NATIONAL AND KAPODISTRIAN UNIVERSITY OF ATHENS

School of Science

Information Technologies in Medicine and Biology

Direction: *Bioinformatics*

Algorithms in Structural Bioinformatics

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Deadline Date: *02/04/2013*
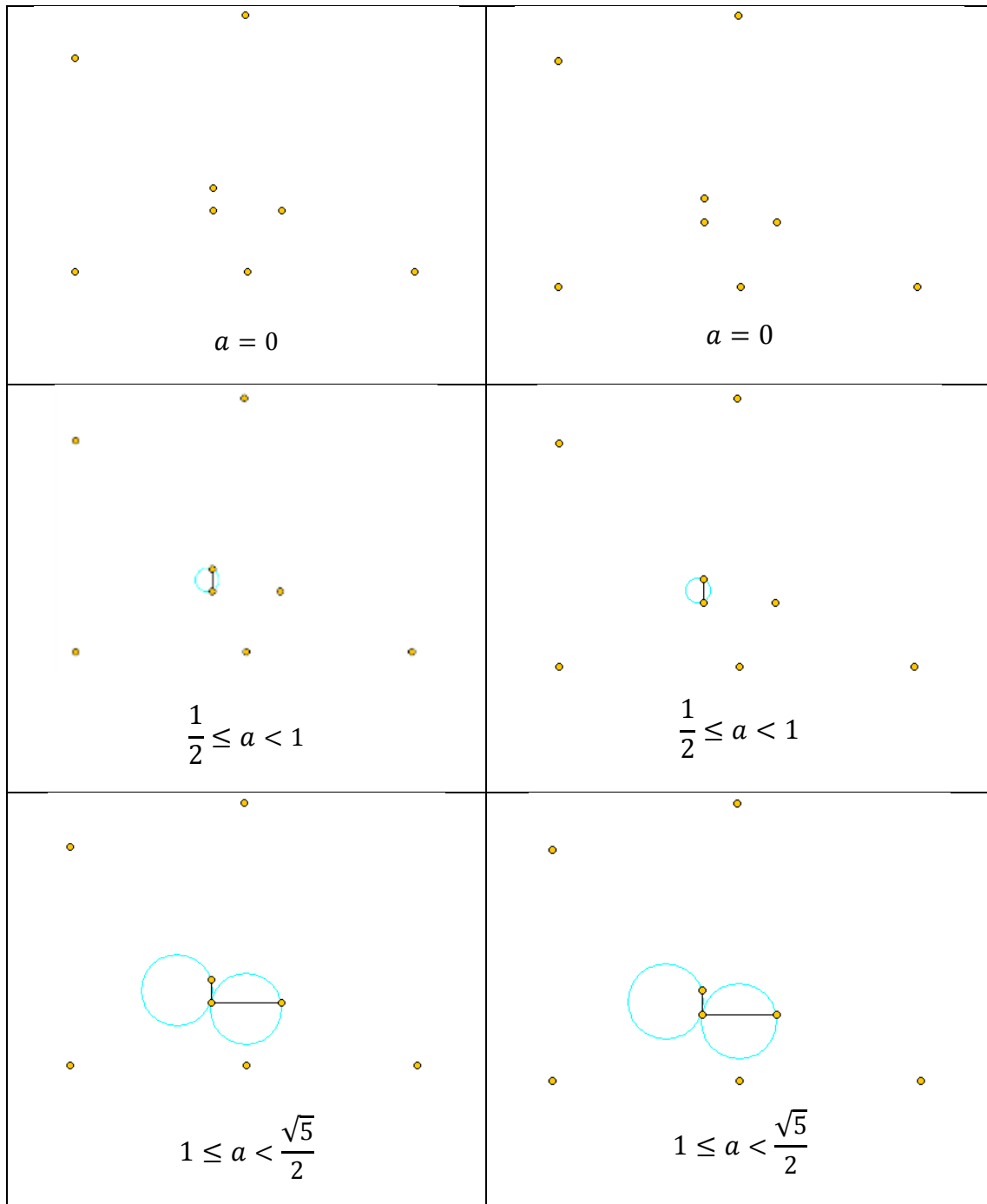
Assignment 4

1. Structural alignment

In this assignment we were asked, given 8 points: (O=(0,0), A=(4,0), B=(3,2), C=(3,3), D=(0,6), E=(4,7), F=(8,0), G=(5,2), to compute the α-shape S_α and the α-complex C_α, as α takes values from 0 to +∞, and indicate the values of α where S_α and C_α change.
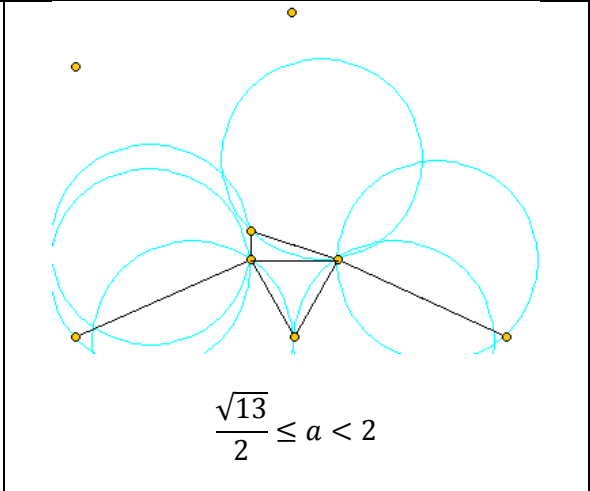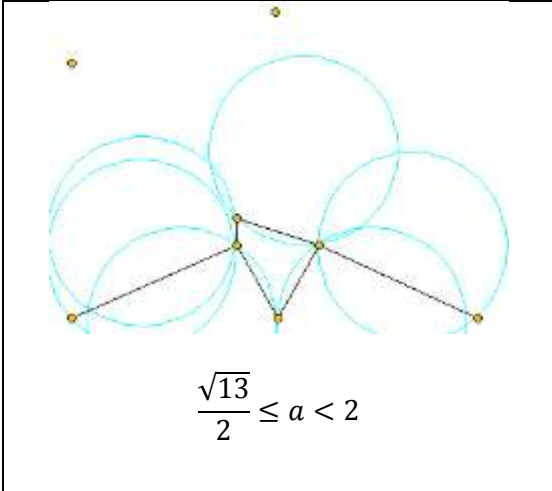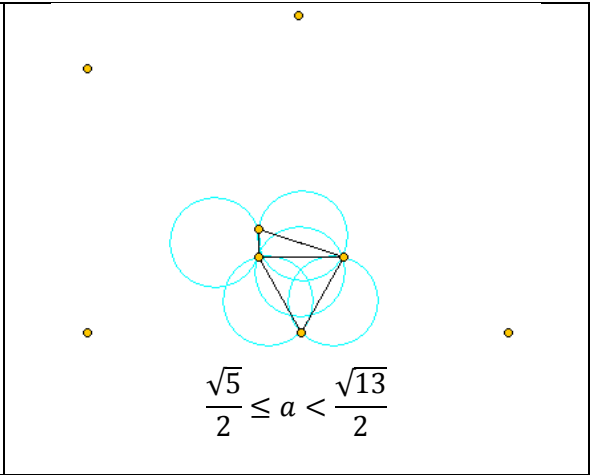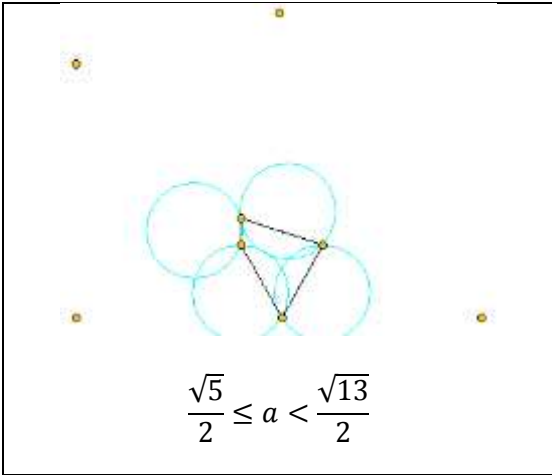
We implemented a C++ program that does this for us and we ran it several times with different α values and each time we noticed the changes from between **edges-facets** and **facets-tetrahedra**. When an alteration happened we notice and keep the value of α.

The final results we concluded in are indicated below and are found in the regions of interest (interval ends) where an alteration in complex occurs:
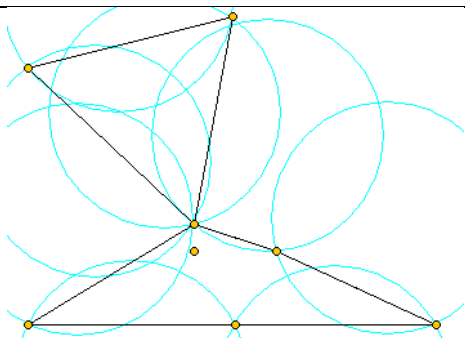
1) $a = 0$
2) $\frac{1}{2} \leq a < 1$
3) $1 \leq a < \frac{\sqrt{5}}{2}$
4) $\frac{\sqrt{5}}{2} \leq a < \frac{\sqrt{13}}{2}$
5) $\frac{\sqrt{13}}{2} \leq a < 2$
6) $2 \leq a < \frac{\sqrt{17}}{2}$
7) $\frac{\sqrt{17}}{2} \leq a < \frac{\sqrt{18}}{2}$
8) $\frac{\sqrt{18}}{2} \leq a < \frac{\sqrt{26}}{2}$
9) $\frac{\sqrt{26}}{2} \leq a < \frac{\sqrt{36}}{2}$
10) $\frac{\sqrt{36}}{2} \leq a < \frac{\sqrt{65}}{2}$
11) $a \geq \frac{\sqrt{65}}{2}$

Additionally to the above, we now extended the exercise using the GUI implementation Applet in Java so that to provide some images too, and not only the above results. The results given from the Applet are shown below:
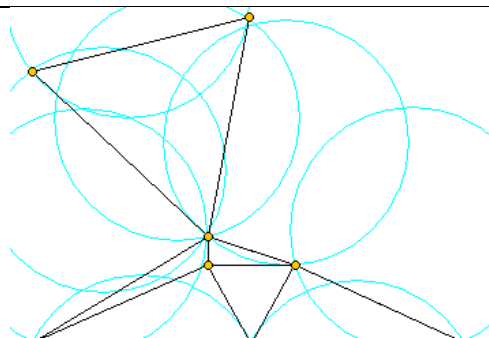
$a = 0$	$a = 0$
$\dfrac{1}{2} \leq a < 1$	$\dfrac{1}{2} \leq a < 1$
$1 \leq a < \dfrac{\sqrt{5}}{2}$	$1 \leq a < \dfrac{\sqrt{5}}{2}$

$$\frac{\sqrt{5}}{2} \le a < \frac{\sqrt{13}}{2}$$
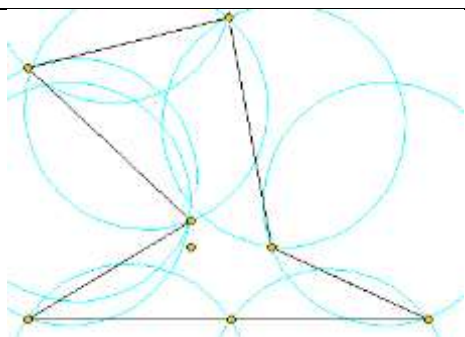
$$\frac{\sqrt{5}}{2} \le a < \frac{\sqrt{13}}{2}$$

$$\frac{\sqrt{13}}{2} \le a < 2$$

$$\frac{\sqrt{13}}{2} \le a < 2$$

$$2 \le a < \frac{\sqrt{17}}{2}$$

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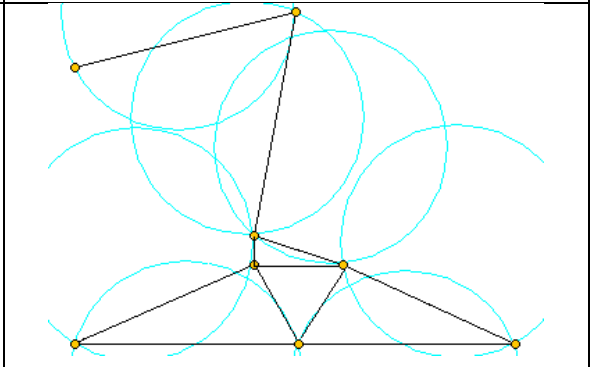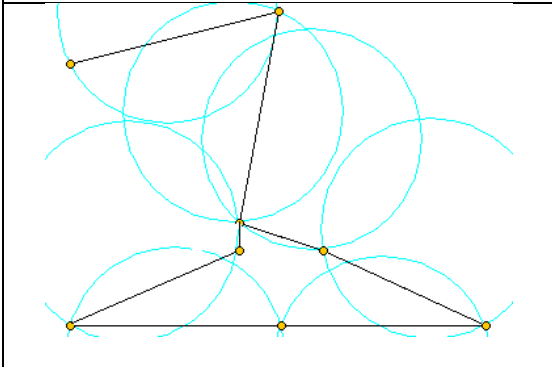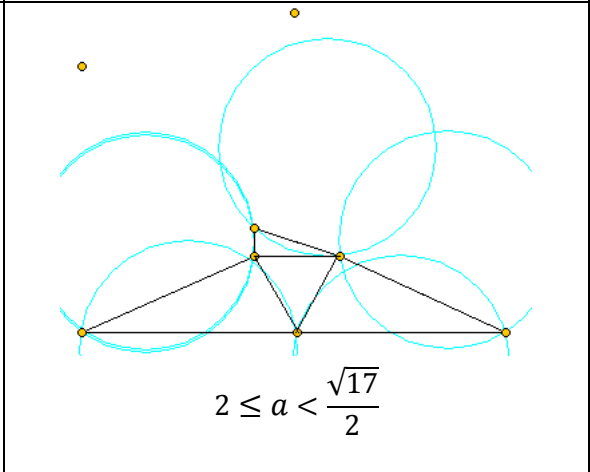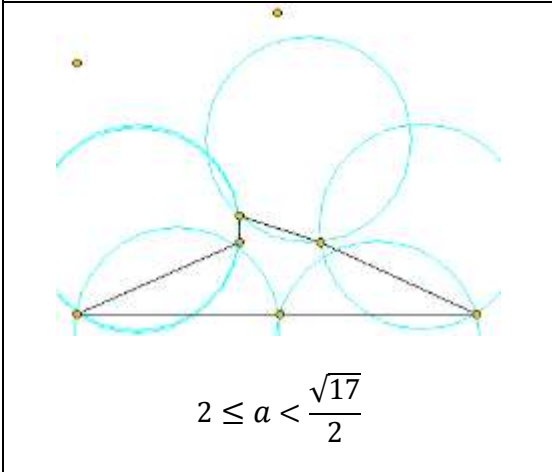
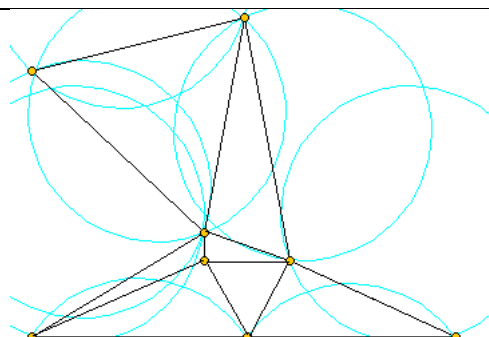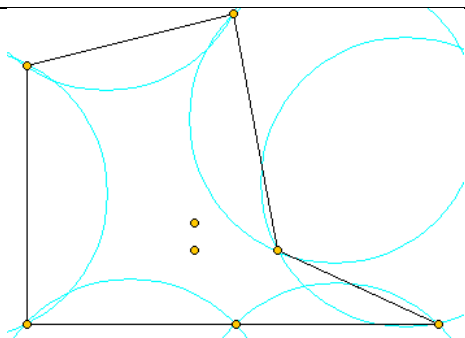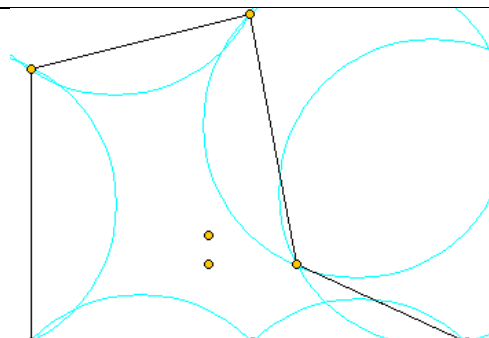| $\dfrac{\sqrt{17}}{2} \leq a < \dfrac{\sqrt{18}}{2}$	$\dfrac{\sqrt{17}}{2} \leq a < \dfrac{\sqrt{18}}{2}$
$\dfrac{\sqrt{18}}{2} \leq a < \dfrac{\sqrt{26}}{2}$	$\dfrac{\sqrt{18}}{2} \leq a < \dfrac{\sqrt{26}}{2}$
$\dfrac{\sqrt{26}}{2} \leq a < \dfrac{\sqrt{36}}{2}$	$\dfrac{\sqrt{26}}{2} \leq a < \dfrac{\sqrt{36}}{2}$
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$$a \geq \frac{\sqrt{65}}{2}$$

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