

# Population Analysis of Massive Black hole Binaries with LISA using Iterative weighted KDE

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LISA Spain Meeting 2024

October 16-17, 2024

Institute of Space Sciences (ICE, CSIC and IEEC)

UAB, Barcelona, Spain

**SISSA**  
Scuola  
Internazionale  
Superiore di  
Studi Avanzati

**INFN**  
Istituto Nazionale di Fisica Nucleare



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European Research Council  
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# Overview

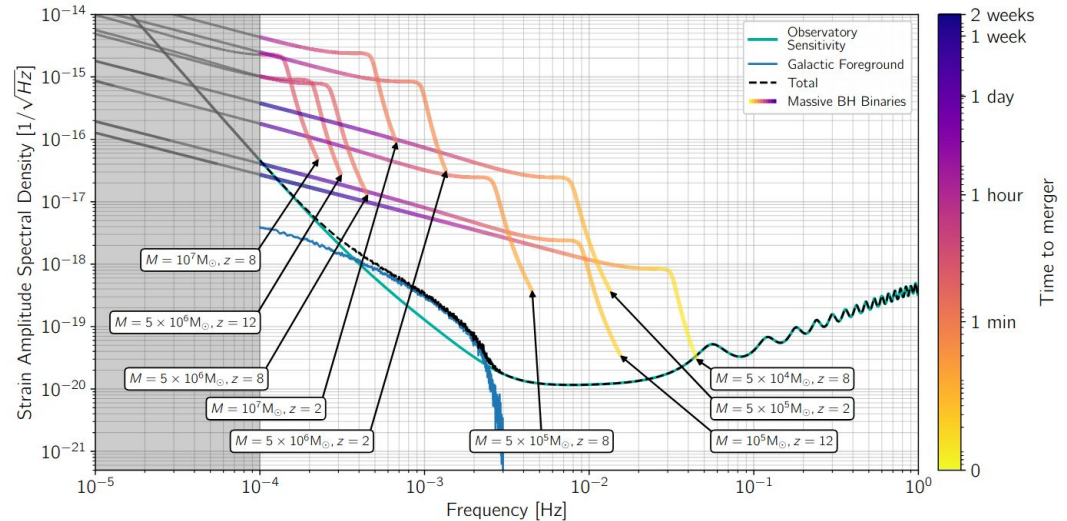
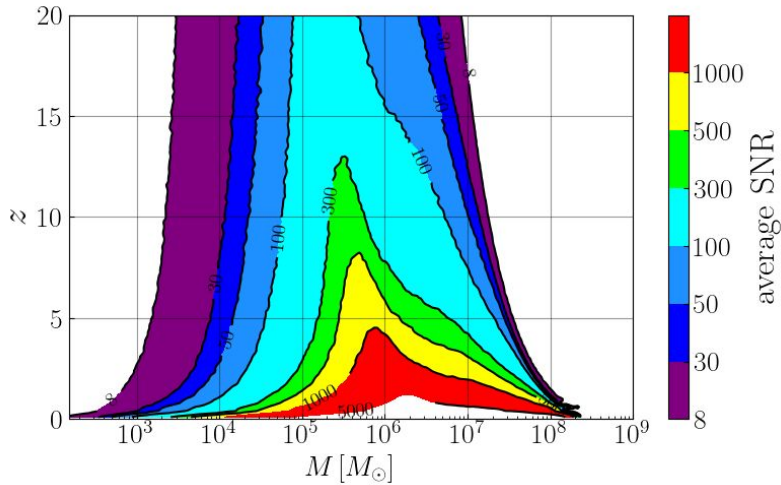
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- Motivation
- Method of KDE with Iterative Reweighting technique
- Applications on Massive BHBs evolve from Pop III star (“light seed”) for LISA
- Future Work

# Motivation

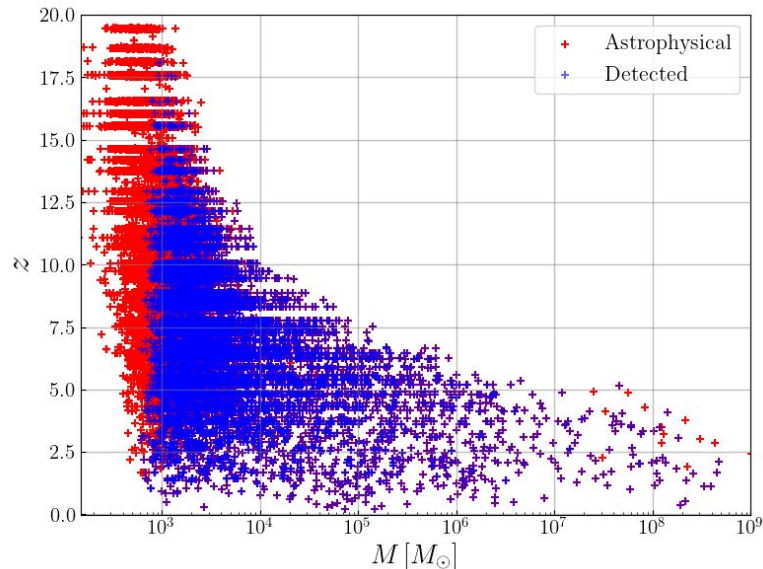
- LISA will see **Massive Black hole Binaries (MBHBs)**, crucial for true understanding of formation, evolution of such systems as well as Galaxy evolution



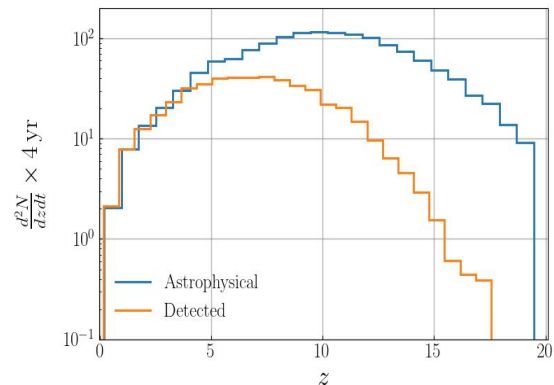
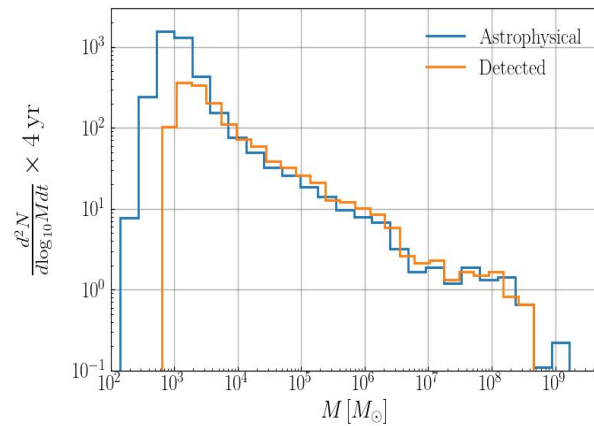
Credit: ESA-SCI-DIR-RP-002, Sep, 2023

# Pop-III (“light seed”) Remnant Binary Black holes

- Low Mass High Redshift events
- Selection effects are crucial



Data from Phys. Rev. D 93, 024003 (2016)



# Our Goal: Non parametric Method with Selection Effects to Reconstruct Astrophysical Rates

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- *Phys.Rev.D* 105 (2022)
- *Astrophys.J.* 960 (2024)

# Kernel Density Estimation (KDE)

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- **Objective:**

- Flexible, and, **non parametric** method
- Prioritize computational simplicity and speed
- Go from a set of detected events to a **rate density with small/quantified uncertainty**
- Addresses same questions as other methods
  - stellar evolution, Black hole and Binary formation channel

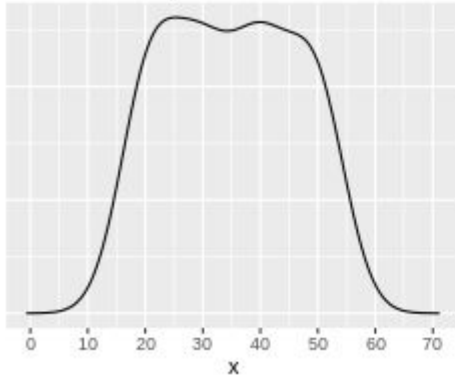
# Kernel Density Estimation (KDE)

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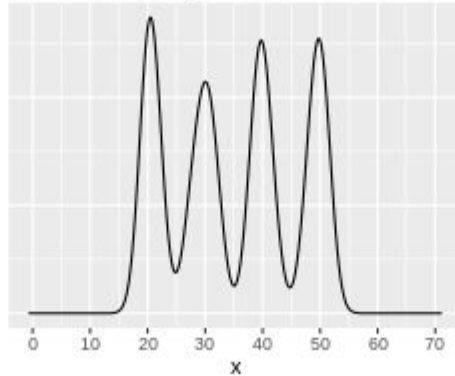
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- Put a blob of density at each event. Ensures data have "fairly high" likelihood
  - but what size of blob (**bandwidth choice**)?

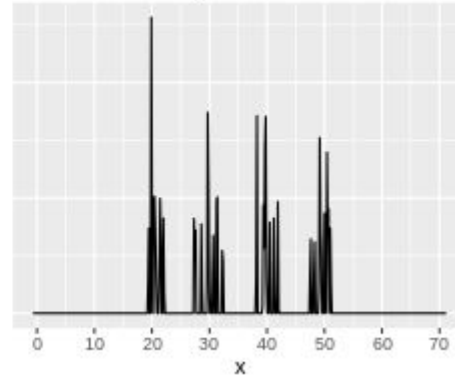
Oversmoothing



What we actually want

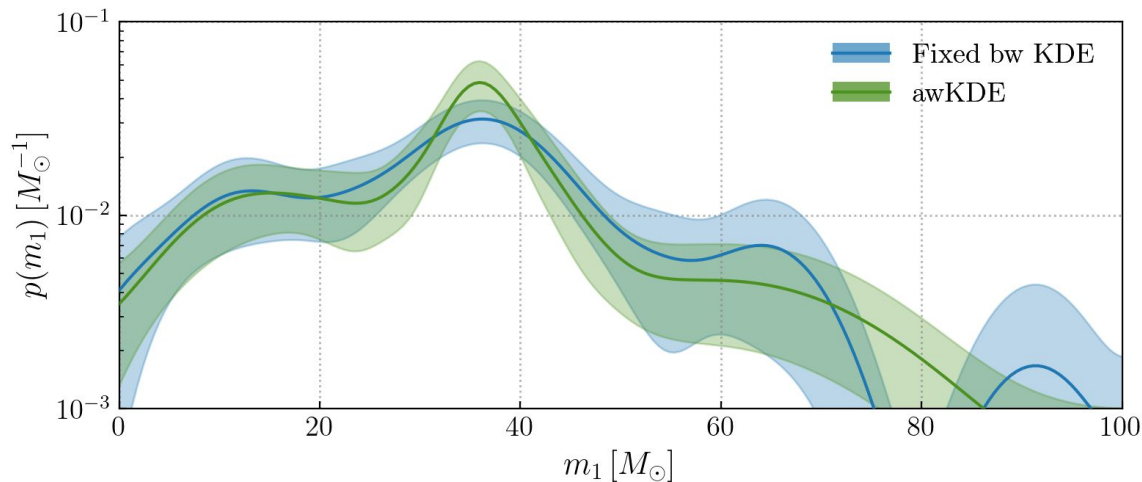


Undersmoothing



# Adaptive Width Kernel Density Estimation (awKDE)

- Under-smoothing makes estimate biased Over-smoothing makes estimate (too) uncertain
- Optimized **adaptive bandwidth**: Adjust **local bw**  $\propto$  to typical **distance between events**





# Adaptive Width Kernel Density Estimation (awKDE)

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- Using an initial global bandwidth choice to make a pilot Gaussian KDE

$$\hat{f}(x) = \frac{1}{\sum_i W_i} \sum_{i=1}^n \frac{W_i}{h\lambda_i} K\left(\frac{x - X_i}{h\lambda_i}\right). \quad \lambda_i = 1 \quad W_i = 1$$

- Derive local (adaptive) bandwidth from pilot KDE & sensitivity parameter,  $0 \leq \alpha \leq 1$

$$\lambda_i = \left(\frac{\hat{f}_0(X_i)}{g}\right)^{-\alpha}, \quad \log g = n^{-1} \sum_{i=1}^n \log \hat{f}_0(X_i)$$

- Final KDE uses this local bandwidth
- For multi-dimensional case linearly transform data to have zero mean and unit covariance

# Choice of KDE Hyper-parameters

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- Determine optimum initial bandwidth and  $\alpha$  by grid search using **maximum likelihood as a figure of merit on leave-one-out cross validation** with

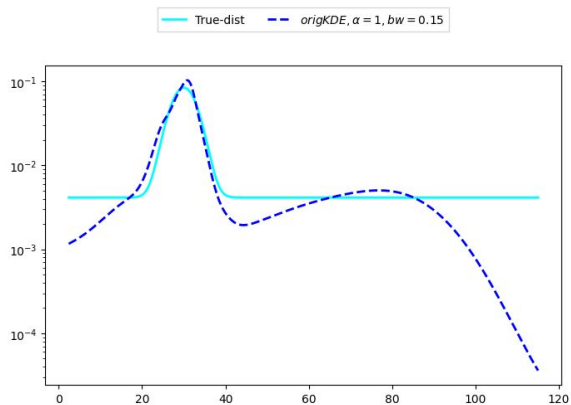
$$\log \mathcal{L}_{LOO} = \sum_{i=1}^n \log \hat{f}_{LOO,i}(X_i)$$

where  $\hat{f}_{LOO,i}$  is the KDE constructed from all samples except  $X_i$

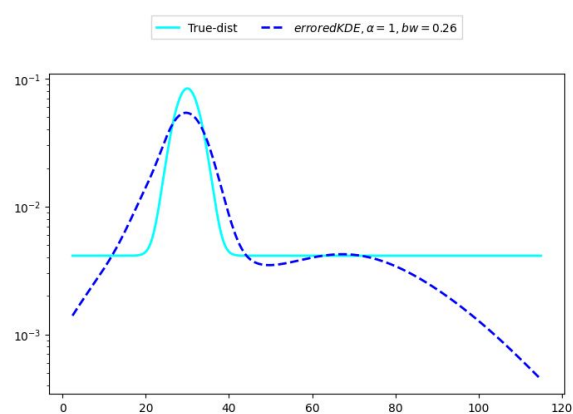
- Linear in logarithm of estimate at observed values and will penalize relative errors
- For **large number of samples** we use **k-fold cross validation** with **5 folds** with same figure of merit

# Parameter Estimation Uncertainties

- Event parameters can't be measured exactly
- Posterior samples are only accurate under default PE-prior population
- Expected to over-disperse population feature



Data without uncertainty



Data with uncertainty

# 'Deconvolving' PE uncertainty via Reweighting

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- Accurate population model requires accurate event values
- Accurate estimate of event value requires population model



- Address by iteration : use previous rate estimate for reweighting PE samples

# Expectation-Maximization Algorithm

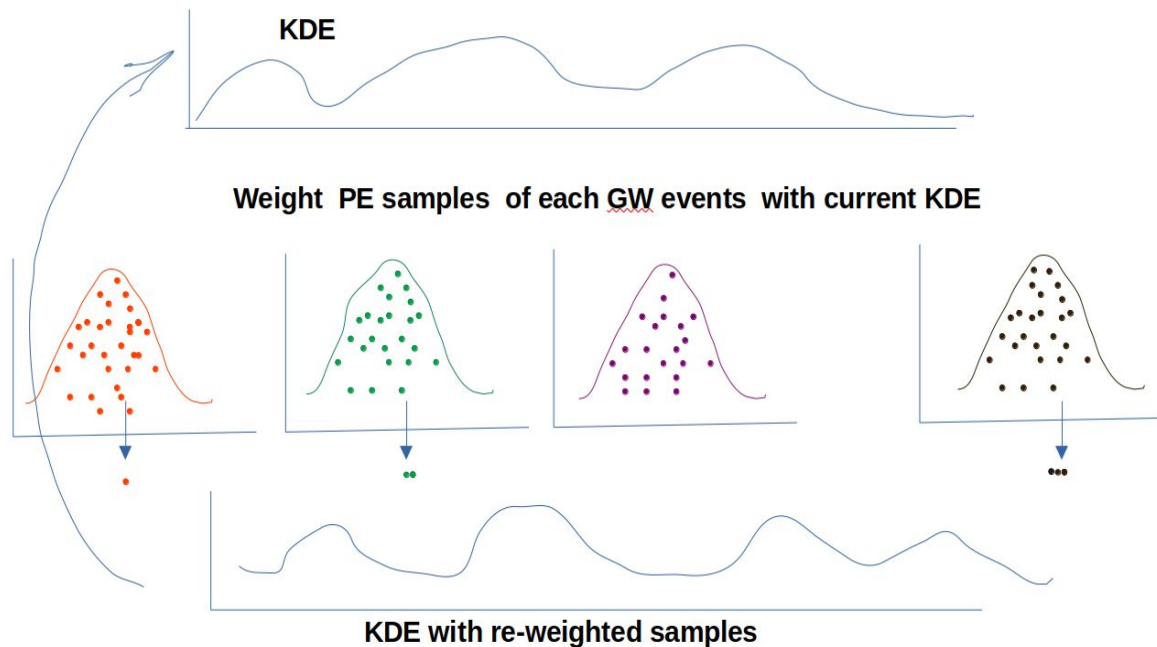
*Astrophys.J.* 960 (2024)

1. Draw Poisson(1) PE samples per event weighted by current estimate of population rate density

2. Optimize an adaptive KDE trained with this sample set

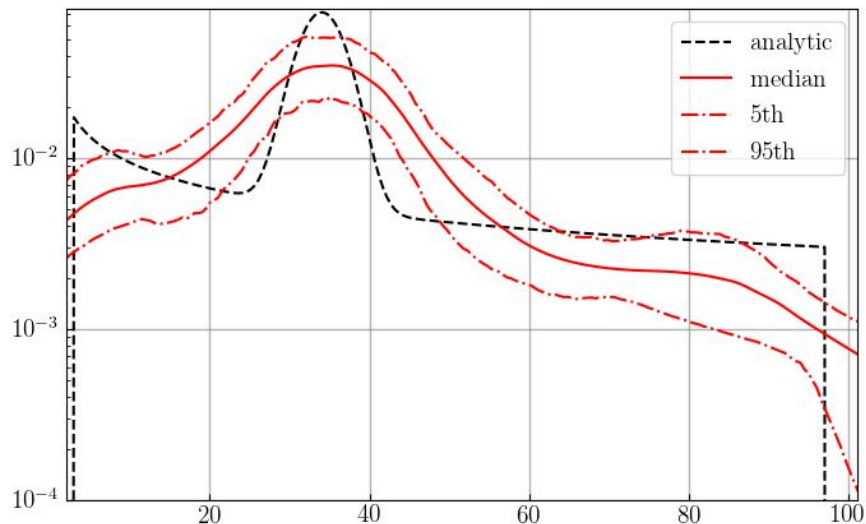
3. Update current rate estimate using the KDE

4. Go to step 1

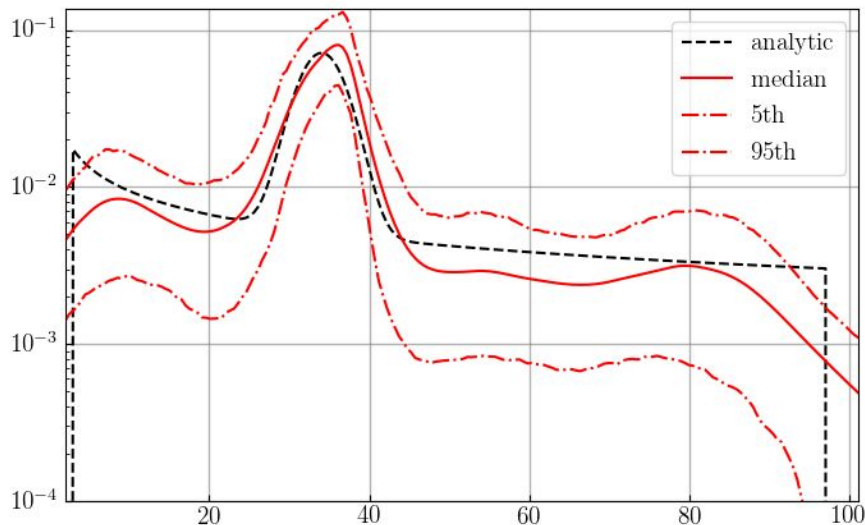


# Test: Expectation-Maximization Algorithm

- 50% of events in Gaussian peak, peak  $\sigma = 3$ , PE error & sample uncertainty 5



Without iterative reweighting



With iterative reweighting

# Selection Effects

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- To get the **rates from density estimate**, account for **selection bias**

$$p_{\text{det}}(\mathbf{x}, \theta) = \int p(\rho > \rho_{\text{th}} | \bar{\rho}(\mathbf{x}, \theta, \psi)) p(\psi) d^n \psi,$$

- KDE parameters  $x : (M, z)$
- Other intrinsic parameters  $\theta : (q, \chi, \dots)$
- Uniform distribution over extrinsic parameters and time of observation  $p(\psi)$

# Rate Estimates including Selection effects

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- **Astrophysical** rate density

$$R_{\text{det}}(x) = \int R(x, \theta) p_{\text{det}}(x, \theta) d^n \theta .$$

$$R(x, \theta) = R(x) p_{\text{pop}}(\theta)$$

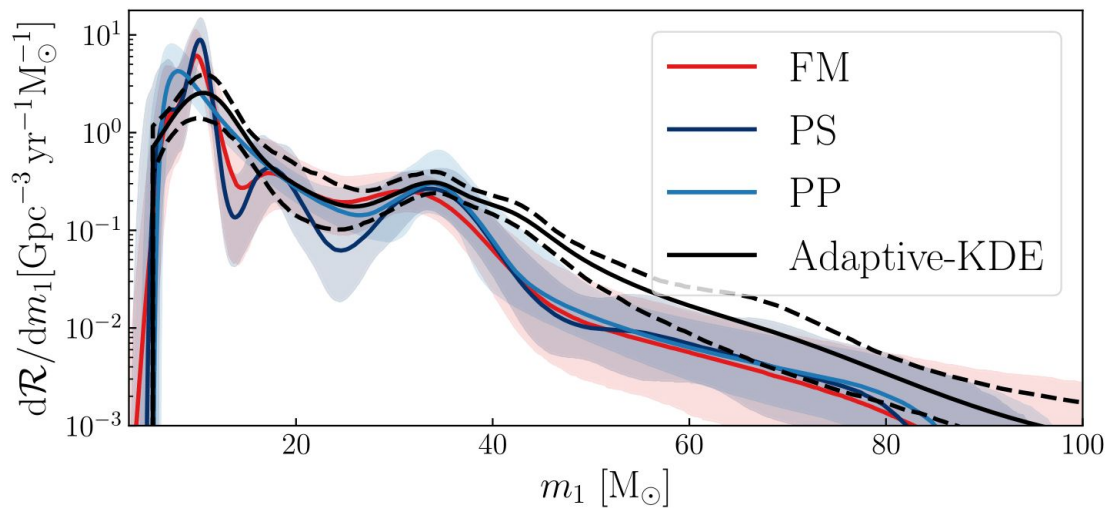
$$\begin{aligned} R_{\text{det}}(x) &= R(x) \int p_{\text{pop}}(\theta) p_{\text{det}}(x, \theta) d^n \theta \\ &\equiv R(x) p_{\text{det}}(x; p_{\text{pop}}) , \end{aligned}$$

$$R(x) = \frac{R_{\text{det}}(x)}{p_{\text{det}}(x; p_{\text{pop}})}$$



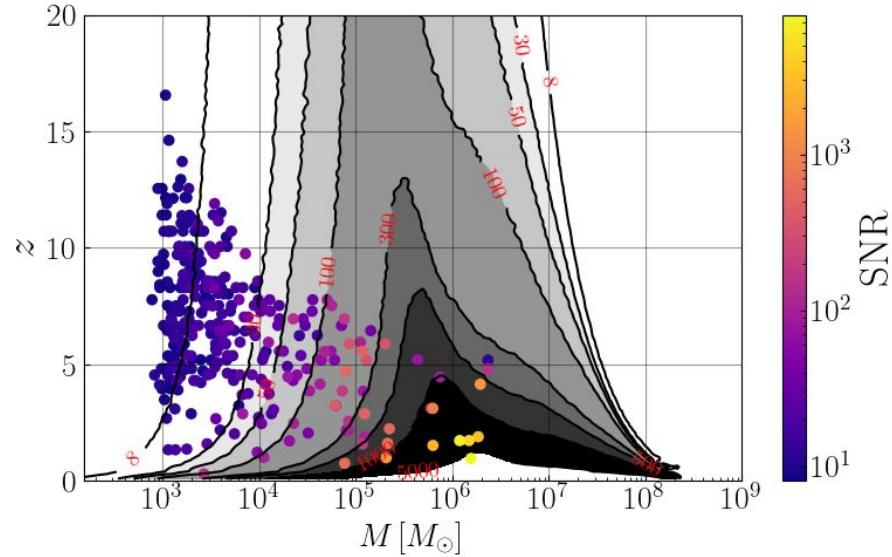
# Application on GWs

- Applied on GWTC-3



- *Phys.Rev.D* 105 (2022)
- *Astrophys.J.* 960 (2024)

# Data: light-seed model popIII (K+16)



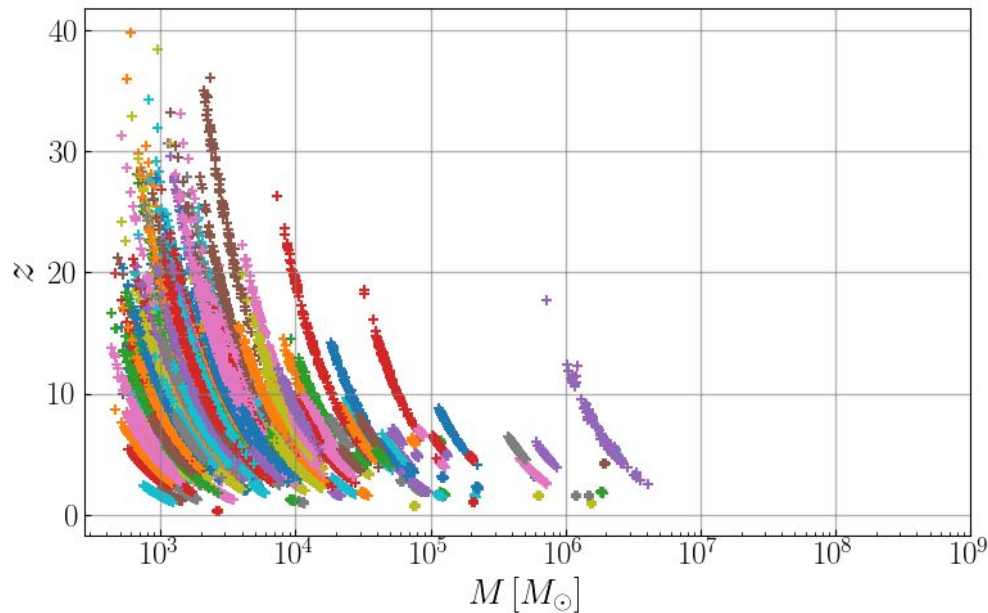
Data from Phys. Rev. D 93, 024003 (2016)

# Parameter Estimation

Light-seed model: popIII-d (K+16)

- Posterior samples (100 per event)
- Included weak lensing effects

$$\sigma_{\text{wl}}(z) = D_L \times 0.066 \left( \frac{1 - (1 + z)^{-0.25}}{0.25} \right)^{1.8}$$



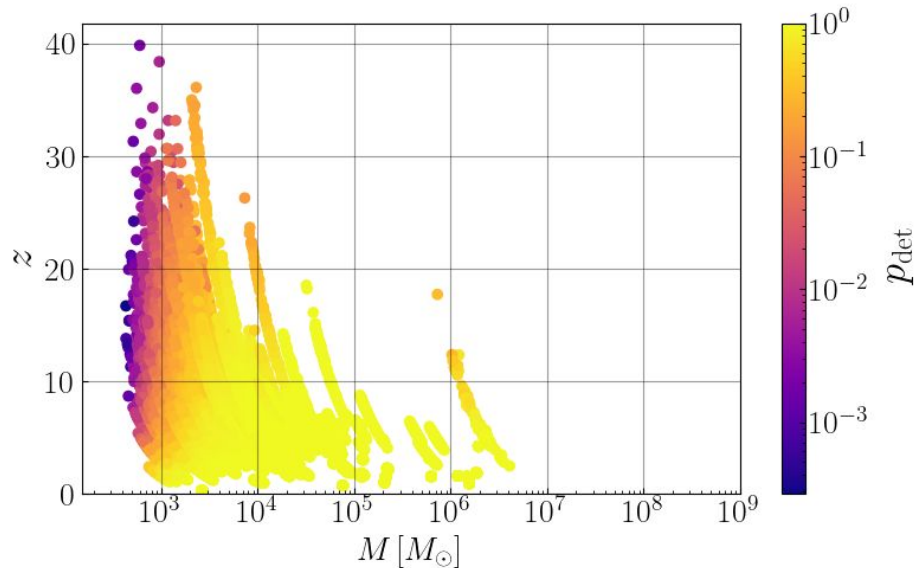
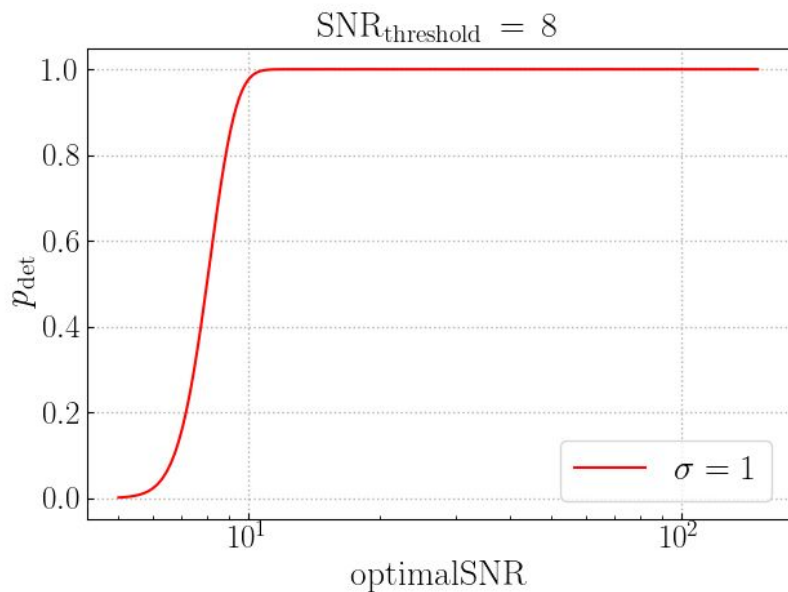
Phys. Rev. D.108 103034 (2023)

# Selection Effects

- Matched-filter SNR (standard Gaussian noise) to get  $P_{\text{det}}$

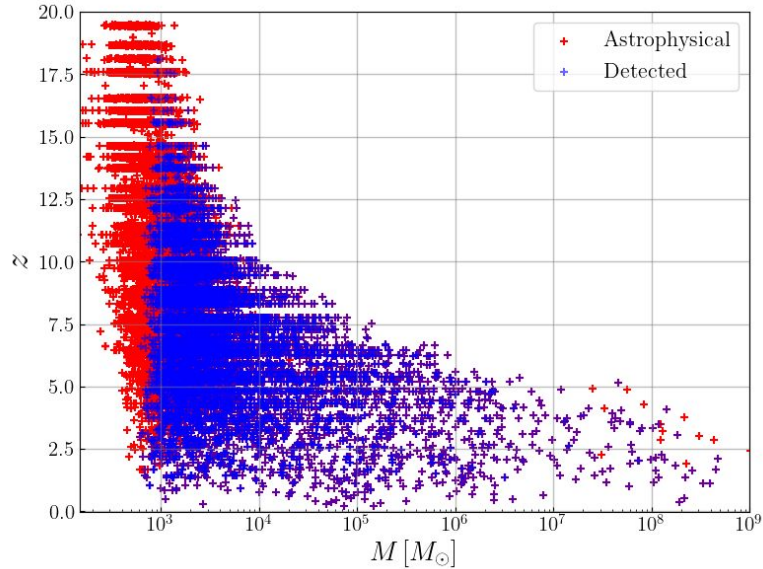
$$p(\rho|\bar{\rho})d\rho = \frac{1}{\sqrt{2\pi}} e^{-(\rho-\bar{\rho})^2/2} d\rho.$$

cap:  $p_{\text{det}} < 1e-3$

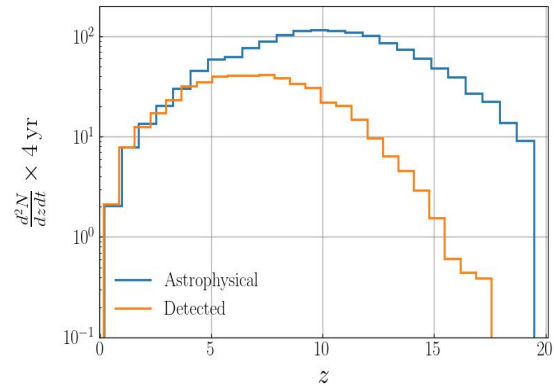
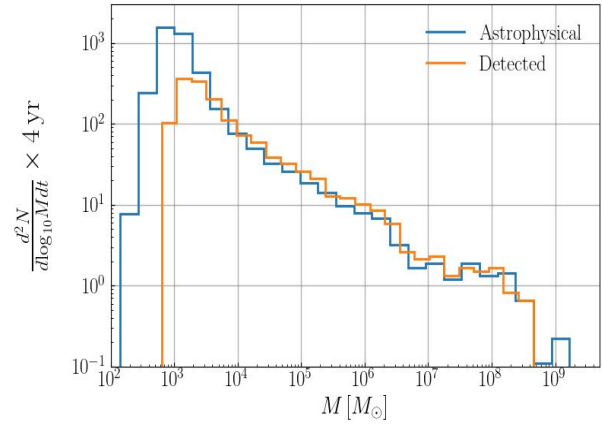


# Testing methods: Model

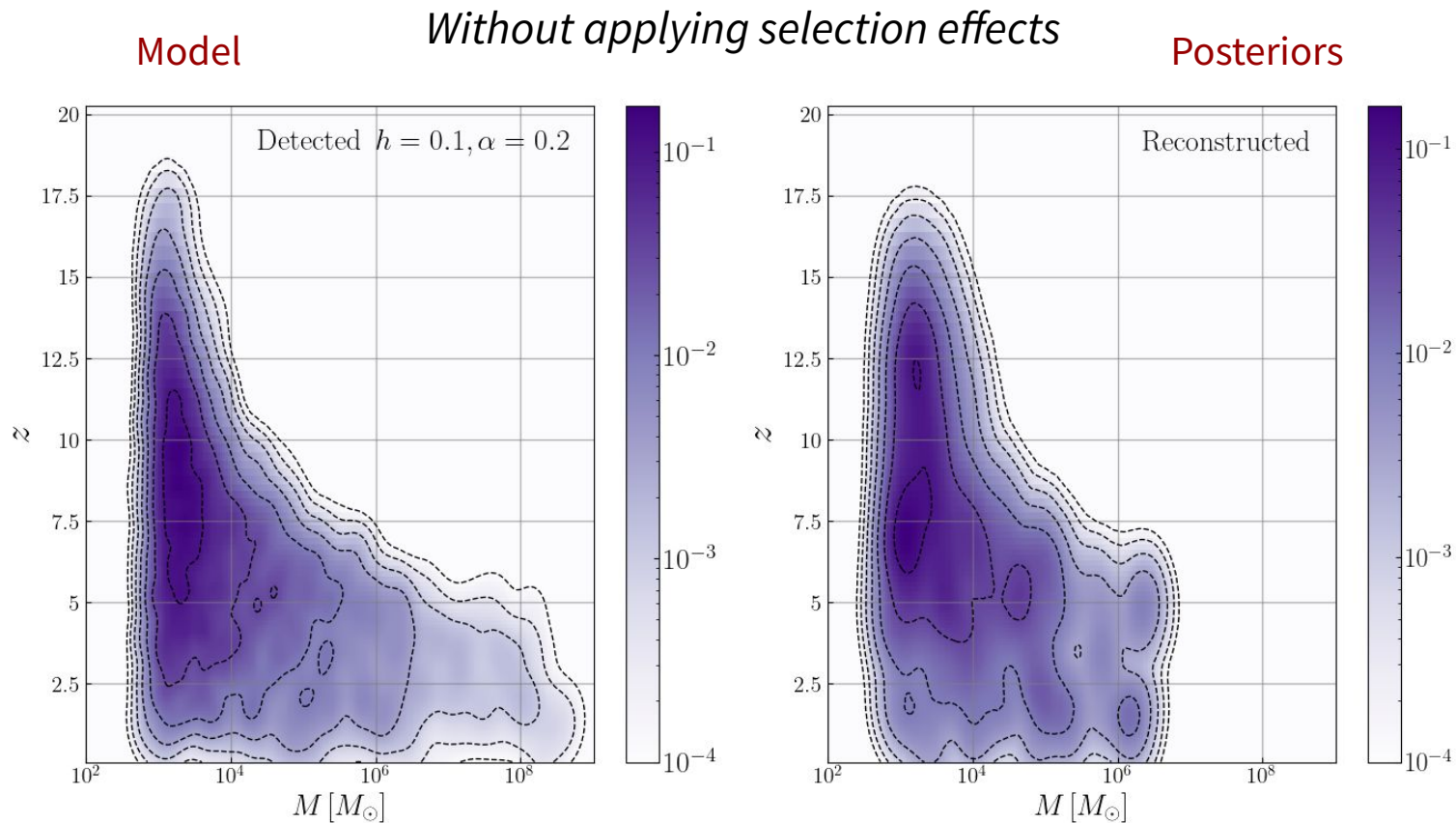
## Light-seed model: popIII-d (K+16)



From Phys. Rev. D 93, 024003 (2016)

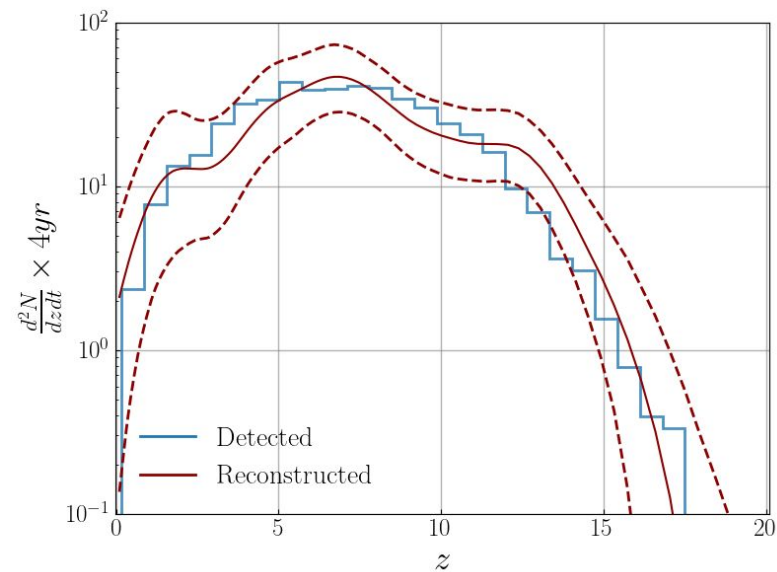
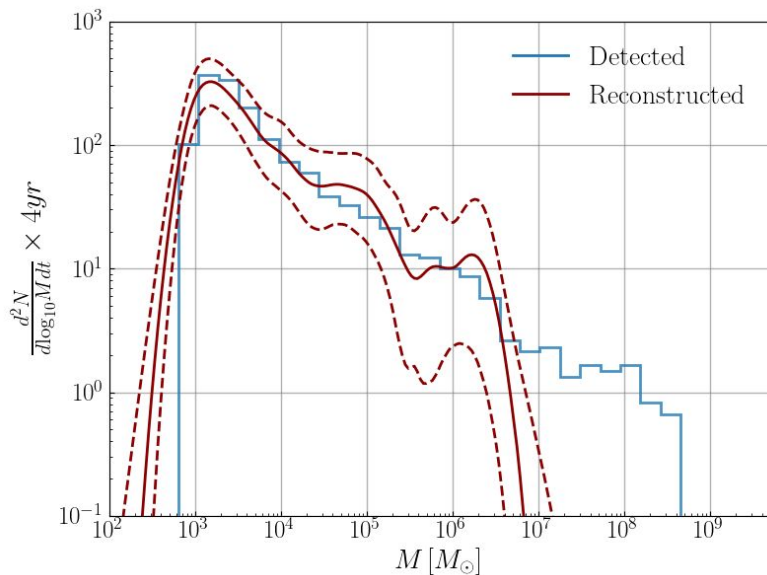


# Results: KDE reconstruction



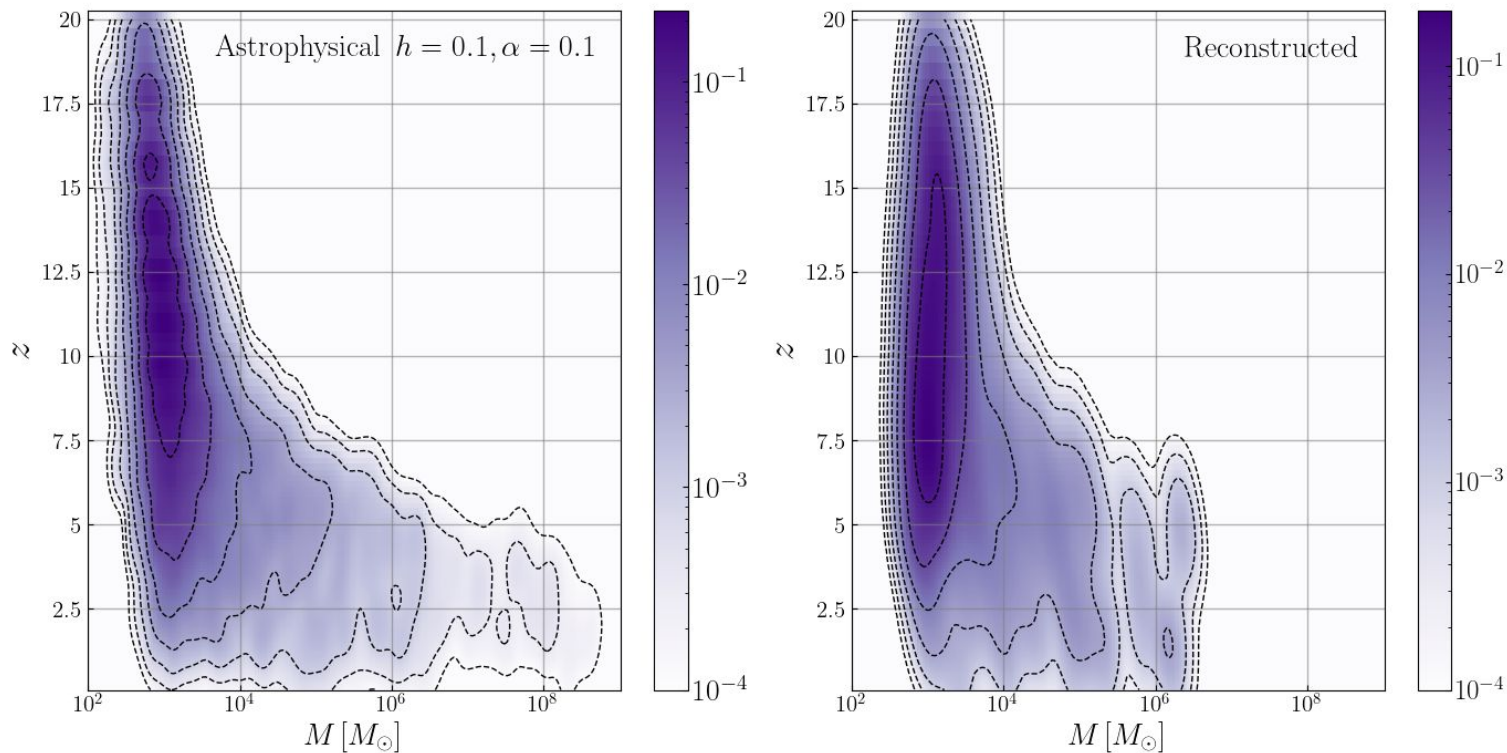
# Results: Rates without Selection effects

Rate = KDE\*Number of events



# Results: KDE reconstruction

*Applying selection effects: weights = 1/pdet*

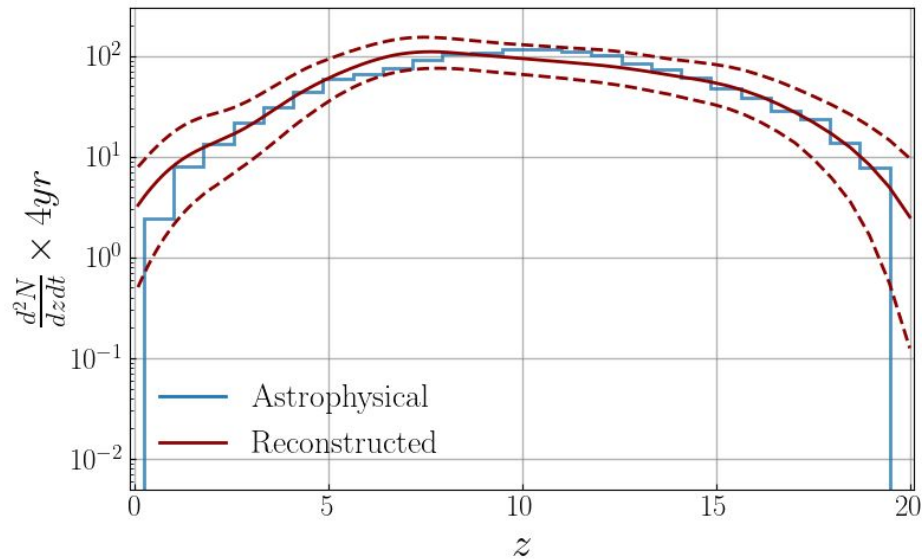
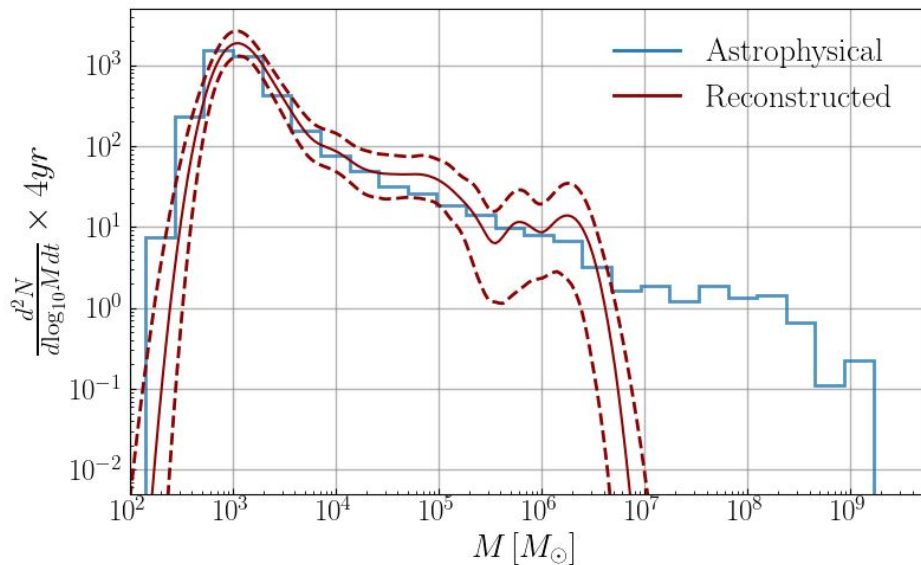




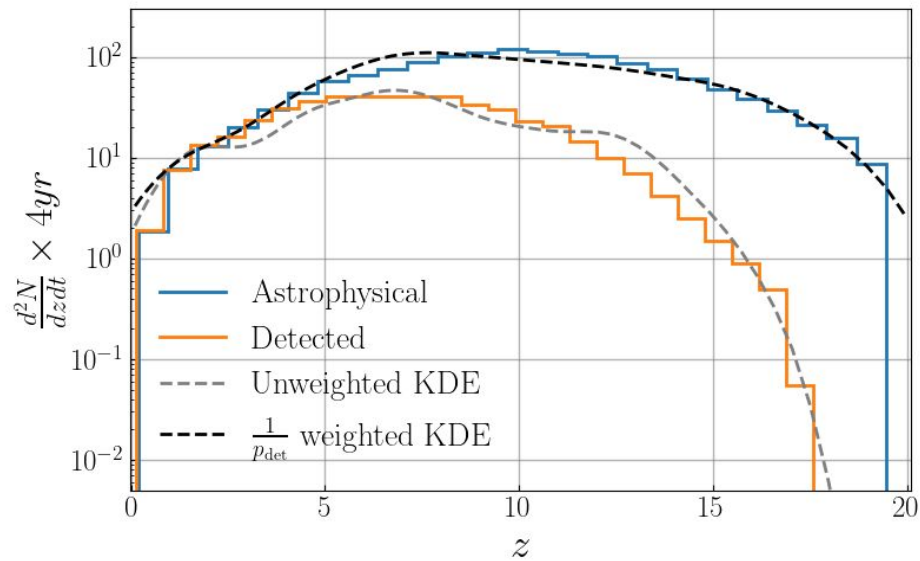
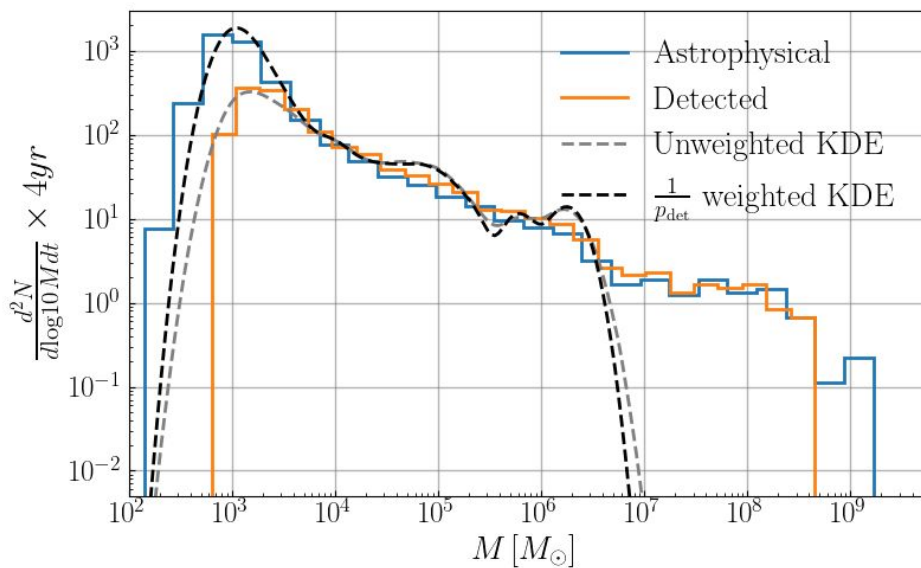
# Results: Rates from KDE with Selection Effects

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# Results



**Future: Test Adaptive KDE with Selection Effects  
For other light seed models**

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# Quick Recap

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- 1) KDE as non parametric model for population analysis
  - a) Adaptive KDE without selection effects
  - b) Weighted KDE with selection effect
  
- 2) Iterative Reweighting to reduce PE uncertainty
  
- 3) Fast, Flexible method for quick Population Analysis
  
- 4) Future: Weighted Adaptive KDE fixing selection effects for small values

# Questions!

# Future Work

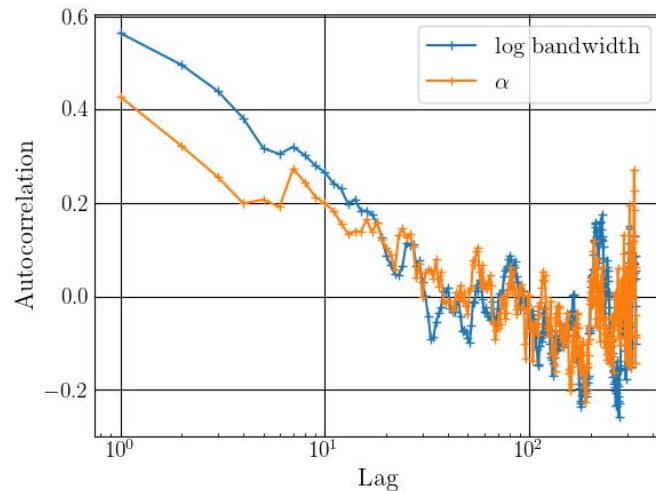
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- Extension of multidimensional iterative awKDE including component spins, mass-ratio
  - Technical issue in optimizing the Gaussian kernel for a multidimensional data set, where it will not be appropriate (or even meaningful, given the different units) to impose equal variances over different parameters as we currently do for (log)  $m_1$  and  $m_2$
  - For more than two dimensions a grid search may not be practicable; more sophisticated methods may be required in order to realize the potential of iterative KDE over a full set of population parameters

# Autocorrelation of KDE 'hyper'parameters

- KDE has global bandwidth (bw) and adaptive ( $\alpha$ ) parameters
- Optimized via CV max likelihood at each iteration
- Monitor evolution to characterize the process
- Autocorrelation close to 0 after ~30 iterations



# Rates and Population Analysis

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## Why:

- From features in population study, **understand the astrophysical origin** of detected events
- **Improve theoretical models**, learn about outliers ,....

## How:

### **Parametric Method:**

Have **functional form**

Good: extrapolation, robust even with few events, Bayes factor, Interpretable

Issues: Bound to specific functional form,  
**New features to be added by hand**

### **Non Parametric Method:**

Good: **Data based, flexible**, can be computationally efficient, provide insights for parametric models

Issues: no extrapolation, no Bayes factor, **no direct connection with physics**

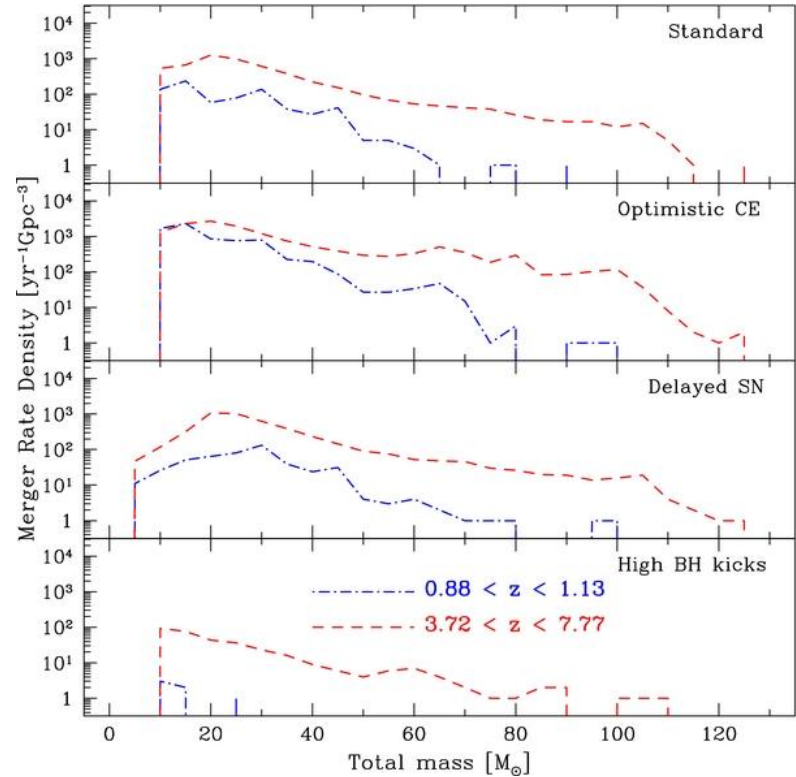


# Population Study

- Population analysis to understand individual events
  - New events exciting as an outlier in population
  
- From features in population study, understand the astrophysical origin of detected events
  - Stellar evolution, formation channel, cosmology

# Astrophysical Models vs Gravitational Wave Detections

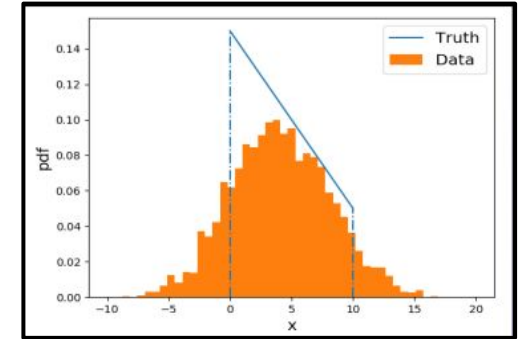
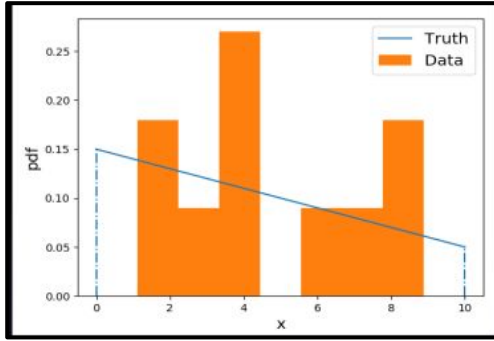
- Astrophysics modelling  
⇒ expected merger  
distribution over redshift,  
masses, spins ...
- Models do not predict  
individual merger parameters
- GW detections ⇒ distribution  
"samples"



Dominik et al. Astrophys.J. 779 (2013) 72

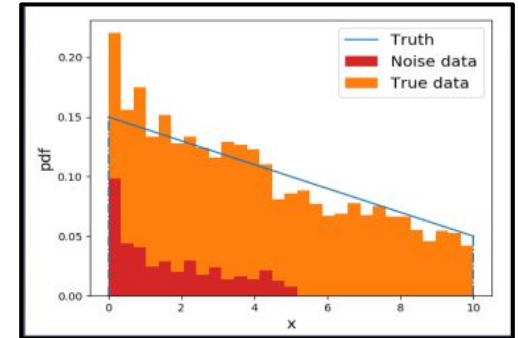
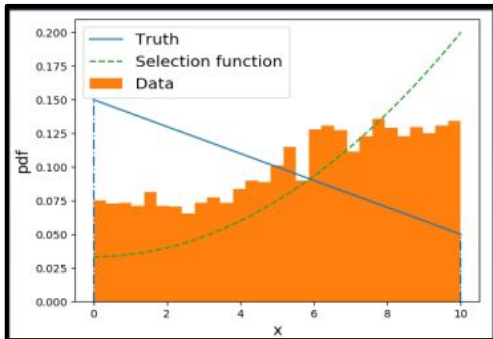
# Hazards of Gravitational Wave Population Analysis

Low event Statistics



Measurement error

Selection bias



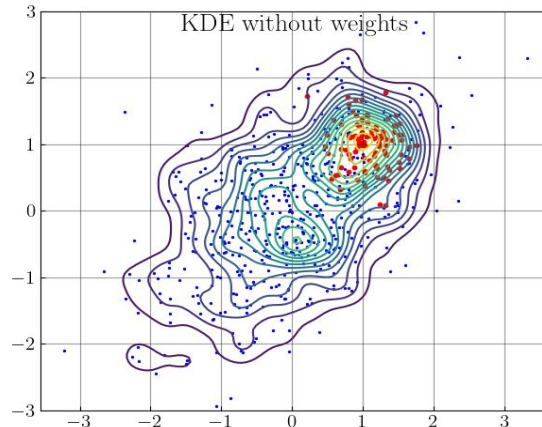
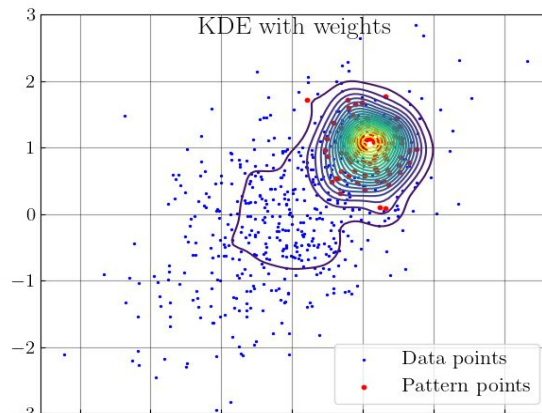
Noise contamination

# Weighted Kernel Density Estimation (Weighted-KDE)

- Using a global bandwidth for a Gaussian KDE with weights based on data points

$$\hat{f}(x) = \frac{1}{\sum_i W_i} \sum_{i=1}^n \frac{W_i}{h\lambda_i} K\left(\frac{x - X_i}{h\lambda_i}\right).$$

$$\sum_i W_i = n, \quad W_i \iff X_i, \quad \lambda_i = 1$$



# Selection Effects

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- To Get the Rates from density estimate, account for selection bias

$$p_{\text{det}}(x, \theta) = \int p(\rho > \rho_{\text{th}} | \bar{\rho}(x, \theta, \psi)) p(\psi) d^n \psi,$$

$$R_{\text{det}}(x) = \int R(x, \theta) p_{\text{det}}(x, \theta) d^n \theta.$$

$$R(x, \theta) = R(x) p_{\text{pop}}(\theta)$$

$$\begin{aligned} R_{\text{det}}(x) &= R(x) \int p_{\text{pop}}(\theta) p_{\text{det}}(x, \theta) d^n \theta \\ &\equiv R(x) p_{\text{det}}(x; p_{\text{pop}}), \end{aligned}$$