Guiding New Physics Searches with Unsupervised Learning

[DS, Jacques - 1807.06038]

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Searches for New Physics Beyond the Standard Model
have been negative so far…

MAYBE:

1. New Physics (NP) is not accessible by LHC

new particles are too light/heavy
or interacting too weakly

2. We have not explored all the possibilities

new physics may be buried under large bkg
or hiding behind unusual signatures

> New Physics ?

“Don’t want to miss a thing” (in data)

closer look at current data
get ready for next run

Model-independent search

searches for specific models may be insensitive
to unexpected / unknown / anomalous processes

> New Statistical Test

Want a statistical test for NP which is:

1. **model-independent:**

   no assumption about underlying physical model to intepret data

   → more general

2. **non-parametric:**

   compare two samples as a whole (not just their means, etc.)

   → fewer assumptions, no max likelihood estim.

3. **un-binned:**

   high-dim feature space partitioned without rectangular bins

   → retain full multi-dim info of data

> Outline

1. Statistical test of dataset compatibility

2. Applications to High-Energy Physics

> Outline

1. Statistical test of dataset compatibility

2. Applications to High-Energy Physics

[a.k.a. "homogeneity test"]

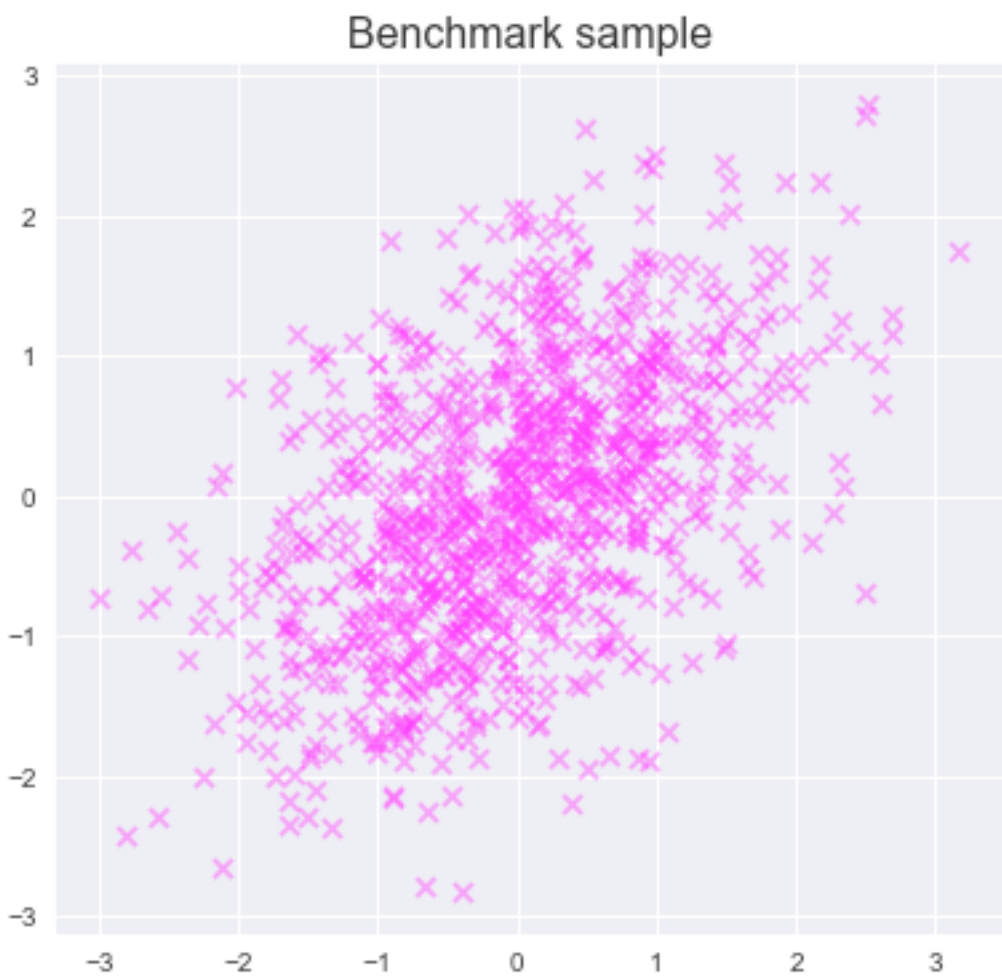
Two sets:

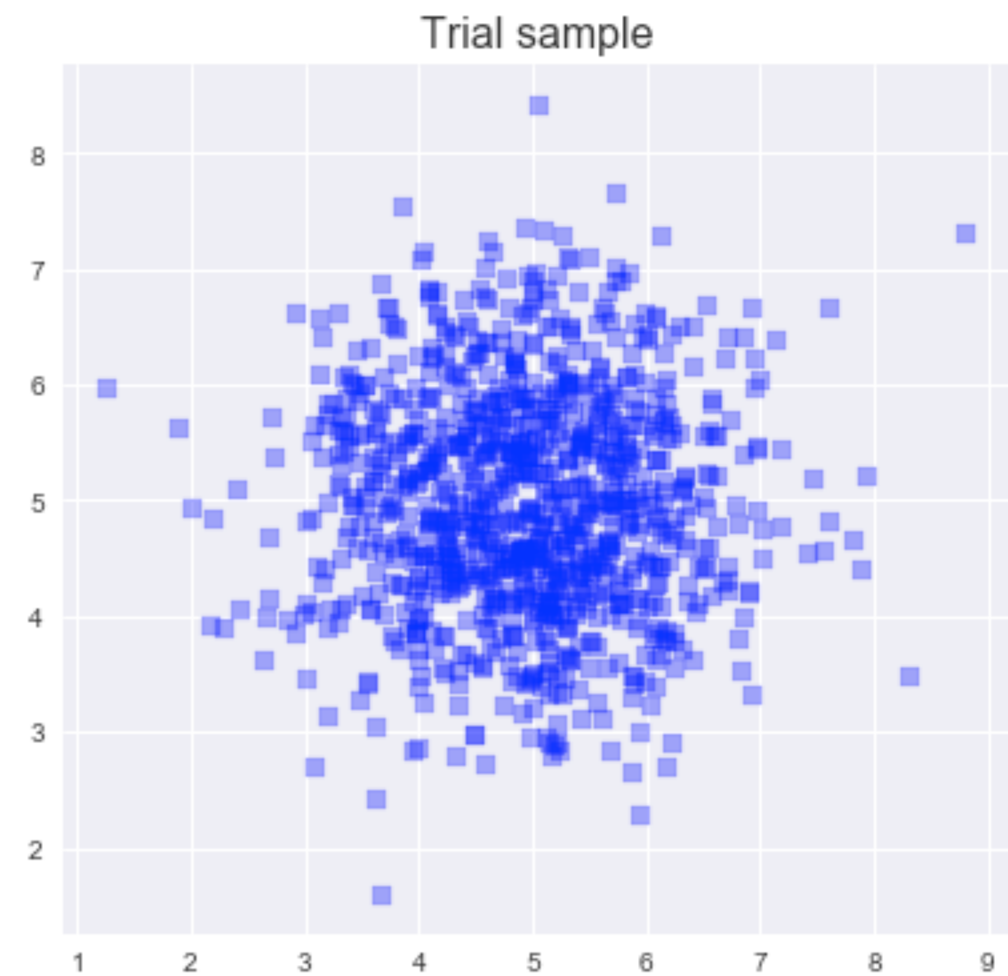
Trial: $\mathcal{T} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N_T}\} \overset{\text{iid}}{\sim} p_T$

Benchmark: $\mathcal{B} = \{\boldsymbol{x}'_1, \ldots, \boldsymbol{x}'_{N_B}\} \overset{\text{iid}}{\sim} p_B$

$\boldsymbol{x}_i, \boldsymbol{x}'_i \in \mathbb{R}^D$

probability distributions p_B, p_T unknown





e.g.: simulated SM bkg real measured data

> Two-sample Test

Two sets:

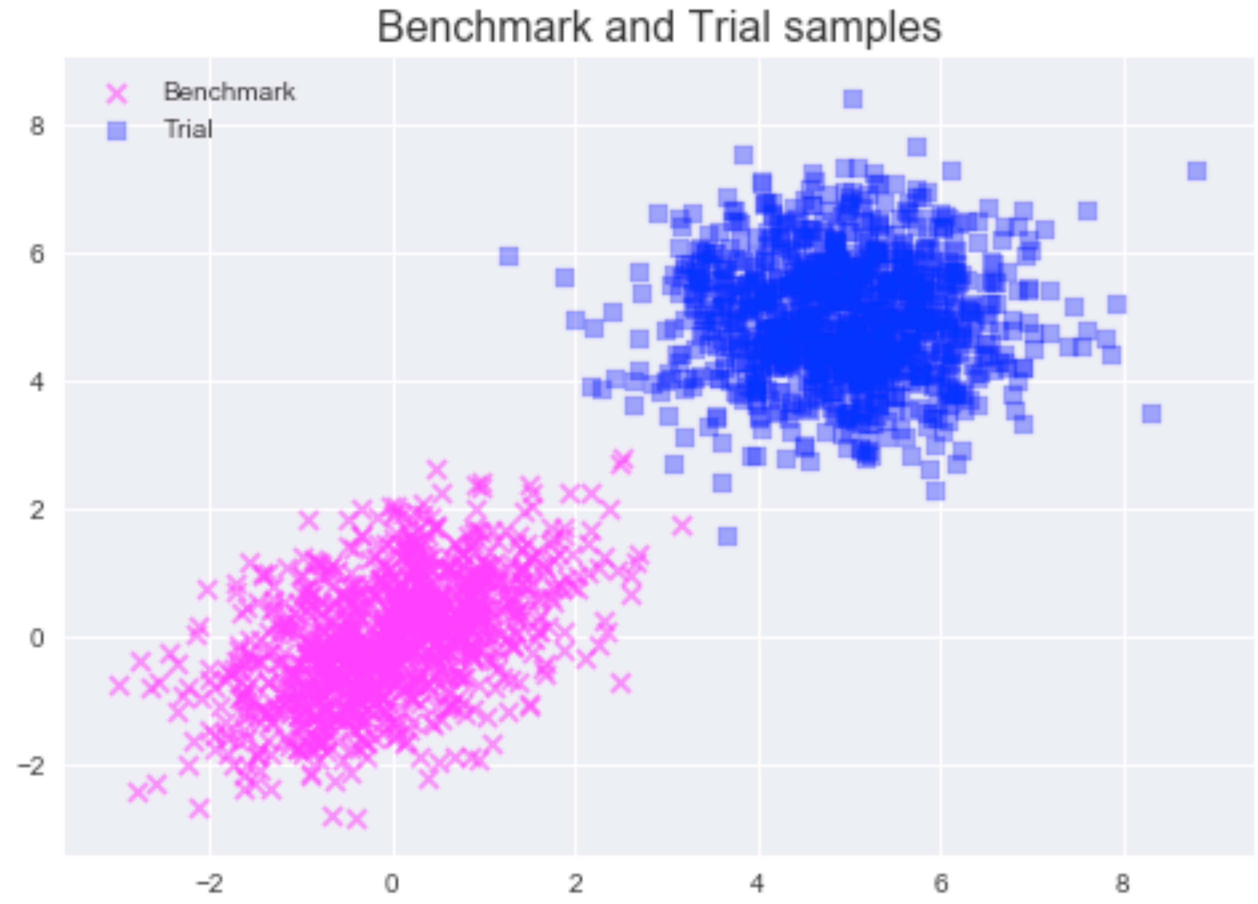
Trial: $\mathcal{T} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N_T}\} \overset{\text{iid}}{\sim} p_T$

Benchmark: $\mathcal{B} = \{\boldsymbol{x}'_1, \ldots, \boldsymbol{x}'_{N_B}\} \overset{\text{iid}}{\sim} p_B$

$\boldsymbol{x}_i, \boldsymbol{x}'_i \in \mathbb{R}^D$

probability distributions p_B, p_T unknown

Are *B,T* drawn from the same prob. distribution?



easy…

Two sets:

Trial: $\mathcal{T} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N_T}\} \overset{\text{iid}}{\sim} p_T$

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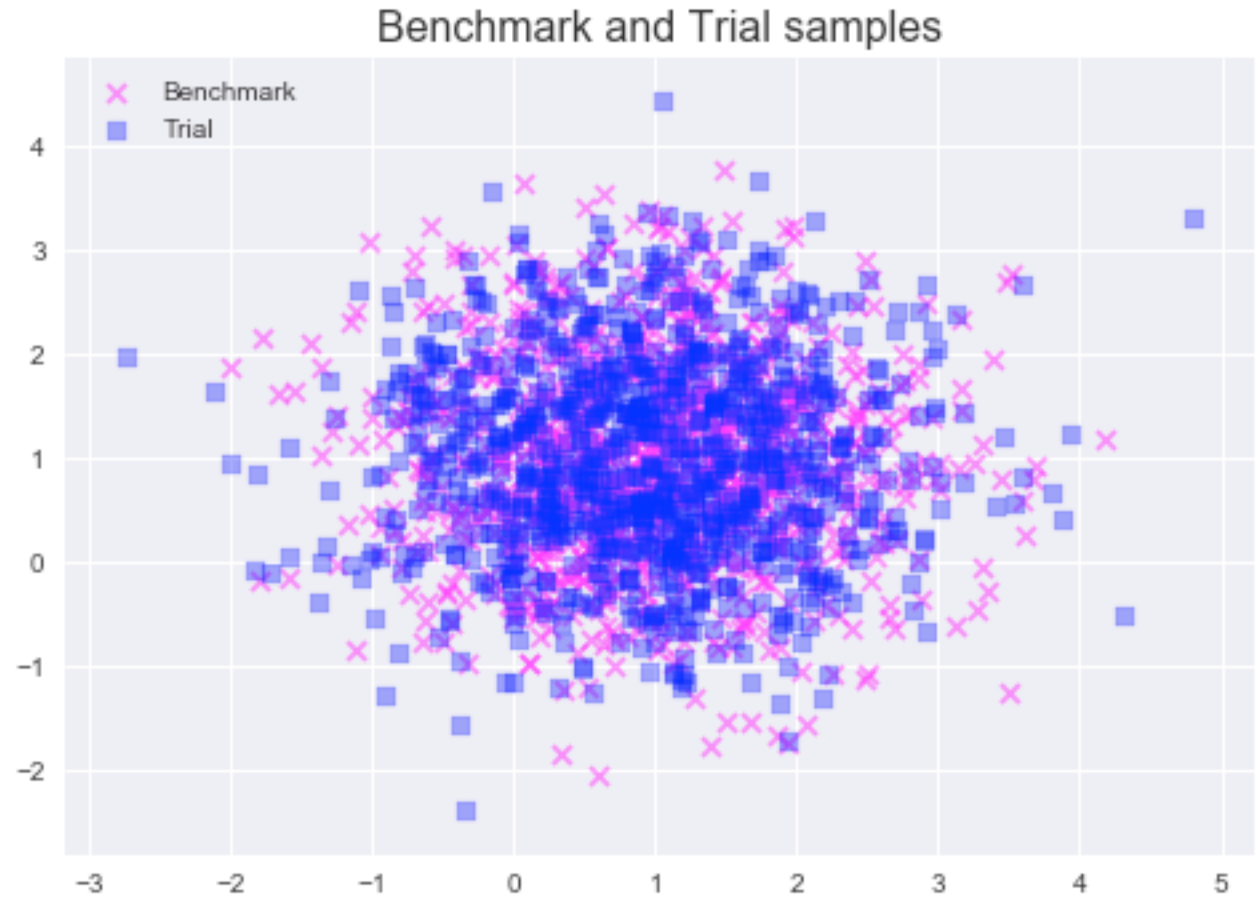


… hard!

RECIPE:

1. Density Estimator

→ reconstruct PDFs from samples

2. Test Statistic (TS)

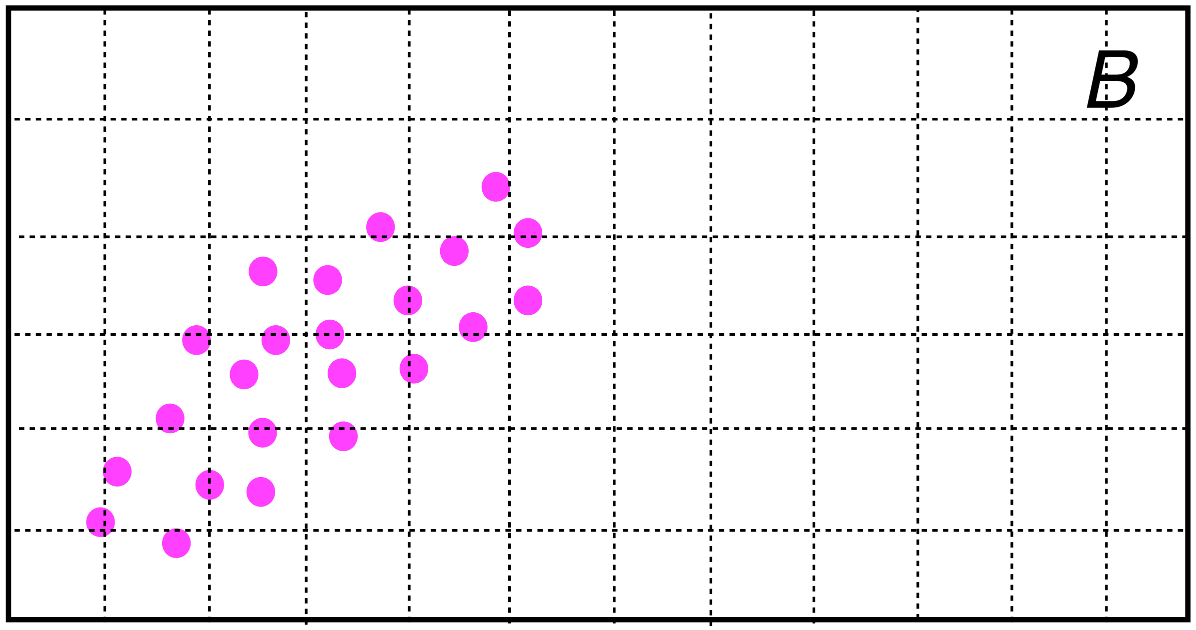
→ measure "distance" between PDFs

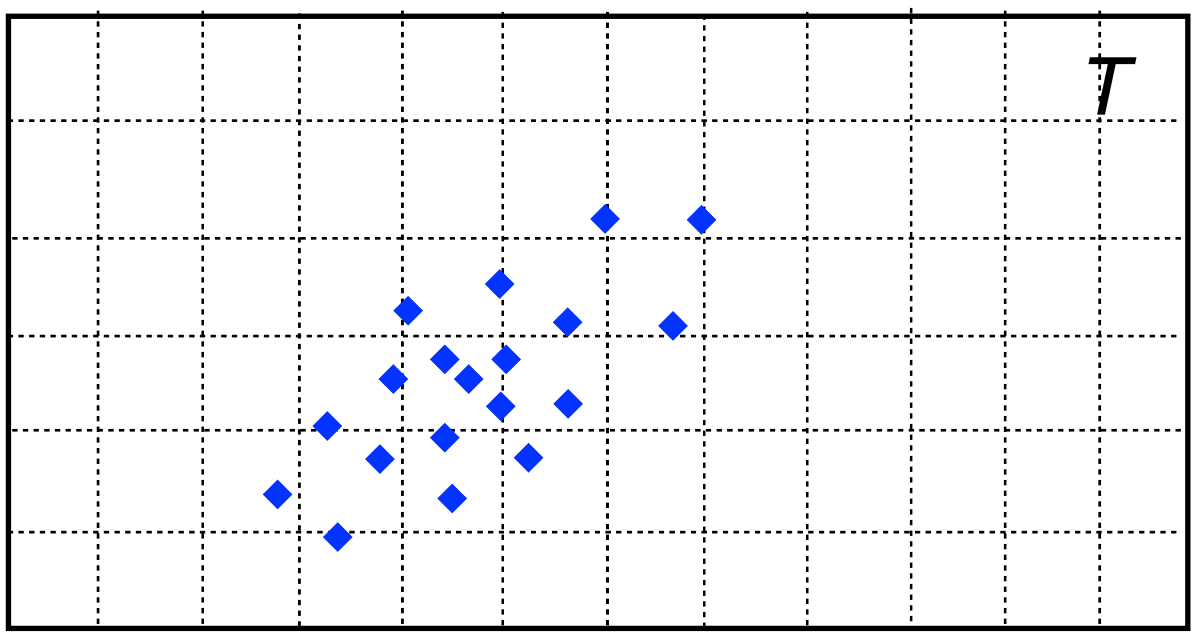
3. TS distribution

→ associate probabilities to TS
under null hypothesis H_0: $p_B = p_T$

4. *p* -value

→ accept/reject H_0





Divide the space in squared bins?

✓ easy

✓ can use simple statistics (e.g. χ^2)

✗ hard/slow/impossible in high-D

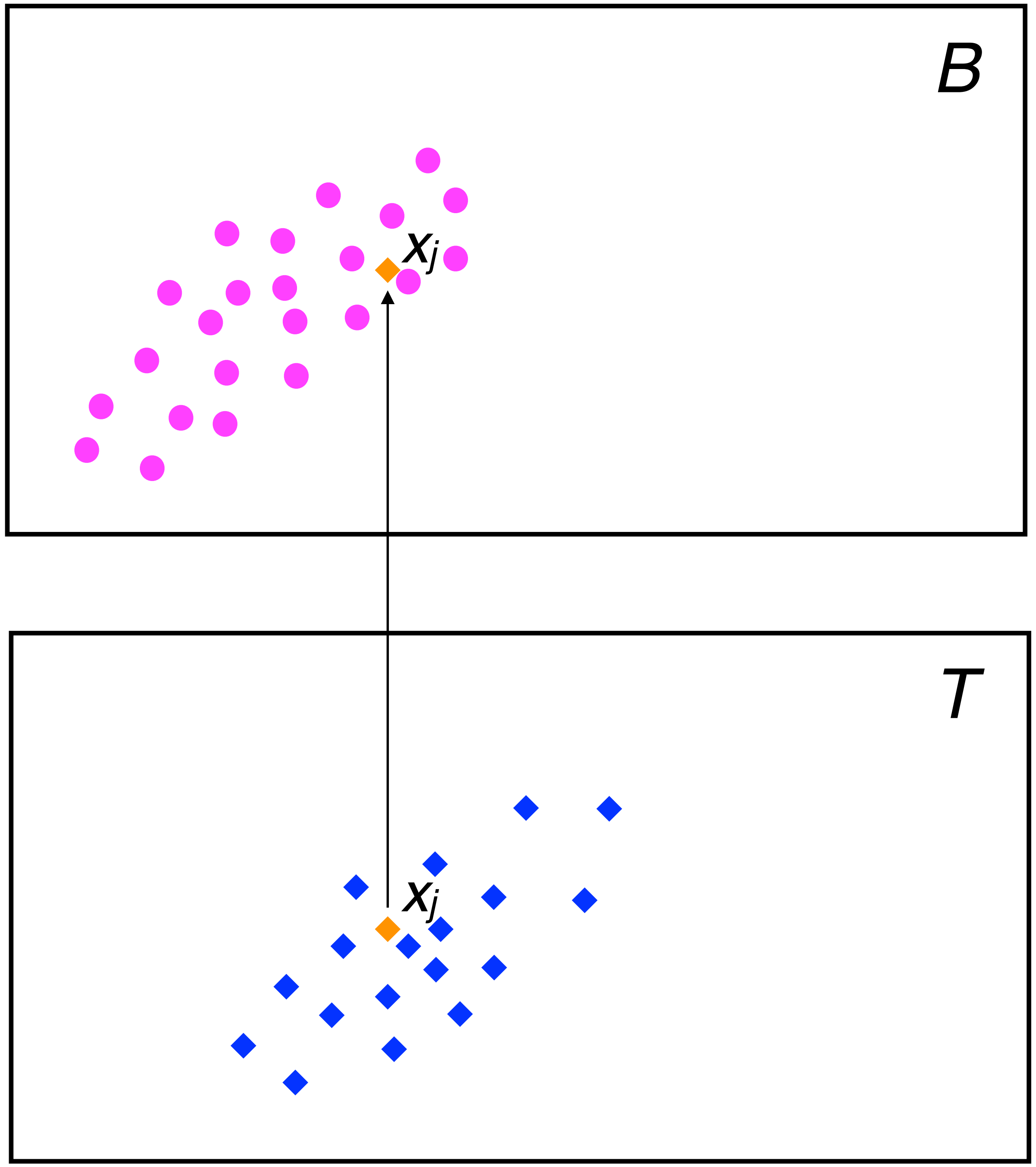
Need un-binned multivariate approach

Find PDFs *estimators*: $\hat{p}_B(\boldsymbol{x}), \hat{p}_T(\boldsymbol{x})$
e.g. based on densities of points:

$$\hat{p}_{B,T}(\boldsymbol{x}) = \frac{\rho_{B,T}(\boldsymbol{x})}{N_{B,T}}$$

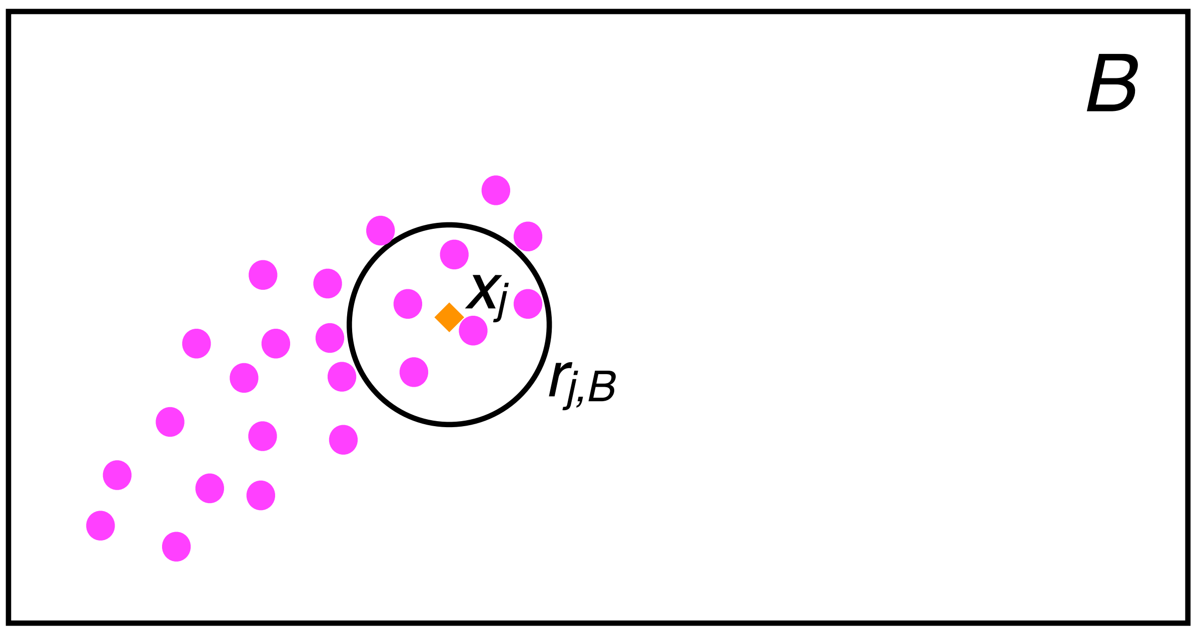
Nearest Neighbors!

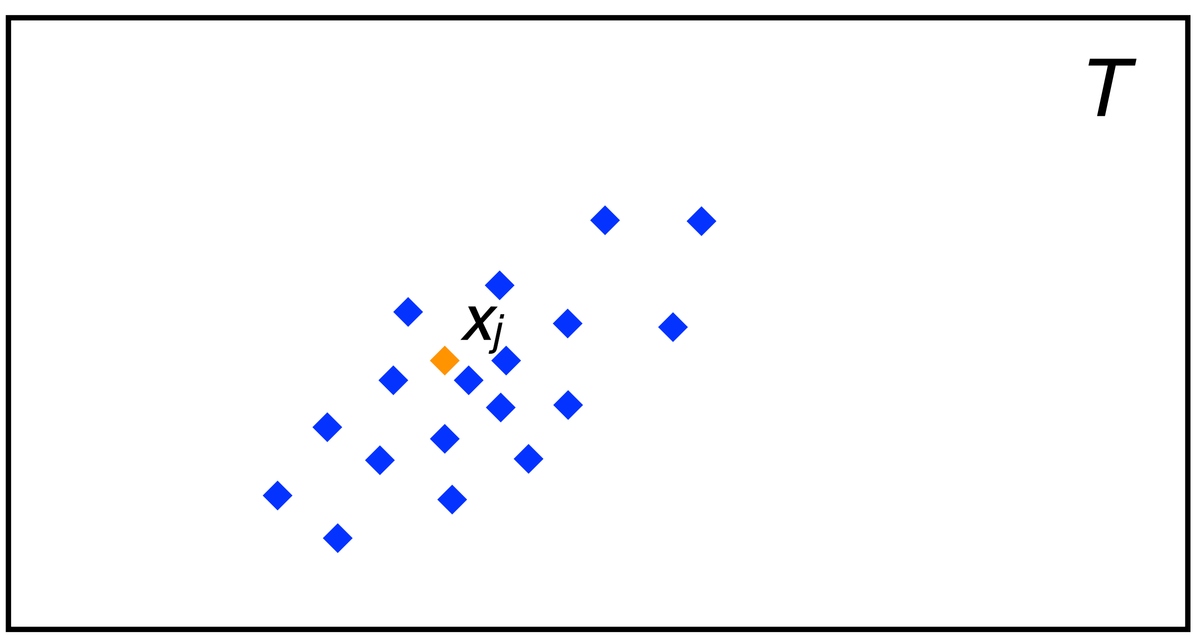
[Schilling - 1986][Henze - 1988]
[Wang et al. - 2005,2006]
[Dasu et al. - 2006][Perez-Cruz - 2008]
[Sugiyama et al. - 2011][Kremer et al, 2015]



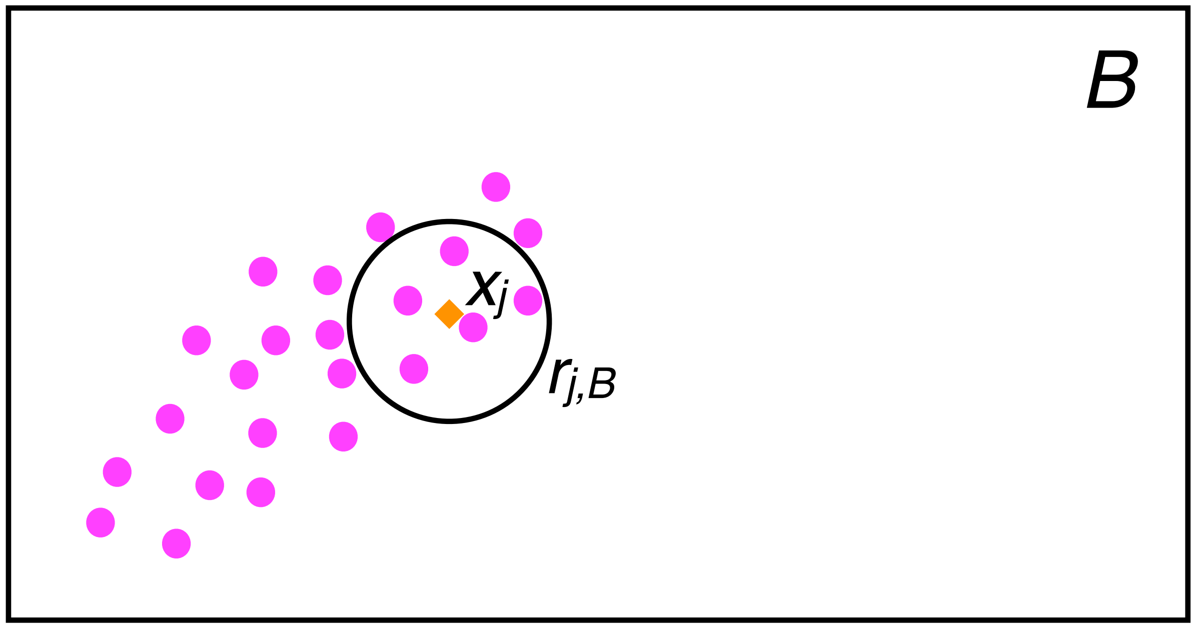
- Fix integer K.
- Choose query point x_j in *T* and draw it in *B.*

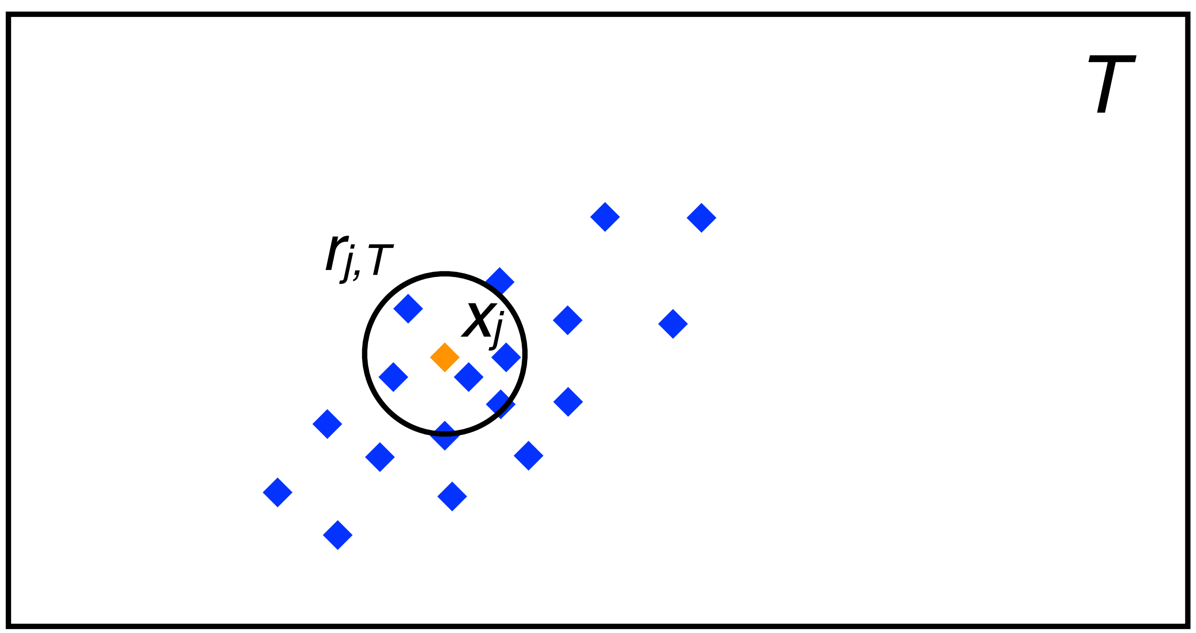
> 1. Density Estimator





- Fix integer K.
- Choose query point x_j in T and draw it in B.
- Find the distance $r_{j,B}$ of the Kth-NN of x_j in B.





- Fix integer K.
- Choose query point x_j in T and draw it in B.
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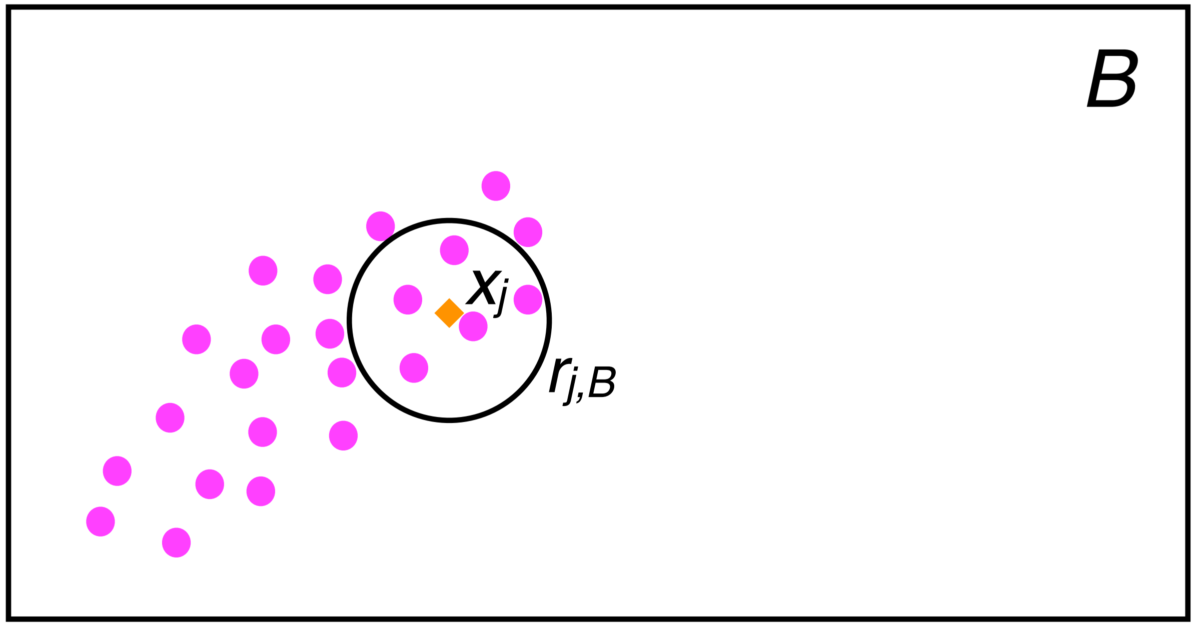
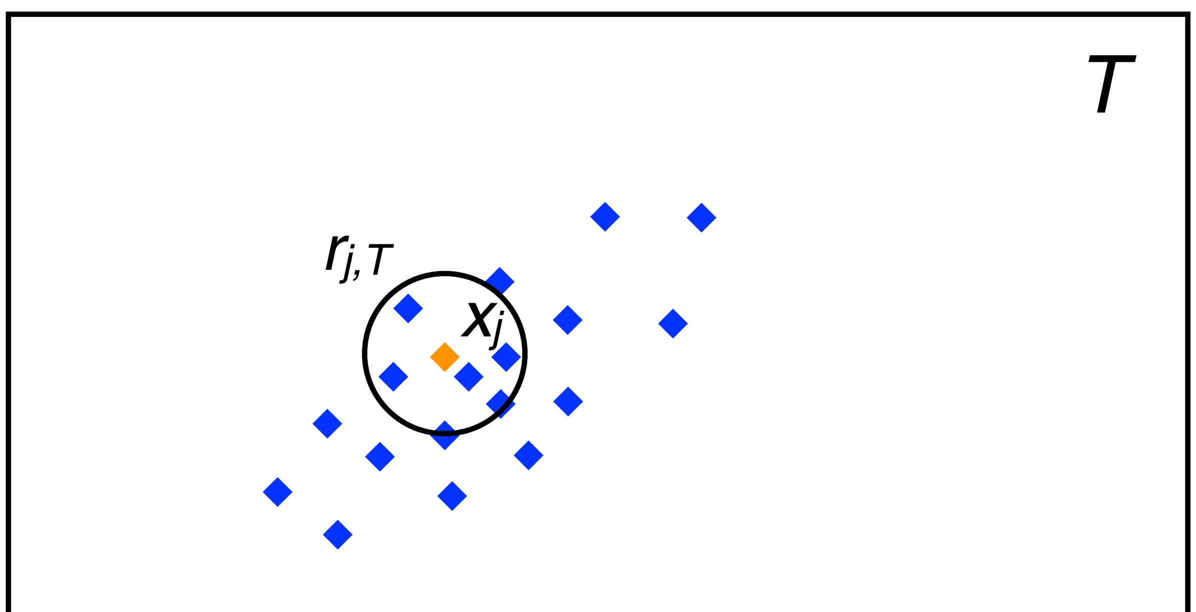
- Find the distance $r_{j,T}$ of the Kth-NN of x_j in T.

> 1. Density Estimator





- Fix integer K.
- Choose query point x_j in T and draw it in B.
- Find the distance $r_{j,B}$ of the Kth-NN of x_j in B.
- Find the distance $r_{j,T}$ of the Kth-NN of x_j in T.
- Estimate PDFs:

$$\hat{p}_B(\boldsymbol{x}_j) = \frac{K}{N_B} \frac{1}{\omega_D r_{j,B}^D}$$

$$\hat{p}_T(\boldsymbol{x}_j) = \frac{K}{N_T - 1} \frac{1}{\omega_D r_{j,T}^D}$$

> 2. Test Statistic

- Measure of the "distance" between 2 PDFs

- Define **Test Statistic**:
  (detect under-/over-densities)

$$\mathrm{TS}(\mathcal{T}) \equiv \frac{1}{N_T} \sum_{j=1}^{N_T} \log \frac{\hat{p}_T(\boldsymbol{x}_j)}{\hat{p}_B(\boldsymbol{x}_j)}$$

- Related to Kullback-Leibler divergence as: $\mathrm{TS}(\mathcal{T}) = \hat{D}_{\mathrm{KL}}(\hat{p}_T || \hat{p}_B)$

$$D_{\mathrm{KL}}(p||q) \equiv \int_{\mathbb{R}^D} p(\boldsymbol{x}) \log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})} d\boldsymbol{x}$$

- From NN-estimated PDFs: $\mathrm{TS}(\mathcal{T}) = \frac{D}{N_T} \sum_{j=1}^{N_T} \log \frac{r_{j,B}}{r_{j,T}} + \log \frac{N_B}{N_T - 1}$

- **Theorem:** this estimator converges to $D_{\mathrm{KL}}(p_B || p_T)$,
  in large sample limit

[Wang et al. - 2005,2006]

> 3. Test Statistic Distribution

How is TS distributed? **Permutation test!**

Assume p_B=p_T. Union set: $\mathcal{U} = \mathcal{T} \cup \mathcal{B} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N_T}, \boldsymbol{x}'_1, \ldots, \boldsymbol{x}_{N_B}\}$

for *n = 1* **to** N_{perm} **do**

- Random reshuffle (sample without replacement) *U*:

$$\mathcal{U}_n = \{\tilde{\boldsymbol{x}}_1, \ldots, \tilde{\boldsymbol{x}}_{N_T+N_B}\}$$

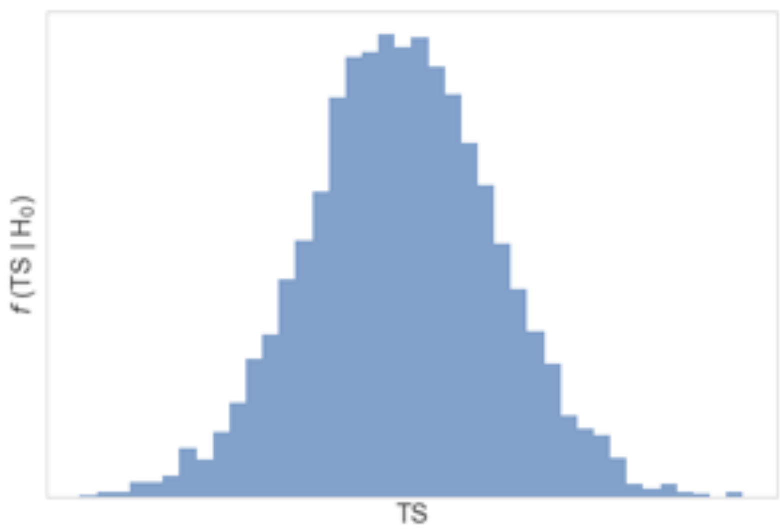
- Assign first N_B points to *B* and remaining points to *T*:

$$\tilde{\mathcal{B}} = \{\tilde{\boldsymbol{x}}_1, \ldots, \tilde{\boldsymbol{x}}_{N_B}\}$$
$$\tilde{\mathcal{T}} = \{\tilde{\boldsymbol{x}}_{N_B+1}, \ldots, \tilde{\boldsymbol{x}}_{N_B+N_T}\}$$

- Compute the test statistic TS_n on: $(\tilde{\mathcal{B}}, \tilde{\mathcal{T}})$

end for

Distribution of TS under H_0: $f(\mathrm{TS}|H_0) \leftarrow \{\mathrm{TS}_n\}$
[asymptotically normal with zero mean]



> 4. *p*-value

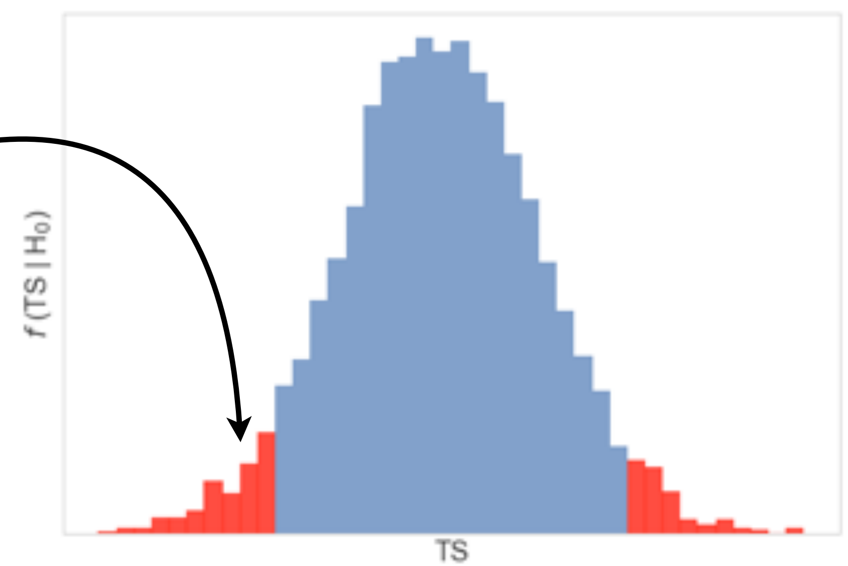
- $\hat{\mu}, \hat{\sigma}$: mean,variance of TS distribution $f(\mathrm{TS}|H_0)$

- Standardize the TS: $\mathrm{TS} \to \mathrm{TS}' \equiv \dfrac{\mathrm{TS} - \hat{\mu}}{\hat{\sigma}}$

- TS' distributed according to $f'(\mathrm{TS}'|H_0) = \hat{\sigma} f(\hat{\mu} + \hat{\sigma}\mathrm{TS}'|H_0)$

- Two-sided *p*-value:

$$p = 2\int_{|\mathrm{TS}'_{\mathrm{obs}}|}^{+\infty} f'(\mathrm{TS}'|H_0) d\mathrm{TS}'$$

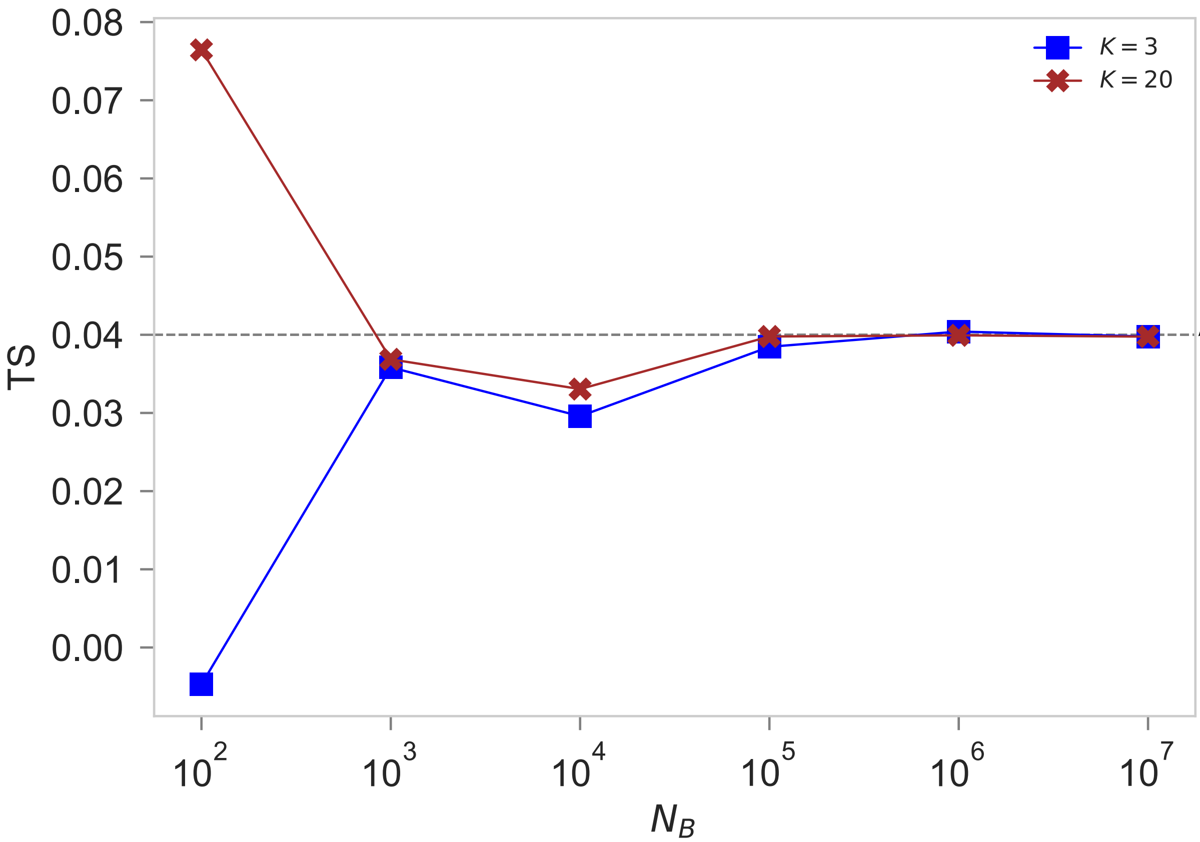


- Equivalent significance: $Z \equiv \Phi^{-1}(1 - p/2)$

> Gaussian Example

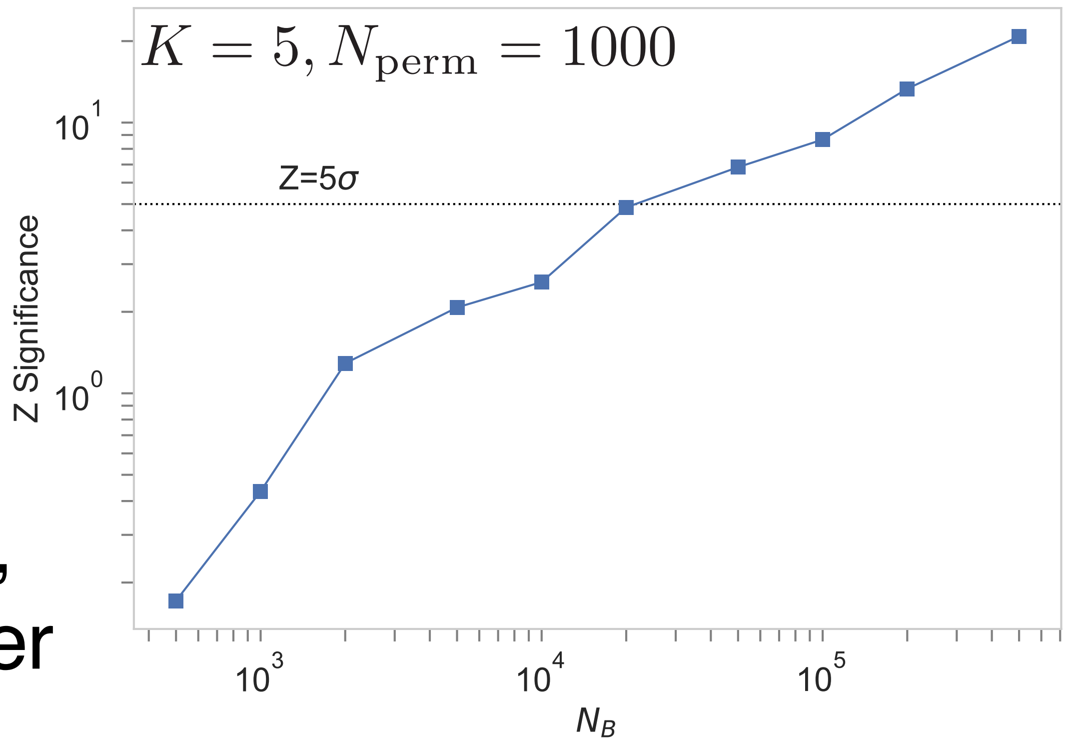
$$p_B = \mathcal{N}(\boldsymbol{\mu}_B, \Sigma_B) \qquad p_T = \mathcal{N}(\boldsymbol{\mu}_T, \Sigma_T) \qquad \Sigma_B = \Sigma_T = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\boldsymbol{\mu}_B = \begin{pmatrix} 1.0 \\ 1.0 \end{pmatrix} \qquad \boldsymbol{\mu}_T = \begin{pmatrix} 1.2 \\ 1.2 \end{pmatrix}$$



exact KL divergence

$$\boldsymbol{\mu}_B = \begin{pmatrix} 1.0 \\ 1.0 \end{pmatrix} \qquad \boldsymbol{\mu}_T = \begin{pmatrix} 1.15 \\ 1.15 \end{pmatrix}$$



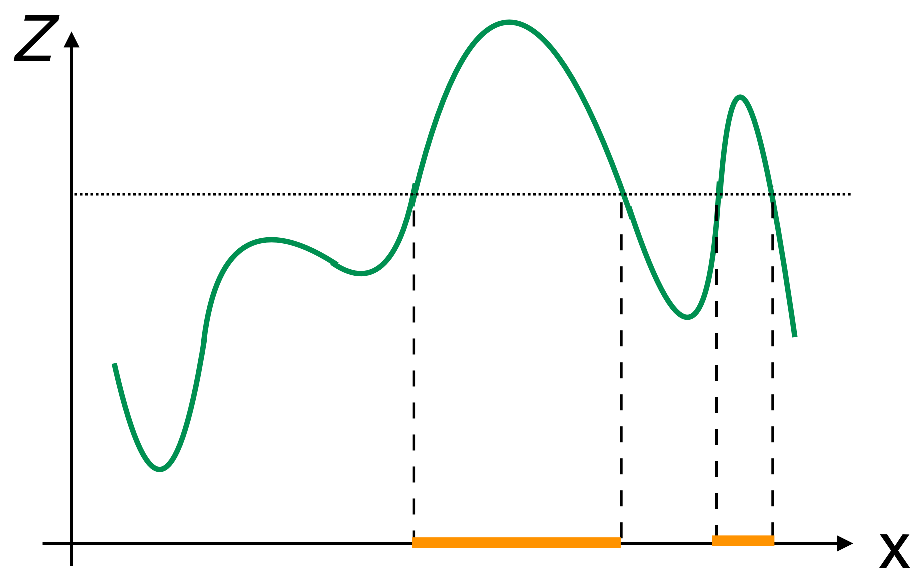
more data, more power

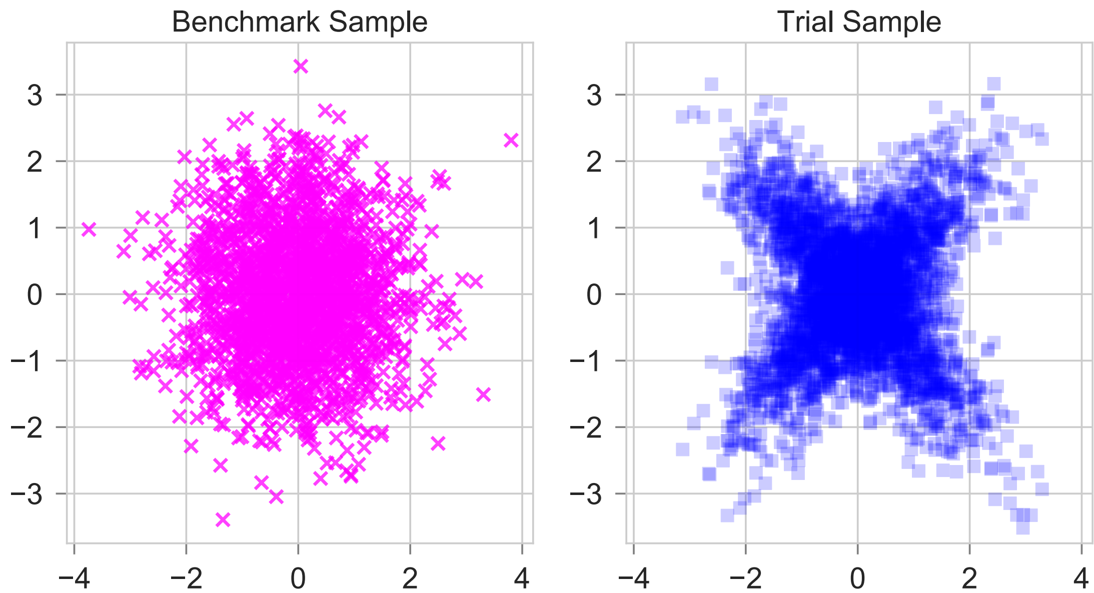
Bonus: Characterize regions with significant discrepancies

1. "Score" field over *T*: $Z(\boldsymbol{x}_j) \equiv \frac{u(\boldsymbol{x}_j) - \bar{u}}{\sigma_u}$

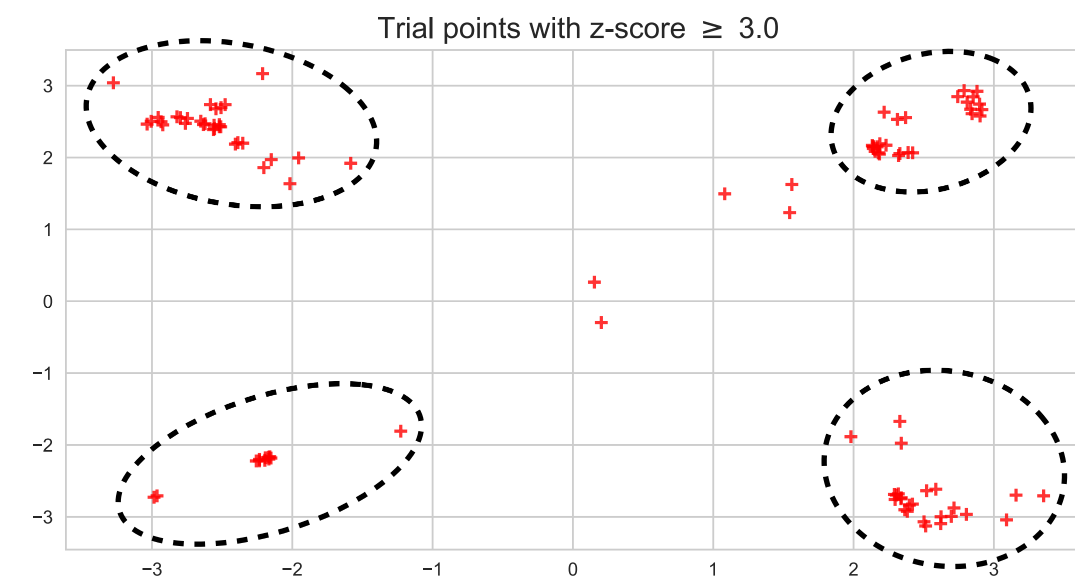
with: $u(\boldsymbol{x}_j) \equiv \log \frac{r_{j,B}}{r_{j,T}}$

$\mathrm{TS}_{\mathrm{obs}} = D\,\bar{u} + \mathrm{const}$





2. Identify points where $Z(\boldsymbol{x}) > c$
   They contribute the most to large $\mathrm{TS}_{\mathrm{obs}}$
   → high-discrepancy (anomalous) regions



3. Apply a clustering algorithm to group them

INPUT:

Trial sample: $\mathcal{T} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N_T}\} \overset{\text{iid}}{\sim} p_T$

Benchmark sample: $\mathcal{B} = \{\boldsymbol{x}'_1, \ldots, \boldsymbol{x}'_{N_B}\} \overset{\text{iid}}{\sim} p_B$

K: number of nearest neighbors

N_{perm}: number of permutations

$\boldsymbol{x}_i, \boldsymbol{x}'_i \in \mathbb{R}^D$

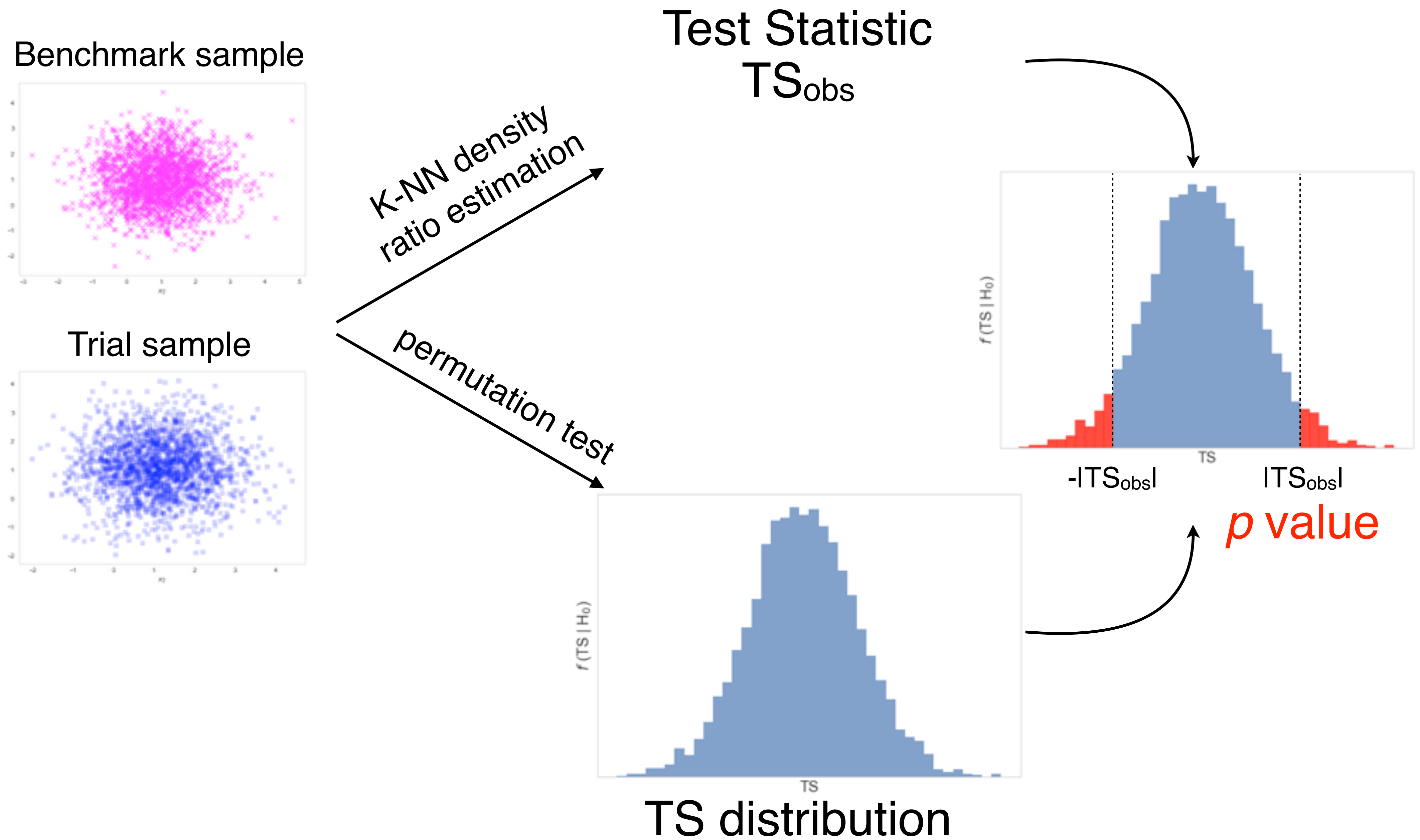
p_B, p_T unknown

OUTPUT:

p-value of the null hypothesis H_0: $p_B = p_T$

[check compatibility between 2 samples]

> NN2ST: Summary



[github.com/de-simone/NN2ST]

> NN2ST: Summary

- ✓ general, model-independent
- ✓ fast, no optimization
- ✓ sensitive to unspecified signals
- ✓ useful when no variable can separate sig/bkg
- ✓ helps finding signal regions, optimal cuts, …

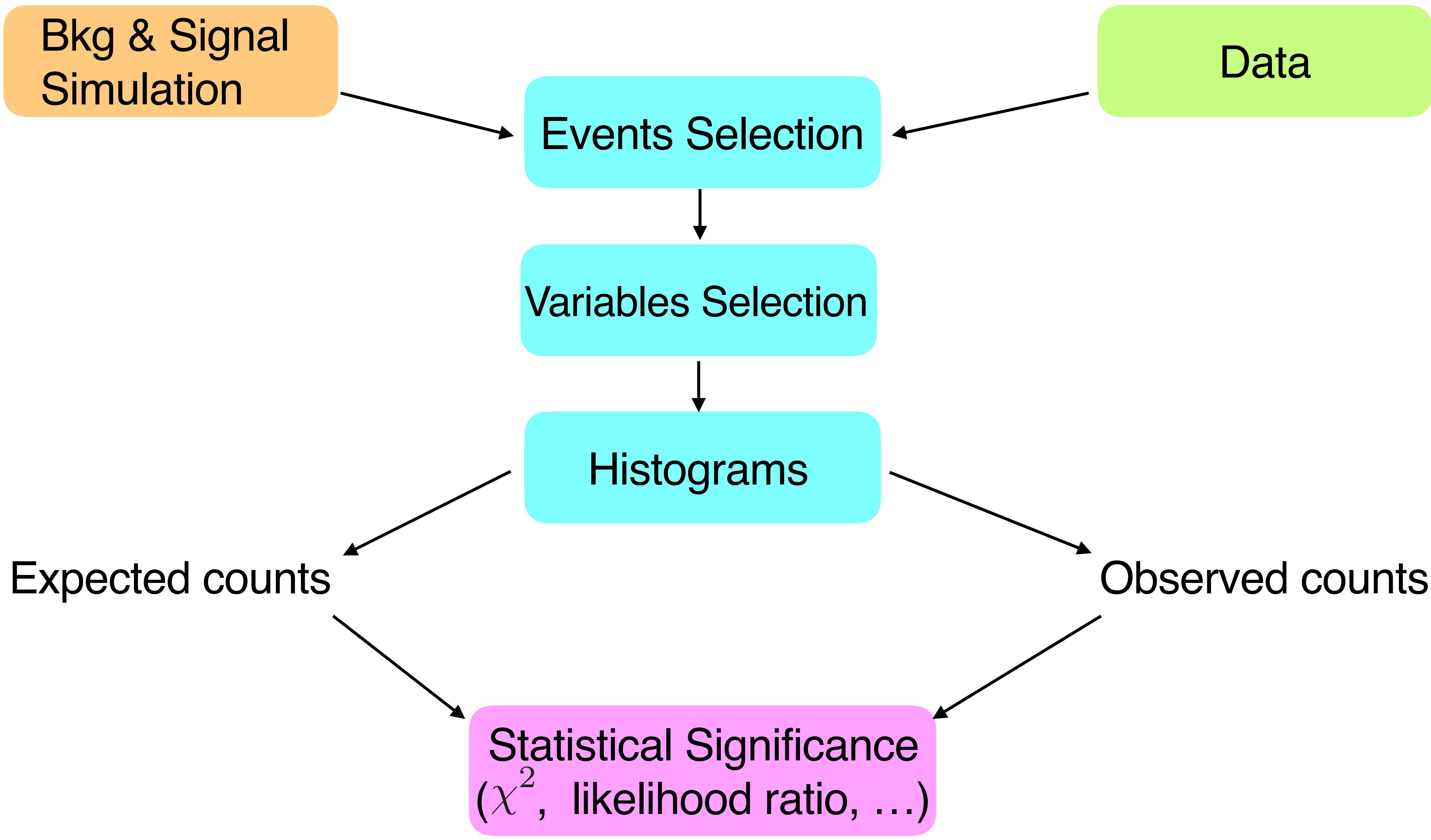
- ✘ need to run for each sample pair
- ✘ permutation test is bottleneck
- ✘ limited by sample accuracies

> Outline

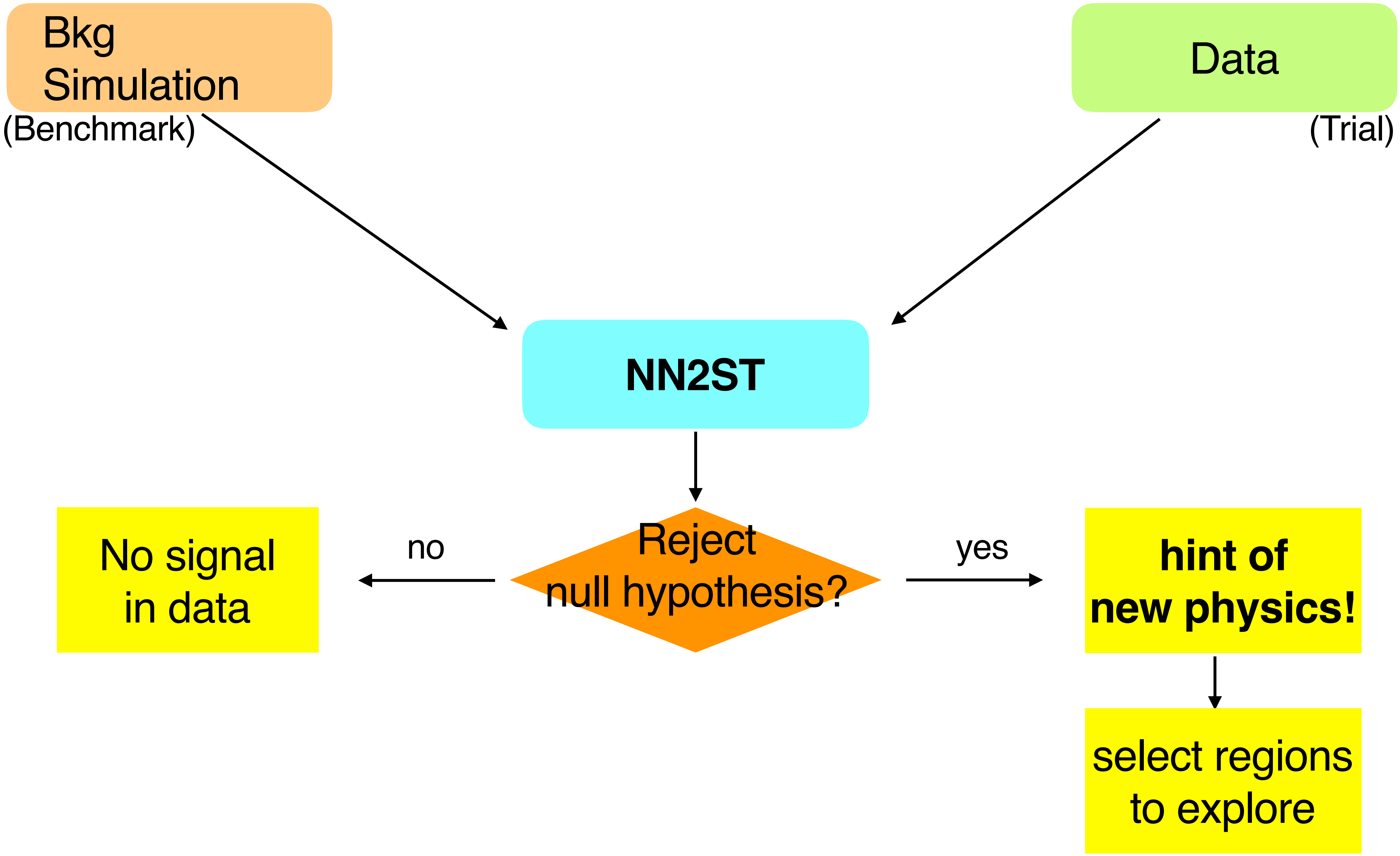
1. Statistical test of dataset compatibility

2. Applications to High-Energy Physics

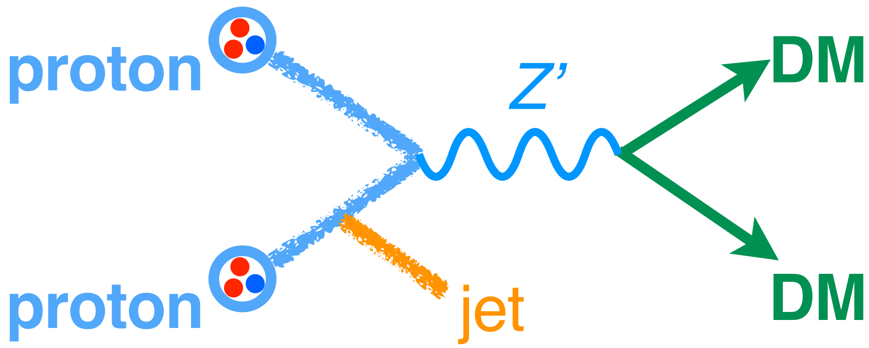
> Standard Analysis Pipeline



> Our Method

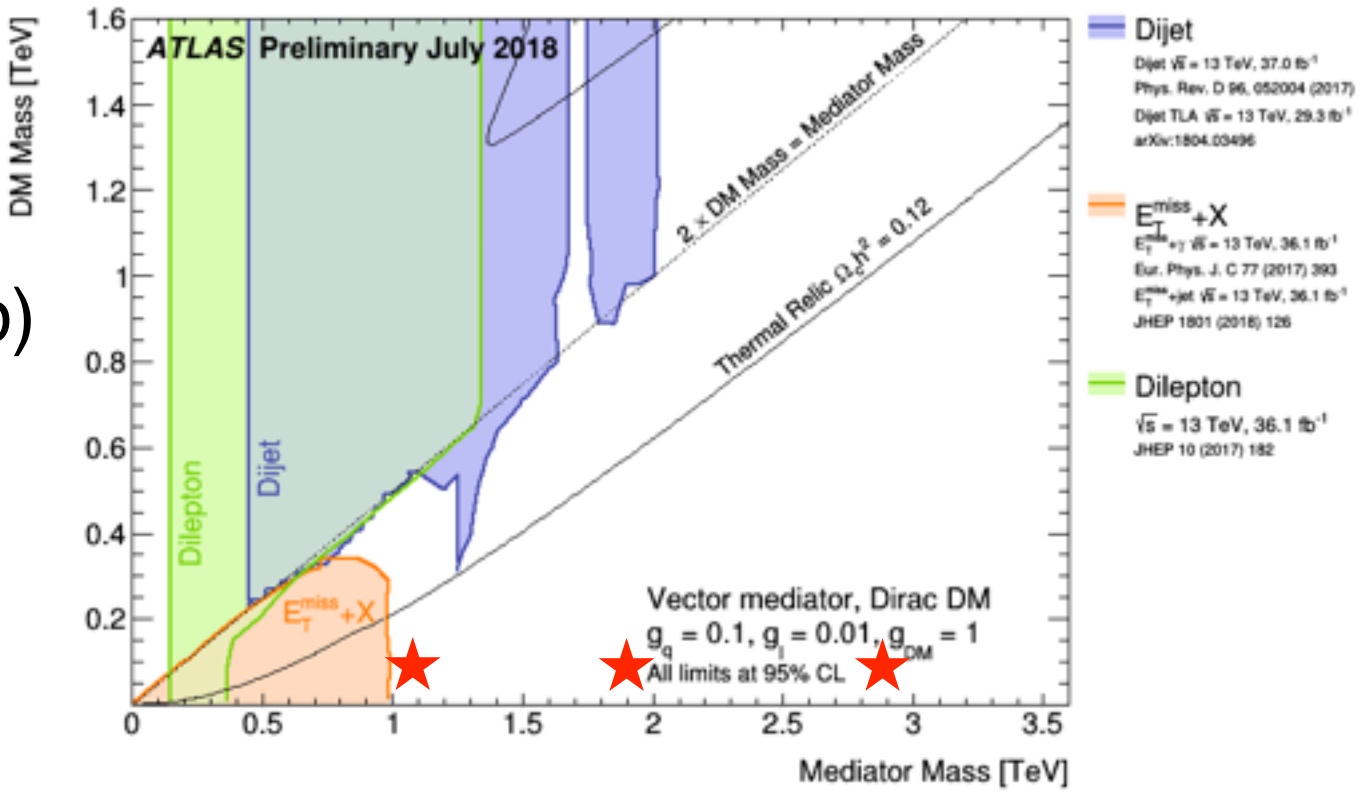

Bkg
Simulation
(Benchmark)
Data
(Trial)
NN2ST
Reject
null hypothesis?
no
No signal
in data
yes
hint of
new physics!
select regions
to explore

> DM search @ LHC



DM + Z'
vector mediator

m_{DM} = 100 GeV
$m_{Z'}$ = 1.2, 2, 3 TeV
g_{DM} = 1, g_q = 0.1
$\sqrt{s} = 13\ \mathrm{TeV}$



- "proof-of-principle" study
- bkg: $Z \to \nu\bar{\nu} + (1,2)\, j$ ($\sigma_{\rm bkg}$=202.6 pb)
  sub-leading bkgs not included
- no full detector effects
  (generic Delphes profile)

Benchmark: **$\mathbf{BKG_1}$**

Trials: **$\mathbf{BKG_2}$ + SIG**

$K = 5$

$N_{perm} = 3000$

8 features:

- n. of jets
- p_T, η of 2 leading jets
- $E_T^{\rm miss}, H_T$
- $\Delta\phi_{E_T^{\rm miss}, j_1}$

B: **BKG_1** (20k events)
T1: **BKG_2** (20k events) **+ SIG_1** (2010 events)
T2: **BKG_2** (20k events) **+ SIG_2** (375 events)
T3: **BKG_2** (20k events) **+ SIG_3** (59 events)

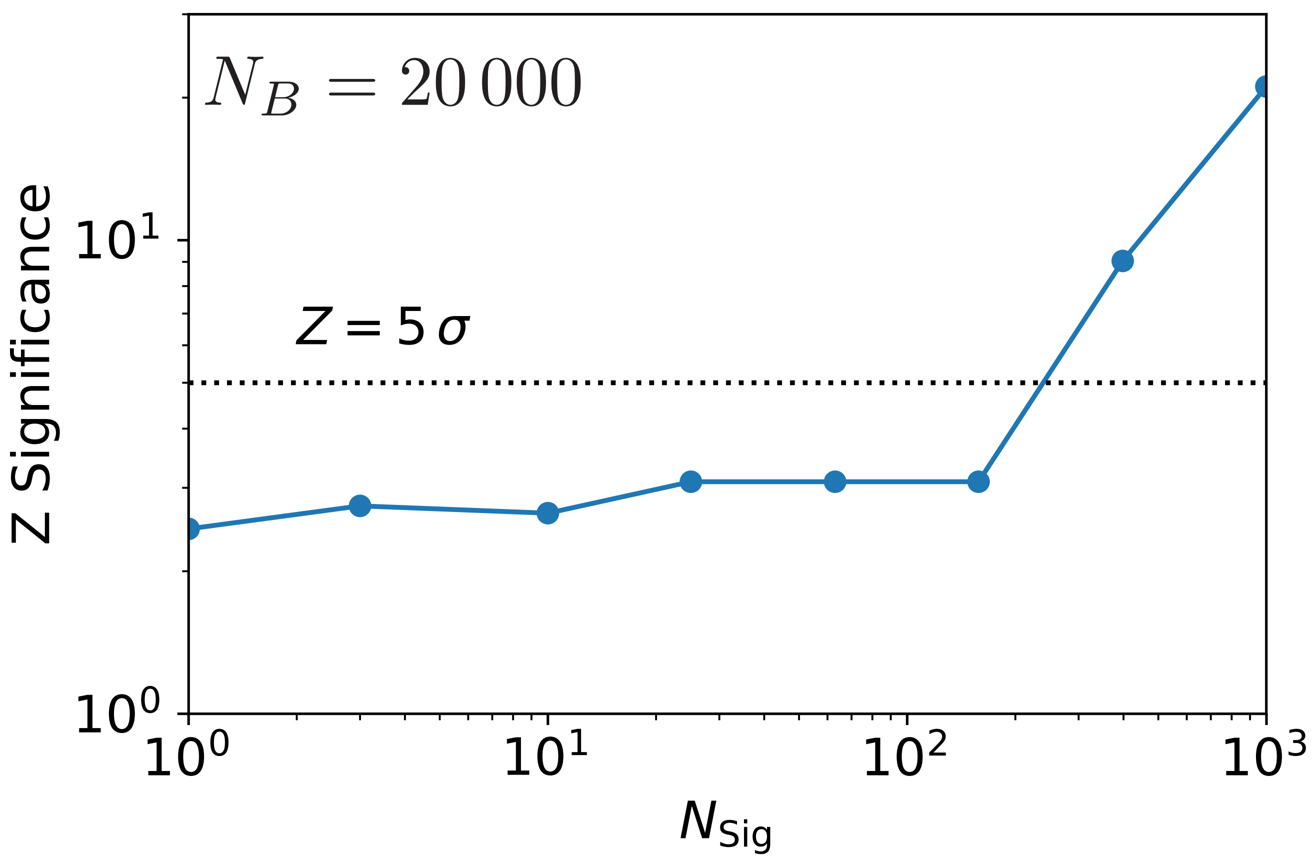
$$N_{\rm sig} = N_B \times \frac{\sigma_{\rm signal}}{\sigma_{\rm bkg}}$$

Sample	$M_{Z'}$	$\sigma_{\rm signal}$	Z
T1	1.2 TeV	20.4 pb	>15 σ
T2	2 TeV	3.8 pb	10 σ
T3	3 TeV	0.6 pb	0.13 σ

too good to be true!

- in real world: expect degradation of results (bkg uncert.)
- **the method has value, it is worth exploring**

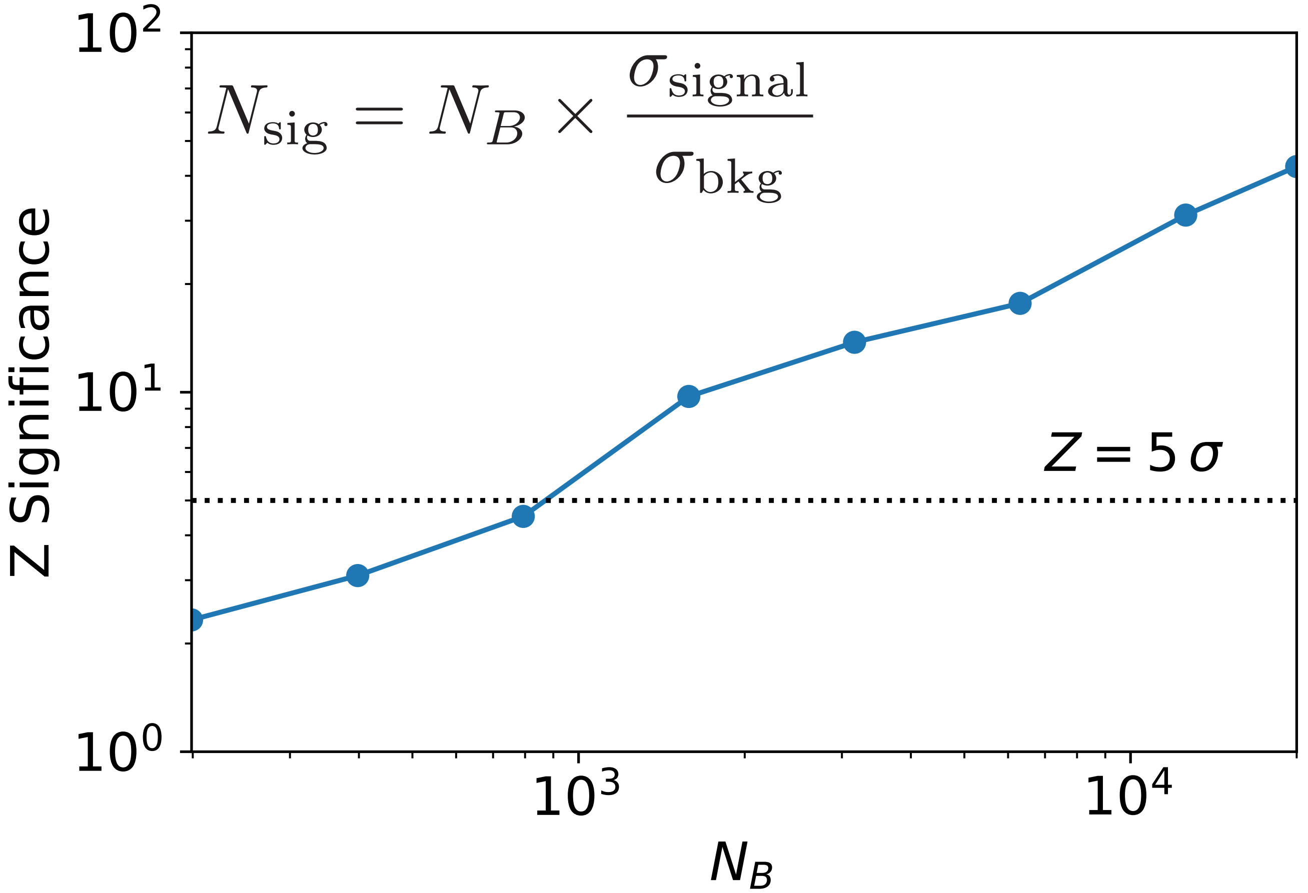
> DM search @ LHC



stronger signal
easier to discover

$$N_T = N_B + N_{\mathrm{sig}}$$

more data,
more power



> Outlook

Directions for future work:

- inclusion and impact of bkg uncertainties

- adaptive choice of K

- identifying discrepant regions in realistic situations
  (with Z-score method)

- validation tool for bkg:
  compatibility between MC sims. and data in control regions

- scalability

- … your suggestions?

> Take-Home Messages

1. New Statistical Test for BSM Physics

- assess degree of compatibility between 2 samples
- rooted on nearest-neighbors, solid math foundations

2. NN2ST as a discovery tool

- powerful and model-independent
- lots of applications

3. NN2ST to guide searches

- identify regions of discrepancies

BACK UP

> Model Selection

how to choose *K*? **Model Selection!**

True: $r(\boldsymbol{x}) = \dfrac{p_T(\boldsymbol{x})}{p_B(\boldsymbol{x})}$ Estimated: $\hat{r}(\boldsymbol{x}) = \dfrac{\hat{p}_T(\boldsymbol{x})}{\hat{p}_B(\boldsymbol{x})}$

Define the mean-square error:

$$\begin{aligned} L(r,\hat{r}) &= \frac{1}{2}\int \left[\hat{r}(\boldsymbol{x}') - r(\boldsymbol{x}')\right]^2 p_B(\boldsymbol{x}')d\boldsymbol{x}' \\ &= \frac{1}{2}\int \hat{r}(\boldsymbol{x}')^2 p_B(\boldsymbol{x}')d\boldsymbol{x}' - \int \hat{r}(\boldsymbol{x})p_T(\boldsymbol{x})d\boldsymbol{x} + \frac{1}{2}\int r(\boldsymbol{x}')^2 p_B(\boldsymbol{x}')d\boldsymbol{x}' \end{aligned}$$

Estimate loss: $\hat{L}(r,\hat{r}) = \dfrac{1}{2N_B}\displaystyle\sum_{\boldsymbol{x}'\in\mathcal{B}} \hat{r}(\boldsymbol{x}')^2 - \dfrac{1}{N_T}\sum_{\boldsymbol{x}\in\mathcal{T}} \hat{r}(\boldsymbol{x})$

Select optimal *K* minimizing the loss.

Alternatively: Point-Adaptive k-NN (PAk) [1802.10549]