Enhancing Isotope Charge Radius Measurement Precision with Statistical Analysis

Yucheng Pan

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Research Experience

Enhancing Isotope Charge Radius Measurement Precision with Statistical Analysis Sep. 2023 - Present

Supervisor: Prof. Ke Deng
Center for Statistical Science, Tsinghua University

Research content:

- Literature review
- Data collection and processing
- Coding, experiments and evaluation

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Laser Spectroscopy

- The nuclear root-mean-square (rms) charge radius is a fundamental quantity for both nuclear structure and reaction calculations.
- Up to now, there are many different experimental methods developed to measure the nuclear charge radius.
- In recent decades, laser spectroscopy techniques outstand in our understanding of exotic nuclei, because of their high precision and sensitivity.

Isotope Shift

There is a small difference between the same spectral line of two isotopes with mass numbers A and A', called the isotope shift (IS),

$$\delta\nu_{IS}^{AA'} = \nu_A - \nu_{A'} \tag{1}$$

resulting from the difference in their mass and volume, and these are two major effects contributing to the isotope shift:

$$\delta\nu_{IS}^{AA'} = \delta\nu_{MS}^{AA'} + \delta\nu_{FS}^{AA'} \tag{2}$$

where $\delta\nu_{MS}^{AA'}$ is the mass shift and $\delta\nu_{FS}^{AA'}$ is the field shift.

Isotope Shift

According to nuclear physics([MPYW+92]), the mass shift can be calculated by

$$\delta\nu_{MS}^{AA'} = K_{MS}\frac{A' - A}{AA'} \tag{3}$$

, and the field shift is

$$\begin{aligned}\delta\nu_{FS}^{AA'} &= F\lambda_{A,A'} \\ &= F(\delta < r^2 >^{AA'} + a\delta < r^4 >^{AA'} + b\delta < r^6 >^{AA'} + ...) \\ &\approx F\delta < r^2 >^{AA'}\end{aligned} \tag{4}$$

which can be considered as a approximate linear function of the nuclear charge distribution.

Main Formula

The main formula for analysis is

$$\delta\nu_{IS}^{AA'} - K_{MS}\frac{A' - A}{AA'} = F\delta < r^2 >^{AA'} \tag{5}$$

where K_{MS} is the mass shift factor, F is the electronic factor, A and A' are the mass numbers of the two isotopes.
$\delta\nu_{IS}^{AA'}$ can be measured by laser spectroscopy, and K_{MS} is always assumed to be known from literature.

King Plot

The common method to measure the nuclear charge radii in physics is the King plot method.

1. Select two reference isotopes with mass numbers of A_0 and A_0' respectively, and calculate the modified isotope shift of transition i: $\delta\nu_{i,modi}^{AA'} \triangleq \delta\nu_i^{AA'} \frac{AA'}{A'-A} \frac{A_0-A_0'}{A_0 A_0'}$
2. Choose a known spectral line j, construct linear regression of $\delta\nu_{i,modi}^{AA'}$ against $\delta\nu_{j,modi}^{AA'}$ for j and target spectral line i.
3. Parameter estimate: $\beta_1 = \frac{F_i}{F_j}$, $\beta_0 = \frac{K_{MS,i}-K_{MS,j}F_i}{F_j} \frac{A_0-A_0'}{A_0 A_0'}$.
4. Use F_j from literature to calculate F_i, then construct linear regression of $\delta\nu_i^{AA'}$ against $\delta < r^2 >^{AA'}$ according to Eq.(5).

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Measurement Error Model

Different from linear regression, there are uncertainties about the predictor variables $\delta < r^2 >^{AA'}$, so a multivariate linear regression model with measurement error is in need.:

$$\begin{aligned} y_{ij}^* &= k_j t_i^* + b_j \\ Y_{ij} &= y_{ij}^* + \epsilon_{ij}^y \\ T_i &= t_i^* + \epsilon_i^t \end{aligned} \tag{6}$$

where y_{ij}^* is the true (ideal) value of the i-th field shift $\delta\nu_{F,j}^{A_{ref},A_i}$ at the j-th spectral line, t_i^* is the true value of the i-th nuclear charge distribution shift $\delta < r^2 >^{A_{ref},A_i}$, and Y_{ij} and T_i are random variables representing the observed values of y_{ij}^* and t_i^*.

Assumption

- $\epsilon_{ij}^{y} \sim \mathcal{N}(0, \sigma_{ij}^2)$
- $\epsilon_{i}^{t} \sim \mathcal{N}(0, \tau_{i}^2)$
- ϵ_{ij}^{y} and ϵ_{i}^{t} are independent
- σ_{ij} and τ_i are known (the uncertainty of the measurements)

Derive that $Y_{ij} \sim \mathcal{N}(k_j t_i^* + b_j, \sigma_{ij}^2)$ and $T_i \sim \mathcal{N}(t_i^*, \tau_i^2)$.

Likelihood Function

To estimate the parameters $\vec{k}$, $\vec{b}$, $\vec{t^*}$, we need to maximize the likelihood function,

$$L(\vec{k}, \vec{b}, \vec{t^*}; \mathbf{Y}, \vec{T}) = \prod_{i=1}^{I} \prod_{j=1}^{J_i} f(y_{ij}|k_j, b_j, t_i^*) \cdot f(t_i|t_i^*) \tag{7}$$

equivalently, maximize the log-likelihood function,

$$\begin{aligned} \log L(\vec{k}, \vec{b}, \vec{t^*}; \mathbf{Y}, \vec{T}) = &- \sum_{i=1}^{I} \sum_{j=1}^{J_i} \frac{(y_{ij} - k_j t_i^* - b_j)^2}{2\sigma_{ij}^2} \\ &- \sum_{i=1}^{I} \frac{(t_i - t_i^*)^2}{2\tau_i^2} + \text{const.} \end{aligned} \tag{8}$$

where I is the number of isotopes collected, J_i is the number of spectral lines collected for the i-th isotope.

MLE

$$\frac{\partial \log L}{\partial k_j} = \sum_{i=1}^{I} \frac{t_i^*(y_{ij} - k_j t_i^* - b_j)}{\sigma_{ij}^2} \tag{9}$$

$$\frac{\partial \log L}{\partial b_j} = \sum_{i=1}^{I} \frac{y_{ij} - k_j t_i^* - b_j}{\sigma_{ij}^2} \tag{10}$$

$$\frac{\partial \log L}{\partial t_i} = \sum_{j=1}^{J_i} \frac{k_j(y_{ij} - k_j t_i^* - b_j)}{\sigma_{ij}^2} - \frac{t_i - t_i^*}{\tau_i^2} \tag{11}$$

However, the closed-form solution of MLE is hard to obtain because of the cross terms of k_j and t_i^* in the partial derivatives. So we have to use numerical optimization algorithms to estimate the parameters.

Optimization Algorithms

- There are many optimization algorithms to numerically find the maximum (or equivalently, minimum) of a function, such as Bisection method, Fixed-point iteration, Newton's method, Quasi-Newton method, gradient descent, majorization-minimization algorithm, etc.
- Here we choose BFGS from the Quasi-Newton method and EM algorithm from the majorization-minimization algorithm, which are widely used, efficient and robust.

Newton's Methods

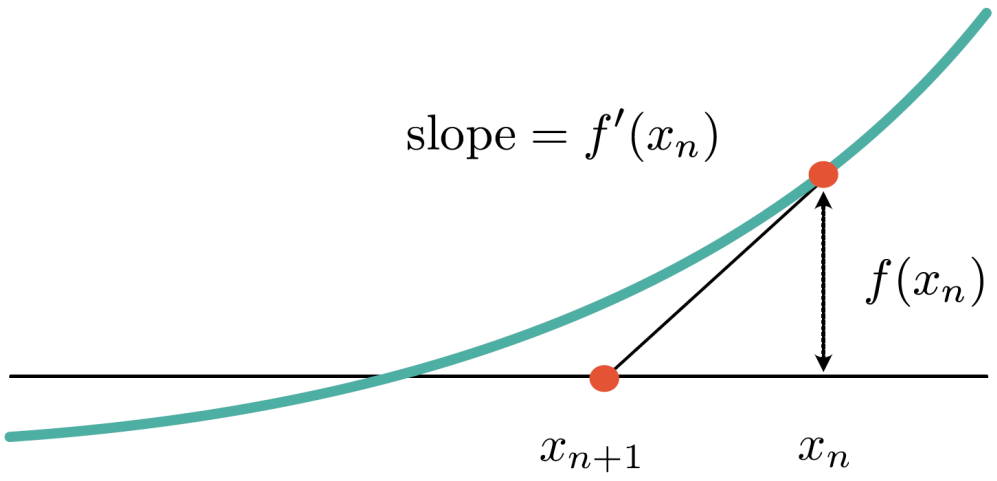

图 1: Newton's method

Iteration rule:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{12}$$

And it can be rewritten in matrix form as

$$x_{n+1} = x_n - (\nabla f(x_n))^{-1} f(x_n) \tag{13}$$

Quasi-Newton Methods

Newton's methods require the derivatives (for maximization, even the Hessian matrix) of the function, which is hard to obtain in practice. And they are sensitive to the initial values.
So Quasi-Newton methods are developed to solve these problems. They use a sequence of approximations to the Hessian matrix

$$x_{n+1} = x_n - \alpha_n M_n^{-1} \nabla f(x_n) \tag{14}$$

where α_n is the step size, which can be determined by backtracking line search, M_n is an approximation to the Hessian matrix, and should satisfy the secant condition

$$M_{n+1}(x_{n+1} - x_n) = \nabla f(x_{n+1}) - \nabla f(x_n) \tag{15}$$

BFGS

BFGS is one of the most popular Quasi-Newton methods. It updates the approximation to the Hessian matrix by

$$M_{n+1} = M_n + \frac{y_n y_n^T}{y_n^T z_n} - \frac{M_n z_n z_n^T M_n}{z_n^T M_n z_n} \tag{16}$$

where $z_n = x_{n+1} - x_n$, $y_n = \nabla f(x_{n+1}) - \nabla f(x_n)$. Equivalently and more efficiently, we can use the Sherman-Morrison formula to update the inverse of the Hessian matrix.

$$H_{n+1} = H_n + \frac{y_n y_n^T}{y_n^T z_n} - \frac{H_n z_n z_n^T H_n}{z_n^T H_n z_n} \tag{17}$$

where $H_n = M_n^{-1}$.

EM

EM is a majorization-minimization algorithm, which is widely used to solve the maximum likelihood estimation problem with latent variables. It can be divided into Estimation (E) step and Maximization (M) step.

- E-step:

$$Q(\theta|\theta^{(t)}) = \mathbb{E}_{\mathbf{Z}|\mathbf{X},\theta^{(t)}}\left[\log L(\theta; \mathbf{X}, \mathbf{Z})\right] \tag{18}$$

  where $\mathbf{Z}$ is the latent variable, and $\mathbf{X}$ is the observed data.

- M-step:

$$\theta^{(t+1)} = \arg\max_{\theta} Q(\theta|\theta^{(t)}) \tag{19}$$

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Experiment

Data is collected and processed from literature [MMK+19], [GRBB+16], [NBI+98], [VLS+96], [MPYW+92], [VSL+92], [PBB+84], [ABG+82], [BBD+80] and [BHKS78].
Parameters estimated from linear regression can be used as a good initial value for the two methods.

$$\hat{k}_j = \frac{\sum_{i=1}^{I_j}(y_{ij} - \overline{y_{\cdot j}})(t_i - \overline{t})}{\sum_{i=1}^{I_j}(t_i - \overline{t})^2} \tag{20}$$

$$\hat{b}_j = \overline{y_{\cdot j}} - \hat{k}_j \overline{t} \tag{21}$$

t_i serves as the latent variable in the EM algorithm. As for the initial value, the t_i with the minimum uncertainty is chosen.

Experiment

As for iteration,

- BFGS: we use the `optim` function in R with the BFGS method.
- EM: Through calculation, the iteration rule is

$$k_j^{(t+1)} = \frac{\overline{y_{ij}\mu_i} - \overline{y_{ij}} \cdot \overline{\mu_i}}{\overline{\mu_i^2 + \epsilon_i^2} - \overline{\mu_i}^2} \tag{22}$$

$$b_j^{(t+1)} = \overline{y_{ij}} - k_j^{(t+1)}\overline{\mu_i} \tag{23}$$

where $t_i \sim \mathcal{N}(\mu_i, \epsilon_i^2)$,

$$\mu_i = \frac{\left(\sum_{j=1}^{J_i} k_j^{(t)}(y_{ij} - b_j^{(t)})/\epsilon_{ij}^2 + t_i/\tau_i^2\right)}{\left(\sum_{j=1}^{J_i}(k_j^{(t)})^2/\epsilon_{ij}^2 + \tau_i^{-2}\right)}, \ \epsilon_i^2 = \frac{1}{\left(\sum_{j=1}^{J_i}(k_j^{(t)})^2/\epsilon_{ij}^2 + \tau_i^{-2}\right)}$$

Evaluation with Bootstrap

- To evaluate the performance of the two methods, the uncertainties of the estimates of isotope radii shift $\delta < r^2 >$ ($\mathbb{E}[t]$) are estimated with bootstrap.
- Simulated data $y_{ij}^{sim} \sim \mathcal{N}(k_j t_i^* + b_j, \sigma_{ij}^2)$ and $t_i^{sim} \sim \mathcal{N}(t_i^*, \tau_i^2)$ with the estimated parameters k, b and t^* of BFGS and EM respectively for 1000 times.
- σ_{ij}^2, τ_i^2 are the same as the original data. We use the same uncertainties because we want to simulate the same experiment process.

Results

A	N_{exp}	τ_{BFGS}	τ_{EM}	τ_{obs}
36	1	**0.018983**	0.020033	0.026401
37	1	0.017364	**0.017195**	0.022672
38	1	**0.005082**	0.006187	0.006395
39	2	**0.005164**	0.006356	0.006438
41	2	**0.002547**	0.004113	0.002800
42	7	**0.000671**	0.000684	0.000700
43	8	**0.000399**	0.000458	0.000400
44	8	**0.000924**	0.000997	0.001000
45	4	**0.004406**	0.004526	0.010000
46	6	**0.002854**	0.003098	0.005000
47	2	**0.004844**	0.005470	0.009487
48	8	**0.002805**	0.004179	0.006000
49	1	**0.007213**	0.007444	0.012649
50	2	0.007339	**0.007309**	0.012369
51	1	**0.008307**	0.008972	0.013342
52	1	**0.010134**	0.011568	0.015811
Avg		**0.006190**	0.006787	0.009467

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Future Work

- More data and experiments of different isotopes
- Utilize the replicated measurements
- Extend the model to higher order polynomial
- Extend the method to other fields
- Try out other statistical computing methods
- Provide a pipeline for evaluation of new measurement and hypothesis test for theoretical values

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Thanks!