

LEARNING NEW PHYSICS FROM DATA: A SYMMETRIZED APPROACH

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INBAR SAVORAY

UC Berkeley & Lawrence Berkeley National Lab

IN COLLABORATION WITH: SHIKMA BRESSLER AND YUVAL ZURGIL

Weizmann Institute of Science

MOTIVATION

- Despite great theoretical and experimental effort, no evidence of New Physics has been found to date.
- Many dedicated searches ruled out a significant portion of the parameter space of theoretically motivated models.
- However, there is still much more to explore:
 - New theoretical models.
 - A lot of data.



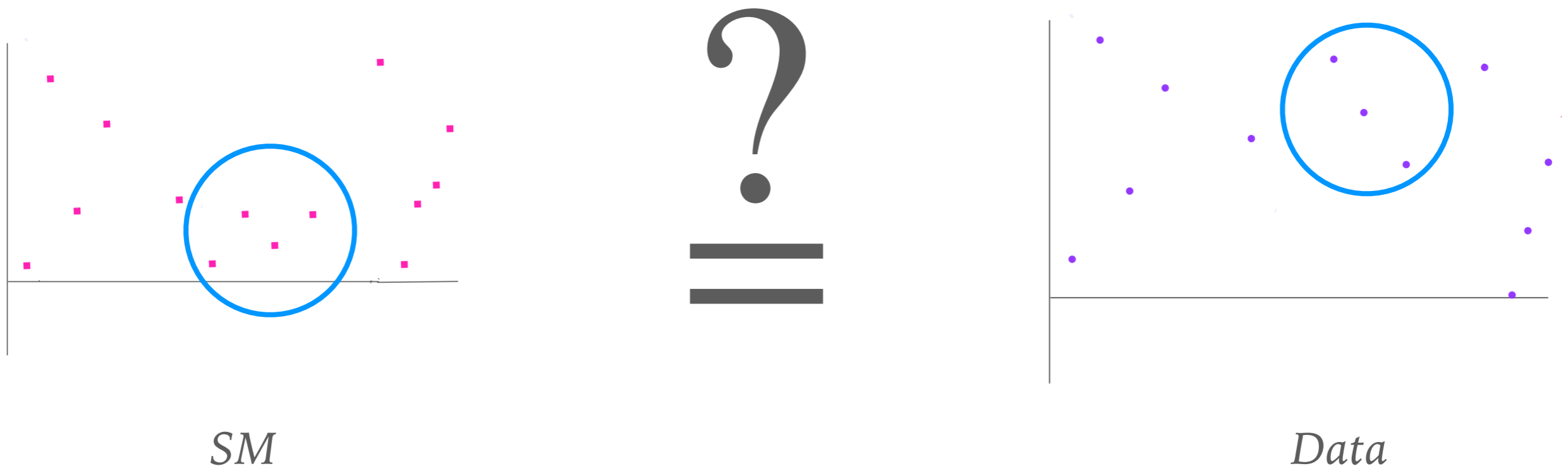
404. That's an error.

The requested URL /newphysics was not found on this server. That's all we know.



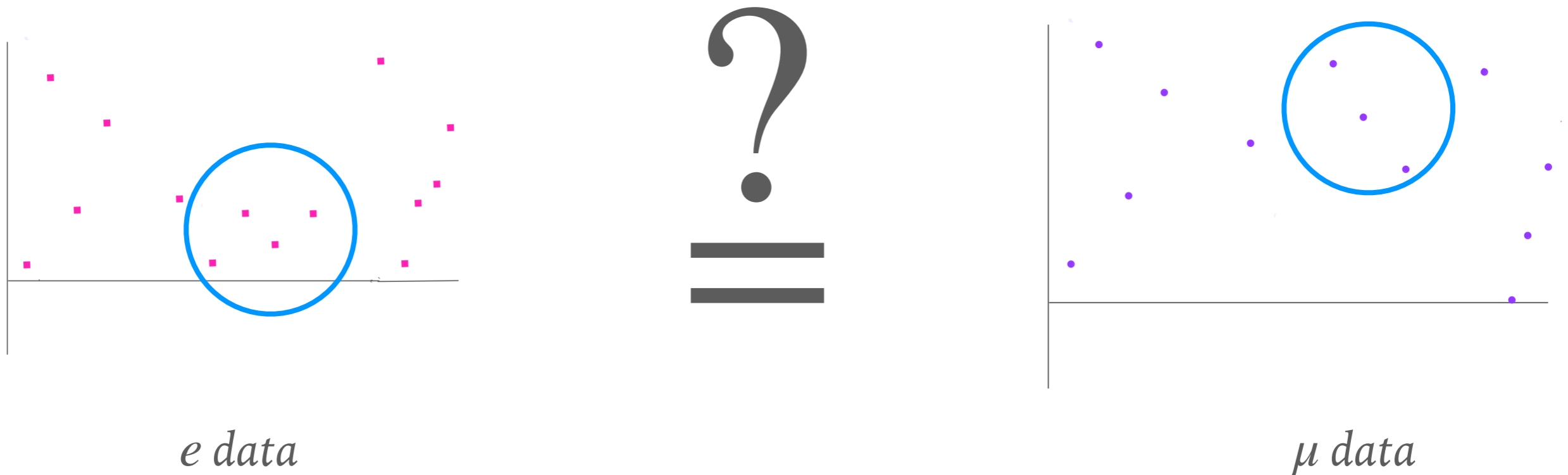
MODEL AGNOSTIC SEARCHES

- **Data-directed paradigm (DDP)** for model agnostic searches:
 - Search for deviations from SM properties (what we do know).
 - Scan the data efficiently.
 - Identify anomalous regions for detailed study.



MODEL AGNOSTIC SEARCHES

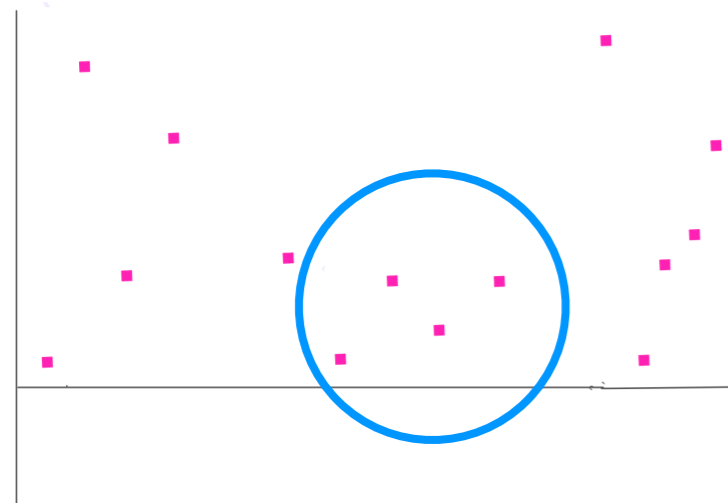
- **SM symmetries** imply relations between different regions of the data, that if violated could point to NP.
- Example - **lepton flavor universality**: $e/\mu/\tau$ should be **interchangeable** (up to H+phase space).
- (Hints: neutrino masses + B-anomalies)



GOAL

- Efficiently scan data for asymmetries between samples that should only differ by statistical fluctuations.
- Model-independent interpretation: minimal assumptions, no detailed simulations (SM&NP).

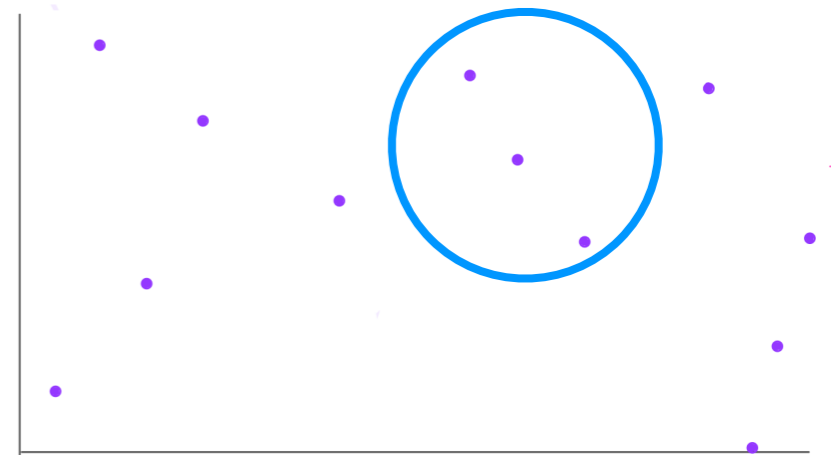
Fast & Robust



e data

?

≡



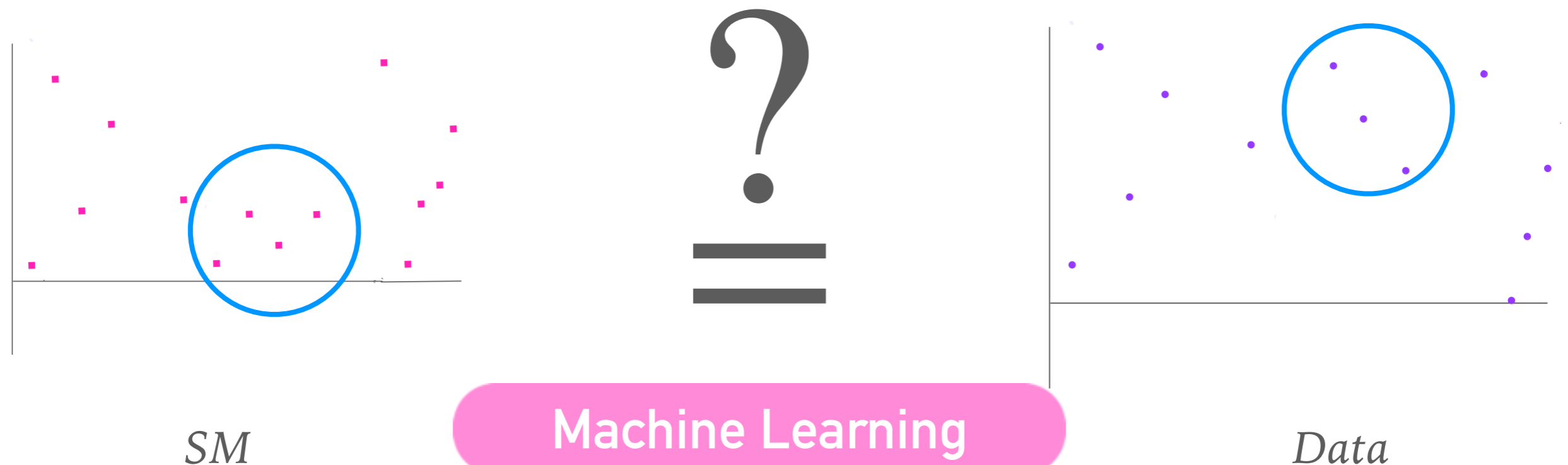
μ data

Flexible

METHOD

- Previous proposal - **“Learning NP from a Machine” (NPLM)**
R. T. D’Agnolo & A. Wulzer, [1806.02350].
- Testing whether an observed dataset is distributed according to a much larger reference SM sample.

Likelihood ratio test



METHOD

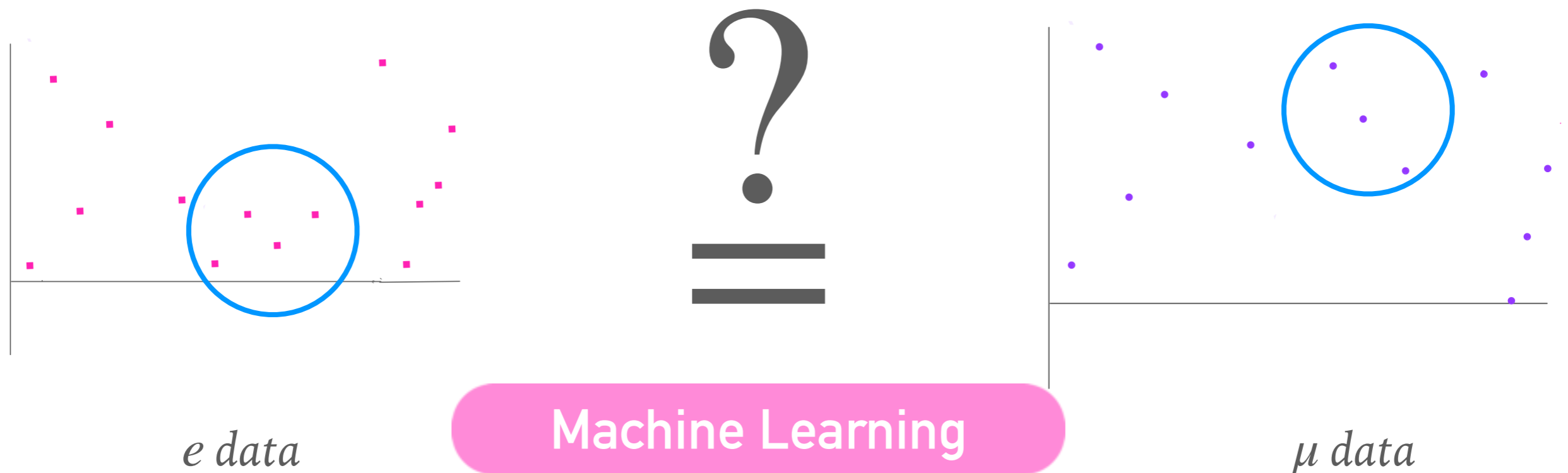
- Previous proposal - **“Learning NP from a Machine” (NPLM)**

R. T. D’Agnolo & A. Wulzer, [1806.02350].

- Testing whether an observed dataset is distributed according to a much larger reference SM sample.

Can it be implemented for small asymmetry searches?

Likelihood ratio test



LIKELIHOOD 101

- Likelihood - probability of obtaining result x had θ been true:

$$\mathcal{L}(\theta | x) = p(x | \theta)$$

- Model fitting
- Hypothesis testing

LIKELIHOOD 101 – MODEL FITTING

- Likelihood - probability of obtaining result x had θ been true:

$$\mathcal{L}(\theta | x) = p(x | \theta)$$

- The model in which the probability of obtaining the observed is the highest is the most likely (MLE)

$$\text{MLE: } \hat{\theta} = \operatorname{argmax} (\mathcal{L} (\theta | x_{\text{obs}}))$$

- Likelihood always maximal if prediction=observed.
- If something occurred, it cannot have zero probability.

LIKELIHOOD 101 - MODEL FITTING

- Likelihood - probability of obtaining result x had θ been true:

$$\mathcal{L}(\theta | x) = p(x | \theta)$$

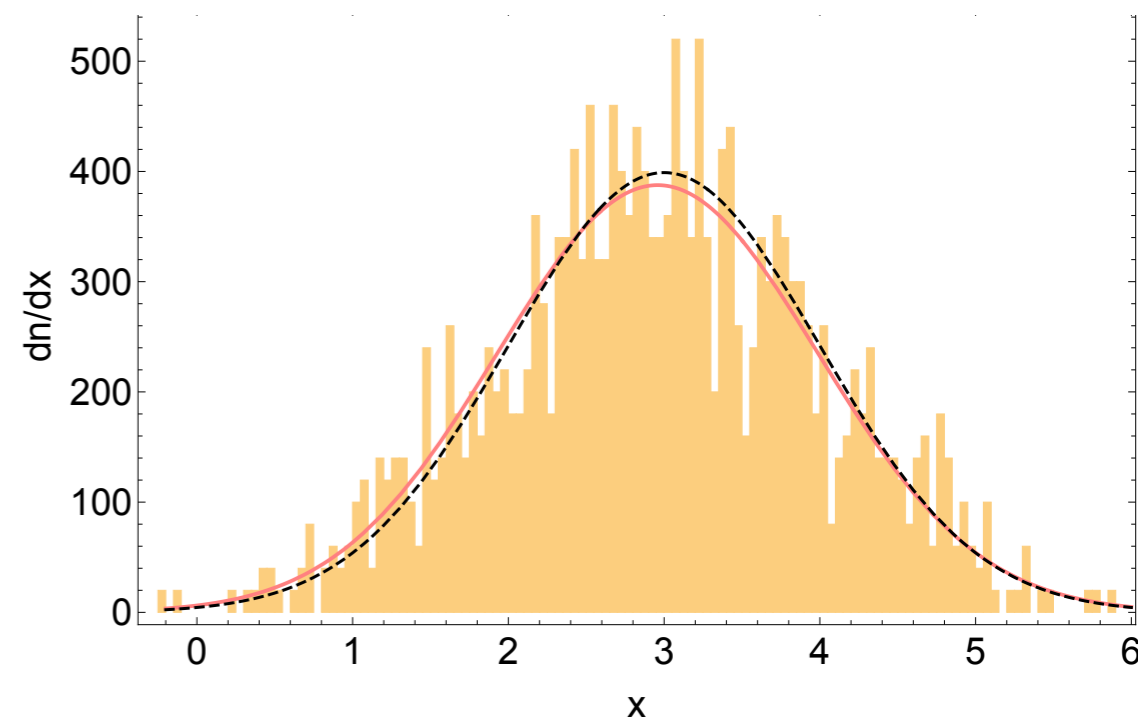
- The model in which the probability of obtaining the observed is the highest is the most likely (MLE)

$$\text{MLE: } \hat{\theta} = \operatorname{argmax} (\mathcal{L} (\theta | x_{\text{obs}}))$$

- Example: Gaussian PDF $\{x_0, \sigma\} = \theta$

$$\mathcal{L} (x_0, \sigma | x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\sum_i (x_i - x_0)^2}{2\sigma^2}}$$

$$\text{MLE: } \hat{x}_0 = \bar{x}, \hat{\sigma} = \sqrt{\frac{1}{N} \sum_i (x_i - \bar{x})^2}.$$

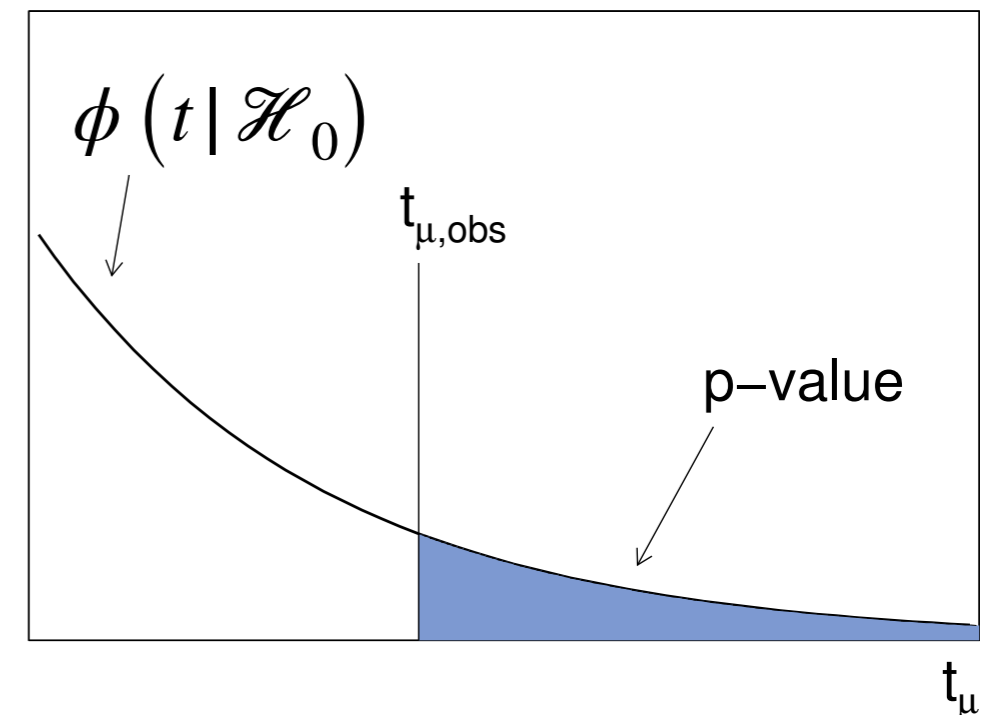


LIKELIHOOD 101 – HYPOTHESES TESTING

- Maximum profile likelihood test of $\mathcal{H}_0 (\mu_0, \nu)$ vs. $\mathcal{H}_1 (\mu, \nu)$

$$t_{\text{obs}} = 2 \log \left(\frac{\max_{\mu, \nu} (\mathcal{L} (\mathcal{H}_1 | x_{\text{obs}}))}{\max_{\nu} (\mathcal{L} (\mathcal{H}_0 | x_{\text{obs}}))} \right) \quad \begin{array}{l} \text{SM+NP} \\ \text{SM} \end{array}$$

- Optimal according to the Neyman-Pearson Lemma.
- Generate toy datasets $\{x_{\text{toy}}\}$ from \mathcal{H}_0
- Find the distribution of t
- Calculate p-value for rejecting \mathcal{H}_0



LIKELIHOOD 101 – HYPOTHESES TESTING

- Maximum profile likelihood test of $\mathcal{H}_0 (\mu_0, \nu)$ vs. $\mathcal{H}_1 (\mu, \nu)$

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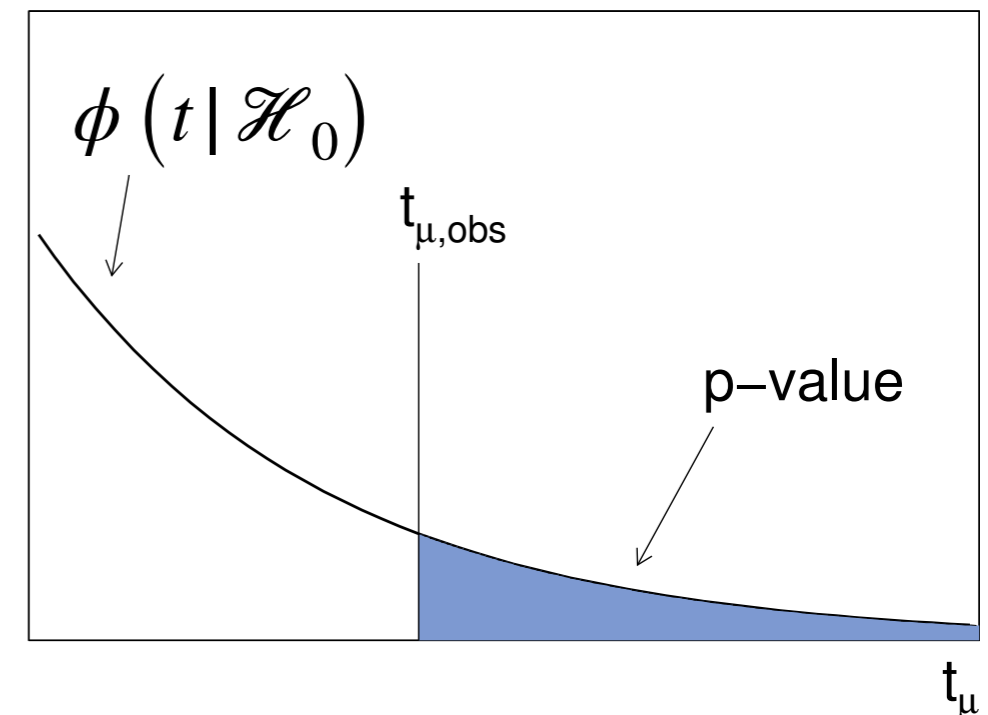
- Optimal according to the Neyman-Pearson Lemma.

- **Asymptotic null-distribution** -
for high enough statistics known
regardless of underlying model:

$$\phi (t | \mathcal{H}_0) \rightarrow \chi_n^2 ,$$

$n = \# \text{dof}$ NP

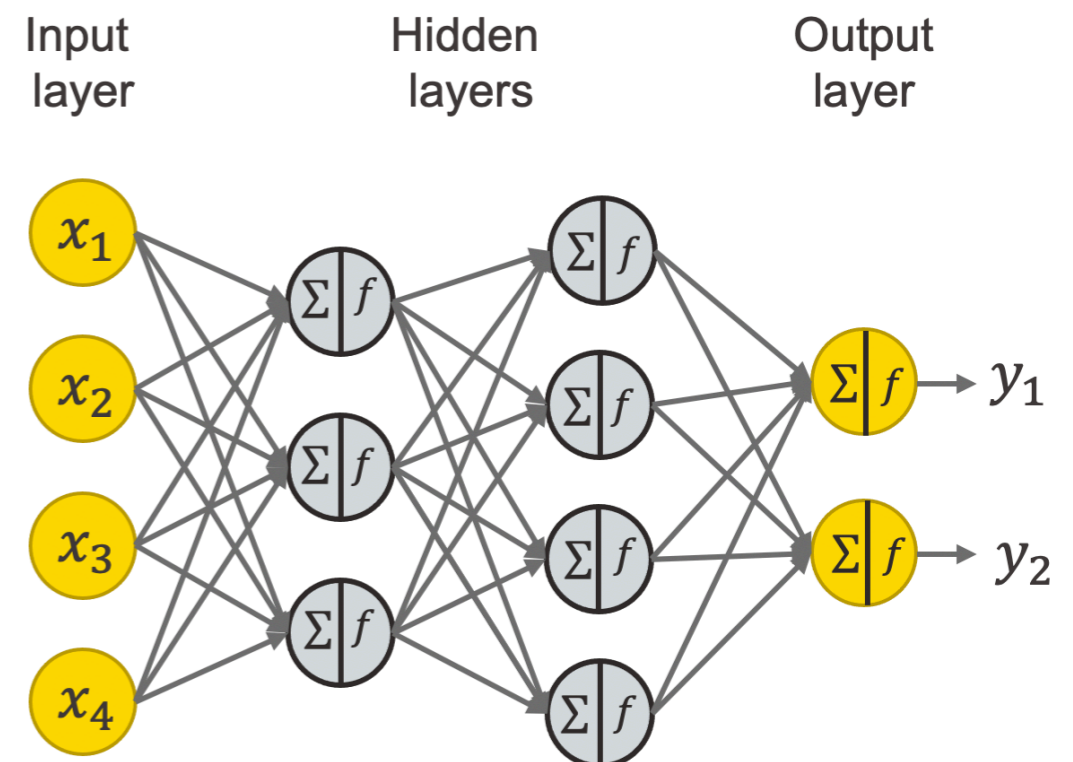
Fast & Robust



MACHINE LEARNING 101

- A family of functions - **expressive, universal approximators**
- Neural Network (NN) - a specific family of functions.
- Training - NN parameters θ found by minimizing some “loss”.

Flexible

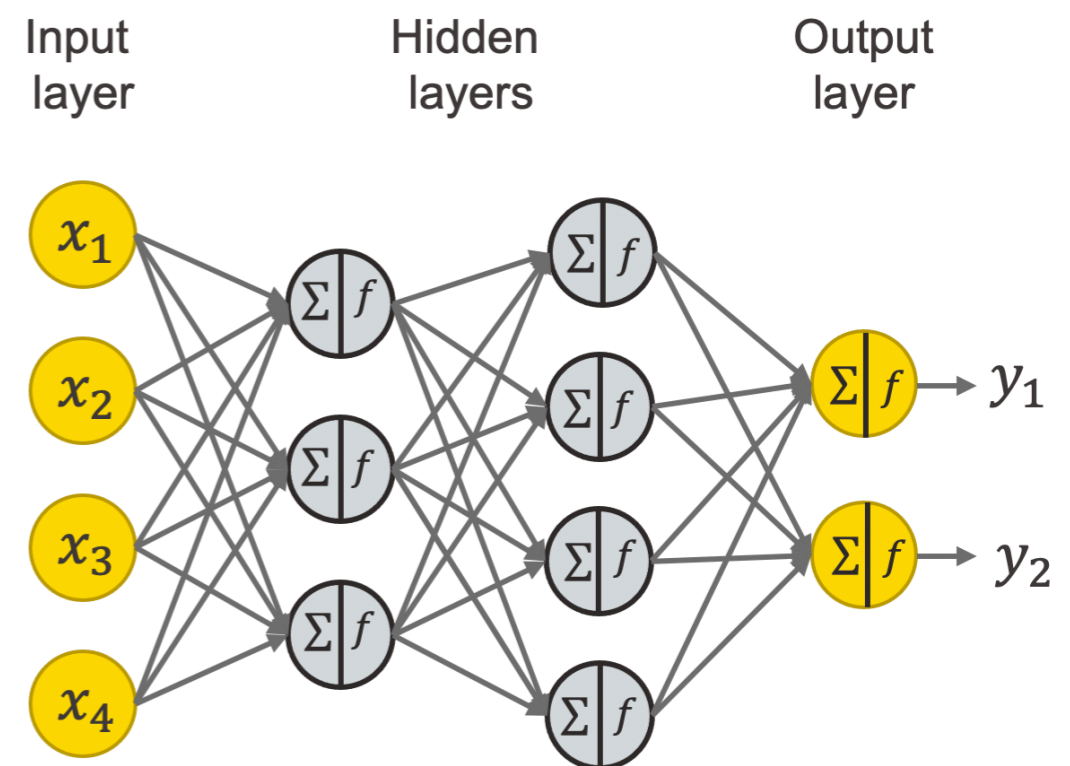


MACHINE LEARNING 101

- A family of functions - **expressive, universal approximators**
- Neural Network (NN) - a specific family of functions.
- Training - NN parameters θ found by minimizing some “loss”.
 - $p(x | \theta) = \mathcal{L}(\mathcal{H}(\theta) | x)$ given by the output of a NN.
 - NN loss = $-\mathcal{L}(\mathcal{H}(\theta) | x_{\text{obs}})$.

$$t_{\text{obs}} = 2 \log \left(\frac{\max_{\mu, \nu} \left(\mathcal{L}(\mathcal{H}_1 | x_{\text{obs}}) \right)}{\max_{\nu} \left(\mathcal{L}(\mathcal{H}_0 | x_{\text{obs}}) \right)} \right)$$

Flexible



NPLM

- Determine if sample \mathbf{A} is drawn from SM or $SM+NP$ distribution.

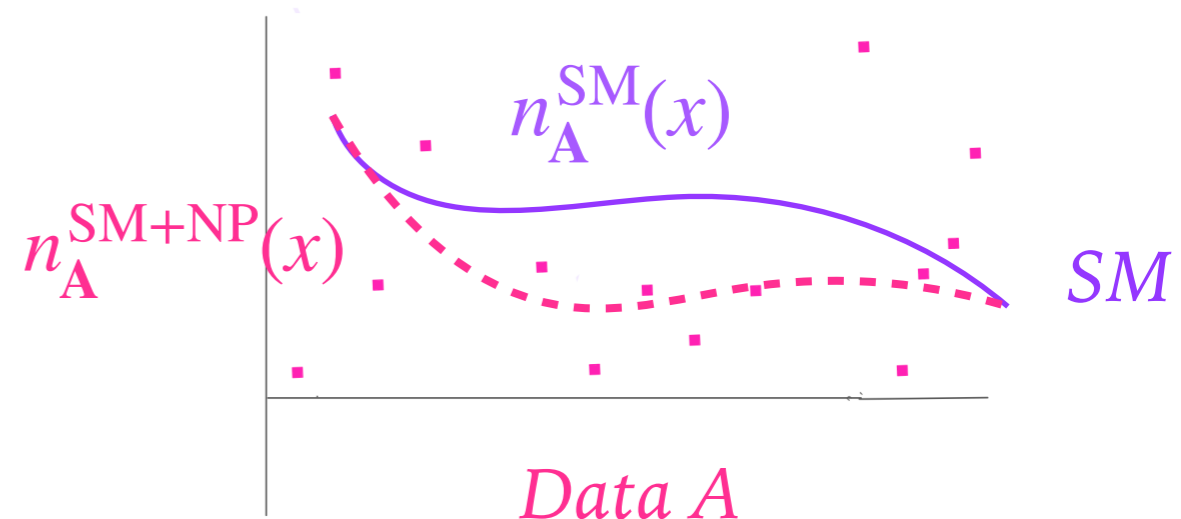
$$\mathcal{H}_0 : n_{\mathbf{A}}(x) = n_{\mathbf{A}}^{SM}(x) , \quad \mathcal{H}_1 : n_{\mathbf{A}}(x) = n_{\mathbf{A}}^{SM+NP}(x) ,$$

- Profile likelihood test $n(x) = Np(x)$

$$t = 2 \log \left(\frac{\max \left(\mathcal{L} \left(\mathcal{H}_1 | \mathbf{A} \right) \right)}{\max \left(\mathcal{L} \left(\mathcal{H}_0 | \mathbf{A} \right) \right)} \right) ,$$

- Poisson likelihood:

$$\mathcal{L} \left(\mathcal{H} | \mathbf{A} \right) = \frac{e^{-N_{\mathbf{A}}(\mathcal{H})}}{\tilde{N}_{\mathbf{A}}!} \prod_{x \in \mathbf{A}} n_{\mathbf{A}}(x | \mathcal{H}) .$$



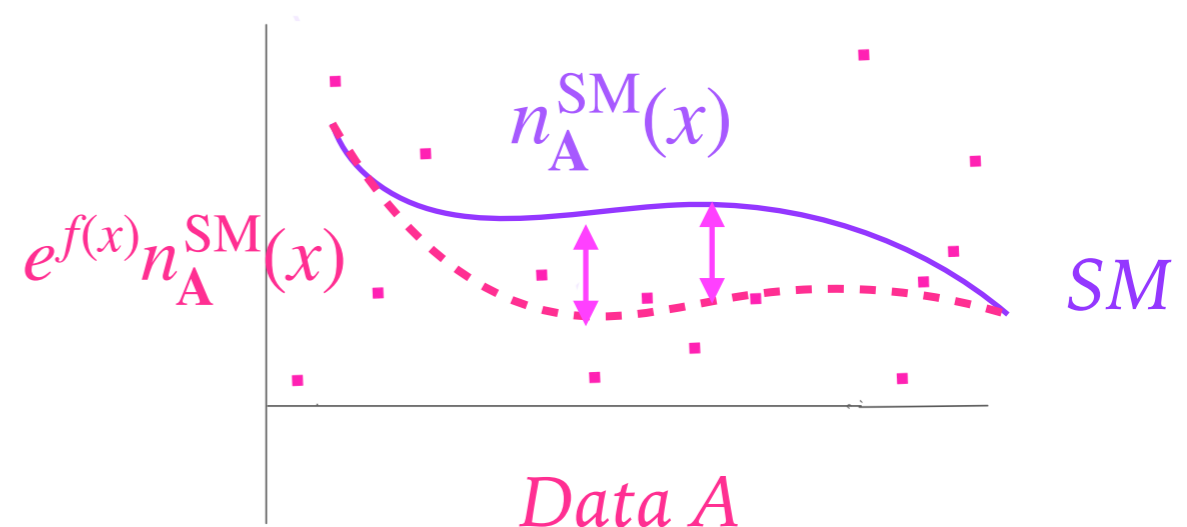
NPLM

- Determine if sample \mathbf{A} is drawn from SM or $SM+NP$ distribution.

$$\mathcal{H}_0 : n_{\mathbf{A}}(x) = n_{\mathbf{A}}^{SM}(x) , \quad \mathcal{H}_1 : n_{\mathbf{A}}(x) = e^{f(x)} n_{\mathbf{A}}^{SM}(x) ,$$

- Profile likelihood test

$$t = 2 \left(- \int \left(e^{\hat{f}(x)} - 1 \right) \hat{n}_{\mathbf{A}}^{SM}(x) dx + \sum_{x \in \mathbf{A}} \hat{f}(x) \right) \quad \text{NP: } f(x) \text{ is an output of a NN maximizing } t$$



NPLM

- Determine if sample **A** is drawn from **SM** or **SM+NP** distribution.

$$\mathcal{H}_0 : n_{\mathbf{A}}(x) = n_{\mathbf{A}}^{\text{SM}}(x) , \quad \mathcal{H}_1 : n_{\mathbf{A}}(x) = e^{f(x)} n_{\mathbf{A}}^{\text{SM}}(x) ,$$

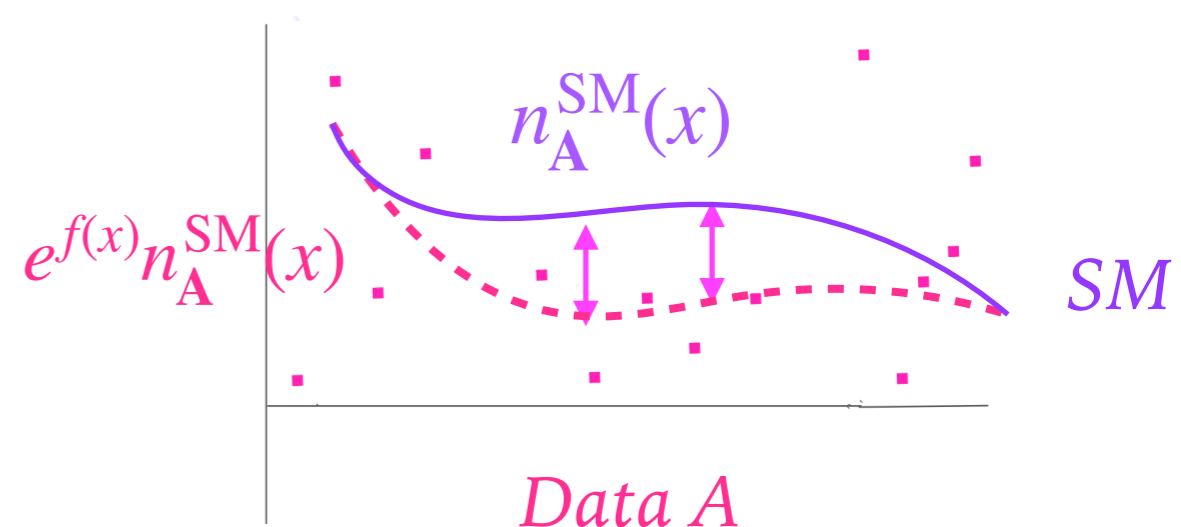
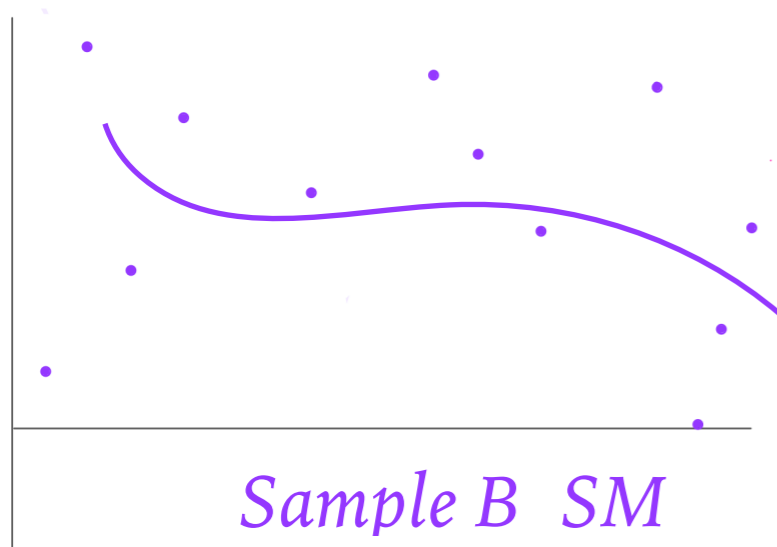
- Profile likelihood test

*SM: fit from
control
sample B*

$$t = 2 \left(- \int \left(e^{\hat{f}(x)} - 1 \right) \hat{n}_{\mathbf{A}}^{\text{SM}}(x) dx + \sum_{x \in \mathbf{A}} \hat{f}(x) \right)$$

*NP: $f(x)$ is an
output of a NN
maximizing t*

- SM dist. given by large sample **B** drawn from it, $\tilde{N}_{\mathbf{B}} \gg \tilde{N}_{\mathbf{A}}$



NPLM

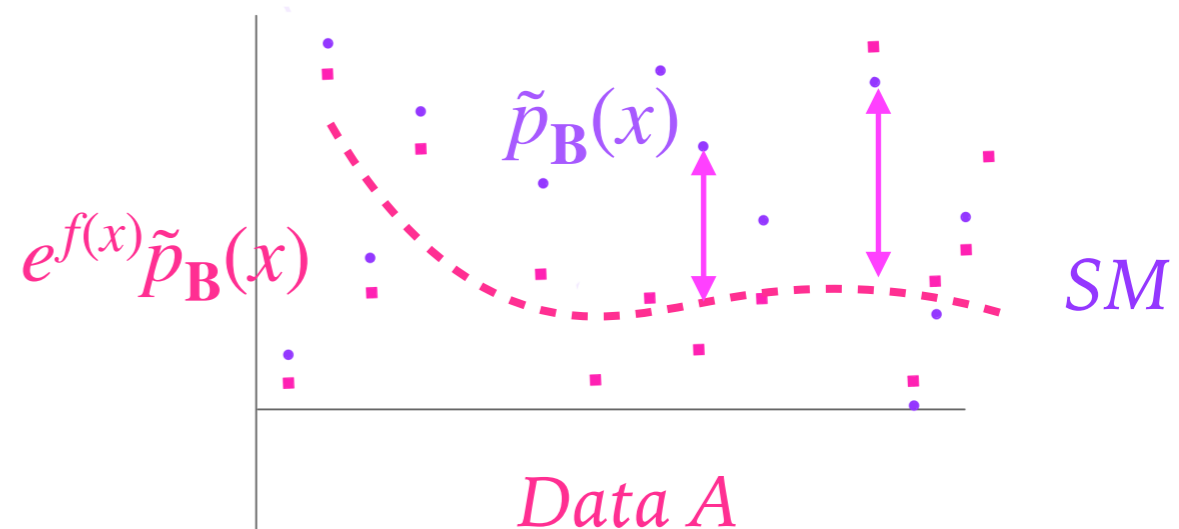
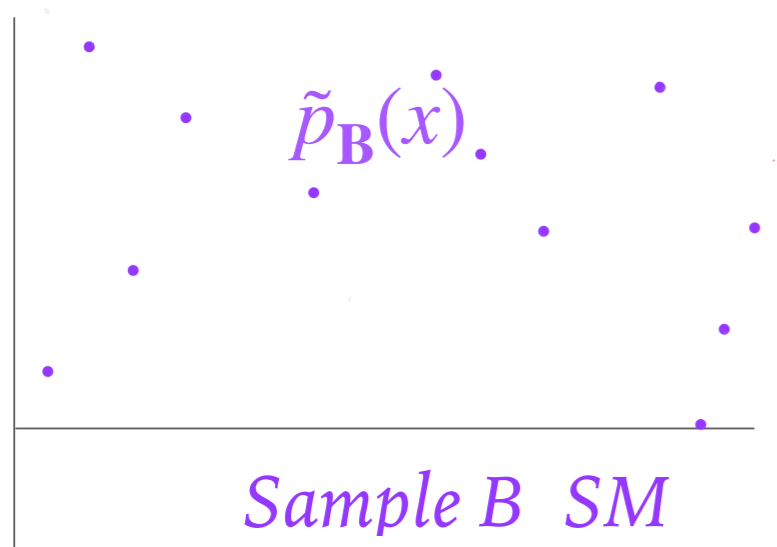
- Determine if sample **A** is drawn from **SM** or **SM+NP** distribution.

$$\mathcal{H}_0 : n_{\mathbf{A}}(x) = N_{\mathbf{A}} \tilde{p}_{\mathbf{B}}(x), \quad \mathcal{H}_1 : n_{\mathbf{A}}(x) = e^{f(x)} N_{\mathbf{A}} \tilde{p}_{\mathbf{B}}(x),$$

- Profile likelihood test

SM: empiric observation B $t = 2 \left(-\frac{N_{\mathbf{A}}}{\tilde{N}_{\mathbf{B}}} \sum_{x \in \mathbf{B}} \left(e^{\hat{f}(x)} - 1 \right) + \sum_{x \in \mathbf{A}} \hat{f}(x) \right)$ *NP: $f(x)$ is an output of a NN maximizing t*

- SM dist. represented by large sample **B** drawn from it, $\tilde{N}_{\mathbf{B}} \gg \tilde{N}_{\mathbf{A}}$



NPLM

- Profile likelihood test loss

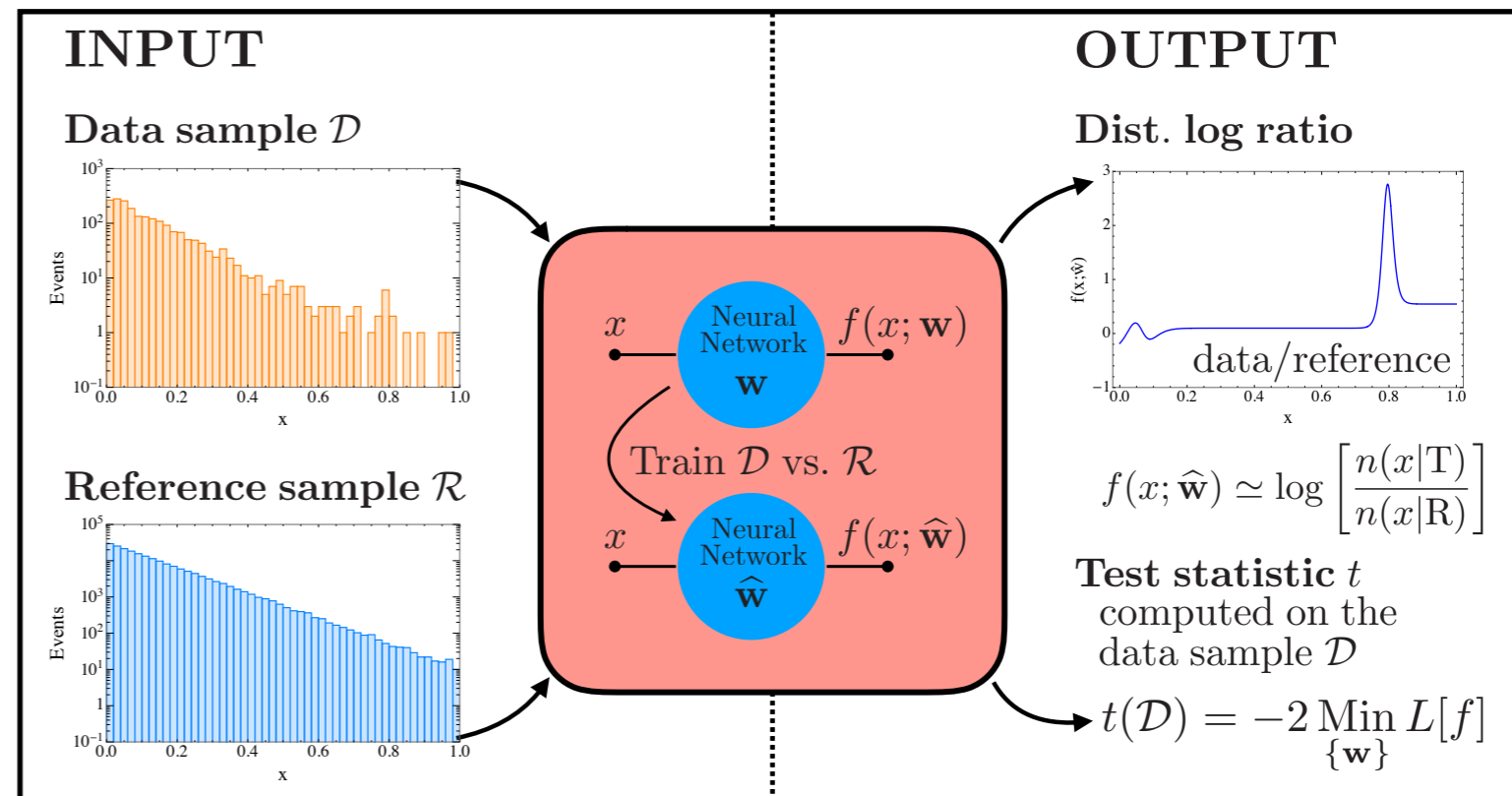
SM: empiric observation B

$$L = - \left(-\frac{N_A}{\tilde{N}_B} \sum_{x \in B} \left(e^{\hat{f}(x)} - 1 \right) + \sum_{x \in A} \hat{f}(x) \right)$$

NP: $f(x)$ is an output of a NN minimizing L

- Interpretation:

- **NP:** deviations of $f(x)$ from zero
- **Significance:** p-value of obtained $t = -2L$

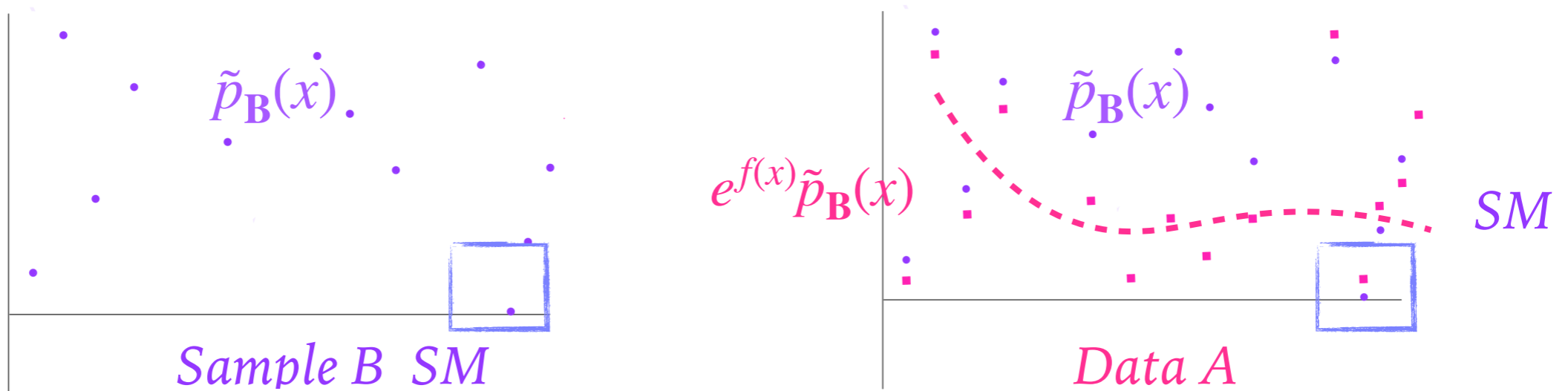


NPLM CHALLENGES: SEVERE WEIGHT-CLIPPING

- Unbounded loss

$$L = - \left(-\frac{N_A}{\tilde{N}_B} \sum_{x \in B} \left(e^{\hat{f}(x)} - 1 \right) + \sum_{x \in A} \hat{f}(x) \right)$$

- For $x_\star \in (A - A \cap B)$, if $f(x_\star) \rightarrow \infty$ then $L \rightarrow -\infty$.



NPLM CHALLENGES: SEVERE WEIGHT-CLIPPING

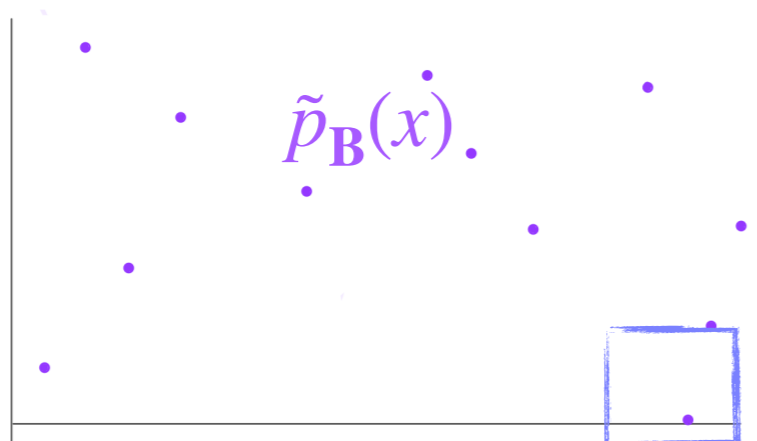
- Unbounded loss

$$L = - \left(-\frac{N_{\mathbf{A}}}{\tilde{N}_{\mathbf{B}}} \sum_{x \in \mathbf{B}} \left(e^{\hat{f}(x)} - 1 \right) + \sum_{x \in \mathbf{A}} \hat{f}(x) \right)$$

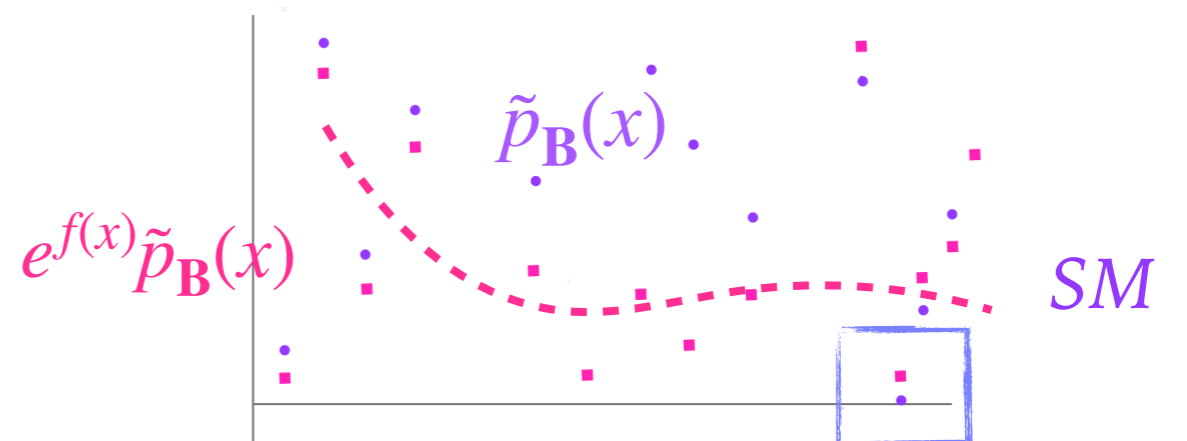
- For $x_{\star} \in (\mathbf{A} - \mathbf{A} \cap \mathbf{B})$, if $f(x_{\star}) \rightarrow \infty$ then $L \rightarrow -\infty$.

- This is a result of a false null-hypothesis.

$$\begin{aligned} \mathcal{H}_1 : \quad n_{\mathbf{A}}(x_{\star}) &= e^{f(x_{\star})} N_{\mathbf{A}} \tilde{p}_{\mathbf{B}}(x_{\star}), \\ \mathcal{H}_0 : \quad n_{\mathbf{A}}(x_{\star}) &= N_{\mathbf{A}} \tilde{p}_{\mathbf{B}}(x_{\star}) = 0, \end{aligned} \quad t = 2 \log \left(\frac{\max(\mathcal{L}(\mathcal{H}_1 | \mathbf{A}))}{\max(\mathcal{L}(\mathcal{H}_0 | \mathbf{A})) = 0} \right)$$



Sample B SM



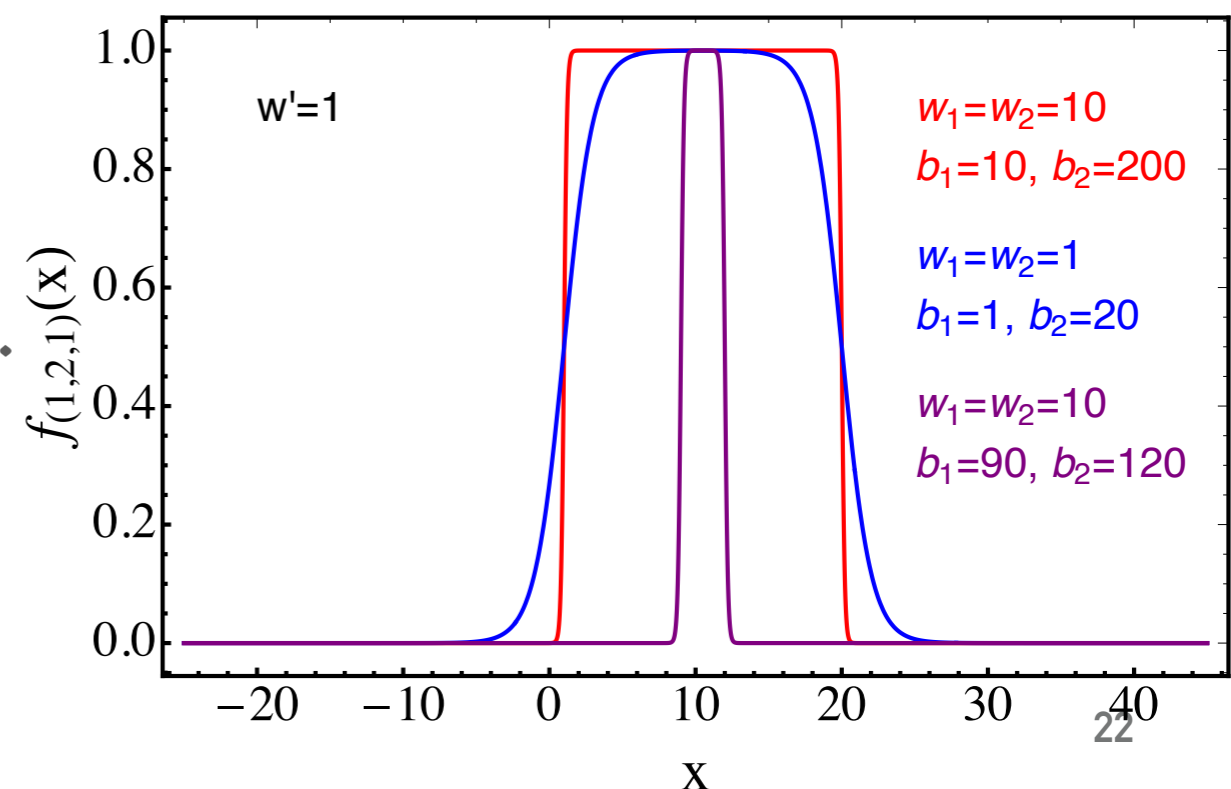
Data A

NPLM CHALLENGES: SEVERE WEIGHT-CLIPPING

- Unbounded loss

$$L = - \left(-\frac{N_A}{\tilde{N}_B} \sum_{x \in B} \left(e^{\hat{f}(x)} - 1 \right) + \sum_{x \in A} \hat{f}(x) \right)$$

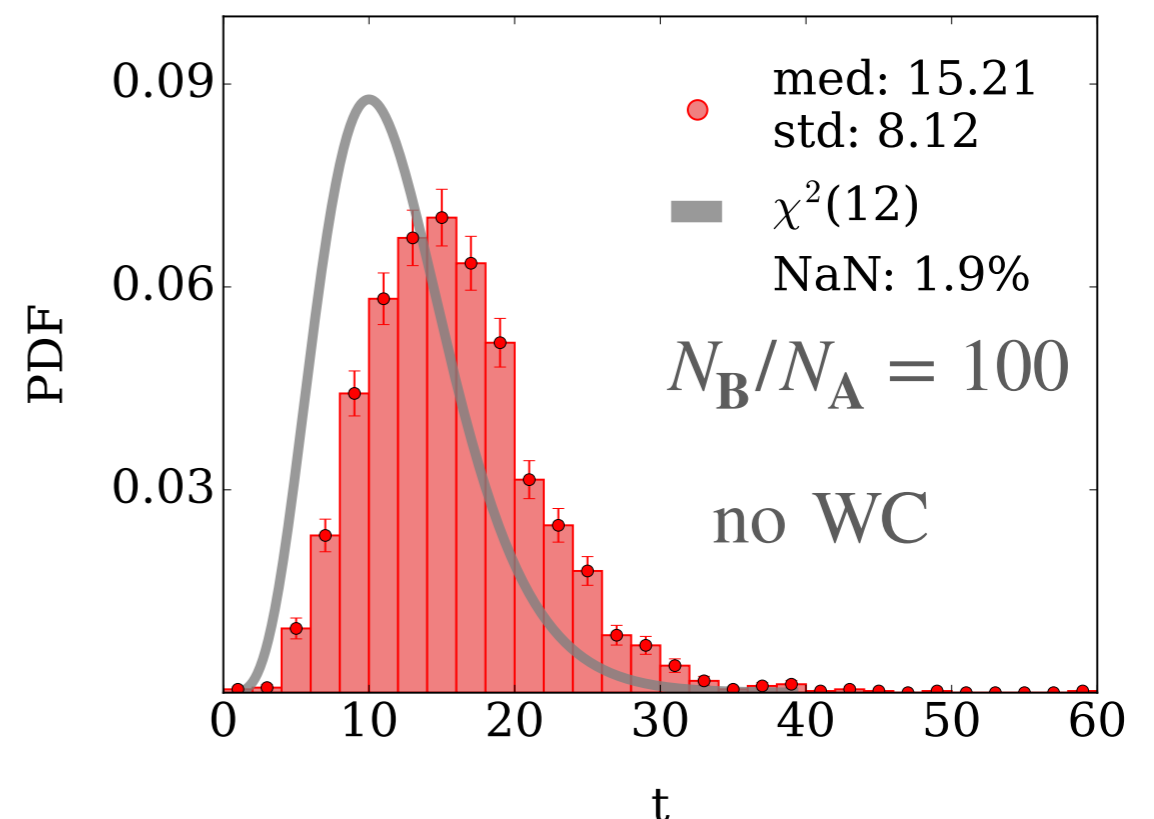
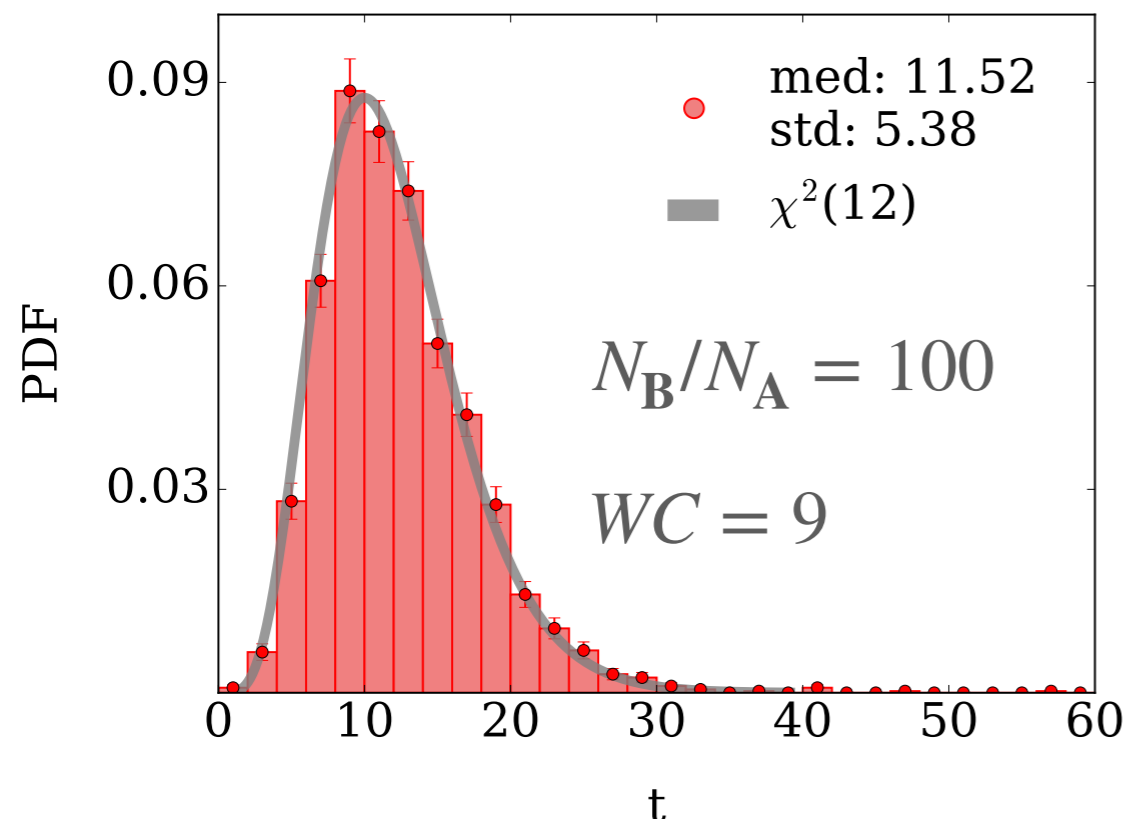
- For $x_\star \in (A - A \cap B)$, if $f(x_\star) \rightarrow \infty$ then $L \rightarrow -\infty$.
- Weight-clipping - setting a max for NN weights (\sim gradients).
 - Not allow divergences on small scales $\Delta x \leq 1/W$.
 - Smooth out local fluctuations.



NPLM CHALLENGES: SEVERE WEIGHT-CLIPPING

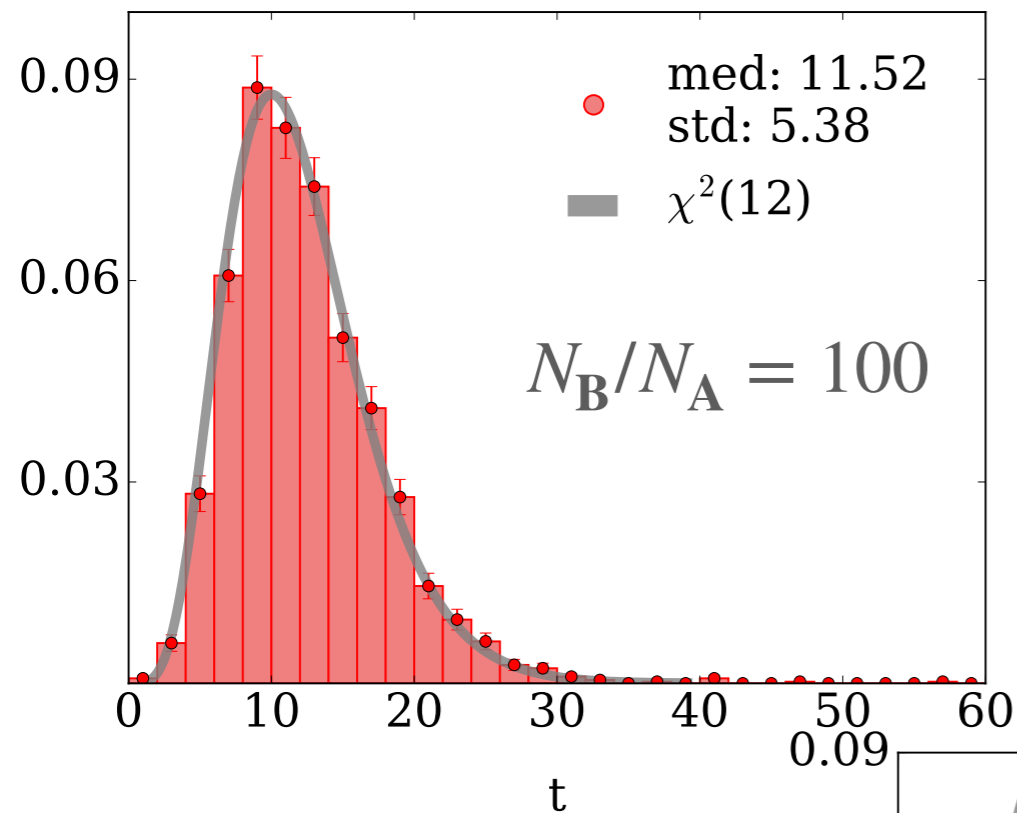
- Weight-clipping - setting a max for NN weights (\sim gradients).
- Determined to reach the asymptotic distribution and avoid divergences.
- **Costly optimization process.**
- **The stricter the WC, the less flexible the NN.**

χ_n^2 predicted
for likelihood
test

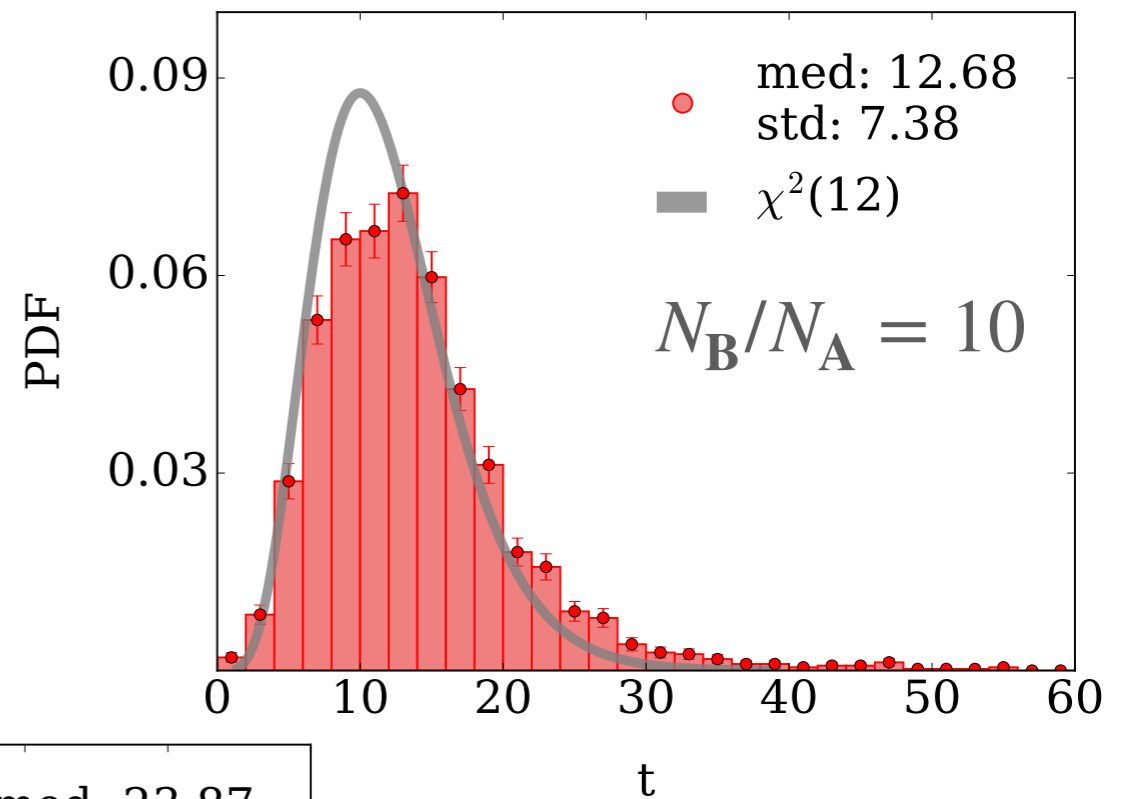


NPLM CHALLENGES: IMBALANCED SAMPLES

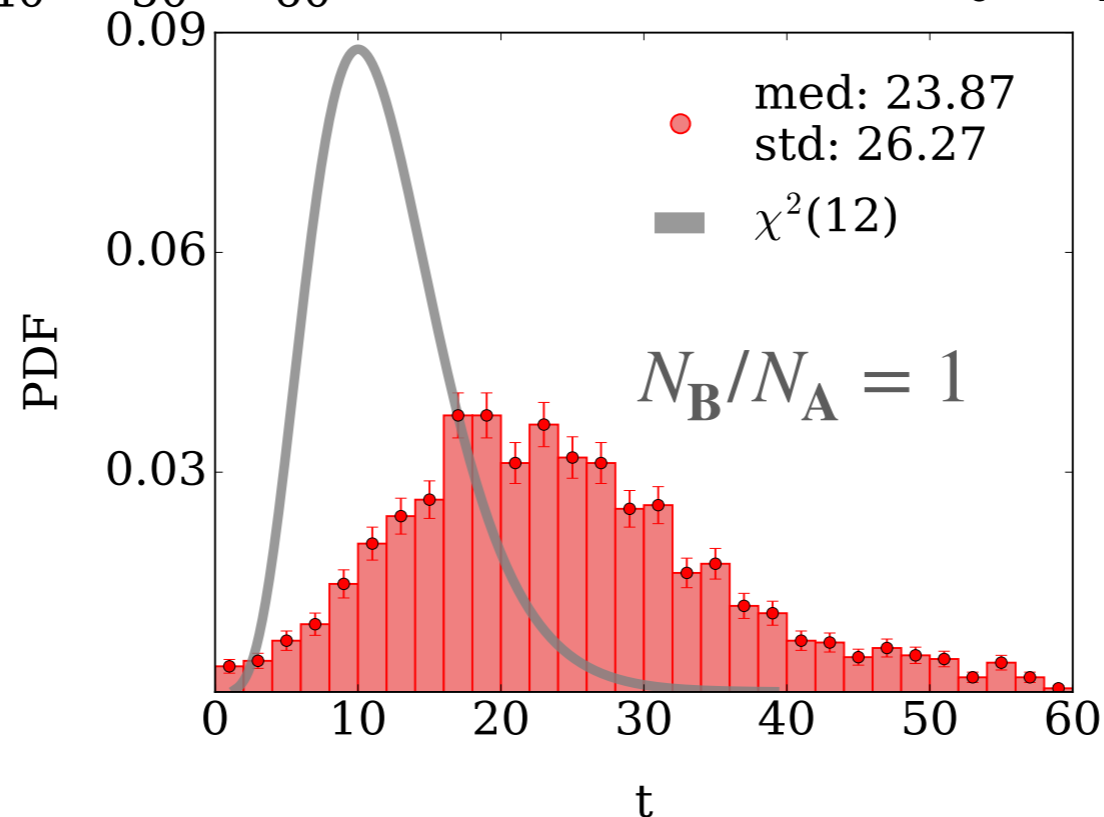
► Requires a large ratio between sample sizes $\tilde{N}_B \gg \tilde{N}_A$



$WC = 9$



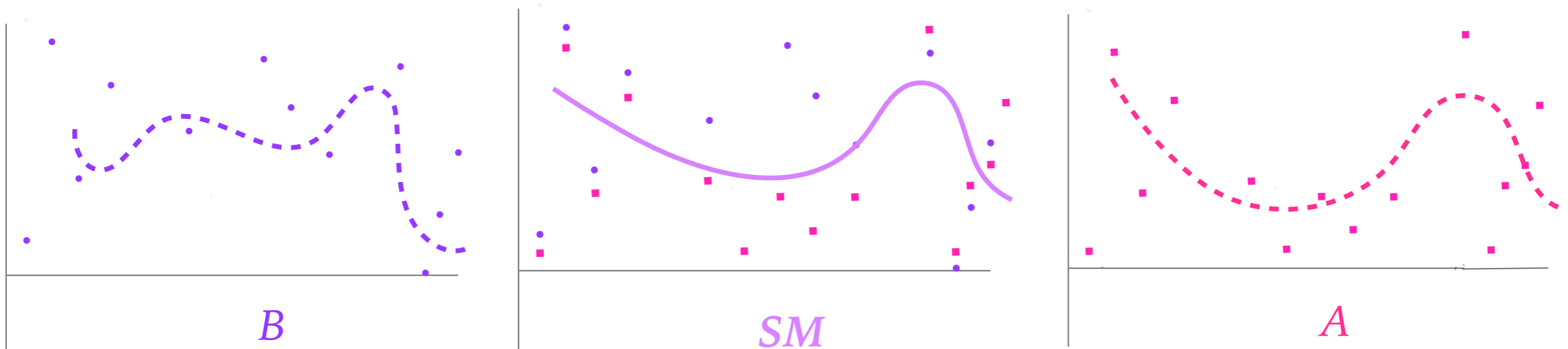
χ_n^2 predicted for
likelihood test



t distribution
for toy data A
and B generated
from the same
PDF

THE SYMMETRIZED FORMALISM

- **Symmetric question:** instead of asking if sample A comes from the distribution of sample B, we ask if A and B come from the same distribution.
- **Symmetric (democratic) modeling:** account for fluctuations in both samples.
- Improved sensitivity for any sample sizes ratio N_A/N_B .
- Avoid artificial singularities.



THE SYMMETRIZED FORMALISM – SYMMETRIC TEST

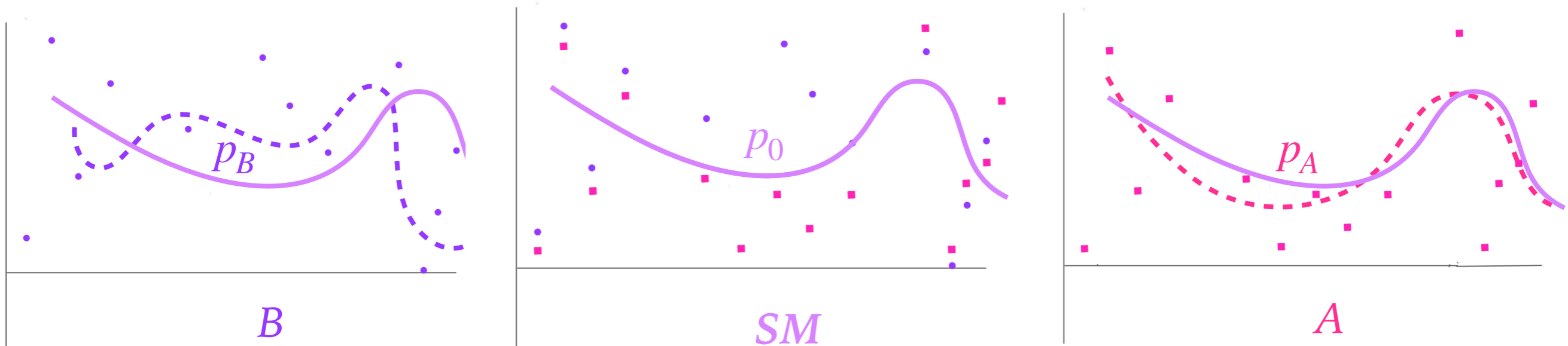
- Determine if samples **A** and **B** are drawn from the same distribution.

$$\mathcal{H}_0 : \quad n_{\mathbf{A}}(x) = N_{\mathbf{A}}p_0(x) , \quad n_{\mathbf{B}}(x) = N_{\mathbf{B}}p_0(x)$$

$$\mathcal{H}_1 : \quad n_{\mathbf{A}}(x) = N_{\mathbf{A}}p_{\mathbf{A}}(x) , \quad n_{\mathbf{B}}(x) = N_{\mathbf{B}}p_{\mathbf{B}}(x) ,$$

- Symmetric test - learn common PDF from both samples, test on both

$$t = 2 \log \left(\frac{\max_{p_{\mathbf{A}}, p_{\mathbf{B}}} \left(\mathcal{L} \left(N_{\mathbf{A}}, p_{\mathbf{A}}(x) \mid \mathbf{A} \right) \mathcal{L} \left(N_{\mathbf{B}}, p_{\mathbf{B}}(x) \mid \mathbf{B} \right) \right)}{\max_{p_0} \left(\mathcal{L} \left(N_{\mathbf{A}}, p_0(x) \mid \mathbf{A} \right) \mathcal{L} \left(N_{\mathbf{B}}, p_0(x) \mid \mathbf{B} \right) \right)} \right)$$



THE SYMMETRIZED FORMALISM – SYMMETRIC TEST

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- NPLM: if $\tilde{N}_{\mathbf{B}} \gg \tilde{N}_{\mathbf{A}}$, learn common PDF from **B** - $\hat{p}_0 \approx \hat{p}_{\mathbf{B}}$, test on **A**

$$t_{N_{\mathbf{B}} \gg N_{\mathbf{A}}} \rightarrow 2 \log \left(\frac{\max_{p_{\mathbf{A}}} \left(\mathcal{L} (N_{\mathbf{A}}, p_{\mathbf{A}}(x) | \mathbf{A}) \right)}{\mathcal{L} (N_{\mathbf{A}}, \hat{p}_{\mathbf{B}}(x) | \mathbf{A})} \right)$$

THE SYMMETRIZED FORMALISM

- Determine if observed samples **A** and **B** are drawn from the same distribution.

$$\mathcal{H}_0 : \quad n_{\mathbf{A}}(x) = N_{\mathbf{A}} e^{f_0} p_0(x) , \quad n_{\mathbf{B}}(x) = N_{\mathbf{B}} e^{g_0} p_0(x)$$

$$\mathcal{H}_1 : \quad n_{\mathbf{A}}(x) = N_{\mathbf{A}} e^{f(x)} p_0(x) , \quad n_{\mathbf{B}}(x) = N_{\mathbf{B}} e^{g(x)} p_0(x) ,$$

- The symmetric null distribution -

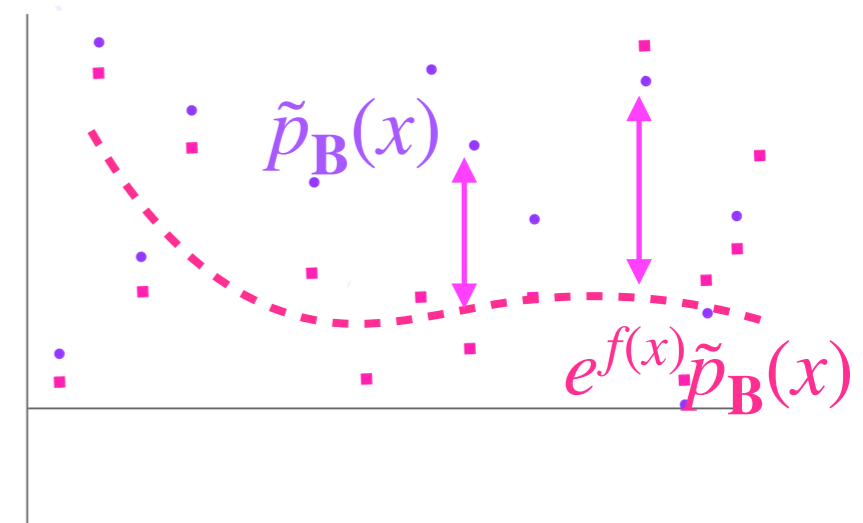
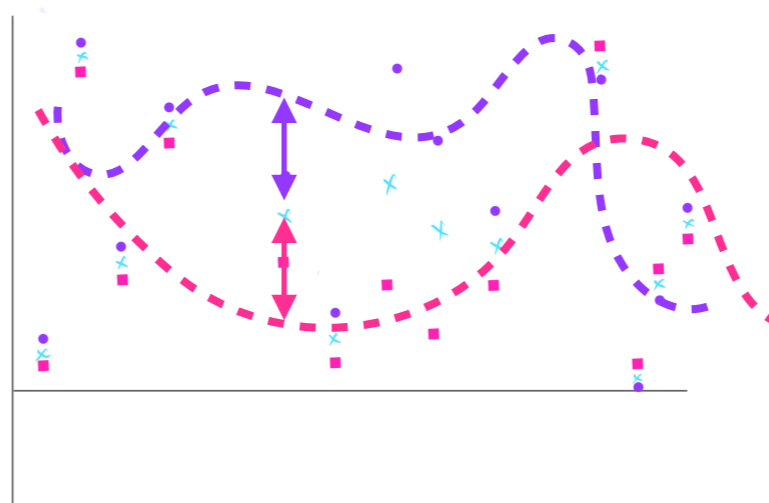
True global MLE \mathcal{H}_0

$$p_0(x) = \frac{\tilde{n}_{\mathbf{A}}(x) + \tilde{n}_{\mathbf{B}}(x)}{\tilde{N}_{\mathbf{A}} + \tilde{N}_{\mathbf{B}}}$$

NPLM

$$p_0(x) = \frac{\tilde{n}_{\mathbf{B}}(x)}{\tilde{N}_{\mathbf{B}}}$$

Approx. global MLE \mathcal{H}_0



THE SYMMETRIZED FORMALISM

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- The symmetric null distribution -

True global MLE \mathcal{H}_0

$$p_0(x) = \frac{\tilde{n}_{\mathbf{A}}(x) + \tilde{n}_{\mathbf{B}}(x)}{\tilde{N}_{\mathbf{A}} + \tilde{N}_{\mathbf{B}}}$$

NPLM

$$p_0(x) = \frac{\tilde{n}_{\mathbf{B}}(x)}{\tilde{N}_{\mathbf{B}}}$$

- The symmetric test statistic -

$$t_{\mathbf{A+B}}(\mathbf{A}) = -2 \min \left[-\frac{1}{\tilde{N}_{\mathbf{A}} + \tilde{N}_{\mathbf{B}}} \sum_{x \in \mathbf{A,B}} \tilde{N}_{\mathbf{A}} (e^{f(x)} - 1) + \sum_{x \in \mathbf{A}} f(x) \right]$$

$$t_{\mathbf{A+B}}(\mathbf{B}) = -2 \min \left[-\frac{1}{\tilde{N}_{\mathbf{A}} + \tilde{N}_{\mathbf{B}}} \sum_{x \in \mathbf{A,B}} \tilde{N}_{\mathbf{B}} (e^{g(x)} - 1) + \sum_{x \in \mathbf{B}} g(x) \right]$$

Approx. global MLE \mathcal{H}_0

$$t_{\mathbf{B}}(\mathbf{A}) = 2 \left(-\frac{N_{\mathbf{A}}}{\tilde{N}_{\mathbf{B}}} \sum_{x \in \mathbf{B}} (e^{\hat{f}(x)} - 1) + \sum_{x \in \mathbf{A}} \hat{f}(x) \right)$$

No divergences

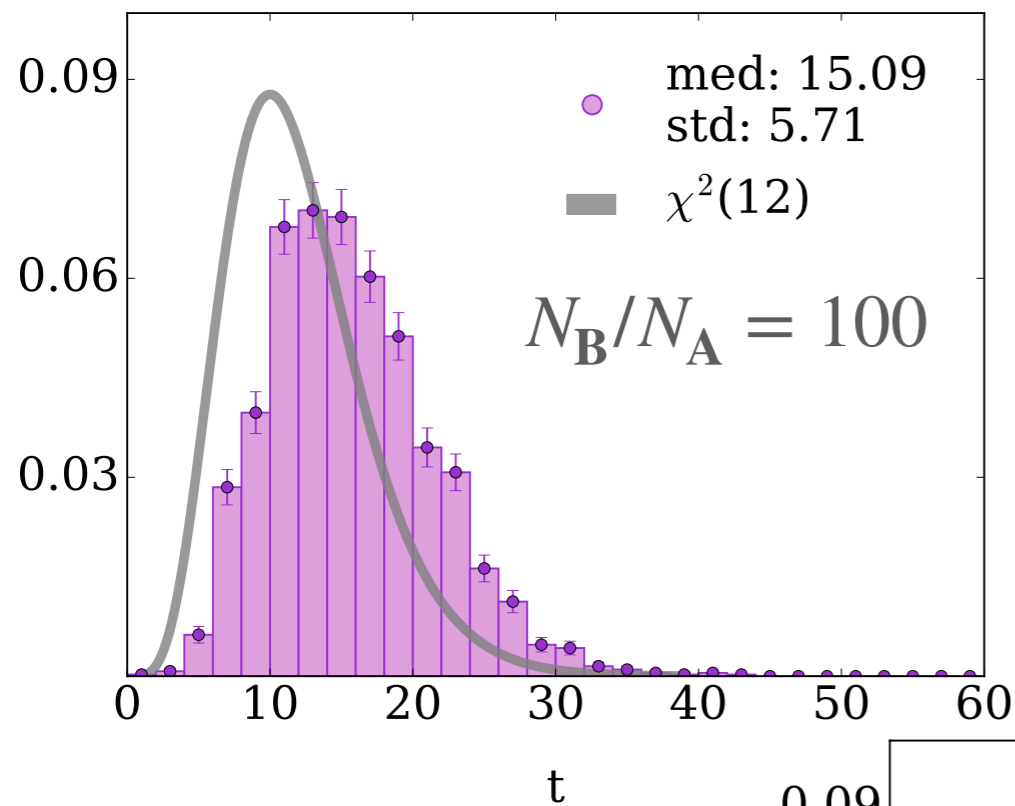
Unbounded

RESULTS

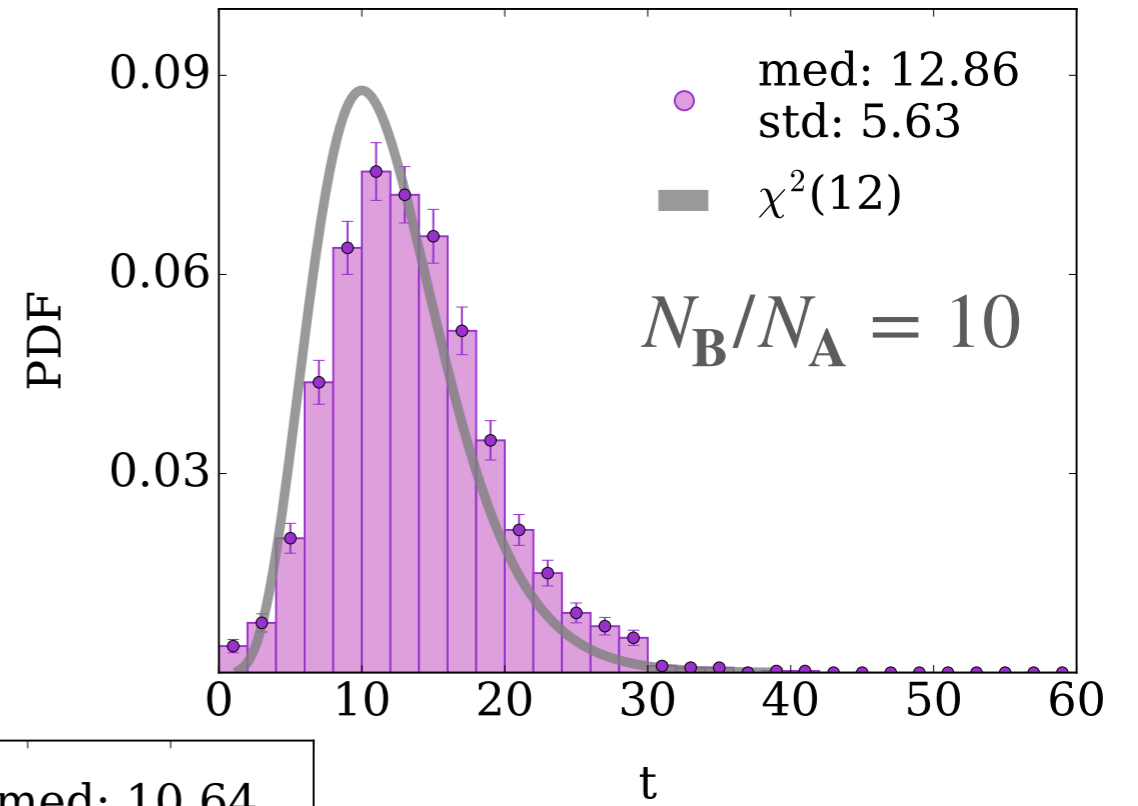
- Toy LFV - $e^\pm\mu^\mp$ samples with $\sim 2.2 \times 10^5$ events.
- 1-d variable: $x = \frac{m_{coll}}{100 \text{ GeV}}$
- Hyper-parameters: 500k epochs, 1 hidden layer of 4 neurons
- Symmetric - \mathbf{A} and \mathbf{B} randomly drawn from the $e\mu$ sample
- Asymmetric - $H \rightarrow \tau e, \tau \rightarrow \mu + X$ added to \mathbf{A} .

RESULTS – THE SYMMETRIC CASE

➤ Good agreement with asymptotic χ_n^2 for any \tilde{N}_B/\tilde{N}_A

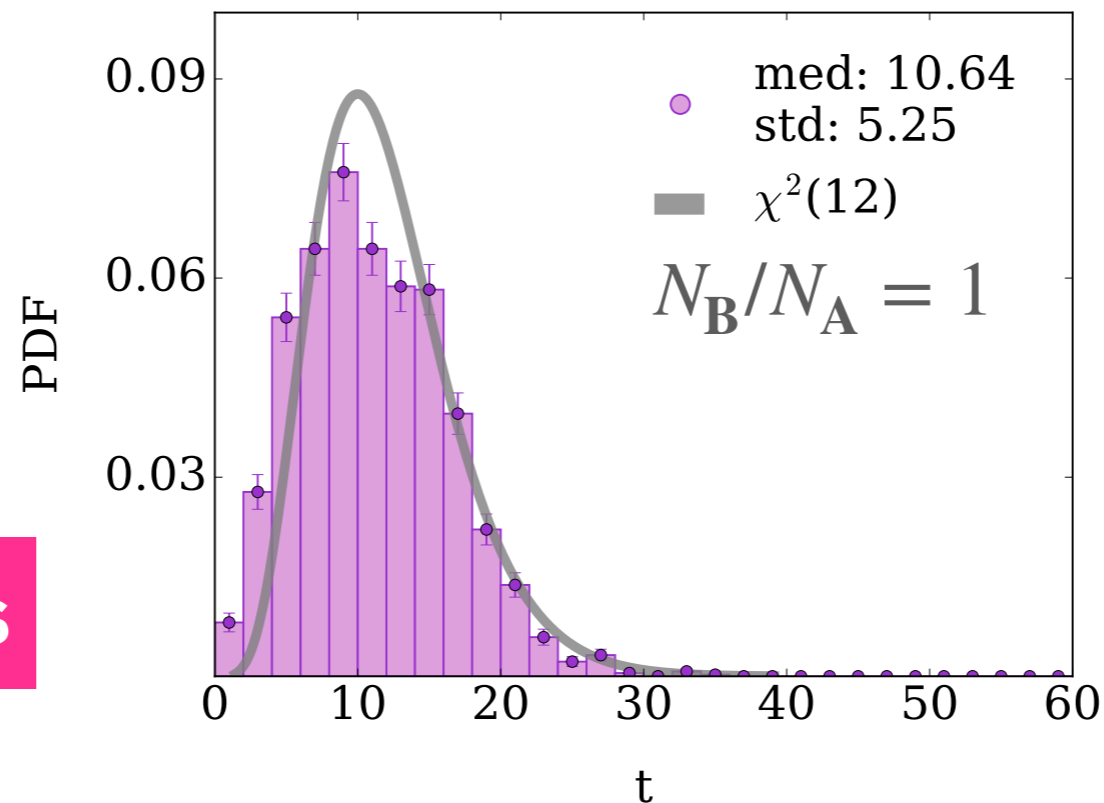


No WC!



χ_n^2 predicted for likelihood test

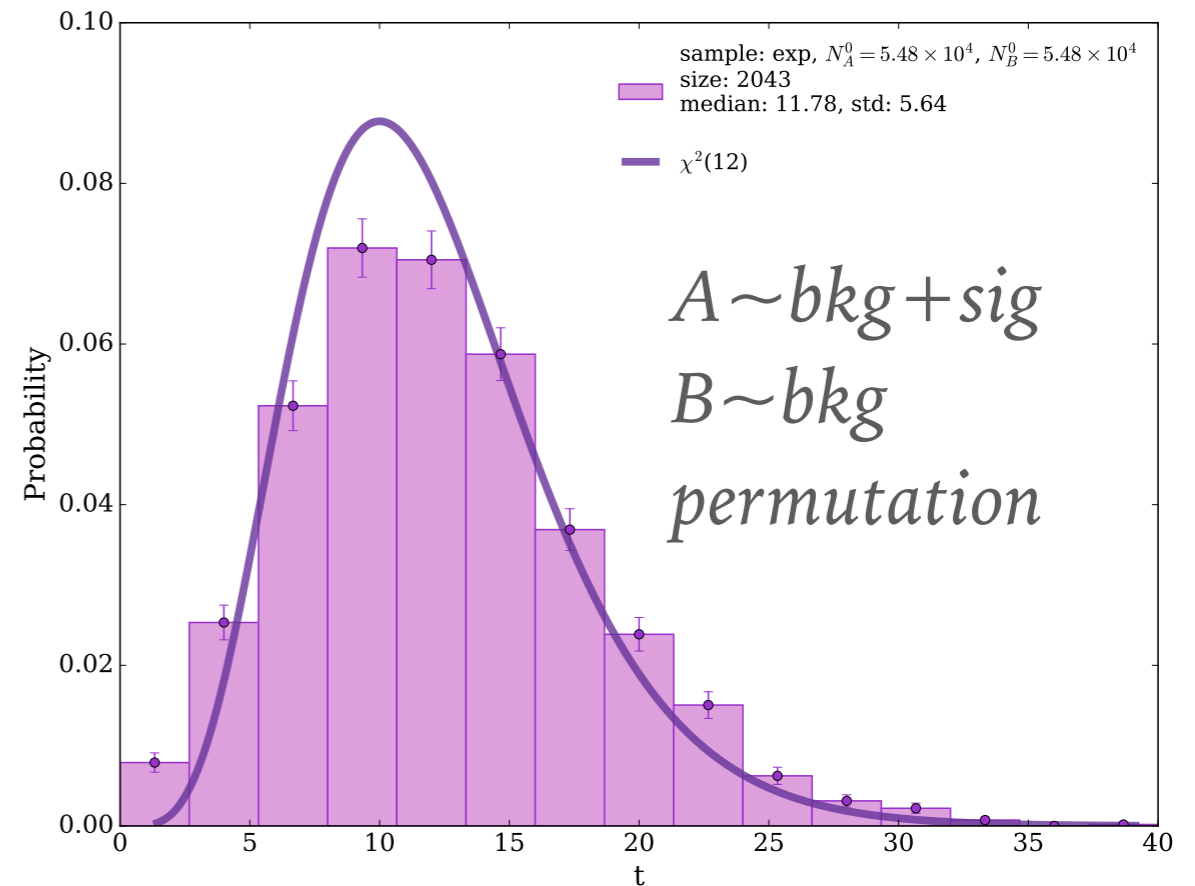
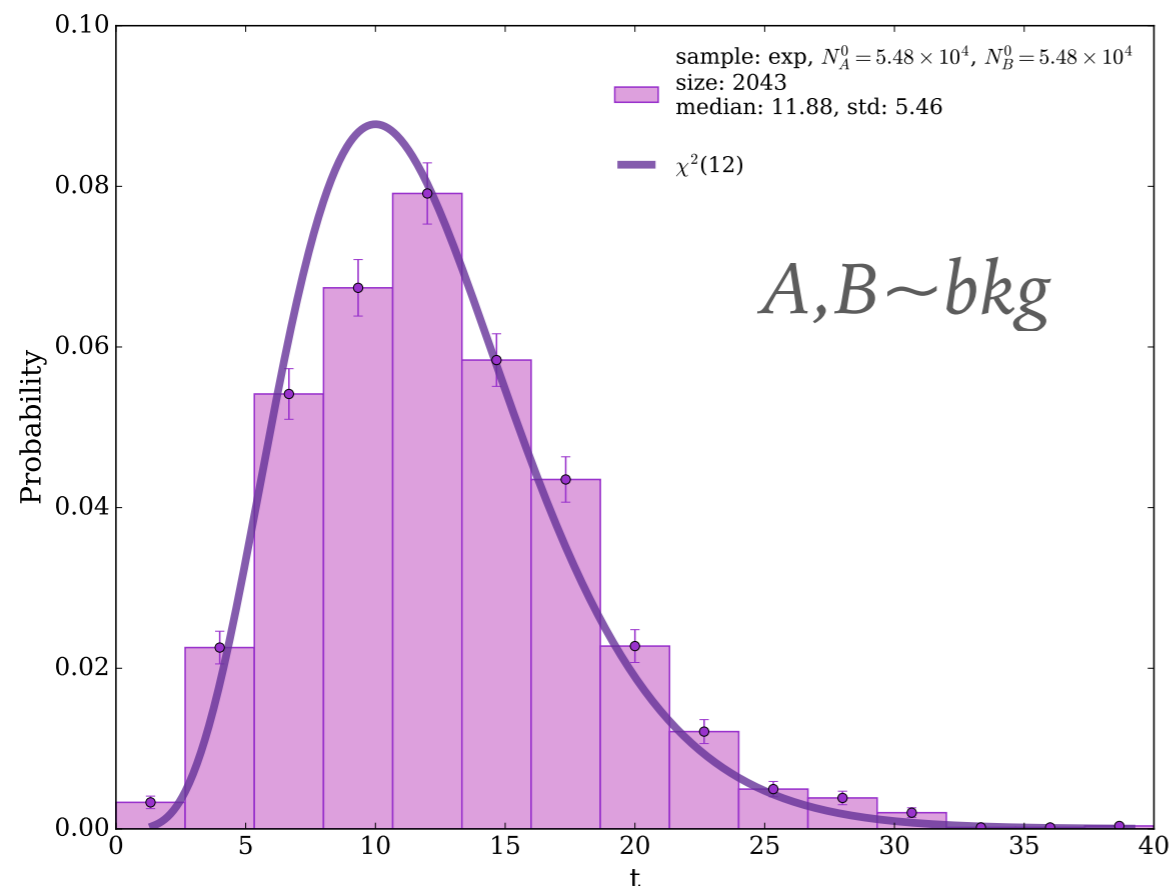
No divergences



t distribution for toy data A and B generated from the same PDF

RESULTS – EMPIRIC SYMMETRIC DISTRIBUTION

- Narrower and predictable background-only distribution.
- Good agreement with asymptotic χ_n^2
- Can generate empiric distribution from permutations of observed A and B



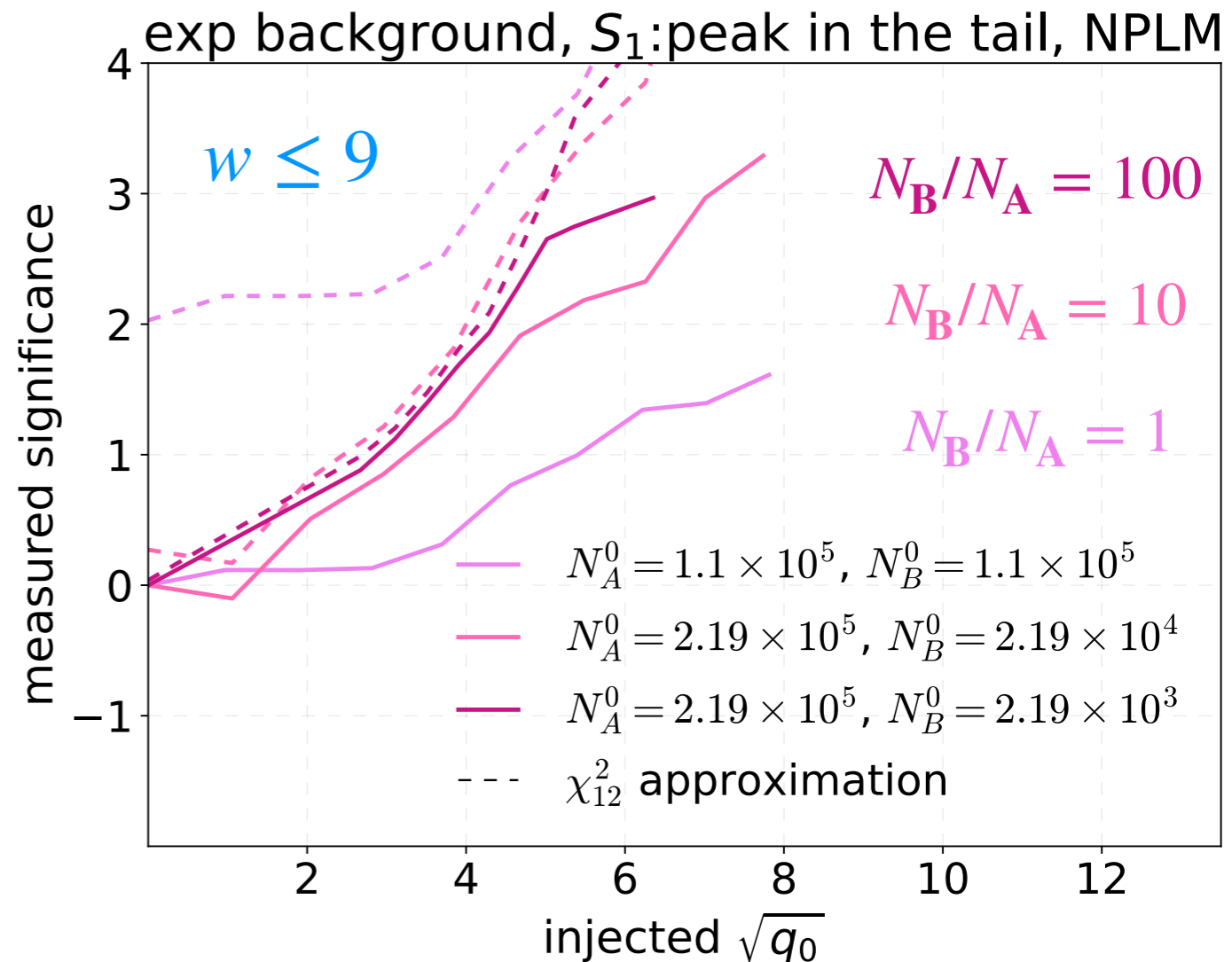
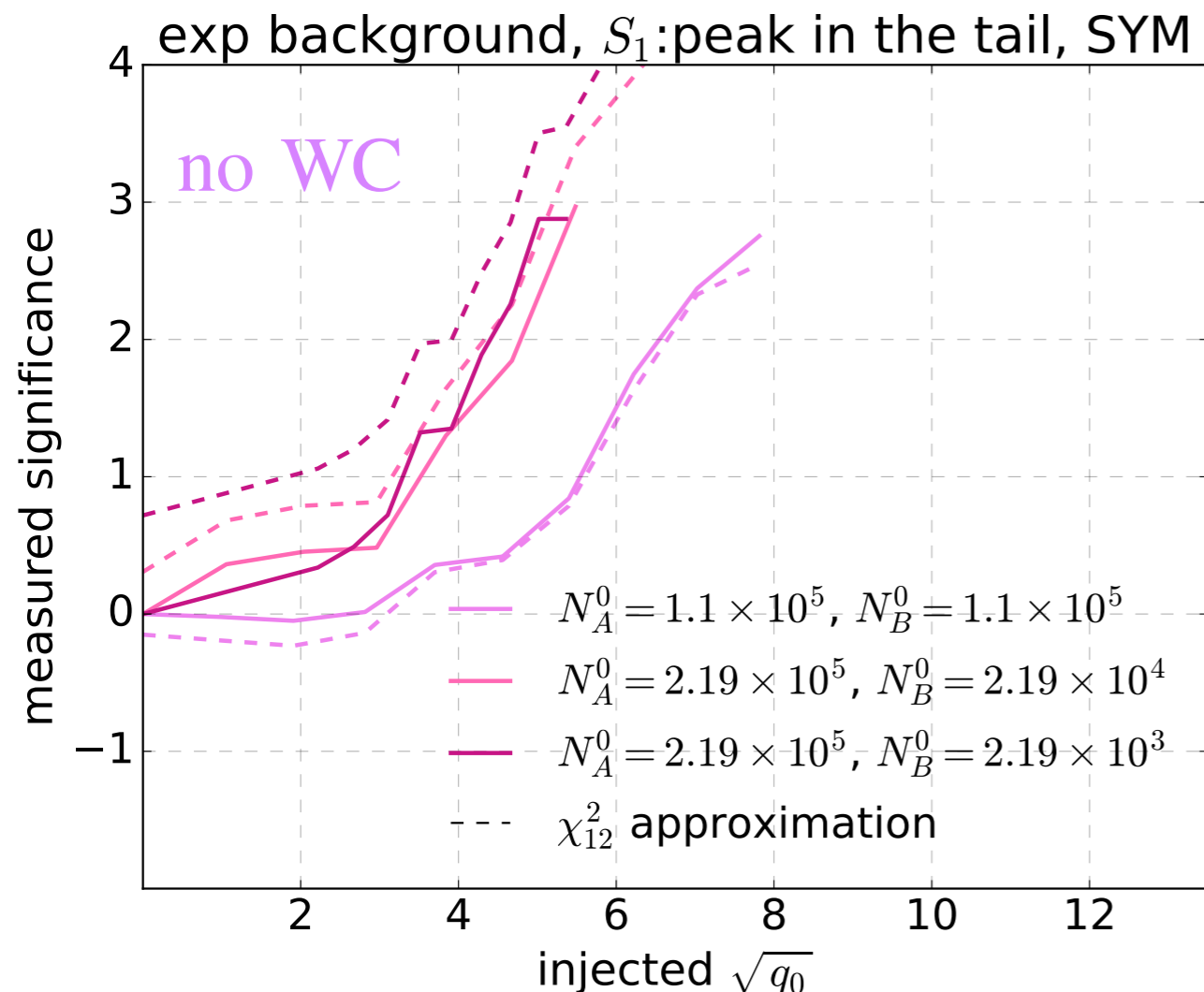
Symmetry assumptions only, no need for detailed SM simulation!

RESULTS - THE ASYMMETRIC CASE

- Better sensitivity due to narrower background-only distribution and relaxed weight-clipping.

$$t_{A+B}(A) + t_{A+B}(B)$$

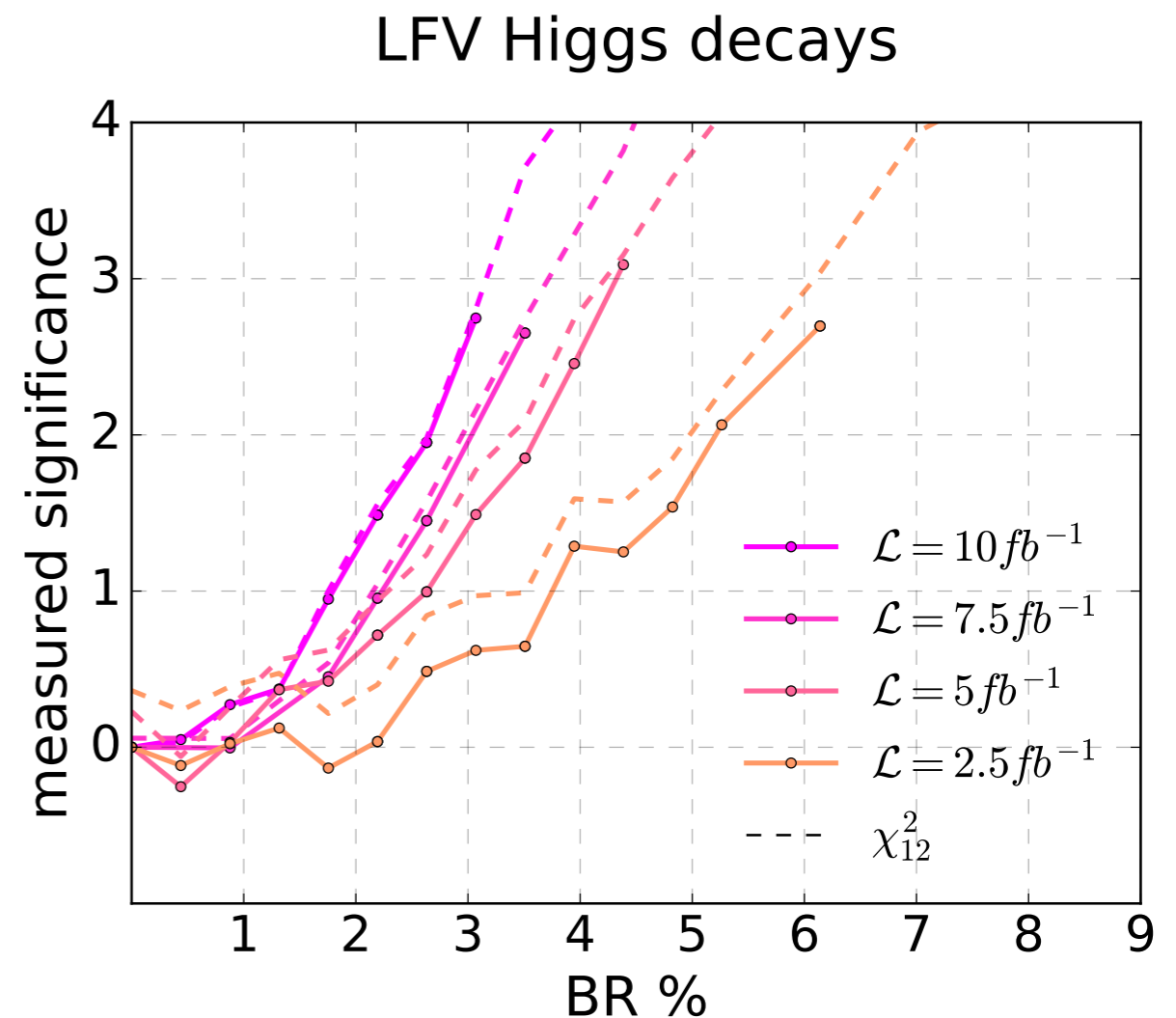
$$t_B(A)$$



RESULTS - THE ASYMMETRIC CASE

- Sensitivity to $BR(H \rightarrow \tau e) \sim 2.6\%$ at $L = 10 \text{ fb}^{-1}$
- Current bound: $BR(H \rightarrow \tau e) \sim 0.2\%$ at $L = 138 \text{ fb}^{-1}$

ATLAS, [2302.05225], CMS, [2105.03007]



CONCLUSIONS

- SM symmetries can be exploited for model-agnostic NP searches that are fully data-based.
- NPLM: ML+likelihood-loss test for deviations of observed data from much larger reference dataset.
- The symmetrized formalism -
 - **Symmetric statistical test** to account for fluctuations in both samples.
 - **Symmetric reference distribution** - assigning non-zero probability to all observed events.
- Allows for searches for differences between samples of arbitrary sizes, and relaxing the tuning of the model parameters.

OPEN QUESTIONS AND FUTURE WORK

- Realistic analysis -

- Including more kinematical variables.

NPLM: R. T. D'Agnolo, G. Grosso, M. Pierini, A. Wulzer & M. Zanetti [1912.12155].

- Including systematic uncertainties.

NPLM: R. T. D'Agnolo, G. Grosso, M. Pierini, A. Wulzer & M. Zanetti [2111.13633].

- Imperfect symmetries - correct for detector effects that violate LFU.

M. Birman, S. Bressler et al, ATLAS [1604.07730].

- Hyper-parameters choice -

- Improve robustness by preventing overfitting.

THANK YOU!

OPEN QUESTIONS AND FUTURE WORK

OPEN QUESTIONS AND FUTURE WORK

➤ Symmetry corrections - electrons and muons are not identical

➤ Different efficiencies

$$n_{e,\mu} = n_{e,\mu}^{\text{truth}} \epsilon_{e,\mu} + f_{e,\mu}$$

➤ Different fake rates

➤ Previous works on restoring the symmetry by re-weighting

$$R^\epsilon = \frac{N_\mu}{N_e}$$

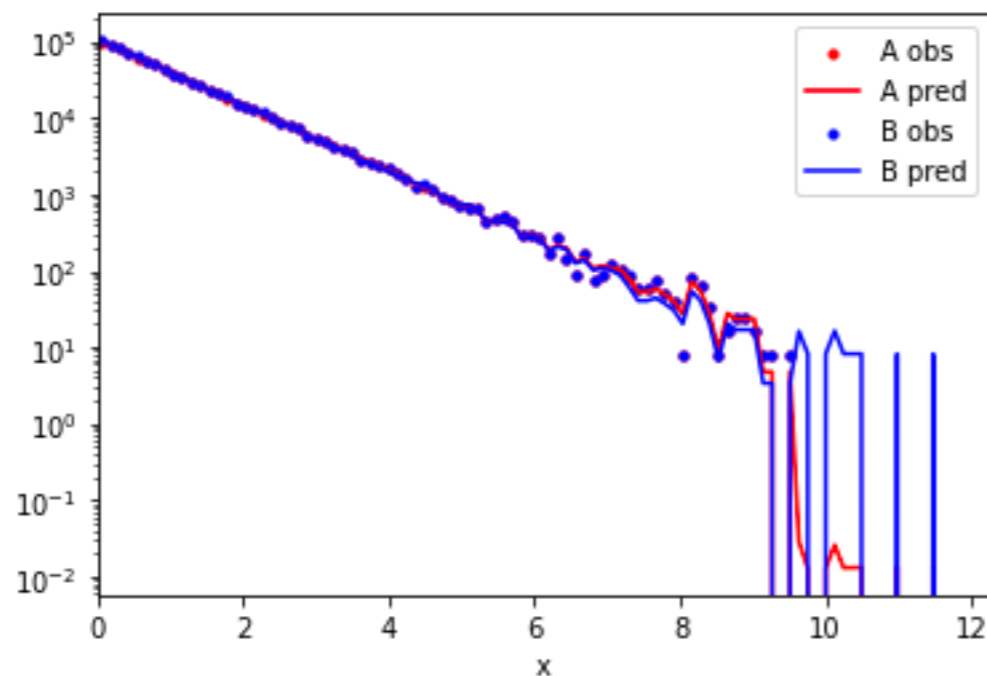
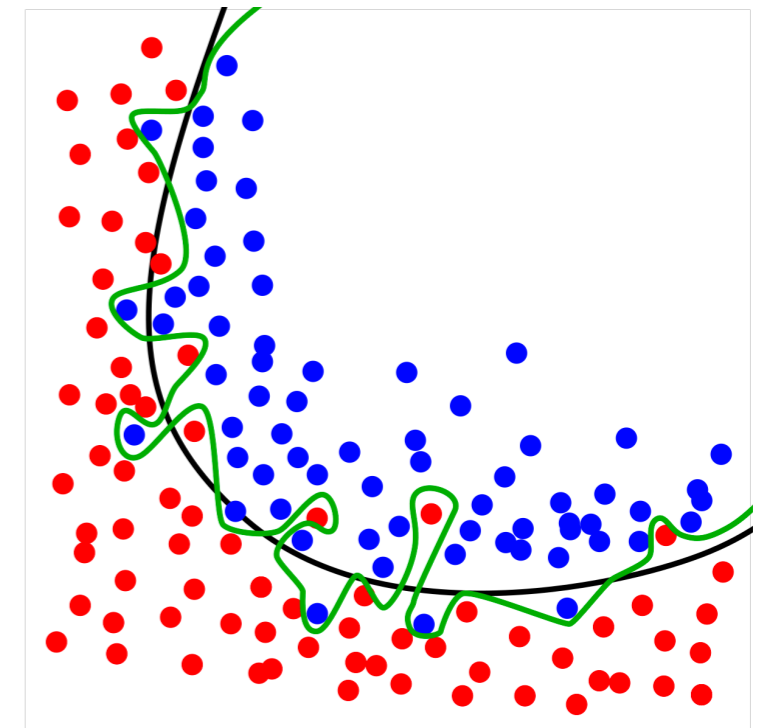
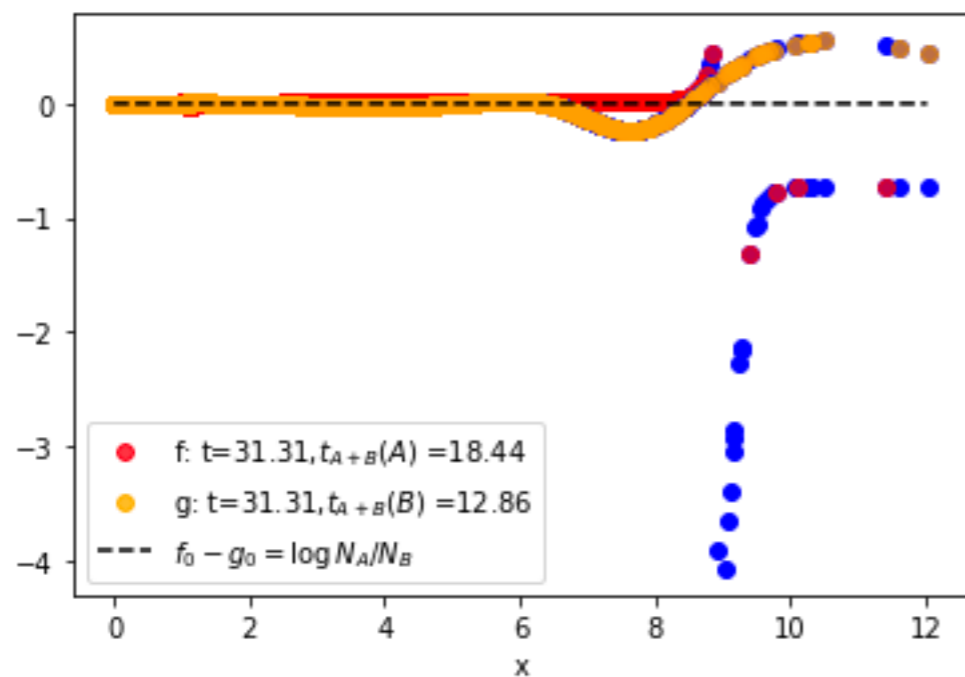
M. Birman, S. Bressler et al, ATLAS[1604.07730]

➤ Can use a similar approach to the symmetrized test?

$$t = 2 \log \left(\frac{\max_{p_e, p_\mu, p_{SM}, \epsilon_e, \epsilon_\mu, f_e, f_\mu} \left(\mathcal{L}(n_e \epsilon_e + f_e | \mathbf{e}_{\text{obs}}) \mathcal{L}(n_\mu \epsilon_\mu + f_\mu | \mu_{\text{obs}}) \mathcal{L}(n^{SM} \epsilon_e + f_e | \mathbf{e}_{\text{sim}}) \mathcal{L}(n^{SM} \epsilon_\mu + f_\mu | \mu_{\text{sim}}) \right)}{\max_{p_0, \epsilon_e, \epsilon_\mu, f_e, f_\mu} \left(\mathcal{L}(n^{SM} \epsilon_e + f_e | \mathbf{e}_{\text{obs}}) \mathcal{L}(n^{SM} \epsilon_\mu + f_\mu | \mu_{\text{obs}}) \mathcal{L}(n^{SM} \epsilon_e + f_e | \mathbf{e}_{\text{sim}}) \mathcal{L}(n^{SM} \epsilon_\mu + f_\mu | \mu_{\text{sim}}) \right)} \right)$$

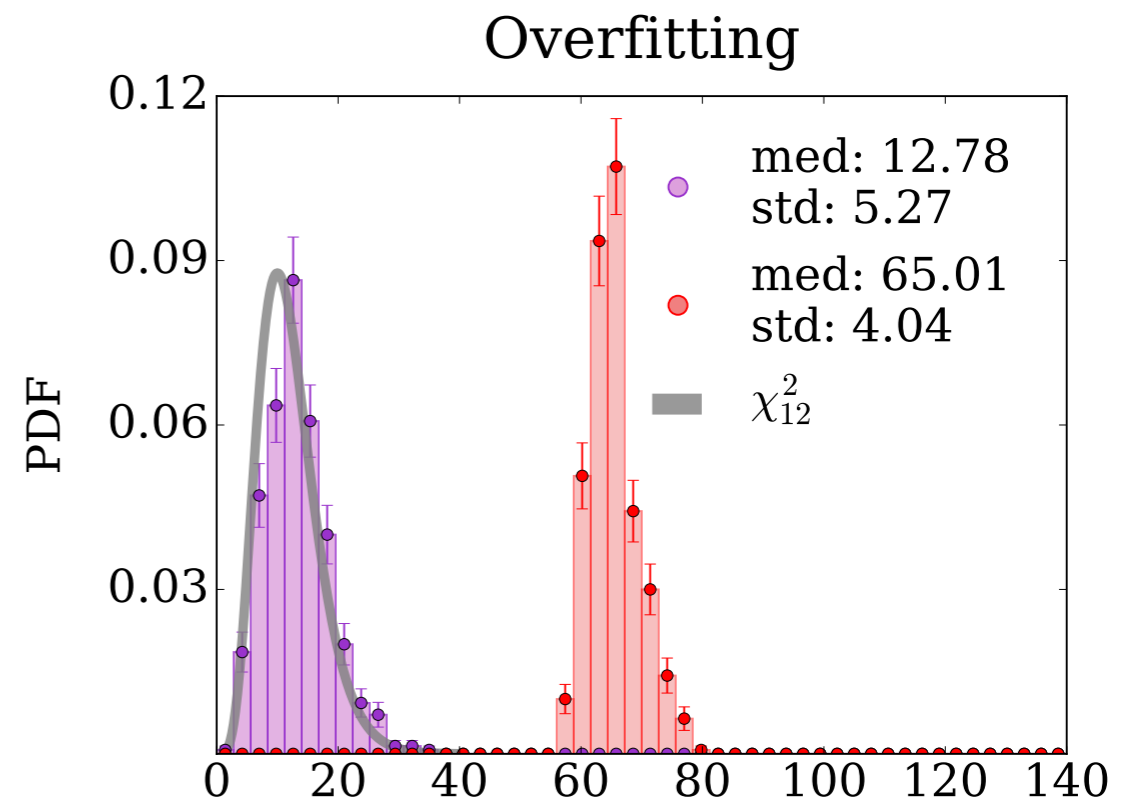
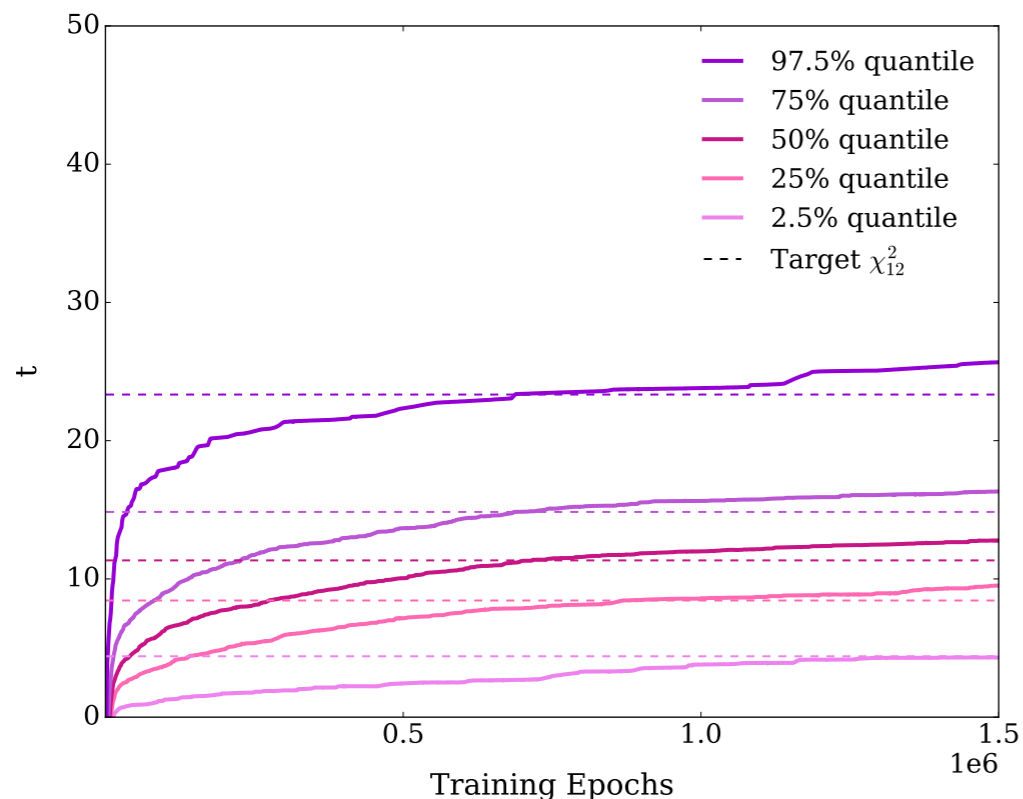
OPEN QUESTIONS AND FUTURE WORK

- Overfitting - too flexible functions are also able to perfectly fit statistical fluctuations.



OPEN QUESTIONS AND FUTURE WORK

- Overfitting - too flexible functions are also able to perfectly fit statistical fluctuations.
- Distribution drifts away from the asymptotic χ^2 for a large number of epochs
- “Slightly” overfit solutions could be severe - locating longest runs



OPEN QUESTIONS AND FUTURE WORK

- Overfitting - potential solutions:
- Different fitting schemes -
 - Smooth functions + averaging.
 - Fit symmetric and asymmetric components instead of A and B.
- Standard ML regularization techniques -
 - Validation set - should understand resulting distribution.
 - Adding a cost term to the loss penalizing high weights/complex models.
 - Understand relation between overfitting and a normal distribution of the parameters under the null hypothesis.