A linear iterative unfolding method for imaging

András László

laszlo.andras@wigner.mta.hu

Wigner Research Centre for Physics, Budapest

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Károly Róbert College, Gyöngyös

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Outline

- BE correlations as an imaging problem
- A linear iterative unfolding algorithm
- Summary

Based on:

[1] A. László: `JPCS` **368** `(2012) 012043`.

[2] A. László: `arXiv:1404.2787`.

BE correlations as an imaging problem

- In Bose-Einstein correlation studies the two-particle momentum correlation function $C(\vec{q})$ is measured experimentally, $\vec{q}$ being the three-momentum difference.
- The two-particle momentum correlation function is of the form

$$C(\vec{q}) - 1 = \int \left(\left| \frac{1}{\sqrt{2}} \Phi_{\vec{q}}(\vec{r}) + \frac{1}{\sqrt{2}} \Phi_{-\vec{q}}(\vec{r}) \right|^2 - 1 \right) S(\vec{r})\, \mathrm{d}^3 r \Big/ \int S(\vec{r}\,')\, \mathrm{d}^3 r'$$

where $\Phi_{\vec{q}}(\vec{r})$ is the fundamental solution of Schrödinger equation with given momentum $\vec{q}$, while

$$S(\vec{r}) = \int s(\vec{\rho} + \frac{1}{2}\vec{r})\, s(\vec{\rho} - \frac{1}{2}\vec{r})\, \mathrm{d}^3 \rho$$

is the two-particle source function (PLB **485** (1999) 407). Here, $s(\vec{\rho})$ is the single particle source function.
- Question: can we reconstruct the normalized two-particle source function $S(\vec{r}) / \int S(\vec{r}\,')\, \mathrm{d}^3 r'$ given the two-particle momentum correlation function $C(\vec{q})$ and the kernel function

$$k_{\vec{q}}(\vec{r}) := \left(\left| \frac{1}{\sqrt{2}} \Phi_{\vec{q}}(\vec{r}) + \frac{1}{\sqrt{2}} \Phi_{-\vec{q}}(\vec{r}) \right|^2 - 1 \right) \qquad ?$$

- For uncharged particles the wave function $\Phi_{\vec{q}}(\vec{r})$ is the plane wave

$$\Phi^0_{\vec{q}}(\vec{r}) \;=\; \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}}$$

in which case the kernel function $k_{\vec{q}}(\vec{r})$ is

$$k^0_{\vec{q}}(\vec{r}) \;=\; \cos(2\vec{q}\cdot\vec{r}),$$

therefore $C(\vec{q})-1$ is the Fourier transform of $S(\vec{r})$ as $S(\vec{r})$ is real and even function.

- For charged particles the wave function $\Phi_{\vec{q}}(\vec{r})$ is the fundamental solution of the Coulomb scattering Schrödinger equation

$$\Phi^C_{\vec{q}}(\vec{r}) \;=\; \mathrm{e}^{-\frac{\pi}{2}\frac{\alpha Z m}{|\vec{q}|}}\,\Gamma\left(1+\mathrm{i}\frac{\alpha Z m}{|\vec{q}|}\right)\,{}_1F_1\left(-\mathrm{i}\frac{\alpha Z m}{|\vec{q}|};1;\mathrm{i}\left(|\vec{q}|\,|\vec{r}|-\vec{q}\cdot\vec{r}\right)\right)\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}}$$

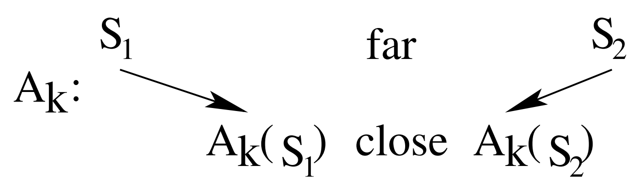
with corresponding kernel function $k^C_{\vec{q}}(\vec{r})$. In that case, $C(\vec{q})-1$ is not simply the Fourier transform of $S(\vec{r})$.

- The stated task belongs to the class of unfolding problems, namely

$$S = ? \quad : \qquad C - 1 = A_k S + n$$

where A_k is the folding operator by the kernel function k and n is the measurement noise (statistical and systematic errors).

- These unfolding problems are analytically invertible (i.e. A_k^{-1} exists), but the task is numerically ill-posed.
- That means: distant source functions S may lead to close images C, whose difference may be shadowed by the measurement noise n.



- Or equivalently: in the equation

$$A_k^{-1}(C - 1) \; = \; S \; + \; A_k^{-1} n$$

the last term is not guaranteed to be small if n was small.

- A naive approach is to discretize the operator A_k and evaluate A_k^{-1} on $C - 1$.
- Some kind of regulatization treatment is needed in order to keep the contribution of the noise term small. This treatment is quite arbitrary.
- In `JPCS` **`368`** `(2012) 012043` and `arXiv:1404.2787` an iterative unfolding method is proposed and mathematical proof of convergence is presented along with error propagation formulae.
- The bias error (approximation error) decreases with increasing iteration order, whereas the propagated statistical and systematic errors increase and thus compete with each-other.
- The regularization is performed via the stopping of the iterative approximation at optimal error content and error estimations can be given there.

A linear iterative unfolding algorithm

JPCS **368** (2012) 012043 and arXiv:1404.2787

- Assume that the source function $S(\vec{r})$ has compact support within $|\vec{r}| \leq R$.
- Let us define the normalization factor

$$K_{k,R} = \max_{|\vec{r}_2| \leq R} \int_{|\vec{r}_1| \leq R} \int k_{\vec{q}}(\vec{r}_1)\, k_{\vec{q}}(\vec{r}_2)\, \mathrm{d}^3 q\, \mathrm{d}^3 r_1 .$$

- Take the iteration scheme in search for S (with $C - 1 = A_k S$):
  - $S_0 = K_{k,R}^{-1} A_k^T (C - 1)$,
  - $S_{N+1} = S_N + \left(S_0 - K_{k,R}^{-1} A_k^T A_k S_N\right)$,
    where A_k^T is the transpose folding by A_k.
- Binwise and monotone L^2 convergence holds whenever $K_{k,R} < \infty$. Proof based on Riesz-Thorin theorem + spectral representation of positive operator over L^2 space.
- Iteration scheme motivated by the "Neuman series" known in functional analysis.
- Resembles to "Landweber iteration" (Am.J.Math. **73** (1951) 615), but regularity condition $\int_{|\vec{r}| \leq R} \int \left|k_{\vec{q}}(\vec{r})\right|^2 \, \mathrm{d}^3 q\, \mathrm{d}^3 r < \infty$ of that result does not hold for our problem.

Upper estimate to the residual term (bias error) at finite iteration order approximation:

- In practical applications, besides fact of convergence, one also may want to know the deviation from limiting pdf at given finite iteration order N.
- Let B be a histogram bin in the domain of the source function S.
- Then,

$$\frac{1}{\mathrm{Vol}(B)} \int_B |S - S_N| (\vec{r})\, \mathrm{d}^3 r$$

$$\leq \; (1+\epsilon) \, \|S_N\|_{L^2} \left\| \frac{1}{\mathrm{Vol(B)}} \left(\chi_B - \chi_{B,N}\right) \right\|_{L^2}$$

for arbitrary $\epsilon > 0$ and large N with χ_B being the box function over the bin B and $\chi_{B,N}$ is the N-th iterative approximation of χ_B in the same manner as S_N of S.

Exact statistical error propagation:

- As the method is linear, exact propagation of covariance matrix of initial histogram $C-1$ is possible.
- Let $\mathcal{C}$ be the covariance matrix of the measured correlation histogram $C-1$. Let $\mathcal{E}$ be the square-root of $\mathcal{C}$, i.e. $\mathcal{C}=\mathcal{E}\mathcal{E}^T$.
- Perform the iteration:
  - $S_0 = K_{k,R}^{-1}A_k^T(C-1)$,
    $\mathcal{E}_0 = K_{k,R}^{-1}A_k^T\mathcal{E}$,
  - $S_{N+1} = S_N + \Big(S_0 - K_{k,R}^{-1}A_k^TA_kS_N\Big)$,
    $\mathcal{E}_{N+1} = \mathcal{E}_N + \Big(\mathcal{E}_0 - K_{k,R}^{-1}A_k^TA_k\mathcal{E}_N\Big)$.
- Then, the statistical covariance matrix in each step of S_N will be $\mathcal{C}_N = \mathcal{E}_N\,\mathcal{E}_N^T$.
- Iteration stop when e.g. L^1 norm of statistical error content exceeds predefined limit.

Properties of systematic error propagation:

- An upper estimation can be proved using spectral representation of operators.
- Let δC be the systematic error on the measured $C-1$ and δS_N the propagated systematic error of S_N.
- Let B be a histogram bin on the domain of S.
- Then,

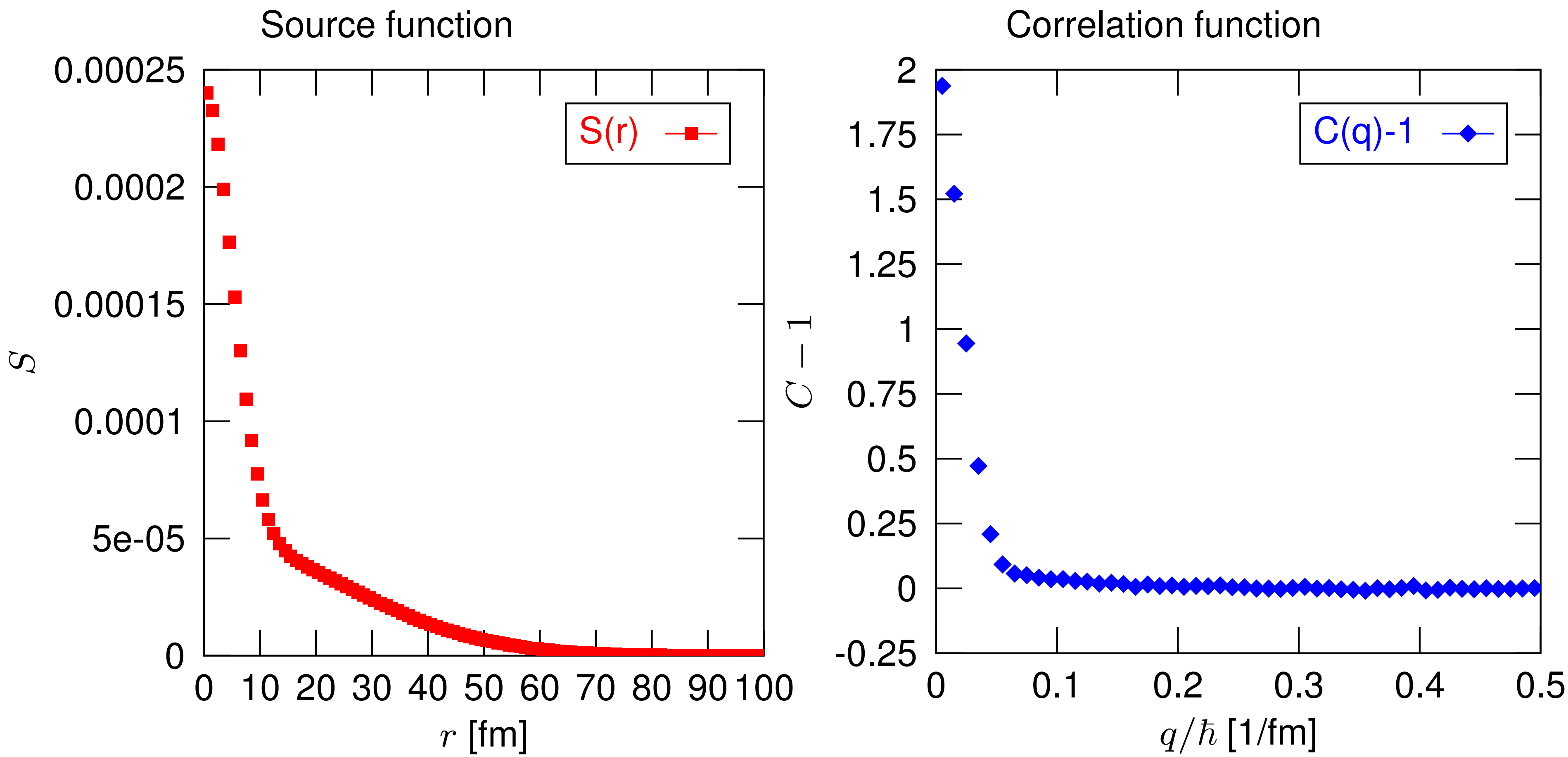
$$\left|\frac{1}{\mathrm{Vol}(B)}\int_B \delta S_N(\vec{r})\;\mathrm{d}^3 r\right|$$

$$\leq \left\|\frac{1}{\mathrm{Vol(B)}} X_{B,N}\right\|_{L^2}\sqrt{\int_{|\vec{r}|\leq R}\left(K_{k,R}^{-1}A_k^T|\delta C|\right)^2\;\mathrm{d}^3 r}$$

where

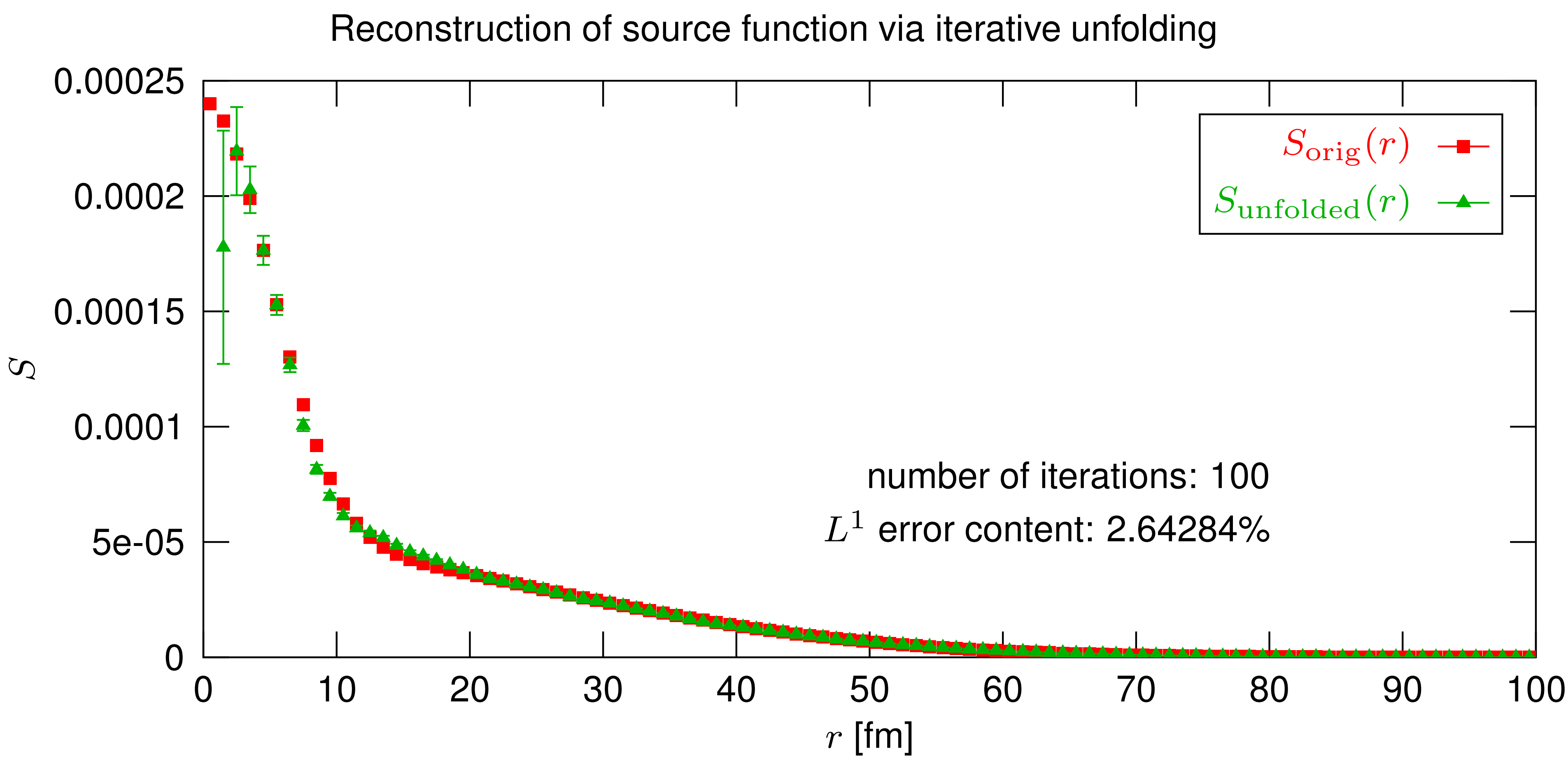
$$X_{B,0}=\chi_B \text{ and } X_{B,N+1}=X_{B,N}+\left(X_{B,0}-K_{k,R}^{-1}A_k^T A_k X_{B,N}\right).$$

Demo example:



Source is superposition of $\sigma = 5\,\mathrm{fm}$ gaussian with a $\sigma = 25\,\mathrm{fm}$ gaussian, along with its correlation function (with a simulated statistics of 100000 entries).

Extraction of source function from correlation via the proposed iterative unfolding:



Better approach would be the following (still some work needed).

- Take the measured correlation function with Coulomb distortion $C^C(\vec{q}) - 1$.
- Inverse Fourier transform it as if there were no Coulomb distortion, i.e. calculate

$$F^{-1}\left(C^C - 1\right)$$

$$= A_{k^0}^{-1}\left(C^C - 1\right).$$

- In order to obtain $S(\vec{r})$, unfold this with the same method against the folding operator

$$A_{F^{-1}(kC)}$$

$$= A_{k^0}^{-1} A_{kC}$$

because this operator has much better spectral properties.

- In this case assumption $|\vec{r}| \leq R$ can be dropped, along with faster convergence.
- For this, analytical or numerical form of the (inverse) Fourier transform of the BE kernel function with Coulomb effect is needed (not yet done).

Summary

- A linear iterative unfolding algorithm is proposed in
  `JPCS` **`368`** `(2012) 012043` and `arXiv:1404.2787`.
- Convergence proved under conditions which also hold for BE imaging problems.
- Estimation of bias errors possible at each finite iteration step.
- Exact propagation of statistical errors due to linearity.
- Upper estimates for propagated systematic errors possible.
- Available application library in C:
  `http://www.rmki.kfki.hu/~laszloa/downloads/libunfold.tar.gz`
- Method could be still improved if (inverse) Fourier transform of the BE kernel function with Coulomb correction is calculated (numerical presentation would be enough).

Thanks to: Máthé Csanád, Ferenc Siklér for discussions.