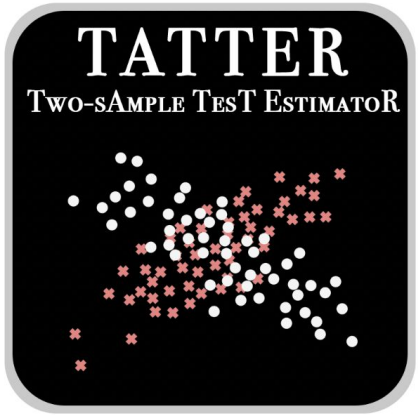
TATTER: A hypothesis testing tool for multi-dimensional data



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Paper: https://www.sciencedirect.com/science/article/pii/S2213133720300998#appA

Github: https://github.com/afarahi/tatter/tree/e8dc8a33d16dbd5855568302d062f5641f319ade

Introduction

- Many different data sets exist from a variety of surveys
    - Large-scale structure, CMB
    - Need a test to determine if data samples from different surveys were generated from the same distribution
    - Done using two-sample hypothesis testing
    - Will quantify if combining two samples is statistically justified
- Can also be used to compare simulations to empirical data

Two-sample hypothesis testing

- Performed on data from two independent samples
  - Testing to see if the difference in the populations is statistically significant
- Null hypothesis (H_0): $p(x) = q(y)$

  Alternative hypothesis (H_A): $p(x) \neq q(y)$

  - Will compute a null distribution assuming the null hypothesis is true
  - If observed value falls in the tail of the null distribution, then the null hypothesis is rejectected
- Many different types exist
  - Use depends on the problem being solved

Previous methods

- Kolmogorov-Smirnov (K-S) test
  - Compares cumulative distribution function of two sets of data
  - Popular choice for this two sample test
  - Non-parametric
  - Does not support multidimensional data distributions
- Kullback-Leibler (K-L) test
  - Quantifies the discrepancy between two samples
    - Measures how much information is lost when distribution q(y) is used to approximate p(x)
  - Is not symmetric
  - Can only use for certain types of pdfs

Introduction to maximum mean discrepancy test (MMD)

- Two-sample estimator that is based on distance
  - Developed to compute the distance between two multi-dimensional distributions
  - Relies on embedding sample into a high dimensional “feature space” through a kernel function (Gretton+, 2012a)
- Test statistic will determine how much test results differ from the null hypothesis
  - Value of zero indicated that two distributions are the same

Design of MMD

- Measure of the Maximum Mean Discrepancy in this work is

$$\widehat{\mathrm{MMD}}_u^2[k, x, y] = \frac{1}{m(m-1)} \sum_{i=1}^{m} \sum_{j \neq i}^{m} k(x_i, x_j) + \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i}^{n} k(y_i, y_j) - \frac{2}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} k(x_i, y_j)$$

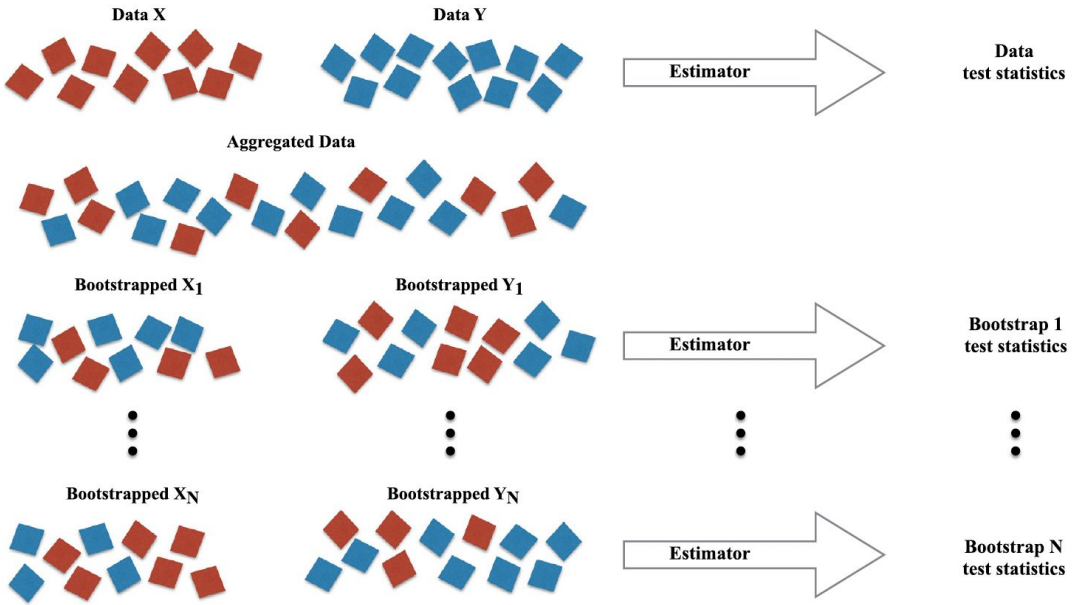
  - $k(x_i, y_j)$ is the kernel
  - x_i and y_j are samples from distributions
  - m and n are size of sample data
    - Gaussian radial basis function

$$k(x, y) = \exp(-\gamma \|x - y\|^2)$$

    - Allows algorithm to capture complex, non-linear interactions

Perform hypothesis testing for MMD

- Compute test statistic on previous slide using two lists drawn from probability distributions p(x) and q(y)
- To compute the null distribution
  - Data sets are combined
  - Randomly draw m points for x_{test} and n points for y_{test}
  - Uses bootstrap algorithm for resampling



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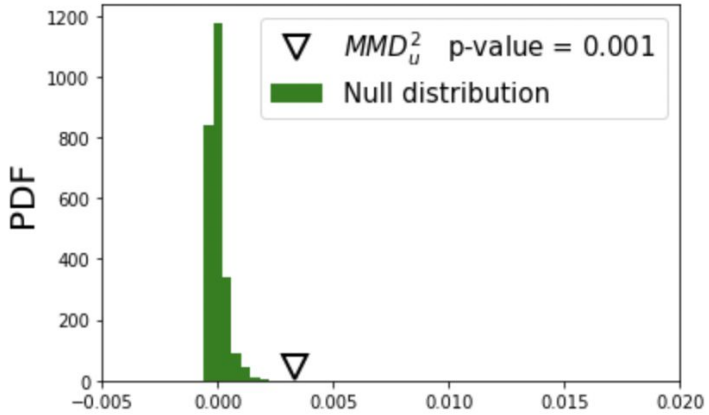
Perform hypothesis testing for MMD cont.

- Compute MMD^2_{null}
- Calculate the p-value using

$$1 - p = \Pr(\mathrm{MMD}^2_{\mathrm{null}}[k, x, y] < \mathrm{MMD}^2_{\mathrm{data}}[k, x, y]).$$

  - P-value < 0.05 indicates that null hypothesis can be rejected



Algorithm 1 Our simulation-based bootstrap algorithm to estimate the null distribution and p-value

Input: $x, y, N_b, k(.,.)$: observed samples, the number of bootstraps, and the kernel function.

Output: $\widehat{\mathrm{MMD}}^2$, Null, p-value: an estimation of the MMD^2 for the observed samples, drawn from the null distribution, and p-value.

initialize the hyper parameters. (γ, see Eq. (4))

$\widehat{\mathrm{MMD}}^2 = \mathrm{MMD}^2(x, y, k)$: compute $\mathrm{MMD}^2(x, y, k)$ with Eq. (2)

Z $\leftarrow$ aggregate observed samples.

for i in $\{1, \cdots, N_b\}$ **do**

  $x_{\mathrm{boot}} \leftarrow$ randomly draw m data points from Z (with replacements)

  $y_{\mathrm{boot}} \leftarrow$ randomly draw n data points from Z (with replacements)

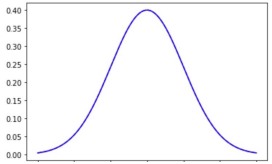
  $\mathrm{Null}[i] \leftarrow \mathrm{MMD}^2(x_{\mathrm{boot}}, y_{\mathrm{boot}}, k)$

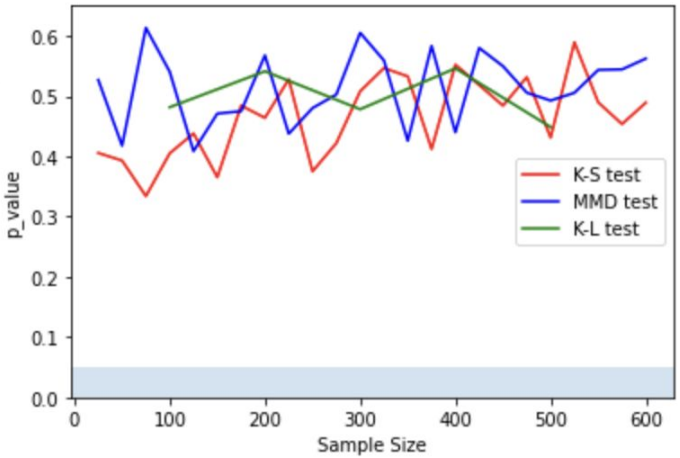
end for

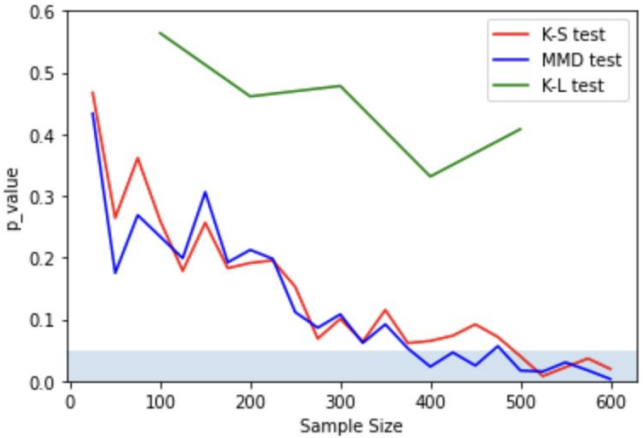
p-value = count(Null > $\widehat{MMD}^2$)/N_b

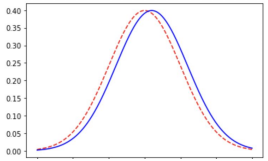
Comparison with other test statistics

- Compare MMD, K-S, and K-L tests on two gaussian distributions
  - Once where means are the same and one where they differ by 0.2
  - Sample size is equal to 1
  - All correctly don't reject the null when the means are the same
  - MMD performance is comparable to K-S test



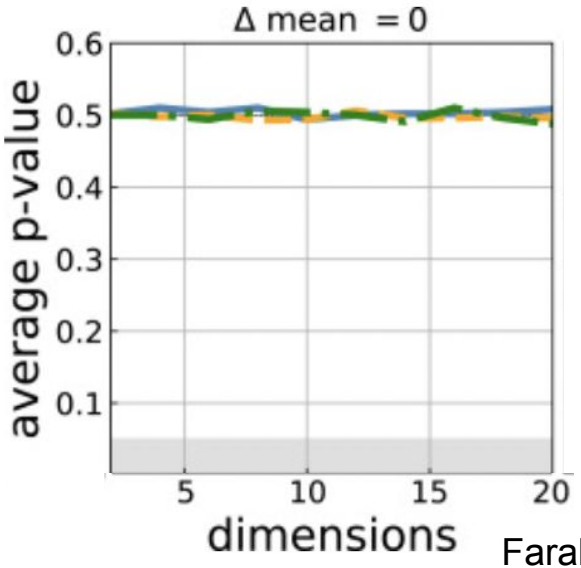


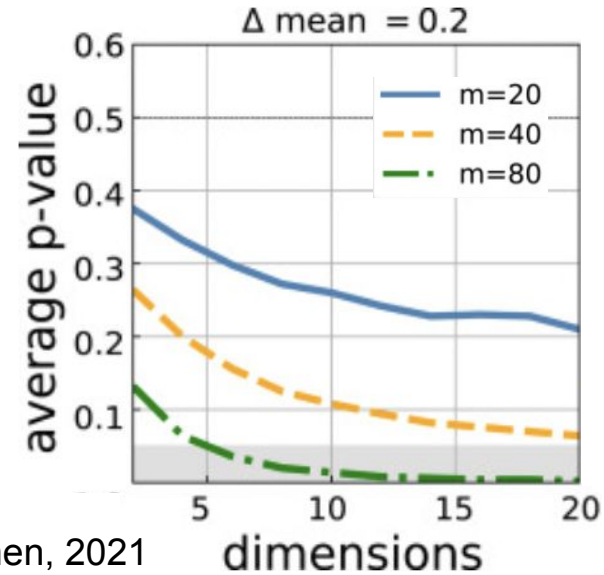




Multi-dimensional data

- MMD is designed to work for multi-dimensional data
  - Short-coming of K-S test





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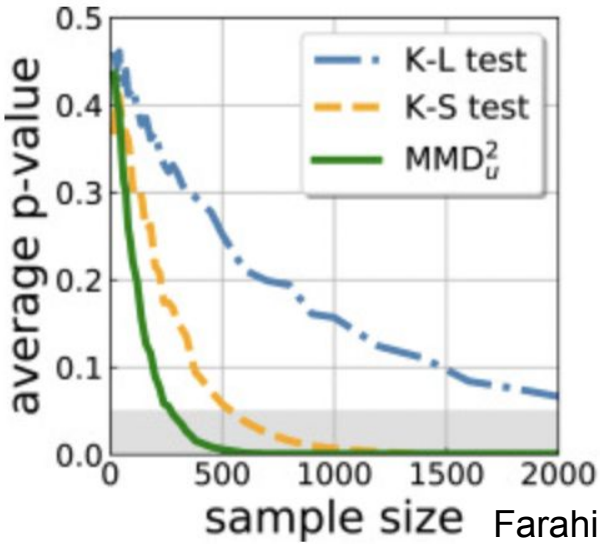
Different Distributions

- MMD is able to distinguish between data sets from different distributions
  - Able to do this without knowing the distributions beforehand



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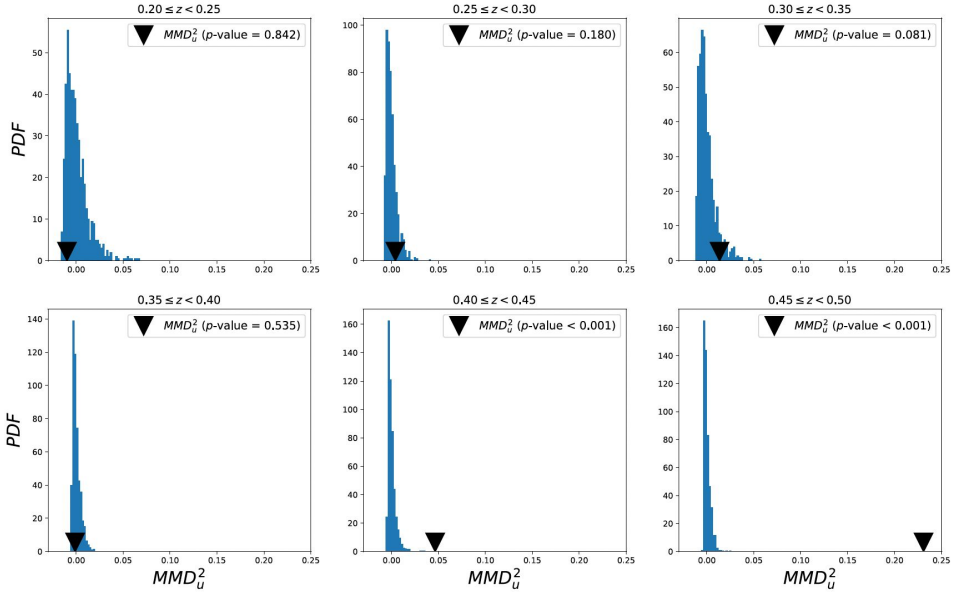
Application to astronomy

- Can be used to assess homogeneity of survey products and learn about systematics
- When looking at samples of galaxy clusters from two surveys
  - If galaxies are chosen in the same way and use the same cluster finding algorithm then distributions should be similar
  - Differences point to unaccounted for systematics
  - Will not be able to combine data samples

Application to astronomy cont.

- Looked at optical richness and redshift from SDSS and DES data
  - Performed MMD test to compare similarity
  - Looks similar at low redshift but differs at high redshift indicating that there are systematics affecting the data



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Summary

- Maximum mean distance test is a new two-sample hypothesis test
    - Accuracy is comparable to other popular tests
    - Can be extended to multi-dimensional data
- Performance is comparable to or better than other two-sample tests used in astronomy (K-S and K-L tests)
- Can be used to determine if astronomical data sets from different surveys can be combined
    - Also as a test for potential systematics