

Classifier-Based Two-Sample Testing for Model-Independent Searches of New Physics

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Two-Sample Testing

Two-sample testing refers to the following hypothesis testing problem:

Let $X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} p_1$ and $Y_1, \dots, Y_m \stackrel{\text{i.i.d.}}{\sim} p_2$

Test $H_0: p_1 = p_2$ vs. $H_1: p_1 \neq p_2$

Lots of classical tests in the univariate case (Kolmogorov–Smirnov, Anderson–Darling, Cramér–von Mises,...)

New in recent years: use classifiers to perform the test in high-dimensional spaces (e.g., Kim et al. (2019, 2021))

- Basic idea: train a classifier to separate X_1, \dots, X_n from Y_1, \dots, Y_m
- If the classifier is able distinguish between the two samples, then that provides evidence against H_0

Model-independent searches of new physics

In our recent work (Chakravarti et al., 2023), we approach the problem of model-independent searches of new physics using classifier-based two-sample testing

→ Provides sensitivity for unexpected or misspecified signals

Available datasets:

Training background: $\mathcal{X} = \{X_1, \dots, X_{m_b}\}$, $X_i \sim p_b$

Experimental data: $\mathcal{W} = \{W_1, \dots, W_n\}$, $W_i \sim q = (1 - \lambda)p_b + \lambda p_s$,

where p_b is a simulator for Standard Model background events and p_s is an unspecified signal distribution with unknown signal strength λ

We only have access to \mathcal{X} and \mathcal{W} ; i.e., no direct access to p_b , q , p_s or λ

Task 1: We want to understand if \mathcal{W} shows evidence for the presence of p_s

Task 2: We want to understand what λ and p_s look like

Model-independent search using a semi-supervised classifier

To test for the presence of p_s , we want to carry out the test

$$H_0: \lambda = 0 \quad \text{vs.} \quad H_1: \lambda > 0$$

without pre-specifying p_s

This can be achieved by performing the two-sample test

$$H_0: p_b = q \quad \text{vs.} \quad H_1: p_b \neq q$$

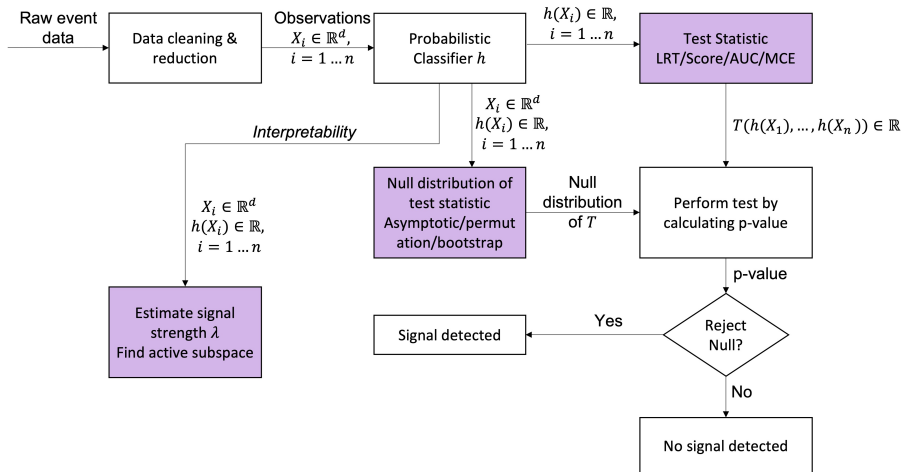
using the data $X_i \sim p_b$ and $W_i \sim q$

To do this in high dimensions, we train a classifier h to separate the background data \mathcal{X} from the experimental data \mathcal{W}

- Under H_0 , the classifier should not be able to separate \mathcal{X} from \mathcal{W}
- So if the classifier is able to differentiate between these two samples, then that provides evidence for the presence of p_s

This approach has close connections to the work by D'Agnolo and Wulzer (2019), D'Agnolo et al. (2021) and D'Agnolo et al. (2022)

Overview of the approach



Classifier-based test statistics

Test statistics based on a classifier \hat{h} that is trained to separate the experimental data \mathcal{W} from the background data \mathcal{X} :

① Likelihood Ratio Test Statistic:

$$\text{LRT} = 2 \sum_i \log \hat{\psi}(W_i),$$

where $\hat{\psi}(z) = \frac{m_b}{n} \frac{\hat{h}(z)}{1-\hat{h}(z)}$ is a classifier-based estimate of the density ratio $\psi = q/p_b$

② Area Under the Curve (AUC) Test Statistic:

$$\hat{\theta} = \frac{1}{m_b n} \sum_i \sum_j \mathbb{I} \left\{ \hat{h}(W_j) > \hat{h}(X_i) \right\}$$

Test $H_0 : \theta = 0.5$ versus $H_1 : 0.5 < \theta < 1$.

③ Misclassification Error (MCE) Test Statistic:

$$\widehat{\text{MCE}} = \frac{1}{2} \left[\frac{1}{m_b} \sum_i \mathbb{I} \left\{ \hat{h}(X_i) > \pi \right\} + \frac{1}{n} \sum_j \mathbb{I} \left\{ \hat{h}(W_j) < \pi \right\} \right], \quad \pi = n/(n+m_b)$$

Test $H_0 : \text{MCE} = 0.5$ versus $H_1 : \text{MCE} < 0.5$.

Calibration of the tests

In order to control the Type I error, we need to obtain the distribution of the test statistics under the null $H_0 : \lambda = 0$

Notice that under the null both \mathcal{X} and \mathcal{W} are samples from p_b

Three approaches:

- 1 **Asymptotics:** Can derive the asymptotic distribution for each of the test statistics; for example, for AUC, Newcombe (2006) showed that

$$\frac{\hat{\theta} - 0.5}{\sqrt{V_0(\hat{\theta})}} \rightsquigarrow N(0, 1),$$

for certain $V_0(\hat{\theta})$ under the null

- 2 **Nonparametric bootstrap:** Sample with replacement from $\mathcal{X} \cup \mathcal{W}$ and randomly label as either X 's or W 's
- 3 **Permutation:** Randomly permute the class labels in $\mathcal{X} \cup \mathcal{W}$

In-sample vs. out-of-sample evaluations

In practice, we need to be careful with in-sample vs. out-of-sample evaluation of the classifier \hat{h}

- For each calibration method, we use half of the data to train the classifier and the other half to evaluate and calibrate the test statistics (sample splitting)
- For the permutation method, we also consider a variant where the classifier is evaluated in-sample, which requires retraining the classifier for each permutation cycle

Power of detecting a signal

Power of detecting a **well-specified** signal in the Kaggle Higgs boson data

Model	Method	Signal Strength (λ)						
		0.15	0.1	0.07	0.05	0.03	0.01	0
Supervised LRT	Asymptotic	100	100	96	62	18	18	6
	Bootstrap	100	96	78	58	6	0	0
	Permutation	100	98	98	86	28	6	0
Supervised Score	Bootstrap	64	66	74	50	18	0	0
	Permutation	94	92	100	92	80	24	12
Semi-Supervised LRT	Asymptotic	100	98	74	38	16	6	2
	Bootstrap	100	98	48	10	2	2	0
	Permutation	100	98	72	38	16	6	2
	Slow Perm	82	8	0	4	2	0	4
Semi-Supervised AUC	Asymptotic	100	96	78	32	14	4	2
	Bootstrap	100	98	70	32	20	6	2
	Permutation	100	98	68	32	20	4	2
	Slow Perm	100	100	94	56	20	8	4
Semi-Supervised MCE	Asymptotic	100	92	60	28	14	2	2
	Bootstrap	100	96	52	28	16	6	4
	Permutation	100	96	52	30	14	6	6
	Slow Perm	100	98	86	58	16	6	2

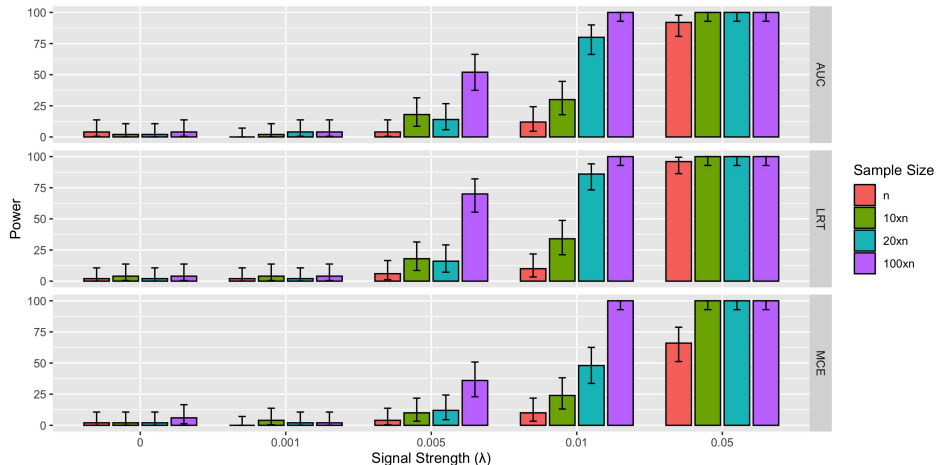
Power of detecting a signal

Power of detecting a **misspecified** signal in the Kaggle Higgs boson data

Model	Method	Signal Strength (λ)						
		0.15	0.1	0.07	0.05	0.03	0.01	0
Supervised LRT	Asymptotic	2	10	2	8	8	6	4
	Bootstrap	0	0	0	0	0	0	0
	Permutation	0	0	0	0	0	2	0
Supervised Score	Bootstrap	0	0	0	0	0	0	0
	Permutation	0	0	0	0	0	2	8
Semi-Supervised LRT	Asymptotic	100	100	100	82	18	4	4
	Bootstrap	100	100	100	60	4	2	0
	Permutation	100	100	100	82	18	4	2
	Slow Perm	100	100	78	22	2	4	6
Semi-Supervised AUC	Asymptotic	100	100	100	78	16	8	4
	Bootstrap	100	100	100	82	20	10	0
	Permutation	100	100	100	80	20	8	2
	Slow Perm	100	100	100	100	34	10	4
Semi-Supervised MCE	Asymptotic	100	100	100	66	24	6	4
	Bootstrap	100	100	100	62	16	6	4
	Permutation	100	100	100	62	14	6	4
	Slow Perm	100	100	100	98	22	8	2

Signal misspecified by transforming $\tau_{\text{pt}}^* = \tau_{\text{pt}} - 0.7(\tau_{\text{pt}} - \min(\tau_{\text{pt}}))$

Power as a function of sample size



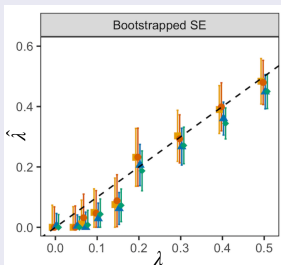
Power of the asymptotic model-independent tests for increasing sample sizes

Interpreting the semi-supervised classifier

We may want to be able to analyze the trained semi-supervised classifier \hat{h} to learn about the properties of the potential signal

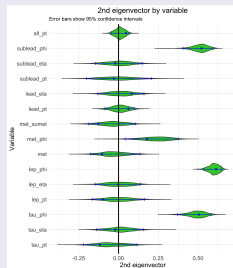
Signal strength

We estimate the signal strength λ from the classifier \hat{h} using the Neyman–Pearson quantile transform



Variable importance

We use the *active subspace* of the classifier to identify variable combinations that help separate the signal from the background



See the backups or Chakravarti et al. (2023) for more on these two approaches

Incorporating systematics

The aforementioned approaches assume that the training background sample \mathcal{X} comes from the true background p_b

However, in practice the simulator for \mathcal{X} is likely to be systematically misspecified

So the “signals” found might simply be due to background mismodeling

It would probably be possible to parameterize the systematics so that $p_b = p_b(\gamma)$, where $\gamma \in \Gamma$ is a nuisance parameter

We would then want to test

$$H_0: q \in \{p_b(\gamma) : \gamma \in \Gamma\} \text{ vs. } H_1: q \notin \{p_b(\gamma) : \gamma \in \Gamma\}$$

D’Agnolo et al. (2022) is an important first contribution toward this direction, but it is not immediately clear how to incorporate the nuisance parameters into the classifier-based test statistics discussed here

→ Will require developing new statistical methodology

Comparison of the two proposed approaches

Our LRT test is closely related to the approach of D'Agnolo et al. (D'Agnolo and Wulzer, 2019; D'Agnolo et al., 2021, 2022)

Let's try to understand what some of the differences are

I find it instructive to focus on the case where we test for the equivalence of two probability densities instead of the equivalence of two Poisson point process intensity functions

So as before, we have two samples

Training background: $\mathcal{X} = \{X_1, \dots, X_{m_b}\}, \quad X_i \stackrel{\text{i.i.d.}}{\sim} p_b$

Experimental data: $\mathcal{W} = \{W_1, \dots, W_n\}, \quad W_i \stackrel{\text{i.i.d.}}{\sim} q$

and we want to perform the test

$$H_0: p_b = q \quad \text{vs.} \quad H_1: p_b \neq q$$

Comparison of the two proposed approaches

The starting point for both Chakravarti et al. and D'Agnolo et al. is the likelihood ratio

$$\text{LRT} = 2 \log \left(\frac{\prod_{i=1}^n q(W_i)}{\prod_{i=1}^n p_b(W_i)} \right) = 2 \log \left(\prod_{i=1}^n \frac{q(W_i)}{p_b(W_i)} \right)$$

The challenge here is that we don't know q and p_b so we need to somehow learn the test statistic from the data, and this is where the two groups differ

Chakravarti et al. train a classifier h to separate \mathcal{X} from \mathcal{W} and use the mathematical fact (see Ben's talk yesterday) that h relates to the ratio q/p_b by

$$\frac{q(z)}{p_b(z)} = \frac{m_b}{n} \frac{h(z)}{1 - h(z)}$$

This effectively corresponds to deriving the alternative hypothesis q using the data and then performing a simple vs. simple test

Comparison of the two proposed approaches

D'Agnolo et al., on the other hand, proceed as follows¹:

Let's write down some flexible parametric form for q so that $q(z) = q(z; \theta)$ for some parameter vector θ

Specifically, let's use

$$q(z; \theta) = \frac{p_b(z) \exp(f(z; \theta))}{\int p_b(x) \exp(f(x; \theta)) dx},$$

where $f(z; \theta)$ is a neural network and θ are the parameters of that neural network

To obtain the test statistic, one would maximize over θ to find the most likely alternative model

$$\text{LRT} = 2 \log \left(\frac{\max_{\theta} \prod_{i=1}^n q(W_i; \theta)}{\prod_{i=1}^n p_b(W_i)} \right)$$

¹I have adapted here their method to probability densities instead of Poisson point process intensity functions

Comparison of the two proposed approaches

Plugging in the assumed form for q allows us to cancel the denominator which gives

$$\begin{aligned} \text{LRT} &= 2 \log \left(\max_{\theta} \frac{\prod_{i=1}^n \exp(f(W_i; \theta))}{\left[\int p_b(x) \exp(f(x; \theta)) dx \right]^n} \right) \\ &= 2 \max_{\theta} \left[\sum_{i=1}^n f(W_i; \theta) - n \log \mathbb{E}_{X \sim p_b} [\exp(f(X; \theta))] \right] \end{aligned}$$

D'Agnolo et al. then replace the expectation by an empirical average based on the background sample

$$\text{LRT} \approx 2 \max_{\theta} \left[\sum_{i=1}^n f(W_i; \theta) - n \log \left(\frac{1}{m_b} \sum_{i=1}^{m_b} \exp(f(X_i; \theta)) \right) \right]$$

The neural network f is trained by using the negative of the expression inside the brackets as the loss function and this yields the test statistic

Comparison of the two proposed approaches

Some remarks:

- Chakravarti et al. use a simple vs. simple likelihood ratio with a data-derived alternative, while D'Agnolo et al. use a simple vs. composite likelihood ratio with maximization over the alternative model parameters
- The test statistics are learned in a fundamentally different way by the two groups
- Chakravarti et al. fit a classifier (output in $[0, 1]$), while D'Agnolo et al. fit a neural network regression function (output in \mathbb{R})
- For D'Agnolo et al., the NN is evaluated in-sample, while Chakravarti et al. had trouble getting the in-sample LRT tests working reliably (but in-sample AUC and MCE tests worked well)

Comparison of the two proposed approaches

Some more remarks:

- For D'Agnolo et al., the two samples \mathcal{X} and \mathcal{W} play an asymmetric role in the training (\mathcal{X} is only used to constrain the normalization), while for Chakravarti et al. the two samples have a symmetric role in the training
- D'Agnolo et al. require $m_b \gg n$, while Chakravarti et al. took $m_b \approx n$
- If the classifier $h(z)$ converges to the true class probability for all z , then Chakravarti et al. consistently estimate the true LRT, while it's not immediately clear to me at least what can be said about the consistency of D'Agnolo et al.
- How does each approach perform with increasing data dimension?

Comparison of the two proposed approaches

Ultimately what matters the most is how these approaches perform on realistic HEP two-sample testing problems

Grosso et al. (2023) have started to investigate this question

- They find that the D'Agnolo et al. approach has more power than a variant of the classifier approach (different from Chakravarti et al., as far as I understand)

One should note that the results here depend also on what classifier is used, what test statistic is used, training hyperparameters, calibration method, in-sample vs. out-of-sample evaluation, sample sizes for \mathcal{X} and \mathcal{W} , dimension of the data,...

Future work will hopefully shed more light on the similarities and differences between D'Agnolo et al. and the classifier-based approaches

Discussion and Conclusions

- Classifiers provide a powerful tool for high-dimensional two-sample testing
- To fully specify the test, one needs to also specify:
 - What test statistic is used?
 - How is the test statistic learned?
 - How is the null distribution obtained?
 - Is the classifier evaluated in-sample or out-of-sample?
 - What classifier is used?
- Different choices above will lead to different two-sample tests with different properties
- An interesting common feature of these tests is that the alternative hypothesis is adaptively learned from the data during classifier training
- Here we focused on using classifier-based two-sample tests for model-independent searches of new physics
 - Such approaches may be able to increase the sensitivity of LHC for unexpected or misspecified signals
- Other use cases: DQM, validation of simulators / generative models,...
- Important avenue for future work: incorporating systematics into the classifier-based tests

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Semi-supervised anomaly detection—towards model-independent searches of new physics. In Journal of Physics: Conference Series, volume 368, page 012032. IOP Publishing, 2012.
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Backup

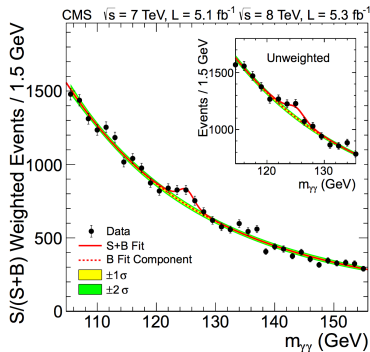
Hypothesis testing for discovery of new physics

Discovery of new phenomena at the LHC usually boils down to testing for the presence of a signal distribution over a background of known Standard Model physics:

- Known physics: $p_b(z)$
- New signal: $p_s(z)$
- Nature: $q(z) = (1 - \lambda)p_b(z) + \lambda p_s(z)$

Want to test $H_0 : \lambda = 0$ vs. $H_1 : \lambda > 0$

If one rejects H_0 at high enough significance level, then one would proceed to claim discovery of new physics



Model-dependent classifier-based tests

Most of these tests are done in the **model-dependent mode**, where the test statistic is optimized to have high power for detecting a specific signal

Relevant datasets:

Training background: $\mathcal{X} = \{X_1, \dots, X_{m_b}\}, \quad X_i \sim p_b$

Training signal: $\mathcal{Y} = \{Y_1, \dots, Y_{m_s}\}, \quad Y_i \sim p_s$

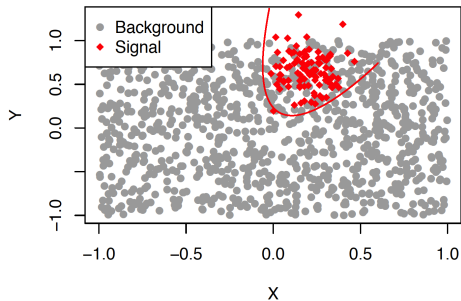
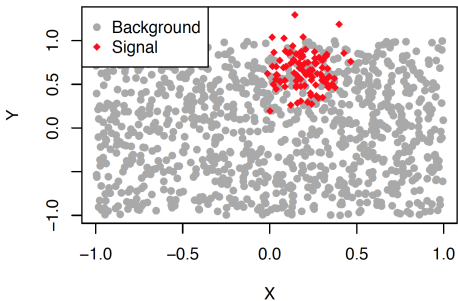
Experimental data: $\mathcal{W} = \{W_1, \dots, W_n\}, \quad W_i \sim q = (1 - \lambda)p_b + \lambda p_s$

Basic idea: use \mathcal{X} and \mathcal{Y} to find the optimal test for detecting p_s in \mathcal{W}

When the data space is high-dimensional, this is usually done using classifiers:

- 1 Train a supervised classifier to separate \mathcal{X} from \mathcal{Y}
- 2 Use the classifier output to test for the presence of signal in \mathcal{W}

Classifier training



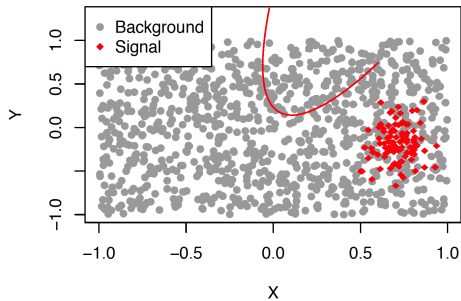
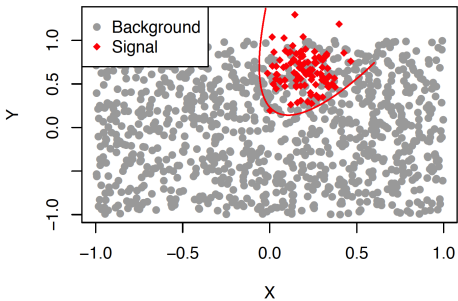
Testing when the signal is misspecified

To perform this test, we need to assume that we can reliably simulate data from both p_b and p_s

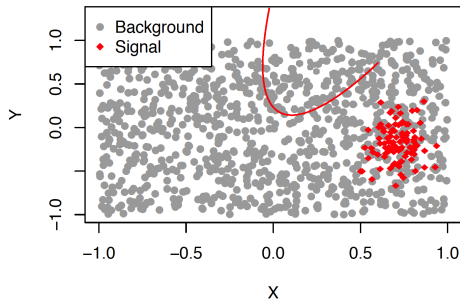
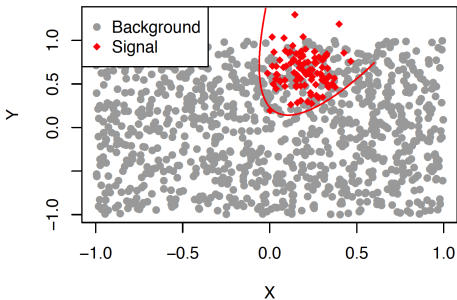
However, when either or both of these simulators are systematically misspecified, the test may not behave as desired

Specifically, if the test is optimized for a misspecified p_s , it may have little to no power for an actual signal

Systematically misspecified signal



Systematically misspecified signal



⇒ How to obtain an omnibus test that would have power for a wide range of signals, even in high-dimensional situations?

Related problems in statistics and ML

The model-independent search problem is closely related to a number of problems studied in statistics and machine learning

Specifically, it can be seen as an example of:

- 1 **Two-sample testing** (e.g., Kim et al. (2019, 2021)):

$$X_i \stackrel{\text{iid}}{\sim} p_1, Y_i \stackrel{\text{iid}}{\sim} p_2, \text{ is } p_1 = p_2?$$

- 2 **Collective anomaly detection** (e.g., Chandola et al. (2009)):

Is there a collection of data points which taken together deviate from the anticipated data?

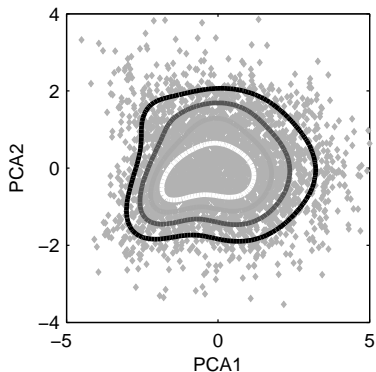
Notice that

model independent search \neq outlier detection

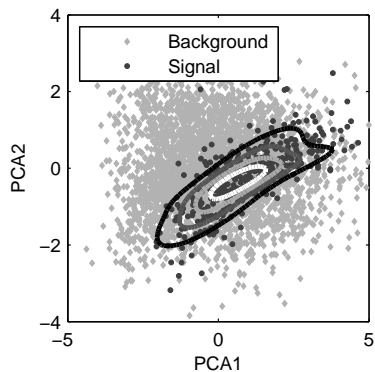
Each signal event is typically indistinguishable from the background on its own; it is the collection of many signal events that defines the excess

Model-independent searches in low-dimensional spaces

In Kuusela et al. (2012) and Vatanen et al. (2012), we used Gaussian mixture models to first fit the background sample and then, given the background model, fit any anomalous signal present in the experimental sample



(a) Background model $p_b(z)$



(b) Signal model $p_s(z)$

This approach works fine in 2–3 dimensions but does not really scale to higher dimensions

Our work (Chakravarti et al., 2023) makes the following contributions:

- 1 We investigate various ways of obtaining a test statistic from the trained classifier \hat{h} as well as various ways of calibrating the tests
- 2 We propose a way to estimate the signal strength λ based on \hat{h}
- 3 We propose a way to interpret \hat{h} using active subspaces

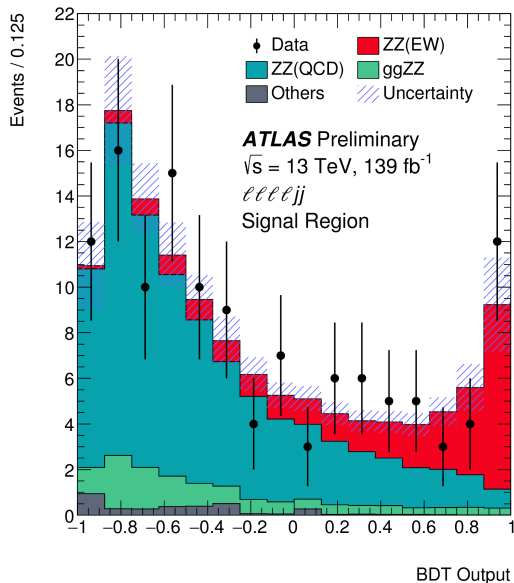
Kaggle Higgs boson data

We explore the performance of these methods using the Kaggle Higgs boson challenge dataset²

- Simulated $H \rightarrow \tau\tau$ events in ATLAS
- Select events with two jets and only consider primitive features (transverse momenta, MET, angles,...)
- 15 variables after accounting for rotational symmetry in ϕ
- 80,806 background events; 84,221 signal events
- Generate 50 “replicates” by sampling without replacement $m_b = 40,403$ background events, $m_s = 20,403$ signal events and $n = 40,403$ experimental events from the original samples
- We use Random Forest as the classifier h throughout

²<https://www.kaggle.com/c/higgs-boson>

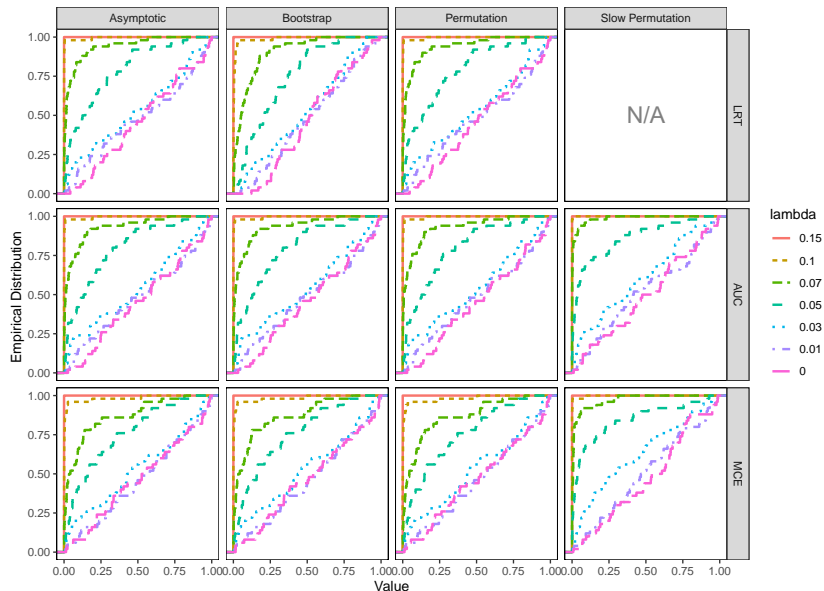
Classifier output



Some options for the test:

- Counting experiment in the highest purity output bin
- Cut on the classifier output; test using the resulting signal-enriched sample
- LRT: Use the connection of the classifier output to the likelihood ratio
- ...

p -value distributions for the semi-supervised tests



Estimating the signal strength

Given a trained semi-supervised classifier \hat{h} , how can we estimate the signal strength λ ?

If we know that $p_s(z) = 0$ for some known z , then this is simple

Since

$$\psi(z) = \frac{q(z)}{p_b(z)} = \left(\frac{1 - \pi}{\pi} \right) \left(\frac{h(z)}{1 - h(z)} \right),$$

we obtain

$$\hat{\lambda} = 1 - \left(\frac{1 - \pi}{\pi} \right) \left(\frac{\hat{h}(z)}{1 - \hat{h}(z)} \right),$$

for any z with $p_s(z) = 0$

However, in the model-independent setting, we may not know when $p_s(z) = 0 \rightarrow$ What to do?

Estimating the signal strength

Need to assume $\inf_z p_s(z)/p_b(z) = 0$ for identifiability; assume also $p_b, q > 0$ everywhere, for simplicity

Define the Neyman–Pearson Quantile Transform of z as:

$$\rho(z) = P_{X \sim p_b} \left(\frac{q(X)}{p_b(X)} \geq \frac{q(z)}{p_b(z)} \right) = P_{X \sim p_b} (\psi(X) \geq \psi(z)) = P_{X \sim p_b} (h(X) \geq h(z))$$

Let g_q be the density function of $\rho(Z)$ when $Z \sim q$

Then it can be shown that g_q is monotonically decreasing and

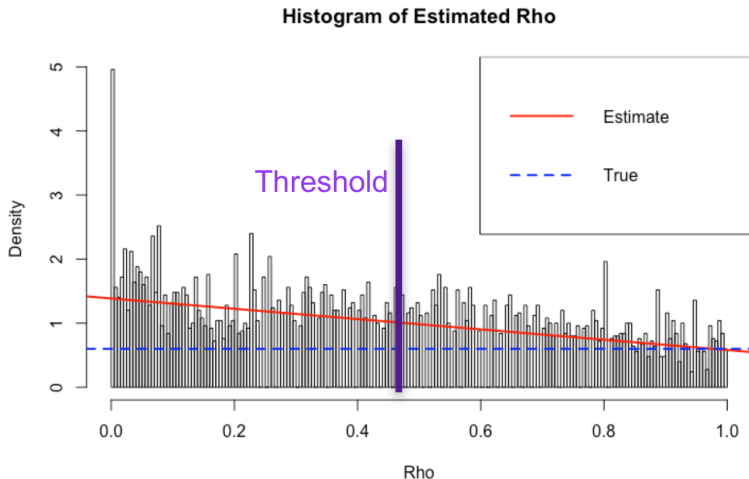
$$g_q(1) = 1 - \lambda$$

which allows us to estimate λ using $\hat{\lambda} = 1 - \hat{g}_q(1)$

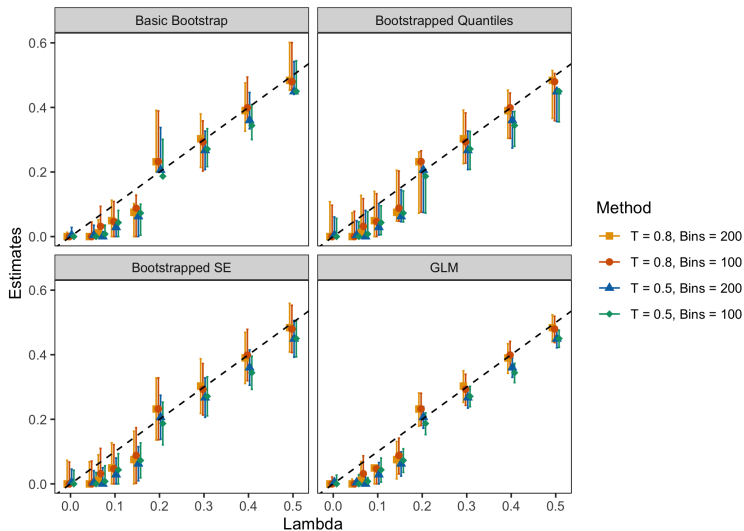
→ We need to estimate a monotone density at its boundary

Estimating the signal strength

In practice, we form a histogram of $\rho(W_i)$ and estimate $g_q(1)$ using a Poisson regression on bins close to 1



Estimating the signal strength



Estimated λ vs. true λ with various uncertainty estimates

Active subspaces for interpreting the classifier

The fitted classifier surface \hat{h} contains information about how the experimental data \mathcal{W} differs from the background data \mathcal{X}

How do we extract this information from \hat{h} ?

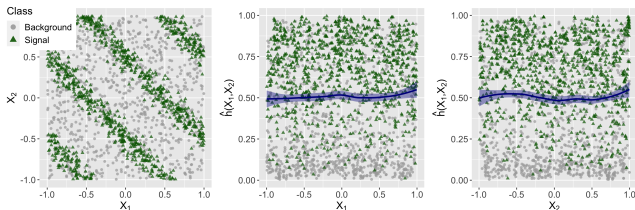
Could look at \hat{h} as a function of each input variable

But this might not reveal information contained in variable dependencies

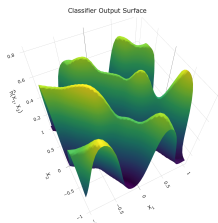
We propose to look at the *active subspace* of \hat{h} instead

Basic idea: perform PCA on the gradients $\nabla \hat{h}(z)$ to reveal those directions in which the classifier surface changes the most

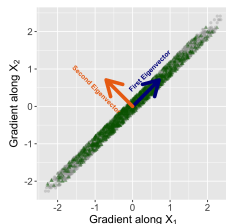
Active subspaces for interpreting the classifier



(a) X_1 versus X_2 , $\hat{h}(X_1, X_2)$ versus X_1 and $\hat{h}(X_1, X_2)$ versus X_2



(b) Smoothed Classifier Surface



(c) PCA of the Standardized Gradients

Active subspaces for interpreting the classifier

In practice, we look at the gradients of

$$H(z) := \text{logit}(\hat{h}(z)) = \log \left(\hat{h}(z) / (1 - \hat{h}(z)) \right)$$

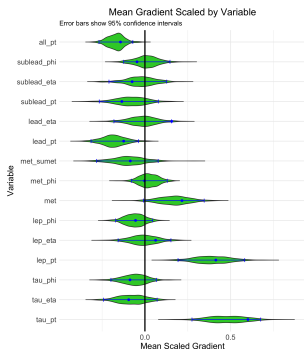
which are estimated by fitting a local linear regression on $H(Z_i)$ where $Z_i \in \mathcal{X} \cup \mathcal{W}$

Furthermore, we standardize the gradients by their estimated standard errors: $G(z) = \frac{\widehat{\nabla H(z)}}{\sqrt{\widehat{\text{Var}}(\nabla H(z))}}$

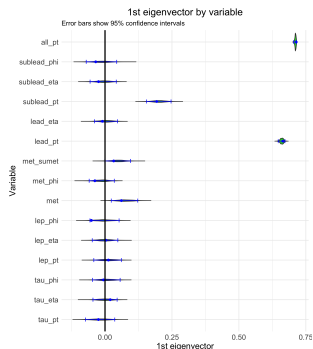
We then perform PCA on $G(Z_i)$: the mean of $G(Z_i)$ describes the slope of $H(z)$ and the principal components of $G(Z_i)$ capture the variation of $H(z)$ around the slope

Uncertainty estimates using bootstrapping

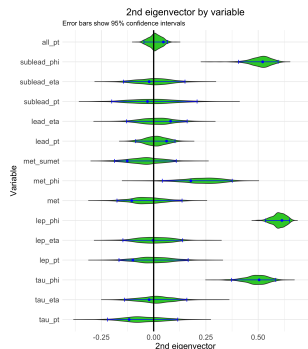
Active subspaces for interpreting the classifier



(a) Mean Gradient



(b) First Eigenvector



(c) Second Eigenvector

Density Ratios and Classifiers

In general, given two densities p and q and samples

$$X_1, \dots, X_n \sim p$$

$$Y_1, \dots, Y_n \sim q$$

Give labels: $Z \left| \begin{array}{cccccc} X_1 & \dots & X_n & Y_1 & \dots & Y_n \\ 1 & \dots & 1 & 0 & \dots & 0 \end{array} \right.$

Classifier ψ :

$$\psi(u) = P(Z = 1|u) = \frac{p}{p+q}$$

and so

$$\frac{p}{q} = \frac{\psi}{1-\psi}.$$

p -value distributions for the supervised tests

