Reversible Jump MCMC for Pile-up Decomposition

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CIDeR-ML meeting

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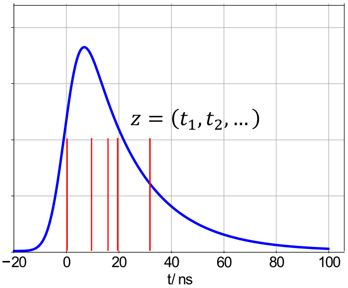
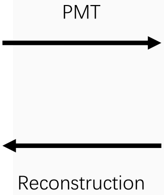
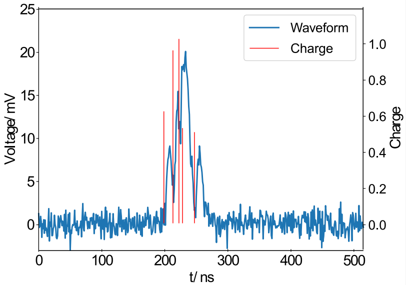
Motivation: pileup is common in observations

PE pulses pile up in waveform (1-D time pileup)



Sample from Poisson process



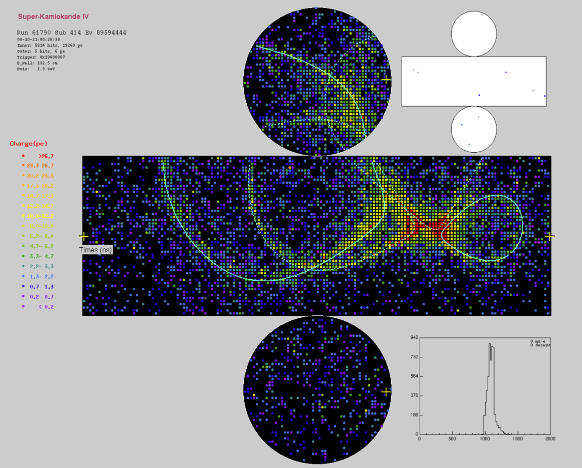


Convolution with single PE waveform

Number of PE (hit time t_i) is a **variable**, $\{N; t_1, \dots, t_N\} \in \mathbb{L}_N = \{N\} \otimes \mathbb{R}^N$

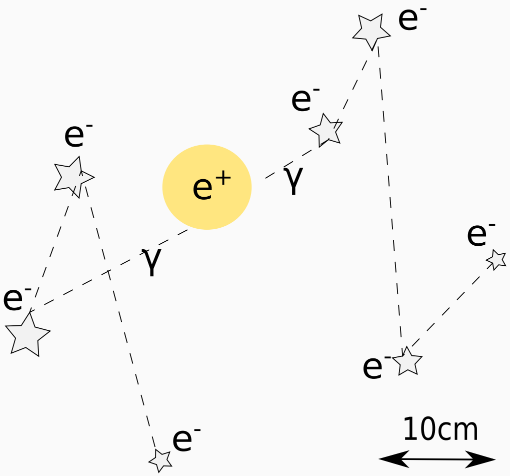
Concerning charge of each PE: $\{N; t_i, q_i\} \in \mathbb{L}_N = \{N\} \otimes \mathbb{R}^{2N}$

Multiple charged particles in a GeV neutrino event o proton decay



Number of rings is a **variable.** $\{N; t_i, \vec{r}_i, \vec{p}_i, \mathrm{PID}_i\} \in \mathbb{L}_N = \{N\} \otimes \mathbb{R}^{8N}$

MeV physics: β^-/$2\beta^-$/4β^-/γ/β^+ discrimination



- β^-: single point source. E.g. solar neutrino CC capture induced single β decay (^{130}Te + $\nu_e \longrightarrow e^-$ + ^{130}I*, ^{130}I $\longrightarrow \beta$ + $\bar{\nu}_e$ + ^{130}Xe); ^{8}B solar neutrino ES. Background of $0\nu\beta\beta$
- $2\beta^-$: $2\nu\beta\beta$, Majorana neutrino $\rightarrow$ $0\nu\beta\beta$
- $4\beta^-$: Dirac neutrino $\rightarrow 0\nu4\beta$
- γ: radioactive calibration source or background (external ^{40}K, ^{208}Tl; n capture γ); NCQE
- β^+: $\bar{\nu}_e$ IBD; β decay with γ

Motivation: pileup is common in observations

- Dark noise PEs mixing with event PEs (sub MeV in LS; MeV in water)
- Cascade event: $\pi/\mu \to e$, ^{212}Bi-^{212}Po, ^{85}Kr, Kaon ($p \to \nu + K$, $K \to \mu/\pi \to e$) in a DAQ window (1-D time pileup)
  $\{x, y, z; N; t_i, E_i\} \in \mathbb{R}^3 \otimes \mathbb{L}_N = \mathbb{R}^3 \otimes \{N\} \otimes \mathbb{R}^{2N}$
- Accidental ^{14}C pileup with other event in organic LS
- Multiple segments in a track
- Multiple tracks
- Bundle muons vs single muon

Mixture model and RJMCMC

Mixture model, and the frequentist way

Master likelihood $\mathcal{L}(\theta; x) = p(x|\theta),\ \theta \in \{N\} \otimes \mathbb{R}^{mN}$, x is observed data (e.g. waveform ADC; PMT charge)

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MLE is performed in $\mathbb{R}^{mN}$ subspace. Techniques like Expectation-Maximization can be useful to further simplify the MLE process.

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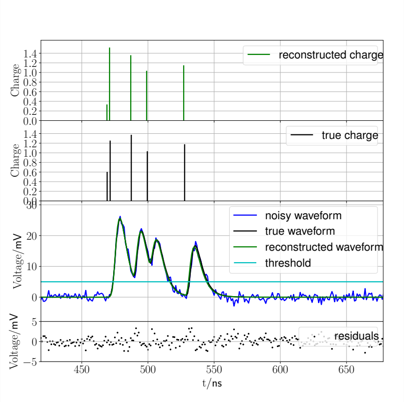
Then we compare mixture models with different N, e.g. likelihood ratio with penalties to constraint number of free parameters.

E.g. SK `fiTQun` adds a penalty term to $\log \mathcal{L} -= a_0 + a_1 \cdot E_{\mathrm{new}},\ a_0 > 0,\ a_1 \geqslant 0$ to discourage adding new ring

Can we use statistical model to replace penalty term?

$$p(w_j|\{t_i, q_i\}, N) = \prod_{j=1}^{W} \frac{1}{\sqrt{2\pi}\sigma_w} \exp\left\{-\frac{[w_j - \sum_{i=1}^{N} q_i V_{\mathrm{PE}}(t_j - t_i)]^2}{2\sigma_w^2}\right\}$$



$j \in 1, \cdots, W$ time grids, w_j waveform, σ_w Gaussian white noise

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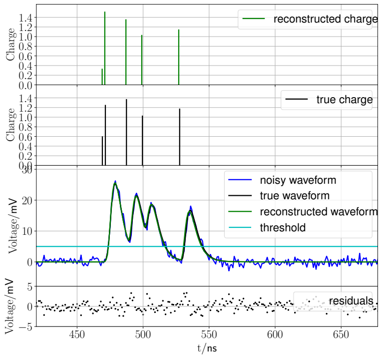

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Prevent overfit w with many small q_i? Constraint q_i with charge model!

$p(\{q_i\}, w_j|\{t_i\}, N) \;=\; p(w_j|\{t_i, q_i\}, N) \prod_{i=1}^{N} p(q_i)$,

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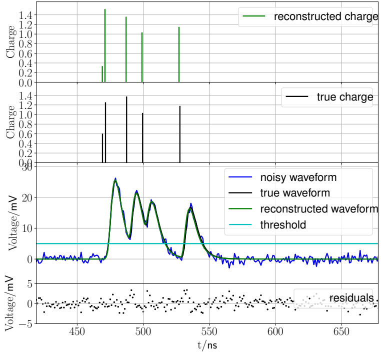

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Modeling N is also useful: $p(N, \{q_i\}, w_j|\{t_i\}) = p(\{q_i\}, w_j|\{t_i\}, N)p(N)$, $N \sim \lambda(\mu)$

The dimension curse for likelihood ratio

Cannot direct compare probabilities across dimensions! $>$, $<$ and ratio is not well-defined when comparing likelihood in $\{N\} \otimes \mathbb{R}^{mN}$ across N!

$\prod_{i=1}^{N} p(q_i)\mathrm{d}q^N$ and $\prod_{i=1}^{N+1} p(q_i)\mathrm{d}q^{N+1}$ lives in different dimensions.

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$p(w_j|\{t_i\}) = \int_{\mathbb{R}^N} \mathrm{d}q^N p(w_j|\{t_i, q_i\}, N) \prod_{i=1}^{N} p(q_i)$ but it only has a closed form if $p(q)$ is Gaussian. Let alone $p(w_j|N) = \int_{\mathbb{R}^N} \mathrm{d}q^N \int_{\mathbb{R}^N} \mathrm{d}t^N p(w_j|\{t_i, q_i\}, N) \prod_{i=1}^{N} p(q_i)p(t_i)$, but it only has a closed form if $p(q)$ is Gaussian.

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However, MC sampling $\{N\} \otimes \mathbb{R}^N$ is possible: naively sample N and then t_i.

Sample posterior with RJMCMC

Posterior $p(N, \{t_i\}|w_j) \propto p(w_j|N, \{t_i\})\pi(N)\pi(t_i)^N$, easy to calculate but difficult to direct sample N and then t_i, can't even calculate $\int p(N|w) = \int_{\mathbb{R}^{\mathbb{N}}} \mathrm{d}t^N p(N, t|w)$

RJMCMC is used to sample in $\{N\} \otimes \mathbb{R}^{mN}$ without knowing marginal distribution $p(N)$ in advance.

$$\min\left\{1, \frac{L(\theta')\pi(\theta')}{L(\theta)\pi(\theta)}\frac{p(\theta' \to \theta)}{p(\theta \to \theta')}\right\} \xrightarrow[\text{RJMCMC}]{\text{From MH to}} \frac{L(\theta')\pi(\theta')}{L(\theta)\pi(\theta)}\frac{g(v)p(\text{choose } \theta' \to \theta)}{g(u)p(\text{choose } \theta \to \theta')}\left|\det\frac{\partial(\theta', v)}{\partial(\theta, u)}\right|$$

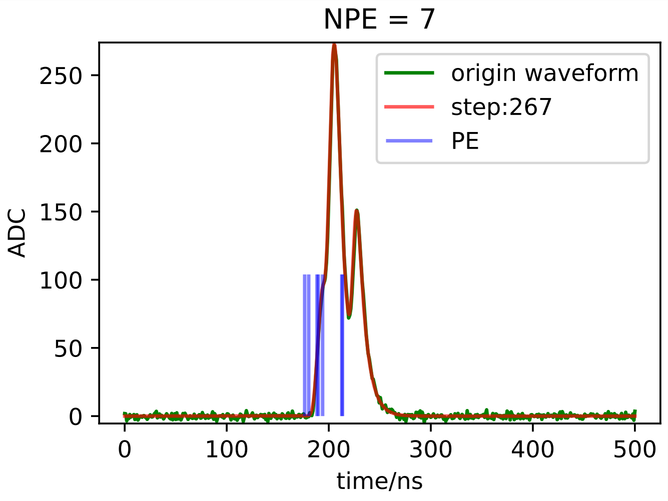
- θ: parameter to be fit; current step θ, next step θ'
- $p(a \to b)$: proposal probability to jump from parameter a to parameter b
- u, v: proposed auxiliary parameters satisfying $\dim u + \dim\theta = \dim v + \dim\theta'$
- $g(u)$ proposal probability to raise u (continuous part)
- $p(\text{choose } \theta' \to \theta)$: discrete part
- implemented jump $f : (\theta, u) \to (\theta', v)$, Jacobian term $|\det(\nabla f)|$

FSMP: RJMCMC on PE reconstruction from waveform

First glimpse on Fast Stochastic Matching Pursuit (FSMP)

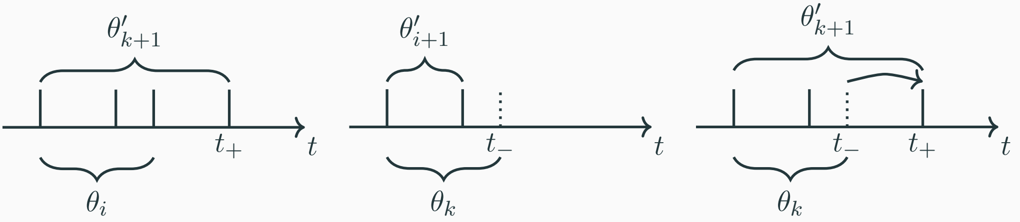
arXiv:2112.06913

arXiv:2403.03156



FSMP: a RJMCMC jumping N and t_i to match waveform

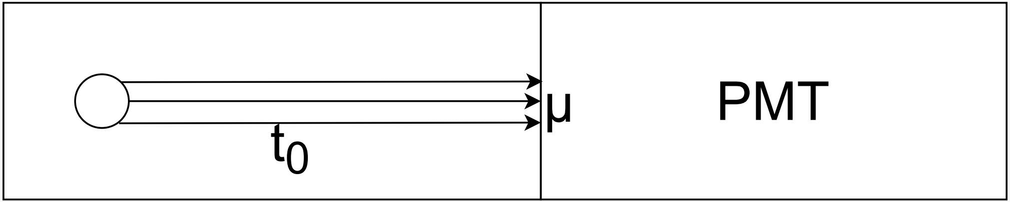
RJMCMC master formula



- $g(u)$: u can be drawn from smeared deconvolution result $h(t)$
- +1 PE $p(\text{choose } +1) = p_+ = 1/4$
- -1 PE at **the** t_-: $p(\text{choose } -t_-) = p_- \frac{1}{N} = 1/(4N)$
- +1 PE $\theta_{i+1} = (\theta_k, t_+) = f(\theta_k, u) = (\theta_k, u)$, f is i.d. transform so $|\det \nabla f| = 1$
- Move t_i from t_- to t_+: $p_{\text{move}} p(\text{choose } t_i) = 1/2 \times 1/N$
- $\alpha_+ = \frac{p(N_k, \{t_i\}_{k+1}|w_j)\pi(N_{k+1})\pi(\{t_i\}_{k+1})}{p(N_k, \{t_i\}_k|w_j)\pi(N_k)\pi(\{t_i\}_k)} \frac{1 \cdot p(\text{choose } -t_-)}{g(u)p(\text{choose } +1)} |\det \nabla f| = \cdots \times \frac{1}{(N+1)h(t_+)}$
- $\alpha_- = \cdots \times Nh(t_-)$

Toward particle reconstruction

A toy detector with one PMT: λ is energy, fly time t_0 is vertex.



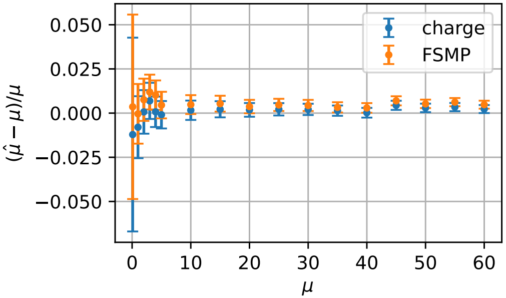
Reconstruct t_0 upon FSMP output vs first hit method

Reconstruct λ upon FSMP output vs $\frac{\text{charge}}{\text{gain}}$

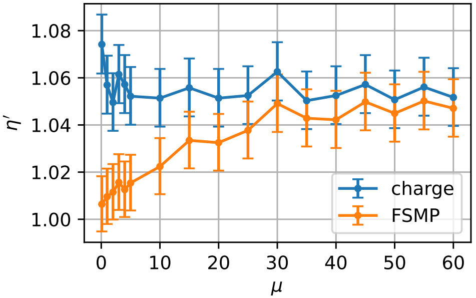
FSMP performance on energy

$$\eta_{\text{theory}} = \frac{1}{\sqrt{\mu}}$$ the theoretical limit of resolution

$$\eta = \frac{\sqrt{\mathrm{Var}[\hat{\mu}]}}{\mathrm{E}[\hat{\mu}]}$$, relative resolution $\eta' = \frac{\eta}{\eta_{\text{theory}}}$,



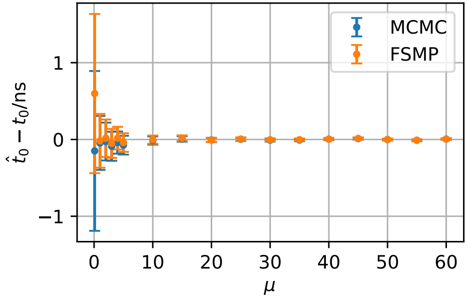
μ relative bias



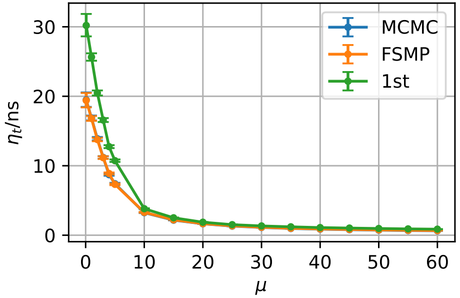
μ relative resolution

FSMP performance on vertex

MCMC: reconstruct t_0 with known PE truth, gives theoretical limit of t_0 resolution.



t_0 absolute bias

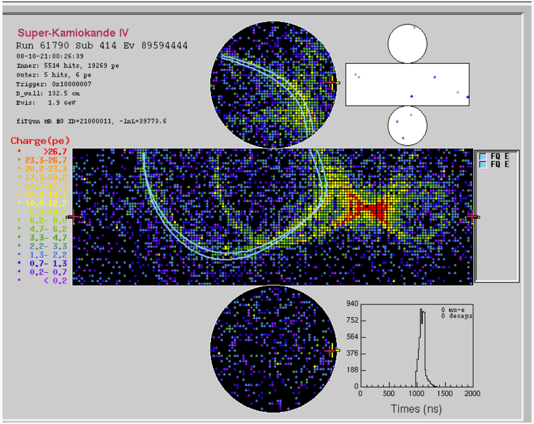


t_0 absolute resolution

RJMCMC-fiTQun

Development history and status until last month

Wiki page: `https://www-sk1.icrr.u-tokyo.ac.jp/sk-local/wiki/index.php/RJMCMC-fiTQun`

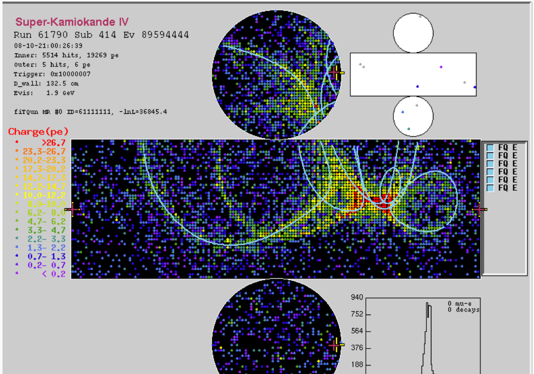


The RJMCMC is very hard to propose new rings with only split-merge steps

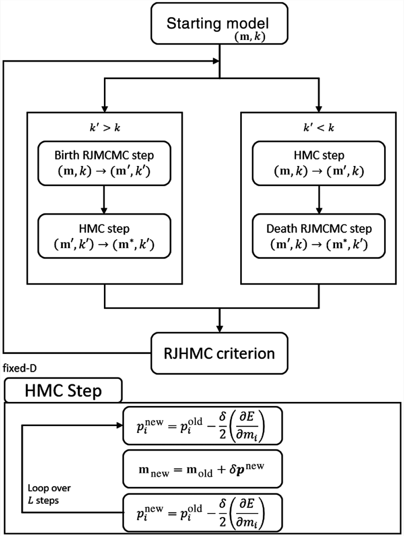
Progress in the last week

I improved the proposal algorithm $h(\vec{r})$ and correctly implemented the birth-death jump

Now RJMCMC can easily jump to multiple rings. But saving more than 6 rings to zbs somehow broke output format and event display fails, so only 6 rings at max.



A dream: RJHMC



Gradient information can be used to guide the MCMC chain: Hamiltonian MC[a].

Extend to cross-dimensional: RJHMC[b]

[a] Duane et al., “Hybrid Monte Carlo”.

[b] Sen and Biswas, “Transdimensional seismic inversion using the reversible jump Hamiltonian Monte Carlo algorithm”.

Detailed plans for workshop

Plan A: traditional RJMCMC written in C++

1. 4.11 Run `skdetsim`, shooting N 0.1-1 GeV electron/muon; check chain fidelity
2. 4.12 Calculate confusion matrix of `RJMCMC-fiTQun` to see the ring counting capabilities
3. 4.13 `fiTQun`1R result as initial state $\rightarrow$ MR result as initial state
4. 4.14-15 Tune prior and estimate chain convergence using Gelman-Rubin method

Plan B: (RJ)HMC written in python

1. 4.14 Prepare for the math formulas of RJHMC
2. 4.15-16 Implement a differentiable `fiTQun`likelihood with opticSIREN
3. 4.16-18 Implement the 1 ring HMC calling differentiable likelihood
4. 4.17-18 Run 1 ring HMC on forward simulation output
5. Future: multi-ring superposition forward simulation, RJHMC