A new unified perspective on the problem of limited Monte Carlo for likelihood calculations

Based on 1712.01293
and "to be published"
(in a few days on arXiv)

ERLANGEN CENTRE FOR ASTROPARTICLE PHYSICS

PHYSTAT-ν CERN 2019

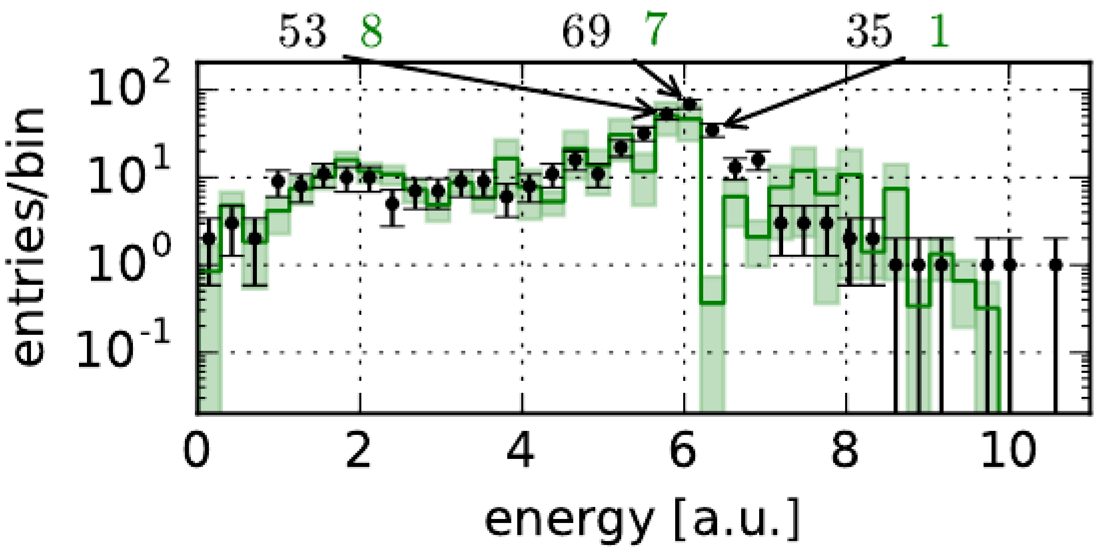
Thorsten Glüsenkamp,

Phystat-ν, CERN, Jan. 2019

The challenge: limited MC in binned likelihoods

Example Poisson (1 bin):

$$\frac{e^{-\sum w_i} \cdot \sum {w_i}^k}{k!}$$



MC ≈ 0.1DATA

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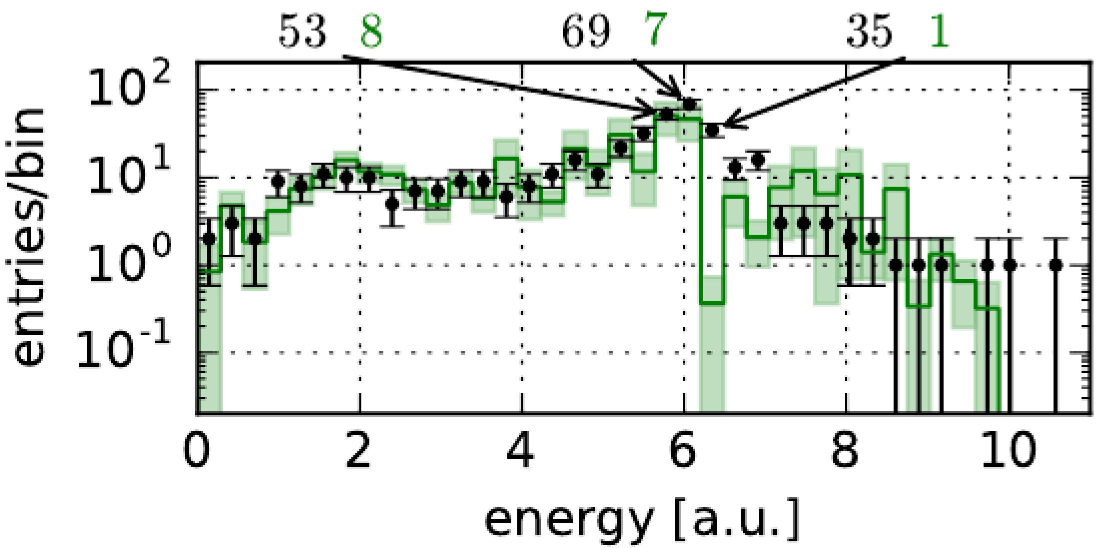

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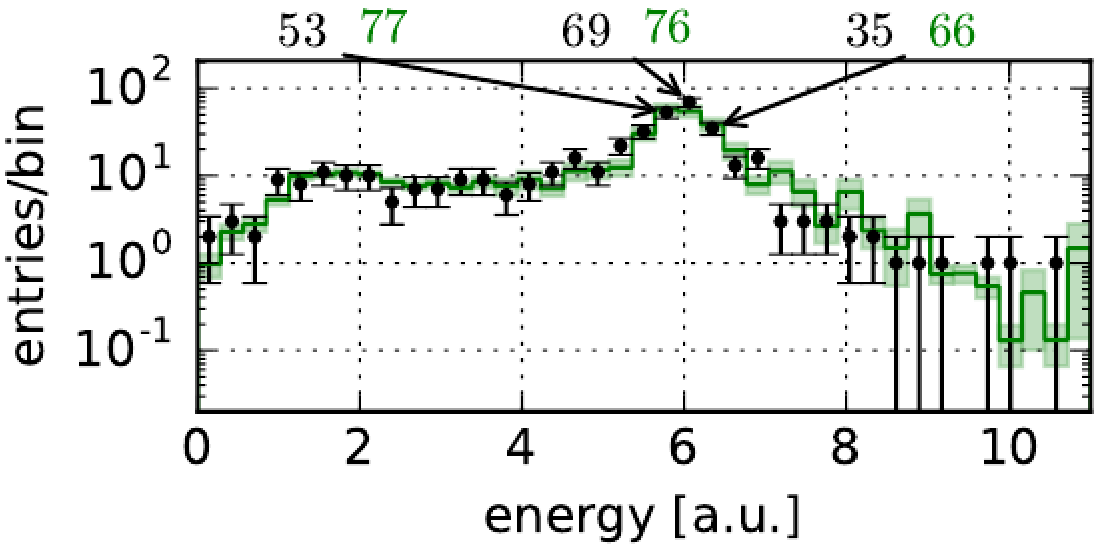

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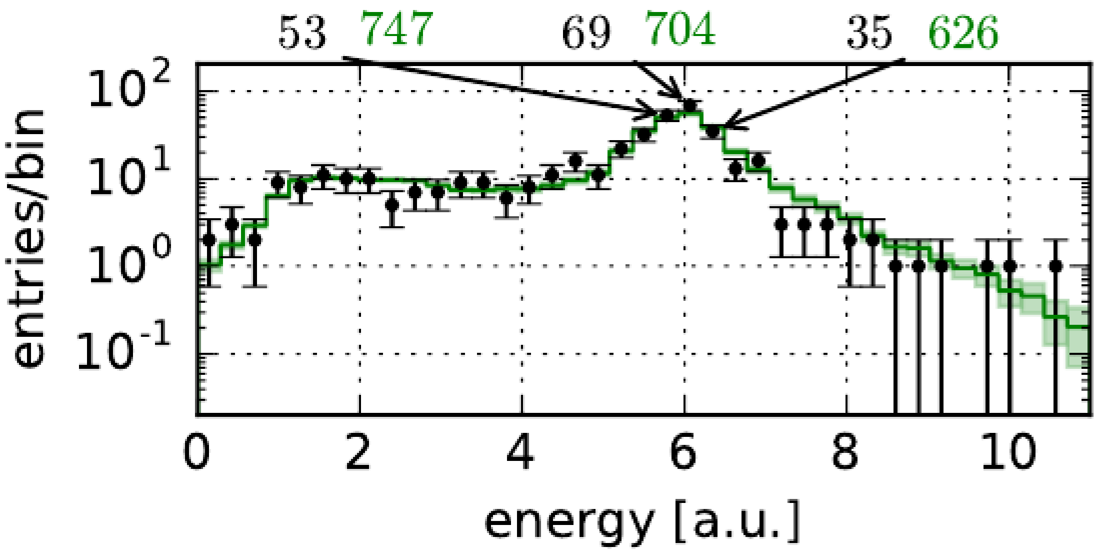

MC ≈ 10 DATA

Barlow, Beeston (93)

that these are damped by a factor N_D/N_j, but we cannot hope that this is small. There is a general rule of thumb that the MC samples should be ten times larger than the data sample, so any effects of finite MC data size are relatively small. Unfortunately many

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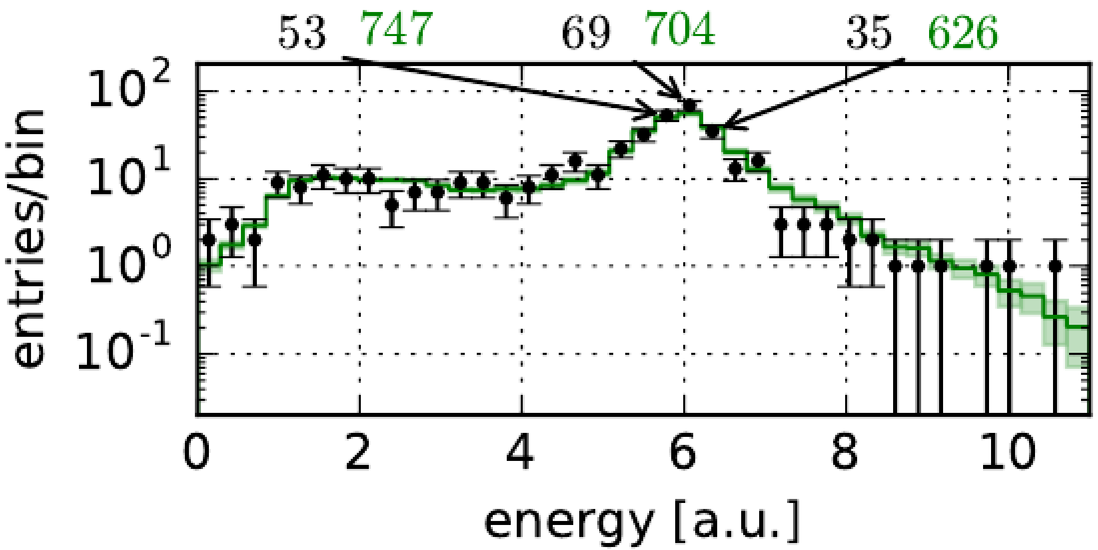

MC $\approx$ 10 DATA

Q: If we cannot get 10X MC, which procedures exist to handle the small MC samples?

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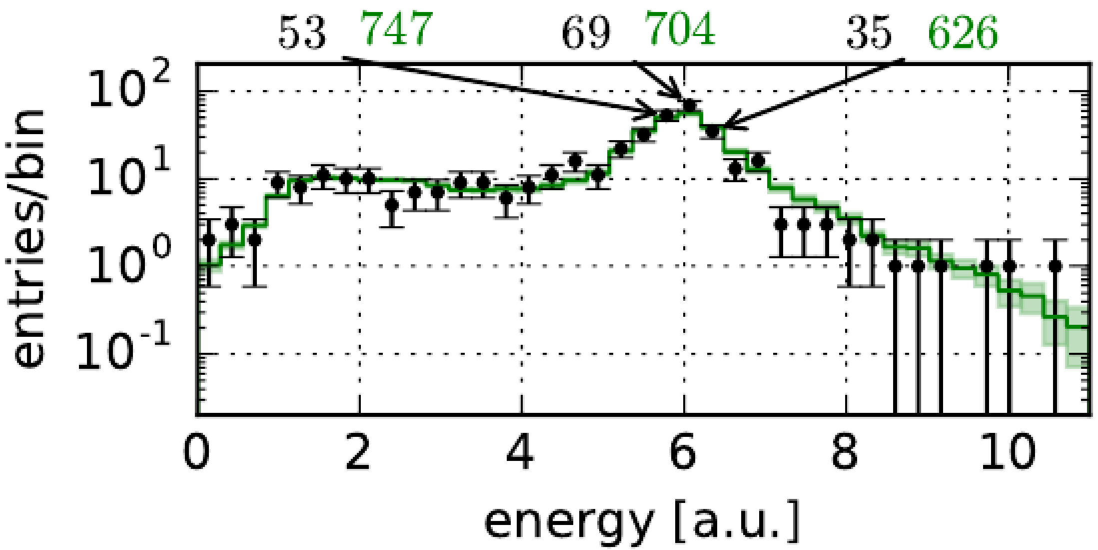

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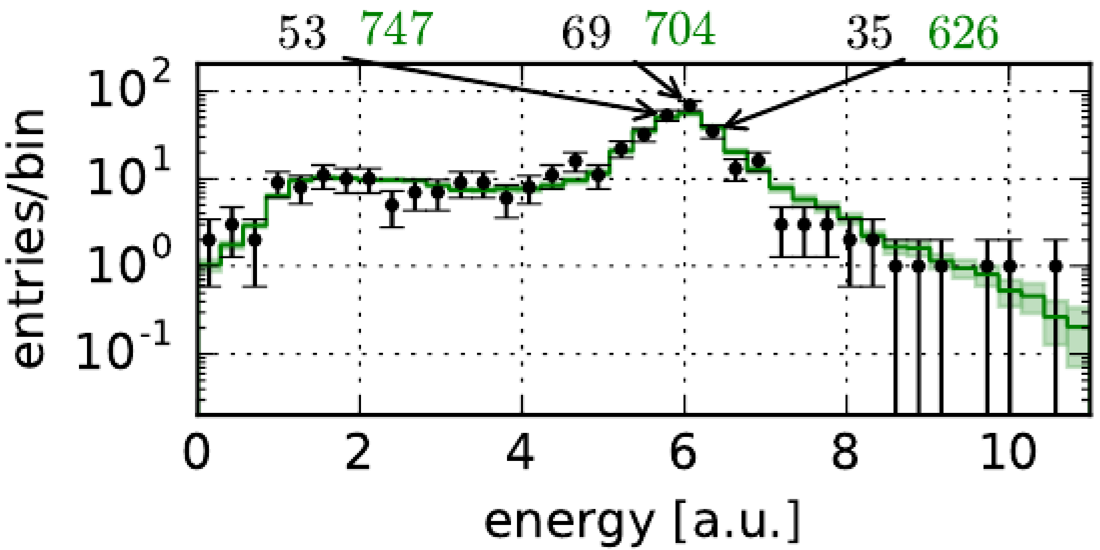

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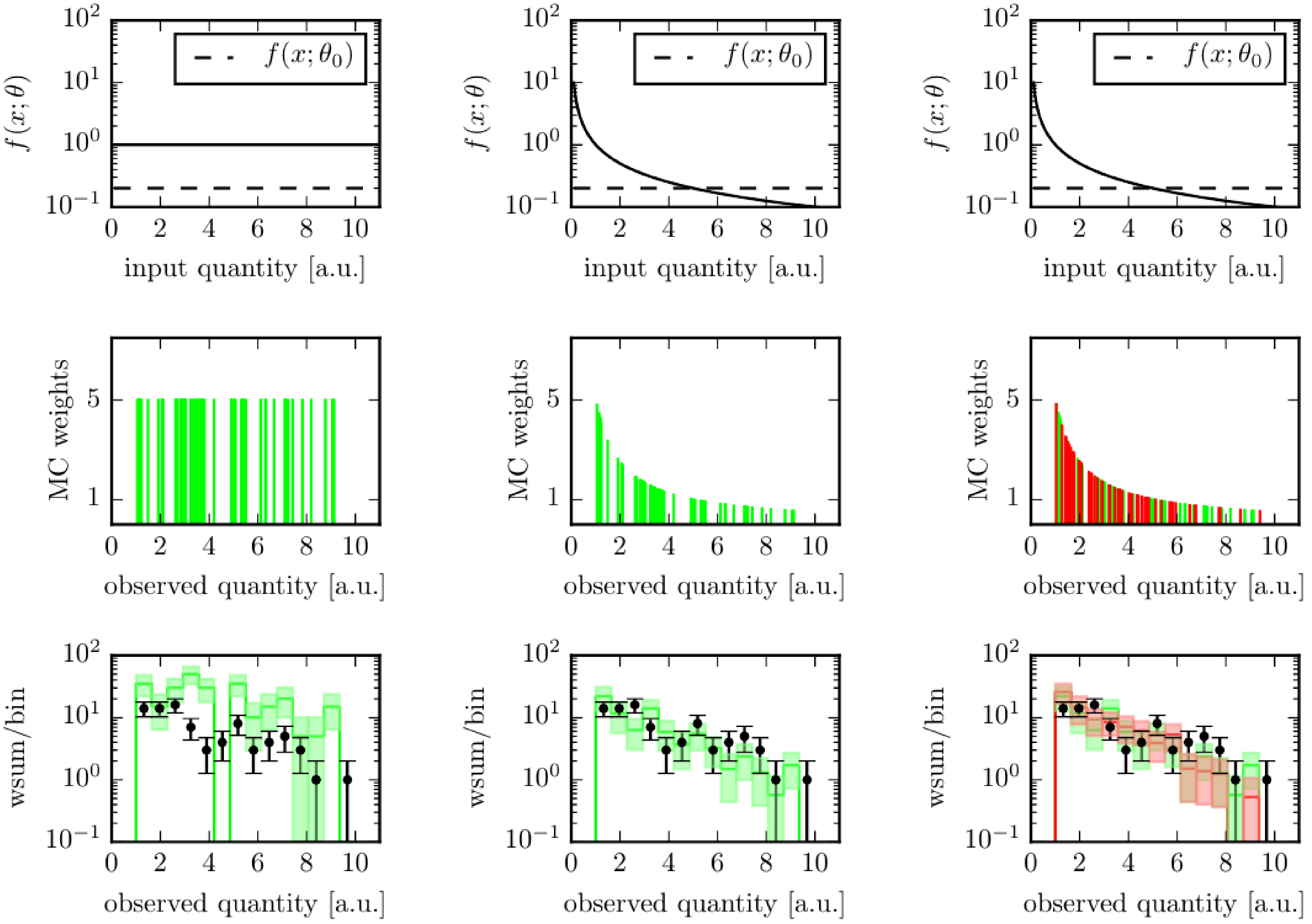
This talk: All approaches fundamentally approximate the CPD – with pros n cons

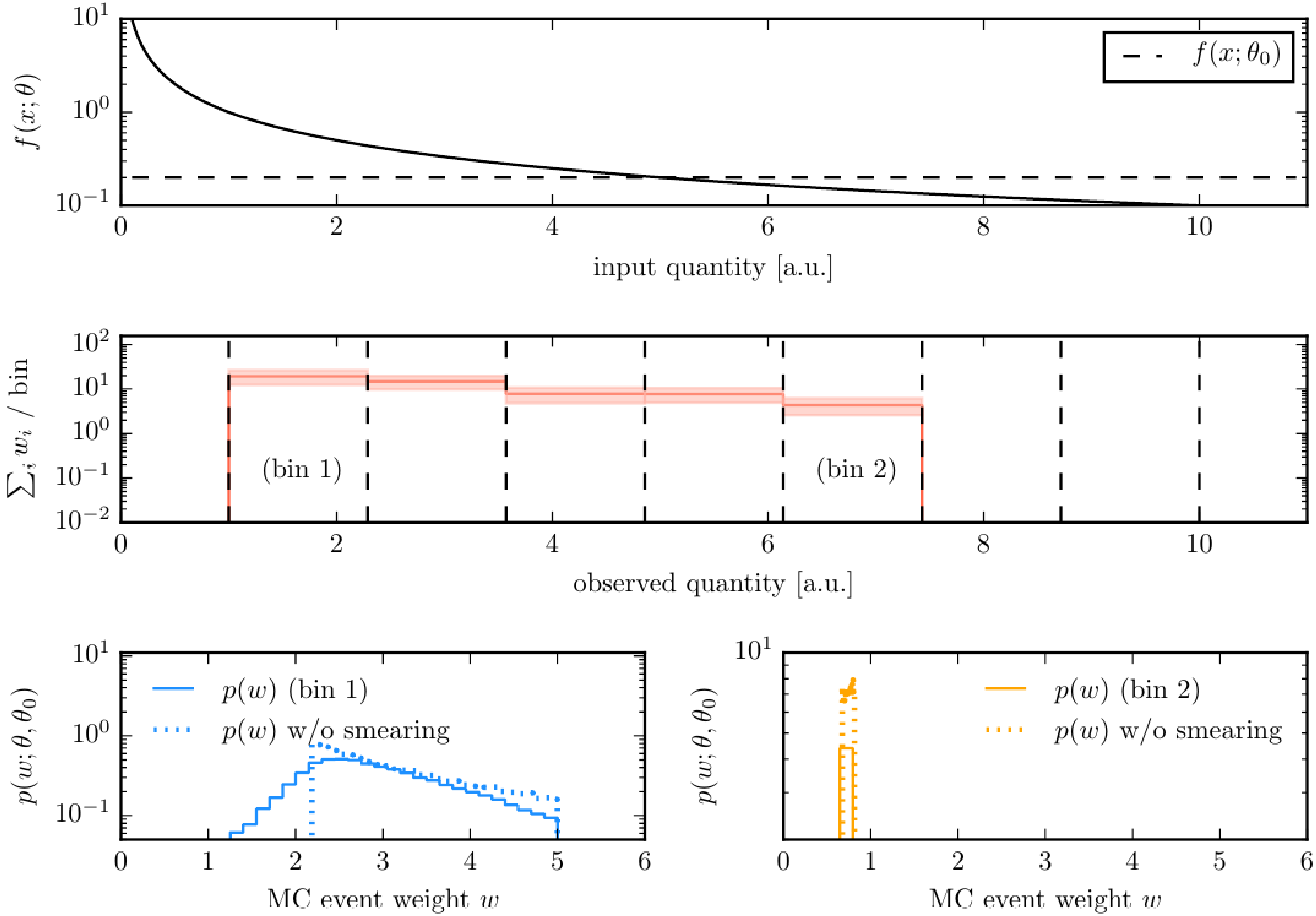
Overview

1. The probability distribution for the sum of weights
   Compound **P**oisson **D**istribution (CPD)
2. Approximations of the CPD in existing approaches
   - Probabilistic approaches have interesting connections to special functions, statistics, B-Splines
3. Some further not-yet discussed solutions
4. Performance Comparisons
5. Summary

3 steps to understand the CPD ..

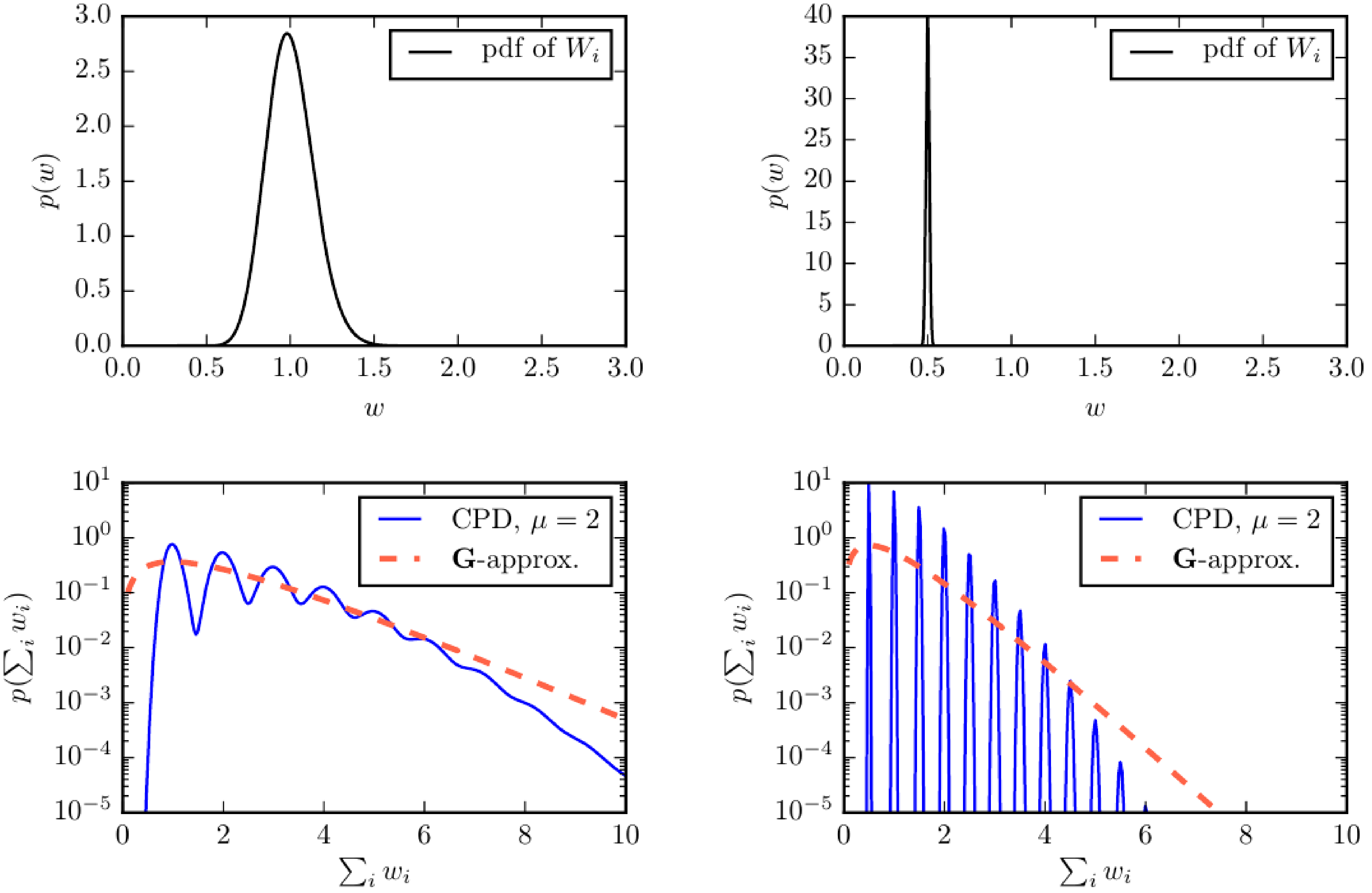


Step1: MC weighting



Step2: the distribution p(w)

Step3 – the CPD



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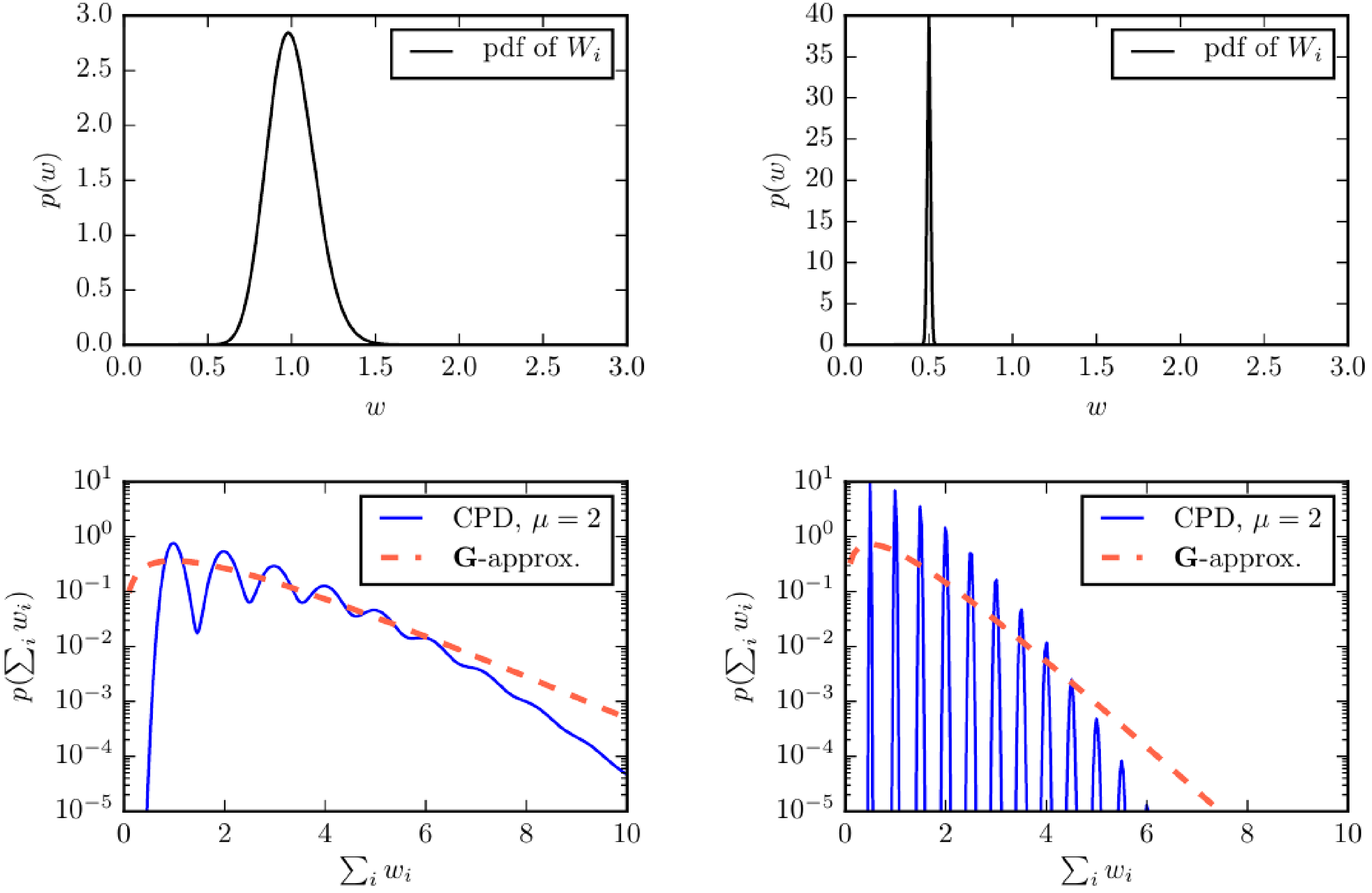

Probability distribution for the sum of weights: $p(\sum w)$

Random variable of CPD: Z

$$Z = \sum_{i=1}^{N} W_i$$

$$N \sim \text{Poisson}$$

$$\widehat{\mu}(Z) = \sum_i w_i$$

$$\widehat{\text{var}}(Z) = \sum_i w_i^2$$

↑

$$\text{E}[Z] = \mu_z = \text{E}[N] \cdot \text{E}[W]$$

$$\text{Var}[Z] = \text{E}[N] \cdot \text{Var}[W] + (\text{E}[W])^2 \cdot \text{Var}[N]$$

What we would like to do:

- Take PDF of the sum of weights (CPD) and integrate the Poisson mean

$$L_{bin,exact} = \int \frac{e^{-\lambda} \cdot \lambda^k}{k!} \cdot p_{CPD}(\lambda) d\lambda$$

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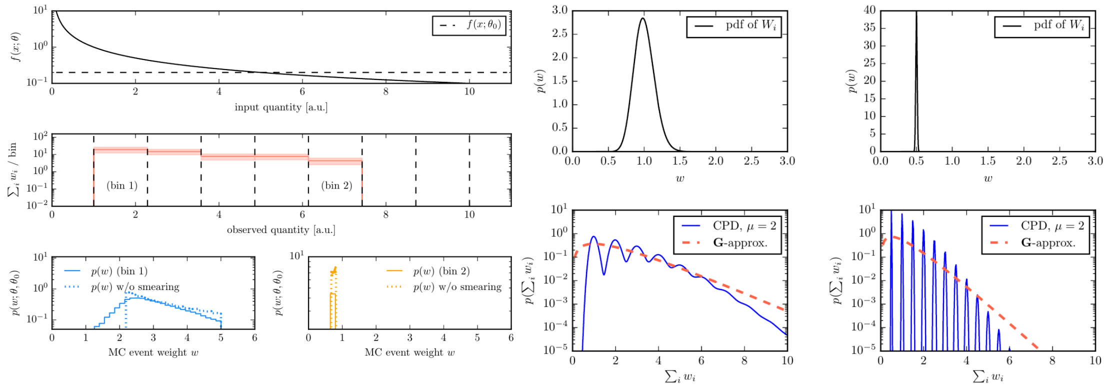

- However: CPD is <u>not tractable</u> (except for equal weights)

One possibility: Approximate and then integrate

Statistics of weighted MC

$$Z = \sum_{i=1}^{N} W_i$$
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Intead of

$$L_{bin,exact} = \int \frac{e^{-\lambda} \cdot \lambda^k}{k!} \cdot p(\lambda)_{CPD} d\lambda$$

Argüelles et al. (2019)

$$\int \mathbf{P}(k;\lambda) \cdot \mathbf{G}(\lambda;\alpha,\beta) d\lambda$$

$$\alpha = \frac{(\sum_i w_i)^2}{\sum_i w_i^2} + a \ , \ \beta = \frac{\sum_i w_i}{\sum_i w_i^2} + b$$

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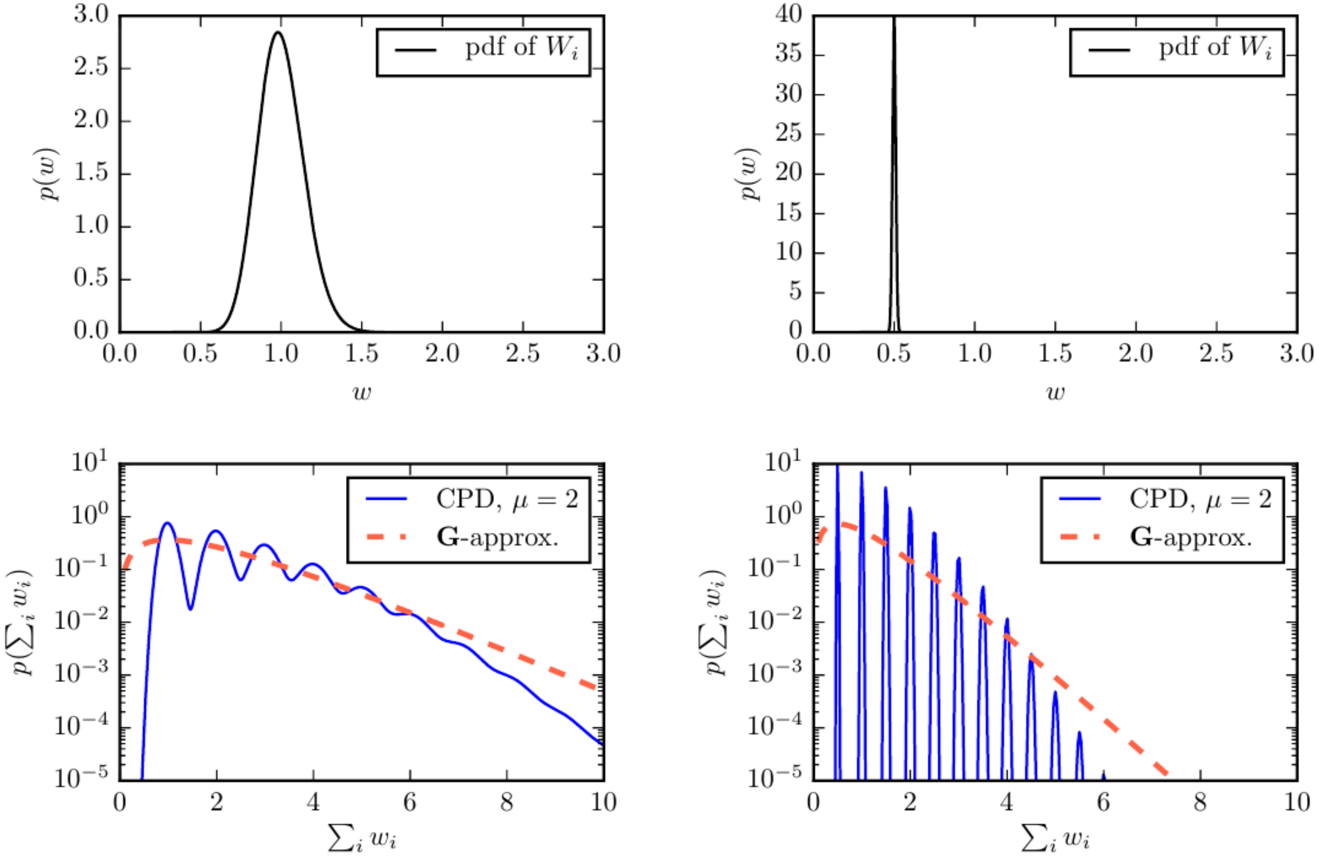
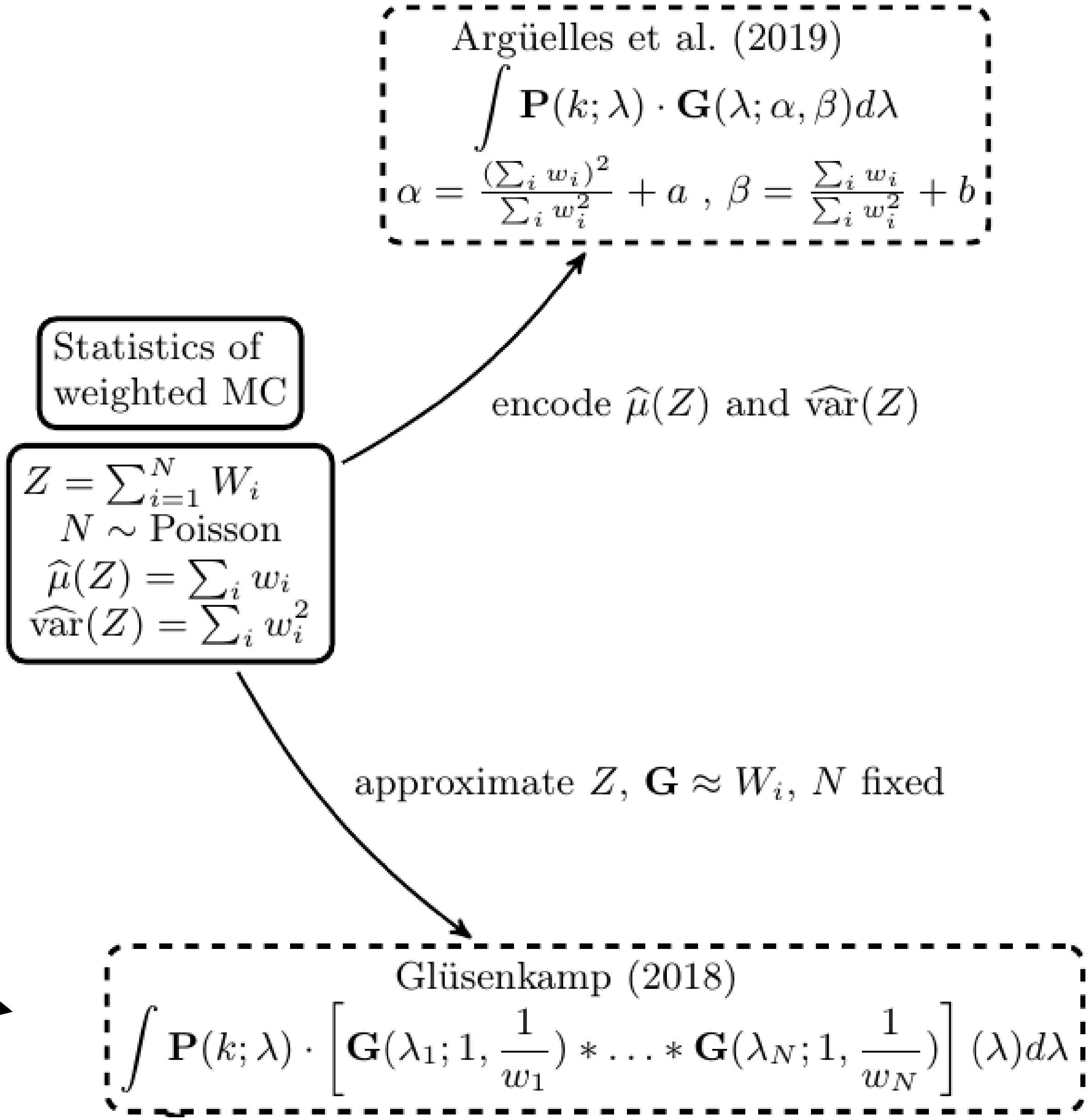
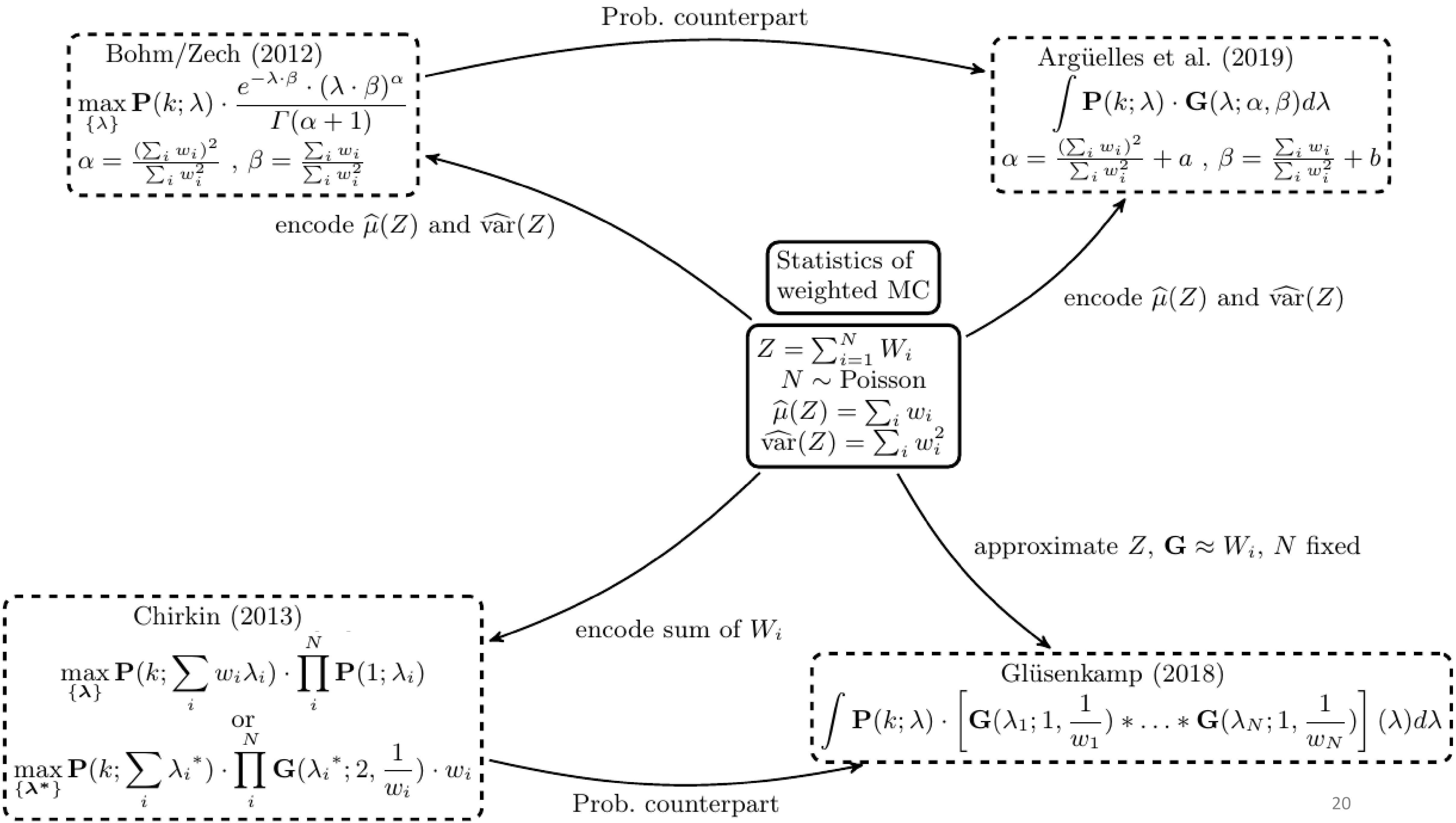


$$P(k; \Sigma\, w_i) = \frac{e^{-\sum w_i} \cdot \sum {w_i}^k}{k!} =$$

$$= \int \frac{e^{-\lambda} \cdot \lambda^k}{k!}\, \delta\left(\lambda - \sum w_i\right) d\lambda$$

$$= \int P(k; \lambda) \cdot [\delta(\lambda - w_1) * \cdots * \delta(\lambda - w_n)](\lambda)\, d\lambda$$





Prob. counterpart
Bohm/Zech (2012)
$\max_{\{\lambda\}} \mathbf{P}(k;\lambda) \cdot \frac{e^{-\lambda \cdot \beta} \cdot (\lambda \cdot \beta)^{\alpha}}{\Gamma(\alpha+1)}$
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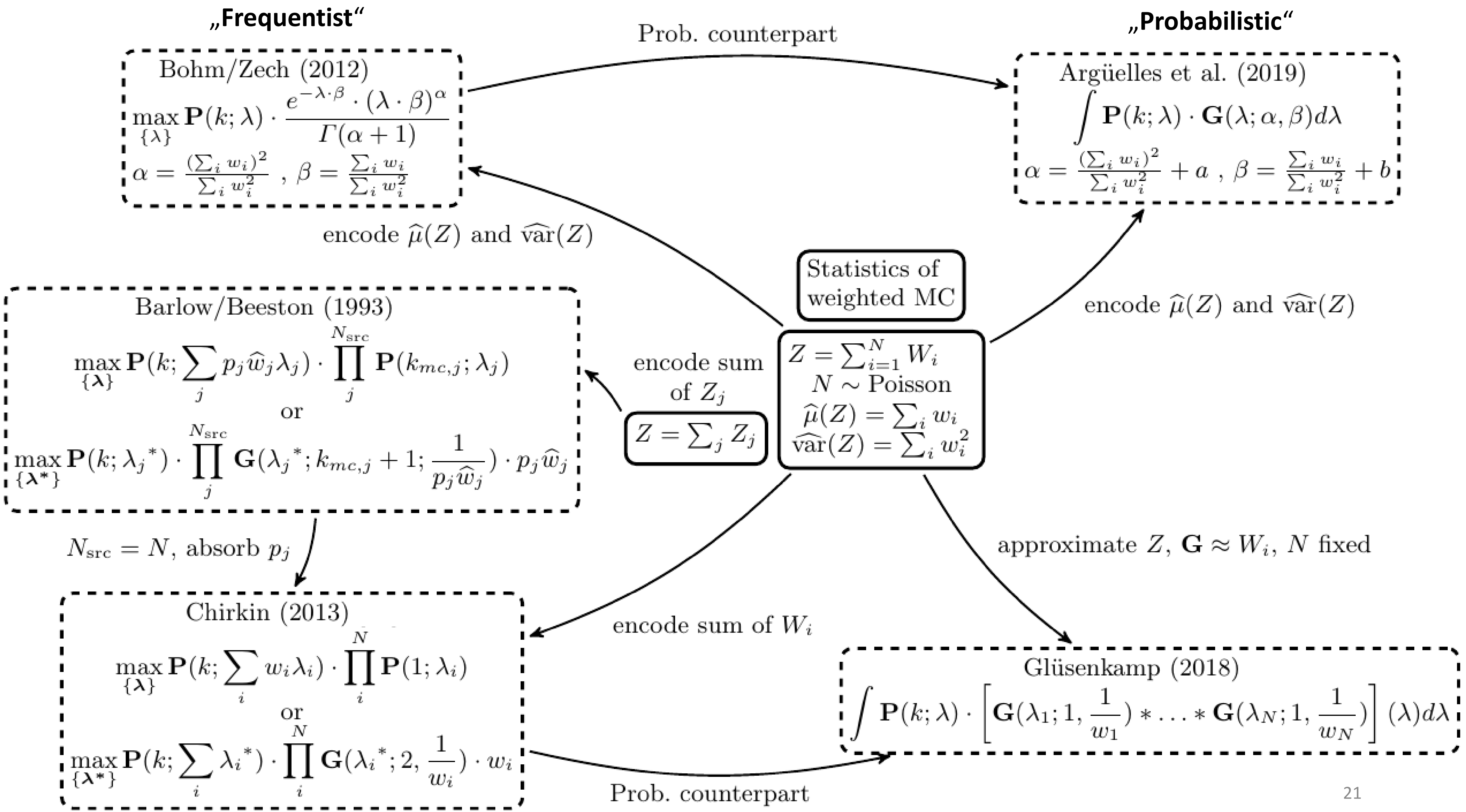
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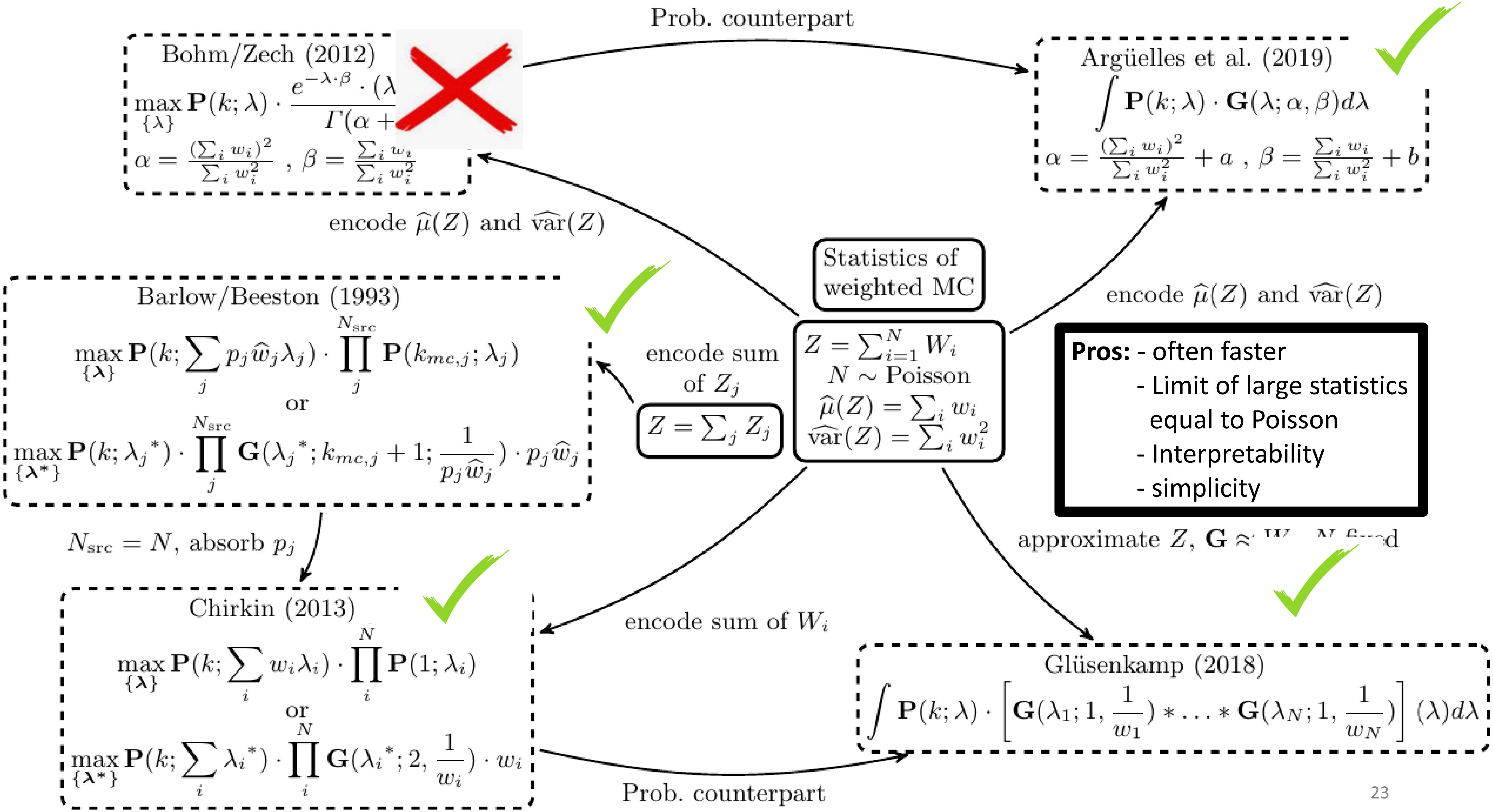

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Pretty much indistinguishable results

Both allow for prior freedom

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How can we calculate this integral

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Di Salvo´08 → $\sim F_D$

↓ *Carlson ´63*

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↓ *Dickey ´82*

$$\sum_{\sum_i k_i = k,\ k_i \geq 0} \prod_i \frac{\Gamma(k_i+\alpha_i)}{k_i! \cdot \Gamma(\alpha_i)} \cdot \beta_i^{\alpha_i} \cdot \left(\frac{1}{1+\beta_i}\right)^{k_i+\alpha_i}$$

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← *Egorychev Rules ´80s*

$$\sim \frac{1}{2\pi i}\cdot\oint_{\rho=\epsilon}\frac{1}{t^{a-c+1}\cdot\prod_i^N (t-1/z_{+1,i})^{b_{+1,i}}}dt$$

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Di Salvo´08 → $\sim F_D$

$$D_k(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{1}{k}\sum_{j=1}^{k}\left[\left(\sum_{i=1}^{N}\alpha_i\cdot\frac{1}{1+\beta_i}^{j}\right)D_{k-j}\right] \quad \text{and } D_0 = 1$$

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$$\int_0^\infty \mathrm{P}(k;\lambda)\cdot\left[\mathrm{G}(\lambda_1;\alpha_1,\beta_1) * \ldots * \mathrm{G}(\lambda_N;\alpha_N,\beta_N)\right](\lambda)\; d\lambda$$

Di Salvo´08 → $\sim F_D$

$$D_k(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{1}{k}\sum_{j=1}^{k}\left[\left(\sum_{i=1}^{N}\alpha_i\cdot\frac{1}{1+\beta_i}^{\,j}\right)D_{k-j}\right] \quad \text{and } D_0 = 1$$

$\sim F_D$ → *Carlson ´63* → $\sim$ Carlson R_n

Exact n-th B-Spline Moment w/ arbitrary knots

Legendre Polynomials and others

....

...

Dickey ´82

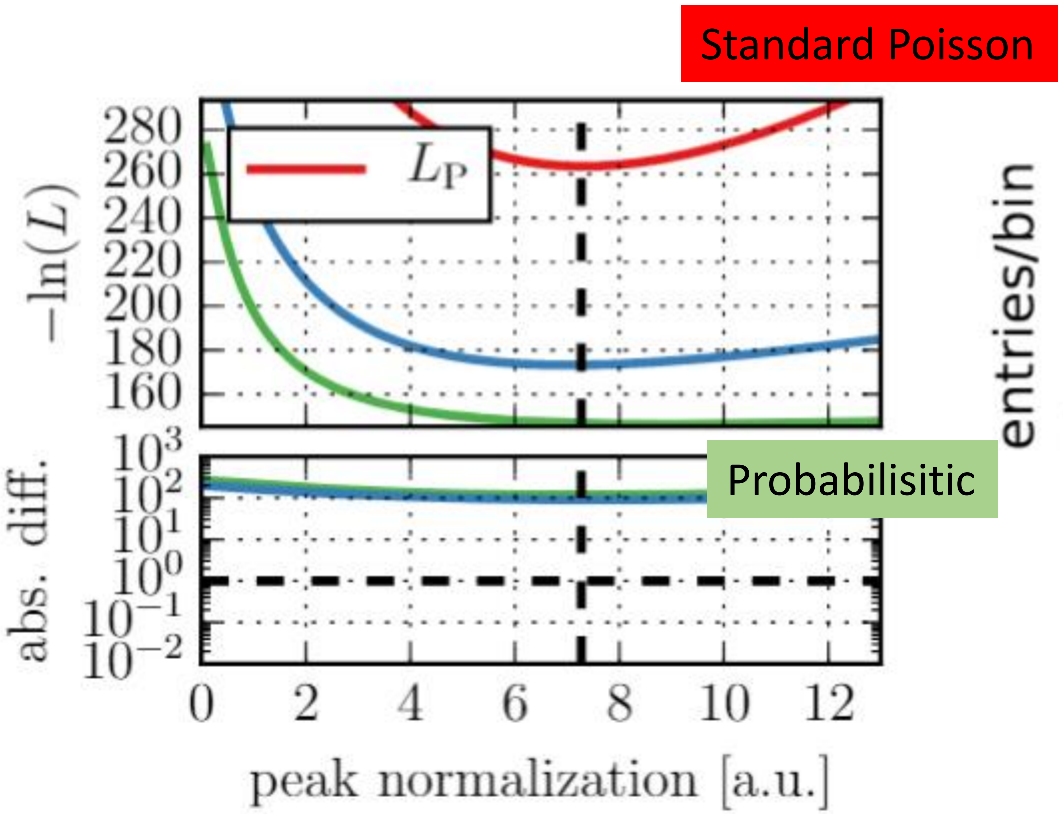
$\sim \frac{1}{2\pi}$ … dt

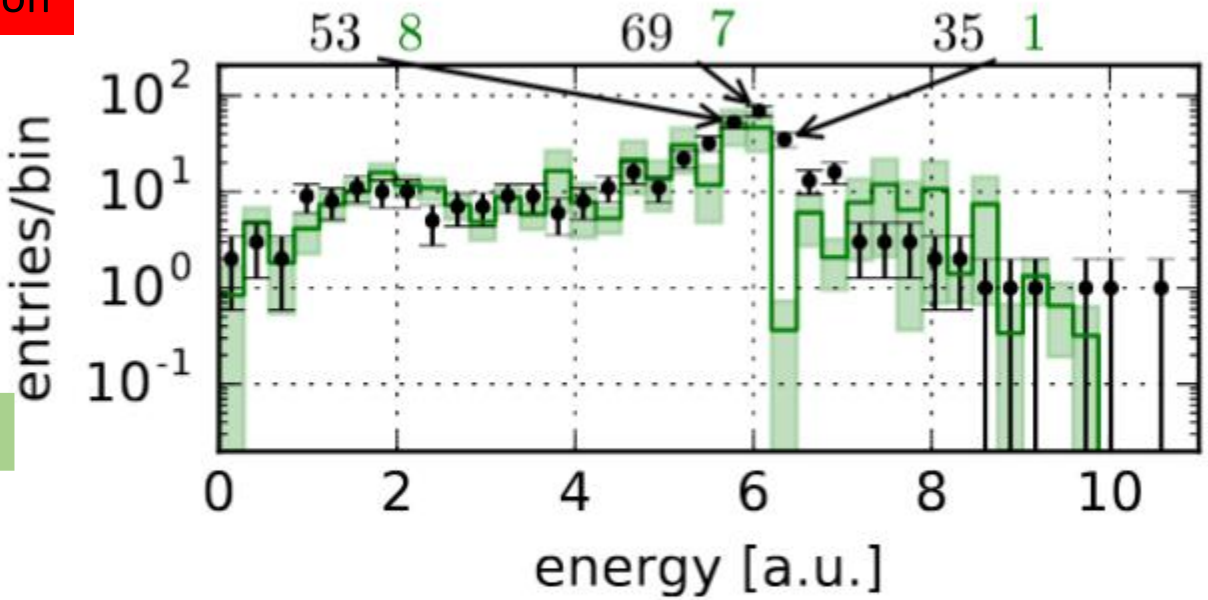
The problem of limited Monte Carlo is connected to these other areas in statistics and special functions

Egorychev Rules ´80s

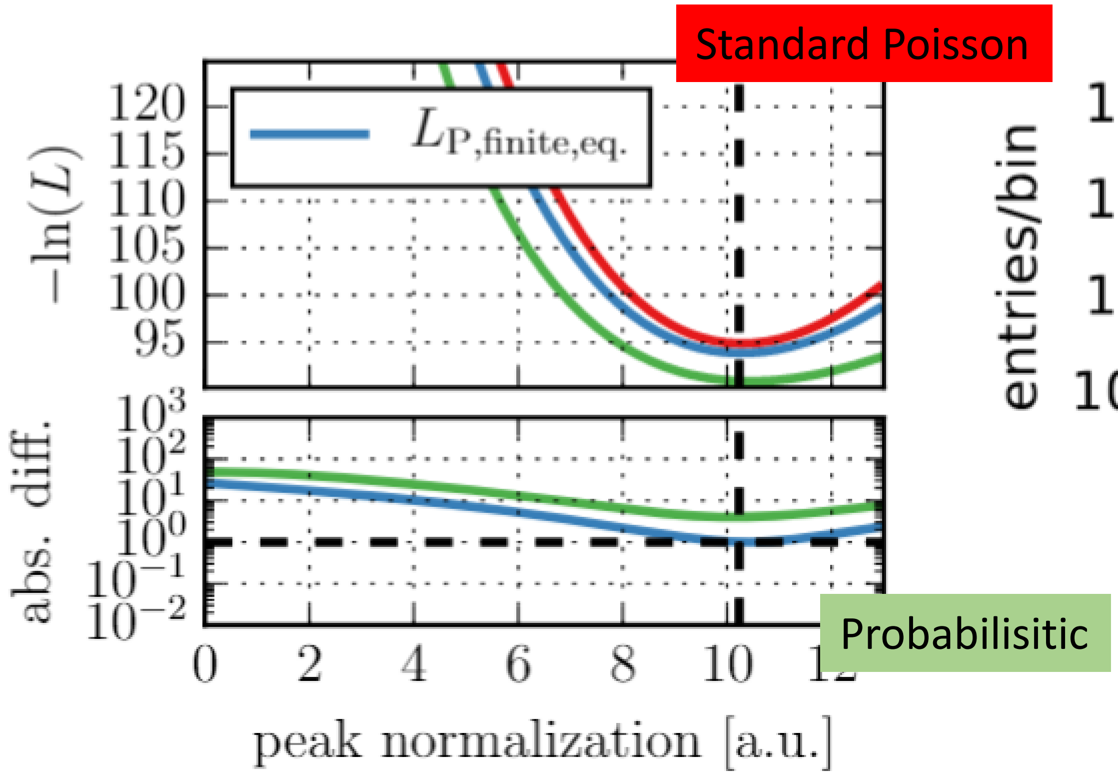
$$\sum_{\sum_i k_i = k,\; k_i \geq 0}\;\prod_i \frac{\Gamma(k_i+\alpha_i)}{k_i!\cdot\Gamma(\alpha_i)}\cdot\beta_i^{\alpha_i}\cdot\left(\frac{1}{1+\beta_i}\right)^{k_i+\alpha_i}$$

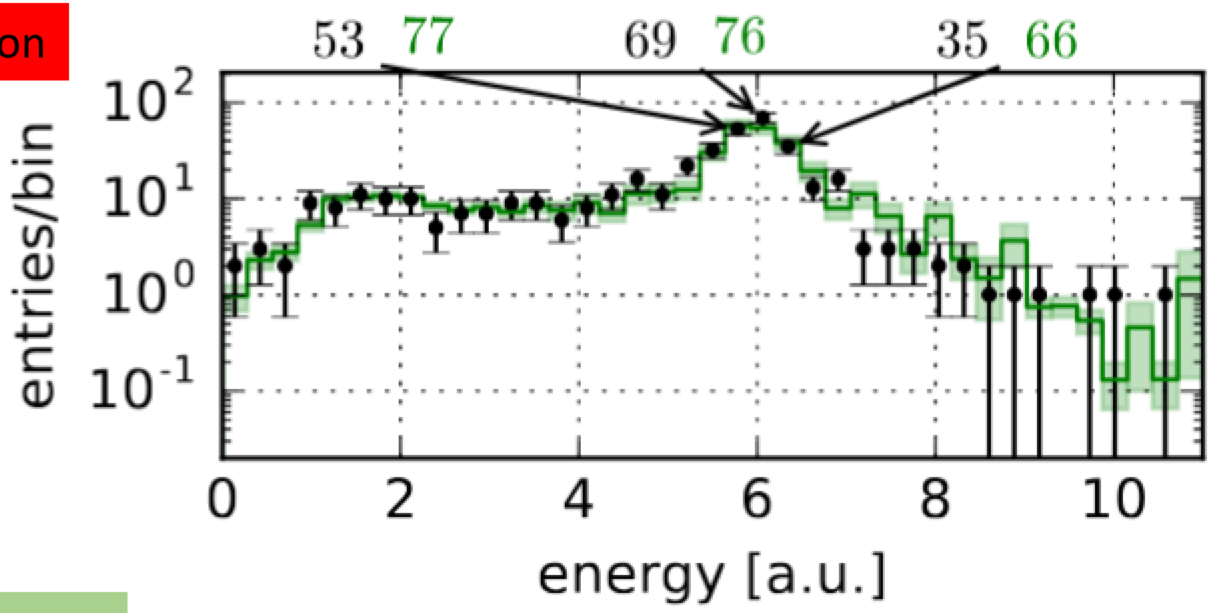
Comparisons





Comparisons





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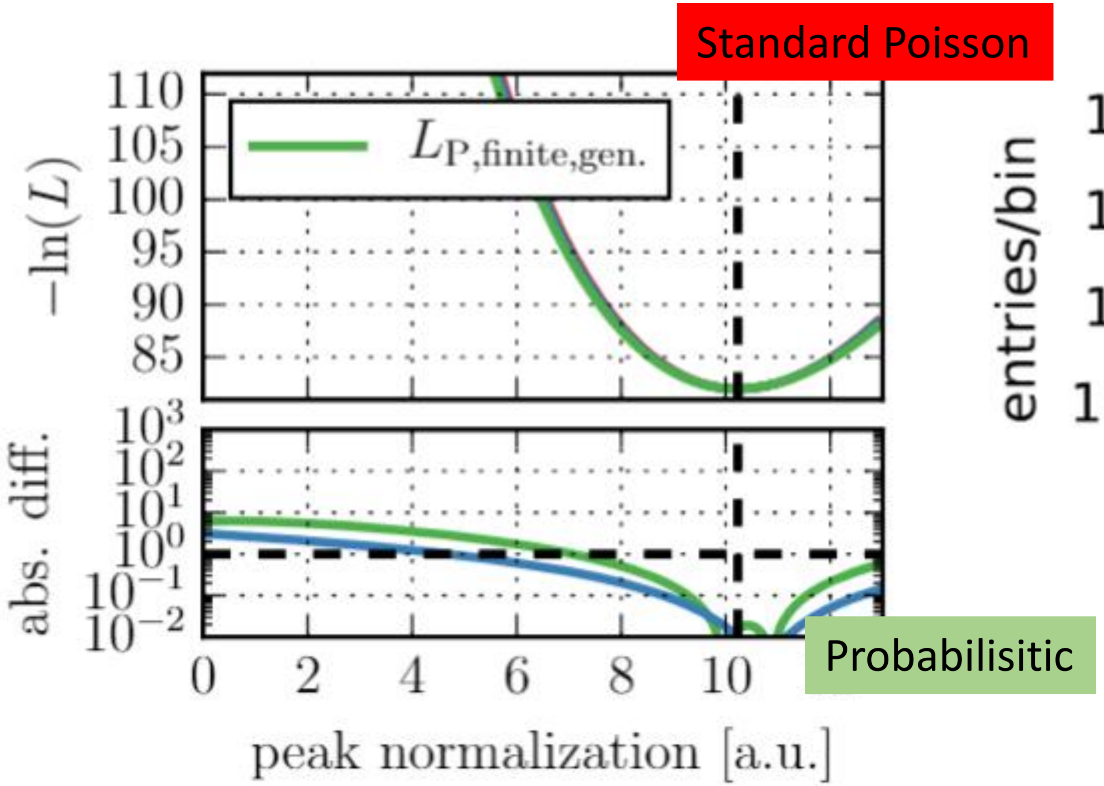
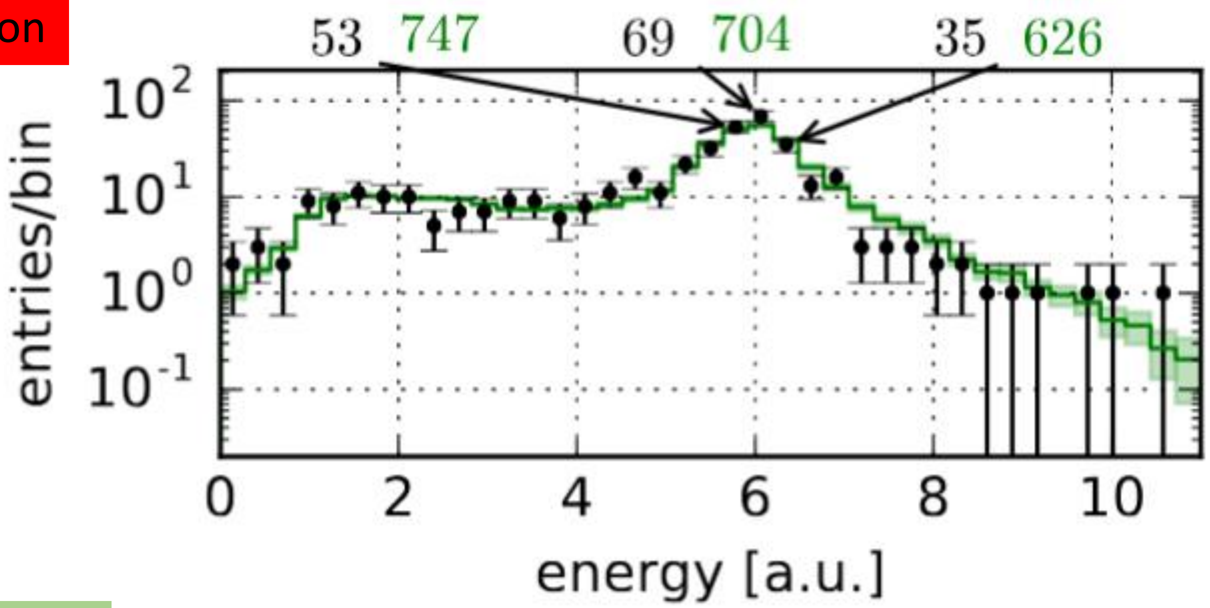
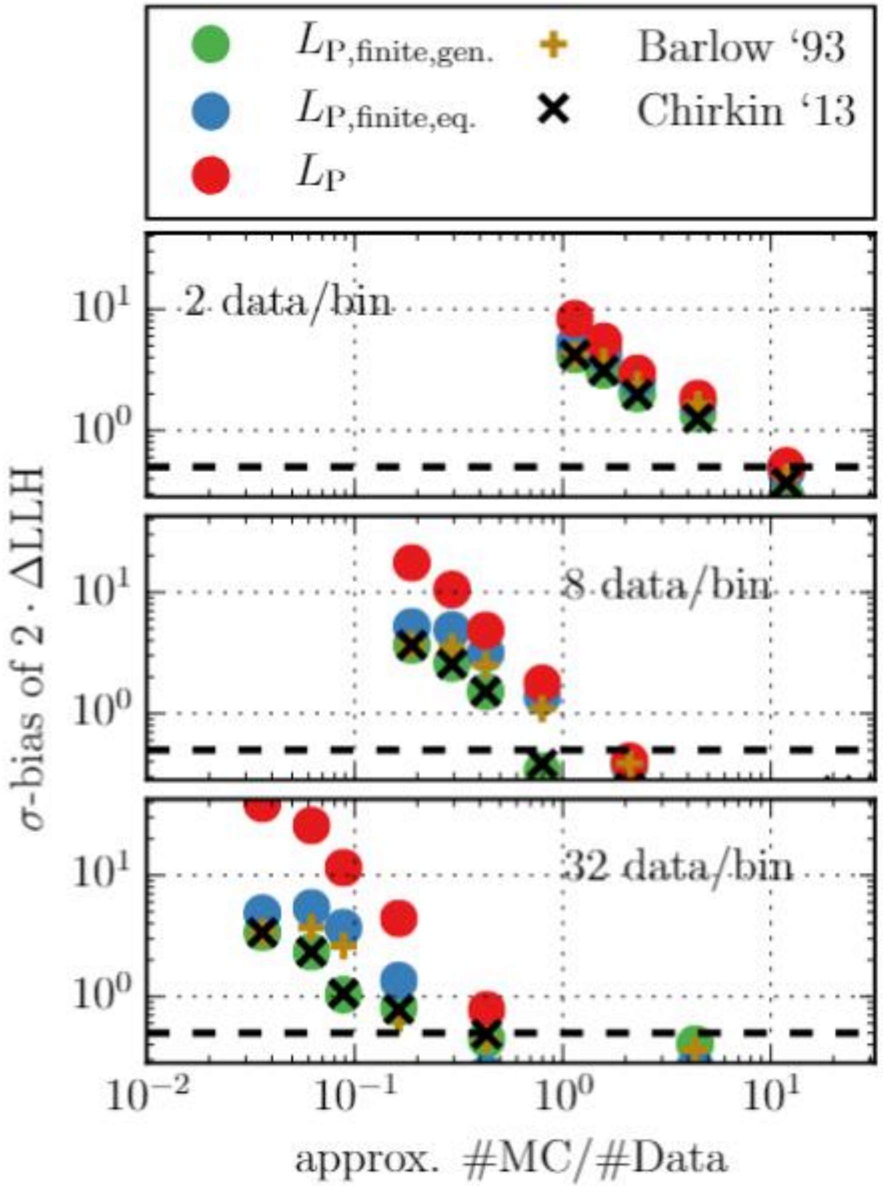
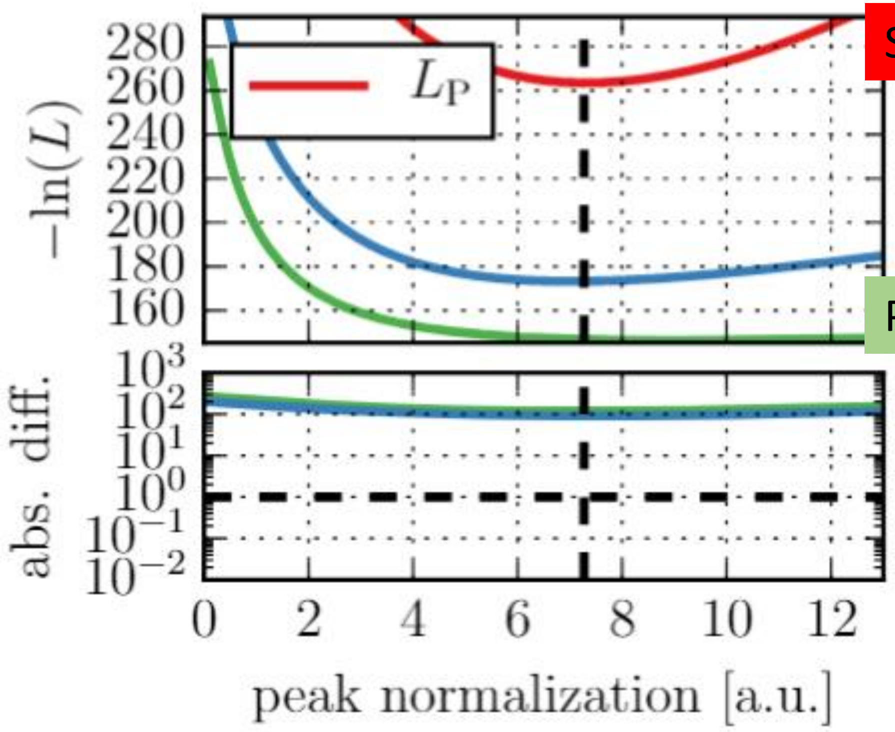




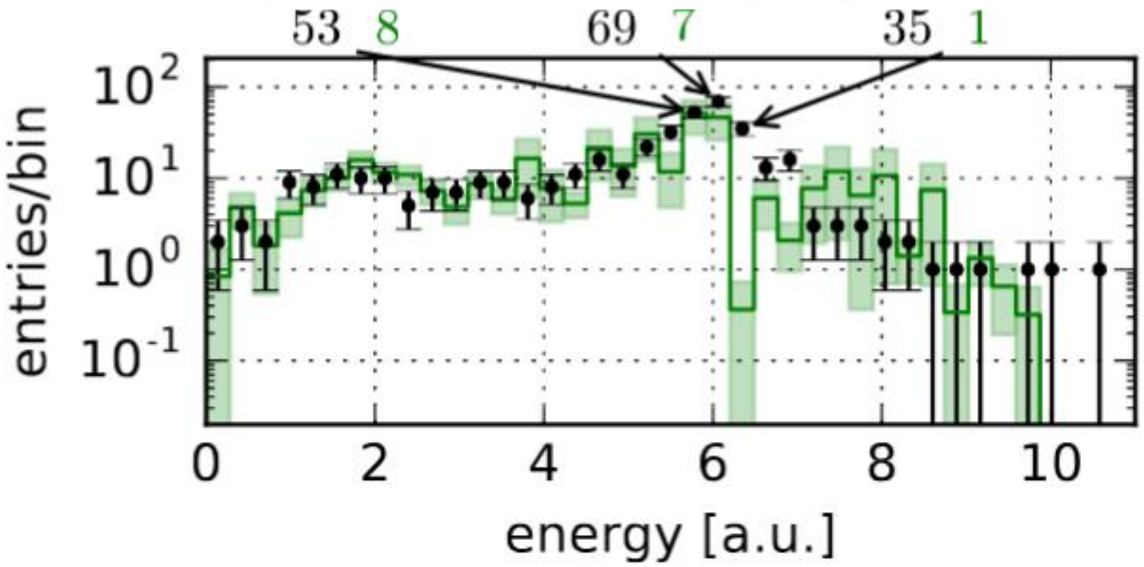
Comparisons



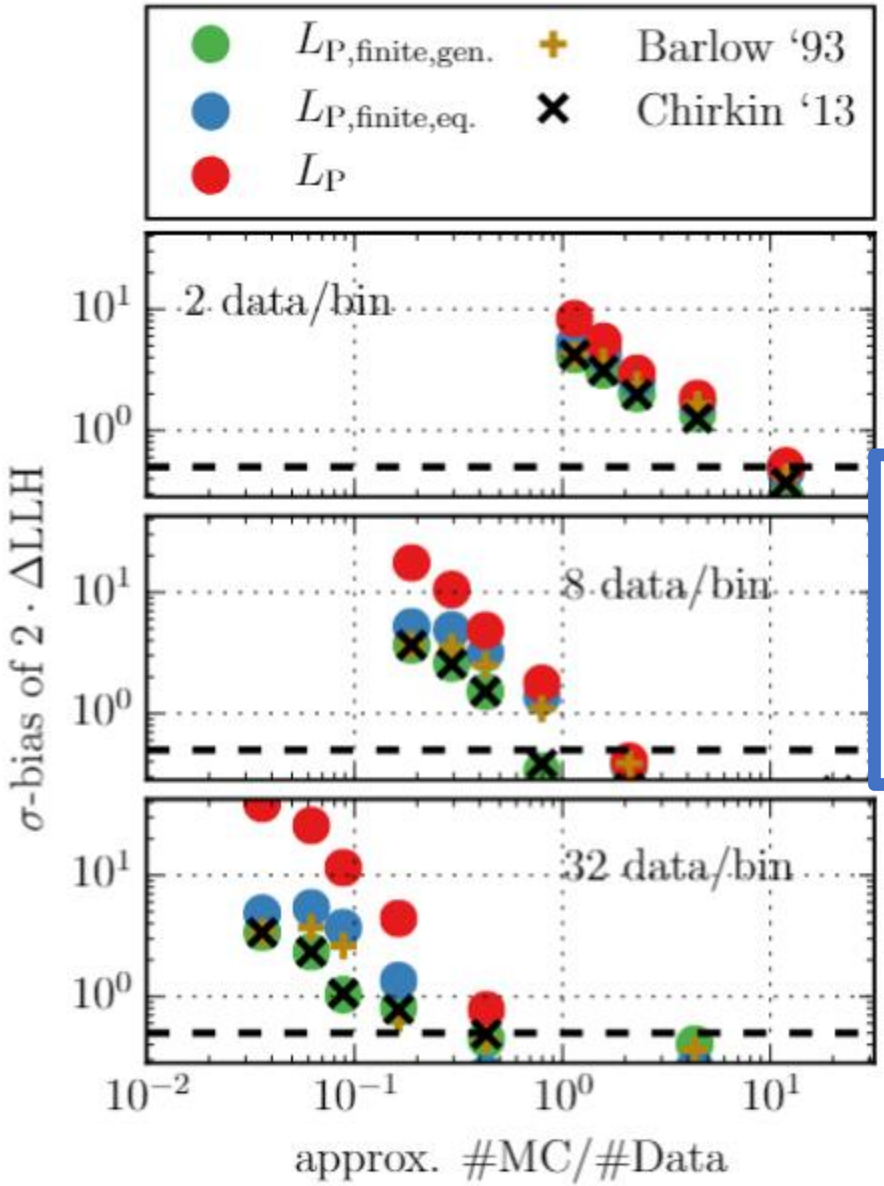


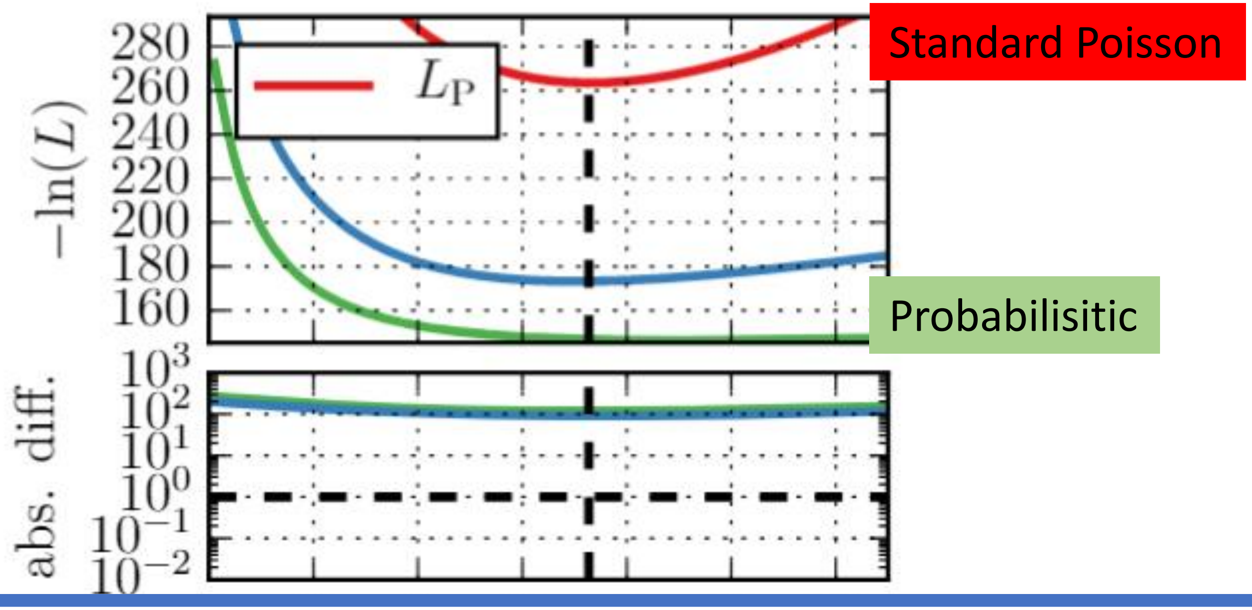
Standard Poisson

Probabilisitic



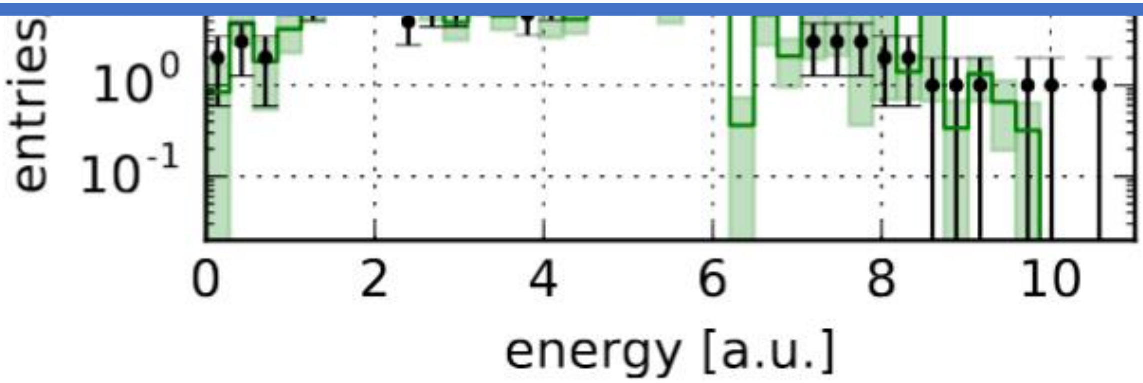
Comparisons



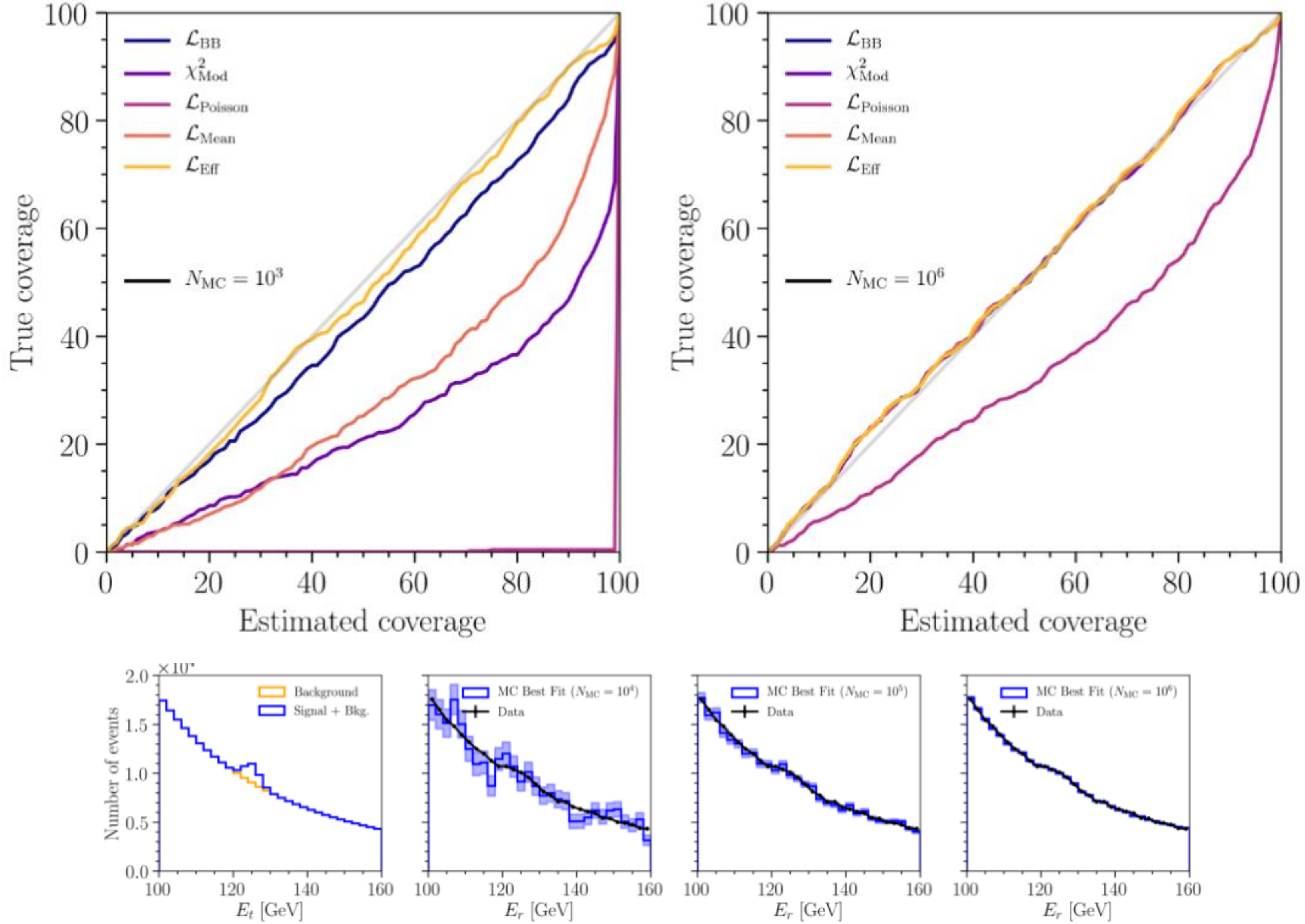


Not a surprise: We have 1 weighted source dataset, Barlow/Beeston averages the weights

Not a realistic situation

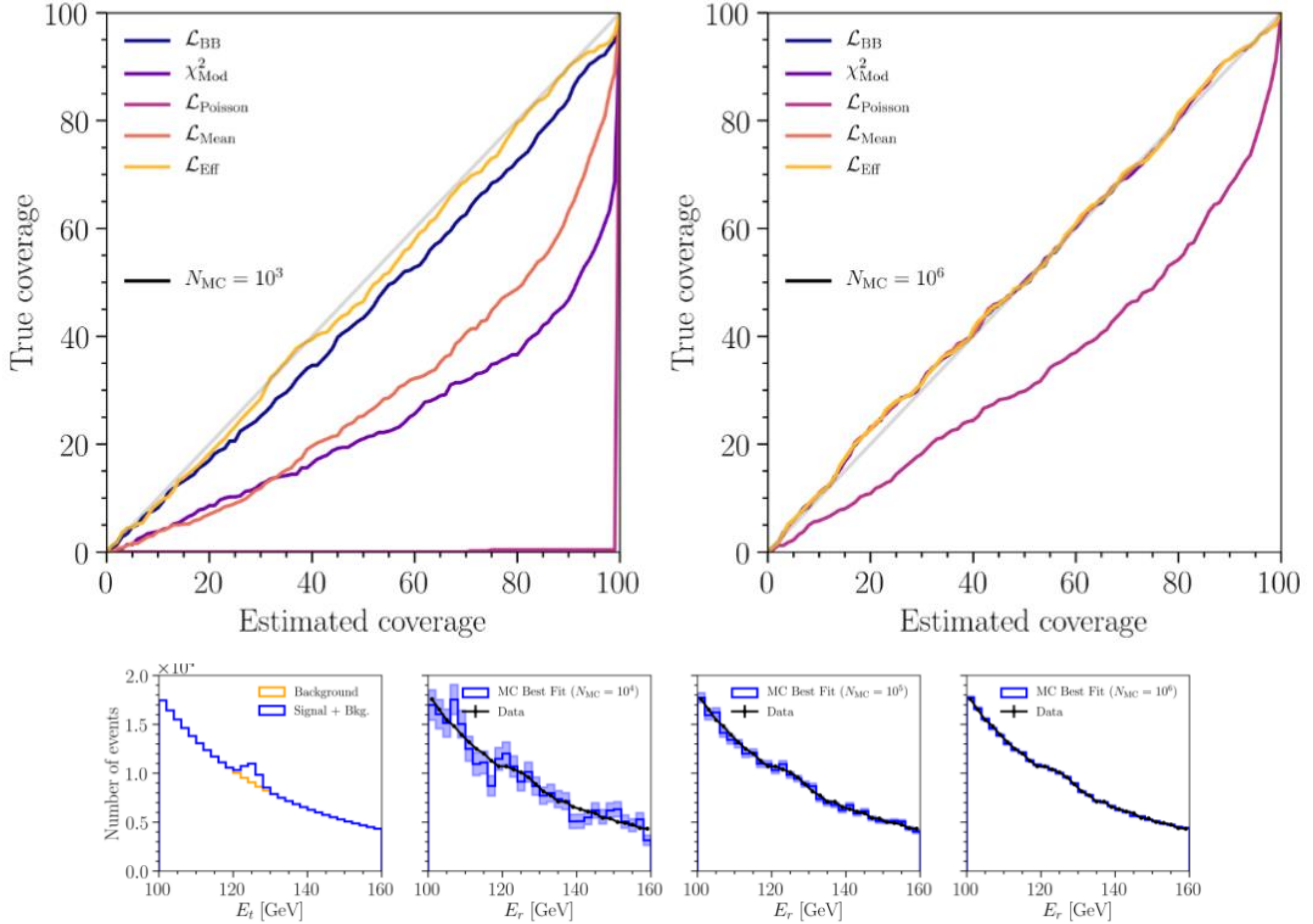


Comparisons



1901.04645

Comparisons



Also works well
with 2 sources (signal+bg)

BUT:
-Requires usage of different hyper parameters (Tuning) "$\mathcal{L}_{Eff}$"/"$\mathcal{L}_{Mean}$"

Signal+Background increase statistics simultaneously
-> also not realistic

At other statistical levels "$\mathcal{L}_{Mean}$" can be better than "$\mathcal{L}_{Eff}$"

1901.04645

We need further generalizations and more tests…

Generalization (1)

$$\int \mathbf{P}(k;\lambda) \cdot [\mathbf{GPG}_1 * \ldots * \mathbf{GPG}_N](\lambda) d\lambda$$

Generalization (2)

$$\int \mathbf{P}(k;\lambda) \cdot [\mathbf{G}_1 * \ldots * \mathbf{G}_{N_{src}}](\lambda) d\lambda$$

Generalization (3)

$$\int \mathbf{P}(k;\lambda) \cdot [\mathbf{GG}_1 * \ldots * \mathbf{GG}_{N_{src}}](\lambda) d\lambda$$

To appear

We need further generalizations and more tests…

Generalization (1)

$$\int \mathbf{P}(k;\lambda)\cdot\left[\mathbf{GPG}_1 * \ldots * \mathbf{GPG}_N\right](\lambda)d\lambda$$

→ Interpretation 1: Apprixmate W_i

Tries to model the CPD better (as CPGD)

Generalization (2)

$$\int \mathbf{P}(k;\lambda)\cdot\left[\mathbf{G}_1 * \ldots * \mathbf{G}_{N_{src}}\right](\lambda)d\lambda$$

Generalization (3)

$$\int \mathbf{P}(k;\lambda)\cdot\left[\mathbf{GG}_1 * \ldots * \mathbf{GG}_{N_{src}}\right](\lambda)d\lambda$$

→ Interpretation 2: Apprixmate CPDs directly

Direct Counterpart of Barlow/Beeston
Model individual source datasets

$$\max_{\{\boldsymbol{\lambda}\}} \mathbf{P}(k;\sum_j p_j \widehat{w}_j \lambda_j)\cdot\prod_j^{N_{\mathrm{src}}} \mathbf{P}(k_{mc,j};\lambda_j)$$

All of these can be exactly calculated!

To appear

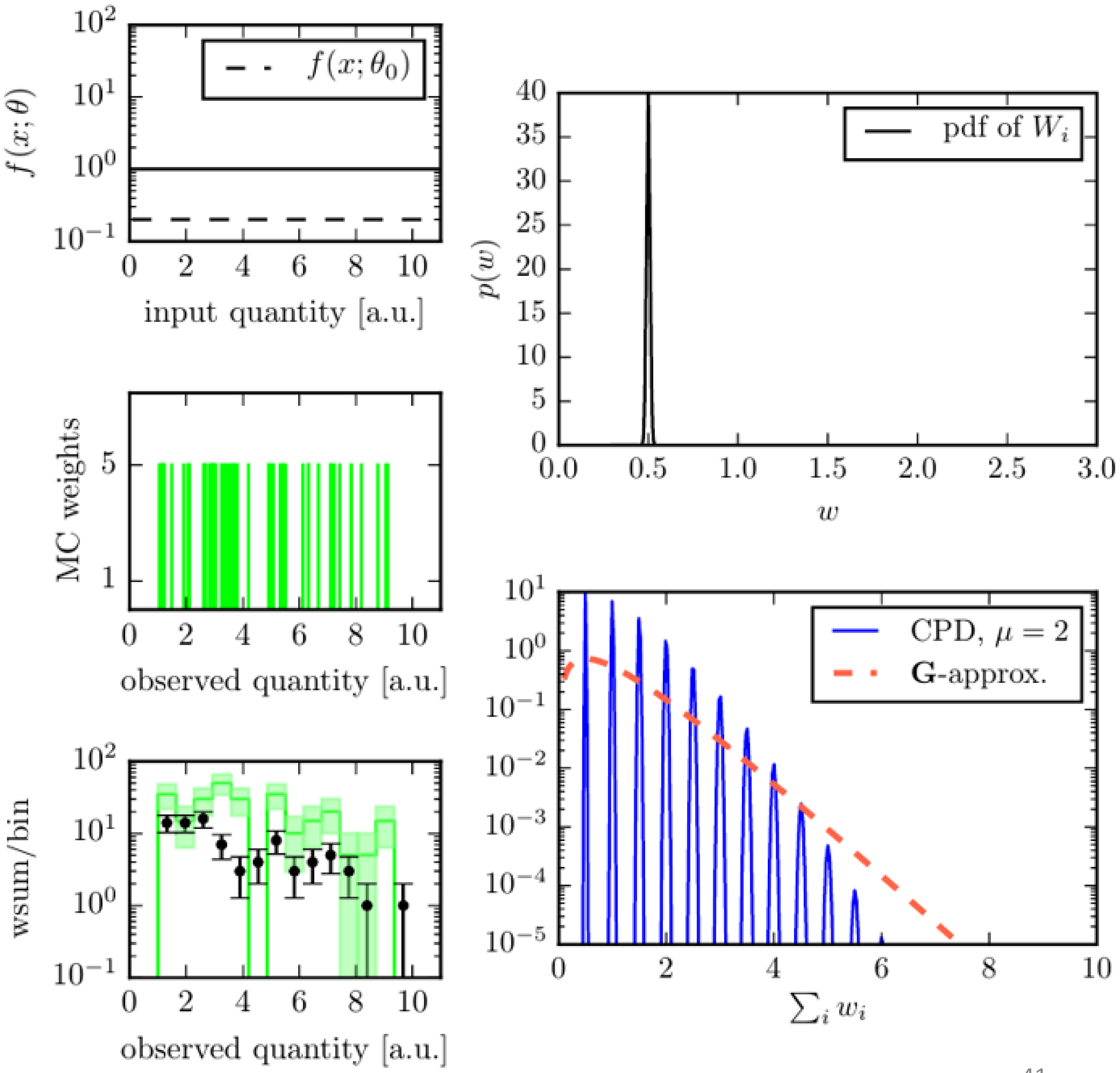
First test: Equal weights

$$L_{bin,exact} = \int \frac{e^{-\lambda} \cdot \lambda^k}{k!} \cdot p_{CPD}(\lambda) d\lambda$$

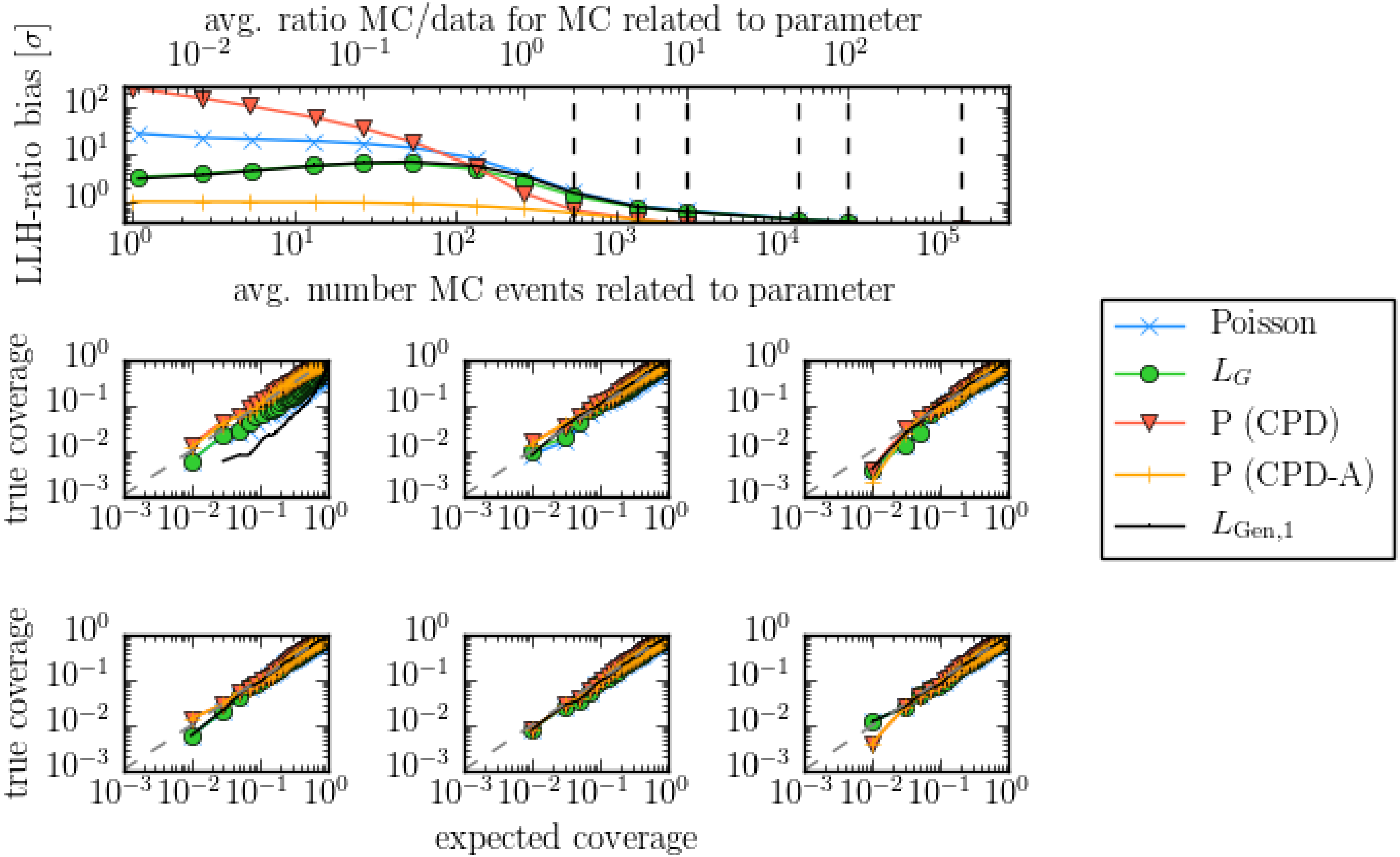
$$= \int \frac{e^{-\lambda} \cdot \lambda^k}{k!} \cdot \sum_{k_{mc}=0}^{\infty} \frac{e^{-\mu} \cdot \mu^{k_{mc}}}{k_{mc}!} \cdot \delta(\lambda - k_{mc} \cdot w) d\lambda$$

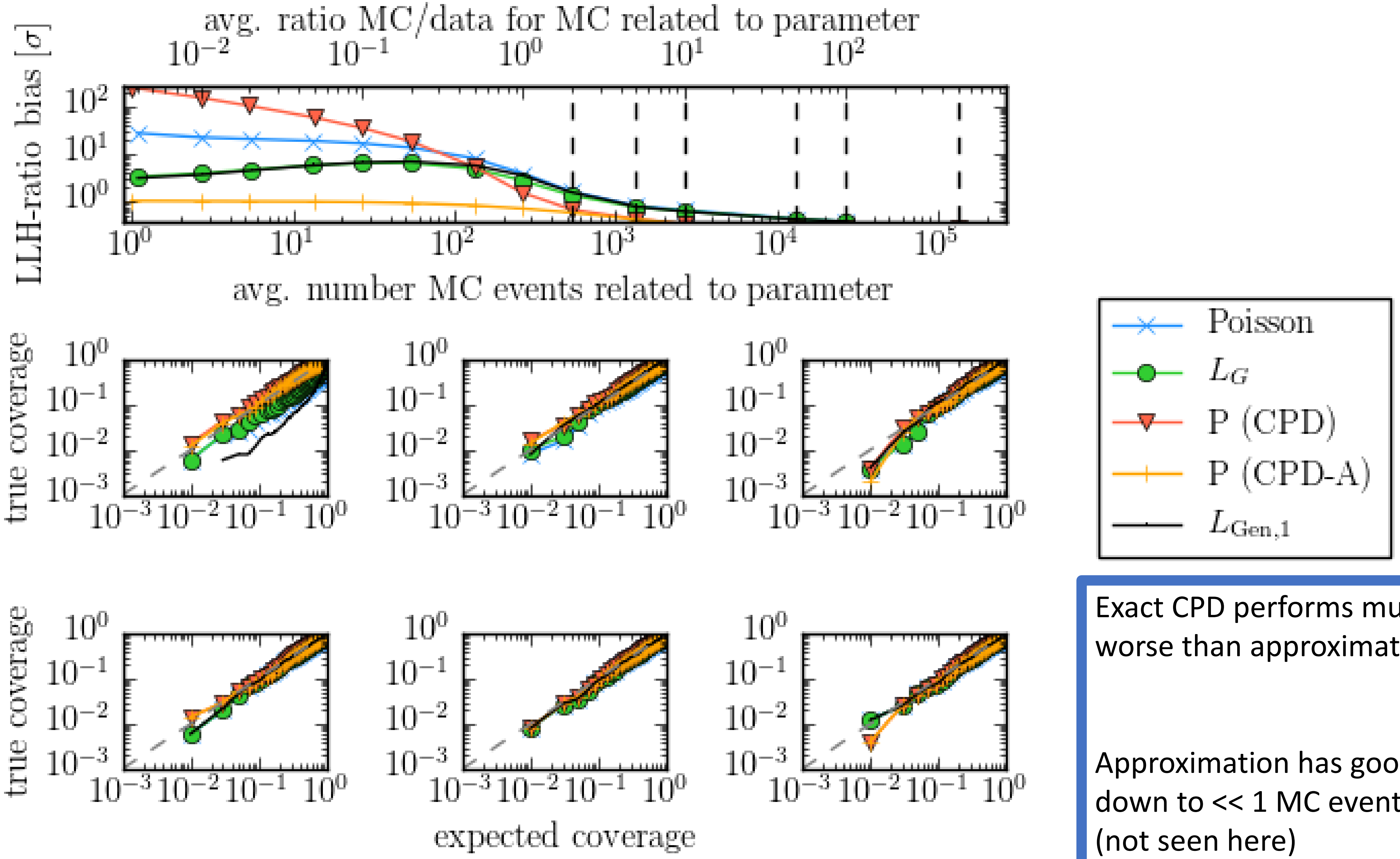
$$= \sum_{k_{mc}=0}^{\infty} \frac{e^{-k_{mc} w} \cdot (k_{mc} w)^k}{k!} \cdot \frac{e^{-\mu} \cdot \mu^{k_{mc}}}{k_{mc}!}$$

We can calculate the CPD exactly
For equal weights, including μ



To appear

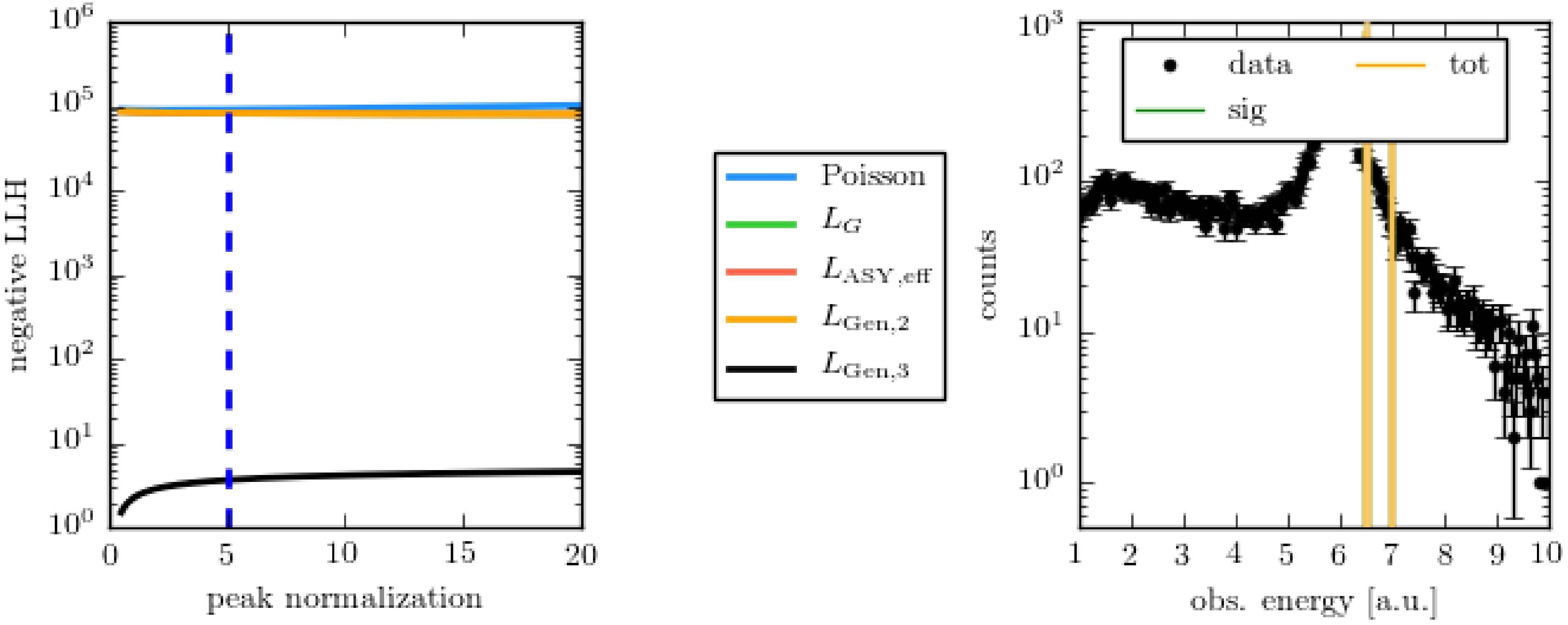

avg. ratio MC/data for MC related to parameter
LLH-ratio bias [σ]
avg. number MC events related to parameter
true coverage
expected coverage
Poisson
L_G
P (CPD)
P (CPD-A)
$L_{\mathrm{Gen},1}$



Exact CPD performs much worse than approximation

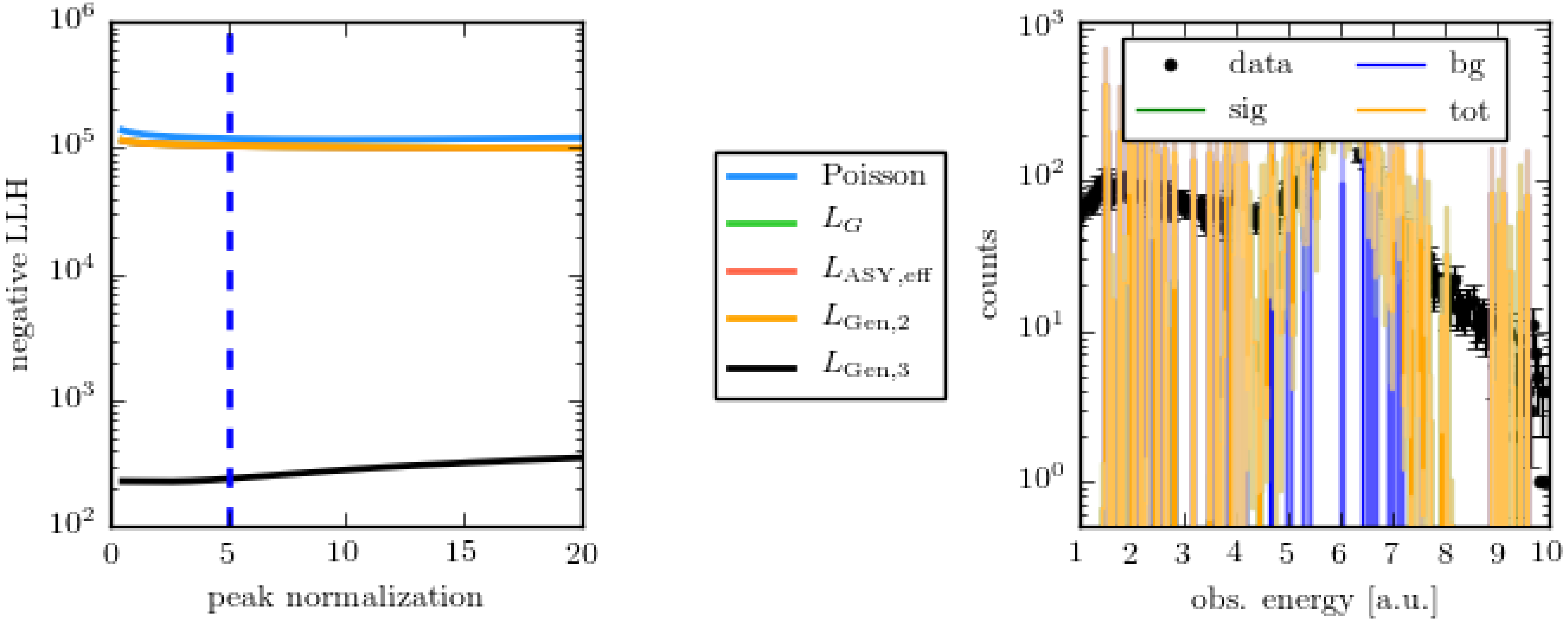
Approximation has good coverage down to << 1 MC event / bin (not seen here)

2nd Test: Increse statistics in both sig/bg



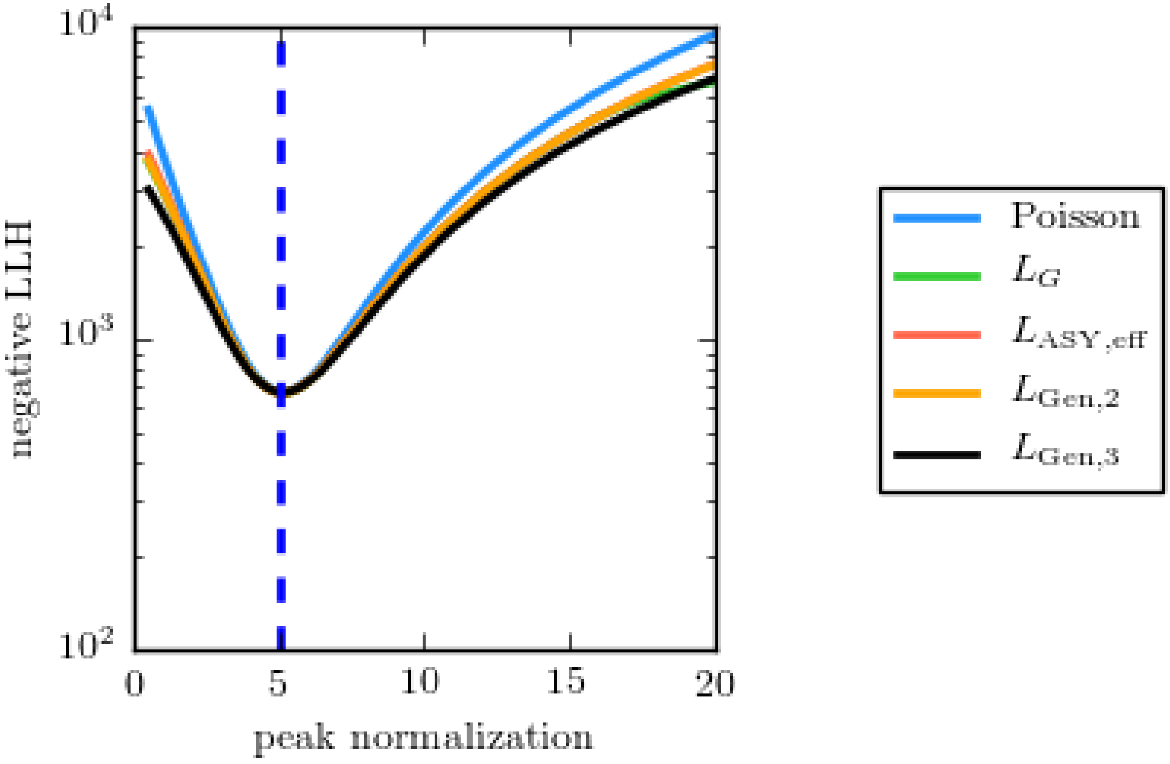
To appear

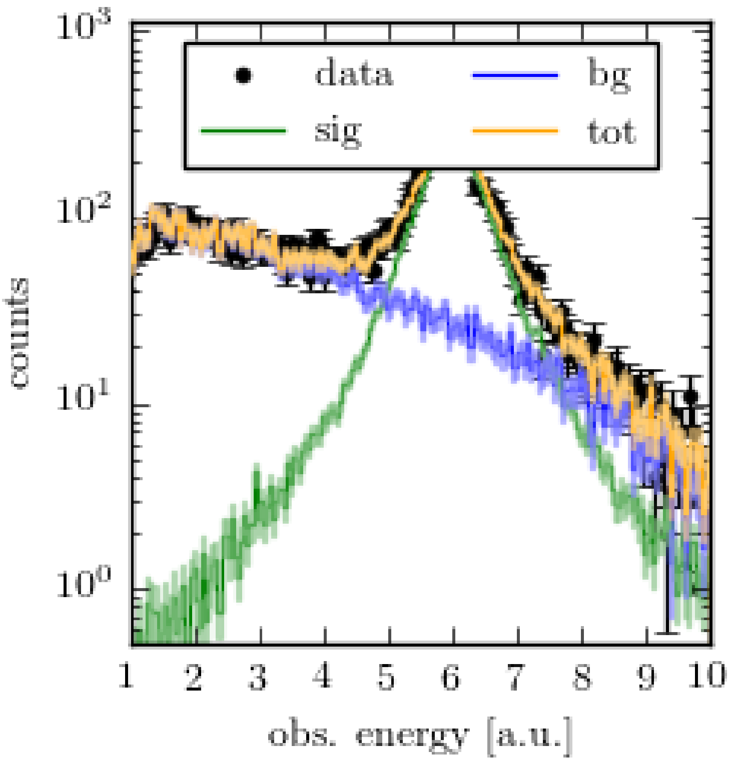
2nd Test: Increse statistics in both sig/bg



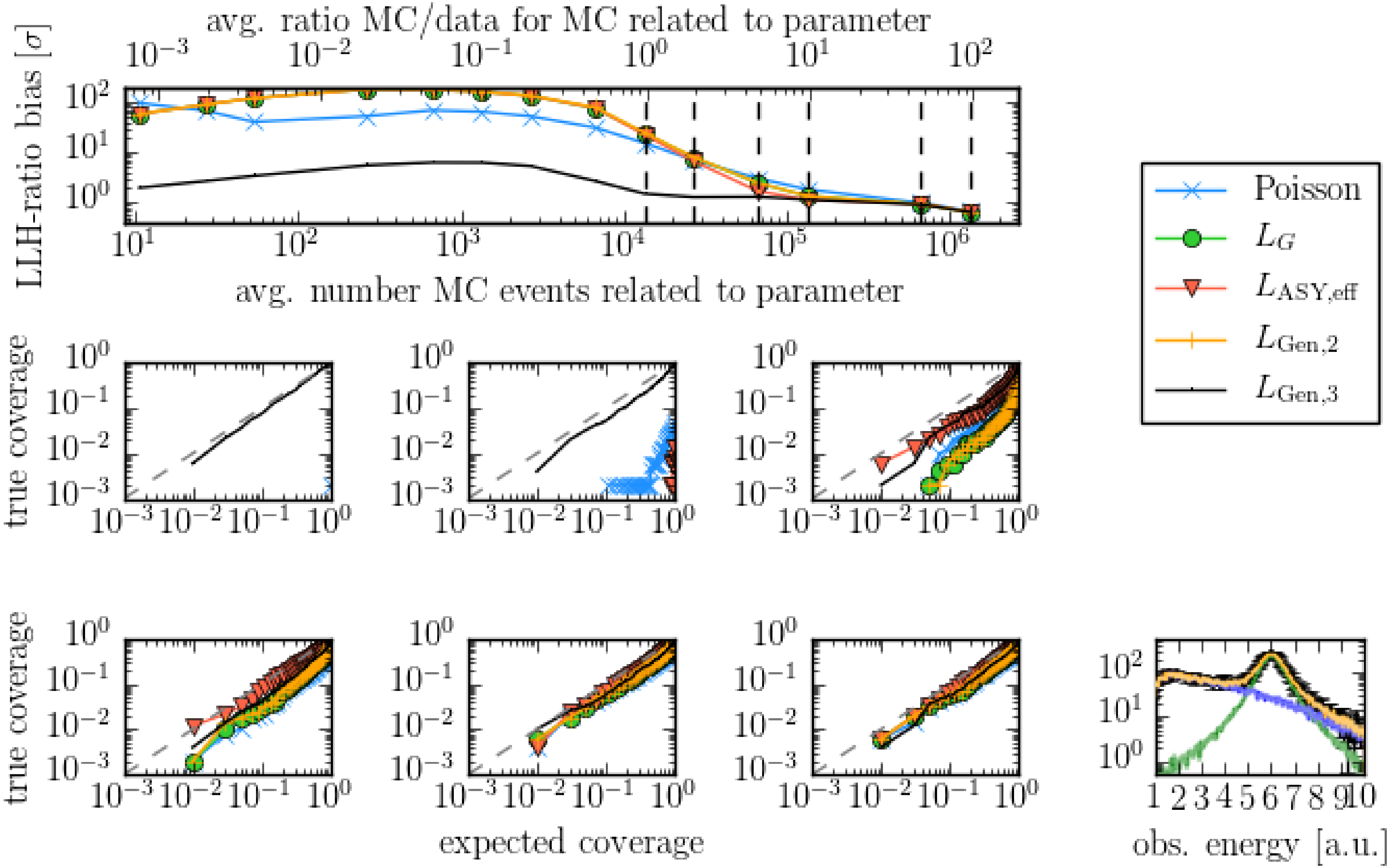
To appear

2nd Test: Increse statistics in both sig/bg

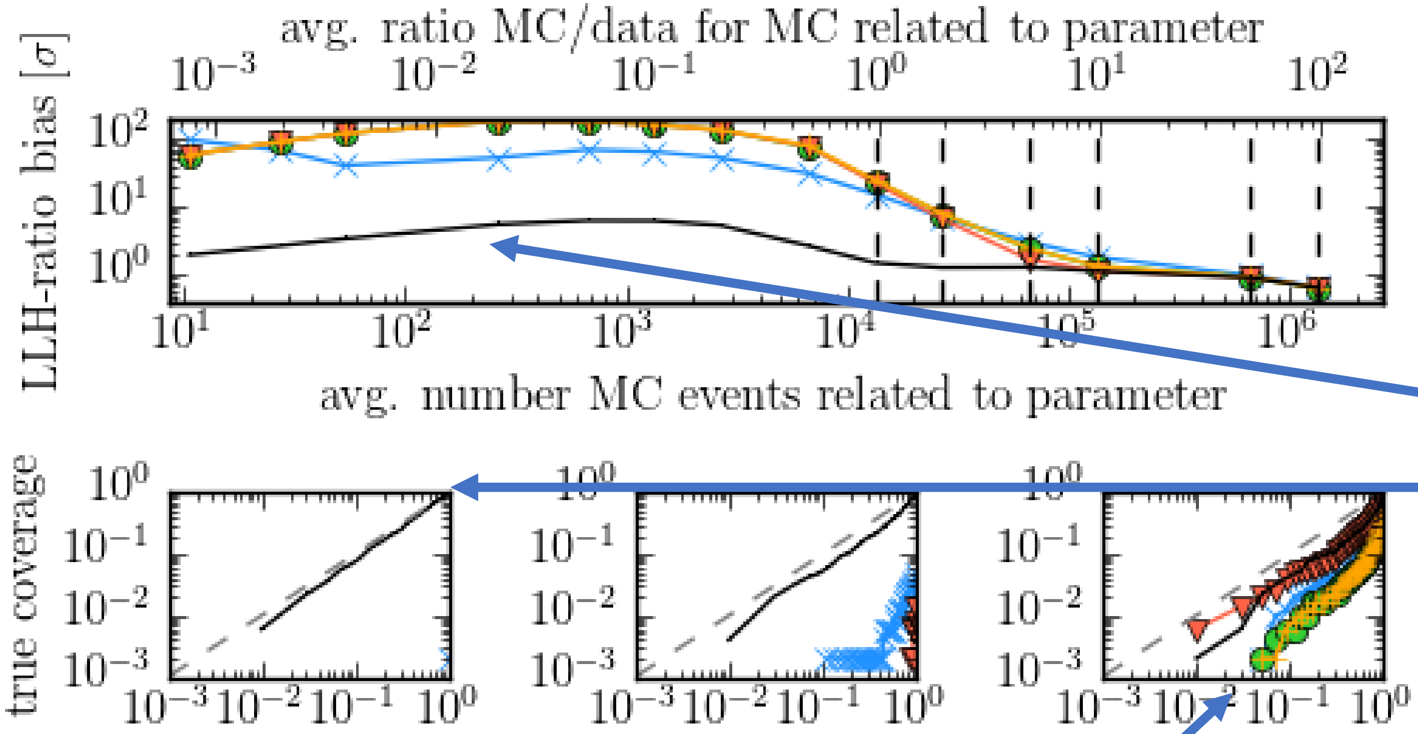


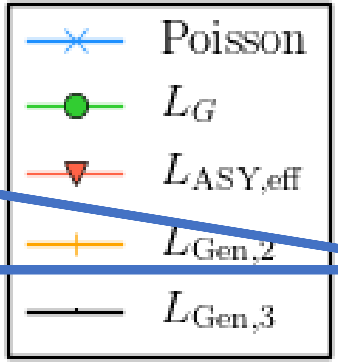


To appear


avg. ratio MC/data for MC related to parameter
LLH-ratio bias [σ]
avg. number MC events related to parameter
true coverage
expected coverage
obs. energy [a.u.]
Poisson
L_G
$L_{\text{ASY,eff}}$
$L_{\text{Gen},2}$
$L_{\text{Gen},3}$

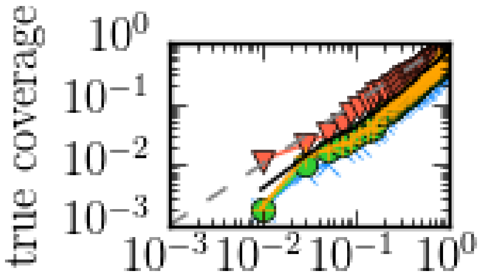
To appear

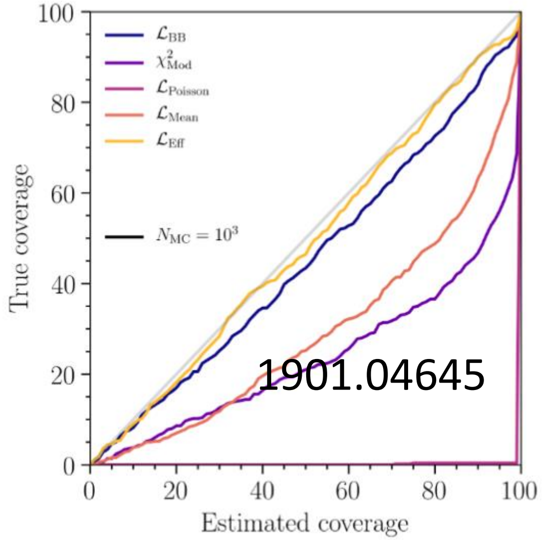




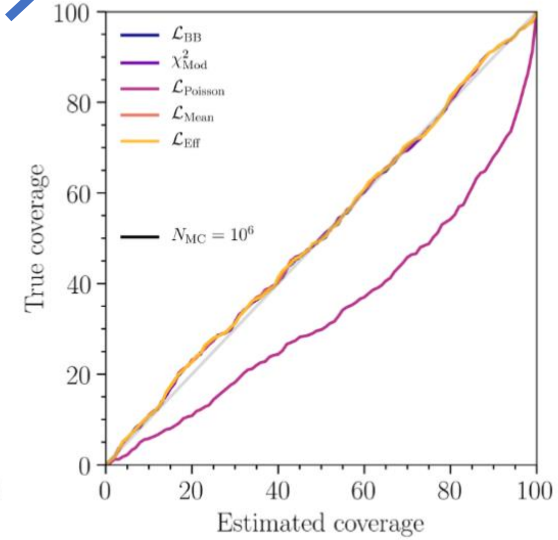
Including uncertainty about number of events greatly reduces bias

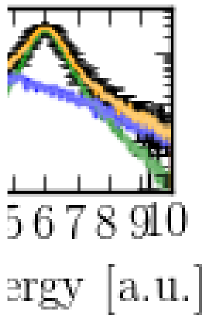
Similar behavior of "$\mathcal{L}_{Eff}$
(forgot Barlow here)





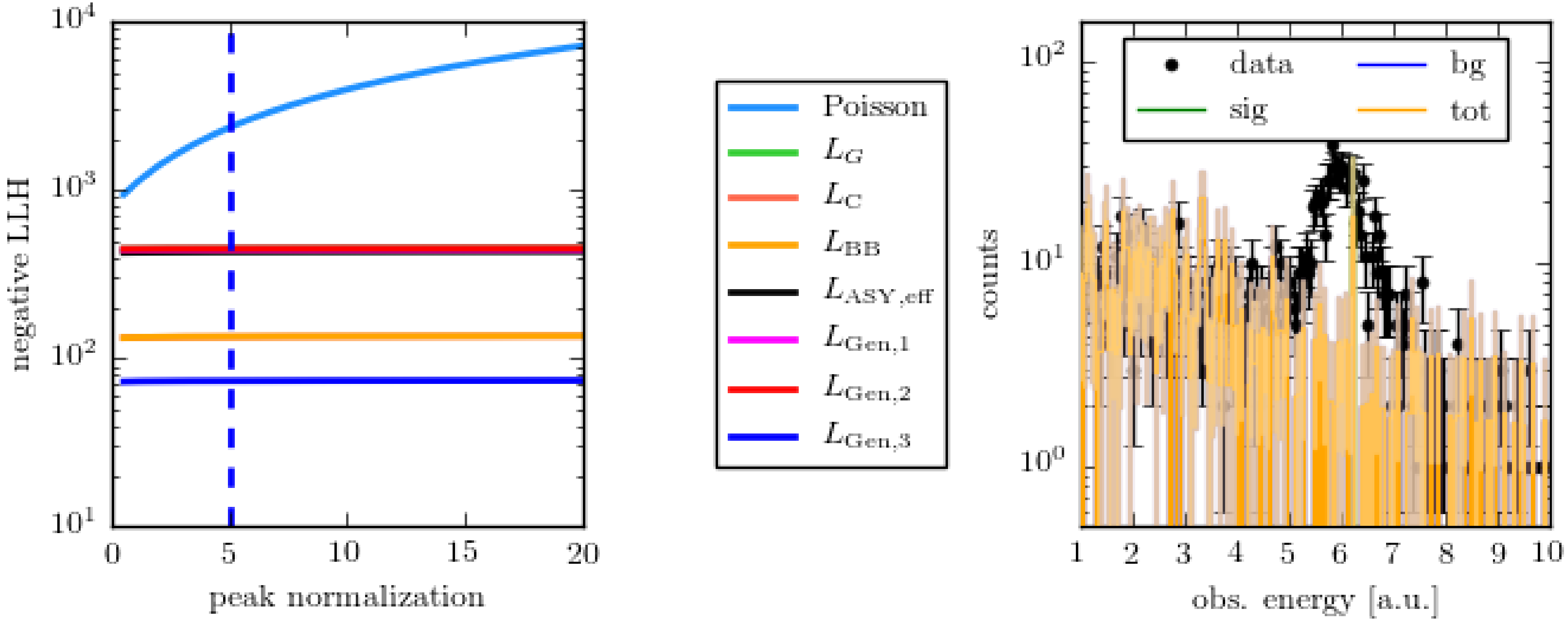
1901.04645



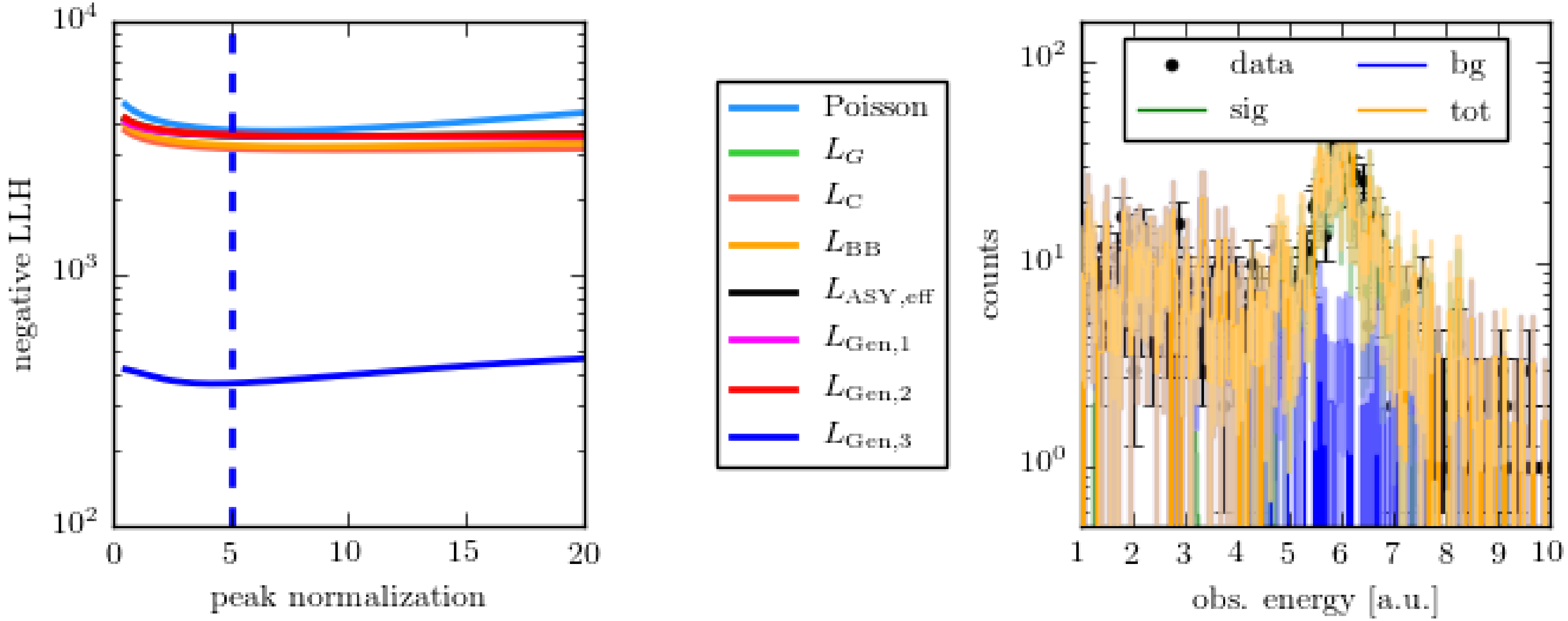


To appear

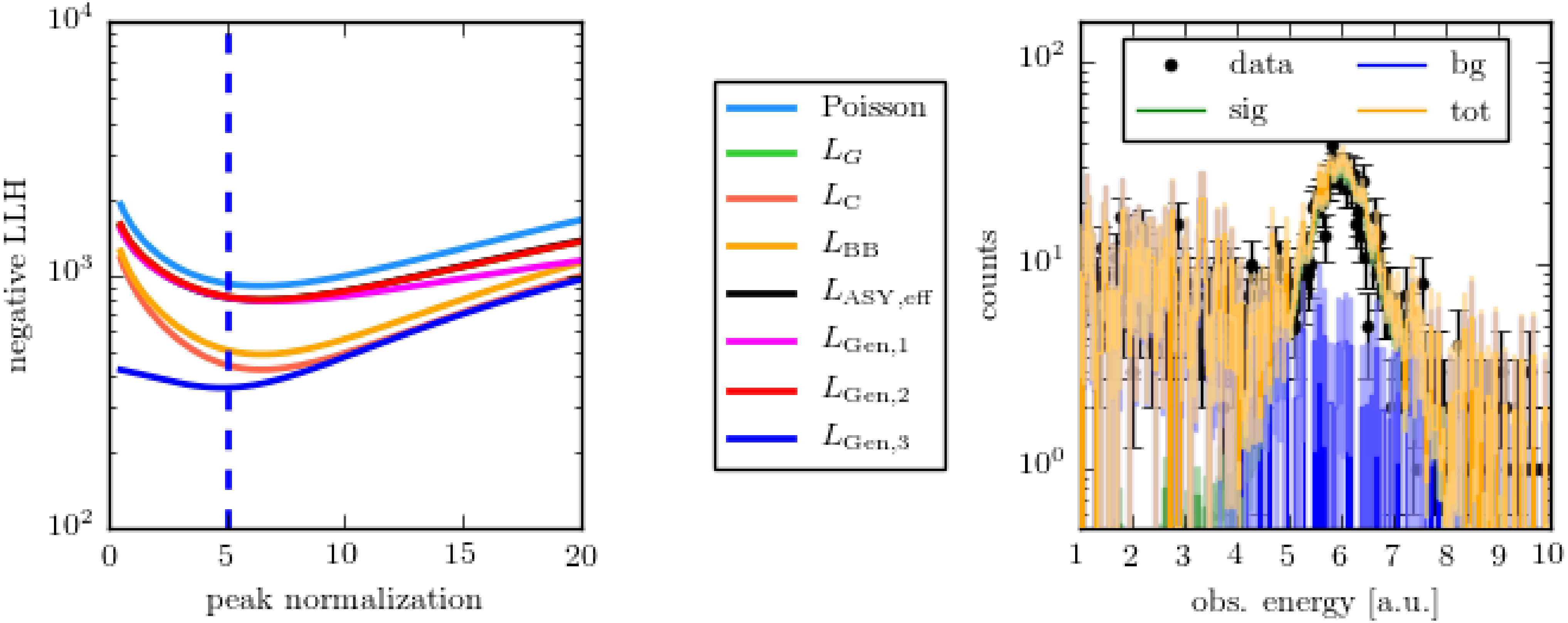
Test 3: Background statistics is limited

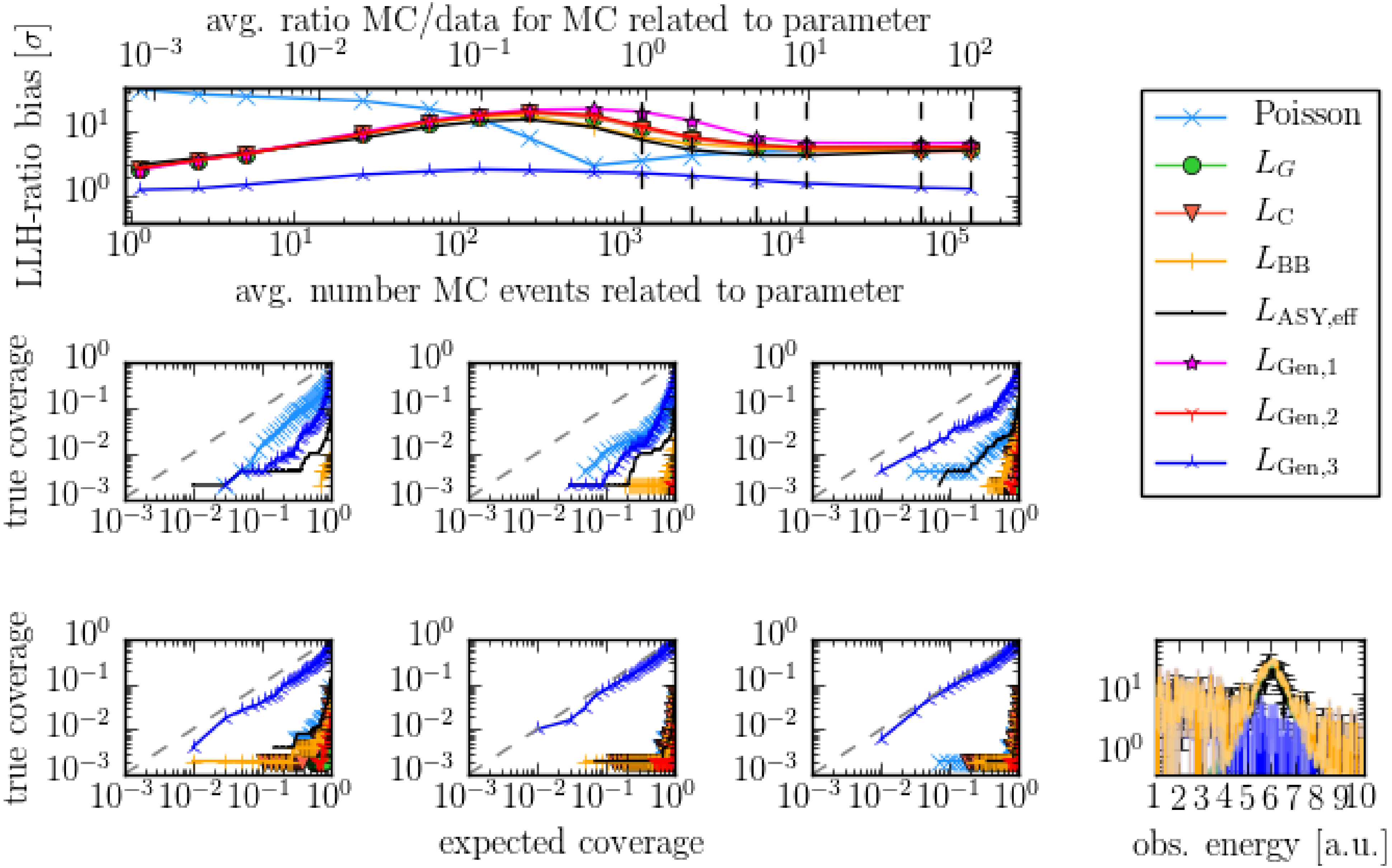


Test 3: Background statistics is limited



Test 3: Background statistics is limited





avg. ratio MC/data for MC related to parameter
LLH-ratio bias [σ]
avg. number MC events related to parameter
Poisson
L_G
L_C
L_{BB}
$L_{ASY,eff}$
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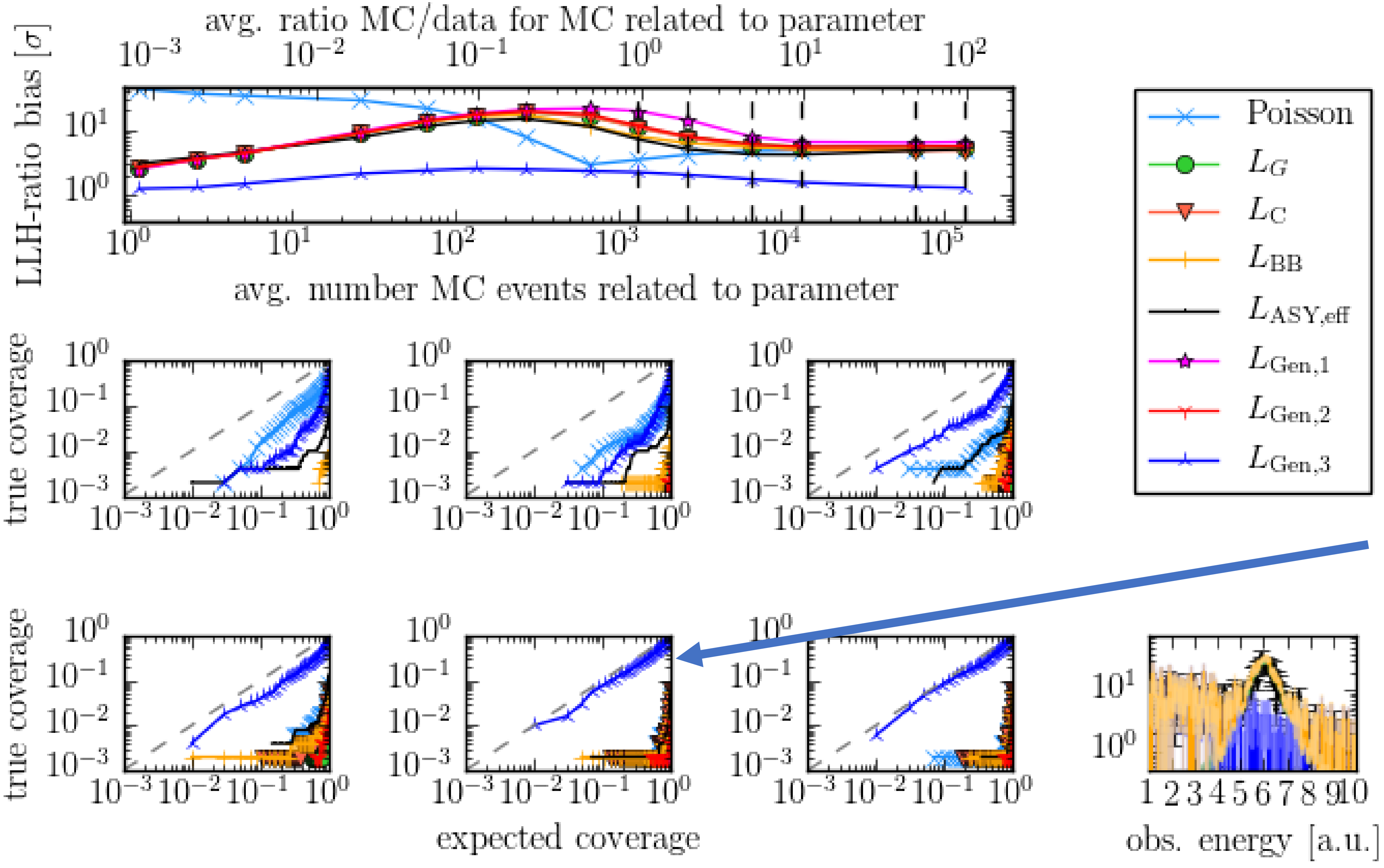

Generalization 3
seems to be the
Only approach
to handle the
Limited background

Summary

- All approaches approximate the CPD + integrate over Poisson mean
  either with nuisance optimization **or** via integration
- exact CPD /equal weights (scaled Poisson) behaves badly in likelihood scans … probably because of multimodality?
- Some advantages of probabilistic approaches:
  Interpretability, simplicity, convergence to Poisson as $n_{MC} \rightarrow \infty$
- There is now a precise probabilistic counterpart of Barlow/Beeston

$$\max_{\{\boldsymbol{\lambda}\}} \mathbf{P}(k; \sum_j p_j \widehat{w}_j \lambda_j) \cdot \prod_j^{N_{\mathrm{src}}} \mathbf{P}(k_{mc,j}; \lambda_j) \longrightarrow \int \mathbf{P}(k; \lambda) \cdot \left[\mathbf{GG}_1 * \ldots * \mathbf{GG}_{N_{src}}\right](\lambda) d\lambda$$

(all of this will be on arXiv in a couple of days)

Useful links

- Barlow et al 93 https://www.sciencedirect.com/science/article/pii/001046559390005W
- Bohm/Zech 2012 https://www.sciencedirect.com/science/article/pii/S0168900212006705?via%3Dihub
- Chirkin 2013 https://arxiv.org/abs/1304.0735
- Glüsenkamp 2018 https://arxiv.org/abs/1712.01293
- Argüelles et al 2019 https://arxiv.org/abs/1901.04645

- Code for probabilistic likelihood implementations (c++/python):
  https://github.com/thoglu/mc_uncertainty
  (will be updated in next days with new formulas)