Convolution/deconvolution of generalized Gaussian kernels with applications to proton/photon physics and electron capture of charged particles

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Abstract. Scatter processes of photons lead to blurring of images produced by CT (computed tomography) or CBCT (cone beam computed tomography). Multiple scatter is described by, at least, one Gaussian kernel. In various tasks, this approximation is crude; we need two/three Gaussian kernels to account for long-range tails (Landau tails), which appear in Molière scatter of protons, energy straggling and electron capture of charged particles passing through matter and Compton scatter. The ideal image (source function) is subjected to Gaussian convolution to yield a blurred image. The inverse problem is to obtain the source image from a detected image. Deconvolution methods of linear combinations of two/three Gaussian kernels with different parameters $c_0, s_0, s_1, s_2$ can be derived via an inhomogeneous Fredholm integral equation of second kind (IFIE2) and Liouville - Neumann series (LNS) to provide the source function $\rho$. Scatter functions $s_0, s_1, s_2$ are best determined by Monte-Carlo. An advantage of LNS is given, if the scatter functions $s_0, s_1, s_2$ depend on coordinates. The convergence criterion can always be satisfied with regard to the above mentioned cases. A generalization is given by an analysis of the Dirac equation and Fermi-Dirac statistics leading to Landau tails applied to Bethe-Bloch equation (BBE) of charged particles and electron capture.

1. Introduction
Multiple scatter can be treated with, at least, one single Gaussian kernel [1], which we abbreviate by $K(s, u - x)$, but it may refer to more space dimensions. The ideal image (source function $\rho$ without any blurring) is subjected to a Gaussian convolution in order to yield an image function $\phi$ (blurred image):

$$\phi = \int K(s, u - x) \cdot \rho(u) du$$

The magnitude of the parameter $s$ represents a measure of the blurring strength that as $s \to 0$ the kernel $K$ tends to the $\delta$-distribution and $\phi$ becomes identical with $\rho$. In many situations the restriction to one Gaussian kernel represents a crude approximation, and we need a linear combination of Gaussian kernels with $K_g$ as a resulting convolution kernel to account for long-range tails, which appear in the Molière multiple scatter theory of protons with accounting for Landau tails [2, 3] or in Compton scatter [1]:

$$K_g = c_0 \cdot K(s_0, u - x) + c_1 \cdot K(s_1, u - x) + c_2 \cdot K(s_2, u - x)$$

$$\phi = \int K_g(s_0, s_1, s_2, c_0, c_1, c_2, u - x) \cdot \rho(u) du.$$  (2)

In every case, the parameters in Eq. (2) have to satisfy $c_0 + c_1 + c_2 = 1$, $c_0 > c_1$, $c_0 > c_2$ and $s_0 < s_1$, $s_0 < s_2$. The restriction to two Gaussian kernels results by setting $c_2 = 0$. If $c_2 \neq 0$, $c_1 < 0$ can also be valid, but $K_g \geq 0$. 

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must exist. The previous study [1] of the inverse task of $K_g$ requires $s_1 \wedge s_2 > s_0 \sqrt{2}$. This restriction may lead to critical cases (proton dosimetry, image processing with CBCT). The LNS method can circumvent this restriction, since it only needs that $s_1 \wedge s_2 > s_0$ is satisfied. The inverse task of Eq. (1) is to determine the ideal source image from a determined image. If the scatter parameters are known, we are able to calculate the idealistic source $q$ by $K^{-1}(s, u – x)$. A possible representation [1] of $K^{-1}$ is given by:

$$K^{-1}(s, u – x) = \sum_{n=0}^{N} c_n(s) \cdot H_{2n}(\frac{s}{s_0}) \cdot K(s, u – x)$$

$$N \rightarrow \infty; \quad c_n = (-1)^n \cdot \frac{s^n}{(2^n \cdot n!)}; \quad (n = 0, 1, \ldots, \infty)$$

Due to many applications of $K^{-1}(s, u – x)$ it represents a proven tool circumventing ill-posed aspects [1, 4 – 7]. $H_{2n}$ refer to Hermite polynomials of even order. The coefficients $c_n$ of the two-point Hermite polynomials of $K^{-1}$ are determined by a Lie series expansion (in practice: $N < \infty$). $K$ and $K^{-1}$ can be derived as Green’s functions [5, 7]. The intention of this study is to derive $K^{-1}_g(s_0, c_0, s_1, c_1, s_2, c_2, u – x)$ of a linear combination of two/three Gaussian convolution kernels according to Eq. (2) and to give some examples via an IFIE2 and related LNS.

2. Methods

The basic formulas of all calculations are the following two operator functions, defined as Lie series:

$$O^{-1} = \exp(\mp \frac{i}{\hbar} \cdot s \cdot \frac{d^2}{dx^2}) = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \cdot (\mp 1)^n \cdot \frac{j^2}{d^2} / dx^{2n}.$$  \hspace{1cm} (4)

$O^{-1}$ and $O^{-1}$ obey the following relation $O^{-1} \cdot O^{-1} = O^{-1} \cdot O^{-1} = 1$ (unit operator). In three dimensions, we have to substitute $d^3/dx^2$ by the 3D Laplace operator $\Delta$. We point out that the operator $O$ results from an operator calculus of the Boltzmann canonical ensemble $\exp(-H/k_B \cdot T)$ connected to a free particle Schrödinger equation $H = - (\hbar^2/2m) \cdot \Delta$. If $q(x)$ represents a source and $\phi(x)$ an image function, the following relationships have to be valid:

$$\phi(x) = O^{-1} \cdot \rho(x) \quad \text{and} \quad \rho(x) = O \cdot \phi(x).$$  \hspace{1cm} (5)

The equivalence between Eq. (5) and Eq. (6) has been previously shown [1]. In Eq. (5) the class of permitted functions is $C^\infty$, whereas in Eq. (6) we can consider the spaces either $L_1$ or $L_2$.

The differential operator formulation of Eq. (2) is:

$$\phi(x) = O^{-1}_f \cdot \rho(x) = [c_0 \cdot O^{-1}_0(s_0) + c_1 \cdot O^{-1}_1(s_1) + c_2 \cdot O^{-1}_2(s_2)] \cdot \rho(x).$$  \hspace{1cm} (7)

In every case, the condition $O^{-1}_f \cdot O^{-1}_f = I$ has to be satisfied. According to a previous study [7] we obtain:

$$O^{-1}_f \cdot \rho = \begin{cases} [c_0 \cdot O^{-1}_0(s_0) + c_1 \cdot O^{-1}_1(s_1) + c_2 \cdot O^{-1}_2(s_2)] \cdot \rho \Rightarrow - O^{-1}_0 \cdot [1 + \frac{\hbar^2}{2m} \cdot \Delta] \cdot \phi \rho = 0 \\ \rho \Rightarrow 0 \end{cases}$$  \hspace{1cm} (8)

We use the following abbreviation: $f(x, y, z) = \frac{1}{c_3} \cdot \int K^{-1}_0(s_0, u – x) \cdot \phi(\tilde{u}) d^3u$.  \hspace{1cm} (9)

Function $f$ incorporates the inhomogeneous part of the Fredholm integral equation of second kind (IFIE2). In order to derive an alternative method to solve the inverse problem of a linear combination of Gaussian convolutions, we consider Eq. (8) with regard to two kernels (the generalization to $c_2 \neq 0$ is stated elsewhere [8]). By that, we obtain the desired formula, which can be transformed to an IFIE2:
Parameters and

In practical problems $N = 4$ is sufficient. The inversion can be obtained via Gompertz functions ($N = 5$):

$$
\rho(\vec{x}) = \frac{\alpha}{\beta} \cdot \int \rho(\vec{u}) \cdot K_f(\sigma, \vec{u} - \vec{x}) d\vec{u}
$$

The LNS procedure consists of iterated procedures, and the resolving kernel $K_{\text{res}}$ is given by:

$$
K_{\text{res}}(\vec{u} - \vec{x}, \lambda) = \left\{ \begin{array}{ll}
\lambda^3 \cdot K_{f}(\vec{u}_0) (L \to \infty) \\
\lambda^3 \cdot K_{f}(\vec{u}_n) (L \to \infty) \\
\end{array} \right.
$$

The solution of the integral equation becomes:

$$
\rho(\vec{x}) = \int K_{\text{res}}(\vec{u} - \vec{x}, \lambda) \cdot f(\vec{u}) d\vec{u}
$$

The application of BBE for the determination of the electronic stopping power is established for the passage of protons through homogeneous media. A particular importance of BBE appears in Monte-Carlo calculations to simulate charged projectile particles along the track. This equation reads:

$$
-dE(z)/dz = \left( \frac{K}{v^2} \right) \left[ \ln \left( \frac{2mv^2}{E_z} \right) - \ln \left( 1 - \beta^2 \right) + a_{\Delta} + a_{\Delta_{\text{surf}}} + a_{\Delta_{\text{block}}} \right] + a_{\Delta_{\text{shell}}} + a_{\Delta_{\text{block}}}
$$

The stopping power is determined by $dE(z)/dz$ and yields:

$$
S(z) = dE(z)/dz = -E(z)/(R_{\text{CSDA}} - z) + \sum_{i=1}^{N} \lambda_i E_i(z) (N \to \infty)
$$

Due to electron capture formula (16) is only applicable to protons, whereas for heavy carbons we have to account for $q'(E)$, which can be described by generalized convolutions, based on Fermi-Dirac statistics. With regard to our task Dirac equation and Fermi-Dirac statistics to describe the particle motion are an adequate starting-point (Eq. $E_F$: energy of the Fermi edge, $d_\pi$ density of states):

$$
\begin{align*}
H_D &= c \alpha \vec{p} + \beta mc^2; \quad \hat{H} = H_D - E_F \\
f_F(\hat{H}) &= \exp \left( \frac{\beta mc^2}{i(h \pi/2)^{1/2} \cdot d_\pi(H_D)} \right)
\end{align*}
$$

The application of Eq. (17) to BBE finally provides the stopping power $S_E$ and $q^2(E)$:
Please note that the parameters [4] must be modified:

\[ \alpha = 0.0069465598; \quad \beta = 0.0008132157; \quad \gamma = -0.00000121069; \quad \delta = 0.000000001051. \]

If \( N = 1 \) and \( q_{\text{eff}} = 0.995 \) the above formula is valid for protons.

3. Applications

Parameters necessary for calculations can be found in [4, 8]. With regard to LNS in image processing we consider an image recorded by CBCT (Figures 1 – 3), 140 kV X-rays.

![Figure 1. Phantom (left side) for a CBCT check.](image1)

![Figure 2. Measured 2D dose distribution (in Hounsfield values).](image2)

The result of deconvolution via LNS is shown in Figure 3; details are given in [8].

![Figure 3. Deconvolution of Figure 2.](image3)

![Figure 4. Identical task in the MV domain (6 MeV, portal imager, IMRT).](image4)

The LNS procedure will now be applied to proton physics (IMPT) and the generalized convolution (Fermi-Dirac statistics) to electron capture. The field-size for IMPT amounts to 4.8 x 4.8 mm², which we have used due to available data of the HCL. It turned out by many studies that in proton therapy scanning methods have a preferred importance, since broad beams a rather difficult to handle due to the varying range of targets and range shifts resulting from heterogeneity of patient tissue [6]. The importance of the deconvolution of very narrow proton beams is demonstrated by Figure 5, which is closely related to
Figure 6. With regard to scanning beams in proton radiotherapy and IMPT the deconvolution can provide reliable information on the necessity of superposition of neighboring proton beamlets to avoid underdos e in DOIs or fluence modulation in IMPT. We also present results of calculations for protons, He and C ions; the initial energy amounts to 400 MeV/nucleon. This appears to be a reasonable restriction with regard to therapeutic conditions. Thus Figure 8 shows that at the end of the projectile track all charged ions nearly behave in the same manner, whereas Figure 7 is restricted to C ions, which start with different initial energies $E_0$.

4. Discussion
The LNS procedure is powerful with regard to the inverse problem of linear combinations of Gaussian convolution kernels. The application of the Fermi-Dirac statistics (instead of Boltzmann) can be handled with linear combinations of shifted Gaussian kernels [4]. Thus desired back calculations can also be carried out with the LNS-procedure, e.g. the calculation of $q^*(E)$ of measured Bragg curves of heavy carbons. By considering the energy dependence of the projectile particle charge $q(E)$, the LET of the stopping power $S(E)$ of charged particles can be accounted for in dose calculations.

Figure 5. Stopping-power of 158 MeV protons (HCL). Figure 6. Transverse profiles at $z = 6$ cm and Bragg peak.

Figure 7. Charge $q(E)$ of C ions; $E_0 = 200, 300$ and 400 MeV/nucleon.

Figure 8. $q(E)$ for 3 nuclei, $E_0 = 400$ MeV/nucleon.

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