A multidimensional function \( y(\vec{r}) \) defined by a sample of points \( \{\vec{r}_i, y_i\} \) is approximated by a differentiable function \( \tilde{y}(\vec{r}) \). The problem is solved by using the Gauss-Hermite folding method developed in the nuclear shell correction method by Strutinsky.

1 Introduction

Our aim is to approximate a sample of points \( \{\vec{r}_i, y_i\} \) which represents a measured or hard to evaluate data by a differentiable function \( y(x) \). We would like to solve this problem using the Gauss-Hermite folding method which idea was originally proposed by V.M. Strutinsky and later-on generalized in Ref. [1]. A detailed description of this method may be found already in text-books, e.g. in Ref. [3]. Having the width of the folding function comparable with the average distance between \( x_i \) points in the \( i \)th direction one can obtain the folded function which goes very close to the data points but increasing its width one can also wash out the fine structure stored in the data. Usually the Strutinsky method was used to realize the second scope. The parameter of the folding procedure will be determined by requirement that the integral in the \( i \)th direction of the folded function should be the same as the integral evaluated with \( \{x_i, y_i\} \) pairs using the trapezium rule. A corresponding Fortran program for the approximation in the \( n \)-dimensional space is listed in Appendix.

2 General folding formulae in the one-dimensional case

We consider an ensemble of \( N \) points \( \{x_i\} \) distributed uniformly in the interval \([a, b]\). To each point \( x_i \) corresponds a point \( y_i \), and we assume there exists a function \( y(x) \) such that:

\[
y_i = y(x_i) .
\]

(1)

Let \( j_n(x, x') \) be a symmetric function of its arguments (i.e. \( j_n(x, x') = j_n(x', x) \)) having the following properties:

\[
\int_{-\infty}^{+\infty} j_n(x, x') \, dx = 1
\]

(2)

and

\[
P_k(x) = \int_{-\infty}^{+\infty} P_k(x') \, j_n(x, x') \, dx',
\]

(3)

1Truly speaking the assumption about the uniform distribution of the points is too strong. It is sufficient to assume that the points \( x_i \) have to cover the whole interval \([a, b]\) and to be ordered i.e. \( x_{i+1} > x_i \).
where \( k \leq n \) are the even natural numbers and \( P_k \) is an arbitrary polynomial of the order \( k \). In the following the function \( j_n(x, x') \) will be called the folding function of the \( n^{th} \) order.

An example of such a folding function can be a combination of the Gauss function and the Hermite polynomials of argument proportional to \( |x - x'| \) frequently used in the Strutinsky shell correction method [1, 3]. More detailed description of the Strutinsky folding function will be given in the next section.

With each discrete point \((x_i, y_i)\), one can associate the function \( \tilde{y}_i(x) \) defined by:

\[
\tilde{y}_i(x) = \int_{-\infty}^{+\infty} y_i \delta(x' - x_i) j_n(x, x') \, dx' ,
\]

(4)

where \( \delta(x) \) is the Dirac \( \delta \)-function, so that

\[
\tilde{y}_i(x) = y_i j_n(x, x_i) .
\]

(5)

Using Eq. (2) it is easy to verify that the integral of the function \( \tilde{y}_i(x) \) is

\[
\int_{-\infty}^{+\infty} \tilde{y}_i(x) \, dx = y_i .
\]

(6)

Let us construct the function \( \tilde{y}(x) \) by summing up all functions \( \tilde{y}_i(x) \) corresponding to each \( x_i \) point

\[
\tilde{y}(x) = \sum_{i=1}^{N} \omega_i \tilde{y}_i(x) .
\]

(7)

The Lebesgue theorem says that the function \( \tilde{y}(x) \) is an approximation of \( y(x) \) if the weights \( \omega_i \) are determined from the assumption that the integrals of the unfolded and folded functions are (nearly) equal:

\[
\int_{a}^{b} y(x) \, dx \approx \int_{-\infty}^{+\infty} \tilde{y}(x) \, dx = \sum_{i=1}^{N} \omega_i y_i .
\]

(8)

The Riemann formula for the integral of the function \( y(x) \) between bounds \( a \) and \( b \) reads:

\[
\int_{a}^{b} y(x) \, dx = \lim_{N \to \infty} \sum_{i=1}^{N} y(x_i) \Delta x_i ,
\]

(9)

where \( \Delta x_i \) is set to:

\[
\Delta x_i = \frac{1}{2} (x_{i+1} - x_{i-1})
\]

(10)

with \( x_0 = a \) and \( x_{N+1} = b \). Comparing Eqs. (8) and (9) one can see that a reasonable choice of the weight is

\[
\omega_i = \Delta x_i .
\]

(11)

If the number \( N \) of sample points \((x_i, y_i)\) large enough than the condition (8) will be fullfiled.

So, finally the folded function \( \tilde{y}(x) \) is given by

\[
\tilde{y}(x) = \sum_{i=1}^{N} y_i \Delta x_i j_n(x, x_i) .
\]

(12)
3 Gauss-Hermite folding function

Let the folding function \( j_n(x, x') \) be a modified Gauss function

\[
j_n(x, x') = \frac{1}{\gamma \sqrt{\pi}} \exp \left\{ - \left( \frac{x-x'}{\gamma} \right)^2 \right\} f_n \left( \frac{x-x'}{\gamma} \right),
\]

where \( \gamma \) is the parameter and \( f_n(\frac{x-x'}{\gamma}) \) is the so-called correction polynomial of the order \( n \) determined by the Strutinsky condition \( \Box \). In the following we would like to evaluate the coefficients of the correction polynomial using some properties of the Hermite polynomials which are orthogonal with the weight equal to the Gauss function.

Let us introduce the variable \( u = (x - x')/\gamma \) which belongs to the interval \( (-\infty, +\infty) \).

The smearing function \( j_n(x, x') \) and the polynomial \( P_n(x) \) \( \Box \) can be now written as

\[
j_n(x, x') = e^{-u^2} \frac{1}{\gamma \sqrt{\pi}} f_n(u),
\]

\[
P_n(x') = P_n(x - \gamma u) \equiv P_n'(u),
\]

and

\[
P_n(x) = P_n(x + \gamma 0) \equiv P_n'(0).
\]

Let us decompose the function \( P_n'(u) \) into series of the Hermite polynomials \( H_i(u) \)

\[
P_n'(u) = \sum_{i=1}^{n} a_i H_i(u).
\]

Now the condition \( \Box \) for \( k = n \) can be written as

\[
P_n'(0) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} P_n'(u) e^{-u^2} f_n(u) du
\]

and inserting the relation \( \Box \) one obtains

\[
\sum_{i=1}^{n} a_i \left\{ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-u^2} H_i(u) f_n(u) du - H_i(0) \right\} = 0.
\]

The last equation should be fulfilled for arbitrary values of \( a_i \neq 0 \) what leads to the following set of equations

\[
\frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-u^2} H_i(u) f_n(u) du = H_i(0),
\]

where \( i = 0, 2, ..., n \). From the other side the correction function \( f_n(u) \) can be also decomposed into series of the Hermite polynomials

\[
f_n(u) = \sum_{k=1}^{n} C_k H_k(u).
\]

Inserting the above relation to Eq. \( \Box \) one obtains

\[
H_i(0) = \sum_{k=1}^{n} C_k \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-u^2} H_i(u) H_k(u) du.
\]
Then using the orthogonality properties of the Hermite polynomials
\[ \int_{-\infty}^{+\infty} e^{-u^2} H_i(u) H_k(u) \, du = 2^i \, i! \, \delta_{ik}, \] (23)

one obtains the coefficients of the correction polynomial (21)
\[ C_i = \frac{1}{2^i i!} H_i(0) \] (24)

The values of the Hermite polynomials at zero-point are
\[ H_i(0) = \begin{cases} 1 & \text{for } i = 0, \\ 2^n (-1)^n (2n - 1)!! & \text{for } i = 2n, \\ 0 & \text{for } i = 2n + 1, \end{cases} \] (25)

so
\[ C_i = \begin{cases} \frac{1}{2^i (2n)!!} & \text{for } i = 0, \\ (-1)^n \frac{(2n-1)!!}{2^n} & \text{for } i = 2n > 0, \\ 0 & \text{for } i = 2n + 1. \end{cases} \] (26)

The first few coefficients \( C_i \) and the corresponding Hermite polynomials are:
\[\begin{align*}
C_0 &= 1 & H_0 &= 1 \\
C_2 &= -\frac{1}{4} & H_2(u) &= 4u^2 - 2 \\
C_4 &= +\frac{1}{32} & H_4(u) &= 16u^4 - 48u^2 + 12 \\
C_6 &= -\frac{1}{384} & H_6(u) &= 64u^6 - 480u^4 + 720u^2 - 120
\end{align*}\] (27)

and the corresponding correction polynomials have the following form
\[\begin{align*}
f_0(u) &= 1, \\
f_2(u) &= \frac{3}{2} - u^2, \\
f_4(u) &= \frac{15}{8} - \frac{5}{2} u^2 + \frac{1}{2} u^4, \\
f_6(u) &= \frac{35}{16} - \frac{35}{8} u^2 + \frac{7}{4} u^4 - \frac{1}{6} u^6.
\end{align*}\] (28)

Finally the function \( \tilde{y}(x) \) approximated by the Gauss-Hermite folding reads:
\[ \tilde{y}(x) = \frac{1}{\gamma \sqrt{\pi}} \sum_{i=1}^{N} y_i \, \Delta x_i \exp \left\{ -\left( \frac{x - x_i}{\gamma} \right)^2 \right\} f_n \left( \frac{x - x_i}{\gamma} \right). \] (29)

As a rule the smearing parameter \( \gamma \) is arbitrary and it can be different at each point \( x_i \). But it should be related to the distance \( \Delta x_i \) between subsequent points if one would like to approximate the function stored in the mesh of \( \{ x_i, y_i \} \) points. Similarly one has to choose the \( \gamma \) parameter of the order of the period-length of the fine structure (e.g. shell effects) in case when one would like to wash out this structure from the function \( y(x) \).
4 Multidimensional case

The extension of the formalism described in the previous sections is straightforward. Let assume that the data points are stored in a m-dimensional array $Y[1 : N_1, 1 : N_2, ..., 1 : N_m]$ which corresponds to the ordinates given by the $m$ one-dimensional arrays $X_i[1 : N_i]$, where $i = 1, 2, ..., m$. It means that each element of $Y[i_1, i_2, ..., i_m]$ corresponds to the coordinate $X_k[i_k]$ with $k = 1, 2, ..., m$.

The ensemble of the Hermite polynomials $H_i(x)$ forms a complete basis of orthogonal functions in which an arbitrary m-dimensional function $F(\vec{r}) \equiv F(x_1, x_2, ..., x_m)$ can be expanded

$$ F(x_1, x_2, ..., x_m) = \sum_{i_1=0}^{\infty} \sum_{i_2=0}^{\infty} \cdots \sum_{i_m=0}^{\infty} C_{i_1i_2...i_m} H_{i_1}(x_1) H_{i_2}(x_2) \cdots H_{i_m}(x_m). \quad (30) $$

The same is true for any polynomial $P_n(x_1, x_2, ..., x_m)$ of the order $n$ but in this case the upper limit of the sums in equation analogous to (30) will be $n$. It means that the folding function in the m-dimensional space is simply the product of the $m$-th one-dimensional foldings performed in each single direction:

$$ J_n(x_1, x_2', ..., x_m') = \prod_{i=1}^{m} j_n(x_i, x_i'). \quad (31) $$

The folded function $\tilde{Y}(x_1, x_2, ..., x_m)$ is given by the equation analogous to (12):

$$ \tilde{Y}(x_1, x_2, ..., x_m) = \sum_{i_1=0}^{\infty} \Delta x_{i_1} \sum_{i_2=0}^{\infty} \Delta x_{i_2} \cdots \sum_{i_m=0}^{\infty} \Delta x_{i_m} \cdot Y[i_1, i_2, ..., i_m] j_n(x_1, X_1[i_1]) \cdots j_n(x_m, X_m[i_m]). \quad (32) $$

The folding function $j_n(x_i, x_i')$ for the Gauss-Hermite smoothing (13) is

$$ j_n(x_i, x_i') = \frac{1}{\gamma_i \sqrt{\pi}} \exp \left\{ -\left( \frac{x_i - x_i'}{\gamma_i} \right)^2 \right\} f_n \left( \frac{x_i - x_i'}{\gamma_i} \right). \quad (33) $$
The Gaussian width $\gamma_i$ can be different in each coordinate. The correction polynomial $f_n$ was already given by Eq. (21) and it is tabulated in (28) for $n=0,2,4,$ and 6.

5 Some data illustrating the quality of the method

The second order ($n = 2$) Gauss-Hermite folding in a four-dimensional space is used. Taking into account higher order correction polynomials (28) one does not increase significantly the quality of the approximation of the function in the middle of the data region but it would need a more careful treatment of the problem at the edges. The folding is performed using the $p$ mesh points closest to the given point in each direction. The tested function are spanned on $21^4$ points. In addition it is assumed that outside the the data region $\{x_i, y_k\}$ the function which should be folded has a constant value (equal to the value of the first or the last point in the given direction depending from which side of the data region one takes the data for folding).

The data in Table 1 are listed for some values of the smearing parameter $\gamma$ in order to see its influence on the accuracy of the approximation. The cosines function in the four-dimensional space is chosen as the test function:

$$Y(x_1, x_2, x_3, x_4) = \cos(r),$$

where $r = \sqrt{x_1^2 + x_2^2 + x_3^2 + x_4^2}$ and the equidistant points $x_n(i) \in (-2\pi, 2\pi)$ for $i = 1, 2, ..., 21$ and $n = 1, 2, 3, 4$. The upper and lower limit are $Y_{\text{max}} = 1$ and $Y_{\text{min}} = -1$ respectively.

Table 1: The approximation of the four-dimensional $\cos(r)$ function by the 2nd order Gauss-Hermite folding on basis of $p = 5$ and $p = 7$ closest to the given points in function of the smearing parameter $\gamma$.

| $1/\gamma$ | $\delta_{\text{avr}}$ | $\delta_{\text{min}}$ | $\delta_{\text{max}}$ | $\delta_{\text{avr}}$ | $\delta_{\text{min}}$ | $\delta_{\text{max}}$ |
|------------|------------------------|-----------------------|------------------------|------------------------|-----------------------|------------------------|
|            | $p = 5$                | $p = 7$               |                        |                        |                        |                        |
| 0.98       | 0.0081                 | -0.0296               | 0.0530                 | 0.0030                 | -0.0073               | 0.0241                 |
| 1.00       | 0.0072                 | -0.0261               | 0.0485                 | **0.0029**             | **-0.0074**           | **0.0242**             |
| 1.02       | 0.0065                 | -0.0233               | 0.0452                 | 0.0030                 | -0.0076               | 0.0249                 |
| 1.04       | 0.0060                 | -0.0210               | 0.0428                 | 0.0032                 | -0.0080               | 0.0260                 |
| 1.06       | 0.0057                 | -0.0192               | 0.0414                 | 0.0035                 | -0.0086               | 0.0276                 |
| 1.08       | **0.0057**             | **-0.0179**           | **0.0409**             | 0.0040                 | -0.0093               | 0.0295                 |
| 1.10       | 0.0059                 | -0.0171               | 0.0411                 | 0.0046                 | -0.0102               | 0.0320                 |

The root mean square deviation

$$\delta_{\text{avr}} = \left( \frac{\sum_{i=1}^{N} \{Y[\vec{r}(i)] \}^2}{N - 1} \right)^{1/2}$$

as well as the maximal in plus difference ($\delta_{\text{max}}$) and the minimal in minus one ($\delta_{\text{min}}$) are evaluated for the $N = 149057$ mesh and inter-mesh points (in the middle) excluding the points which lie on two outer layers (i.e two first or last rows or columns). Such a choice of the test nodes was made in order to eliminate the influence of the border condition on the deviation $\delta_{\text{avr}}$. 

6
Some other examples of the accuracy of the 2\textsuperscript{nd} order Gauss-Hermite approximations are listed in Table 2. The function written in the first column are tabulated at 21 equidistant points in the each coordinate in the 4-dimensional space in the interval written in the 2\textsuperscript{nd} column. The smearing parameter $\gamma = 0.93$ or $\gamma = 1$ is chosen in case of the $p = 5$ or $p = 7$ point basis used when folding, respectively. It is seen in Tables 1 and 2 that in all considered cases the root mean square deviation ($\delta_{\text{avr}}$) is of the order $10^{-6}$ or less of the maximal difference $Y_{\text{max}} - Y_{\text{min}}$ between the data points.

### Table 2: A few examples of the approximation accuracy in the four-dimensional space.

| Function $Y$          | Range       | $Y_{\text{min}}$ | $Y_{\text{max}}$ | $p$ | $\delta_{\text{avr}}$ | $\delta_{\text{min}}$ | $\delta_{\text{max}}$ |
|-----------------------|-------------|-------------------|-------------------|-----|-----------------------|-----------------------|-----------------------|
| $\sin(r)/r$           | $-2\pi : 2\pi$ | -0.2172          | 1                 | 5   | 0.0011                | -0.0029               | 0.0128                |
|                       |             |                   |                   | 7   | 0.0005                | -0.0012               | 0.0059                |
| $x_1^2 + x_2^2 + x_3^2 + x_4^2$ | $-2 : 2$   | 0                 | 8                 | 5   | 0.0053                | -0.0218               | 0.0102                |
|                       |             |                   |                   | 7   | 0.0013                | -0.0017               | 0.0014                |
| $(x_1 \cdot x_2 \cdot x_3 \cdot x_4)^2$ | $-2 : 2$   | 0                 | 256               | 5   | 0.0076                | -0.2491               | 0.1161                |
|                       |             |                   |                   | 5   | 0.0017                | -0.0191               | 0.0102                |
| $x_1 \cdot x_2 \cdot x_3 \cdot x_4$          | $-2 : 2$   | -16               | 16                | 5   | 0.0014                | -0.0180               | 0.0180                |
|                       |             |                   |                   | 7   | 0.0001                | -0.0017               | 0.0017                |

### 6 Summary and conclusions

A new method of the smooth approximation of a function defined on a sample of points in a multidimensional space is proposed. The folding of the discrete data points using the Gauss-Hermite method of Strutinsky is performed. Depending on the width of the Gauss function the folded function can be very close to the approximated data or can give its average behavior only.

The folded function and all its derivatives are continuous. This significantly increases the range of applicability of the method. Our approximation of the discrete data can be used e.g. when solving transport equations or other type of equations of motion in a multidimensional space, what is a frequent problem in economy, meteorology and environment protection problems as well as in molecular or nuclear dynamics.

The proposed approximation of the data can be also used in the computer graphic art. It can wash out the fine structure from a photography keeping unchanged its average background. One can also think about the use of the new folding method when one evaluates the cross-sections of a multidimensional data which one has e.g. in the X-ray tomography.

### References

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7 Appendix

The source of the fortran program for the 2nd order Gauss-Hermite approximation:

```
ghost.f
C--- The 2nd order Gauss-Hermite folding (a la V.M. Strutinsky) of a function
C defined on a sample of equidistant points in the n-dimensional space
C-------------------------------------------------------------------------
C
C subroutine ghost(nna,npts,xdn,dx,y,yref,gamma,x,fun,dfun)
parameter (ndim=4,id=2,nid=2*id+1)
dimension y(npts),xdn(ndim),dx(ndim),x(ndim),dfun(ndim),nna(ndim)
C C The data points which should be approximated by the function fun(x) have
C to be stored in the main program as the n-dimensional array:
C dimension y(nna(1),nna(2),...,nna(ndim)),
C where nna(i) is the number of points related to the x_i coordinate.
C The total number of points in y is npts=nna(1)*nna(2)*...*nna(ndim).
C The equidistant grid beginning at xdn(i) with step dx(i) is assumed
C for each coordinate. The value and gradient of the approximated function
C in the the point x(ndim) are stored in fun and dfun respectively.
C REMARK: In order to increase the accuracy of the approximation one
C preforms the folding of the differences y(i)-yref, where yref is the
C function value around which the approximation should be the best.
C A reasonable choice of yref is the average of the input points i.e.
C yref=(sum y(i))/npts. The folding is performed using 2*id+1 points
C closest to point x in each direction and gamma is the smearing width.
C (C) Copr. 2004 Krzysztof Pomorski, email: pomorski@kf.umcs.lublin.pl
C
dimension f(ndim,nid),df(ndim,nid),fdf(ndim),ni(ndim),nnn(ndim)
gami=1./gamma
fun=0.
nnn(1)=1
do 2 i=1,ndim
dfun(i)=0.
   if(i.gt.1) nnn(i)=nnn(i-1)*nna(i-1)
   xx=(x(i)-xdn(i))/dx(i)+1.
   ni(i)=int(xx+0.5)
   fnorm=0.
do 1 j=1,nid
t=gami*(xx-(ni(i)+j-id-1))
gauss=exp(-t**2)
f(i,j)=gami*gauss*(1.5-t**2)
   fnorm=fnorm+f(i,j)
do 2 j=1,nid
   f(i,j)=f(i,j)/fnorm
   df(i,j)=gami**2*gauss*(2.*t**3-5.*t)/dx(i)
do 2 j=1,nid
   f(i,j)=f(i,j)/fnorm
   nbox=nid**ndim
   do 6 k=1,nbox
      l=1
      ff=1.
do 3 m=1,ndim
         icur=k-l
         nn=nid***(ndim-1)
do 5 i=nn,m-1,-1
            j=icur/nn+1
            ff=ff*f(i,j)
do 5
   do 6 k=1,ndim
      do 4 i=1,ndim
         if(m.eq.i) dfdf(m)=dfdf(m)+df(i,j)
do 4
      do 4 i=1,ndim
         if(m.ne.i) dfdf(m)=dfdf(m)+f(i,j)*
            min(nna(i),max(l,ni(i)+j-id-1))-1
      icur=icur-(j-1)*nn
   do 6
   fun=fun+(y(l)-yref)*ff
   do 6 m=1,ndim
   dfun(m)=dfun(m)+(y(l)-yref)*dfdf(m)
fun=fun+yref
return
end
```