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Algorithms of Scientific Computing II

Exercise 4 - Methods for Long-Range Potentials

1) Error estimation

In this exercise we want to analyse the error in the calculation of long-range potentials with the tree methods from the lecture. Assume, that the kernel G of the potential Φ behaves like a $\frac{1}{r}$-potential.

In the lecture it was stated, that the relative local approximation error in the calculation of Φ is $O(\theta^{p+1})$. Prove that!

Use the θ-criterion from the lecture:

$$\frac{diam}{\|x - y_0^\nu\|} \leq \theta$$

ANSWER:

A few foregoing considerations: For the infimum of the kernel (for a given x choose y so that the kernel is minimized) and the supremum of the $(p+1)$-th derivative we use the following abbreviations:

$$g_{min}^\nu(x) = \inf_{y \in \Omega_\nu} G(x,y) \tag{1}$$

$$g_{max}^{\nu,p+1}(x) = \sup_{y \in \Omega_\nu} \max_{\|j\|_1 = p+1} \frac{1}{j!} |G_{0,j}(x,y)| \tag{2}$$

The potential considered behaves like $\frac{1}{r}$. So there are constants c_1 and c_2 for which holds:

$$c_1 \cdot \frac{1}{\|x-y\|} \leq G(x,y) \tag{3}$$

$$c_2 \cdot \frac{1}{\|x-y\|^{\|j\|_1+1}} \geq |G_{0,j}(x,y)| \tag{4}$$

In the following we want to substitute y by y_0 in the left sides of the inequations. With the theta-criterion and the triangle inequation we can deduce the following correlation:

$$\frac{1}{\|x-y\|} \geq \frac{1}{\|x-y_o^\nu\| + \|y_o^\nu - y\|} \geq \frac{1}{\|x-y_o^\nu\| + \theta\|x-y_o^\nu\|} = \frac{1}{1+\theta} \cdot \frac{1}{\|x-y_o^\nu\|}$$

With (3) follows:

$$c_1 \cdot \frac{1}{(1+\theta)\|x-y_o^\nu\|} \quad \leq \quad G(x,y)$$

As the left side of the inequation does not depent on y any more, the kernel function on the right side can be substituted by the kernel function for an arbitrary y (as the inequation holds for all y). Thus, we substitute $G(x,y)$ in the right side by $g_{min}^\nu(x)$:

$$c_1 \cdot \frac{1}{(1+\theta)\|x-y_o^\nu\|} \quad \leq \quad g_{min}^\nu(x) \tag{5}$$

Analogously we can deal with inequation (4). In the first step we use the reverse triangle inequality (for a triangle with edges a, b and c holds: $a \geq b - c$, thus $\frac{1}{a} \leq \frac{1}{b-c}$):

$$\frac{1}{\|x-y\|} \leq \frac{1}{\|x-y_o^\nu\| - \|y_o^\nu - y\|} \leq \frac{1}{\|x-y_o^\nu\| - \theta\|x-y_o^\nu\|} = \frac{1}{1-\theta} \cdot \frac{1}{\|x-y_o^\nu\|}$$

$$c_2 \cdot \frac{1}{(1-\theta)^{\|j\|_1+1}\|x-y_o^\nu\|^{\|j\|_1+1}} \quad \geq \quad G(x,y)$$

$$c_2 \cdot \frac{1}{(1-\theta)^{p+2}\|x-y_o^\nu\|^{p+2}} \quad \geq \quad g_{max}^{\nu,p+1}(x) \tag{6}$$

These considerations lead to approximations for $g_{min}^\nu(x)$ and $g_{max}^{\nu,p+1}$. They will be used later on.

For the estimation of the error we start with the potential. The formula for the potential governing a domain Ω_ν with respect to a point x reads:

$$\Phi_\nu(x) = \int_{\Omega_\nu} G(x,y)\rho(y)dy \tag{7}$$

In the lecture the taylor series for the kernel has been shown:

$$G(x,y) = \sum_{\|j\|_1 \leq p} \frac{1}{j!} G_{0,j}(x,y_0)(y-y_0)^j + R_p(x,y) \tag{8}$$

The remainder term of the kernel $R_p(x,y)$ can be estimated with the lagrangian form:

$$R_p(x,y) = \sum_{\|j\|_1 = p+1} \frac{1}{j!} G_{0,j}(x, y_0 + \xi(y-y_0))(y-y_0)^j \tag{9}$$

Thereby it holds: $0 \leq \xi \leq 1$ With (9), (8) and (7) follows for the absolute error of the calculation of the potential

$$e_\nu^{abs}(x) = \int_{\Omega_\nu} \rho(y) \sum_{\|j\|_1 = p+1} \frac{1}{j!} G_{0,j}(x, y_0 + \xi(y-y_0))(y-y_0)^j dy \tag{10}$$

The relative error corresponds to the absolute error (10) divided by the potential (7):

$$\begin{aligned} e_\nu^{rel}(x) &= \frac{e_\nu^{abs}(x)}{\Phi_\nu(x)} \\ &= \frac{\int_{\Omega_\nu} \rho(x) \sum_{\|j\|_1 = p+1} \frac{1}{j!} G_{0,j}(x, y_0 + \xi(y-y_0))(y-y_0)^j dy}{\int_{\Omega_\nu} G(x,y)\rho(y)dy} \end{aligned}$$

For a positive ρ and positive kernel with (1) and (2) follows:

$$\begin{aligned} e_\nu^{rel}(x) &\leq \frac{\int_{\Omega_\nu} \rho(y) \sum_{\|j\|_1 = p+1} \frac{1}{j!} |G_{0,j}(x, y_0 + \xi(y-y_0))| \cdot |(y-y_0)^j| dy}{\int_{\Omega_\nu} G(x,y)\rho(y)dy} \\ &\leq c \cdot \frac{g_{max}^{\nu,p+1}(x) \cdot diam^{p+1}}{g_{min}^{\nu}(x)} \end{aligned}$$

Inserting estimations (5) and (6) gives us:

$$\begin{aligned} e_\nu^{rel}(x) &\leq c \cdot \frac{(1+\theta)\|x - y_o^\nu\| \cdot diam^{p+1}}{(1-\theta)^{p+2}\|x - y_o^\nu\|^{p+2}} \\ &= c \cdot \frac{(1+\theta)}{(1-\theta)^{p+2}} \cdot \left(\frac{diam}{\|x - y_o^\nu\|^{p+1}} \right)^{p+1} \\ &\leq c \cdot \frac{(1+\theta)}{(1-\theta)^{p+2}} \cdot \theta^{p+1} \end{aligned}$$

If we assume that θ is very small, $(1+\theta)$ and $(1-\theta)$ approach 1:

$$e_\nu^{rel}(x) \quad \leq \quad c \cdot \theta^{p+1}$$

2) Complexity of the Barnes-Hut-Method

In the lecture the costs for the d-dimensional Barnes-Hut-Method were given as $O(\theta^{-d} N log N)$. First derive the costs for the twodimensional Barnes-Hut-Method. Then explain descriptively (without proof), why the formula is also correct for 3d.

ANSWER:

The "outer loop" of the Barnes-Hut-algorithm iterates over all particles and calculates the force effective on every particle. As there are N particles in total, for each of those particles the costs have to be $O(\theta^{-d} \cdot log\ N)$. For the given complexity of $O(\theta^{-d} \cdot N \cdot log\ N)$ we assume that the tree is not degenerated, thus the tree has $O(log\ N)$ levels. If we can show, that at each level the costs are $O(\theta^{-d})$, the formula is proven valid.

We start out from the twodimensional case. First we consider an arbitrary level and determine the number of nodes (i.e. particles of pseude-particles) we have to consider.Those are exactly the nodes for which the parent node didn't fulfill the θ-criterion. For the parent node it has to hold:

$\frac{diam}{|distance|} > \theta$. Thus it follows for the distance:

$$|distance| < \frac{diam}{\theta} \tag{11}$$

We will now try to determine an upper bound for the number of parent cells which fulfill that condition. Therefor we consider only one coordinate axis first.

Not considering the absolute value, (11) can be rewritten as $-\frac{diam}{\theta} < distance < \frac{diam}{\theta}$. Thus the "area" of the distance is $2 \cdot \frac{diam}{\theta}$. As one node coveres an area with the diameter $diam$ there can be only

$$\frac{2 \cdot \frac{diam}{\theta}}{diam} = \frac{2}{\theta}$$

nodes next to each other, for which the θ-criterion does not hold. In the second axis there are just as many. Thus there are

$$\left(\frac{2}{\theta}\right)^2 = 4 \cdot \theta^{-2}$$

nodes in total, which don't fulfill the θ-criterion. Those are the parent nodes we have to consider at the current level. That number still has to be multiplied by 4, what doesn't change the order.

Thus the maximum computational costs on each level are $O(\theta^{-2})$. As there area $log\ N$ levels in total and N particles, the total computational costs sum up to $O(\theta^{-2} \cdot N \cdot log\ N)$.

For three dimensions it is easy to see that there are not $c \cdot \theta^{-2}$ any more for which the θ-criterion is fulfilled, but only $c \cdot \theta^{-3}$, as we are dealing now with a cubic area.