Deconvolution of 3-D Gaussian kernels

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Abstract

Ulmer and Kaissl formulas for the deconvolution of one-dimensional Gaussian kernels are generalized to the three-dimensional case. The generalization is based on the use of the scalar version of the Grad’s multivariate Hermite polynomials which can be expressed through ordinary Hermite polynomials.

Keywords: Deconvolution, Gaussian kernels, Multivariate Hermite polynomials, Hermite polynomials, Laguerre polynomials.

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1. Introduction

Mathematical problem of deconvolution of Gaussian kernels was considered in [1]. In one-dimensional case, such a deconvolution (inverse problem) is equivalent to the solution of the Fredholm-type integral equation

\[ \phi(x) = \int_{-\infty}^{\infty} K(x - \xi; \sigma) \rho(\xi) \, d\xi, \]  

(1)

where \( \phi(x) \) is the known function, typically a detector response in a some measurement process of the unknown signal \( \rho(\xi) \) which is blurred by the finite resolution \( \sigma \) of the detector. This blurring is described by the Gaussian kernel

\[ K(x - \xi; \sigma) = \frac{1}{\sigma \sqrt{\pi}} e^{-(x-\xi)^2/\sigma^2}. \]  

(2)

The integral transform (Gaussian convolution) \( \square \) arises in various problems of applied physics, for example in calculations of transverse profiles of photon, proton or electron beams in medical applications \( \square, \square, \square, \square \).
Usually the integral equation (1) is solved by a Fourier transform method. It is well known that, due to a presence of a fast growing Gaussian function in the deconvolution integral in this case, this method may imply ill-posed inverse problems \[1\]. Therefore alternative methods of deconvolution of Gaussian kernels, avoiding ill-posed inverse problems, were developed \[1, 2\].

In particular, Ulmer and Kaissl provide in \[1\] two different expressions for the inverse kernel \( K^{-1}(x - \xi; \sigma) \) defined through the relation

\[
\rho(x) = \int_{-\infty}^{\infty} K^{-1}(x - \xi; \sigma) \phi(\xi) d\xi. \tag{3}
\]

In the next section we reproduce their results by a method which can be easily generalized to the three-dimensional case.

2. Deconvolution of 1-D Gaussian kernels

Our starting point will be an identity \[5\]

\[
K(x; \sigma) = e^{\frac{\sigma^2}{4} \frac{d^2}{dx^2}} \delta(x), \tag{4}
\]

which can be easily proved by using the Fourier integral representation of the Dirac’s delta function:

\[
\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ipx} dp. \tag{5}
\]

Because of (4), we can write

\[
\phi(x) = \int_{-\infty}^{\infty} \rho(\xi) e^{\frac{\sigma^2}{4} \frac{d^2}{d\xi^2}} \delta(x - \xi) d\xi = \int_{-\infty}^{\infty} \delta(x - \xi) e^{\frac{\sigma^2}{4} \frac{d^2}{d\xi^2}} \rho(\xi) d\xi = e^{\frac{\sigma^2}{4} \frac{d^2}{dx^2}} \rho(x). \tag{6}
\]

Therefore the integral transform (1) can be written in the operator form

\[
\phi(x) = \hat{K} \rho(x), \quad \hat{K} = e^{\frac{\sigma^2}{4} \frac{d^2}{dx^2}}. \tag{7}
\]
Hence its inverse is given by

\[ \rho(x) = \hat{K}^{-1} \phi(x), \quad \hat{K}^{-1} = e^{-\frac{x^2}{4} \frac{d^2}{dx^2}}. \]  

(8)

Now we apply the same trick as in (6):

\[ \rho(x) = \int_{-\infty}^{\infty} \delta(x - \xi) e^{-\frac{x^2}{4} \frac{d^2}{dx^2}} \phi(\xi) = \int_{-\infty}^{\infty} \phi(\xi) e^{-\frac{\xi^2}{4} \frac{d^2}{dx^2}} \delta(x - \xi), \]

which is the same as

\[ \rho(x) = \int_{-\infty}^{\infty} \phi(\xi) e^{-\frac{\xi^2}{2} \frac{d^2}{dx^2}} \delta(x - \xi). \]  

(9)

but, because of (4), we have

\[ e^{-\frac{\xi^2}{4} \frac{d^2}{dx^2}} \delta(x - \xi) = e^{-\frac{x^2}{2} \frac{d^2}{dx^2}} e^{\frac{\xi^2}{4} \frac{d^2}{dx^2}} \delta(x - \xi) = e^{-\frac{x^2}{2} \frac{d^2}{dx^2}} K(x - \xi; \sigma). \]  

(10)

Therefore

\[ \rho(x) = \int_{-\infty}^{\infty} \phi(\xi) e^{-\frac{x^2}{2} \frac{d^2}{dx^2}} K(x - \xi; \sigma), \]

which shows that

\[ K^{-1}(x - \xi; \sigma) = e^{-\frac{x^2}{2} \frac{d^2}{dx^2}} K(x - \xi; \sigma) = \sum_{n=0}^{\infty} \frac{(-\sigma^2)^n}{2^n n!} \frac{d^{2n}}{dx^{2n}} K(x - \xi; \sigma). \]  

(11)

Thanks to the Rodrigues formula for Hermite polynomials [6]

\[ H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \]

(12)

derivatives of the Gaussian function in (11) can be expressed through Hermite polynomials:

\[ \frac{d^{2n}}{dx^{2n}} K(x - \xi; \sigma) = \sigma^{-2n} H_{2n} \left( \frac{x - \xi}{\sigma} \right) K(x - \xi; \sigma), \]  

(13)
and we finally obtain
\[
K^{-1}(x - \xi; \sigma) = \sum_{n=0}^{\infty} \frac{(-1)^n}{2^n n!} H_{2n} \left( \frac{x - \xi}{\sigma} \right) K(x - \xi; \sigma). \tag{14}
\]

Another version of the inverse Gaussian kernel can be obtained by the use of the following identity
\[
e^{-\frac{a^2}{2} \frac{d^2}{dx^2}} \delta(x - \xi) = \delta(x - \xi) + \left( e^{-\frac{a^2}{2} \frac{d^2}{dx^2}} - e^{-\frac{a^2}{4} \frac{d^2}{dx^2}} \right) e^{\frac{a^2}{4} \frac{d^2}{dx^2}} \delta(x - \xi). \tag{15}
\]

Using this identity and the identity (4) in (9), we get
\[
\rho(x) = \int_{-\infty}^{\infty} \phi(\xi) \left[ \delta(x - \xi) + \left( e^{-\frac{a^2}{2} \frac{d^2}{dx^2}} - e^{-\frac{a^2}{4} \frac{d^2}{dx^2}} \right) e^{\frac{a^2}{4} \frac{d^2}{dx^2}} \delta(x - \xi) \right] d\xi = \int_{-\infty}^{\infty} \phi(\xi) \left[ \delta(x - \xi) + \sum_{n=1}^{\infty} \frac{(-\sigma^2)^n}{4^n n!} \left( 2^n - 1 \right) \frac{d^{2n}}{dx^{2n}} K(x - \xi; \sigma) \right]. \tag{16}
\]

Therefore, in light of (13), we have
\[
K^{-1}(x - \xi; \sigma) = \delta(x - \xi) + \sum_{n=1}^{\infty} \frac{(-1)^n}{4^n n!} \left( 2^n - 1 \right) H_{2n} \left( \frac{x - \xi}{\sigma} \right) K(x - \xi; \sigma). \tag{17}
\]

Equations (14) and (17) were first obtained (with some typos) in [1].

3. Deconvolution of 3-D Gaussian kernels

Generalization to the three-dimensional case is now straightforward. All what is needed is to change the differential operator \( \frac{d^2}{dx^2} \) by its three-dimensional version (Laplacian) \( \Delta = \nabla^2 \), change \( x \) and \( \xi \) by the corresponding three-dimensional vectors \( \mathbf{r} \) and \( \mathbf{\xi} \), and use a three-dimensional Gaussian kernel
\[
K(\mathbf{r} - \mathbf{\xi}; \sigma) = \frac{1}{\sigma^3 \sqrt{\pi^3}} e^{-\frac{(\mathbf{r} - \mathbf{\xi})^2}{2\sigma^2}}. \tag{18}
\]

Then, instead of (11), we will end up with the equation
\[
K^{-1}(\mathbf{r} - \mathbf{\xi}; \sigma) = e^{-\frac{\sigma^2}{2} \Delta} K(\mathbf{r} - \mathbf{\xi}; \sigma) = \sum_{n=0}^{\infty} \frac{(-\sigma^2)^n}{2^n n!} \Delta^n K(\mathbf{r} - \mathbf{\xi}; \sigma). \tag{19}
\]
However now the action of the powers of Laplacian $\Delta = \nabla^2$ on the three-
dimensional Gaussian function cannot be as simply expressed in terms of the
Hermite polynomials, as in the one-dimensional case. In [2] the following
approach was suggested. Using

$$K(r - \xi; \sigma) = K(x - \xi_x; \sigma) K(y - \xi_y; \sigma) K(z - \xi_z; \sigma),$$

and

$$e^{-\frac{r^2}{2}} \Delta = e^{-\frac{x^2}{2}} \frac{\partial^2}{\partial x^2} e^{-\frac{y^2}{2}} \frac{\partial^2}{\partial y^2} e^{-\frac{z^2}{2}} \frac{\partial^2}{\partial z^2},$$

we get from the first equation of (19)

$$K^{-1}(r - \xi; \sigma) = F_1 F_2 F_3 K(r - \xi; \sigma),$$

where

$$F_1 = \sum_{n_1=0}^{\infty} \frac{(-1)^{n_1}}{2^{n_1} n_1!} H_{2n_1} \left(\frac{x - \xi_x}{\sigma}\right), \quad F_2 = \sum_{n_2=0}^{\infty} \frac{(-1)^{n_2}}{2^{n_2} n_2!} H_{2n_2} \left(\frac{y - \xi_y}{\sigma}\right),$$

$$F_3 = \sum_{n_3=0}^{\infty} \frac{(-1)^{n_3}}{2^{n_3} n_3!} H_{2n_3} \left(\frac{z - \xi_z}{\sigma}\right).$$

Yet this form of inverse kernel doesn’t seem convenient in applications. Es-
pecially if we note that a more straightforward generalization of equations
(14) and (17) is possible if we use multivariate and tensorial generalization of
Hermite polynomials introduced by Grad [7, 8]. Grad’s definition generalizes
the Rodrigues formula for the univariate Hermite polynomials (12):

$$H^{(n)}_{i_1 i_2 \cdots i_n} (r) = (-1)^n e^{r^2} \nabla_{i_1} \nabla_{i_2} \cdots \nabla_{i_n} e^{-r^2}. \quad (23)$$

Using this definition, we easily get straightforward generalization of the equation
(14) in the form

$$K^{-1}(r - \xi; \sigma) = \sum_{n=0}^{\infty} \frac{(-1)^n}{2^n n!} H_{2n} \left(\frac{(r - \xi)^2}{\sigma^2}\right) K(r - \xi; \sigma),$$

where

$$H_{2n} \left(\frac{(r - \xi)^2}{\sigma^2}\right) = \delta_{i_1 i_2} \delta_{i_3 i_4} \cdots \delta_{i_{2n-1} i_{2n}} H^{(2n)}_{i_1 i_2 \cdots i_{2n-1} i_{2n}}(r - \xi; \sigma).$$

5
is the completely contracted version of the multivariate Hermite polynomials (the so called scalar, or irreducible, Hermite polynomials [9]).

Analogously, the generalization of the equation (17) looks like

\[ K^{-1}(r - \xi; \sigma) = \delta(r - \xi) + \sum_{n=1}^{\infty} \frac{(-1)^n}{4^n n!} (2^n - 1) \mathcal{H}_{2n} \left( \frac{(r - \xi)^2}{\sigma^2} \right) K(r - \xi; \sigma). \]  

(26)

4. Calculation of scalar Hermite polynomials

Scalar Hermite polynomials can be expressed in terms of the classical (associated) Laguerre polynomials [9, 10]. Below we elaborate this connection and show that, in fact, Scalar Hermite polynomials can be expressed through the ordinary Hermite polynomials.

Let us introduce the following operators [11]

\[ \hat{E} = \frac{1}{2} r^2, \quad \hat{F} = -\frac{1}{2} \Delta, \quad \hat{H} = r \cdot \nabla + \frac{3}{2}. \]  

(27)

Using the commutator

\[ [\nabla_i, r] = \frac{r_i}{r}, \]

it can be easily checked that these operators obey commutation relations of the sl(2, \mathbb{C}) Lie algebra [11]:

\[ [\hat{H}, \hat{E}] = 2\hat{E}, \quad [\hat{H}, \hat{F}] = -2\hat{F}, \quad [\hat{E}, \hat{F}] = \hat{H}. \]  

(28)

It is clear from (23) and (25) that

\[ \mathcal{H}_{2n}(r^2) = e^{r^2} \Delta^n e^{-r^2} = e^{r^2} \Delta^n e^{-r^2}(1) = \left( e^{r^2} \Delta e^{-r^2} \right)^n(1), \]  

(29)

where \( \hat{r} \) is just a multiplication operator: \( \hat{r} g(r) = rg(r) \) for any function \( g(r) \), and an expression \( A(1) \) means that the operator \( \hat{A} \) acts on the function \( g(r) = 1 \). The trick used here is borrowed from [12] and it is useful because the last expression in (29) allows to use the operator identity (Baker-Hausdorff formula) [13]

\[ e^\hat{A} \hat{B} e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!} [\hat{A}, [\hat{A}, \hat{B}]] + \frac{1}{3!} [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] + \cdots \]  

(30)
With the help of the commutation relations (28), we can easily check that in the case of the last expression in (29) the corresponding Baker-Hausdorff series (30) in fact terminates and we end up with

\[ e^{r^2 \Delta} e^{-r^2} = e^{2\hat{E}}(-2\hat{F})e^{-2\hat{E}} = -2\hat{F} - 4\hat{H} + 8\hat{E}. \]  

(31)

Analogously, we have

\[ e^{-\frac{1}{4}} (4r^2)^n = e^{-\frac{1}{4}} (4r^2)^n e^{\frac{1}{4}} (1) = \left( e^{-\frac{1}{4}} (4r^2) e^{\frac{1}{4}} \right)^n (1), \]

(32)

and

\[ e^{-\frac{1}{4}} (4r^2) e^{\frac{1}{4}} = e^{\frac{1}{2}} \hat{F} (8\hat{E}) e^{-\frac{1}{2}} \hat{F} = 8\hat{E} - 4\hat{H} - 2\hat{F}. \]

(33)

Comparing (33) and (31), we see from (29) and (32) that

\[ H_{2n}(r^2) = e^{-\frac{1}{4}} (4r^2)^n = e^{-\frac{1}{4}} (2r)^{2n}. \]

(34)

Note that the relation (34) is completely analogous to an alternative expression for the usual Hermite polynomials \[14]\]

\[ H_n(x) = e^{-\frac{1}{4} \frac{d}{dx}} (2x)^n. \]

(35)

Although in some calculations (35) is more useful than the Rodrigues formula, it was little known for a long time (see, for example, \[15, 16\]).

Using

\[ \Delta r^n = \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dr^n}{dr} \right) = n(n + 1) r^{n-2}, \]

it can be proved by induction that

\[ \Delta^m r^{2n} = \frac{(2n + 1)!}{(2n - 2m + 1)!} r^{2(n-m)}, \quad \text{if} \quad n \geq m, \]

(36)

and \[\Delta^m r^{2n} = 0, \quad \text{if} \quad m > n.\] Then (34) gives

\[ H_{2n}(r^2) = \sum_{m=0}^{\infty} \frac{(-1)^m 4^{n-m}}{m!} \Delta^m r^{2n} = \sum_{m=0}^{n} \frac{(-1)^m 4^{n-m}}{m!} \frac{(2n + 1)!}{(2n - 2m + 1)!} r^{2(n-m)}, \]

which, after introduction of a new summation index \[i = n - m,\] can be rewritten as follows:

\[ H_{2n}(r^2) = (-1)^n \sum_{i=0}^{n} \frac{(-1)^i 4^i (2n + 1)!}{(n-i)! (2i + 1)!} r^{2i}. \]

(37)
In particular, we get for the first few scalar Hermite polynomials:

\[ H_2(r^2) = 2(2r^2 - 3), \]
\[ H_4(r^2) = 4(4r^4 - 20r^2 + 15), \]
\[ H_6(r^2) = 8(8r^6 - 84r^4 + 210r^2 - 105), \]
\[ H_8(r^2) = 16(16r^8 - 288r^6 + 1512r^4 - 2520r^2 + 945). \] (38)

In light of the Legendre duplication formula \[17\]

\[ (2z + 1)! = 2^{2z+1} \frac{\pi^{-1/2}}{z!} \frac{(z + \frac{1}{2})!}{(n + \frac{1}{2})!}, \] (39)

we have

\[ \frac{4^i (2n + 1)!}{(n - i)! (2i + 1)!} = \frac{2^{2n} n!}{i!} \frac{(n + \frac{1}{2})!}{(n - i)! (i + \frac{1}{2})!} = \left( \frac{n + \frac{1}{2}}{n - i} \right) \frac{2^{2n} n!}{i!}, \]

and (37) takes the form

\[ H_{2n}(r^2) = (-1)^n 2^{2n} n! \sum_{i=0}^{n} \frac{(-1)^i}{i!} \frac{(n + \frac{1}{2})!}{(n - i)!} (r^2)^i. \] (40)

On the other hand, the associated Laguerre polynomials \( L_n^k \) satisfy \[14\]

\[ L_n^k(x) = \sum_{i=0}^{n} \frac{(-1)^i}{i!} \frac{(n + k)!}{(n - i)!} x^i. \] (41)

Comparing (40) and (41), we see that

\[ H_{2n}(r^2) = (-1)^n 2^{2n} n! L_n^{1/2}(r^2). \] (42)

However \[14\]

\[ L_n^{1/2}(r^2) = \frac{(-1)^n}{2^{2n+1} n!} H_{2n+1}(r), \] (43)

and we finally get a simple expression for the scalar Hermite polynomials in terms of ordinary Hermite polynomials:

\[ H_{2n}(r^2) = \frac{H_{2n+1}(r)}{2r}. \] (44)
5. Concluding remarks

As we see, the use of Grad’s multivariate Hermite polynomials allows to perform a straightforward generalization of Ulmer and Kaissl formulas for the inverse problem of a Gaussian convolution to the three-dimensional case. In this generalization, the scalar Hermite polynomials play the same role as ordinary Hermite polynomials in the Ulmer and Kaissl’s one-dimensional formulas. The scalar Hermite polynomials by themselves can be expressed in terms of associated Laguerre polynomials and through them, rather surprisingly, through ordinary Hermite polynomials. The latter connection becomes less mysterious thanks to the new generating functions for even- and odd-Hermite polynomials [18]:

\[
F(x, t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_{2n}(x) = \frac{1}{\sqrt{1 + 4t}} \exp \left( \frac{4tx^2}{1 + 4t} \right),
\]

\[
G(x, t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_{2n+1}(x) = \frac{2x}{\sqrt{(1 + 4t)^3}} \exp \left( \frac{4tx^2}{1 + 4t} \right). \tag{45}
\]

Indeed, since

\[
(2r)^{2n} = 4^n (x^2 + y^2 + z^2)^n = \sum_{n_1+n_2+n_3=n} \frac{n!}{n_1! n_2! n_3!} (2x)^{2n_1} (2y)^{2n_2} (2z)^{2n_3},
\]

(20), (34) and (35) imply that (44) is equivalent to the curious identity

\[
\sum_{n_1+n_2+n_3=n} \frac{n!}{n_1! n_2! n_3!} H_{2n_1}(x) H_{2n_2}(y) H_{2n_3}(z) = \frac{H_{2n+1}(r)}{2r}, \tag{46}
\]

which, however, is a simple consequence of the generating functions (45), because

\[
F(x, t) F(y, t) F(z, t) = \frac{G(r, t)}{2r}.
\]

The task of deconvolution arises in many fields, such as geophysics, signal and image processing, underwater acoustics, astrophysics, high-energy physics, etc. A general theory is beautiful, although very abstract [19]. For more practical-minded introduction, see [20]. Naturally many algorithms of deconvolution were developed. Our aim in this note was not to suggest one
more practical algorithm and test its robustness, but indicate that the algorithm described in [1] can be naturally generalized for the three-dimensional case.

We hope that this refinement of the Ulmer and Kaissl method can find some practical applications. Besides many applications in medical radiation physics [2], Ulmer and Kaissl method was applied to get a (one-dimensional) inverse integral kernel for diffusion in a harmonic potential of an overdamped Brownian particle [21]. The method (its three-dimensional version described in this article) was also used to obtain a non-local generalization of the Schrödinger equation due to quantum-gravity effects [22]. It can be also useful in some problems of non-local gravity [23, 24].

Finally, the relation (44), which expresses scalar Hermite polynomials in terms of ordinary Hermite polynomials can be useful in plasma physics (in [9, 10] scalar Hermite polynomials were expressed through the Laguerre polynomials but the connection with the ordinary Hermite polynomials was not noticed).

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