Simulations on the Sphere: Distribution of Points and Calculations of Energy

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1. Introduction

1.1. Definitions

1) An arrangement of n points on the sphere has the *maximum property* if the minimal distance between any two points of the set is maximal.
2) If n points are placed on a sphere and moreover a force is assumed to act according to a certain law one can consider equilibrium configurations or stable equilibria only. If this happens we shall call the arrangement of n points an *equilibrium configuration.*

1.2. Questions

1) Suppose the vertices of a platonic solid are placed on the unit sphere. Does this provide an example of an arrangement with
   - the maximum property or
   - an equilibrium configuration?
2) In what way do specific force laws give rise to different equilibrium configurations?

2. Methods

All our results are based on two types of simulations.

- Stochastic simulation: the points on the sphere are subject to random displacements and the evolution towards a desired optimum is controlled by selection. Clearly this idea is inspired by Darwinian Evolution. Figure 1 shows a typical process of the points trying to reach an optimized situation.
- Deterministic simulation: Chose some hypothetical repelling force acting between the points. Letting the points move we would expect that they end up in an equilibrium configuration. Our simulation is time discrete and in each one of the steps we chose a single point P_k, and determine the resulting force caused by all the other points P_i , $i \neq k$, at the given moment. The new position of P_k is now computed by applying a shift along the resulting force and projecting the end position back to the sphere. Figure 2 shows how the points move directly to their destination.

3. Experiences and results

Our experimental setup proved to be advantageous because the two independent methods allow cross validation of results. The deterministic simulation excels in runtime behaviour. Its drawback is the dependence on a specific physical law. In contrast, the selection criteria of the stochastic simulation may easily be adapted to various criteria. However the runtimes usually exceed the ones of the deterministic simulation.

3.1. Repelling springs and Hooke's law

We discovered the following surprising fact: An equilibrium position is attained if and only if the center of gravity of n points coincides with the center of the sphere. Moreover the resulting energy attains a maximum of size $2n^2$. For instance the platonic solids are equilibrium configurations but moving four of the vertices of a cube to the North Pole and four to the South Pole gives another equilibrium configuration. The deformation can be achieved in such a way, that the center of gravity stays at the center of the sphere. The conclusion is that in this case the energy of the configuration is not a suitable invariant for finding arrangements with the maximum property.

Using the Darwinian approach it became clear that the cube cannot satisfy the maximum property. Furthermore, it was doubtful whether the dodecahedron provided an arrangement with the maximum property. The investigation of this case prompted the next steps in our project.

- Definition of new invariants, e.g.
- Incidence matrix, distance matrix, eigenvalues
- Coulomb's law and potential
- total lengths of the edges using the convex hull
- convex hull
- surface and volume
- graphical display
- GUI (as shown in figure 3)

3.2. Experiences

Increasing the number of vertices, naturally leads to an increase in runtime. Our progress depended crucially on improvements of the runtime behaviour. Consequently, all our simulations were based on extremal energy criteria rather than the maximum property.
E.g. , the runtime for the convex hull operation grows with a power of four in the number of points. There only is an alternative, if the simulation optimize the point arrangement such a long time, that we expect a nearly perfect regular distribution, we are able to use another method to create the convex hull where the runtime grows only with a power of three.

3.3. Coulomb-Energy

The logic result would be such that the energy increases with amount of points and not visa versa. The deterministic simulation is based on the principle that the points repulse each other. A higher distance therefore leads to a smaller energy. One could imagine pressure springs between the points. To compute such a comparable value the elements of the distance matrix real edges exponentiate with factor -1. The energy-value is therefore higher with 2 points being positioned closed to each other compared to being far apart. This calculated value will be divided by the amount of edges of the figure for getting the Coulomb-Energy per edge. The Coulomb-Energy of the solids are visible in table 6.

3.4. Applications

It has definitely been disproved, that all the platonic solids (see picture 4) provide examples of maximum property. This can be proven by two examples, these are n=8 and n=20. By n=8 points the result of our simulations is not a platonic solid (a cube), it represents an antiprism based on two squares. The antiprism was already known to Rutishauser who found the example by elementary space geometry in 1945 [R]. While it was clear, that this configuration was superior to the cube, it remained open whether this example has the maximum property. This antiprism is shown in figure 5.

The second example is the dodecahedron. Both simulations done with 20 points don't result in the expected platonic solid; they result in a Polyeder, which consists of isosceles triangles. This solid is specifically interesting in relation to its energetic situation. With the, descript in chapter 4, energy measurement method Coulomb-energy for each edge, one realizes that the solid has compared with the dodecahedron a surplus in energy of 30%. The Polyeder has also an essential higher volume and a higher surface compared with the dodecahedron. See for more Details at figure 6.

3.5. Investigations on more ambitious cases, Fullerenes corresponding to C24, C60, C120.

None of C24, C60, C120 provides an optimum configuration for neither the Coulomb potential nor the maximum property. The C60 and the solid with the maximum property for n = 60 are compared in picture 7. We found that in each case triangles dominated the surface of the favourite solids. In the case of the cube and C24 quadrilaterals popped up on the surface of the best arrangements found by simulation: the previously mentioned antiprism based on two squares and a platonic involving six squares. Also solids with odd number of points are composed of triangles. These are shown in figure 8 to 11.

Other examples for configurations with maximum property but also containing quadrilaterals are figures with n = {40, 48}.

4. Discussion

Our method is based on floating point operations. Therefore the scope of our results is limited. We are able to disprove certain claims by computing counterexamples. However we cannot verify the maximum property nor any equilibrium configuration beyond the scope of numerical approximations.

5. Open Ends

An obvious generalization comes to mind: Instead of a sphere, any 2-surfaces could serve to contain a distribution of n points, and analogous questions could be asked. Placing dots on a torus, or even on the fur of a cheetah could be analyzed.

Both types of simulation could be adapted to deal with this more general setup. It then becomes essential to focus on two possible interpretations of our questions. The distance between 2 points could be measured along a straight line in R^3 or along a geodesic line on the surface itself. The case of the trefoil-knot might serve to illustrate the differences between the two ways of looking at the problem.

6. Final remarks

The collection of our Matlab programs forms a workbench which proved to be useful for experimental researches in our area of interests. The subject is an attractive one for young scientists because it leads to blend ideas from biology, physics, geometry, numeric, and computer science.

We wish to thank the foundation "Schweizer Jugend forscht", who delegated our project at the European Union Contest for Young Scientists, for helpful support and to the Kantonsschule Baden who built the base to work at such a project. We especially want to thank H.R. Schneebeli who supported us during the whole project and increased the quality of the work, as well the quality of the report dramatically.

7. Annex

7.1. The Step size control

In both simulations it is possible to control the step size by changing the value of a constant K. In the stochastic simulation the constant k is used to control the maximal possible random movement of a point in each step, while in the deterministic simulation the constant k controls the strength of the repelling force between the points.

The purpose of this chapter is to analyze the speed of the two simulations in reaching the target result, this being the best possible result and the timely dependency of reaching this target from the size of the constant k.

To be able to answer this question there has been a random distribution of points (4, 6 and 12). Both methods have than been optimized, by using different constants, until a previously required accuracy has been reached. This required accuracy represents the allowed tolerance of theoretically optimized distances. The steps to reach this defined accuracy were counted.

For more than 12 points, the calculation would be very time intensive and more complex. This based at the circumstances that the solids could have different distances. This is the reason that for this problem you will find only a few examples in the displayed results.

7.1.1. Efficiency of the deterministic simulation

The deterministic simulation has shown that, when using a bigger value of constant k, the defined result has been reached in less time. Table 1 displays the average number of required steps, when using the deterministic simulation with 4 points and a few different constants. This data is displayed in diagram 1 in such a way that the linear increase of the necessary steps is easily recognizably. As visualized in the table, constants of 1/25 require massively more steps. The diagram therefore only shows a maximum number of 100 steps.

By using a constant of 1000, the deterministic simulation reaches an accuracy of 99% with an average of 6 steps. Two additional steps have already drastically increased the accuracy by a factor 10. The result, when using 15 steps, has reached an accuracy of 6 positions behind the comma. The deterministic method is, when using such big constants, extremely efficient.

Applying constants such as K=10^6 or K=10^10 resulted in the same amount of steps as when using K=1000. For calculations with more than 60 points the constant should be reduced, to avoid extreme high movements initiated trough the strong repulsion of the many points.

With 12 points the deterministic simulation takes slightly longer. Table 2 shows the necessary steps to reach an accuracy of 10^-2 to 10^-6.
It shows that there is an increase in steps, the calculation time however is still well below one second.

The data in table 1 as well in table 2 shows that the number of steps is proportional to the logarithm of the increase of accuracy. This characteristic is extremely helpful trough to the fact that a massive increase in accuracy not necessary lead to a higher computing time.

7.1.2. Efficiency of the stochastic simulation

The number of the selected constant is much more decisive when using the stochastic simulation compared to the deterministic one. Table 3 shows the amount of steps for 4 points and different constants to reach a defined accuracy.

"XXX" represents the fact, that the simulation hasn't been able to compute a result with the required accuracy and not exceeding 10^5 steps. For 4 points it seems that a constant in the area of 1/25 is most ideal to reach an accuracy of 99%. A higher accuracy would anyway not be recognizable by the human eye. For reaching a higher accuracy a smaller constant must be chosen. Most ideal would be a continued adoption of the constant to the accuracy of the current distances between the points. In generally it's visible that the necessary number of steps to reach e certain accuracy proceeds highly exponential. Another remark is that the stochastic simulation is controlled randomly and does lead to some diffusion. Table 4 shows the number of required steps when applying 12 points.

Interesting is the fact, that it requires less steps when using a constant of 1/625 with a reduced accuracy, compared to 4 points. Three times more points need nevertheless around the same amount of steps. The stochastic simulation does require a higher computing time compare to the deterministic simulation. This however could change when using high numbers of points with a high accuracy, the stochastic approach would than become more efficient. To prove such would require further researches and a lot of computing power.

7.2. The n^2-law

The first analyses of the results have shown the following: If all distances between all points are squared and summarized, this than reflects the conclusion of the number of points to be squared.

$$\sum_{j \neq i}^{n} \| \vec{P_i} - \vec{P_j} \|^2 = 2n^2$$

This characteristic goes for all possible dimensions as long the center of gravity of the figure is positioned on the zero point.

$$\| \vec{Z_k} \| = 1$$

$$\vec{Z_1} = \vec{e} = [0|0|1]$$

$$\sum_{j=1}^{n} \vec{Z_j} = \vec{0}$$

$$\sum_{k=1}^{n} \| \vec{Z_k} - \vec{e} \|^2 = \sum_{k=1}^{n} ((\vec{Z_k} - \vec{e}) \cdot (\vec{Z_k} - \vec{e}))$$

$$\Rightarrow \underbrace{\sum_{k=1}^{n} \| \vec{Z_k} - \vec{e} \|^2}_{n} - 2\vec{e} * (\underbrace{\sum_{k=1}^{n} (\vec{Z_k})}_{0} + \underbrace{\sum_{k=1}^{n} (1)}_{n}) = 2n$$

The sum of the distance between and the North Pole $\vec{e}$ and all other $n-1$ points does also result in $2n$. The distances of the other points need to be included resulting in $n * 2n = 2n^2$. This result must be divided by factor 2 since each distance has been accounted for twice, first from P_k to P_i and second from P_i to P_k. Therefore it remains n^2.

The following is the proof that the n^2-law is accurate for figures for which the center of gravity is positioned zero point.

$$\sum_{i=1}^{n}(\sum_{k=1}^{n} \| \overrightarrow{Z_k} - \overrightarrow{Z_i} \|^2) = 2n^2 - 2\underbrace{(\sum_{i=1}^{n} \overrightarrow{Z_i})}_{\vec{s}} \cdot \underbrace{(\sum_{k=1}^{n} \overrightarrow{Z_i})}_{\vec{s}}$$

For simplification $\sum_{i=1}^{n}(\overrightarrow{Z_i})$ abbreviated with $\vec{s}$. $\| \vec{s} \|$ must be positive and additional a conclusion of the above result is:

$$2n^2 - 2 * \| \vec{s} \|^2 \leq 2n^2$$

This goes for all possible figures with n points on the unit sphere. When the sum of the squares of all distances between all points should equal exactly $2n^2$, also $2n^2 - 2 * \| \vec{s} \|^2 = 2n^2$ s must equal 0, also $\sum_{i=1}^{n}(\overrightarrow{Z_i}) = \vec{0}$.
Or expressed differently the sum of all position vectors to the points must result in the zero vector that means the center of gravity of this figure must be positioned in the zero point.

7.3. Surface and Volume

The value of the surface and the volume of a solid seem to be an ideal invariance. The higher the value the more optimal is the distribution of the points. The higher the number of points, the surface and the volume between these points approach the value of the unit sphere (4*pi respectively 4/3*pi). The surface and volume for some examples is entered in table 5. This data includes the percentage portion of the unit sphere. The value of the surface divided with the volume results in a value which displays the enclosed volume of the associated surface. For the sphere this value would be exactly 3 and the more a Polyeder resembles a sphere the value decreases to 3.

7.4. Higher exponents

The simulation also has been run with other formula than the Coulomb-law. But the simulation never got a plausible result whereby there were no further investigations in this affair.

7.5. Graphical display

The simulations give us the coordinates of the results but it is nearly impossible to analyse the figures without a graphical output as well. With the help of the plot-command [H] in Matlab the points can be visualized and another program builds a sphere. This sphere is visualized by showing 8 lines of latitude, the equator, and the 0° meridian.

To get a better overview over the points, the configuration gets moved around the z- and the y- axis, in such a way that moves one point to [0|0|1]. After that, the configuration gets moved around the z-axis, to have a second point lying on the x-z-layer. With this procedure, we can make sure that same configurations result in the same graphical output.

7.6. Subprograms

These subprograms were a part of the simulations to overtake some functions.

Subprogram	Input	Output
Abst	Point, distribution configuration	Sum of the distances of the point to the points of the distribution configuration
Pnet	Distribution configuration	Incidence matrix
Pnet2	Regular distribution matrix	Incidence matrix
Dmat	Distribution configuration	Distance matrix
Rot3	Distribution configuration	Turned distribution matrix, with point 1 on the North pole and point 2 at the prime meridian
Dpyr	Number of points	Distribution configuration with points 1 and 2 on the North and South pole and the other ones regular on the equator.
Diag0	Distance matrix	Distance matrix where the diagonal is set to zero.
Pweg	Number of points	Way coordinates of the points on their way from their start to the target.
Surf2	Distribution configuration	The surface of the solid
Vol	Distribution configuration	The volume of the solid
Kugel2	Void	Creates s window with a sphere, where the solids can be drawn.
Show	Distribution configuration	Shows the points of the distribution configuration in a 3D coordinate system.
Name	Distribution configuration	Set the number of the points of the distribution configuration in a 3D coordinate system at their positions.
Cnct	Incidence matrix, distribution configuration	Connects the points of the distribution matrix related to the incidence matrix.
Hull	Incidence matrix, distribution configuration	Interpolates the points of the distribution matrix related to the incidence matrix with triangles.

8. Sources

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