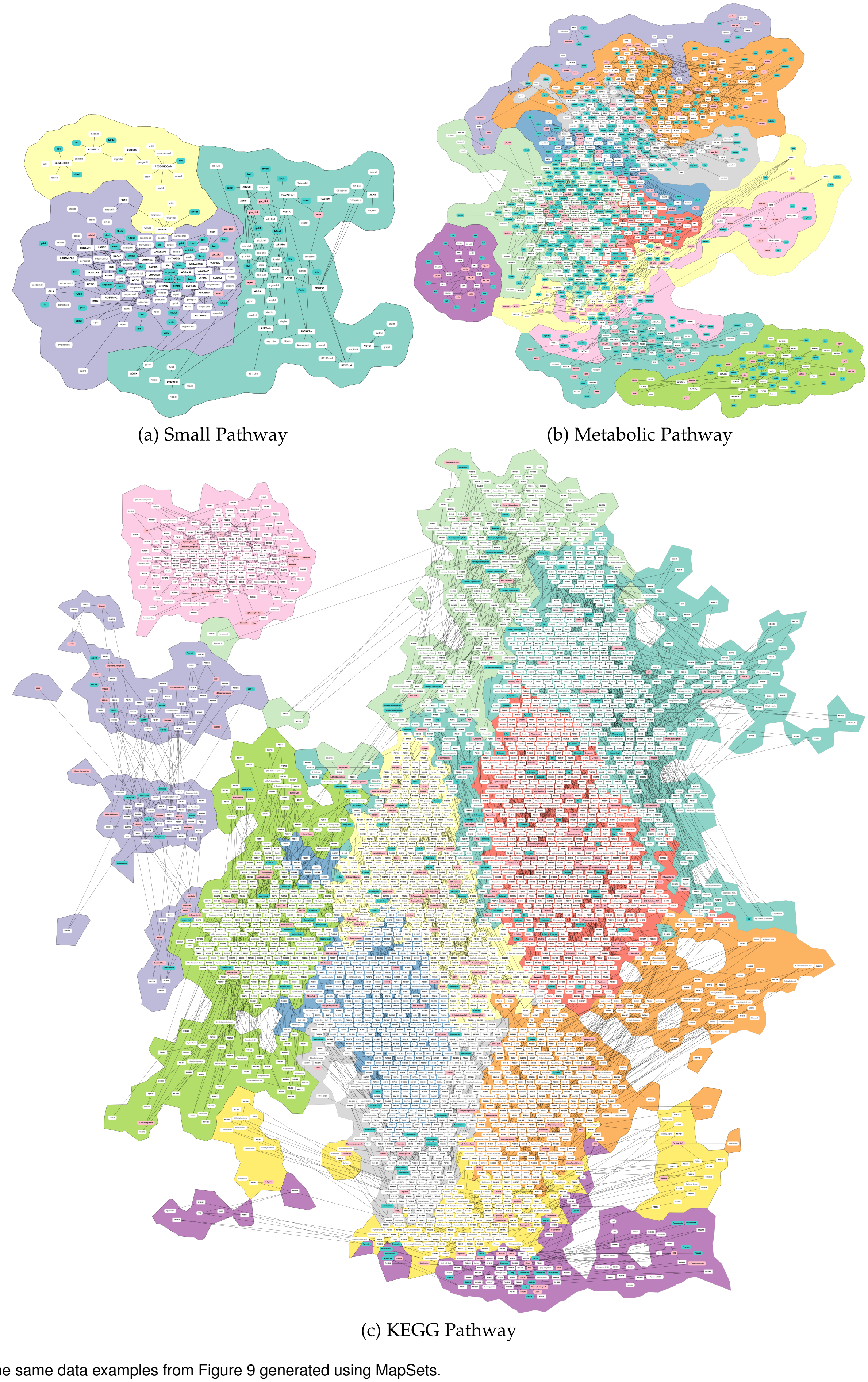
11 SUPPLEMENTARY MATERIALS

In the supplementary materials, we show several experimental results generated from the existing state-of-the-art approaches and using our approach.

11.1 Comparison with the results generated by Existing Approaches

We compare results from MapSets, Metabopolis, and our approach with larger images. Figure 8 shows the results by MapSets [25]. Although MapSets also allow to move vertices to make contiguous clusters possible, MapSets is a bottom-up approach, and thus cannot always guarantee the generation of contiguous clusters. Figure 9 shows the results by Metabopolis [64]. As we can see here, some sparse regions contain less information due to the constraints of using an octilinear layout, in comparison to the results produced by the current approach shown in Figure 10.

We also compare the variations of MapSets with our approach (see Figure 11), including the approach that keeps the fixed node positions and flexible node positions. The contiguous results are generated using GMap Web (http://gmap.cs.arizona.edu) due to the accessibility of the implementation.

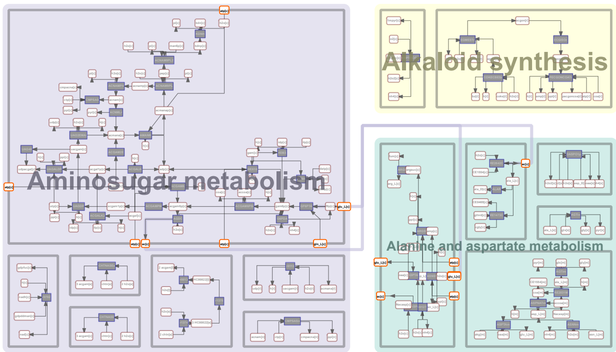


(a) Small Pathway

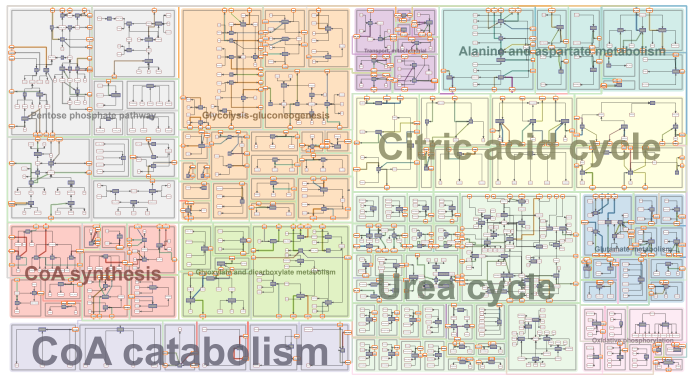
(b) Metabolic Pathway

(c) KEGG Pathway

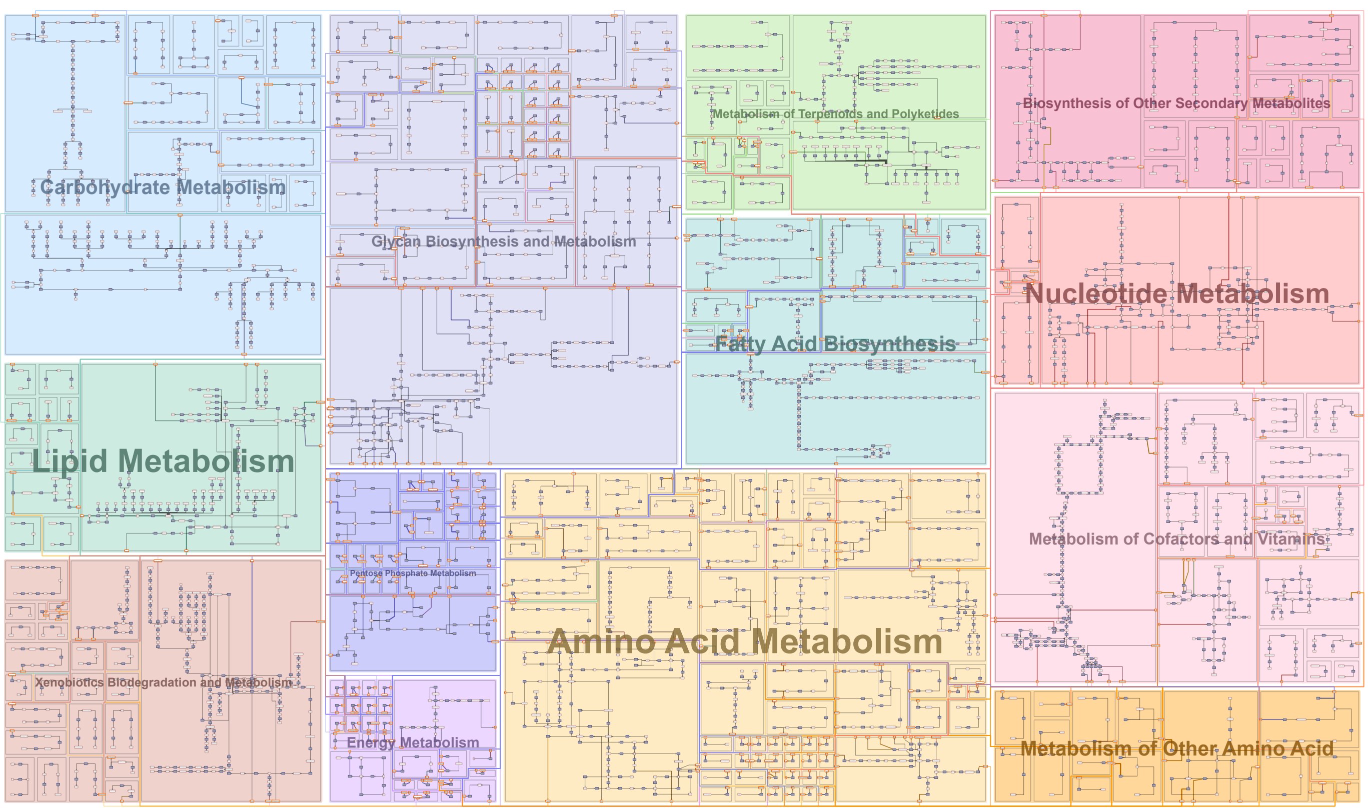
Fig. 8. The same data examples from Figure 9 generated using MapSets.



(a) Small Pathway

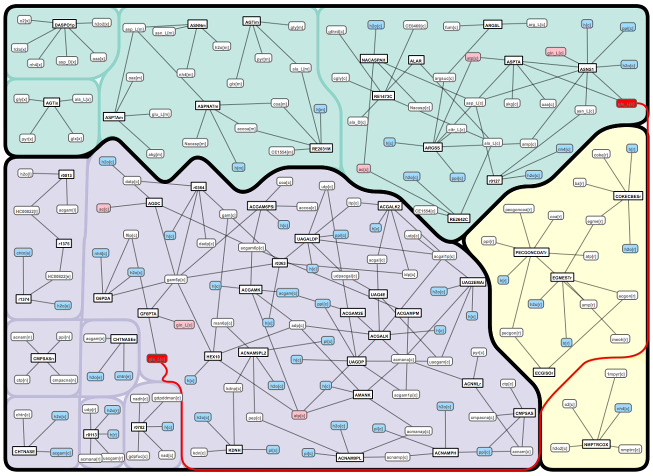


(b) Metabolic Pathway

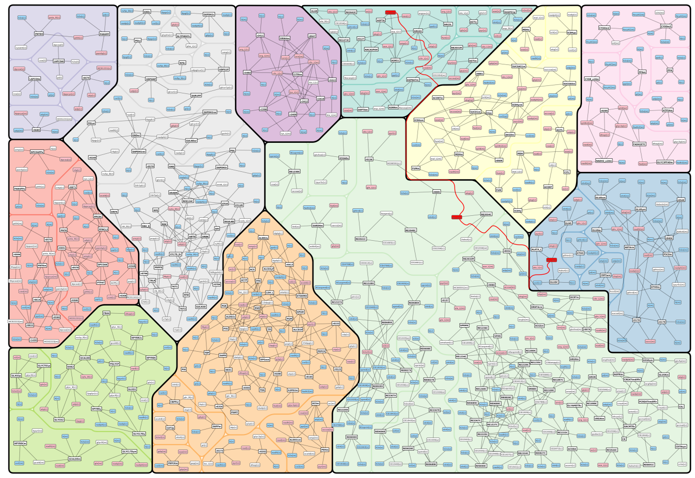


(c) KEGG Pathway

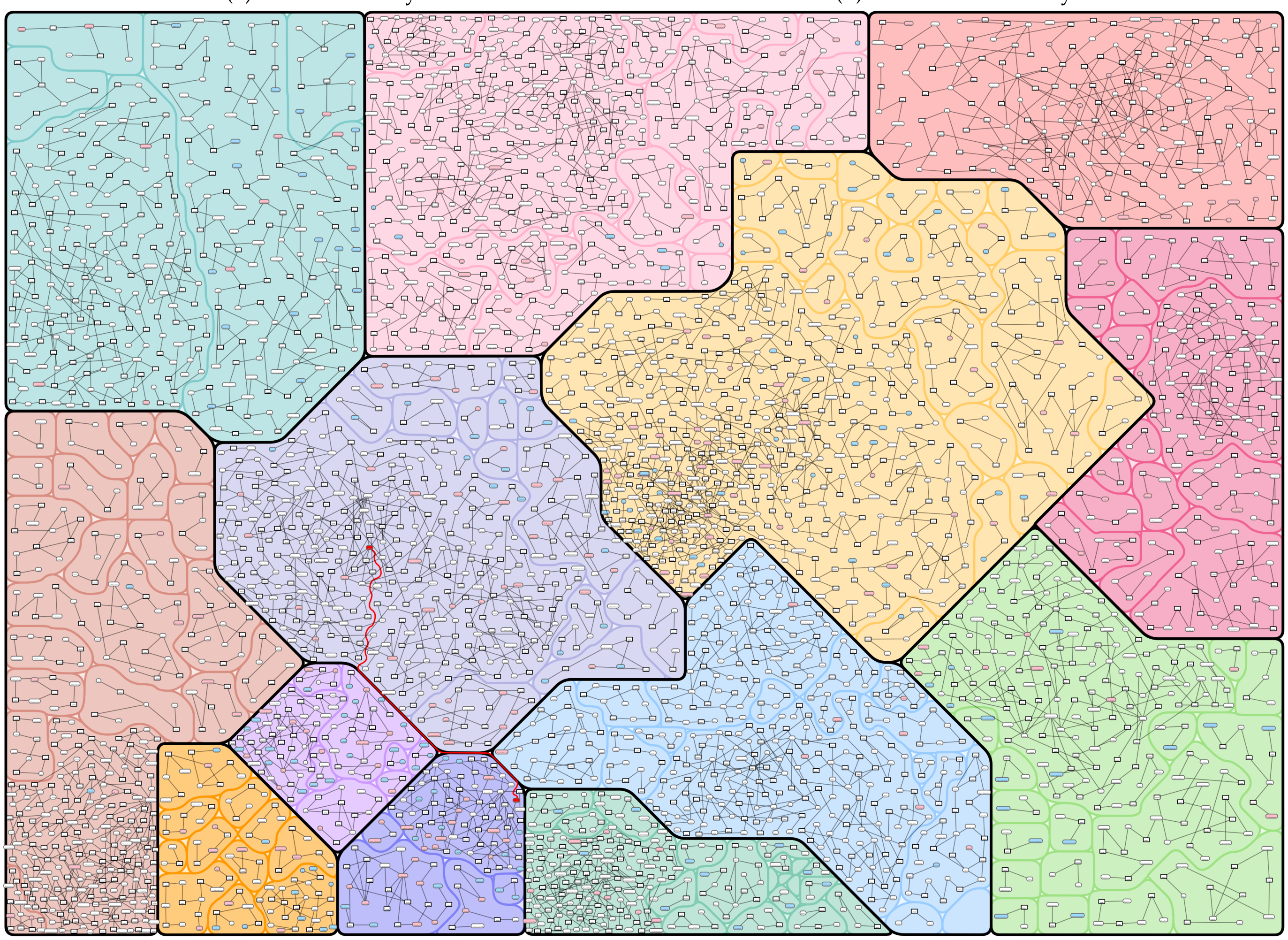
Fig. 9. Example results generated by using Metabopolis [64].



(a) Small Pathway



(b) Metabolic Pathway



(c) KEGG Pathway

Fig. 10. The same data examples from Figure 9 generated using the present system.

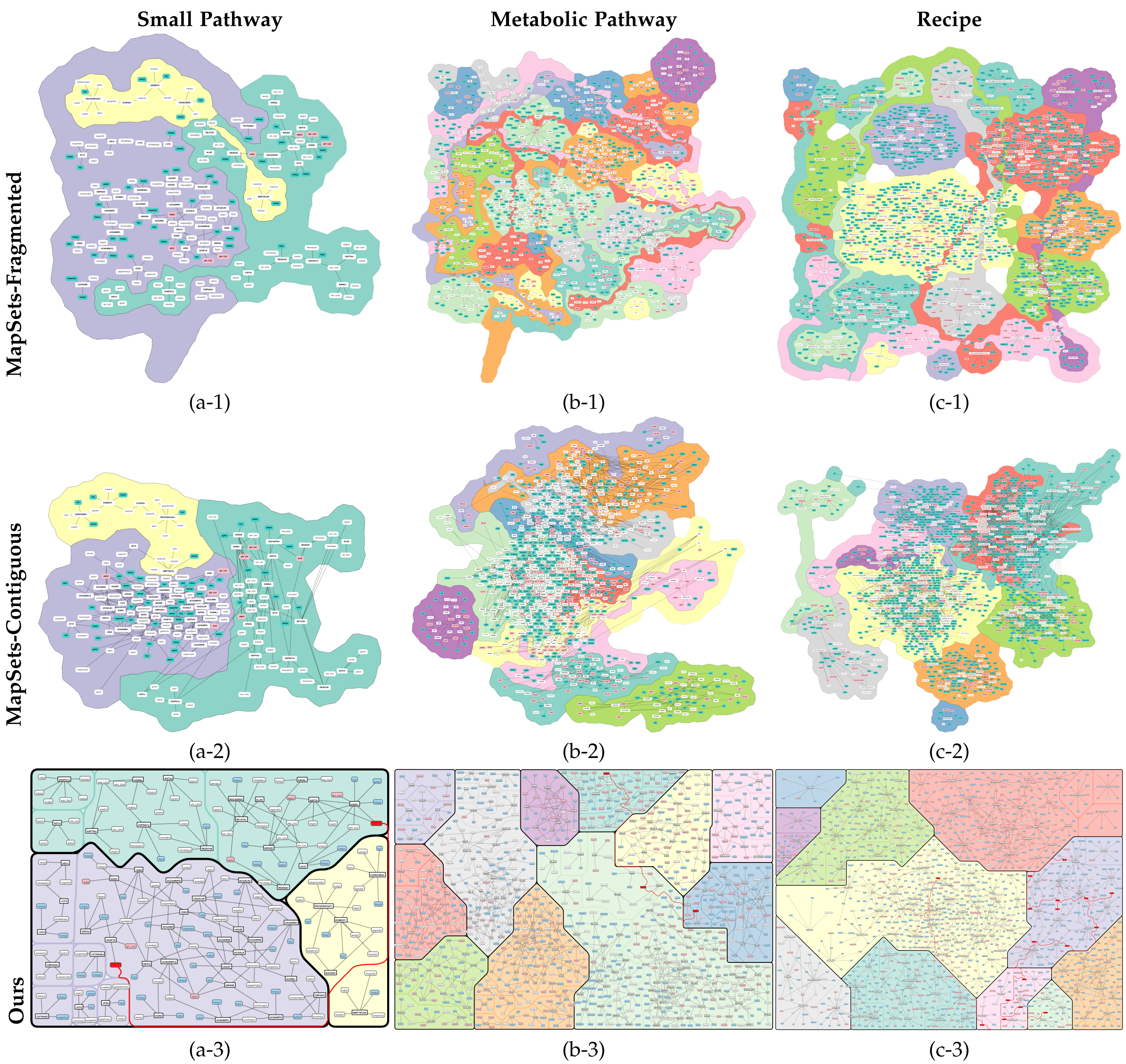


Fig. 11. Results generated using MapSets [25] with its (1) fixed position, (2) contiguous map, and (3) our area balancing algorithms. The layout of (1) was computed using the graphviz library (version 2.40.1) on the local machine described in the main paper (Section 7), and (2) were generated using GMap Web (http://gmap.cs.arizona.edu). As described previously in the main paper, each color in the diagrams indicates a single cluster, even if it is non-contiguous in some cases.

11.2 The Effect of Parameters and the Resulting Overlaps in the Maps

In this section, we present several images that show the effect of different parameters that contributed to our approach, as well as the corresponding overlaps in the images. Figures 12–16 show the results in category-level, Figures 17–21 depict the results in component-level, Figures 22–26 present the results in topology-level, and Figures 27–32 are the results in detail-level. The test begins from the default setting, and each page shows three different scales of a parameter when it is altered in our force-based approach. The left column contains the normal visualization results, while in the right column, we highlight the overlapped pixels of the vertexts and the intersected edges. In the caption, we show the values of the parameters, as well as the overlapped pixels and the number of edge crossings. The forces in this level do not explicitly influence the overlaps or edge crossings shown in the final results, but they provide a good estimation to achieve this goal.

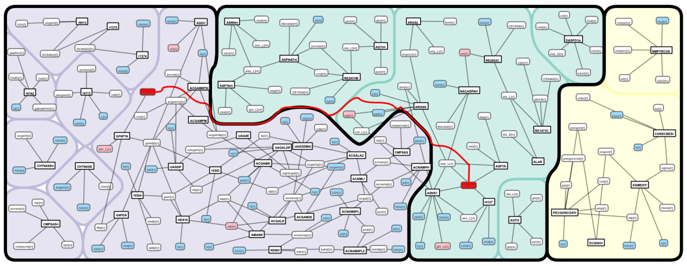
In the category-level (Figures 12–16), the approach aims to partition the canvas in a balanced fashion based on the proportional size of the canvas prepared for the category information. In Figures 12–13, we show the effect of the conventional attractive and repulsive forces. In Figures 14–15, we show the effect of the angular forces, which have less influence on the achieving area balancing. Figure 16 presents the influence of Voronoi centroid forces. In the category-level, Voronoi centroid forces show their significance to allocate balanced space, in order to avoid vertext overlaps.

Figures 17–21 show the results in the component-level. In this level, the adjustment of the parameter influences the relative positioning of the component centers to give an appropriate initial position to begin with. In Figures 12–13, we show the effect of the conventional attractive and repulsive forces. In Figures 14–15, we show the effect of the angular forces. Figure 21 presents the influence of Voronoi centroid forces. In the component-level, attractive forces show their significance to keep similar components as neighbors as well as providing a good initial positioning for the vertices in the next level.

Figures 22–26 show the results in the topology-level. In this level, the approach aims to distribute each component in a balanced fashion. In Figures 22–23, we show the effect of the conventional attractive and repulsive forces. In Figures 24–25, we show the effect of the angular forces. Figure 26 presents the influence of Voronoi centroid forces. In the topology-level, Voronoi centroid forces again show their significance of our balancing strategy to allocate balanced space. Figure 26 (a-1) shows a bad example if the Voronoi centroid forces have been removed. The vertexts become densely packed together.

In detail-level (Figures 27–32), our approach successfully finds a balanced vertext distribution. In Figures 27–28, we show the effect of the conventional attractive and repulsive forces. In Figures 29–30, we show the effect of the angular forces. Figure 31 presents the influence of Voronoi centroid forces. In Figure 32, we present the effect of forces to avoid vertext overlaps. In the detail-level, the angular forces and overlap removal forces show their importance to reduce overlaps (Figure 32 (a-2)–(c-2)), and Voronoi centroid forces is still essential for achieving area balancing.

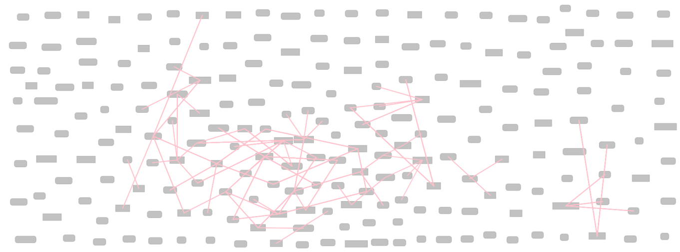
The below Figures 12–32 show a sequence of images, which demonstrate the influence of the proposed parameters to the final visualization.



(a-1)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

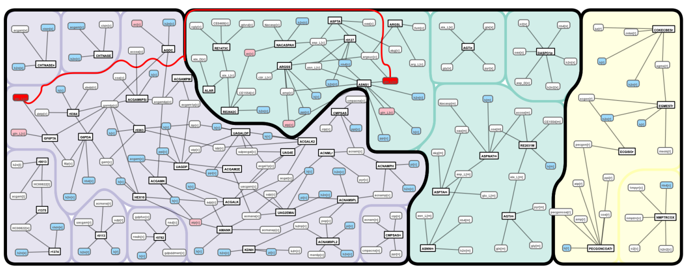
overlapped pixels = 0, total pixels = 1103350, edge crossings = 78.



(a-2)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

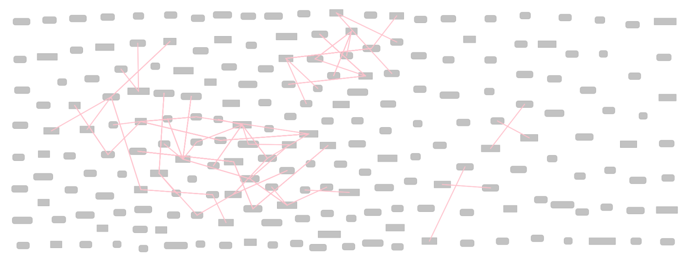
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 78.



(b-1)

$k_a = 0.2, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

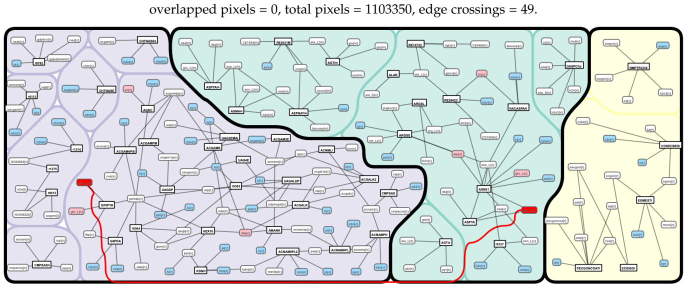
overlapped pixels = 0, total pixels = 1103350, edge crossings = 49.



(b-2)

$k_a = 0.2, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

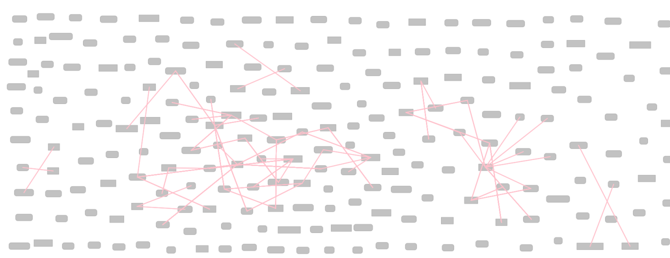
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 49.



(c-1)

$k_a = 0.3, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 70.

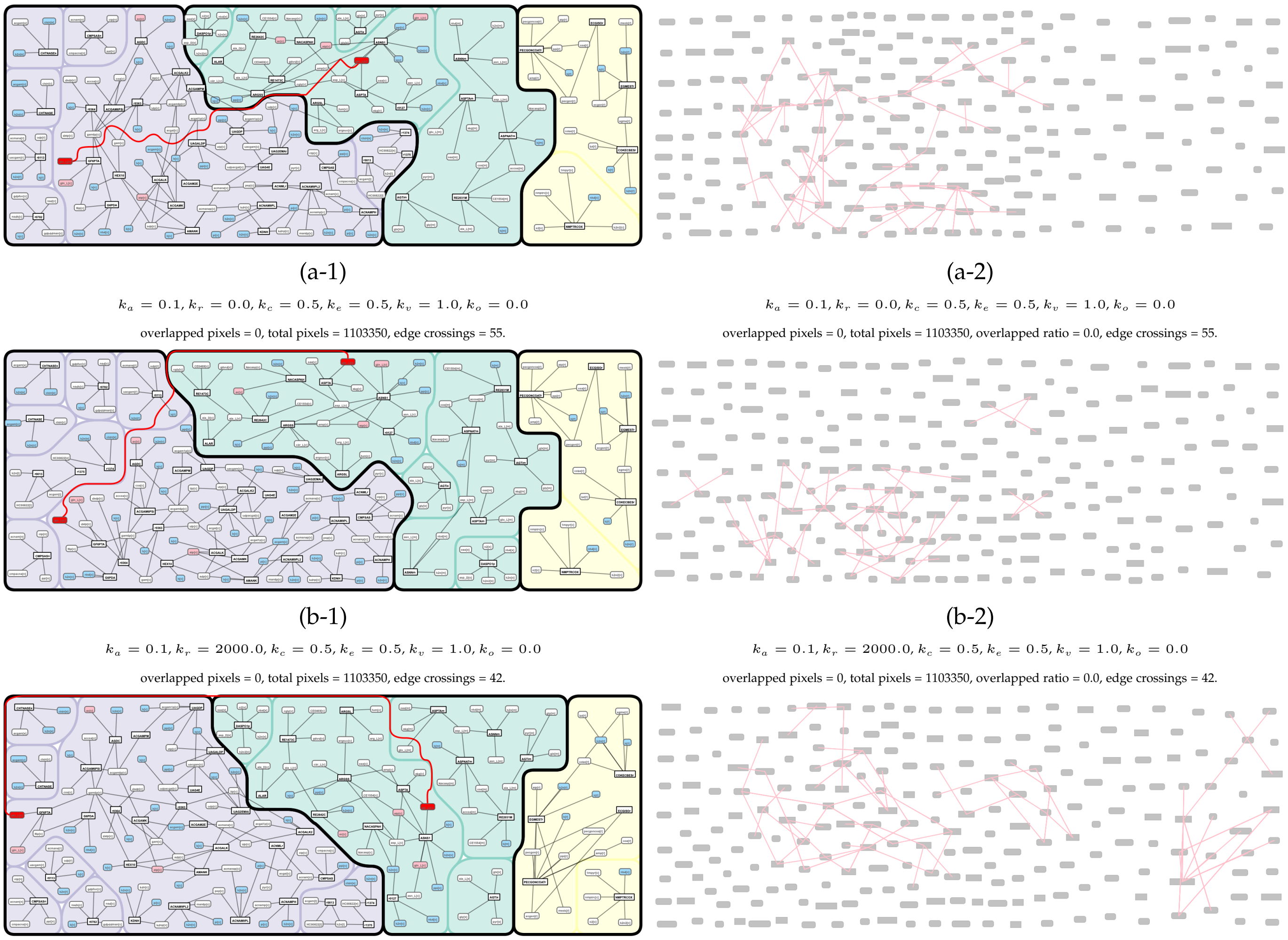


(c-2)

$k_a = 0.3, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 70.

Fig. 12. The effect of parameters and the resulting overlaps in the category-level step. The increase of k_a brings the vertices in the skeleton graph close to each other. The adjustment of the parameter at this stage influences the area and the structure of the category contours.



(a-1)

$k_a = 0.1, k_r = 0.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 55.

(a-2)

$k_a = 0.1, k_r = 0.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 55.

(b-1)

$k_a = 0.1, k_r = 2000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 42.

(b-2)

$k_a = 0.1, k_r = 2000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 42.

(c-1)

$k_a = 0.1, k_r = 4000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

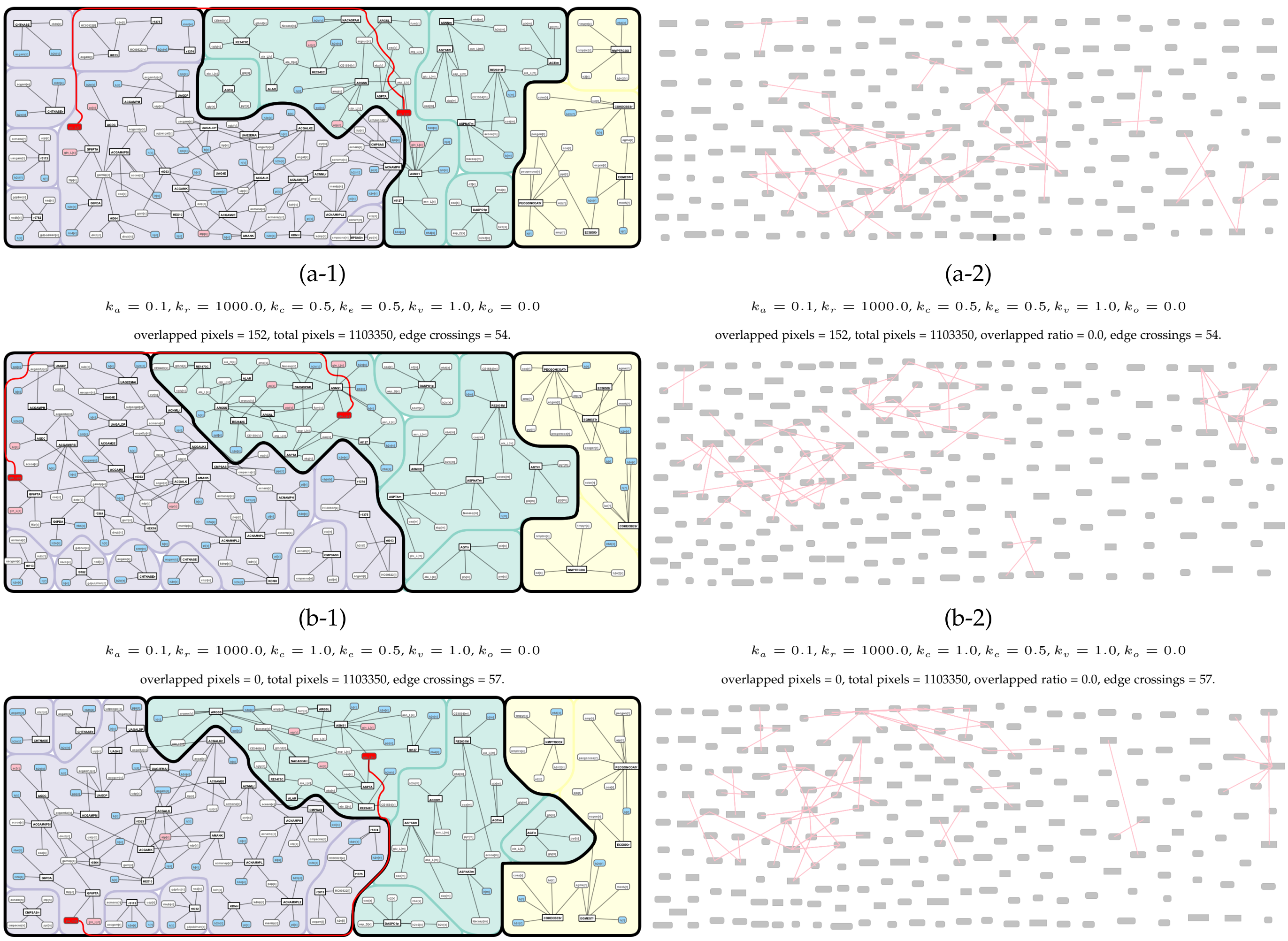
overlapped pixels = 0, total pixels = 1103350, edge crossings = 53.

(c-2)

$k_a = 0.1, k_r = 4000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 53.

Fig. 13. The effect of parameters and the resulting overlaps in the category-level step. The increase of k_r preserves the minimum distance between vertices in the skeleton graph. The adjustment of the parameter at this stage influences the area and the structure of the category contours.



(a-1)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 152, total pixels = 1103350, edge crossings = 54.

(a-2)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 152, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 54.

(b-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 57.

(b-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 57.

(c-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

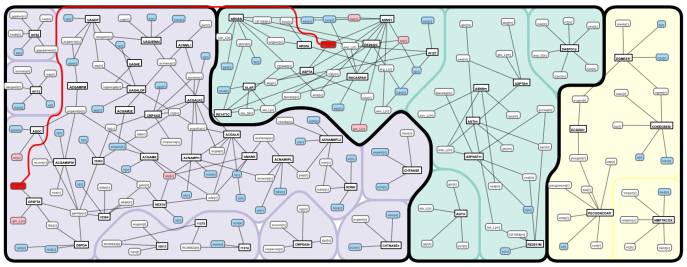
overlapped pixels = 0, total pixels = 1103350, edge crossings = 59.

(c-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 59.

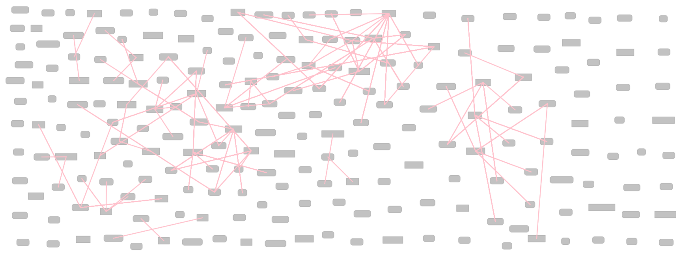
Fig. 14. The effect of parameters and the resulting overlaps in the category-level step. The increase of k_c preserves the minimum distance between a pair of edges spanned from a vertex in the skeleton graph. The adjustment of the parameter at this stage influences the area and the structure of the category contours. The influence of the parameters at this stage should be small.



(a-1)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

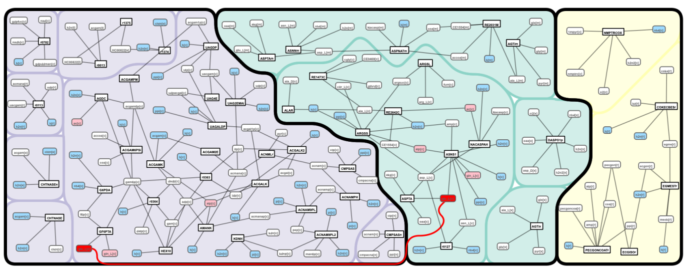
overlapped pixels = 0, total pixels = 1103350, edge crossings = 161.



(a-2)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

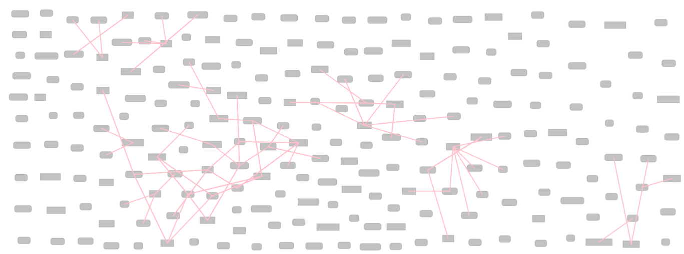
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 161.



(b-1)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 1.0, k_v = 1.0, k_o = 0.0$

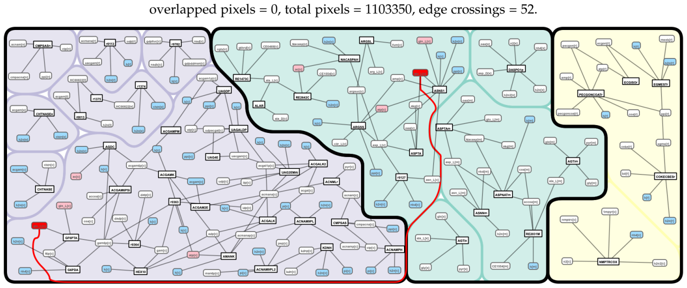
overlapped pixels = 0, total pixels = 1103350, edge crossings = 52.



(b-2)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 1.0, k_v = 1.0, k_o = 0.0$

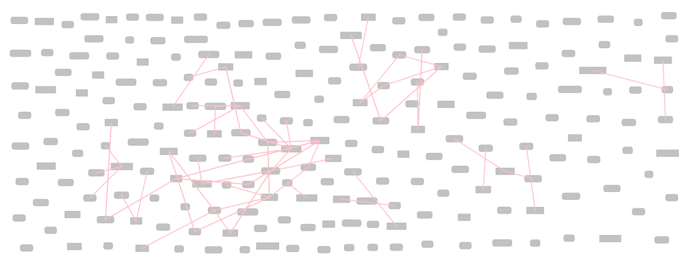
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 52.



(c-1)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 1.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 50.

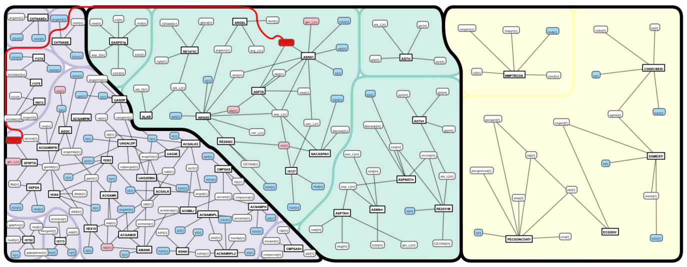


(c-2)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 1.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 50.

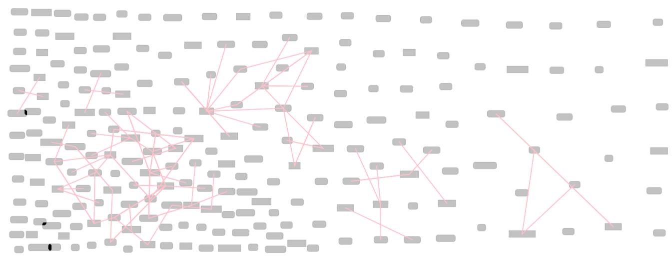
Fig. 15. The effect of parameters and the resulting overlaps in the category-level step. The increase of k_e preserves the minimum angular resolution between a pair of edges spanned from a vertex in the skeleton graph. The adjustment of the parameter at this stage influences the area and the structure of the category contours. The influence of the parameters at this stage should be small.



(a-1)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 0.0, k_o = 0.0$

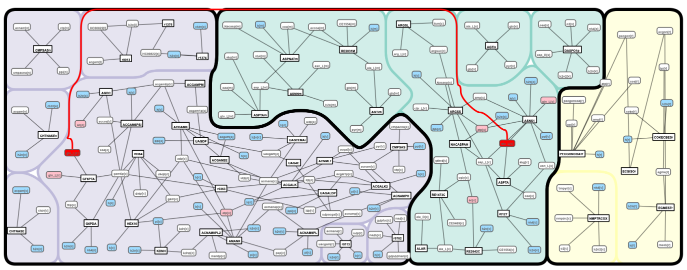
overlapped pixels = 241, total pixels = 1103350, edge crossings = 62.



(a-2)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 0.0, k_o = 0.0$

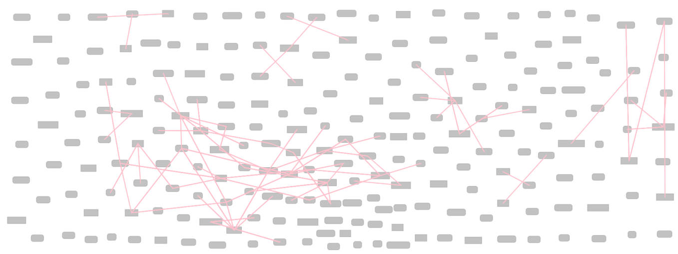
overlapped pixels = 241, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 62.



(b-1)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

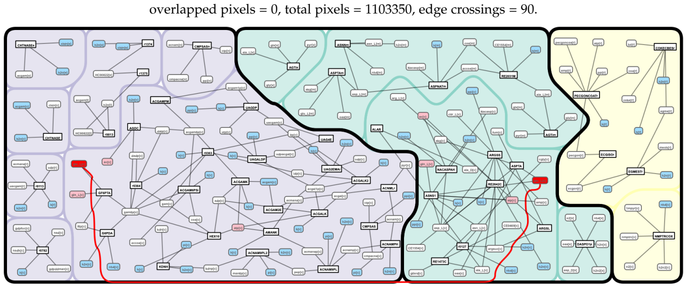
overlapped pixels = 0, total pixels = 1103350, edge crossings = 90.



(b-2)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

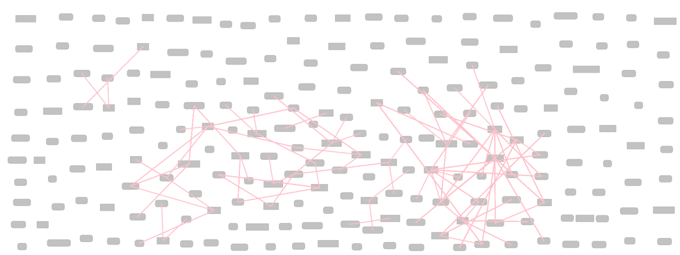
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 90.



(c-1)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 2.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 164.

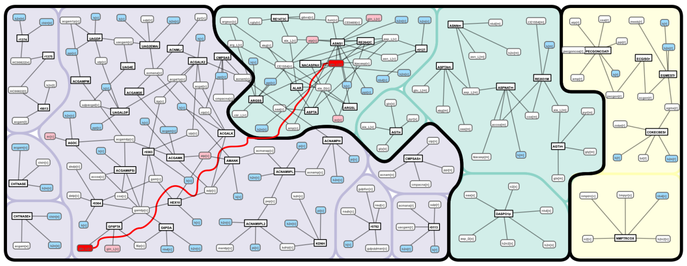


(c-2)

$k_a = 0.1, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 2.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 164.

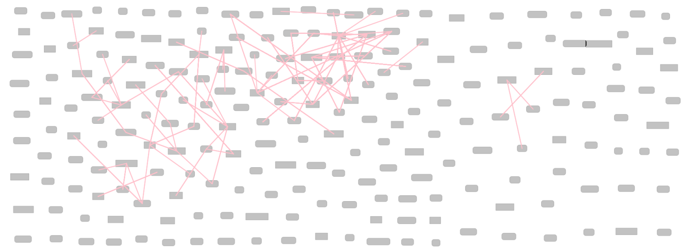
Fig. 16. The effect of parameters and the resulting overlaps in the category-level step. The increase of k_v preserves the minimum area assigned to each vertex in the skeleton graph. The adjustment of the parameter at this stage influences the area and the structure of the category contours. This parameter is especially important for area balancing and avoid vertext overlaps.



(a-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

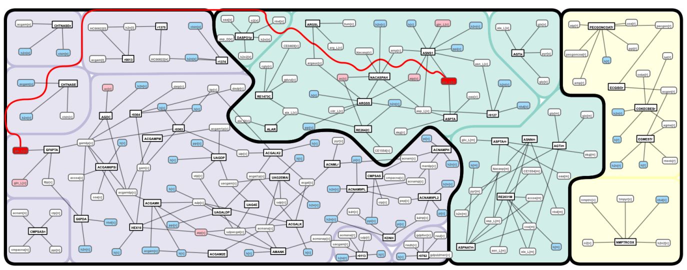
overlapped pixels = 28, total pixels = 1103350, edge crossings = 150.



(a-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

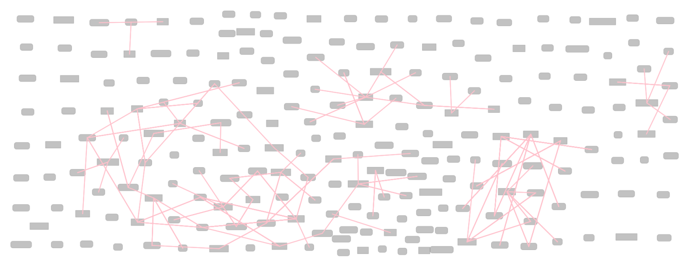
overlapped pixels = 28, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 150.



(b-1)

$k_a = 2.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

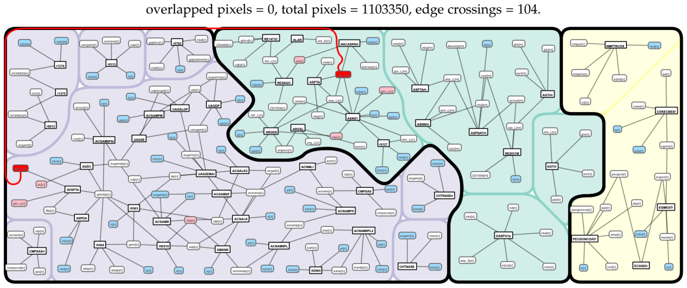
overlapped pixels = 0, total pixels = 1103350, edge crossings = 104.



(b-2)

$k_a = 2.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

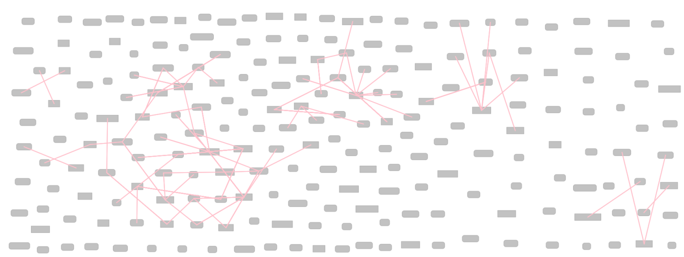
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 104.



(c-1)

$k_a = 3.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 59.

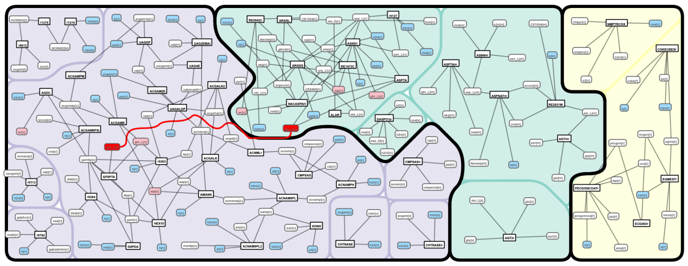


(c-2)

$k_a = 3.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 59.

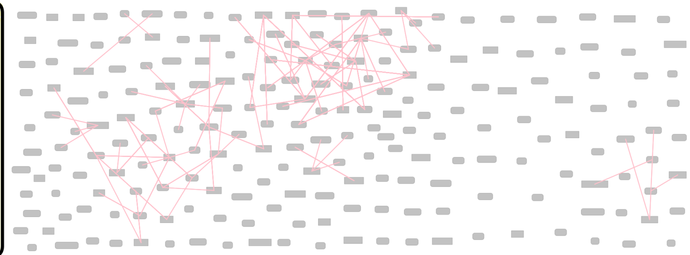
Fig. 17. The effect of parameters and the resulting overlaps in the component-level step. The increase of k_a brings the vertices in the skeleton graph close to each other. The adjustment of the parameter at this stage influences the relative positioning of the component centers.



(a-1)

$k_a = 1.0, k_r = 0.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

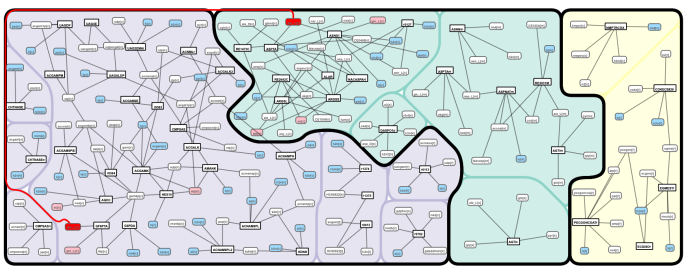
overlapped pixels = 0, total pixels = 1103350, edge crossings = 127.



(a-2)

$k_a = 1.0, k_r = 0.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

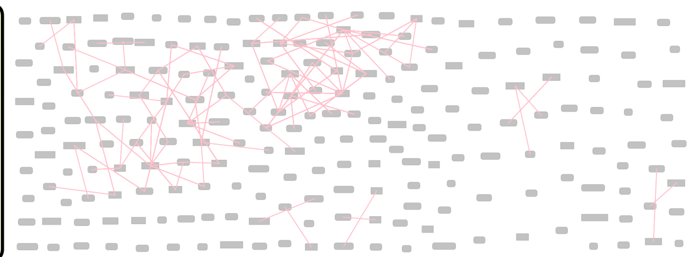
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 127.



(b-1)

$k_a = 1.0, k_r = 2000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

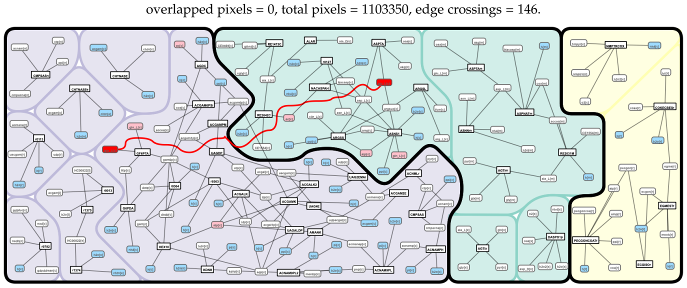
overlapped pixels = 0, total pixels = 1103350, edge crossings = 146.



(b-2)

$k_a = 1.0, k_r = 2000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

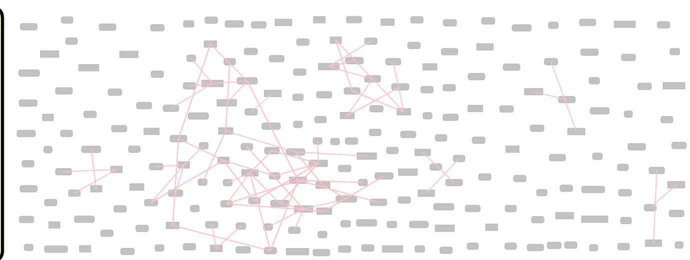
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 146.



(c-1)

$k_a = 1.0, k_r = 4000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 66.

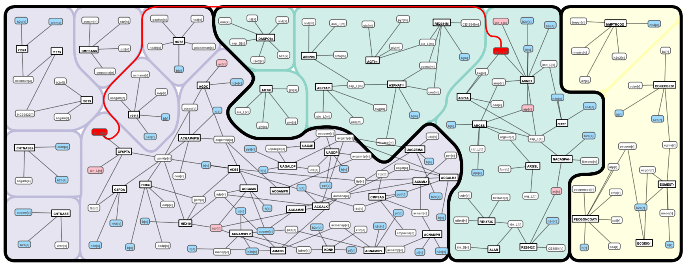


(c-2)

$k_a = 1.0, k_r = 4000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 66.

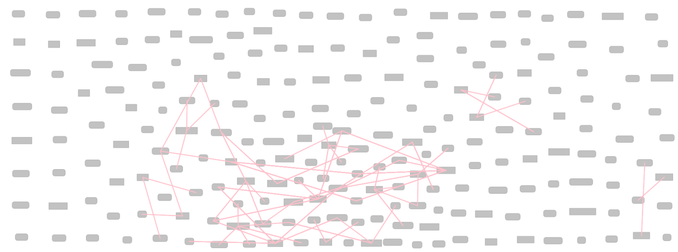
Fig. 18. The effect of parameters and the resulting overlaps in the component-level step. The increase of k_r preserves the minimum distance between vertices in the skeleton graph. The adjustment of the parameter at this stage influences the relative positioning of the component centers.



(a-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

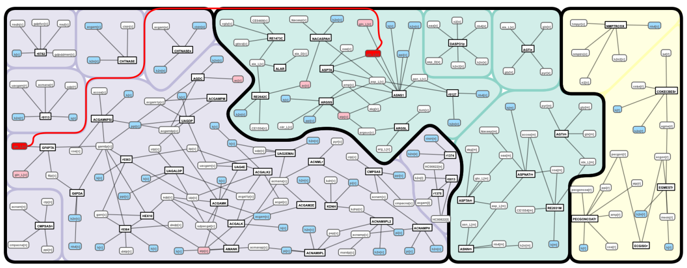
overlapped pixels = 0, total pixels = 1103350, edge crossings = 75.



(a-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

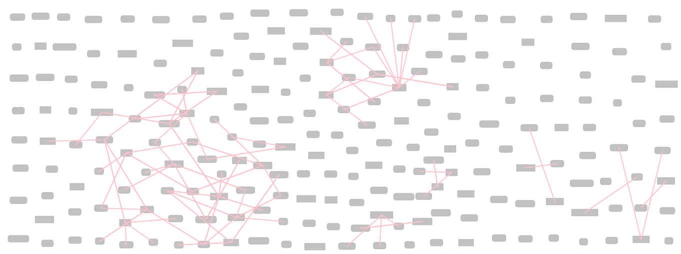
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 75.



(b-1)

$k_a = 1.0, k_r = 1000.0, k_c = 1.0, k_e = 0.5, k_v = 1.0, k_o = 0.0$

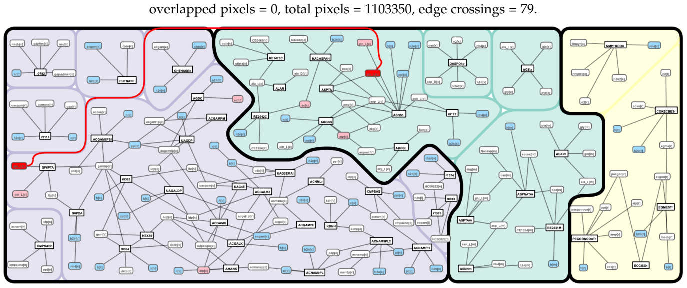
overlapped pixels = 0, total pixels = 1103350, edge crossings = 79.



(b-2)

$k_a = 1.0, k_r = 1000.0, k_c = 1.0, k_e = 0.5, k_v = 1.0, k_o = 0.0$

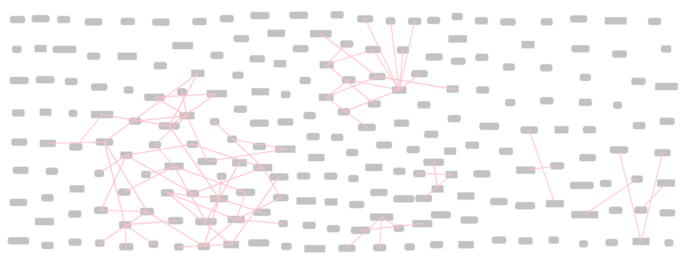
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 79.



(c-1)

$k_a = 1.0, k_r = 1000.0, k_c = 1.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 79.

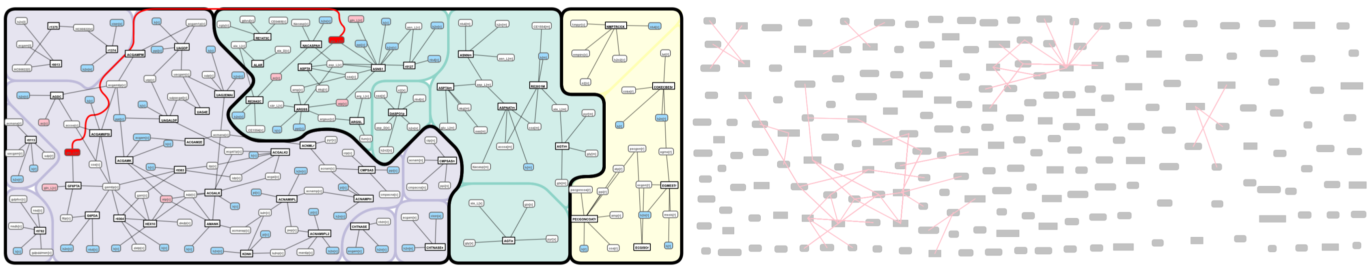


(c-2)

$k_a = 1.0, k_r = 1000.0, k_c = 1.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 79.

Fig. 19. The effect of parameters and the resulting overlaps in the component-level step. The increase of k_c preserves the minimum distance between a pair of edges spanned from a vertex in the skeleton graph. The adjustment of the parameter at this stage influences the relative positioning of the component centers. The influence of the parameters at this stage should be small.



(a-1)

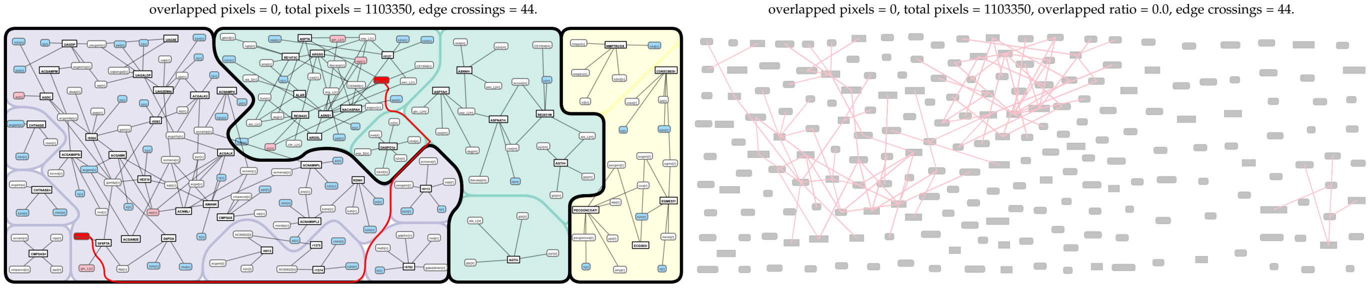
$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 44.

(a-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 44.



(b-1)

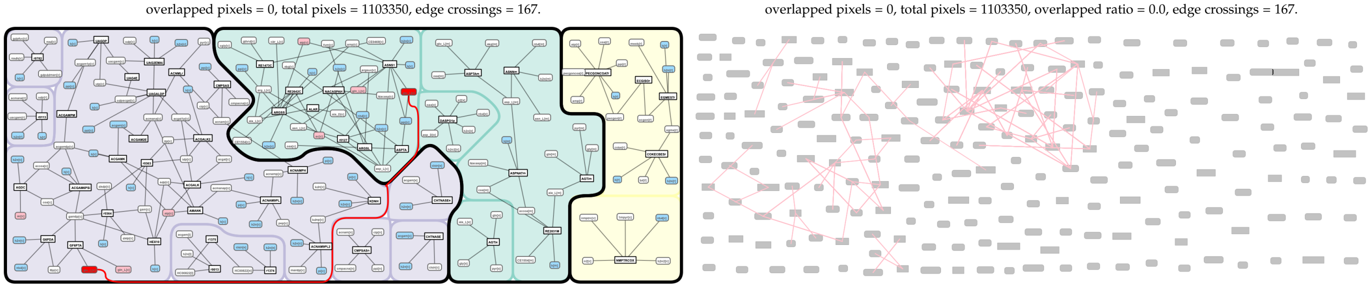
$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 1.0, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 167.

(b-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 1.0, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 167.



(c-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 1.5, k_v = 1.0, k_o = 0.0$

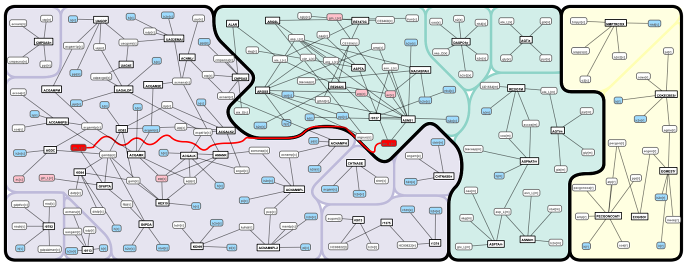
overlapped pixels = 28, total pixels = 1103350, edge crossings = 114.

(c-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 1.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 28, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 114.

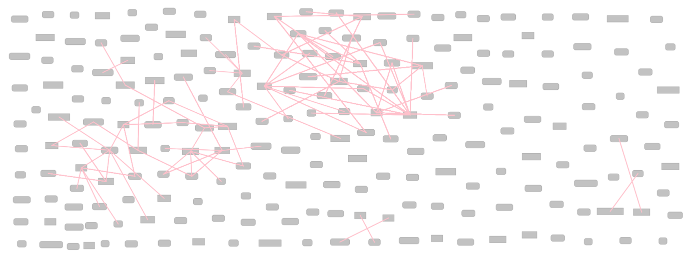
Fig. 20. The effect of parameters and the resulting overlaps in the component-level step. The increase of k_e preserves the minimum angular resolution between a pair of edges spanned from a vertex in the skeleton graph. The adjustment of the parameter at this stage influences the relative positioning of the component centers. The influence of the parameters at this stage should be small.



(a-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 0.0, k_o = 0.0$

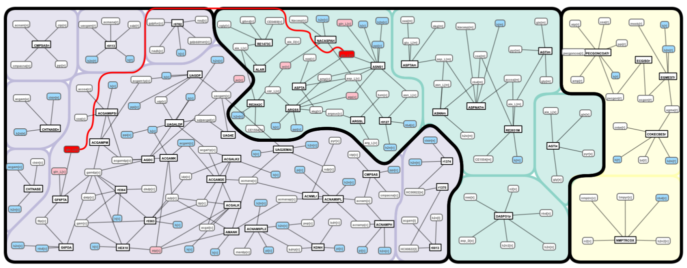
overlapped pixels = 0, total pixels = 1103350, edge crossings = 155.



(a-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 0.0, k_o = 0.0$

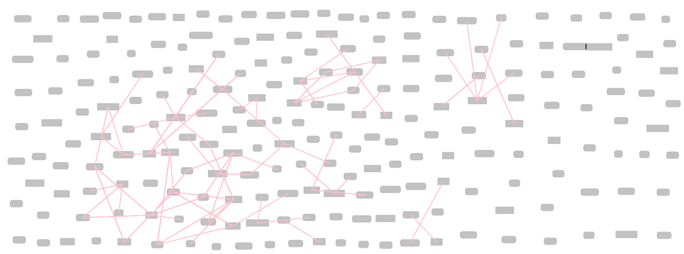
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 155.



(b-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

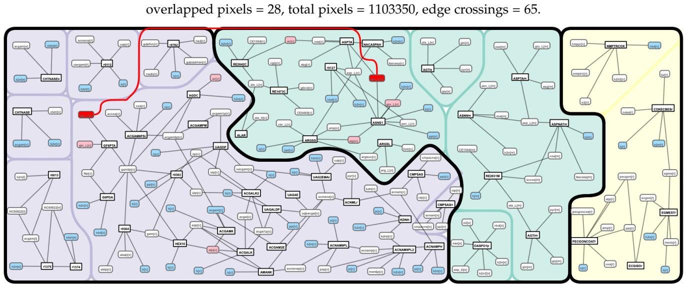
overlapped pixels = 28, total pixels = 1103350, edge crossings = 65.



(b-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

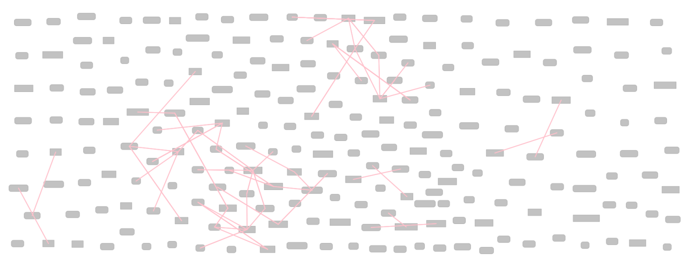
overlapped pixels = 28, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 65.



(c-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 2.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 41.

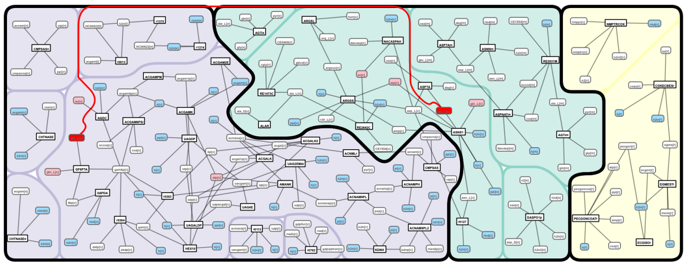


(c-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 2.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 41.

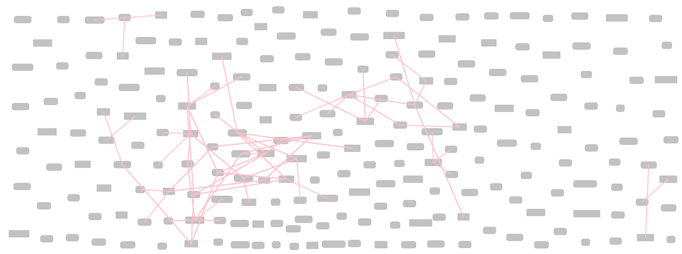
Fig. 21. The effect of parameters and the resulting overlaps in the component-level step. The increase of k_v preserves the minimum area assigned to each vertex in the skeleton graph. The adjustment of the parameter at this stage influences the relative positioning of the component centers, which will be used as initial position of vertices in the next level.



(a-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

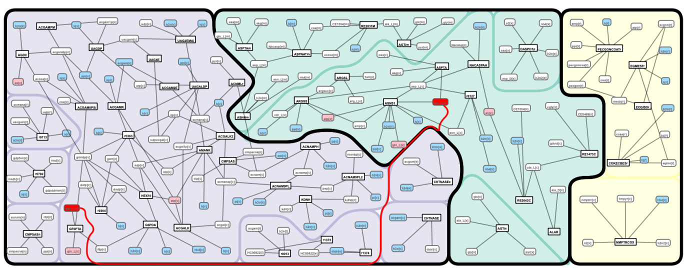
overlapped pixels = 0, total pixels = 1103350, edge crossings = 78.



(a-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

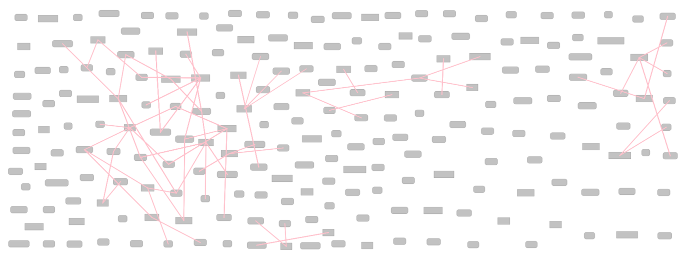
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 78.



(b-1)

$k_a = 2.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

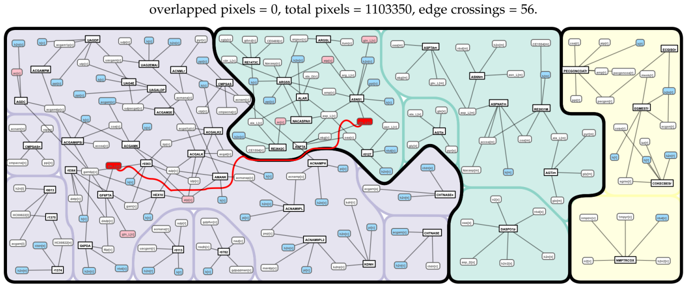
overlapped pixels = 0, total pixels = 1103350, edge crossings = 56.



(b-2)

$k_a = 2.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

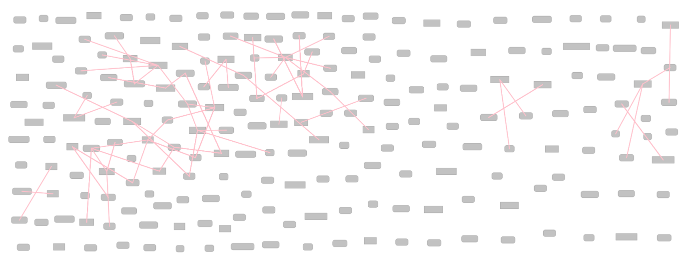
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 56.



(c-1)

$k_a = 3.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 54.

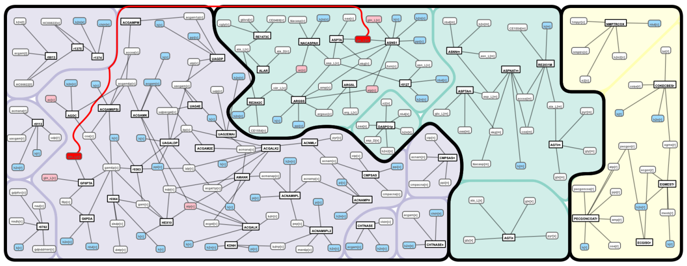


(c-2)

$k_a = 3.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 54.

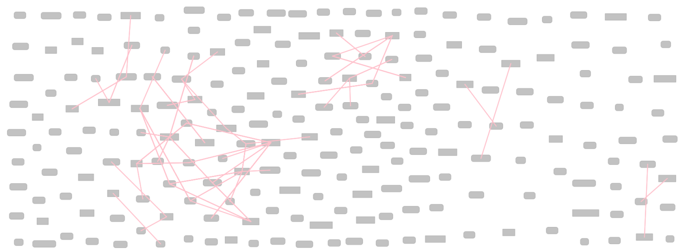
Fig. 22. The effect of parameters and the resulting overlaps in the topology-level step. The increase of k_a brings the vertices in the skeleton graph close to each other. The adjustment of the parameter at this stage influences the relative positioning of the component distribution.



(a-1)

$k_a = 1.0, k_r = 0.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

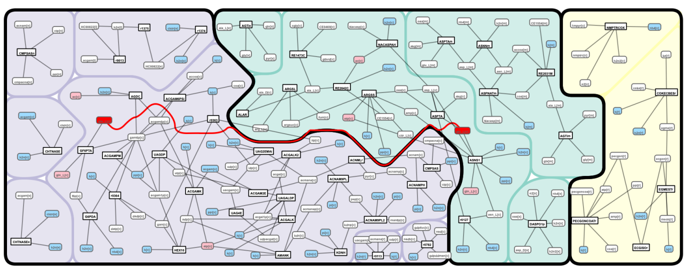
overlapped pixels = 0, total pixels = 1103350, edge crossings = 51.



(a-2)

$k_a = 1.0, k_r = 0.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

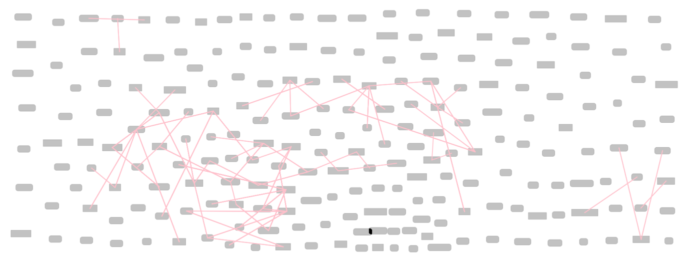
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 51.



(b-1)

$k_a = 1.0, k_r = 2000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

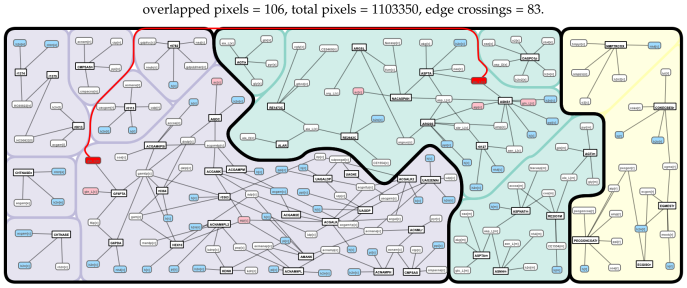
overlapped pixels = 106, total pixels = 1103350, edge crossings = 83.



(b-2)

$k_a = 1.0, k_r = 2000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

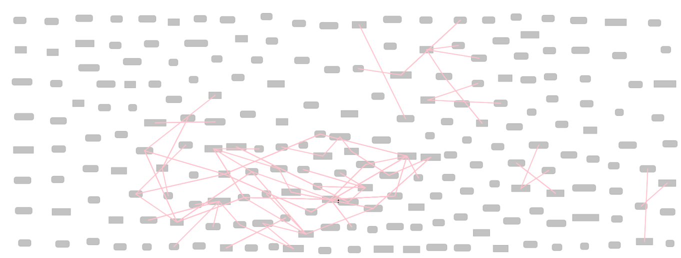
overlapped pixels = 106, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 83.



(c-1)

$k_a = 1.0, k_r = 4000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 26, total pixels = 1103350, edge crossings = 66.

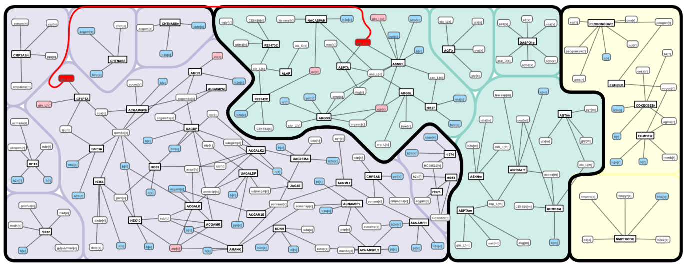


(c-2)

$k_a = 1.0, k_r = 4000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 26, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 66.

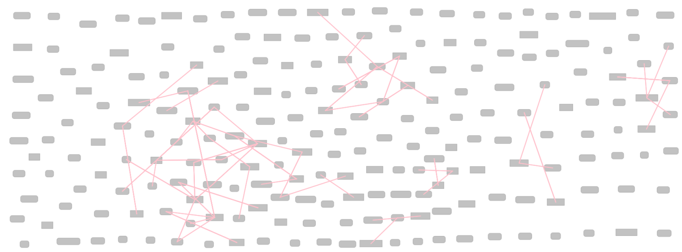
Fig. 23. The effect of parameters and the resulting overlaps in the topology-level step. The increase of k_r preserves the minimum distance between vertices in the skeleton graph. The adjustment of the parameter at this stage influences the relative positioning of the component distribution.



(a-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

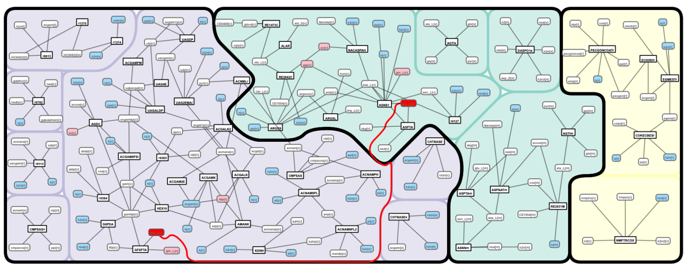
overlapped pixels = 0, total pixels = 1103350, edge crossings = 52.



(a-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

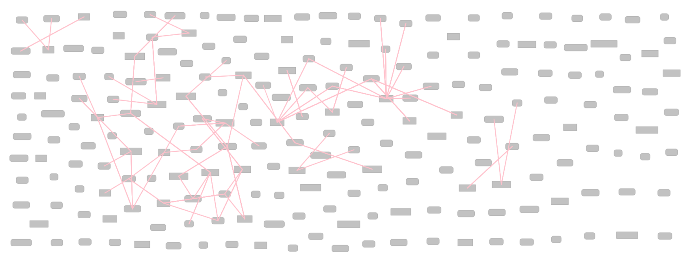
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 52.



(b-1)

$k_a = 1.0, k_r = 1000.0, k_c = 1.0, k_e = 0.5, k_v = 1.0, k_o = 0.0$

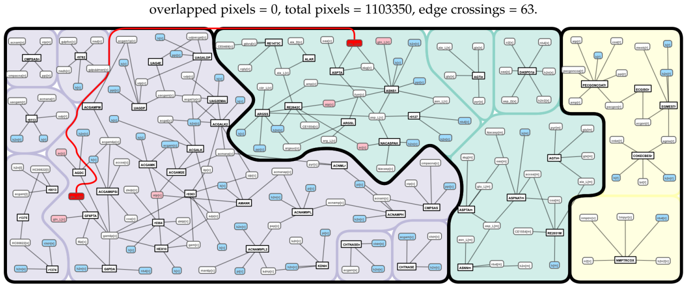
overlapped pixels = 0, total pixels = 1103350, edge crossings = 63.



(b-2)

$k_a = 1.0, k_r = 1000.0, k_c = 1.0, k_e = 0.5, k_v = 1.0, k_o = 0.0$

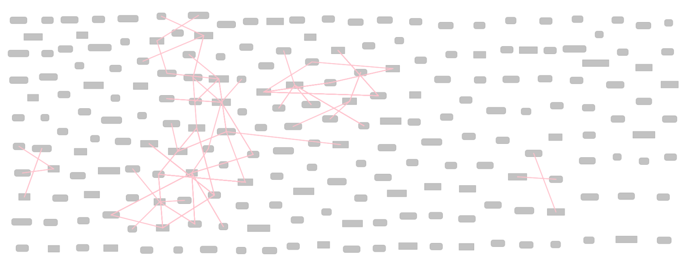
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 63.



(c-1)

$k_a = 1.0, k_r = 1000.0, k_c = 1.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 50.

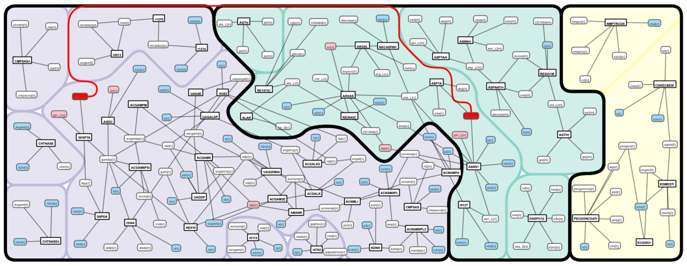


(c-2)

$k_a = 1.0, k_r = 1000.0, k_c = 1.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 50.

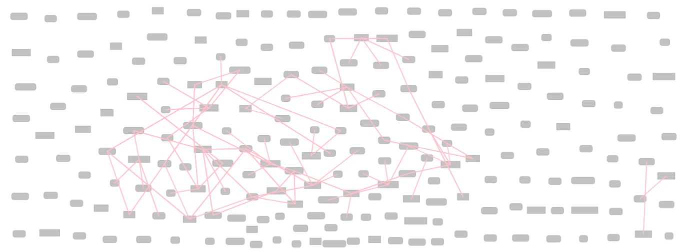
Fig. 24. The effect of parameters and the resulting overlaps in the topology-level step. The increase of k_c preserves the minimum distance between a pair of edges spanned from a vertex in the skeleton graph. The adjustment of the parameter at this stage influences the relative positioning of the component distribution. The influence of the parameters at this stage should be small.



(a-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

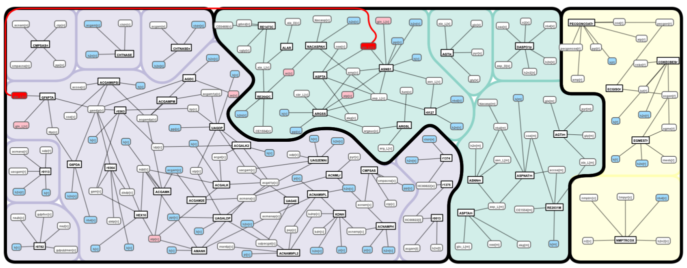
overlapped pixels = 0, total pixels = 1103350, edge crossings = 80.



(a-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

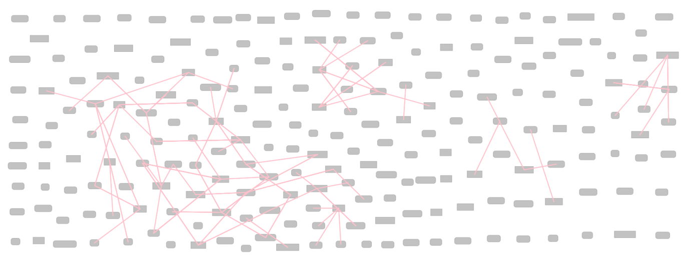
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 80.



(b-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 1.0, k_v = 1.0, k_o = 0.0$

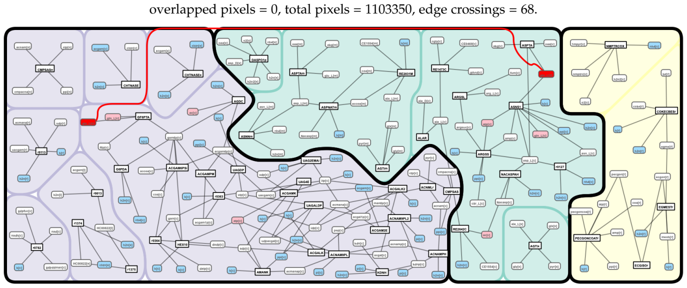
overlapped pixels = 0, total pixels = 1103350, edge crossings = 68.



(b-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 1.0, k_v = 1.0, k_o = 0.0$

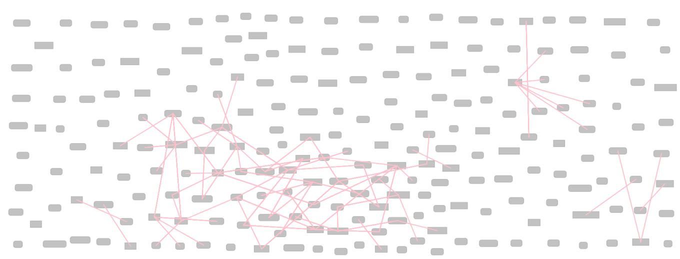
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 68.



(c-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 1.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 101.

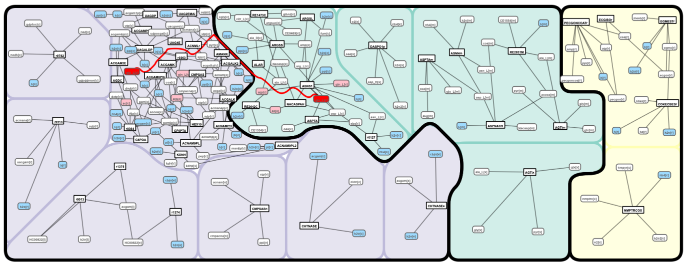


(c-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 1.5, k_v = 1.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 101.

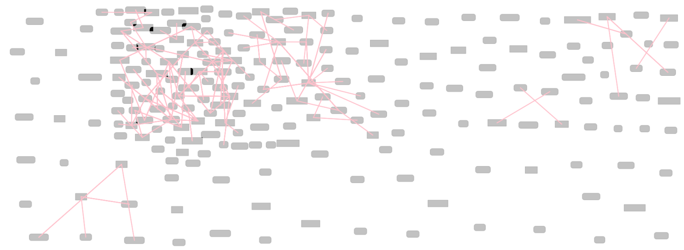
Fig. 25. The effect of parameters and the resulting overlaps in the topology-level step. The increase of k_e preserves the minimum angular resolution between a pair of edges spanned from a vertex in the skeleton graph. The adjustment of the parameter at this stage influences the relative positioning of the component distribution. The influence of the parameters at this stage should be small.



(a-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 0.0, k_o = 0.0$

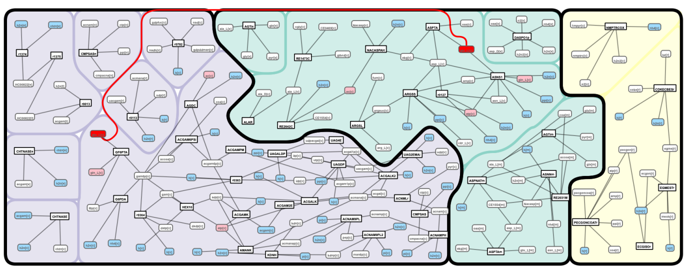
overlapped pixels = 425, total pixels = 1103350, edge crossings = 143.



(a-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 0.0, k_o = 0.0$

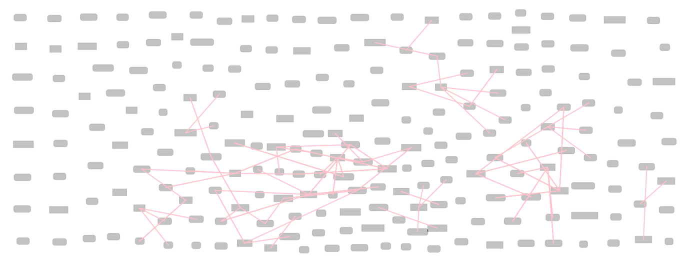
overlapped pixels = 425, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 143.



(b-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

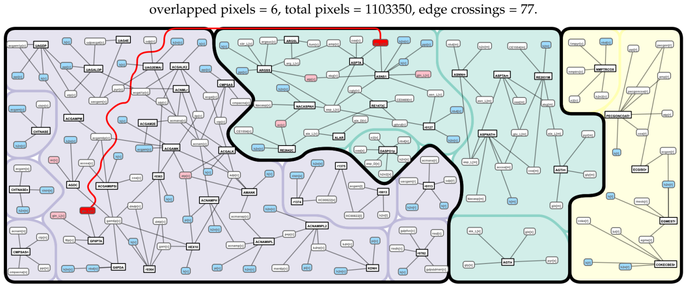
overlapped pixels = 6, total pixels = 1103350, edge crossings = 77.



(b-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 1.0, k_o = 0.0$

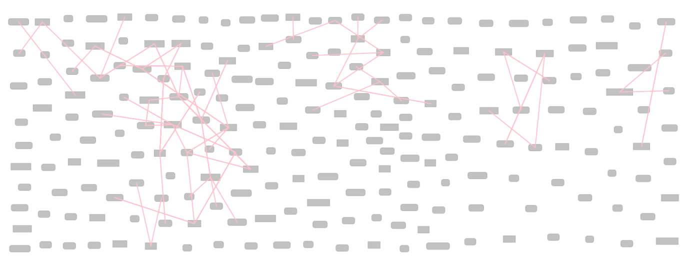
overlapped pixels = 6, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 77.



(c-1)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 2.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 59.

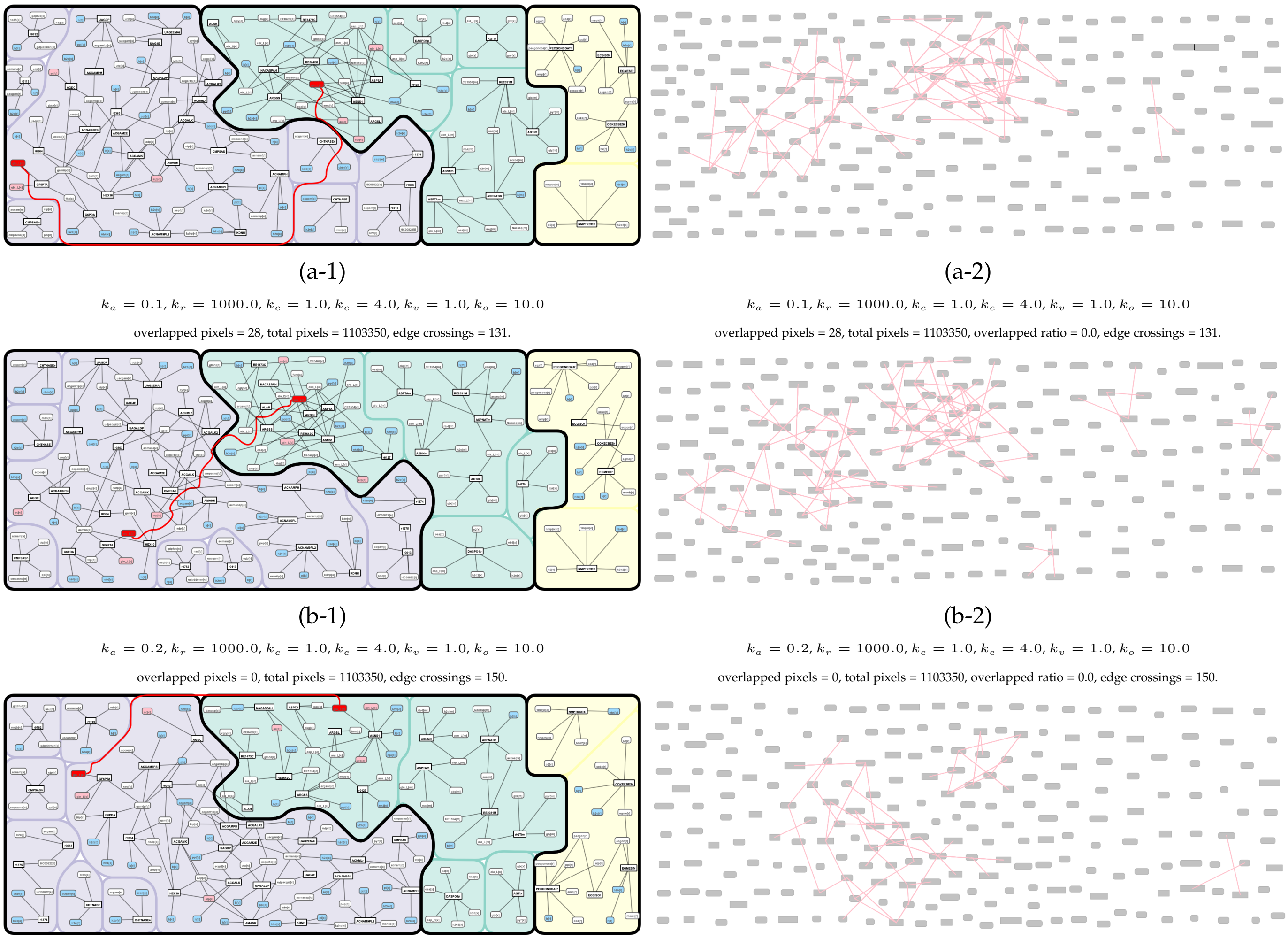


(c-2)

$k_a = 1.0, k_r = 1000.0, k_c = 0.5, k_e = 0.5, k_v = 2.0, k_o = 0.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 59.

Fig. 26. The effect of parameters and the resulting overlaps in the topology-level step. The increase of k_v preserves the minimum area assigned to each vertex in the skeleton graph. The adjustment of the parameter at this stage influences the relative positioning of the component distribution.



(a-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 28, total pixels = 1103350, edge crossings = 131.

(a-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 28, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 131.

(b-1)

$k_a = 0.2, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 150.

(b-2)

$k_a = 0.2, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 150.

(c-1)

$k_a = 0.3, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

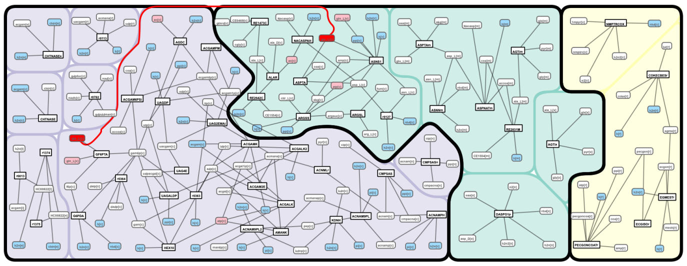
overlapped pixels = 0, total pixels = 1103350, edge crossings = 39.

(c-2)

$k_a = 0.3, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 39.

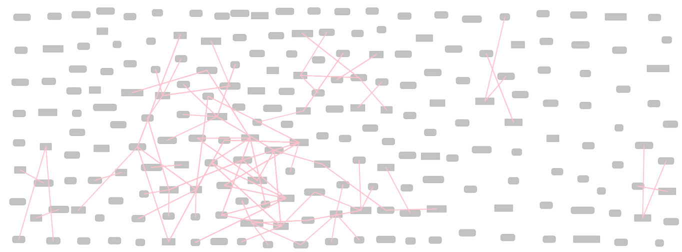
Fig. 27. The effect of parameters and the resulting overlaps in the detail-level step. The increase of k_a brings the vertices in the final subgraphs close to each other. The adjustment of the parameter at this stage influences the final vertext distribution.



(a-1)

$k_a = 0.1, k_r = 0.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

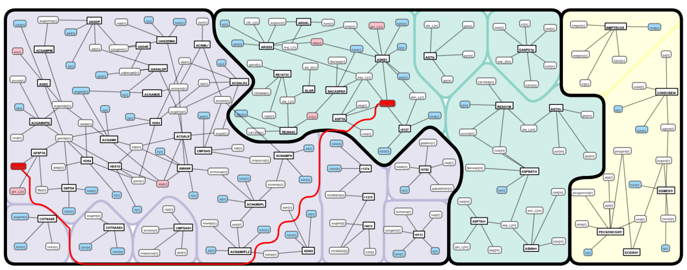
overlapped pixels = 0, total pixels = 1103350, edge crossings = 105.



(a-2)

$k_a = 0.1, k_r = 0.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

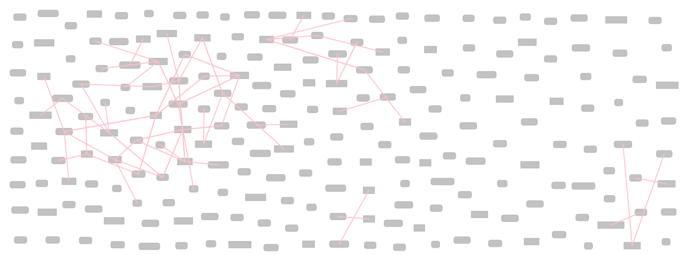
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 105.



(b-1)

$k_a = 0.1, k_r = 2000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

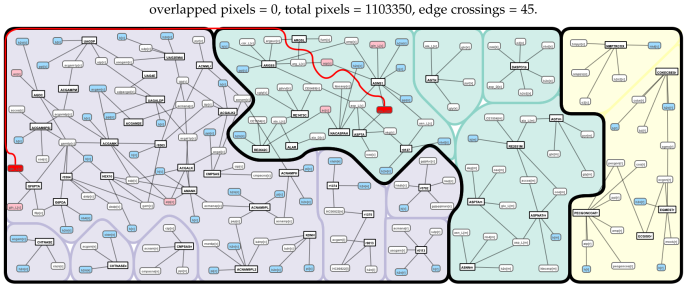
overlapped pixels = 0, total pixels = 1103350, edge crossings = 45.



(b-2)

$k_a = 0.1, k_r = 2000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

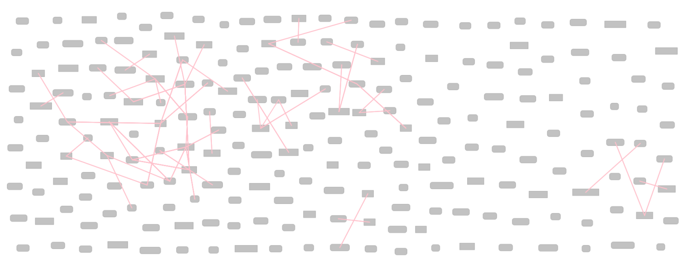
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 45.



(c-1)

$k_a = 0.1, k_r = 4000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 41.

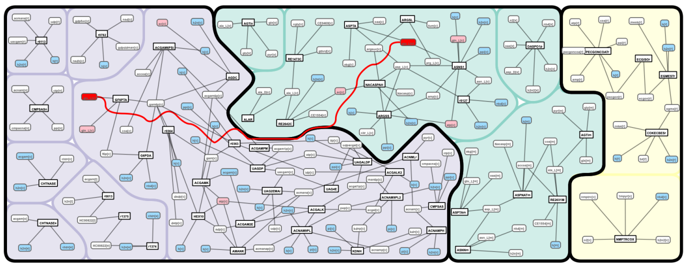


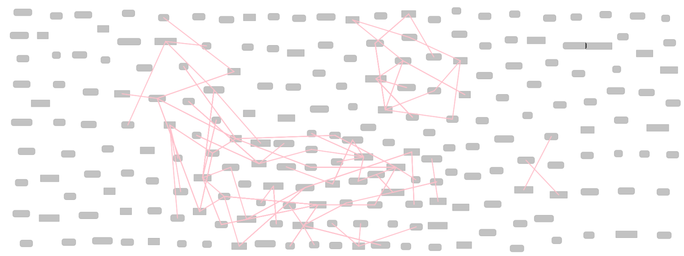
(c-2)

$k_a = 0.1, k_r = 4000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 41.

Fig. 28. The effect of parameters and the resulting overlaps in the detail-level step. The increase of k_r preserves the minimum distance between vertices in the final subgraphs. The adjustment of the parameter at this stage influences the final vertext distribution.





(a-1)

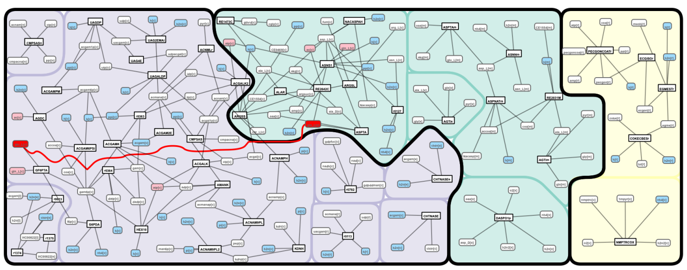
$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

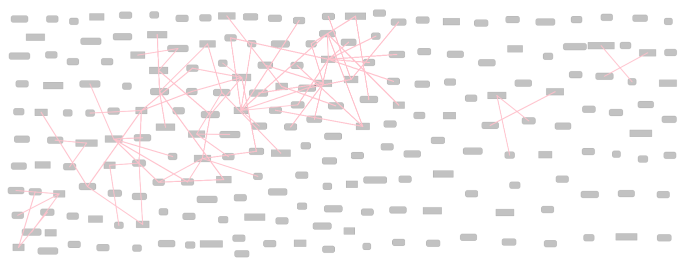
overlapped pixels = 28, total pixels = 1103350, edge crossings = 76.

(a-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 28, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 76.





(b-1)

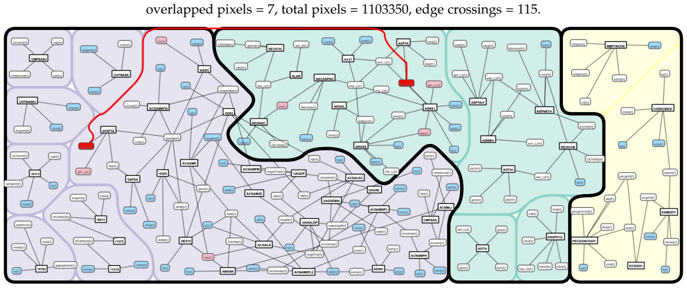
$k_a = 0.1, k_r = 1000.0, k_c = 2.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

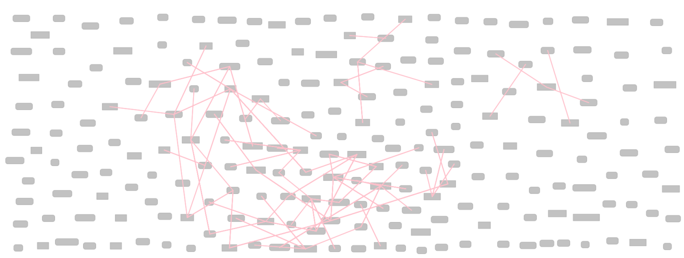
overlapped pixels = 7, total pixels = 1103350, edge crossings = 115.

(b-2)

$k_a = 0.1, k_r = 1000.0, k_c = 2.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 7, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 115.





(c-1)

$k_a = 0.1, k_r = 1000.0, k_c = 3.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

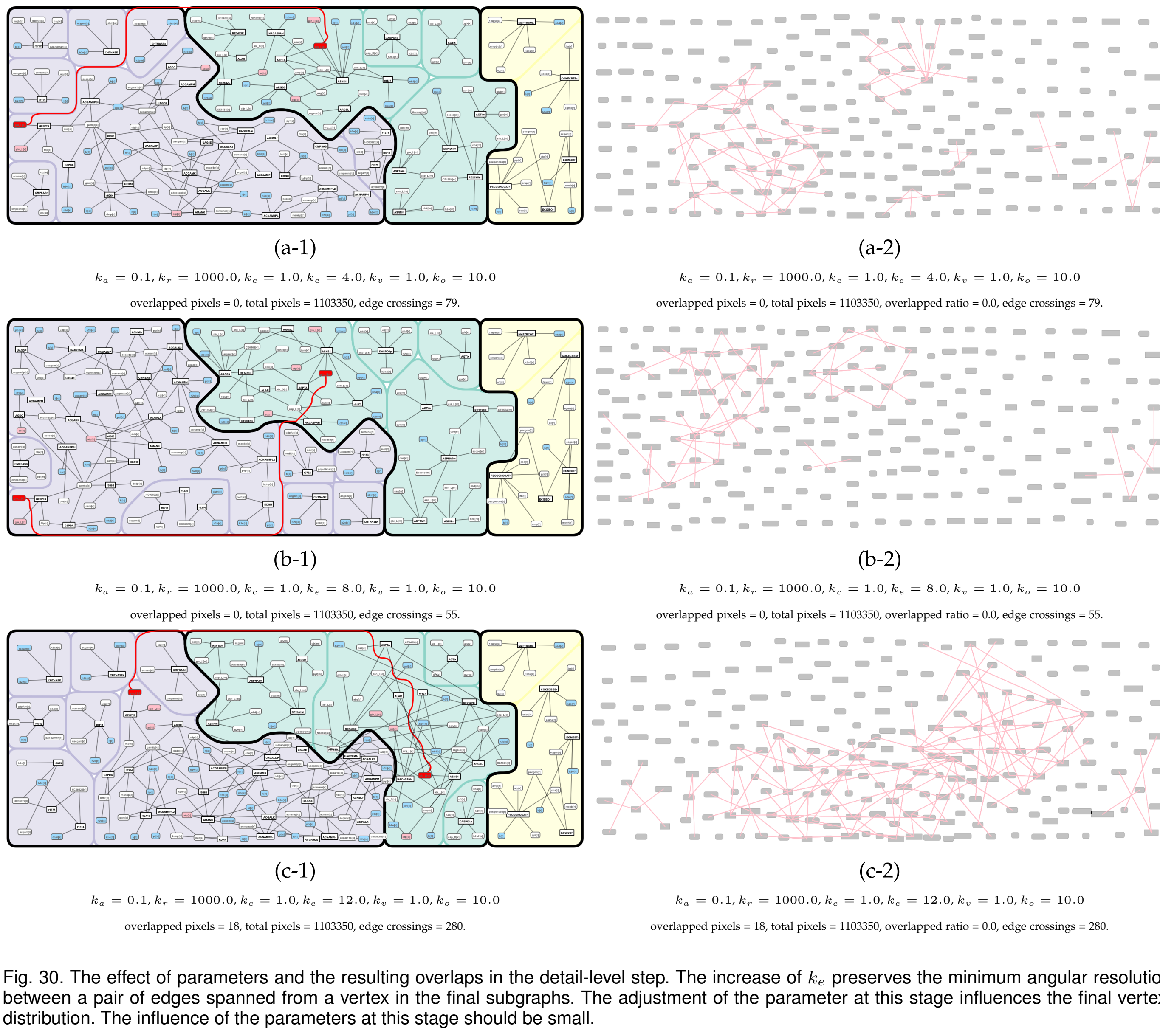
overlapped pixels = 0, total pixels = 1103350, edge crossings = 88.

(c-2)

$k_a = 0.1, k_r = 1000.0, k_c = 3.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 88.

Fig. 29. The effect of parameters and the resulting overlaps in the detail-level step. The increase of k_c preserves the minimum distance between a pair of edges spanned from a vertex in the final subgraphs. The adjustment of the parameter at this stage influences the final vertext distribution. The influence of the parameters at this stage should be small.



(a-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 79.

(a-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 79.

(b-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 8.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 55.

(b-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 8.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 55.

(c-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 12.0, k_v = 1.0, k_o = 10.0$

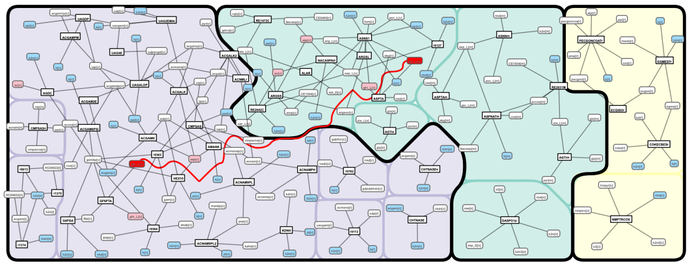
overlapped pixels = 18, total pixels = 1103350, edge crossings = 280.

(c-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 12.0, k_v = 1.0, k_o = 10.0$

overlapped pixels = 18, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 280.

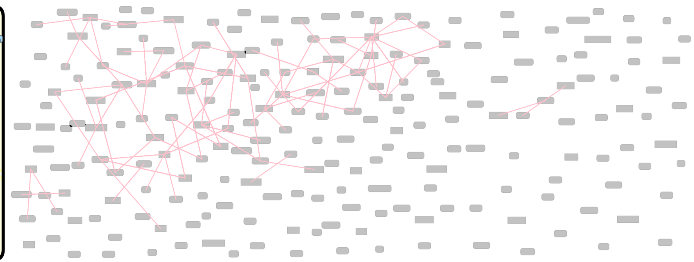
Fig. 30. The effect of parameters and the resulting overlaps in the detail-level step. The increase of k_e preserves the minimum angular resolution between a pair of edges spanned from a vertex in the final subgraphs. The adjustment of the parameter at this stage influences the final vertext distribution. The influence of the parameters at this stage should be small.



(a-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 0.0, k_o = 10.0$

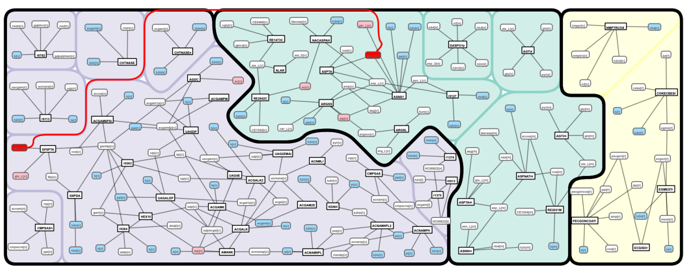
overlapped pixels = 41, total pixels = 1103350, edge crossings = 96.



(a-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 0.0, k_o = 10.0$

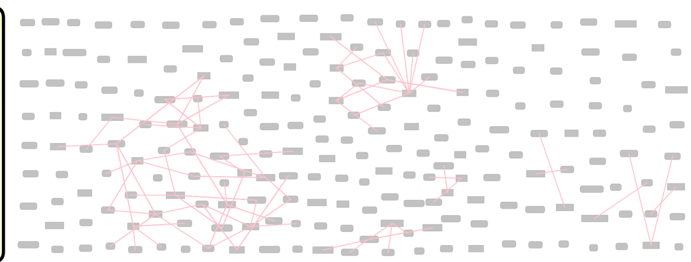
overlapped pixels = 41, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 96.



(b-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

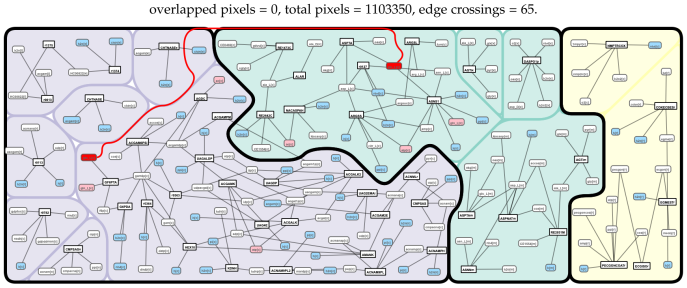
overlapped pixels = 0, total pixels = 1103350, edge crossings = 65.



(b-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

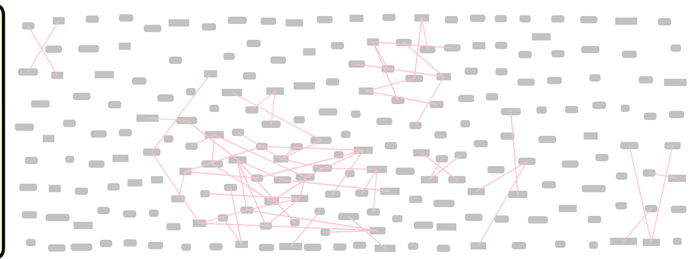
overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 65.



(c-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 2.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, edge crossings = 67.

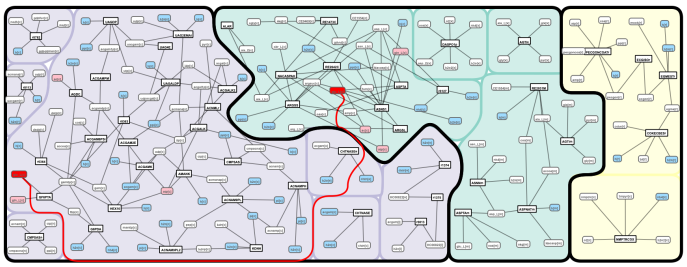


(c-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 2.0, k_o = 10.0$

overlapped pixels = 0, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 67.

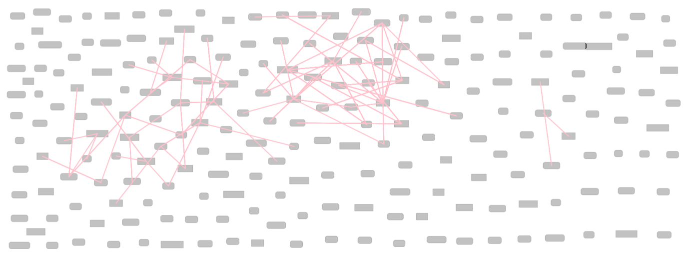
Fig. 31. The effect of parameters and the resulting overlaps in the detail-level step. The increase of k_v preserves the minimum area assigned to each vertex in the final subgraphs. The adjustment of the parameter at this stage influences the final vertext distribution.



(a-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

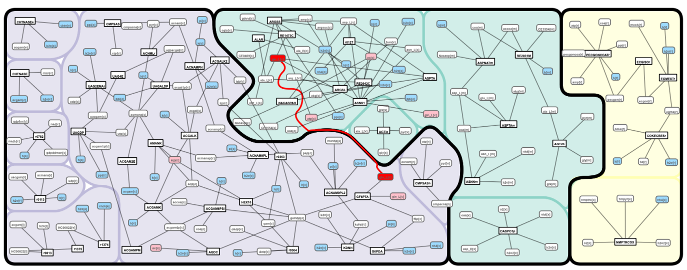
overlapped pixels = 28, total pixels = 1103350, edge crossings = 131.



(a-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 10.0$

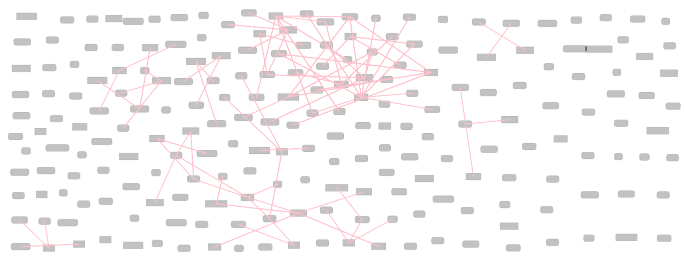
overlapped pixels = 28, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 131.



(b-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 20.0$

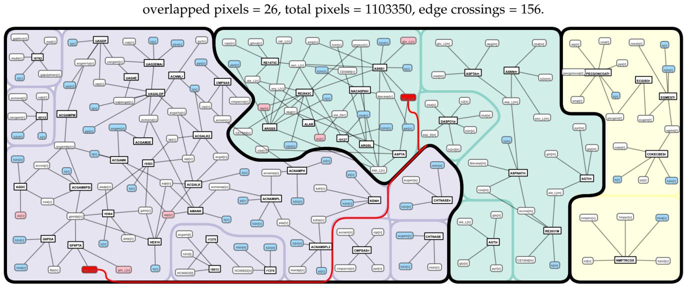
overlapped pixels = 26, total pixels = 1103350, edge crossings = 156.



(b-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 20.0$

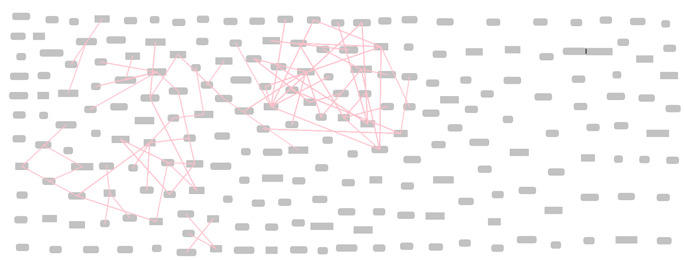
overlapped pixels = 26, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 156.



(c-1)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 30.0$

overlapped pixels = 25, total pixels = 1103350, edge crossings = 120.



(c-2)

$k_a = 0.1, k_r = 1000.0, k_c = 1.0, k_e = 4.0, k_v = 1.0, k_o = 30.0$

overlapped pixels = 25, total pixels = 1103350, overlapped ratio = 0.0, edge crossings = 120.

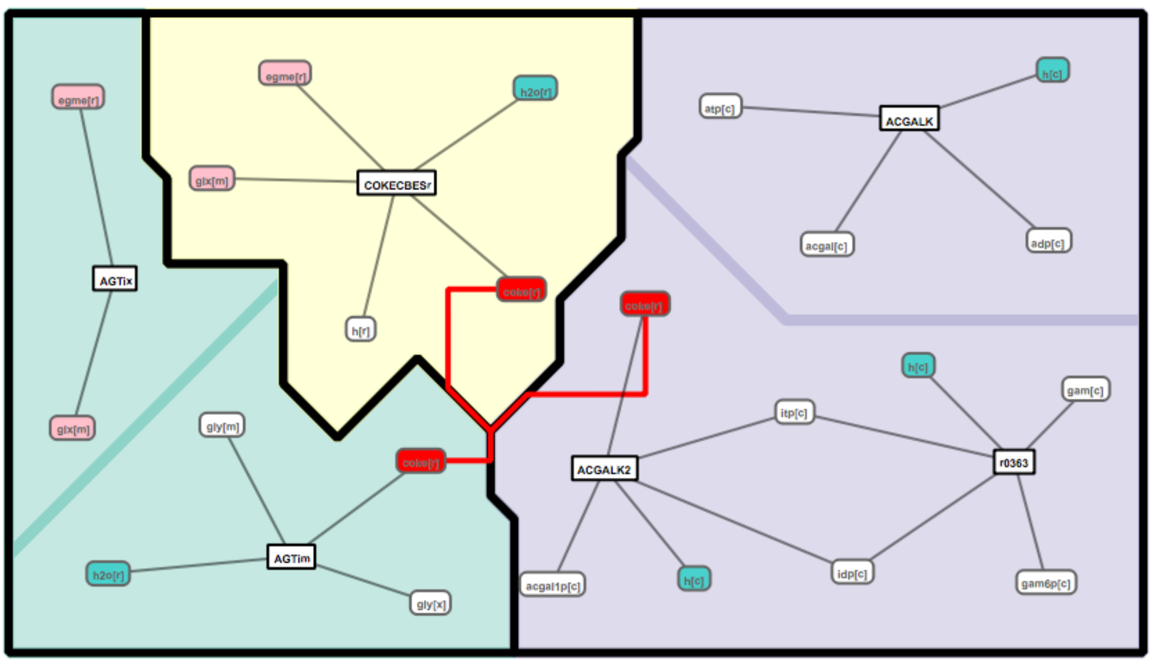
Fig. 32. The effect of parameters and the resulting overlaps in the detail-level step. The increase of k_o aims to remove the overlaps between each pair of vertexts in the final subgraphs. The adjustment of the parameter at this stage influences the final vertext distribution, especially avoiding the overlaps of vertexts.

11.3 User Study with Domain Experts and Discussion

Here we have included the questions that we asked and discussed with the domain experts. The findings have been summarized in Section 9.2.

This is a survey to evaluate the layout of clustered graphs generated using our new algorithm. During the survey, you will be asked several questions regarding layout quality. Please answer the questions as completely as possible. Scientific questions are on this page and personal info is on the second page. The survey takes about 15 minutes.

From now on, we will show several pathway diagrams, which describe biological interactions of molecules in a cell. There are two types of vertices: metabolites (labels with rounded corners) and reactions (labels with sharp corners). The edges indicate relationships between metabolites and reactions. The underlying background color represents the functional groups where metabolites and reactions belong to (e.g. “glutamate metabolism”, “citric acid cycle”, “urea cycle”, …)



Our design goal is to untangle a scale-free network and create a readable visual representation of a pathway diagram. This is achieved by incorporating three strategies,

including
(1) balanced vertex placement over the screen space,
(2) nice space partitioning with simplified boundaries, and

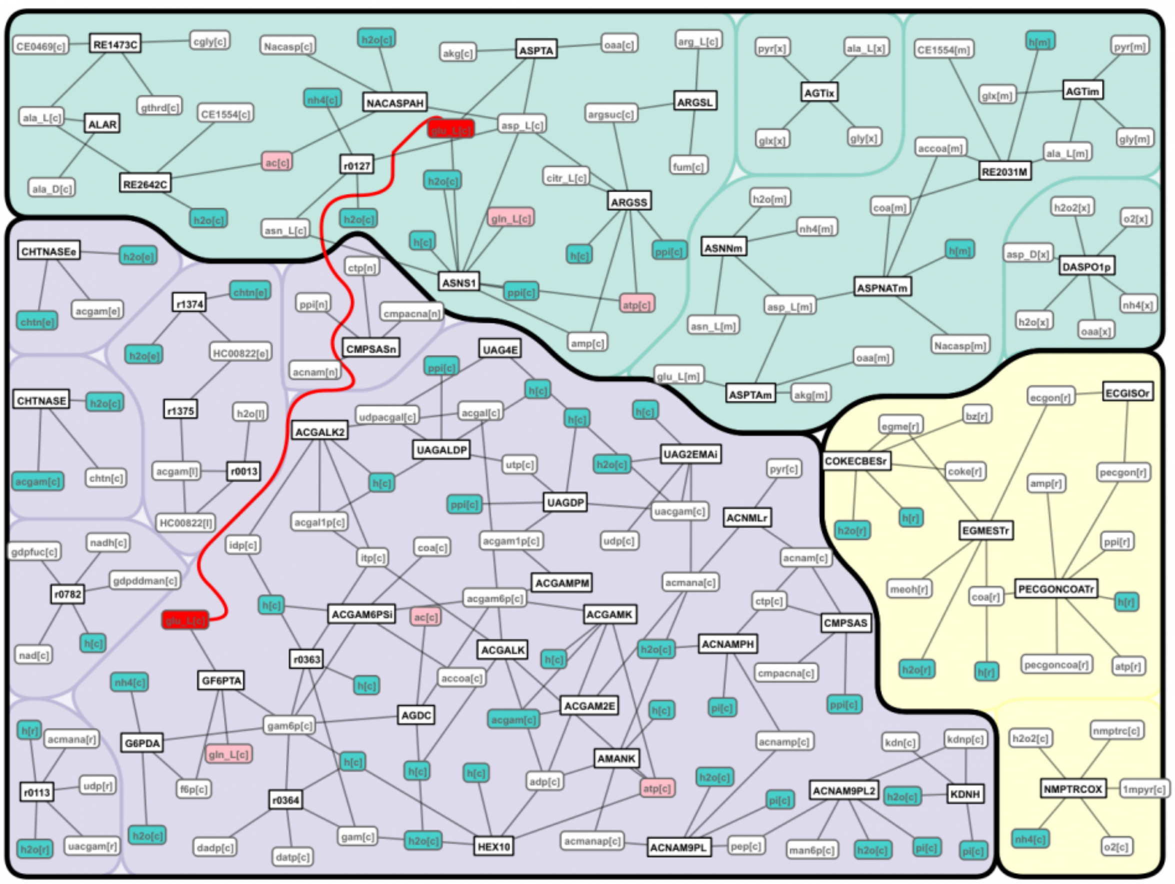
(3) vertex duplication scheme coupled with visual integration.

We borrowed the idea from a manually crafted pathway diagram where metabolites participate in many reactions are duplicated, creating disjoint clustered graphs and eliminating high-degree vertices. Due to this criterion, the metabolites in the above diagram are classified into 3 categories based on their frequency in the network: common=blue (e.g. H2O), special=pink (e.g. adp), and singular=white (e.g. gly). We also incorporate a spanning tree metaphor (coke[r] = red) to connect identical metabolites to accentuate corresponding adjacent neighbors.

In the following, we will show two examples.

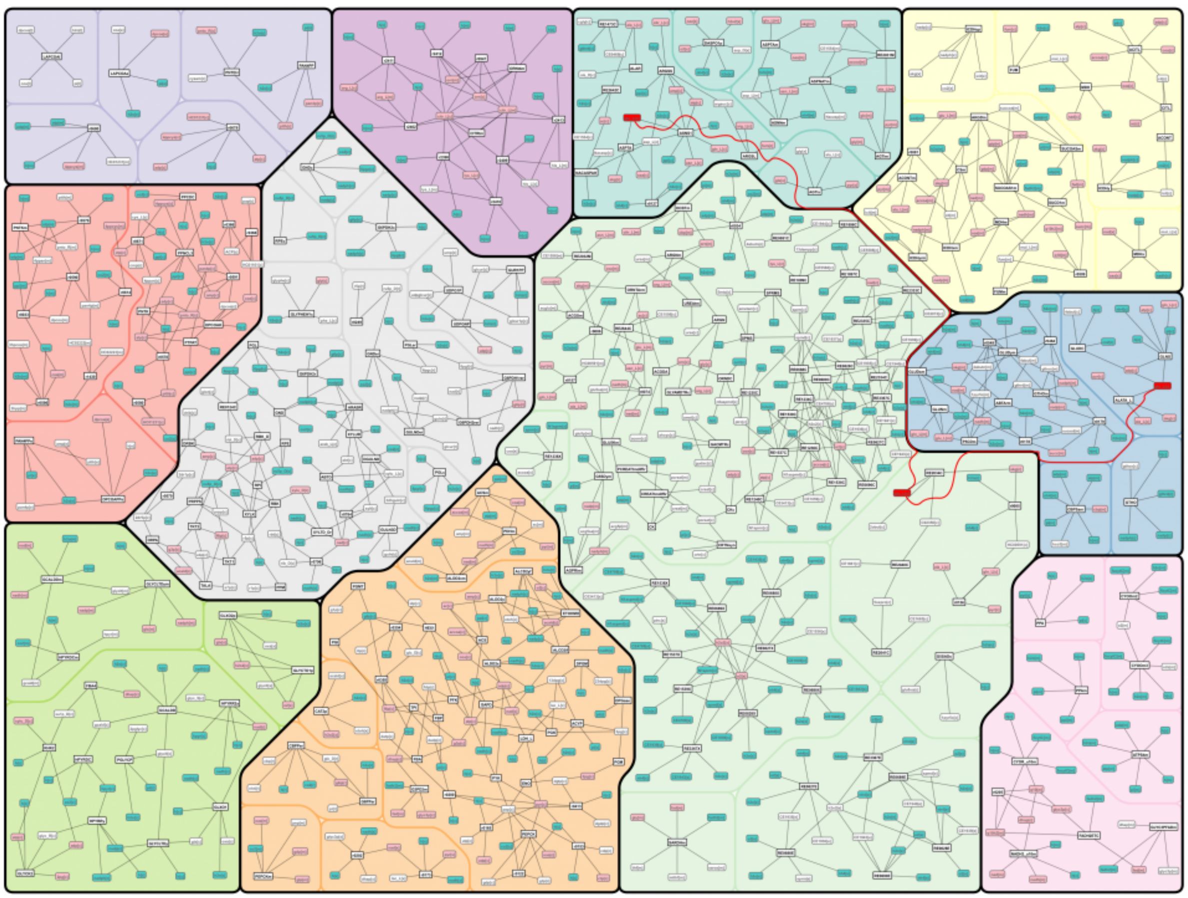
The first diagram represents a collection of pathways in human metabolism. Each connected component is enclosed with a contour.

Please investigate the following larger diagrams and answer the upcoming questions.
You can also open or download the images through the following links:
http://7zgbnh.myvserver.online/download/small-ours.png



This is another example.
The diagram represents a collection of pathways in human metabolism, including "Alanine and aspartate metabolism" (green) , "Citric acid cycle" (yellow), "CoA catabolism" (purple), "CoA synthesis" (red), "Glutamate metabolism" (blue), "Glycolysis-gluconeogenesis" (orange), "Glyoxylate and dicarboxylate metabolism" (grass green), "Oxidative phosphorylation" (pink), "Pentose phosphate pathway" (gray), "Transport, mitochondrial" (deep purple), and "Urea cycle" (light green). Each connected component is enclosed with a contour.

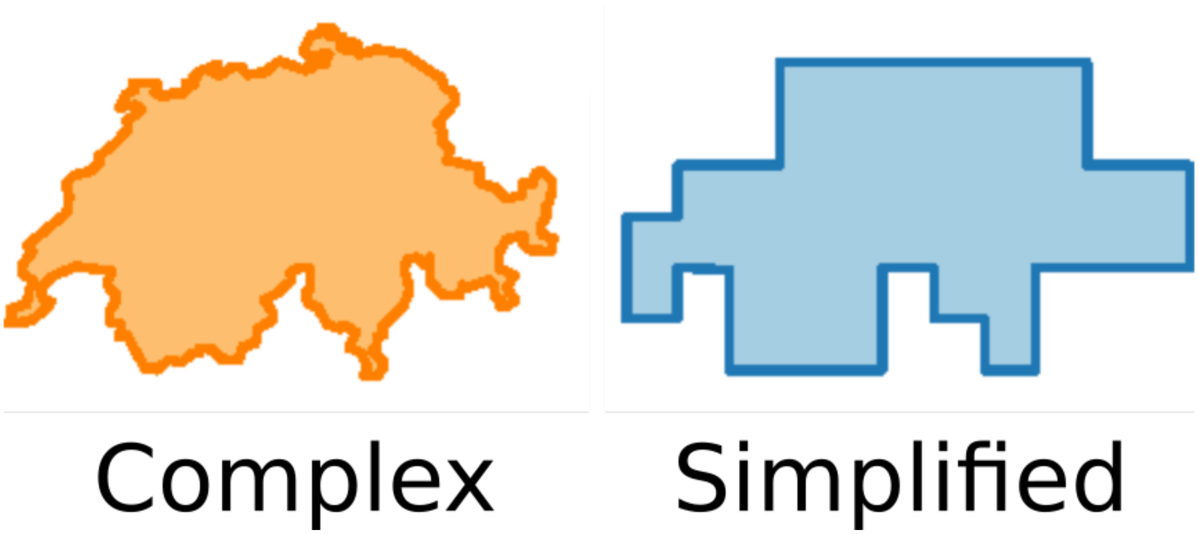
Please investigate the following larger diagrams and answer the upcoming questions.
You can also open or download the images through the following links:
http://7zgbnh.myvserver.online/download/metabolic-ours.png



Do you prefer to arrange textual labels to be:
(1) evenly distributed over the screen space,
(2) avoid textual label overlaps,
(3) retain strongly connected structures?

Please order these three criteria from most important to least important and explain why one is more important than the other. If you consider any criteria is not necessary, please mention it explicitly and explain why.

Do you think
having arbitrary boundaries to enclose each functional group helps clarify the types of metabolites and reactions? Do you prefer the boundary having a simplified or a complex contour shape? Please explain why.



Please write down your comments for the above question.

Based on your previous experience, is it permissible to duplicate unimportant/common vertices(e.g.,h2o) to reduce the visual clutter in a pathway diagram? Please explain why. If you think duplicating those vertices is a clear no go, could you also suggest other solutions?

Does connecting duplicated vertices with a spanning tree (red thick line) helps point out these duplicated vertices and their corresponding neighbors? Please explain why do you think yes or no.

One advantage of this approach is to fully lay out the graph based on the input aspect-ratio (width/height ratio of an image), do you think this is a useful function for you? For example, *during the network analysis* or *when putting the image in a report*.

Would you try the technique to lay out your graph if it is publicly available? Please explain why.

Please elaborate on the unsatisfactory portion of the layout. Why do you think these are critical for you?

Please enter any additional feedback regarding the layout. It would be great if can incorporate your wishes to improve our technique.

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Please fill in your basic personal information. Please note that we will keep the following information confidential and you can request to remove the personal information at any moment. We may put your personal information on scientific publication, so please let us know if you would like to appear anonymously.

Please enter your name and affiliation. e.g., Hsiang-Yun WU, TU Wien, Austria.

The years you have been working with pathway datasets. e.g., 10 years.

What is your education status?

- Ph.D.
- Senior researcher
- Professor
- Other

What is your major expertise?

- Biology
- Bioinformatics
- Chemistry
- Other

Thank you very much for your cooperation.
If you have any question, feel free to contact the following address.

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URL2: http://yun-vis.net/

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