

μ Bias Note

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1 Origin of FBMP's Bias

1.1 Model

$$\begin{aligned} \begin{bmatrix} \mathbf{w} \\ \mathbf{q}' \end{bmatrix} \middle| \mathbf{z} &\sim \text{Normal} \left(\begin{bmatrix} \mathbf{V}_{\text{PE}} \mathbf{z} \\ \mathbf{z} \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma} & \mathbf{V}_{\text{PE}} \mathbf{Z} \\ \mathbf{Z} \mathbf{V}_{\text{PE}}^\top & \mathbf{Z} \end{bmatrix} \right) \\ \boldsymbol{\Sigma} &= \mathbf{V}_{\text{PE}} \mathbf{Z} \mathbf{V}_{\text{PE}}^\top + \sigma_\epsilon^2 \mathbf{I}_M \end{aligned} \quad (1)$$

$$\begin{aligned} \nu &= \log[p(\mathbf{w}, \mathbf{z})] = \log[p(\mathbf{w}|\mathbf{z})p(\mathbf{z})] \\ &= -\frac{1}{2}(\mathbf{w} - \mathbf{V}_{\text{PE}} \mathbf{z})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{w} - \mathbf{V}_{\text{PE}} \mathbf{z}) - \frac{1}{2} \log \det \boldsymbol{\Sigma} - \frac{N}{2} \log 2\pi \\ &\quad + \sum_i \log \text{Poisson}(z_i, p_i) \end{aligned} \quad (2)$$

1.2 Approximation

- Poisson \rightarrow Bernoulli, $z_i = 0, \mathbf{Z}_{ii} = 0$ or $z_i = 1, \mathbf{Z}_{ii} = \sigma^2$
- SPE approximation
 - For delta approximation, SPE \rightarrow delta SPE, $\mathbf{V}_{PE} = \begin{bmatrix} \mathbf{I} \\ \mathbf{O} \end{bmatrix}$, $w_i \sim \text{Normal}(1, \sigma^2 + \sigma_\epsilon^2)$
 - For flat approximation, SPE \rightarrow flat SPE, $\mathbf{V}_{PE} = \frac{1}{\sqrt{M}} \mathbf{J}_{M,N}$, $w_i \sim \text{Normal}(\frac{N}{\sqrt{M}}, \frac{N}{\sqrt{M}} \sigma^2 + \sigma_\epsilon^2)$, $\sum_i^M w_i \sim \text{Normal}(N\sqrt{M}, M^{\frac{3}{2}} N \sigma^2 + M \sigma_\epsilon^2)$
- flat prior, $\begin{cases} \lambda & \text{if } z_i = 1 \\ 1 - \lambda & \text{if } z_i = 0 \end{cases}$

1.3 Evaluation

for a certain (\mathbf{w}, \mathbf{z}) , let $K = \{i | z_i = 1\}$, $|K| = n$

1.3.1 Delta Approximation

$$\boldsymbol{\Sigma} = \begin{bmatrix} \mathbf{Z} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix} + \sigma_\epsilon^2 \mathbf{I}_M \quad (3)$$

$$\det \boldsymbol{\Sigma} = \prod_i (z_i \sigma^2 + \sigma_\epsilon^2) \quad (4)$$

$$\boldsymbol{\Sigma}_{ij}^{-1} = \begin{cases} \frac{1}{z_i \sigma^2 + \sigma_\epsilon^2} & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \quad (5)$$

Thus,

$$-2\nu = \sum_{i \in K} \frac{(w_i - 1)^2}{\sigma^2 + \sigma_\epsilon^2} + \sum_{i \in \bar{K}} \frac{w_i^2}{\sigma_\epsilon^2} \quad (6)$$

$$+ n \log(\sigma^2 + \sigma_\epsilon^2) + (N - n) \log \sigma_\epsilon^2 \quad (7)$$

$$- 2n \log \lambda - 2(N - n) \log(1 - \lambda) + \text{const} \quad (8)$$

Additionally,

$$\sum_{i \in K} \frac{(w_i - 1)^2}{\sigma^2 + \sigma_\epsilon^2} \sim \chi^2(n) \quad (9)$$

$$\frac{w_i^2}{\sigma_\epsilon^2} = \frac{1}{\sigma_\epsilon^2} ((\sigma^2 + \sigma_\epsilon^2) \frac{(w_i - 1)^2}{\sigma^2 + \sigma_\epsilon^2} + 2(w_i - 1) + 1) \quad (10)$$

Calculate expectation on distribution of \mathbf{w} and \mathbf{z} with $|K| = |\mathbf{z}| = n$,

$$-2E(\nu)_n = n + (N - n) \frac{\sigma^2 + \sigma_\epsilon^2}{\sigma_\epsilon^2} + (N - n) \frac{1}{\sigma_\epsilon^2} \quad (11)$$

$$+ n \log(\sigma^2 + \sigma_\epsilon^2) + (N - n) \log \sigma_\epsilon^2 \quad (12)$$

$$- 2n \log \lambda - 2(N - n) \log(1 - \lambda) + \text{const} \quad (13)$$

Thus,

$$-2D(\nu)_n = -2E(\nu)_n - (-2E(\nu)_{n-1}) \quad (14)$$

$$= 1 - \frac{\sigma^2 + \sigma_\epsilon^2}{\sigma_\epsilon^2} - \frac{1}{\sigma_\epsilon^2} \quad (15)$$

$$+ \log(\sigma^2 + \sigma_\epsilon^2) - \log \sigma_\epsilon^2 \quad (16)$$

$$- 2 \log \lambda + 2 \log(1 - \lambda) \quad (17)$$

Remember that $\sigma^2 \gg \sigma_\epsilon^2$ and $\lambda \ll 1$, set $x = \sigma^2/\sigma_\epsilon^2$, then,

$$D(\nu)_n \approx \frac{1}{2}x - \frac{1}{2} \log x + \log \lambda \quad (18)$$

while $x \gg 1$, $\frac{1}{2}x - \frac{1}{2} \log x \gg 1$, the sign of $D(\nu)_n$ is defined by the relative magnitude of $\frac{1}{2}x - \frac{1}{2} \log x$ and $\log \lambda$.

1.3.2 Flat Approximation

$$\mathbf{\Sigma} = \frac{1}{M} \sigma^2 \sum_i^N z_i \mathbf{J}_M + \sigma_\epsilon^2 \mathbf{I}_M \quad (19)$$

$$= \frac{\sigma^2 n}{M} \mathbf{J}_M + \sigma_\epsilon^2 \mathbf{I}_M \quad (20)$$

$$\det \mathbf{\Sigma} = (\sigma_\epsilon^2 + \sigma^2 \sum_i^N z_i) \sigma_\epsilon^{2(M-1)} \quad (21)$$

$$= (\sigma_\epsilon^2 + \sigma^2 n) \sigma_\epsilon^{2(M-1)} \quad (22)$$

$$\mathbf{\Sigma}^{-1} = \frac{1}{\sigma_\epsilon^2} (\mathbf{I}_M - \frac{1}{M} \frac{\sigma^2 \sum_i^N z_i}{\sigma^2 \sum_i^N z_i + \sigma_\epsilon^2} \mathbf{J}_M) \quad (23)$$

$$= \frac{1}{\sigma_\epsilon^2} (\mathbf{I}_M - \frac{1}{M} \frac{1}{1 + \frac{\sigma_\epsilon^2}{\sigma^2 n}} \mathbf{J}_M) \quad (24)$$

set $M^* = M(1 + \frac{\sigma_\epsilon^2}{\sigma^2 n})$, regarding $\sigma \gg \sigma_\epsilon$, thus $M^* \approx M$, and

$$\mathbf{\Sigma}^{-1} = \frac{1}{\sigma_\epsilon^2} (\mathbf{I}_M - \frac{1}{M^*} \mathbf{J}_M) \quad (25)$$

Thus,

$$-2\nu = \frac{1}{\sigma_\epsilon^2} [\sum_i^M (w_i - \frac{n}{\sqrt{M}})^2 - \frac{1}{M^*} (\sum_i^M w_i - n\sqrt{M})^2] \quad (26)$$

$$+ \log(\sigma^2 n + \sigma_\epsilon^2) \quad (27)$$

$$- 2n \log \lambda - 2(N - n) \log(1 - \lambda) + \text{const} \quad (28)$$

Additionally,

$$(w_i - \frac{n}{\sqrt{M}})^2 = (w_i - \frac{N}{\sqrt{M}})^2 \quad (29)$$

$$+ 2(w_i - \frac{N}{\sqrt{M}}) \frac{N-n}{\sqrt{M}} + \frac{(N-n)^2}{M} \quad (30)$$

$$(\sum_i^M w_i - n\sqrt{M})^2 = (\sum_i^M w_i - N\sqrt{M})^2 \quad (31)$$

$$+ 2(\sum_i^M w_i - N\sqrt{M})(N-n)\sqrt{M} + (N-n)^2 M \quad (32)$$

$$\sum_i^M \frac{(w_i - \frac{N}{\sqrt{M}})^2}{\frac{N}{\sqrt{M}}\sigma^2 + \sigma_\epsilon^2} \sim \chi^2(M) \quad (33)$$

$$\frac{(\sum_i^M w_i - N\sqrt{M})^2}{M^{\frac{3}{2}}N\sigma^2 + M\sigma_\epsilon^2} \sim \chi^2(1) \quad (34)$$

Calculate expectation on distribution of \mathbf{w} and \mathbf{z} with $|n| = |\mathbf{z}| = n$,

$$-2E(\nu)_n = \frac{1}{\sigma_\epsilon^2} [(\frac{N}{\sqrt{M}}\sigma^2 + \sigma_\epsilon^2)M + (N-n)^2] \quad (35)$$

$$- \frac{1}{M^*} (M^{\frac{3}{2}}N\sigma^2 + M\sigma_\epsilon^2 + (N-n)^2 M) \quad (36)$$

$$+ \log(\sigma^2 n + \sigma_\epsilon^2) \quad (37)$$

$$- 2n \log \lambda - 2(N-n) \log(1-\lambda) + \text{const} \quad (38)$$

$$= \frac{1}{\sigma_\epsilon^2} [(N\sqrt{M}\sigma^2 + (N-n)^2)(1 - \frac{M}{M^*}) + (M - \frac{M}{M^*})\sigma_\epsilon^2] \quad (39)$$

$$+ \log(\frac{\sigma^2}{\sigma_\epsilon^2} n + 1) \quad (40)$$

$$- 2n \log \lambda - 2(N-n) \log(1-\lambda) + \text{const} \quad (41)$$

Thus,

$$E(\nu)_n' = -\frac{1}{2} \{ \frac{1}{\sigma_\epsilon^2} [2(n-N)(1 - \frac{M}{M^*})] \quad (42)$$

$$+ (N\sqrt{M}\sigma^2 + (N-n)^2 + \sigma_\epsilon^2) \frac{M}{M^{*2}} M^{*'}] \quad (43)$$

$$+ \frac{1}{n + \frac{\sigma_\epsilon^2}{\sigma^2}} \} + \log \lambda - \log(1-\lambda) \quad (44)$$

$$M^{*'} = -\frac{M\sigma_\epsilon^2}{\sigma^2 n^2} \quad (45)$$

when $n = N$,

$$E(\nu)'_n|_N = -\frac{1}{2}\left[\frac{1}{\sigma_\epsilon^2}(N\sqrt{M}\sigma^2 + \sigma_\epsilon^2)\frac{M}{M^{*2}}M^{*'} \right. \quad (46)$$

$$\left. + \frac{1}{N + \frac{\sigma_\epsilon^2}{\sigma^2}}\right] + \log \lambda - \log(1 - \lambda) \quad (47)$$

$$= \frac{1}{2} \frac{N}{(N + \frac{\sigma_\epsilon^2}{\sigma^2})^2} (\sqrt{M} - 1) \quad (48)$$

$$+ \log \lambda - \log(1 - \lambda) \quad (49)$$

Remember that $M \gg 1$, then,

$$C = \frac{1}{2} \frac{N}{(N + \frac{\sigma_\epsilon^2}{\sigma^2})^2} (\sqrt{M} - 1) > 0 \quad (50)$$

the sign of $E(\nu)'_n|_N$ is defined by the relative magnitude of C and $\log \lambda$.

1.4 Discussion

When the time bin is very thin, $\log \lambda \ll 0$, $D(\nu)_n < 0$. When Bernoulli approximation fails, $D(\nu)_n > 0$.

While we may reasonably assume $E(\nu)_n$ will be its maximum when $n = N_{PE}$, considering the fact that RGS in FBMP has imperfect ergodicity, the bias will be positive given $D(\nu)_n > 0$ (or $E(\nu)'_n|_N > 0$) as RGS will **not** stop immediately when $n = N_{PE}$. Given $D(\nu)_n < 0$ (or $E(\nu)'_n|_N < 0$), the bias will be negative.

2 Phenomenon

2.1 P-FBMP with magic time bin

```

1 mu_t = abs(wave.sum() / gmu)
2 if Tau > 10:
3     n = min(math.ceil(20 / mu_t), 5)
4 else:
5     n = min(math.ceil(4 / mu_t), 3)
6 A, wave_r, tlist, t0_t, t0_delta, cha, left_wave, right_wave = wff.
    initial_params(wave[:, wff.nshannon], spe_pre[ent[i] ['ChannelID'
    ]], Mu, Tau, Sigma, gmu, Thres['lucyddM^ast'], p, nsp, nstd,
    is_t0=True, is_delta=False, n=n, nshannon=1)
7 mu_t = abs(wave_r.sum() / gmu)
8 def optit0mu(t0, mu, n, xmmse_star, psy_star, c_star, la):
9     ys = np.log(psy_star) - np.log(poisson.pmf(c_star, la)).sum(
        axis=1)
10    ys = np.exp(ys - ys.max()) / np.sum(np.exp(ys - ys.max()))
11    t0list = np.arange(t0 - 3 * Sigma, t0 + 3 * Sigma + 1e-6, 0.2)

```

```

mulist = np.arange(max(1e-8, mu - 3 * np.sqrt(mu)), mu + 3 * np
    .sqrt(mu), 0.1)
13 b_mu = [max(1e-8, mu - 5 * np.sqrt(mu)), mu + 5 * np.sqrt(mu)]
    tlist_pan = np.sort(np.unique(np.hstack(np.arange(0, window)[: ,
        None] + np.arange(0, 1, 1 / n))))
15 As = np.zeros((len(xmmse_star), len(tlist_pan)))
    As[:, np.isin(tlist_pan, tlist)] = c_star
17 assert sum(np.sum(As, axis=0) > 0) > 0

19 def likelihood(x):
    a = x[0] * wff.convolve_exp_norm(tlist_pan - x[1], Tau,
        Sigma) / n + 1e-8 # use tlist_pan not tlist
21 li = -special.logsumexp(np.log(poisson.pmf(As, a)).sum(axis
    =1), b=ys)
    return li

23 likemu = np.array([likelihood([mulist[j], t0]) for j in range(
    len(mulist))])
25 liket0 = np.array([likelihood([mu, t0list[j]]) for j in range(
    len(t0list))])
    mu, t0 = opti.fmin_l_bfgs_b(likelihood, x0=[mulist[likemu.
        argmin()], t0list[liket0.argmax()]], approx_grad=True,
        bounds=[b_mu, b_t0], maxfun=50000)[0]
27 return mu, t0

29 truth = pelist[pelist['TriggerNo'] == ent[i]['TriggerNo']]
    time_fbmp_start = time.time()
31 factor = np.sqrt(np.diag(np.matmul(A.T, A)).mean())
    A = np.matmul(A, np.diag(1. / np.sqrt(np.diag(np.matmul(A.T, A)))))
33 la = mu_t * wff.convolve_exp_norm(tlist - t0_t, Tau, Sigma) / n + 1
    e-8
    xmmse, xmmse_star, psy_star, nu_star, nu_star_bk, T_star, d_tot_i,
        d_max_i, num_i = wff.fbmpr_fxn_reduced(wave_r, A, la, spe_pre[
            cid]['std'] ** 2, (gsigma * factor / gmu) ** 2, factor, len(la)
        , stop=5, truth=truth, i=i, left=left_wave, right=right_wave,
            tlist=tlist, gmu=gmu, para=p)
35 time_fbmp = time_fbmp + time.time() - time_fbmp_start
    c_star = np.zeros_like(xmmse_star).astype(int)
37 for k in range(len(T_star)):
    t, c = np.unique(T_star[k][xmmse_star[k][T_star[k]] > 0],
        return_counts=True)
39 c_star[k, t] = c
    maxindex = 0

41 xmmse_most = xmmse_star[maxindex]
43 pet = np.repeat(tlist[xmmse_most > 0], c_star[maxindex][xmmse_most
    > 0])
    cha = np.repeat(xmmse_most[xmmse_most > 0] / factor / c_star[
        maxindex][xmmse_most > 0], c_star[maxindex][xmmse_most > 0])
45 mu, t0 = optit0mu(t0_t, mu_t, n, xmmse_star, psy_star, c_star, la)
47 mu_i, t0_i = optit0mu(t0_t, mu_t, n, xmmse_most[None, :], np.array
    ([1]), c_star[maxindex][None, :], la)

```

Motivation: demonstrate magic time binning on μ bias

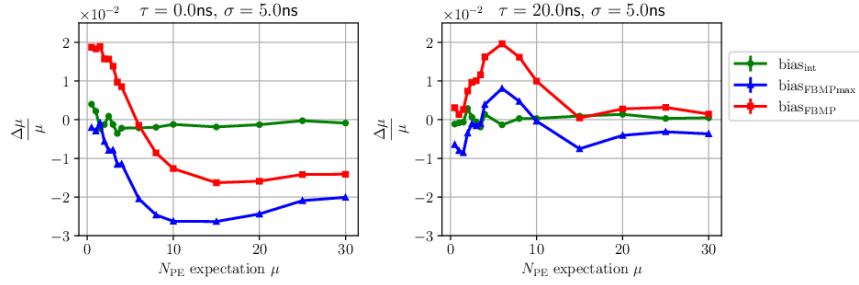
Progress: magic time bin is

```

1 mu_t = abs(wave.sum() / gmu)
2 if Tau > 10:
3     n = min(math.ceil(20 / mu_t), 5)
4 else:
5     n = min(math.ceil(4 / mu_t), 3)

```

Result: relative μ bias are less than 2.5%



2.2 P-FBMP only fitting

```

1 def optit0mu(t0, mu, n, xmmse_star, psy_star, c_star, la):
2     ys = np.log(psy_star) - np.log(poisson.pmf(c_star, la)).sum(
3         axis=1)
4     ys = np.exp(ys - ys.max()) / np.sum(np.exp(ys - ys.max()))
5     t0list = np.arange(t0 - 3 * Sigma, t0 + 3 * Sigma + 1e-6, 0.2)
6     mulist = np.arange(max(1e-8, mu - 3 * np.sqrt(mu)), mu + 3 * np.
7         sqrt(mu), 0.1)
8     b_mu = [max(1e-8, mu - 5 * np.sqrt(mu)), mu + 5 * np.sqrt(mu)]
9     tlist_pan = np.sort(np.unique(np.concatenate([np.unique(np.
10         hstack(np.arange(1, window-1)[: , None] + np.arange(0, 1, 1
11         / n))), tlist])))
12     As = np.zeros((len(xmmse_star), len(tlist_pan)))
13     As[:, np.isin(tlist_pan, tlist)] = c_star
14     tlist_edge = np.concatenate([[tlist_pan[0] - np.diff(tlist_pan)
15         [0] / 2], (tlist_pan[1:] + tlist_pan[:-1]) / 2, [tlist_pan
16         [-1] + np.diff(tlist_pan)[-1] / 2]])
17     diff = np.diff(tlist_edge)
18     assert As.sum() == c_star.sum()
19     assert sum(np.sum(As, axis=0) > 0) > 0
20
21 def likelihood(x):
22     a = x[0] * wff.convolve_exp_norm(tlist_pan - x[1], Tau,
23         Sigma) * diff + 1e-8 # use tlist_pan not tlist
24     li = -special.logsumexp(np.log(poisson.pmf(As, a)).sum(axis
25         =1), b=ys)
26     return li
27
28 likemu = np.array([likelihood([mulist[j], t0]) for j in range(
29     len(mulist))])

```



```

21     liket0 = np.array([likelihood([mu, t0list[j]]) for j in range(
        len(t0list))])
    mu, t0 = opti.fmin_l_bfgs_b(likelihood, x0=[mulist[likemu.
        argmin()], t0list[liket0.argmax()]], approx_grad=True,
        bounds=[b.mu, b.t0], maxfun=50000)[0]
23     return mu, t0

25 truth = pelist[pelist['TriggerNo'] == ent[i]['TriggerNo']]

27 tlist = truth['HitPosInWindow'][truth['HitPosInWindow'] <
    right_wave - 1]
    if len(tlist) == 1:
29         tlist_edge = np.array([tlist[0] - 0.5, tlist[0] + 0.5])
    else:
31         tlist_edge = np.concatenate([[tlist[0] - np.diff(tlist)[0] /
            2], (tlist[1:] + tlist[:-1]) / 2, [tlist[-1] + np.diff(
                tlist)[-1] / 2]])
        t_auto = (np.arange(left_wave, right_wave) / wff.nshannon[:, None]
            - tlist)
33 A = p[2] * np.exp(-1 / 2 * (np.log((t_auto + np.abs(t_auto)) / p[0]
        / 2) / p[1]) ** 2)

35 t0_t = t0.truth[i]['T0']
    mu_t = len(truth)
37 la = mu_t * np.array([integrate.quad(lambda t : wff.
        convolve_exp_norm(t - t0_t, Tau, Sigma), tlist_edge[i],
            tlist_edge[i+1])[0] for i in range(len(tlist))]) + 1e-8

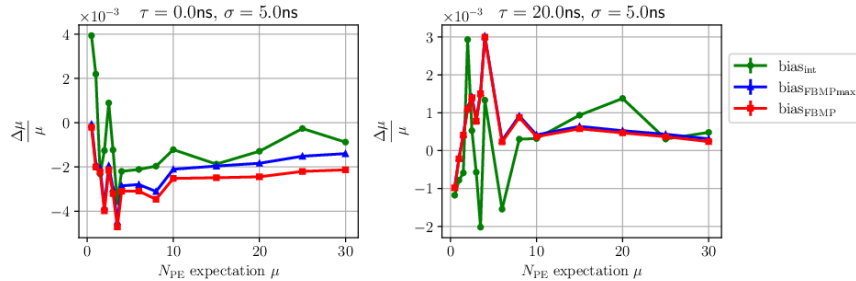
39 c_star_truth = np.ones_like(tlist)
    wav_ans = np.sum([np.where(pp > truth['HitPosInWindow'][j], wff.spe
        (pp - truth['HitPosInWindow'][j], tau=p[0], sigma=p[1], A=p[2])
            * truth['Charge'][j] / gmu, 0) for j in range(len(truth))],
        axis=0)
41 mu, t0 = optit0mu(t0_t, mu_t, n, np.empty(len(la))[None, :], np.
    array([1]), c_star_truth[None, :], la)

```

Motivation: to validate fitting process

Progress: Use true HitPosInWindow as tlist, true T0 as t0_t, length of HitPosInWindow as mu_t. Without FBMP RGS, directly fit μ and t_0 .

Result: fitting process is not related to bias of μ .



2.3 P-FBMP with truth prior

```

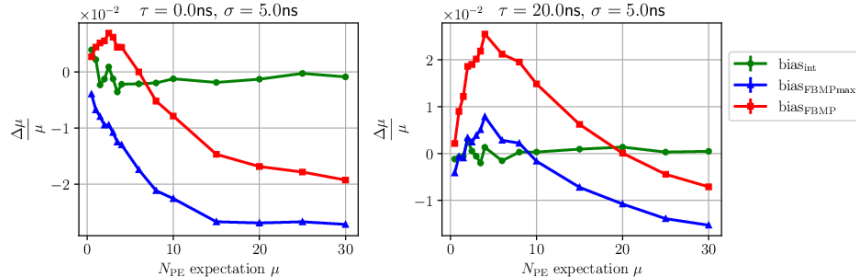
tlist = truth['HitPosInWindow'][truth['HitPosInWindow'] <
    right_wave - 1]
2 if len(tlist) == 1:
    tlist_edge = np.array([tlist[0] - 0.5, tlist[0] + 0.5])
4 else:
    tlist_edge = np.concatenate([[tlist[0] - np.diff(tlist)[0] /
        2], (tlist[1:] + tlist[:-1]) / 2, [tlist[-1] + np.diff(
        tlist)[-1] / 2]])
6 t_auto = (np.arange(left_wave, right_wave) / wff.nshannon[:, None]
    - tlist
A = p[2] * np.exp(-1 / 2 * (np.log((t_auto + np.abs(t_auto)) / p[0]
    / 2) / p[1]) ** 2)
8 t0_t = t0_truth[i]['T0']
mu_t = len(truth)
10 factor = np.sqrt(np.diag(np.matmul(A.T, A)))
A = np.matmul(A, np.diag(1. / np.sqrt(np.diag(np.matmul(A.T, A)))))
12 la = mu_t * np.array([integrate.quad(lambda t : wff.
    convolve_exp_norm(t - t0_t, Tau, Sigma), tlist_edge[i],
    tlist_edge[i+1])[0] for i in range(len(tlist))]) + 1e-8
xmmse, xmmse_star, psy_star, nu_star, nu_star_bk, T_star, d_tot_i,
d_max_i, num_i = wff.fbmp_rfxn_reduced(wave_r, A, la, spe_pre[
    cid]['std'] ** 2, (gsigma * factor / gmu) ** 2, factor, len(la)
    , stop=5, truth=truth, i=i, left=left_wave, right=right_wave,
    tlist=tlist, gmu=gmu, para=p)
14 c_star = np.zeros_like(xmmse_star).astype(int)
for k in range(len(T_star)):
16     t, c = np.unique(T_star[k][xmmse_star[k][T_star[k]] > 0],
        return_counts=True)
        c_star[k, t] = c
18 mu = np.average(c_star.sum(axis=1), weights=psy_star)
t0 = t0_t

```

Motivation: to prove difference between artificial prior and truth prior (derived from simulation) used in FBMP is not the origin of μ bias.

Progress: Use true HitPosInWindow as tlist, true T0 as t0_t, length of HitPosInWindow as mu_t. la is vector of integral in each time bins.

Result: prior used in FBMP is not the origin of μ bias.



2.4 P-FBMP using different bin width

```

1 mu_t = abs(wave.sum() / gmu)
A, wave_r, tlist, t0_t, t0_delta, cha, left_wave, right_wave = wff.
    initial_params(wave[:, wff.nshannon], spe_pre[ent[i]['ChannelID'
    ]], Tau, Sigma, gmu, Thres['lucyddM^\ast'], p, nsp, nstd, is_t0=
    True, is_delta=False, n=n, nshannon=1)
3 mu_t = abs(wave_r.sum() / gmu)
def optit0mu(t0, mu, n, xmmse_star, psy_star, c_star, la):
5     ys = np.log(psy_star) - np.log(poisson.pmf(c_star, la)).sum(
        axis=1)
    ys = np.exp(ys - ys.max()) / np.sum(np.exp(ys - ys.max()))
7     t0list = np.arange(t0 - 3 * Sigma, t0 + 3 * Sigma + 1e-6, 0.2)
    mulist = np.arange(max(1e-8, mu - 3 * np.sqrt(mu)), mu + 3 * np
        .sqrt(mu), 0.1)
9     b_mu = [max(1e-8, mu - 5 * np.sqrt(mu)), mu + 5 * np.sqrt(mu)]
    tlist_pan = np.sort(np.unique(np.hstack(np.arange(0, window)[: ,
        None] + np.arange(0, 1, 1 / n))))
11     As = np.zeros((len(xmmse_star), len(tlist_pan)))
    As[:, np.isin(tlist_pan, tlist)] = c_star
13     assert sum(np.sum(As, axis=0) > 0) > 0

15     def likelihood(x):
        a = x[0] * wff.convolve_exp_norm(tlist_pan - x[1], Tau,
            Sigma) / n + 1e-8 # use tlist_pan not tlist
17         li = -special.logsumexp(np.log(poisson.pmf(As, a)).sum(axis
            =1), b=ys)
        return li

19     likemu = np.array([likelihood([mulist[j], t0]) for j in range(
        len(mulist)])])
21     liket0 = np.array([likelihood([mu, t0list[j]]) for j in range(
        len(t0list)])])
    mu, t0 = opti.fmin_l_bfgs_b(likelihood, x0=[mulist[likemu.
        argmin()], t0list[liket0.argmax()]], approx_grad=True,
        bounds=[b_mu, b_t0], maxfun=50000)[0]
23     return mu, t0

25 truth = pelist[pelist['TriggerNo'] == ent[i]['TriggerNo']]

27 factor = np.sqrt(np.diag(np.matmul(A.T, A)))
A = np.matmul(A, np.diag(1. / np.sqrt(np.diag(np.matmul(A.T, A)))))
29 la = mu_t * wff.convolve_exp_norm(tlist - t0_t, Tau, Sigma) / n + 1
    e-8
    xmmse, xmmse_star, psy_star, nu_star, nu_star_bk, T_star, d_tot_i,
    d_max_i, num_i = wff.fbmpr_fxn_reduced(wave_r, A, la, spe_pre[
    cid]['std'] ** 2, (gsigma * factor / gmu) ** 2, factor, len(la)
    , stop=5, truth=truth, i=i, left=left_wave, right=right_wave,
    tlist=tlist, gmu=gmu, para=p)
31 time_fbmp = time_fbmp + time.time() - time_fbmp_start
c_star = np.zeros_like(xmmse_star).astype(int)
33 for k in range(len(T_star)):
    t, c = np.unique(T_star[k][xmmse_star[k][T_star[k]] > 0],
        return_counts=True)
35     c_star[k, t] = c
    maxindex = 0
37

```

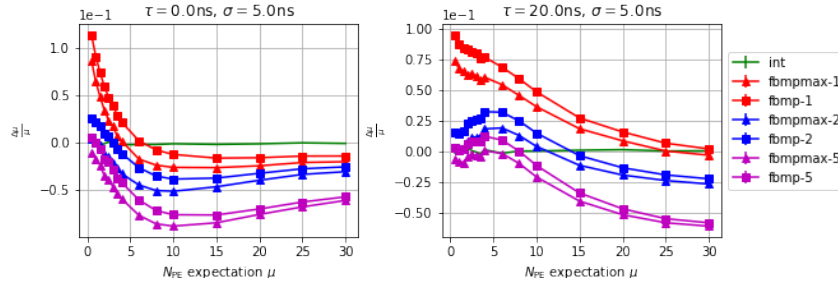
```

xmmse_most = xmmse_star[maxindex]
39 pet = np.repeat(tlist[xmmse_most > 0], c_star[maxindex][xmmse_most
> 0])
cha = np.repeat(xmmse_most[xmmse_most > 0] / factor[xmmse_most > 0]
/ c_star[maxindex][xmmse_most > 0], c_star[maxindex][
41 xmmse_most > 0])
mu, t0 = optit0mu(t0_t, mu_t, n, xmmse_star, psy_star, c_star, la)
43 mu_i, t0_i = optit0mu(t0_t, mu_t, n, xmmse_most[None, :], np.array
([1]), c_star[maxindex][None, :], la)

```

Motivation: to demonstrate the bin width's influence on μ bias.

Progress: $1/n$ is the bin width, $n = \{1, 2, 5\}$



2.5 N_{PE} estimation in one bin

```

1 def getm(i, p):
    N = 10000
    bias = np.empty(N)
    np.random.seed(i)
    Mu = 10
    gmu = 160
    gsigma = 40
    npan = np.arange(1, 50)
    9 for i in range(N):
        n = poisson.ppf(1 - uniform.rvs(scale=1-poisson.cdf(0, Mu),
size=1), Mu).astype(int)
        11 cha = norm.ppf(1 - uniform.rvs(scale=1-norm.cdf(0, loc=gmu,
scale=gsigma), size=n), loc=gmu, scale=gsigma)
        cha = cha.sum()
        13 if p:
            weight = poisson.pmf(npan, Mu) * norm.pdf(cha, loc=gmu
* npan, scale=gsigma * np.sqrt(npan))
        15 else:
            weight = norm.pdf(cha, loc=gmu * npan, scale=gsigma *
np.sqrt(npan))
        17 weight = weight / weight.sum()
        bias[i] = np.sum(npan * weight) - n
        19 m = bias.mean()
        return m
21 slices = np.arange(1000).T.tolist()

```

```

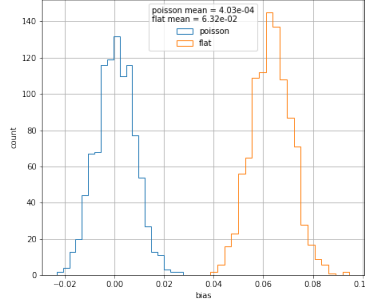
23 with Pool(100) as pool:
    resultpoisson = np.hstack([pool.starmap(getm, zip(slices, [True]
    ] * len(slices)))]])
25 with Pool(100) as pool:
    resultflat = np.hstack([pool.starmap(getm, zip(slices, [False]
    * len(slices)))]])

```

Motivation: to estimate bias of μ based on toy simulation in one bin

Progress: set μ . Sampling: $n \sim \text{Poisson}(n|\mu)$, $q_i \sim \text{Gaussian}(q_i|1, \sigma_q^2)$, $i = \{1, 2, \dots, n\}$, $Q = \sum_i q_i$. Estimation: $p(n|Q) = \frac{\text{Poisson}(n|\mu) \cdot \text{Gaussian}(Q|n, n\sigma_q^2)}{\sum_{j=1}^n \text{Poisson}(j|\mu) \cdot \text{Gaussian}(Q|j, j\sigma_q^2)}$
or $p(n|Q) = \frac{\text{Gaussian}(Q|n, n\sigma_q^2)}{\sum_{j=1}^n \text{Gaussian}(Q|j, j\sigma_q^2)}$

Result: when using Poisson prior, there is **no** bias, when using flat prior, there is bias.



2.6 N_{PE} estimation based on toy simulation

```

1 n = 10000
  npe = 30
3 noi = True
  if noi:
5     std = 1.
  else:
7     std = 1e-4
  window = 200
9 np.random.seed(0)
  wdt = np.dtype([( 'No', np.uint32), ( 'WaveformM^ast', np.float,
  window)])
11 waves = np.empty(n).astype(wdt)
  tlist = np.repeat(np.array([0, 1, 1]), npe / 3)
13 sams = [np.vstack((tlist, wff.charge(npe, gmu=gmu, gsigma=gsigma,
  thres=0))).T for i in range(n)]
  pan = np.arange(0, window)
15 t0 = 0.5
  for i in tqdm(range(n)):
17     wave = np.sum([np.where(pan > sams[i][j, 0], wff.spe(pan - sams
    [i][j, 0], tau=p[0], sigma=p[1], A=p[2]) * sams[i][j, 1] /
    gmu, 0) for j in range(len(sams[i]))]), axis=0)

```

```

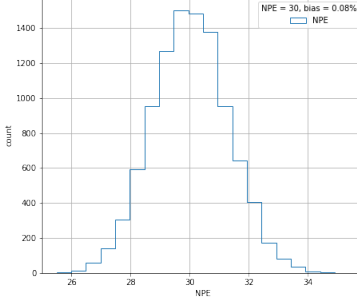
19         if noi:
20             wave = wave + np.random.normal(0, std, size=window)
21             waves[i]['WaveforM^ast'] = wave
22 waves['No'] = np.arange(n).astype(np.uint32)
23 sdt = np.dtype([( 'No', np.uint32), ( 'HitPosInWindow', np.float64),
24                 ( 'Charge', np.float64)])
25 pelist = np.empty(sum([len(sams[i]) for i in range(n)]).astype(
26     sdt))
27 pelist['No'] = np.repeat(np.arange(n), [len(sams[i]) for i in range(
28     n)]).astype(np.uint32)
29 pelist['HitPosInWindow'] = np.hstack([sams[i][:, 0] for i in range(
30     n)])
31 pelist['Charge'] = np.hstack([sams[i][:, 1] for i in range(n)])
32 mu = np.empty(n)
33 for i in tqdm(range(n)):
34     wave = waves[i]['WaveforM^ast'].astype(np.float64) * spe_pre
35     [0]['epulse']
36     truth = pelist[pelist['No'] == waves[i]['No']]
37     tlist = np.unique(truth['HitPosInWindow'])
38
39     t_auto = np.arange(0, window)[: , None] - tlist
40     A = p[2] * np.exp(-1 / 2 * (np.log((t_auto + np.abs(t_auto)) /
41         p[0] / 2) / p[1]) ** 2)
42     mu_t = npe
43     factor = np.sqrt(np.diag(np.matmul(A.T, A)))
44     A = np.matmul(A, np.diag(1. / np.sqrt(np.diag(np.matmul(A.T, A)
45         ))))
46     la = mu_t * np.array([1, 2]) / 3
47
48     xmmse, xmmse_star, psy_star, nu_star, nu_star_bk, T_star,
49         d_tot_i, d_max_i, num_i = wff.fbmpf_xn_reduced(wave, A, la
50         , std ** 2, (gsigma * factor / gmu) ** 2, factor, len(la),
51         stop=5)
52
53     c_star = np.zeros_like(xmmse_star).astype(int)
54     for k in range(len(T_star)):
55         t, c = np.unique(T_star[k][xmmse_star[k][T_star[k]] > 0],
56             return_counts=True)
57         c_star[k, t] = c
58
59     mu[i] = np.average(c_star.sum(axis=1), weights=psy_star)

```

Motivation: try to understand the relation between convolution process and bias

Progress: there is no μ , set N_{PE} as 30, set *HitPosInWindow* to $[0, 1]$, set time profile prior as $[1/3, 2/3]$, sample *Charge*. Use FBMP to generate posterior distribution of N_{PE} .

Result: there is **no** bias on this configuration



2.7 N_{PE} ergodic estimation based on toy simulation

```

1  spemode = 'spe'
   # spemode = 'delta'
3  # spemode = 'flat'
   prior = False
5  plot = False

7  n = 500
   gmu = 160.
9  gsigma = gmu / 4
   window = 200
11 npe = 3
   assert window > npe

13 def spe(t, mode='spe'):
15     if mode == 'spe':
16         return wff.spe((t + np.abs(t)) / 2, p[0], p[1], p[2])
17     elif mode == 'delta':
18         return np.where(t == 0, gmu, 0)
19     elif mode == 'flat':
20         return np.ones_like(t) / window * gmu

21 noi = True
23 if noi:
24     std = 1
25 else:
26     std = 1e-4
27 np.random.seed(0)
   wdtp = np.dtype([( 'No', np.uint32), ( 'Waveform', np.float, window)
   ])
29 waves = np.empty(n).astype(wdtp)

31 tlist = np.arange(npe)

33 p = spe_pre[0][ 'parameters' ]
   sams = [np.vstack((tlist, wff.charge(npe, gmu=gmu, gsigma=gsigma,
   thres=0))).T for i in range(n)]
35 pan = np.arange(window)
   for i in tqdm(range(n)):
37     # wave = np.sum([np.where(pan >= sams[i][j, 0], spe(pan - sams[
   i][j, 0], mode=spemode) * sams[i][j, 1] / gmu, 0) for j in

```

```

range(len(sams[i])), axis=0)
wave = np.sum([spe(pan - sams[i][j, 0], mode=spemode) * sams[i]
               ][j, 1] / gmu for j in range(len(sams[i]))], axis=0)
39 if noi:
    wave = wave + np.random.normal(0, std, size=window)
41 waves[i]['Waveform'] = wave
waves['No'] = np.arange(n).astype(np.uint32)
43 sdt = np.dtype([( 'No', np.uint32), ( 'HitPosInWindow', np.float64),
    ( 'Charge', np.float64)])
pelist = np.empty(sum([len(sams[i]) for i in range(n)]).astype(
    sdt))
45 pelist['No'] = np.repeat(np.arange(n), [len(sams[i]) for i in range(
    n)]).astype(np.uint32)
pelist['HitPosInWindow'] = np.hstack([sams[i][:, 0] for i in range(
    n)])
47 pelist['Charge'] = np.hstack([sams[i][:, 1] for i in range(n)])

49 # npe = 3
aver_npe = np.empty(n)
51 for i in tqdm(range(n)):
    wave = waves[i]['Waveform'].astype(np.float64)[:window] *
        spe_pre[0]['epulse']
53 truth = pelist[pelist['No'] == waves[i]['No']]
tlist = np.unique(truth['HitPosInWindow'])

55 t_auto = np.arange(window)[: , None] - tlist
57 A = spe(t_auto, spemode)
mu_t = npe
59 factor = np.sqrt(np.diag(np.matmul(A.T, A)))
A = A / factor
61 la = mu_t * np.ones_like(tlist) / len(tlist)

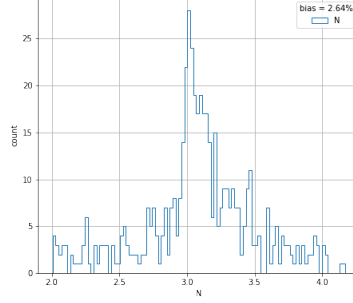
63 samnum = int(10 ** 3)
ind = np.array([[i // 100, i // 10 % 10, i % 10] for i in range(
    samnum)])
65 nu = np.empty(samnum)
for j in range(samnum):
67 nu[j] = wff.nu_direct(wave, A, ind[j], factor, (gsigma *
    factor / gmu) ** 2, std ** 2, la, prior=prior)
    nu[j] = nu[j] + poisson.logpmf(ind[j], mu=la).sum()
69 prob = np.exp(nu - nu.max()) / np.sum(np.exp(nu - nu.max()))
aver_npe[i] = np.average(ind.sum(axis=1), weights=prob)

```

Motivation: see the estimation of N_{PE} when ergodic in model space

Progress: there is no μ , set N_{PE} as 3, set $tlist$ to $[0, 1, 2]$. Use ergodic process to generate posterior distribution of N_{PE} .

Result: there is **still** bias on this configuration



2.8 Influence of lucyddm tlist initialization on μ bias

```

n = 2
2 A, wave_r, tlist, t0_t, t0_delta, cha, left_wave, right_wave = wff.
   initial_params(wave[:, wff.nshannon], spe_pre[ent[i]['ChannelID',
   ]], Tau, Sigma, gmu, Thres['lucyddM'\ast], p, nsp, nstd, is_t0=
   True, is_delta=False, n=n, nshannon=1)

4 truth = pelist[pelist['TriggerNo'] == ent[i]['TriggerNo']]

6 c_star_truth = np.sum([np.where(tlist - 0.5 / n < truth['
   HitPosInWindow'])[j], 1, 0) * np.where(tlist + 0.5 / n > truth['
   HitPosInWindow'])[j], 1, 0) for j in range(len(truth))], axis=0)

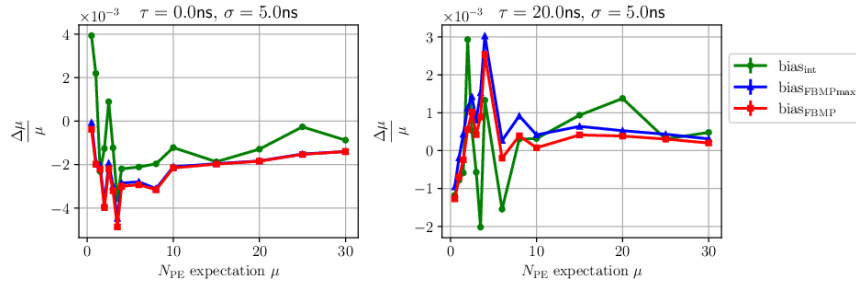
8 mu = c_star_truth.sum()
   t0 = t0_t

```

Motivation: to test the influence of lucyddm time bin initialization on μ bias

Progress: lucyddm initialization, estimate μ as number of truth *HitPosInWindow* in *tlist*

Result: there is **no** bias from lucyddm *tlist* initialization



2.9 Influence of lucyddm wave_r initialization on μ bias

```

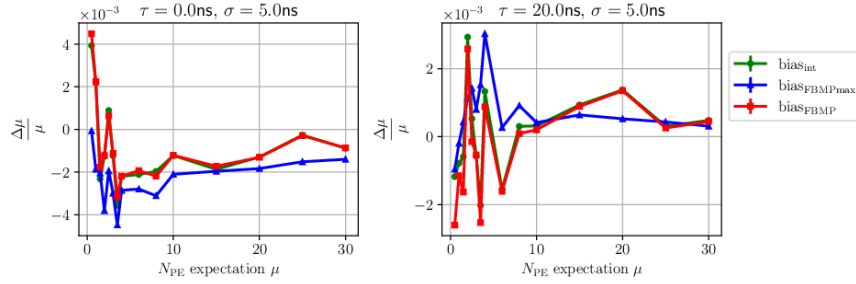
1 mu_t = abs(wave.sum() / gmu)
  n = 2
3 A, wave_r, tlist, t0_t, t0_delta, cha, left_wave, right_wave = wff.
  initial_params(wave[:, wff.nshannon], spe_pre[ent[i]['ChannelID'
  ]], Tau, Sigma, gmu, Thres['lucyddM^ast'], p, nsp, nstd, is_t0=
  True, is_delta=False, n=n, nshannon=1)
  mu_t = abs(wave_r.sum() / gmu)
5 mu = mu_t
  t0 = t0_t

```

Motivation: to test the influence of waveform cut in lucyddm initialization on μ bias

Progress: lucyddm initialization, estimate μ as number of integral of truncated waveform **wave_r**

Result: there is **no** bias from lucyddm waveform cut initialization



2.10 Iterative P-FBMP

```

mu_t = abs(wave.sum() / gmu)
2 if Tau > 10:
    n = min(math.ceil(20 / mu_t), 5)
4 else:
    n = min(math.ceil(4 / mu_t), 3)
6 A, wave_r, tlist, t0_t, t0_delta, cha, left_wave, right_wave = wff.
  initial_params(wave[:, wff.nshannon], spe_pre[ent[i]['ChannelID'
  ]], Tau, Sigma, gmu, Thres['lucyddM^ast'], p, nsp, nstd, is_t0=
  True, is_delta=False, n=n, nshannon=1)
  mu_t = abs(wave_r.sum() / gmu)
8 def optit0mu(t0, mu, n, xmmse_star, psy_star, c_star, la):
    ys = np.log(psy_star) - np.log(poisson.pmf(c_star, la)).sum(
      axis=1)
10    ys = np.exp(ys - ys.max()) / np.sum(np.exp(ys - ys.max()))
    t0list = np.arange(t0 - 3 * Sigma, t0 + 3 * Sigma + 1e-6, 0.2)
12    mulist = np.arange(max(1e-8, mu - 3 * np.sqrt(mu)), mu + 3 * np.
      sqrt(mu), 0.1)
    b_mu = [max(1e-8, mu - 5 * np.sqrt(mu)), mu + 5 * np.sqrt(mu)]
14    tlist_pan = np.sort(np.unique(np.hstack(np.arange(0, window)[: ,
      None] + np.arange(0, 1, 1 / n))))
    As = np.zeros((len(xmmse_star), len(tlist_pan)))
16    As[:, np.isin(tlist_pan, tlist)] = c_star

```

```

18     assert sum(np.sum(As, axis=0) > 0) > 0

19     def likelihood(x):
20         a = x[0] * wff.convolve_exp_norm(tlist_pan - x[1], Tau,
            Sigma) / n + 1e-8 # use tlist_pan not tlist
            li = -special.logsumexp(np.log(poisson.pmf(As, a)).sum(axis
            =1), b=ys)
22         return li

23     likemu = np.array([likelihood([mulist[j], t0]) for j in range(
        len(mulist))])
        liket0 = np.array([likelihood([mu, t0list[j]]) for j in range(
            len(t0list))])
26     mu, t0 = opti.fmin_l_bfgs_b(likelihood, x0=[mulist[likemu.
        argmin()], t0list[liket0.argmax()]], approx_grad=True,
        bounds=[b.mu, b.t0], maxfun=50000)[0]
        return mu, t0

28     truth = pelist[pelist['TriggerNo'] == ent[i]['TriggerNo']]
30     time_fbmp_start = time.time()
        factor = np.sqrt(np.diag(np.matmul(A.T, A)).mean())
32     A = np.matmul(A, np.diag(1. / np.sqrt(np.diag(np.matmul(A.T, A)))))

34     t0_bk = np.inf
        mu_bk = np.inf
36     interc_i = 0
        while abs(mu_bk - mu_t) > 1e-3 or abs(t0_bk - t0_t) > 1e-3:
38         interc_i += 1
            t0_bk = t0_t
            mu_bk = mu_t
40         la = mu_t * wff.convolve_exp_norm(tlist - t0_t, Tau, Sigma) / n
            + 1e-8
42         xmmse, xmmse_star, psy_star, nu_star, nu_star_bk, T_star,
            d_tot_i, d_max_i, num_i = wff.fbmpr_fxn_reduced(wave_r, A,
            la, spe_pre[cid]['std'] ** 2, (gsigma * factor / gmu) ** 2,
            factor, len(la), stop=5, truth=truth, i=i, left=left_wave,
            right=right_wave, tlist=tlist, gmu=gmu, para=p)
        time_fbmp = time_fbmp + time.time() - time_fbmp_start
44         c_star = np.zeros_like(xmmse_star).astype(int)
            for k in range(len(T_star)):
46             t, c = np.unique(T_star[k][xmmse_star[k][T_star[k]] > 0],
                return_counts=True)
                c_star[k, t] = c

48         mu_t, t0_t = optit0mu(t0_t, mu_t, n, xmmse_star, psy_star,
            c_star, la)
50         if interc_i >= 10:
            break

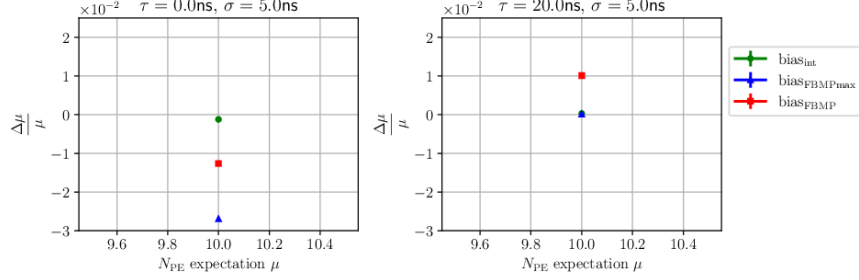
52     mu = mu_t
54     t0 = t0_t
        mu_i, t0_i = optit0mu(t0_t, mu_t, n, xmmse_most[None, :], np.array
            ([1]), c_star[maxindex][None, :], la)

```

Motivation: demonstrate whether iteration can reduce μ bias

Progress: set $\mu = 10$ to save time, iteration after FBMP sampling and fitting until μ and t_0 are stable

Result: iteration can **not** reduce μ bias



2.11 Waveform simulation with fixed *HitPosInWindow*

Waveform simulation:

```

1 np.random.seed(a0 + round(Tau + Sigma))
npe = poisson.ppf(1 - uniform.rvs(scale=1-poisson.cdf(0, mu), size=
    a1 - a0), mu).astype(int)
3 t0 = np.random.uniform(100., 500., size=a1 - a0)
sams = [np.vstack((np.arange(npe[i]) + t0[i], wff.charge(npe[i],
    gmu=gmu, gsigma=gsigma, thres=0))).T for i in range(a1 - a0)]
5 wdtp = np.dtype([('TriggerNo', np.uint32), ('ChannelID', np.uint32),
    ('WaveforM^ast', np.float, window * wff.nshannon)])
waves = np.empty(a1 - a0).astype(wdtp)
7 pan = np.arange(0, window, 1 / wff.nshannon)
for i in range(a1 - a0):
9     wave = np.sum([np.where(pan > sams[i][j, 0], wff.spe(pan - sams
        [i][j, 0], tau=p[0], sigma=p[1], A=p[2]) * sams[i][j, 1] /
        gmu, 0) for j in range(len(sams[i]))], axis=0)
    if args.noi:
11         wave = wave + np.random.normal(0, std, size=window * wff.
            nshannon)
    waves[i][ 'WaveforM^ast'] = wave
13 tdtp = np.dtype([('TriggerNo', np.uint32), ('ChannelID', np.uint32),
    ('T0', np.float64)])
t = np.empty(a1 - a0).astype(tdtp)
15 t[ 'TriggerNo'] = np.arange(a0, a1).astype(np.uint32)
t[ 'T0'] = t0
17 t[ 'ChannelID'] = 0
waves[ 'TriggerNo'] = np.arange(a0, a1).astype(np.uint32)
19 waves[ 'ChannelID'] = 0
sdtp = np.dtype([('TriggerNo', np.uint32), ('PMTId', np.uint32), ('
    HitPosInWindow', np.float64), ('Charge', np.float64)])
21 pelist = np.empty(sum([len(sams[i]) for i in range(a1 - a0)]).
    astype(sdtp))
pelist[ 'TriggerNo'] = np.repeat(np.arange(a0, a1), [len(sams[i])
    for i in range(a1 - a0)]).astype(np.uint32)
23 pelist[ 'PMTId'] = 0
pelist[ 'HitPosInWindow'] = np.hstack([sams[i][:, 0] for i in range(
    a1 - a0)])

```

```

25 pelist[ 'Charge' ] = np.hstack([sams[i][:, 1] for i in range(a1 - a0)
    ])

```

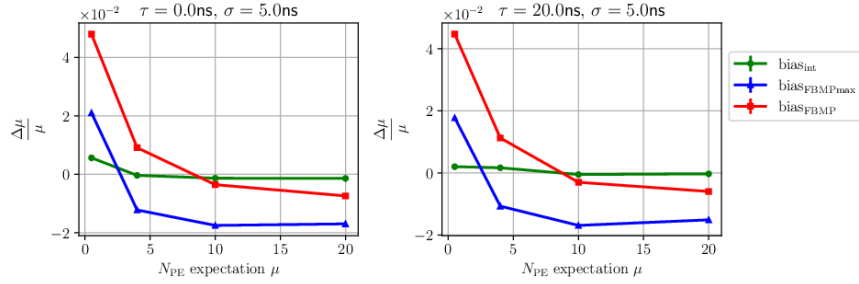
P-FBMP:

```

1  mu_t = abs(wave.sum()) / gmu
2  if Tau > 10:
3      n = min(math.ceil(20 / mu_t), 5)
4  else:
5      n = min(math.ceil(4 / mu_t), 3)
6  A, wave_r, tlist, t0_t, t0_delta, cha, left_wave, right_wave = wff.
    initial_params(wave[:, wff.nshannon], spe_pre[ent[i][ 'ChannelID'
    ]], Tau, Sigma, gmu, Thres[ 'lucyddM^ast' ], p, nsp, nstd, is_t0=
    True, is_delta=False, n=n, nshannon=1)
7
8  truth = pelist[ pelist[ 'TriggerNo' ] == ent[i][ 'TriggerNo' ] ]
9
10 tlist = truth[ 'HitPosInWindow' ][ truth[ 'HitPosInWindow' ] <
    right_wave - 1 ]
11 if len(tlist) == 0:
12     tlist = np.array([300])
13 t_auto = (np.arange(left_wave, right_wave) / wff.nshannon)[: , None]
    - tlist
14 A = p[2] * np.exp(-1 / 2 * (np.log((t_auto + np.abs(t_auto)) / p[0]
    / 2) / p[1]) ** 2)
15
16 t0_t = t0_truth[i][ 'T0' ]
17 mu_t = len(truth)
18 factor = np.sqrt(np.diag(np.matmul(A.T, A)))
19 A = np.matmul(A, np.diag(1. / np.sqrt(np.diag(np.matmul(A.T, A)))))
20 la = mu_t * np.ones(len(tlist)) / len(tlist)
21 xmmse, xmmse_star, psy_star, nu_star, nu_star_bk, T_star, d_tot_i,
    d_max_i, num_i = wff.fbmpr_fxn_reduced(wave_r, A, la, spe_pre[
    cid][ 'std' ] ** 2, (gsigma * factor / gmu) ** 2, factor, len(la)
    , stop=5, truth=truth, i=i, left=left_wave, right=right_wave,
    tlist=tlist, gmu=gmu, para=p)
22 time_fbmp = time_fbmp + time.time() - time_fbmp_start
23 c_star = np.zeros_like(xmmse_star).astype(int)
24 for k in range(len(T_star)):
25     t, c = np.unique(T_star[k][xmmse_star[k][ T_star[k] ] > 0],
        return_counts=True)
26     c_star[k, t] = c
27 maxindex = 0
28
29 xmmse_most = xmmse_star[maxindex]
30 pet = np.repeat(tlist[xmmse_most > 0], c_star[maxindex][xmmse_most
    > 0])
31 cha = np.repeat(xmmse_most[xmmse_most > 0] / factor[xmmse_most > 0]
    / c_star[maxindex][xmmse_most > 0], c_star[maxindex][
    xmmse_most > 0])
32
33 mu = np.average(c_star.sum(axis=1), weights=psy_star)
34 t0 = t0_t
35 mu_i = len(cha)
36 t0_i = t0_t

```

Motivation: to further reduce the influence of binning
Progress: when PE number is N_{PE} , set *HitPosInWindow* relatively (to t_0)
 $\{0, 1, \dots, N_{PE} - 1\}$, sample *Charge* then P-FBMP process with truth prior.
Result: there is still bias with fixed *HitPosInWindow*



2.12 Waveform simulation with fixed *HitPosInWindow*, without prior

Waveform simulation:

```
sams = [np.vstack((np.arange(npe[i]) + t0[i], wff.charge(npe[i],
    gmu=gmu, gsigma=gsigma, thres=0))).T for i in range(a1 - a0)]
```

P-FBMP:

```
1 def fbmpr_fxn_reduced(y, A, p1, sig2w, sig2s, mus, D, stop=0, truth
2   =None, i=None, left=None, right=None, tlist=None, gmu=None,
3   para=None, prior=True):
4   '''
5   3 p1: prior probability for each bin.
6   sig2w: variance of white noise.
7   sig2s: variance of signal x_i.
8   mus: mean of signal x_i.
9   '''
10  # Only for multi-gaussian with arithmetic sequence of mu and
11  sigma
12  M, N = A.shape
13
14  p = 1 - poisson.pmf(0, p1).mean()
15  # Eq. (25)
16  if prior:
17      nu_true_mean = -M / 2 - M / 2 * np.log(sig2w) - p * N / 2 *
18      np.log(sig2s / sig2w + 1) - M / 2 * np.log(2 * np.pi)
19      + N * np.log(1 - p) + p * N * np.log(p / (1 - p))
20      nu_true_stdv = np.sqrt(M / 2 + N * p * (1 - p) * (np.log(p
21      / (1 - p)) - np.log(sig2s / sig2w + 1) / 2) ** 2)
22  else:
```

```

17     nu_true_mean = -M / 2 - M / 2 * np.log(sig2w) - p * N / 2 *
        np.log(sig2s / sig2w + 1) - M / 2 * np.log(2 * np.pi)
        nu_true_stdv = np.sqrt(M / 2 + N * p * (1 - p) * (np.log(
19         sig2s / sig2w + 1) / 2) ** 2)
    nu_stop = (nu_true_mean + stop * nu_true_stdv).max()

21    psy_thresh = 1e-4
    # upper limit of number of PEs.
23    P = max(math.ceil(min(M, p1.sum() + 3 * np.sqrt(p1.sum()))), 1)

25    T = np.full((P, D), 0)
    nu = np.full((P, D), -np.inf)
27    xmmse = np.zeros((P, D, N))
    cc = np.zeros((P, D, N))
29    d_tot = D

31    # nu_root: nu for all s_n=0.
    if prior:
33        nu_root = -0.5 * np.linalg.norm(y) ** 2 / sig2w - 0.5 * M *
            np.log(2 * np.pi) - 0.5 * M * np.log(sig2w) + np.log(
                poisson.pmf(0, p1)).sum()
    else:
35        nu_root = -0.5 * np.linalg.norm(y) ** 2 / sig2w - 0.5 * M *
            np.log(2 * np.pi) - 0.5 * M * np.log(sig2w)
    # Eq. (29)
37    cx_root = A / sig2w
    # Eq. (30) sig2s = 1 sigma^2 - 0 sigma^2
39    betaxt_root = sig2s / (1 + sig2s * np.einsum('ij,ij->j', A,
        cx_root, optimize=True))
    # Eq. (31)
41    if prior:
        nuxt_root = nu_root + 0.5 * (betaxt_root * (y @ cx_root +
            mus / sig2s) ** 2 - mus ** 2 / sig2s + np.log(
                betaxt_root / sig2s)) + np.log(poisson.pmf(1, p1) /
                poisson.pmf(0, p1))
43    else:
        nuxt_root = nu_root + 0.5 * (betaxt_root * (y @ cx_root +
            mus / sig2s) ** 2 - mus ** 2 / sig2s + np.log(
                betaxt_root / sig2s))
45    pan_root = np.zeros(N)

47    # Repeated Greedy Search
    for d in range(D):
49        nuxt = nuxt_root.copy()
        z = y.copy()
51        cx = cx_root.copy()
        betaxt = betaxt_root.copy()
53        pan = pan_root.copy()
        for p in range(P):
55            # look for duplicates of nu and nuxt, set to -inf.
            # only inspect the same number of PEs in Row p.
            nuxtshadow = np.where(np.sum(np.abs(nuxt - nu[p:(p+1),
57                :d]).T) < 1e-4, axis=0), -np.inf, nuxt)
            nustar = max(nuxtshadow)
            istar = np.argmax(nuxtshadow)
            nu[p, d] = nustar
61            T[p, d] = istar

```

```

63     pan[istar] += 1
64     # Eq. (33)
65     cx -= np.einsum('n,m,mp->np', betaxt[istar] * cx[:,
66         istar], cx[:, istar], A, optimize=True)
67
68     # Eq. (34)
69     z -= A[:, istar] * mus[istar]
70     assist = np.zeros(N)
71     t, c = np.unique(T[:p+1, d], return_counts=True)
72     assist[t] = mus[t] * c + sig2s[t] * c * np.dot(z, cx[:,
73         t])
74     cc[p, d][t] = c
75     xmmse[p, d] = assist
76
77     # Eq. (30)
78     betaxt = sig2s / (1 + sig2s * np.sum(A * cx, axis=0))
79     # Eq. (31)
80     if prior:
81         nuxt = nustar + 0.5 * (betaxt * (z @ cx + mus /
82             sig2s) ** 2 - mus ** 2 / sig2s + np.log(betaxt
83             / sig2s)) + np.log(poisson.pmf(pan + 1, mu=p1))
84             / poisson.pmf(pan, mu=p1))
85     else:
86         nuxt = nustar + 0.5 * (betaxt * (z @ cx + mus /
87             sig2s) ** 2 - mus ** 2 / sig2s + np.log(betaxt
88             / sig2s))
89     # nuxt[t] = -np.inf
90
91     if max(nu[:, d]) > nu_stop:
92         d_tot = d + 1
93         break
94     nu_bk = nu[:, :d_tot].copy()
95     nu = nu[:, :d_tot].T.flatten()
96
97     indx = np.argsort(nu)[::-1]
98     d_max = math.floor(indx[0] // P) + 1
99     num = min(math.ceil(np.sum(nu > nu.max() + np.log(psy_thresh))),
100         d_tot * P)
101     nu_star = nu[indx[:num]]
102     nu_star_bk = nu_bk.T.flatten()[indx[:num]]
103     # psy_star = np.exp(nu_star - nu.max()) / np.sum(np.exp(nu_star
104         - nu.max()))
105     T_star = [np.sort(T[:, (indx[k] % P) + 1, indx[k] // P]) for k in
106         range(num)]
107     xmmse_star = np.empty((num, N))
108     for k in range(num):
109         xmmse_star[k] = xmmse[indx[k] % P, indx[k] // P]
110
111     psy_star = np.exp(nu_star - nu.max()) / np.sum(np.exp(nu_star -
112         nu.max()))
113
114     xmmse = np.average(xmmse_star, weights=psy_star, axis=0)
115
116     return xmmse, xmmse_star, psy_star, nu_star, nu_star_bk, T_star
117         , d_tot, d_max, num

```



```

prior = False
2 truth = pelist[pelist['TriggerNo'] == ent[i]['TriggerNo']]

4 tlist = truth['HitPosInWindow'][truth['HitPosInWindow'] <
    right_wave - 1]
if len(tlist) == 0:
6     tlist = np.array([300])
t_auto = (np.arange(left_wave, right_wave) / wff.nshannon)[: , None]
    - tlist
8 A = p[2] * np.exp(-1 / 2 * (np.log((t_auto + np.abs(t_auto)) / p[0]
    / 2) / p[1]) ** 2)

10 t0_t = t0_truth[i]['T0']
mut = len(truth)
12 factor = np.sqrt(np.diag(np.matmul(A.T, A)))
A = A / factor
14 la = mut * np.ones(len(tlist)) / len(tlist)
xmmse, xmmse_star, psy_star, nu_star, nu_star_bk, T_star, d_tot_i,
d_max_i, num_i = wff.fbmp_fxn_reduced(wave_r, A, la, spe_pre[
    cid]['std'] ** 2, (gsigma * factor / gmu) ** 2, factor, len(la)
    , stop=5, truth=truth, i=i, left=left_wave, right=right_wave,
    tlist=tlist, gmu=gmu, para=p, prior=prior)

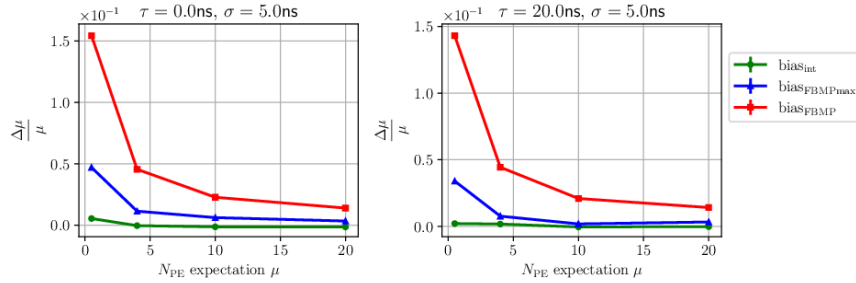
16 mu = np.average(c_star.sum(axis=1), weights=psy_star)
18 t0 = t0_t
mu_i = len(cha)
20 t0_i = t0_t

```

Motivation: to further reduce the influence of prior

Progress: set *HitPosInWindow* relatively (to t_0) $\{0, 1, \dots, N_{PE} - 1\}$, P-FBMP process **without** truth prior.

Result: all biases **are larger** than 0



2.13 P-FBMP without prior and with Gaussian normalization term

```

prior = False
2 space = True
n = 2

```

```

4 | tlist_pan = np.sort(np.unique(np.hstack(np.arange(0, window)[: ,
      None] + np.linspace(0, 1, n, endpoint=False) - (n // 2) / n)))
      b_t0 = [0., 600.]
6 |
8 | def likelihood(mu, t0, As_k, nu_star_k):
      a = wff.convolve_exp_norm(tlist_pan - t0, Tau, Sigma) / n + 1e
        -8 # use tlist_pan not tlist
      # a *= mu / a.sum()
10 |     a *= mu
      li = -special.logsumexp(np.log(poisson.pmf(As_k, mu=a)).sum(
        axis=1) + nu_star_k)
12 |     return li

14 | def sum_mu_likelihood(mu, t0_list, As_list, nu_star_list):
      return np.sum([likelihood(mu, t0_list[k], As_list[k],
        nu_star_list[k]) for k in range(len(t0_list))])

16 | def optit0mu(mu, t0, nu_star, As, mu_init=None):
      l = len(t0)
      mulist = np.arange(max(1e-8, mu - 2 * np.sqrt(mu)), mu + 2 * np
        .sqrt(mu), 1e-1)
20 |     b_mu = [max(1e-8, mu - 5 * np.sqrt(mu)), mu + 5 * np.sqrt(mu)]
      # psy_star = [np.exp(nu_star[k] - nu_star[k].max()) / np.sum(np
        .exp(nu_star[k] - nu_star[k].max())) for k in range(l)]
22 |     t0list = [np.arange(t0[k] - 3 * Sigma, t0[k] + 3 * Sigma + 1e
        -6, 0.2) for k in range(l)]
      sigmamu = None
      logLv_mu = None
      if mu_init is None:
26 |         mu_init = np.empty(l)
          for k in range(l):
28 |             mu_init[k] = mulist[np.array([likelihood(mulist[j], t0[
                k], As[k], nu_star[k]) for j in range(len(mulist))
                ]).argmin()]
              t0_init = t0list[k][np.array([likelihood(mu_init[k],
                t0list[k][j], As[k], nu_star[k]) for j in range(len
                (t0list[k]))]).argmin()])
30 |             likelihood_x = lambda x, As, nu_star: likelihood(x[0],
                x[1], As, nu_star)
              t0[k] = opti.fmin_l_bfgs_b(likelihood_x, args=(As[k],
                nu_star[k]), x0=[mu_init[k], t0_init], approx_grad=
                True, bounds=[b_mu, b_t0], maxfun=50000)[0][1]
32 |             Likelihood = lambda mu: np.sum([likelihood(mu, t0[k], As[k]
                ], nu_star[k]) for k in range(l)])
              mu, fval, _ = opti.fmin_l_bfgs_b(Likelihood, x0=[np.mean(
                mu_init)], approx_grad=True, bounds=[b_mu], maxfun
                =50000)

34 |     else:
      def Likelihood(mu, t0_list, As_list, nu_star_list):
36 |         with Pool(min(args.Ncpu // 3, cpu_count())) as pool:
              result = np.sum(pool.starmap(likelihood, zip([mu] *
                l, t0_list, As_list, nu_star_list)))
38 |         return result
      mu, fval, _ = opti.fmin_l_bfgs_b(Likelihood, args=[t0, As,
        nu_star], x0=[np.mean(mu_init)], approx_grad=True,
        bounds=[b_mu], maxfun=50000, factr=100.0, pgtol=1e-10)
40 |     print('Mu fitting info is ', -)

```

```

42     sigmamumu_est = np.sqrt(mu / N)
    mulist = np.sort(np.append(np.arange(max(1e-8, mu - 2 *
        sigmamumu_est), mu + 2 * sigmamumu_est, sigmamumu_est / 50),
        mu))
    partial_sum_mu_likelihood = partial(sum_mu_likelihood,
        t0_list=t0, As_list=As, nu_star_list=nu_star)
44     with Pool(min(args.Ncpu // 3, cpu_count())) as pool:
        logLv_mu = np.array(pool.starmap(
            partial_sum_mu_likelihood, zip(mulist)))
46
    mu_func = interp1d(mulist, logLv_mu, bounds_error=False,
        fill_value='extrapolate')
48     logLv_delta = np.vectorize(lambda mu_t: np.abs(mu_func(mu_t)
        - fval - 0.5))
    # sigmamumu = abs(opti.fmin_l_bfgs_b(logLv_delta, x0=[mulist[
        np.abs(logLv_mu - fval - 0.5).argmin()]], approx_grad=
        True, bounds=[[mulist[0], mulist[-1]]], maxfun=500000)
        [0] - mu) * np.sqrt(1)
50     sigmamumu_l = abs(opti.fmin_l_bfgs_b(logLv_delta, x0=[mulist[
        mulist <= mu][np.abs(logLv_mu[mulist <= mu] - fval -
        0.5).argmin()]], approx_grad=True, bounds=[[mulist[0],
        mulist[-1]]], maxfun=500000)[0] - mu) * np.sqrt(1)
    sigmamumu_r = abs(opti.fmin_l_bfgs_b(logLv_delta, x0=[mulist[
        mulist > mu][np.abs(logLv_mu[mulist > mu] - fval - 0.5)
        .argmin()]], approx_grad=True, bounds=[[mulist[0],
        mulist[-1]]], maxfun=500000)[0] - mu) * np.sqrt(1)
52     sigmamumu = (sigmamumu_l + sigmamumu_r) / 2
    print('Finite difference sigmamumu is {:.4}'.format(sigmamumu.
        item()))
54
    # derivative_mu2 = nd.Derivative(Likelihood, step=1e-10, n
        =2, full_output=True)
56     # s, info = derivative_mu2(mu, t0_list=t0, As_list=As,
        nu_star_list=nu_star)
    # print('Mu derivative info is', info)
58     # sigmamumu = 1 / np.sqrt(s) * np.sqrt(1)
    return mu, t0, [sigmamumu, mulist, logLv_mu, fval]
60
time_fbmp_start = time.time()
62     cid = ent[i]['ChannelID']
    assert cid == 0
64     wave = ent[i]['Waveform'].astype(np.float64) * spe_pre[cid]['epulse
        ']
66     # initialization
    mu_t = abs(wave.sum()) / gmu)
68     A, y, tlist, t0_t, t0_delta, cha, left_wave, right_wave = wff.
        initial_params(wave[:, wff.nshannon], spe_pre[ent[i]['ChannelID'
        ]], Tau, Sigma, gmu, Thres['lucyddm'], p, is_t0=True, is_delta=
        False, n=n, nshannon=1)
    mu_t = abs(y.sum()) / gmu)
70
    truth = pelist[pelist['TriggerNo'] == ent[i]['TriggerNo']]
72
    # Eq. (9) where the columns of A are taken to be unit-norm.
74     mus = np.sqrt(np.diag(np.matmul(A.T, A)))
    A = A / mus

```

```

76 p1 = mu_t * wff.convolve_exp_norm(tlist - t0_t, Tau, Sigma) / n + 1
    e-8
    # p1 = cha / cha.sum() * mu_t + 1e-8
78 p1 = p1 / p1.sum() * mu_t
    sig2w = spe_pre[cid]['std'] ** 2
80 sig2s = (gsigma * mus / gmu) ** 2
    xmmse_star, nu_star, T_star, c_star, d_max_i, num_i = wff.
        fbmpr_fxn_reduced(y, A, sig2w, sig2s, mus, len(p1), p1=p1,
            truth=truth, i=i, left=left_wave, right=right_wave, tlist=tlist
            , gmu=gmu, para=p, prior=prior, space=space)
82 time_fbmp[i - a0] = time.time() - time_fbmp_start

84 la_truth = Mu * wff.convolve_exp_norm(tlist - t0_truth[i]['T0'],
    Tau, Sigma) / n + 1e-8
    nu_space_prior = np.array([wff.nu_direct(y, A, c_star[j], mus,
        sig2s, sig2w, la_truth, prior=True, space=True) for j in range(
        num_i)])
86
    maxindex = nu_star.argmax()
88 xmmse_most = np.clip(xmmse_star[maxindex], 0, np.inf)
    pet = np.repeat(tlist[xmmse_most > 0], c_star[maxindex][xmmse_most
        > 0])
90 cha = np.repeat(xmmse_most[xmmse_most > 0] / mus[xmmse_most > 0] /
    c_star[maxindex][xmmse_most > 0], c_star[maxindex][xmmse_most >
        0])

92 As = np.zeros((num_i, len(tlist_pan)))
    As[:, np.isin(tlist_pan, tlist)] = c_star
94 assert sum(np.sum(As, axis=0) > 0) > 0

96 spacefactor = 0
    priorfactor = 0
98 if not space:
        spacefactor = np.array([-0.5 * np.log(np.linalg.det(wff.Phi(y,
            A, c_star[j], mus, sig2s, sig2w, p1))) for j in range(num_i
            )])
100 if prior:
        priorfactor = -poisson.logpmf(c_star, p1).sum(axis=1)
102 nu_star = nu_star + priorfactor + spacefactor
    # nu_star = np.log(np.exp(nu_star - nu_star.max()) / np.sum(np.exp(
        nu_star - nu_star.max()))))
104 mu, t0, _ = optit0mu(mu_t, [t0_t], [nu_star], [As])
    mu_i, t0_i, _ = optit0mu(mu_t, [t0_t], [np.array([0.])], [As[
        maxindex][None, :]])

```

```

1 def fbmpr_fxn_reduced(y, A, sig2w, sig2s, mus, D, p1, truth=None, i
    =None, left=None, right=None, tlist=None, gmu=None, para=None,
    prior=False, space=True, plot=False):
    ,,,
3     p1: prior probability for each bin.
    sig2w: variance of white noise.
5     sig2s: variance of signal x_i.
    mus: mean of signal x_i.
    ,,,
7     # Only for multi-gaussian with arithmetic sequence of mu and

```

```

9         sigma
M, N = A.shape

11     psy_thresh = 1e-1
# upper limit of number of PEs.
13     P = max(math.ceil(min(M, p1.sum() + 3 * np.sqrt(p1.sum()))), 1)

15     T = np.full((P, D), 0)
nu = np.full((P, D), -np.inf)
17     xmmse = np.zeros((P, D, N))
cc = np.zeros((P, D, N))

19     # nu_root: nu for all s_n=0.
# no Gaussian space factor
21     nu_root = -0.5 * np.linalg.norm(y) ** 2 / sig2w - 0.5 * M * np.
        log(2 * np.pi)
23     if space:
        nu_root -= 0.5 * M * np.log(sig2w)
25     if prior:
        nu_root += poisson.logpmf(0, p1).sum()
27     # Eq. (29)
cx_root = A / sig2w
29     # Eq. (30) sig2s = 1 sigma^2 - 0 sigma^2
betaxt_root = sig2s / (1 + sig2s * np.einsum('ij, ij->j', A,
        cx_root, optimize=True))
31     # Eq. (31)
# no Gaussian space factor
33     nuxt_root = nu_root + 0.5 * (betaxt_root * (y @ cx_root + mus /
        sig2s) ** 2 - mus ** 2 / sig2s)
    if space:
35         nuxt_root += 0.5 * np.log(betaxt_root / sig2s)
    if prior:
37         nuxt_root += poisson.logpmf(1, p1) - poisson.logpmf(0, p1)
pan_root = np.zeros(N)

39     # Repeated Greedy Search
for d in range(D):
41         nuxt = nuxt_root.copy()
43         z = y.copy()
        cx = cx_root.copy()
45         betaxt = betaxt_root.copy()
        pan = pan_root.copy()
47         for p in range(P):
            # look for duplicates of nu and nuxt, set to -inf.
            # only inspect the same number of PEs in Row p.
49             nuxtshadow = np.where(np.sum(np.abs(nuxt - nu[p:(p+1),
                :d].T) < 1e-4, axis=0), -np.inf, nuxt)
51             nustar = max(nuxtshadow)
            istar = np.argmax(nuxtshadow)
53             nu[p, d] = nustar
            T[p, d] = istar
55             pan[istar] += 1
            # Eq. (33)
57             cx -= np.einsum('n,m,mp->np', betaxt[istar] * cx[:,
                istar], cx[:, istar], A, optimize=True)

59     # Eq. (34)

```

```

61     z -= A[:, istar] * mus[istar]
        assist = np.zeros(N)
        t, c = np.unique(T[:p+1, d], return_counts=True)
63     assist[t] = mus[t] * c + sig2s[t] * c * np.dot(z, cx[:,
        t])
        cc[p, d][t] = c
65     xmmse[p, d] = assist

67     # Eq. (30)
        betaxt = sig2s / (1 + sig2s * np.sum(A * cx, axis=0))
69     # Eq. (31)
        # no Gaussian space factor
71     nuxt = nustar + 0.5 * (betaxt * (z @ cx + mus / sig2s)
        ** 2 - mus ** 2 / sig2s)
        if space:
73         nuxt += 0.5 * np.log(betaxt / sig2s)
        if prior:
75         nuxt += poisson.logpmf(pan + 1, mu=p1) - poisson.
            logpmf(pan, mu=p1)
            nuxt[np.isnan(nuxt)] = -np.inf
77     # nuxt[t] = -np.inf
    nu = nu.T.flatten()

79
    indx = np.argsort(nu)[::-1]
    d_max = math.floor(indx[0] // P) + 1
81    num = min(math.ceil(np.sum(nu > nu.max() + np.log(psy_thresh))),
        , D * P)
83    nu_star = nu[indx[:num]]
    psy_star = np.exp(nu_star - nu_star.max()) / np.sum(np.exp(
        nu_star - nu_star.max()))
85    T_star = [np.sort(T[:, (indx[k] % P) + 1, indx[k] // P]) for k in
        range(num)]
    xmmse_star = np.empty((num, N))
87    for k in range(num):
        xmmse_star[k] = xmmse[indx[k] % P, indx[k] // P]

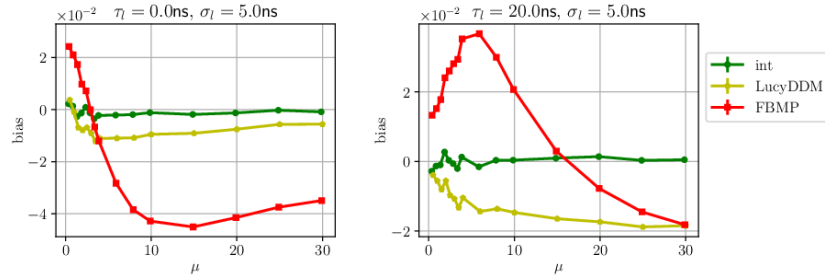
89
    c_star = np.zeros_like(xmmse_star, dtype=int)
91    for k in range(num):
        t, c = np.unique(T_star[k], return_counts=True)
93    c_star[k, t] = c

```

Motivation: to reduce the influence of prior

Progress: *HitPosInWindow* is sampled from time profile, P-FBMP process
without prior.

Result: μ bias persists.



2.14 P-FBMP with lucy prior and with Gaussian

```

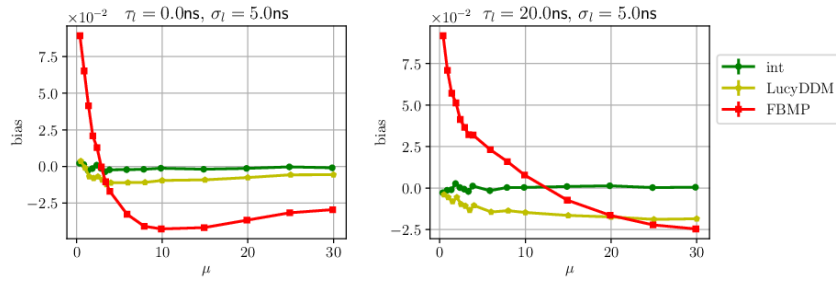
1 prior = True
  space = True
3 la = cha / cha.sum() * mu_t + 1e-8

```

Motivation: to show the relation between lucy prior and μ bias.

Progress: Use `cha` (derived from `lucyddm`) as `la` and the bin width is fixed to $1/2$.

Result: bias still exists when using lucy prior.



2.15 P-FBMP with profile prior and with Gaussian

```

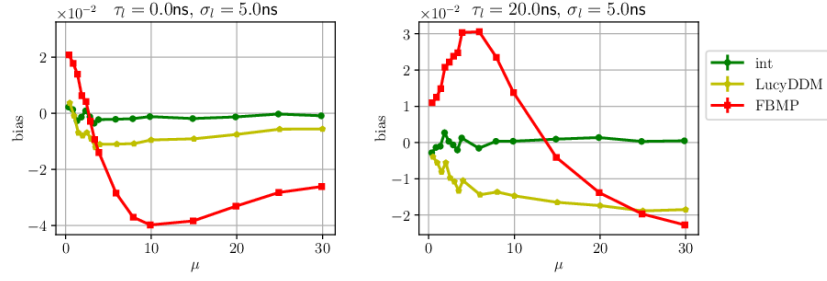
1 prior = True
  space = True
3 la = mu_t * wff.convolve_exp_norm(tlist - t0_t, Tau, Sigma) / n + 1
  e-8

```

Motivation: to show the relation between profile prior and μ bias.

Progress: Use time profile as `la` and the bin width is fixed to $1/2$.

Result: bias still exists when using profile prior.



2.16 P-FBMP without prior and without Gaussian normalization term

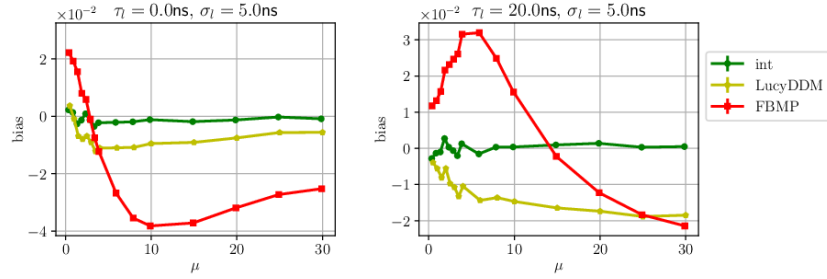
P-FBMP:

```
1 prior = False
  space = False
```

Motivation: to show the μ bias when Gaussian normalization term $-\frac{1}{2} \log \det \Sigma$ in model selecting metric ν is removed, additionally, without prior.

Progress: not calculate $-\frac{1}{2} \log \det \Sigma$ in ν when RGS.

Result: μ bias persists.



2.17 P-FBMP with lucy prior and without Gaussian normalization term

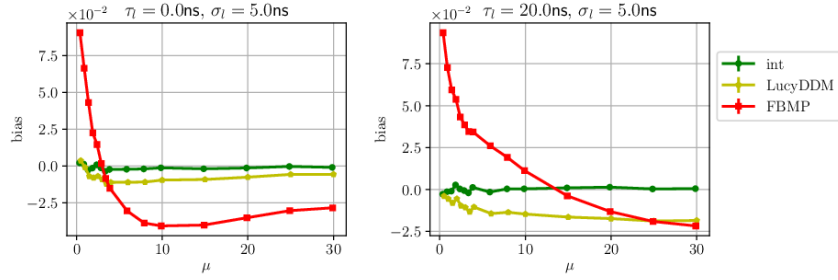
P-FBMP:

```
2 prior = True
  space = False
  la = cha / cha.sum() * mu_t + 1e-8
```

Motivation: to show the μ bias without Gaussian normalization term and with lucy prior.

Progress: not calculate $-\frac{1}{2} \log \det \Sigma$ in ν when RGS.

Result: μ bias persists.



2.18 P-FBMP with profile prior and without Gaussian normalization term

P-FBMP:

```

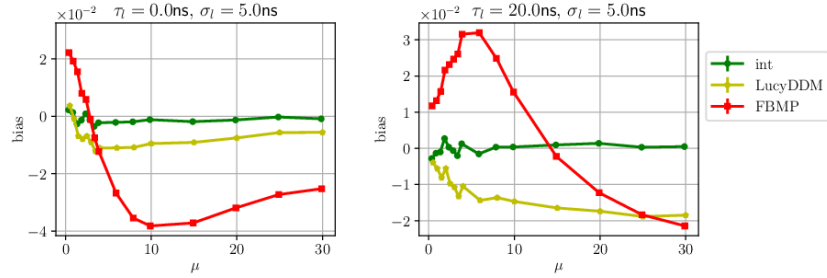
1 prior = True
  space = False
3 la = mu_t * wff.convolve_exp_norm(tlist - t0_t, Tau, Sigma) / n + 1
  e-8

```

Motivation: to show the μ bias without Gaussian normalization term and with profile prior.

Progress: not calculate $-\frac{1}{2} \log \det \Sigma$ in ν when RGS.

Result: μ bias persists.



2.19 P-FBMP μ estimation with α correction

```

1 prior = False
  nsp = 4
3 nstd = 3
  mu_t = abs(wave.sum()) / gmu
5 n = 5
A, wave_r, tlist, t0_t, t0_delta, cha, left_wave, right_wave = wff.
  initial_params(wave[:, wff.nshannon], spe_pre[ent[i]['ChannelID',
  ]], Tau, Sigma, gmu, Thres['lucyddm'], p, nsp, nstd, is_t0=True
  , is_delta=False, n=n, nshannon=1)

```

```

7 | mu_t = abs(wave_r.sum() / gmu)
   | def optit0mu(t0, mu, n, psy_star, c_star, la):
9 |     ys = np.log(psy_star)
   |     if prior:
11 |         ys = ys - poisson.logpmf(c_star, la).sum(axis=1)
   |         ys = np.exp(ys - ys.max()) / np.sum(np.exp(ys - ys.max()))
13 |         t0list = np.arange(t0 - 3 * Sigma, t0 + 3 * Sigma + 1e-6, 0.2)
   |         mulist = np.arange(max(1e-8, mu - 3 * np.sqrt(mu)), mu + 3 * np
   |             .sqrt(mu), 0.1)
15 |         b_mu = [max(1e-8, mu - 5 * np.sqrt(mu)), mu + 5 * np.sqrt(mu)]
   |         tlist_pan = np.sort(np.unique(np.hstack(np.arange(0, window)[: ,
   |             None] + np.linspace(0, 1, n, endpoint=False) - (n // 2) /
   |             n)))
17 |         As = np.zeros((len(psy_star), len(tlist_pan)))
   |         As[:, np.isin(tlist_pan, tlist)] = c_star
19 |         assert sum(np.sum(As, axis=0) > 0) > 0
   |         def likelihood(x):
21 |             a = wff.convolve_exp_norm(tlist_pan - x[1], Tau, Sigma) / n
   |                 + 1e-8 # use tlist_pan not tlist
   |             a = a / a.sum() * x[0]
23 |             li = -special.logsumexp(np.log(poisson.pmf(As, a)).sum(axis
   |                 =1), b=ys)
   |             return li
25 |         likemu = np.array([likelihood([mulist[j], t0]) for j in range(
   |             len(mulist)])])
   |         liket0 = np.array([likelihood([mu, t0list[j]]) for j in range(
   |             len(t0list)])])
27 |         mu, t0 = opti.fmin_l_bfgs_b(likelihood, x0=[mulist[likemu.
   |             argmin()], t0list[liket0.argmax()]], approx_grad=True,
   |             bounds=[b_mu, b_t0], maxfun=50000)[0]
   |         return mu, t0
29 | # 1st FBMP
   | time_fbmp_start = time.time()
31 | # Eq. (9) where the columns of A are taken to be unit-norm.
   | factor = np.sqrt(np.diag(np.matmul(A.T, A)))
33 | A = A / factor
   | # la = mu_t * wff.convolve_exp_norm(tlist - t0_t, Tau, Sigma) / n +
   |     1e-8
35 | la = cha / cha.sum() * mu_t + 1e-8
   | la = la / la.sum() * mu_t
37 | xmmse, xmmse_star, psy_star, nu_star, nu_star_bk, T_star, d_max_i,
   |     num_i = wff.fbmpr_fxn_reduced(wave_r, A, spe_pre[cid]['std'] **
   |         2, (gsigma * factor / gmu) ** 2, factor, len(la), pl=la, stop
   |         =5, truth=truth, i=i, left=left_wave, right=right_wave, tlist=
   |         tlist, gmu=gmu, para=p, prior=prior)
   | time_fbmp = time_fbmp + time.time() - time_fbmp_start
39 | c_star = np.zeros_like(xmmse_star).astype(int)
   | for k in range(len(T_star)):
41 |     t, c = np.unique(T_star[k], return_counts=True)
   |     c_star[k, t] = c
43 | la_truth = len(truth) * wff.convolve_exp_norm(tlist - t0_truth[i][ ,
   |     T0'], Tau, Sigma) / n + 1e-8
   | if prior:
45 |     nu_star_prior = nu_star - poisson.logpmf(c_star, mu=la).sum(
   |         axis=1)
   | nu_star_prior = nu_star + poisson.logpmf(c_star, mu=la_truth).sum(
   |     axis=1)

```

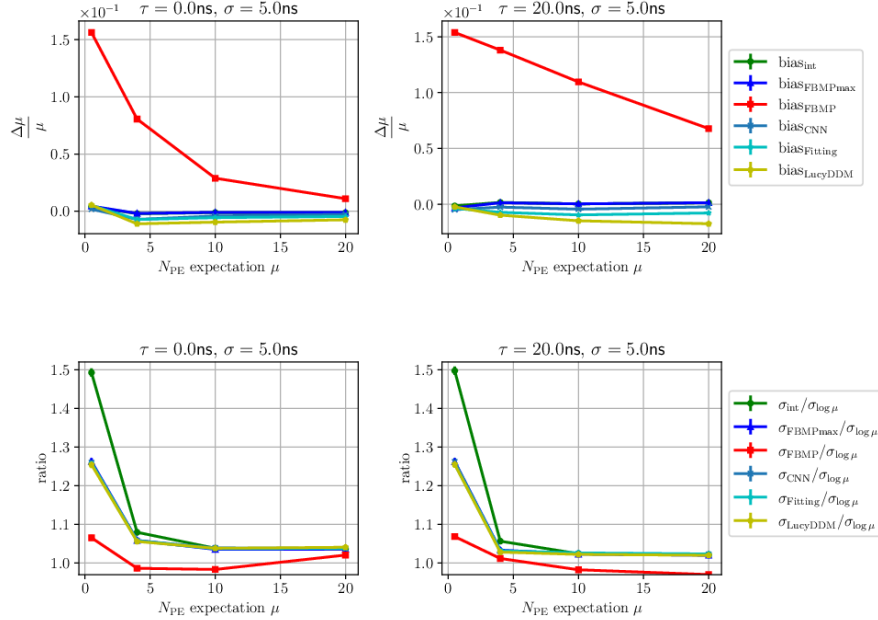
```

47 maxindex = psy_star.argmax()
49 xmmse_most = np.clip(xmmse_star[maxindex], 0, np.inf)
pet = np.repeat(tlist[xmmse_most > 0], c_star[maxindex][xmmse_most
> 0])
51 cha = np.repeat(xmmse_most[xmmse_most > 0] / factor[xmmse_most > 0]
/ c_star[maxindex][xmmse_most > 0], c_star[maxindex][
xmmse_most > 0])
53 mu = np.average(c_star.sum(axis=1), weights=psy_star)
t0 = t0_t
55 output = np.array([(xmmse_most / factor)[(tlist > t - 0.5) & (tlist
< t + 0.5)].sum() for t in range(WindowSize)])
alpha = opti.fmin_l_bfgs_b(lambda alpha: wff.rss_alpha(alpha,
output, wave, mnecpu), x0=[0.01], approx_grad=True, bounds=[[1e
-20, np.inf]], maxfun=50000)[0]
57 cha = cha * alpha
mu_i = cha.sum()
59 t0_i = t0_t

```

Motivation: show the performance of α on FBMP.

Progress: FBMP_{\max} is μ estimation with α correction, FBMP is simple weighted average of N_{PE} of each \mathbf{z} .



3 Correction

3.1 ELBO

Induce **ELBO**(Evidence lower bound). We want to minimize $\text{KL}_q(q(\mathbf{z})|p(\mathbf{z}|\mathbf{w}))$,

$$\text{ELBO} = \log p(\mathbf{w}) - \text{KL}_q(q(\mathbf{z})|p(\mathbf{z}|\mathbf{w})) \quad (51)$$

$$= E_q(\log(p(\mathbf{w}|\mathbf{z}))) - \text{KL}_q(q(\mathbf{z})|p(\mathbf{z})) \quad (52)$$

$$= E_q(\log(p(\mathbf{w}|\mathbf{z}))) - E_q(\log \frac{q(\mathbf{z})}{p(\mathbf{z})}) \quad (53)$$

$$= E_q(\log(p(\mathbf{w}|\mathbf{z})p(\mathbf{z}))) - E_q(\log q(\mathbf{z})) \quad (54)$$

$$= E_q(\nu) + S_q \quad (55)$$

where S is entropy.

Let

$$q(\mathbf{z})_{\boldsymbol{\theta}} = \begin{cases} \frac{\exp \nu(\mathbf{z})}{\sum_{\mathbf{z} \in \mathcal{Z}'} \exp \nu(\mathbf{z})} & \text{if } \mathbf{z} \in \mathcal{Z}' \\ 0 & \text{if } \mathbf{z} \notin \mathcal{Z}' \end{cases} \quad (56)$$

Additionally,

$$\text{ELBO} = \log \sum_{\mathbf{z} \in \mathcal{Z}'} \exp \nu \quad (57)$$

On the other hand, let

$$q(\mathbf{z})_{\boldsymbol{\theta}} = \begin{cases} \frac{f(\boldsymbol{\theta}, \mathbf{z})}{\sum_{\mathbf{z} \in \mathcal{Z}'} f(\boldsymbol{\theta}, \mathbf{z})} & \text{if } \mathbf{z} \in \mathcal{Z}' \\ 0 & \text{if } \mathbf{z} \notin \mathcal{Z}' \end{cases} \quad (58)$$

$$\forall \mathbf{z} \in \mathcal{Z}', f(\boldsymbol{\theta}, \mathbf{z}) > 0 \quad (59)$$

But, $f(\boldsymbol{\theta}, \mathbf{z}) = \exp(\nu + g(\boldsymbol{\theta}, |\mathbf{z}|))$ are bad.

$$\text{ELBO}'_{\boldsymbol{\theta}} = \left(\sum_{\mathbf{z} \in \mathcal{Z}'} \frac{e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}}{\sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}} \nu \right) \quad (60)$$

$$- \sum_{\mathbf{z} \in \mathcal{Z}'} \frac{e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}}{\sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}} \log \frac{e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}}{\sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}} \Big)' \quad (61)$$

$$= \left(- \sum_{\mathbf{z} \in \mathcal{Z}'} \frac{e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}}{\sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}} g(\boldsymbol{\theta}, |\mathbf{z}|) \right) \quad (62)$$

$$+ \sum_{\mathbf{z} \in \mathcal{Z}'} \frac{e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}}{\sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}} \log \sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)} \Big)' \quad (63)$$

$$= - \sum_{\mathbf{z} \in \mathcal{Z}'} \frac{e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}}{\sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}} g'(\boldsymbol{\theta}, |\mathbf{z}|) \quad (64)$$

$$- \sum_{\mathbf{z} \in \mathcal{Z}'} \left(\frac{e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}}{\sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}} \right)' g(\boldsymbol{\theta}, |\mathbf{z}|) \quad (65)$$

$$+ \frac{(\sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)})'}{\sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}} \quad (66)$$

$$= - \sum_{\mathbf{z} \in \mathcal{Z}'} \left(\frac{e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}}{\sum_{\mathbf{z} \in \mathcal{Z}'} e^{\nu+g(\boldsymbol{\theta},|\mathbf{z}|)}} \right)' g(\boldsymbol{\theta}, |\mathbf{z}|) \quad (67)$$

when $\forall \mathbf{z}, g(\boldsymbol{\theta}, |\mathbf{z}|) = 0$, $\text{ELBO}'_{\boldsymbol{\theta}} = 0$.

It is hard to use **ELBO** to correct the bias of μ .