Project: Integration in two dimensions - calculations of electrostatic interaction

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1 Introduction

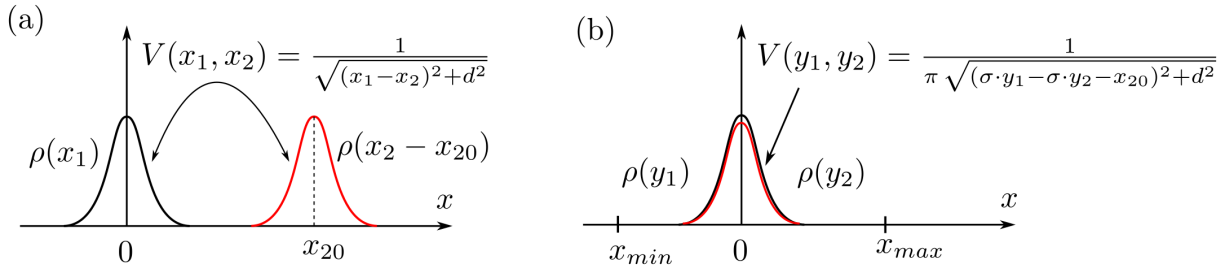

Figure 1: Positions of two gaussian-type densities in real space (a) and after changing the variables (b). The points x_{min} and x_{max} in (b) mark the boundaries of integration interval used for Legendre quadrature.

Two one-dimensional charged particles interact electrostatically. The charge densities are defined as gaussians

$$\rho(x_1) = \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{x_1^2}{\sigma^2}} \tag{1}$$

$$\rho(x_2) = \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{(x_2-x_{20})^2}{\sigma^2}} \tag{2}$$

where σ is the width of gaussians, x_1 and x_2 are the individual positions of particles and x_{20} is the distance of second particle from the origin of coordinate system. Interaction potential is modelled by following expression

$$V(x_1,x_2) = V(|x_1-x_2|) = \frac{1}{\sqrt{(x_1-x_2)^2+d^2}} \tag{3}$$

where: d is a scaling factor removing singularity.
Our task is to calculate the total electrostatic interaction energy, for this purpose we define an integral

$$C = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\, \rho(x_1)\rho(x_2)V(x_1,x_2) \tag{4}$$

$$= \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\, \frac{e^{-\frac{x_1^2}{\sigma^2}} e^{-\frac{(x_2-x_{20})^2}{\sigma^2}}}{\sqrt{(x_1-x_2)^2+d^2}} \tag{5}$$

At first look one may recognize the composition of two integrals with gaussians as weighting functions suggesting the use of Hermite quadratures in numerical calculations. However, before it happens we

must "fit" the weighting functions to the standard form, at present both exponents are scaled and the second one is also shifted. To get rid of these obstacles we first change the variables $(x_1, x_2) \to (y_1, y_2)$

$$\begin{cases} y_1 = \frac{x_1}{\sigma} \\ y_2 = \frac{x_2 - x_{20}}{\sigma} \end{cases} \implies \begin{cases} x_1 = \sigma y_1 \\ x_2 = \sigma y_2 + x_{20} \end{cases} \implies \begin{cases} dx_1 = \sigma dy_1 \\ dx_2 = \sigma dy_2 \end{cases} \tag{6}$$

Now we may transform the integral replacing the old variables with new ones

$$C = \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \, e^{-y_1^2} e^{-y_2^2} \frac{1}{\pi\sqrt{(\sigma \cdot y_1 - \sigma \cdot y_2 - x_{20})^2 + d^2}} \tag{7}$$

Quick analysis of the product of functions appearing in this double-integral tells us that now two gaussian-like densities are centered at the same point $y_1 = y_2 = 0$ but their interaction was rescaled. This case is shown in figure 1(b).
To make the equation 7 more transparent we rewrite it in a more general form

$$C = \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \, w(y_1) \, w(y_2) \, f(y_1, y_2) \tag{8}$$

$$w(y_1) = e^{-y_1^2} \tag{9}$$

$$w(y_2) = e^{-y_2^2} \tag{10}$$

$$f(y_1, y_2) = \frac{1}{\pi\sqrt{(\sigma \cdot y_1 - \sigma \cdot y_2 - x_{20})^2 + d^2}} \tag{11}$$

Now we are ready to replace the integral Eq.8 with compositon of two one-dimensional quadratures

$$S = \sum_{i_1=0}^{n_1-1} \sum_{i_2=0}^{n_2-1} A_{i_1} A_{i_2} f_{i_1,i_2} \tag{12}$$

where: n_1 and n_2 are the numbers of integration nodes, A_{i_1} and A_{i_2} are the weights of quadratures and $f_{i_1,i_2} = f(y_{i_1}, y_{i_2})$, indices 1 and 2 symbolize the particles. Since both integrals in Eq.8 cover the same interval $(-\infty, \infty)$ as well as the weighting functions defined in Eqs. 9 and 10 are the same, we notice that we may use the same sequence of Gauss-Hermite nodes and weights in both quadratures (Eq.12). Moreover, by inspecting Fig.1(b) we may conclude that limitation the integration interval width from infinite $(-\infty, \infty)$ to a finite one (x_{min}, x_{max}), provided that the weighting functions vanishes at the new boundaries, we might use the Gauss-Legendre quadrature as well.

2 Practical part

1. Write a computer program which will calcluate the potential interaction utilizing the two-dimensional quadrature given in Eq.12 with Gauss-Hermite and Gauss-Legendre nodes and weights. You may obtain the nodes and weights by using the routine **gauss_nodes_weights.c**. In calculations assume following parameters: $\sigma = 2$, $d = 0.5$, $x_{20} = 2$, $n_1 = n_2 = n$, $x_{min} = -5$, $x_{max} = 5$. Use the same sequence of nodes and weights for both directions.
2. Calculate the integral for different number of nodes $n = 1, 2, 3, \ldots, 100$. Write data to file and prepare the figure showing the dependence of integral's value on the number of nodes $C(n)$ for Gauss-Hermite and Gauss-Legendre quadratures. Prepare additional figure showing the dependence of $|C(n) - C(n-1)|$ (obviously start from $n = 2$), use logharitmic scale for this difference.

3. For one of the Gauss-type quadratures of your choice fix the number of nodes which guarantees acceptable numerical convergence of integral's value, e.g. $n = 80$ and calculate the dependence of integral on the interparticle distance x_{20}. Scan the region $x_{20} \in [0.1, 40]$ with small step $\Delta x_{20} = 0.1$. Write data to file and prepare the figure showing dependence $C(x_{20})$, compare it with the Coulomb interaction $1/x_{20}$ of two point-like charges.

3 Computational hints

In project you may use the routine **gauss_nodes_weights.c** downloding it form module webpage

```
void gauss_nodes_weights(int k, int n, double *nodes, double *weights)
```

It provides the nodes and weights for Gauss-Legendre ($k = 0$), Gauss-Laguerre ($k = 1$) and Gauss-Hermite ($k = 2$) quadratures. For Gauss-Legendre it requires of passing the boundaries of interval $[a, b]$ in first two entries of array *nodes*: **nodes[0]=a** and **nodes[1]=b**, nodes and weights are automatically rescaled to fit this interval. Parameter **n** must be the same as the number of nodes/weights. Routine requires linking with **Lapacke** library, so compile it adding **-llapacke -lm**, the header **lapacke.h** is included in source file. Example of using the routine in **C**

```
int k,n;
double  *nodes,*weights;

nodes=(double*)malloc(n*sizeof(double));
weights=(double*)malloc(n*sizeof(double));

gauss_nodes_weights(k,n,nodes,weights);

>>>>>>>  calculations   <<<<<<<<<<<<<<<<<<<

free(nodes);
free(weights);
```

and in **C++** with vectors

```
int k,n;
vector<double> nodes(n);
vector<double> weights(n);

gauss_nodes_weights(k,n,&nodes[0], &weights[0]);

>>>>>>>  calculations   <<<<<<<<<<<<<<<<<<<
```

4 Example results

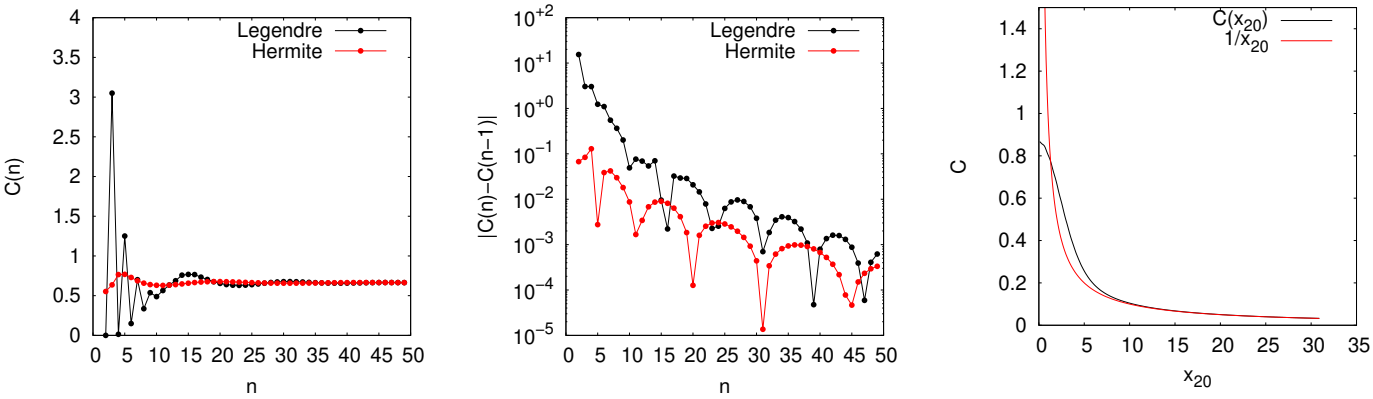

Figure 2: (left) Dependence of interaction potential calculated with Legendre and Hermite quadratures on number of nodes in one-dimensional quadrature, and, (middle) corresponding difference $|C(n) - C(n-1)|$. (right) Dependence of calculated interaction potential between two gaussian-type densities (black) and Coulomb potential of two point-like charges (red) on the distance between centers of densities $C(x_{20})$.