. (2010.09745)], etc)

Solution: Make cuts on transformed classifier output T(h(X)) instead, where T(h(X)) is independent of the protected variable M for background data.

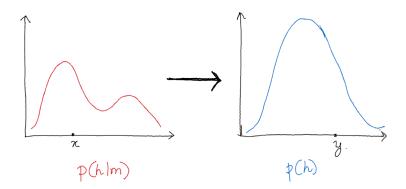
Solution: Make cuts on transformed classifier output T(h(X)) instead, where T(h(X)) is independent of the protected variable M for background data.

• Objective: Minimize $(T(h(X)) - h(X))^2$ subject to T(h(X)) independent of M = m(X), given $X \sim \mathcal{B}$

Solution: Make cuts on transformed classifier output T(h(X)) instead, where T(h(X)) is independent of the protected variable M for background data.

- Objective: Minimize $(T(h(X)) h(X))^2$ subject to T(h(X)) independent of M = m(X), given $X \sim \mathcal{B}$
- When T(h(X))|M has the same distribution as T(h(X)), then T(h(X)) is independent of M.
- The optimal transport map T_a from $p(h(x)|M=a,\mathcal{B})$ to the marginal $p(h(x)|\mathcal{B})$ is the solution.

The optimal transport map T_a from $p(h(x)|M=a,\mathcal{B})$ to the marginal $p(h(x)|\mathcal{B})$ is the solution.



The optimal transport map T_a from $p(h(x)|M=a,\mathcal{B})$ to the marginal $p(h(x)|\mathcal{B})$ is the solution.

- h(X) is univariate.
- Closed form solution to Optimal Transport problem.

$$T_a(h(X)) = G^{-1}(F_{h|M}(h(X)|M=a))$$

where G is the marginal cdf of h(X) and $F_{h|M}$ is the conditional distribution of h(X) given m(X) = a and X is from the background distribution.

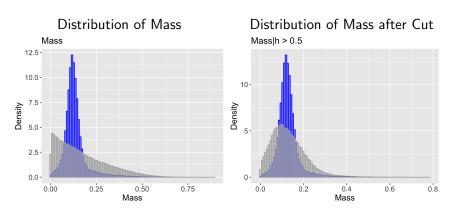
Solution is found by estimating G and $F_{h|M}$.

We call this Classifier Decorrelated through Optimal Transport (CDOT).

Sculpting problem solved!

Example: Protected variable: Mass, Cut: Classfier output h > 0.5.

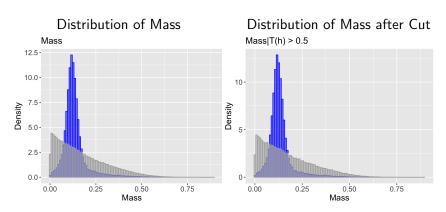
Grey: BG, Blue: SG



Sculpting problem solved!

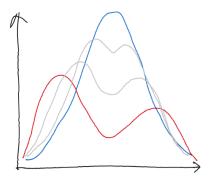
Example: Protected variable: Mass, Cut: Classfier output h > 0.5.

Grey: BG, Blue: SG



Geodesic path of Optimal Transport

Solutions can span from h(X) to T(h(X)).



$$\beta h(X) + (1 - \beta) T(h(X)), \quad \beta \in [0, 1].$$

Discussion on existing decorrelation methods

- DisCo Fever [Kasieczka, Shih (2001.05310)]:
 - Based on "distance correlation", which is 0 iff variables are independent.
 - ▶ Added as a regularization term to the classifier loss function.

Discussion on existing decorrelation methods

- DisCo Fever [Kasieczka, Shih (2001.05310)]:
 - Based on "distance correlation", which is 0 iff variables are independent.
 - ▶ Added as a regularization term to the classifier loss function.
- MoDe [Kitouni et al. (2010.09745)]:
 - Regularization term is based on Legendre moments of conditional CDF of h|M.
 - ▶ MoDe loss with *I*th moment is optimal when the mass dependence of the classifier is at most an *I*th order polynomial.
 - I = 0 case is minimized iff variables are independent.

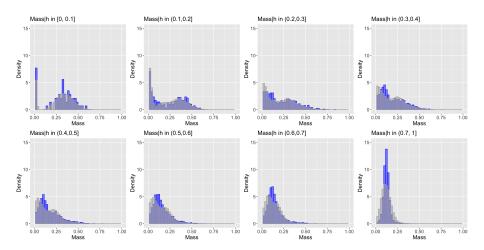
Discussion on existing decorrelation methods

- DisCo Fever [Kasieczka, Shih (2001.05310)]:
 - Based on "distance correlation", which is 0 iff variables are independent.
 - ▶ Added as a regularization term to the classifier loss function.
- MoDe [Kitouni et al. (2010.09745)]:
 - Regularization term is based on Legendre moments of conditional CDF of h|M.
 - ▶ MoDe loss with *I*th moment is optimal when the mass dependence of the classifier is at most an *I*th order polynomial.
 - I = 0 case is minimized iff variables are independent.
- Cuts derived from quantile regression [Moreno et al. (PhysRevD.102.012010)]:
 - Performs quantile regression to find cut = $\hat{Q}_{h|M}(\alpha)$.
 - $P(h > \operatorname{cut}|M) = 1 \alpha \ \forall \ m.$
 - ▶ Binning is a function of *m* and hence random.

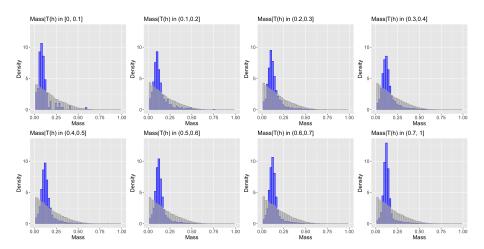
WTagging dataset

- Boosted hadronic W tagging dataset: benchmark for studying decorrelation methods.
- Bump hunt is performed on the mass of one W candidate jet and another (possibly W candidate) jet, mJJ.
- Classification is performed on ten representative jet substructure features.
- Details can be found in DDT [Dolen et al. (JHEP 2016)], DisCo Fever [Kasieczka, Shih (2001.05310)], and MoDe [Kitouni et al. (2010.09745)] papers.

WTagging dataset: before OT transformation

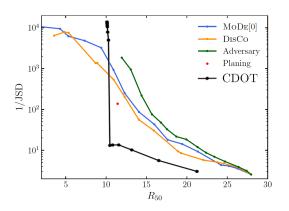


WTagging dataset: after OT transformation



WTagging dataset: comparison

JSD: Jensen–Shannon divergence, *R*50: the background rejection power (inverse false positive rate) at 50% signal efficiency.



CDOT achieves superior signal-to-background ratio for strongly decorrelated classifiers.

Original figure without CDOT taken from the MoDe [Kitouni et al. (2010.09745)] paper.

Simulated Data

- Data was generated using the MadGraph particle physics software.
- 4b represents events that were identified as having four b-jets.
- 3b represents events which were identified as having four jets, of which exactly three are b-jets.
- Signal sample produced at 400 GeV.
- We train the supervised classifier h on the pT, energy, η and ϕ variables of the four jets.
- More details: [Manole et al. (2208.02807)]

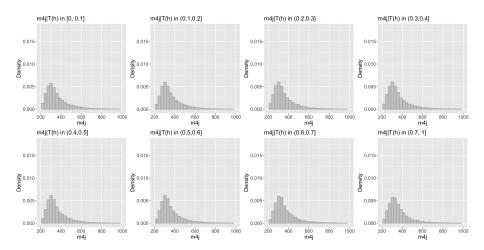
```
MC Background: 3b (50,000)
```

MC Signal: 400 signal (44, 196)

Experimental: 4b + 400 signal (60,000)

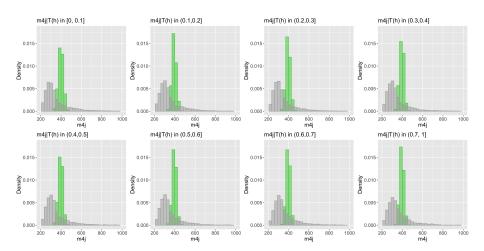
Simulated Data: OT and classifier trained on 3b data

CDOT trained on the 3b data and signal.



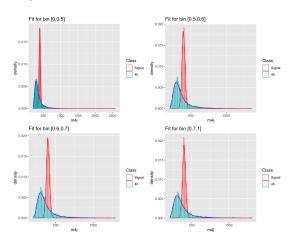
Simulated Data: robust on 4b data with signal

CDOT trained on the 3b data and signal shows robustness on 4b data.



BG joint estimation and bump hunt

- Fit a joint model for all the bins to estimate the BG distribution.
- Assume signal model is known.
- Perform bump hunt.



Summary

- Used a supervised classifier trained on MC simulations to perform cuts on the data.
- Used Optimal Transport to make the classifier cuts independent of the protected variables (resonant features).
- Fit the BG distribution of the protected variable jointly for the different cuts.
- Compared CDOT to other decorrelation methods.
- Checked that the procedure is robust to background misspecification.

Future work

- Find the ideal test for bump hunting jointly in all the bins.
- Compare the decorrelation method to when used with quantile regression.
- Analyze to find what perturbations in background the method is robust towards.

Thank you!



Contact email: p.chakravarti@ucl.ac.uk