Efficient Calibration of Scintillation Time Constants Via Bayesian Optimization (BO)

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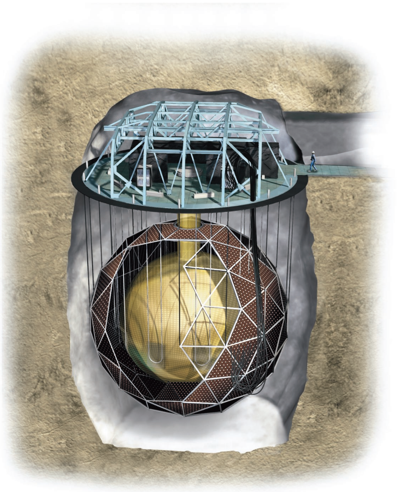
Introduction to SNO+ Experiment

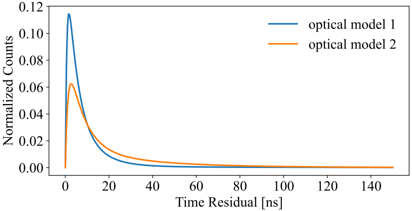
- Located in Sudbury, Canada.
- Searching for Neutrinoless double beta decay ($0\nu\beta\beta$) search and sensitive to neutrino oscillation measurements
- Liquid scintilator experiment filled with 780 tonnes of LAB + 2.2g/L PPO + 2.2mg/L bisMSB
- $\sim$2 km rock overburden + 7000 tonnes of ultra pure water to shield against cosmic muons
- PMT hit time information is essential for reconstructing time, position, energy and classifier values



Motivation of Scintillation Timing Tuning Using In-situ Backgrounds

Accurate scintillation emission timing profiles are required to produce reliable prediction of hit times

- Issues
  1. Ex-situ scintillation timing measurements failed to produce reliable predictions
  2. No simple fitting framework to optimize timing parameters (fitting latent variables than directly measured quantities)
- Solutions
  1. Use in-situ backgrounds
  2. Rely on mc and data comparison
     - Time Residual $= t^i_{res} = t^i_{hit} - t^i_{time\ of\ flight} - t_{event}$
     - If simulated physics perfectly, t_{res} directly represents emission profile
     - Problem reduces to choosing an optimization method that best calibrates MC timing parameters to match data



Toy emission profile in different optics

Bayesian Optimization For Scintillation Timing Tuning

Empirical Scintillation Timing Parametrization:

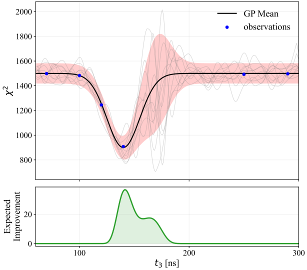
$$P(t) = \sum_{i=1}^{4} A_i \frac{e^{-\tau/\tau_i} - e^{-\tau/\tau_r}}{\tau_i - \tau_r}$$

4 sets of [scaling components (A_i), decay constants (τ_i)] + rise time constant (τ_r) + Reemission Time Constant ($\tau_{Reem,bisMSB}$) $\Rightarrow$ 10 parameters to optimize $\times$ 2 (for β and α particle types)

- Old Method: Grid Search over 10 parameters independently to match t_{res} distribution in data and mc
  - Not efficient and does not consider correlation between features
- New Method: Bayesian Optimization to optimize all parameters simultaneously
  - Considers correlations and reduces the number of iterations needed to find optimal parameters
  - Uncertainty-aware

Introduction to Bayesian Optimization (BO)

- Surrogate Function:
  - Used Gaussian Process (GP) as probalistic model to approximate the objective function based on observed data points.
  - Provides a mean prediction and uncertainty estimate in full parameter space.
- Acquisition Function:
  - Given mean and uncertainty from surrogate, return the most valuable sampling point.
  - Expected Improvement (EI) is chosen to balance exploration and exploitation to find the most worthwhile sample point.
- BO uses the surrogate to predict χ^2 in feature space and proposes next points from the acquisition function until convergence is reached.

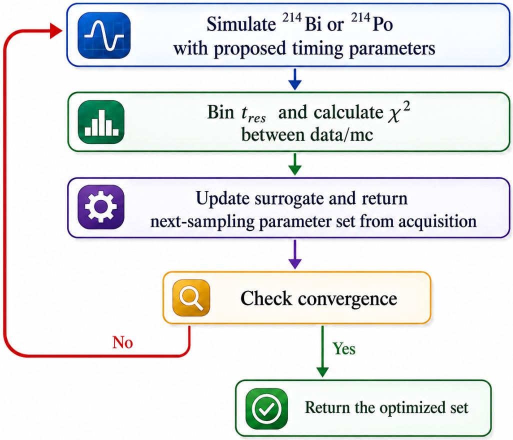


Toy example of surrogate (red) and acquisition (green) function in BO

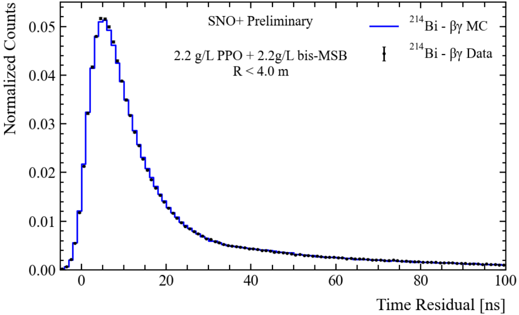
Work Flow

Internal ^{214}Bi ($\beta - \gamma$ decay) and ^{214}Po (α decay) radioactive backgrounds are chosen to measure the β and α emission profiles

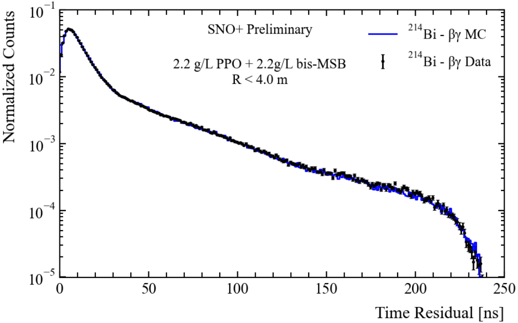
- High Purity and High Statistics
- γ propagation is handled by simulation $\rightarrow$ emission profile of $\beta - \gamma$ is similar to β



Fit Result - β Particle



Best fit t_{res} distribution for β particle

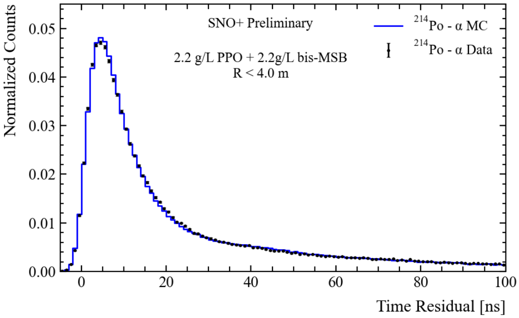


Log Scale

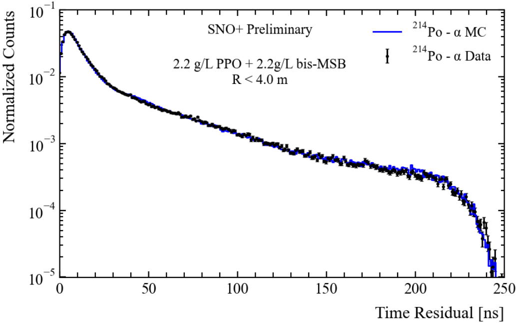
Fit Parameters (β)

τ_1 [ns]	5.28	τ_2 [ns]	13.11	τ_3 [ns]	60.00	τ_4 [ns]	425.45
A_1	0.620	A_2	0.254	A_3	0.061	A_4	0.065
τ_r [ns]	0.83	$\tau_{\text{Reem,bisMSB}}$ [ns]	1.99				

Fit Result - α Particle



Best fit t_{res} distribution for α particle

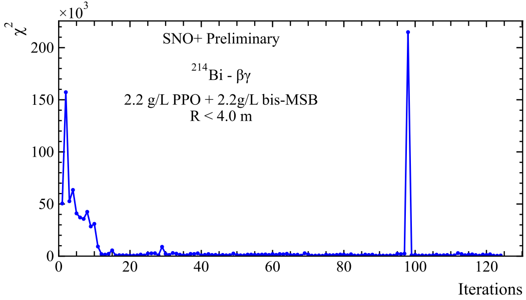


Log Scale

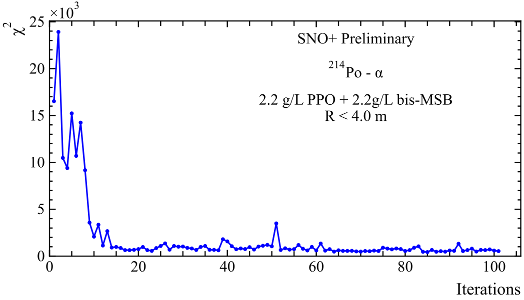
Fit Parameters (α)

τ_1 [ns]	5.01	τ_2 [ns]	21.68	τ_3 [ns]	201.08	τ_4 [ns]	387.68
A_1	0.551	A_2	0.270	A_3	0.109	A_4	0.070
τ_r [ns]	1.16						

Loss Function



β case



α case

BO achieves convergence within $\mathcal{O}(100)$ iterations, roughly a tenfold reduction compared to grid-search method

Conclusion

- Bayesian Optimization is a powerful technique for optimizing parameters when the evaluation process is computationally expensive
- In Scintillation Timing Tuning, BO can efficiently find optimal parameters by modeling the objective function and guiding the search process while considering uncertainties and the correlations between parameters
- Results indicate the advantage of BO in terms of convergence speed and efficiency

Backup Slides

- - Backup - -

Surrogate Function

- In this GP, an RBF kernel is chosen to model the covariance between points in the feature space

$$k_{RBF}(x, x') = \sigma_f^2 \exp\left(-\frac{1}{2l^2}\sum_{i=1}^{d}(x_i - x_i')^2\right)$$

(Hyperparameters: l: length scale between two points x_i, x_i'; σ_f^2: horizontal scale)

- Surrogate utilizes the RBF kernel to keep smoothness
- Posterior mean and variance are calculated based on observed data points

$$\mu(\vec{X}) = \hat{K}_{m,p}\left(\hat{K}_{m,m} + \sigma^2 I\right)^{-1}\hat{F}$$

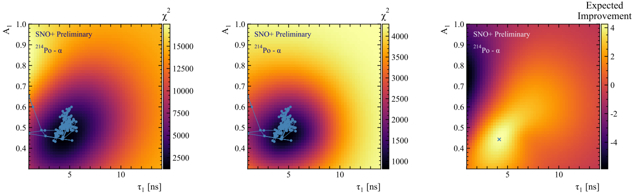
$$\Sigma = \hat{K}_{p,p} - \hat{K}_{p,m}\left(\hat{K}_{m,m} + \sigma^2 I\right)^{-1}\hat{K}_{m,p}$$

(K: covariance, p: proposal points, m: measured points)

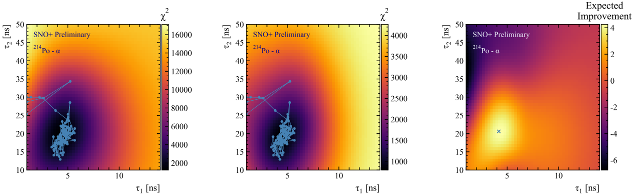
Acquisition Function

- Expected Improvement (EI) is chosen as the acquisition function to balance exploration and exploitation in the optimization process
- Improvement:
  $I(x) = \max(0, \mu_{\text{min}} - \mu(x)) \Rightarrow$ Relative improvement compared to the best measured case μ_{min}
- Expected Improvement:
  $< I(x) >= \mathbb{E}[\max(0, \mu_{\text{min}} - \mu(x))] = \int_{-\infty}^{\infty} I(x) N(\mu(x), \sigma^2(x)) dy(x)$
  $\Rightarrow$ Expected improvement considering the uncertainty of surrogate prediction at each single point
- Select next sample values having the highest EI across the space

Example Correlation Cases in α Timing Tuning



From left to Right: χ^2 Prediction, Uncertainty and EI between τ_1 and A_1



From left to Right: χ^2 Prediction, Uncertainty and EI between τ_1 and τ_2

BO can consider the correlation between parameters and optimize them simultaneously