Force Directed Graph Drawing Algorithms

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1 Introduction

The drawing of graphs, that satisfy some predefined conditions, is one of the most important topics in different fields of applications such as information visualisation or chip production. There are a lot of different techniques of drawing the „nice“ graphs. In this work we present two algorithms from class of force-directed graph drawing algorithms [6]. In the first section we consider the approach by T. Kamada and S. Kawai [5] from 1988 and in the second section the multi-scale algorithm by D. Harel and Y. Koren [3], which can be considered as extension of each force-directed graph drawing algorithm to deal with bigger graphs. In the last section we report the results of our implementations of both algorithms and compare them with the results from the underlying papers.

2 Algorithm by Kamada and Kawai

We implemented an algorithm for drawing general undirected graphs from [5]. In the following we refer to this algorithm as KKA (Kamada Kawai algorithm).
KKA visualizes connected, unweighted, undirected graphs as a 2 dimensional picture where the edges are drawn as straight lines between the vertices. The authors state objectives for their graph drawing algorithm:

1. uniform distribution of vertices and edges
2. preserve symmetric structures
3. low number of edge crossings

The first two objectives are more important for human understanding than the third one. Hence, the goal of KKA is to find a state where the vertices and edges are distributed uniformly. The objectives 2 and 3 often follow from that.
We can now describe an optimal drawing of a graph mathematically. We want to minimize the sum of the differences between the desirable (Euclidian) distances and the actual distances between all pairs of vertices. Now let $G = (V, E)$ be a undirected graph with $n = |V|$ vertices. We define $p_1, \dots, p_n$ as the projections into the 2 dimensional plane of the vertices $v_1, \dots, v_n \in V$. The appropriate mapping $L : V \to \mathbb{R}^2$ is called a layout of a graph G. We now define the energy function

$$E(p_1, \dots, p_n) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{1}{2} k_{ij} \{|p_i - p_j| - l_{ij}\}^2 \tag{1}$$

which models the imbalance of our drawing. We define $(d_{ij})_{i,j=1,\dots,n}$ as the matrix of pairwise distances between all vertices and $(l_{ij})_{i,j=1,\dots,n} = l \times d$ as a scaled distance matrix, where

constant l expresses the desired length of edges. The matrix $(k_{ij})_{i,j=1,\dots,n}$ is a weight matrix and its entries are defined by $k_{ij} = K/d_{ij}^2$, where K is some constant. Since our graphs are undirected, the matrices d, l and k are symmetric.
We want to find a local minimum of E, which is equal to the equilibrium state of the system. Consequently we are looking for p_m with

$$\frac{\partial E}{\partial p_m} = 0 \quad for\ m = 1, \dots, n.$$

This yields in $2n$ nonlinear equations. We set $p_m = (x_m, y_m)$ and solve the equation for every m by using the two-dimensional Newton-Raphson Method. The means we iterate

$$\begin{pmatrix} x_m^{t+1} \\ y_m^{t+1} \end{pmatrix} = \begin{pmatrix} x_m^t + \delta x \\ y_m^t + \delta y \end{pmatrix}.$$

and stop when $\Delta_m := \sqrt{\frac{\partial E}{\partial x_m}^2 + \frac{\partial E}{\partial y_m}^2}$ is smaller than a predefined ϵ for all m. The increments δx and δy are defined by

$$\begin{aligned} \frac{\partial^2 E}{\partial x_m^2}(x_m^t, y_m^t)\delta x + \frac{\partial^2 E}{\partial x_m \partial y_m}(x_m^t, y_m^t)\delta y &= -\frac{\partial E}{\partial x_m}(x_m^t, y_m^t), \\ \frac{\partial^2 E}{\partial y_m \partial x_m}(x_m^t, y_m^t)\delta x + \frac{\partial^2 E}{\partial y_m^2}(x_m^t, y_m^t)\delta y &= -\frac{\partial E}{\partial y_m}(x_m^t, y_m^t). \end{aligned} \tag{2}$$

This leads to the algorithm:

Algorithm 1 Kamada Kawai [5]

```
Compute the matrices d, l and k
initialize p_1, ..., p_n
while (max Δ_i > ε) do
    m = argmax Δ_i
    while Δ_m > ε do
        compute δx and δy
        iterate x_m = x_m + δx, y_m = y_m + δy
        compute Δ_m
    end while
    compute Δ_i for i = 1, ..., n
end while
```

3 A fast multi-scale algorithm by D. Harel and Y. Koren

The second algorithm we implemented is from D. Harel and Y. Koren [3] (further HKA), which also handles the problem of drawing an undirected graph $G = (V, E)$ with straight line edges.

The issue, the authors were dealing with, is the low speed of the most at the time force-directed drawing algorithms due to optimization of the quadratic energy function. This makes them almost inapplicable for large graphs with more than 1000 vertices. To cope with the speed problem the authors continued the approach from [2] and suggested new faster multi-scale algorithm.

The idea of their algorithm is very simple: instead of considering the whole graph G at ones, one builds an approximation sequence of coarse graphs $G^{k_1}, G^{k_2}, \ldots, G^{k_l},\ k_1 < k_2 < \cdots < k_l = |V|$ (*multi-scale representation of* G) and applies one of the simple force-directed drawing algorithms to draw those graphs nicely. Beautification of each scale provides a locally nice layout of G and the sequence of all locally nice layouts approximates the nice layout of G. We refer to the paper [3] for theoretical background of multi-scale representation of a graph, locally and globally nice layouts and describe here only the algorithm presented by the authors.

Algorithm

To build a coarse graph of a given graph G the authors suggest to cluster vertices of G in k groups, so that the distance between vertices in the same group is minimized. This corresponds to the simple observation, that the vertices, which are close to each other according to graph distances, should also be drawn closer.

The algorithm 2 provides a simple heuristic approach for the k-clustering problem. In the new coarser graph the vertices in one cluster will be merged together in a single vertex - corresponding cluster center.

Algorithm 2 K-Centers$(G(V, E), k)$ [3]

1: $S = \{v\}$ for some arbitrary $v \in V$
2: **for** $i = 2$ to k **do**
3: find u, such that $min_{s \in S} d_{us} > min_{s \in S} d_{ws}\ \forall w \in V$
4: $S = S \cup \{u\}$
5: **end for**
6: **return** S

For local layout beautification the KKA (see section 2) with two small changes was selected. First, the algorithm is running in predefined number of iterations without testing the condition in line 5, see algorithm 1. The second change is, that we consider only r-neighbourhood of each vertex, where r-neighbourhood of a vertex v is defined as $N^r(v) = \{u \in V | 0 \leq d_{uv} < r\}$. That means, that the energy function has now the form (compare to formula (1)):

$$E(p_1, \ldots, p_n) = \sum_{i \in V} \sum_{j \in N^r(i)} \frac{1}{2} k_{ij} \{|p_i - p_j| - l_{ij}\}^2 \tag{3}$$

The described variation of the Kamada and Kawai algorithm is summarized in algorithm 3.

Algorithm 3 LocalLayoutG($d_{V\times V}$, L, k, $Iterations$) [3]

1: **for** every $i = 1$ to $Iterations \cdot |V|$ **do**
2: $v = argmax_u\ \Delta_u^k$
3: compute δ_v^k by solving equations (2)
4: $L(v) = L(v) + (\delta_v^k(x), \delta_v^k(y))$
5: **end for**

The complete algorithm of Harel and Koren is listed below:

Algorithm 4 LayoutG(V,E) [3]

1: Set constants Rad, $Iterations$, $Ratio$, $MinSize$
2: Compute the all-pairs shortest length $d_{V\times V}$
3: Set up random layout L
4: $k = MinSize$
5: **while** $k \leq |V|$ **do**
6: $centers = \mathbf{K-Centers}(G(V,E), k)$
7: $radius = \max_{v\in centers} \min_{u\in centers} d_{vu} \cdot Rad$
8: **LocalLayout**$(d_{centers\times centers}, L(centers), radius, Iterations)$
9: **for** every $v \in V$ **do**
10: $L(v) = L(centers(v)) + rand$
11: **end for**
12: $k = k \cdot Ratio$
13: **end while**
14: **return** L

Notice, that there es a random noise ($(0,0) < rand < (1,1)$) added at line 10 to coordinates of vertices.

In the following section we represent the result of thr evaluation of both algorithms in our implementation on the examples from thr corresponding papers.

4 Implementation

The both described algorithms were implemented in Python (version 2.7.6) and included in a simple GUI for better visualisation purposes (see fig.1). The GUI was designed with QT Creator 3.2.2 and then bound with Python using PyQt version 4.11. The results of the evaluation were obtained on two different laptops, but we mention by each table with performance results the hardware specification of the corresponding laptop.

In our code we used the following additional libraries : *numpy* (version 1.8.2), *matplotlib* (version 1.3.1) and *scipy* (version 0.13.3). Our implementation is unfortunately poorly optimized, so that better optimized versions will probably perform better. Anyway we did some optimization, as the initial implementation contained a lot of loops, which are rather slow in Python. So we used a vectorization to get rid of loops in the realisation of described the algorithms.

It is also worth mentioning that the calculation of pairwise distance between all vertices of a given graph is extremely time consuming. In our implementation we first followed the idea in [5] and used Floyd's algorithm [1] for shortest paths. Since this has complexity $O(|V|^3)$ we also implemented a version of Dijkstras algorithm. For graphs with more than 1000 vertices we decided to use a heavily optimized version of Dijkstras algorithm from the *scipy* library. In both papers [5] and [3], where the algorithms were presented, this problem did not arise, because

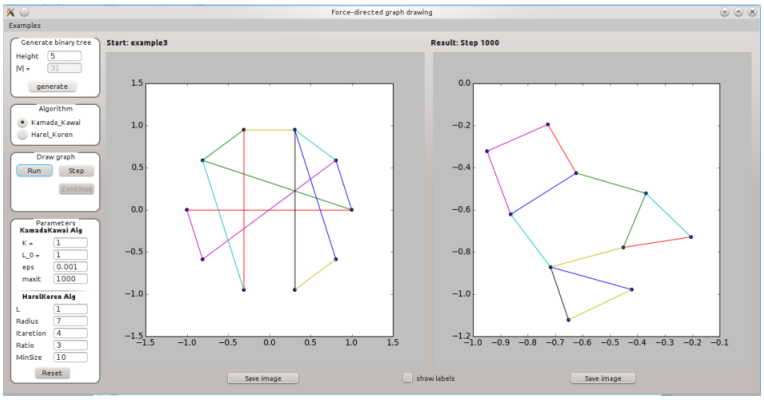


Figure 1: GUI

the first one only considers graphs with fewer vertices and in the second paper an additional library for efficient algorithms on graphs was used.

5 Evaluation results

As start layout we initialize vertices of the graph uniformly on a circle with radius L_0 (see [5]). That means viewed as complex variables we can write

$$p_m = L_0 \times e^{2pi*i*m/n},$$

but as it was mentioned in corresponding papers [5] and [3], the initial position of the vertices has no influence on the end result, as far vertices are not placed on a single line. Additionally, for some examples we load the initial positions of vertices from the corresponding input file (example of the 3elt graph from the collection of J.Petit [7])

We tested both algorithm with different graphs from [5] and [3].

Algorithm of Kamada and Kawai

In fig. 2 we show the initial state of a graph, the first two steps [1] and the state the graph converges to after 49 steps. In the first step the vertex v_2 gets moved to the middle. In the second step the vertex v_6 gets moved. After this we already have a graph without edge crossing. In the following steps the movements are smaller and lead to a symmetric graph, where all the edges have the same length.
We also reproduced the results from fig.3 b and fig. 5 in [5] (compare fig. 3 and fig. 4). It is interesting to see, that for the non symmetric graph on Fig 4 the algorithm did not succeed to reach the local minimum in the predefined number of iterations (1000). If we allow the algorithm to continue, it will only rotate the graph along its center without any changes in it's form.

In fig. 5 we plotted the result drawings of a binary tree achieved by both algorithms. The result achieved by KKA looks slightly better. We believe that for graphs with less than 100 vertices KKA is generally preferable.

Our performance results with KKA can be seen in table 1. Run time on an Intel Core i3-2310M CPU @ 2.10GHz × 4 . Parameters were set to $K = 1$, $L_0 = 1$, $\epsilon = 0.001$. We also included the results of HKA on the same graphs, which is faster, but it requires a careful

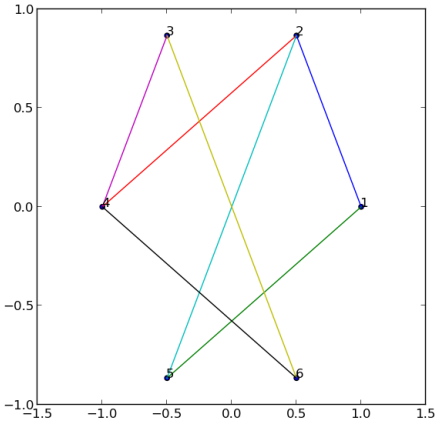
[1] we refer to one iteration of the outer loop as one step

Algorithm:		KKA with loops		KKA optimized		HKA	
Graph	$\|V\|$	Time	Iterations	Time	Iterations	Time	Iterations
Small Graph	6	0.169s	47	0.05s	53	-	-
Pyramid Graph	10	0.370s	45	0.05	46	0.021s	1
Non Symmetric Graph	10	FC	FC	FC	FC	0.024s	1
Binary Graph	7	0.136s	30	0.038s	31	-	-
Binary Graph	15	1.97s	131	0.11s	100	-	-
Binary Graph	31	17.745s	323	0.50s	366	0.032s	1

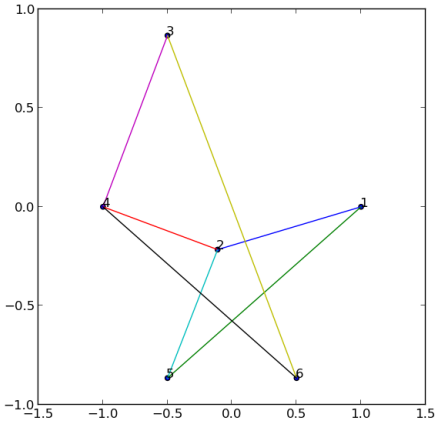
Table 1: Results of KKA

setting of parameters to reach nice drawings results. We omitted the results in cases, where the applying of the HKA was not successful.

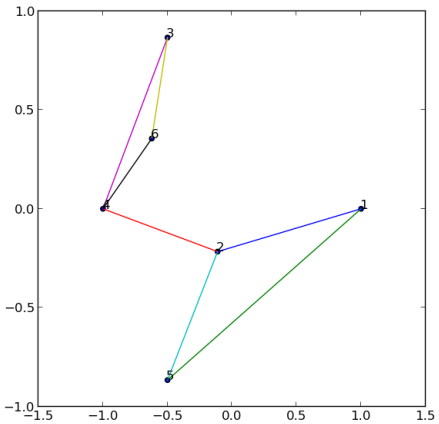
The table also illustrates the importance of vectorisation when working in python.



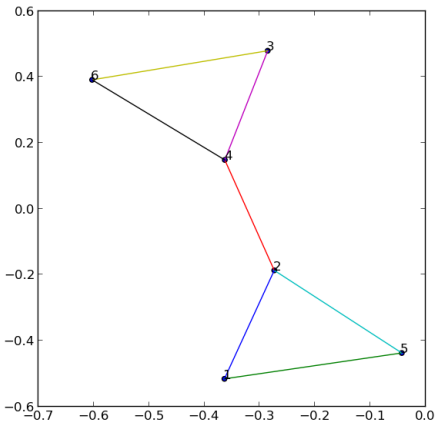
(a) Initial State



(b) Step 1

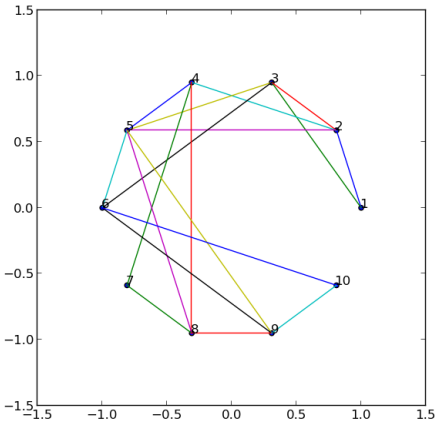


(c) Step 2

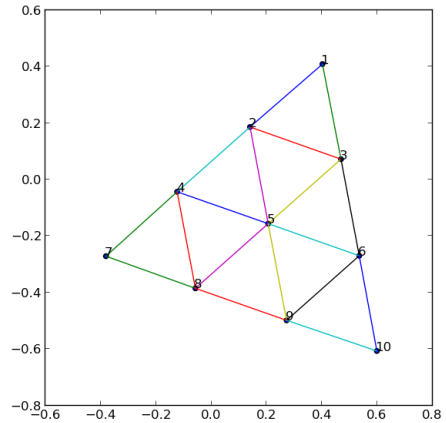


(d) Step 49

Figure 2: Drawing of a small graph in 4 different states, compare fig.2 in [5]

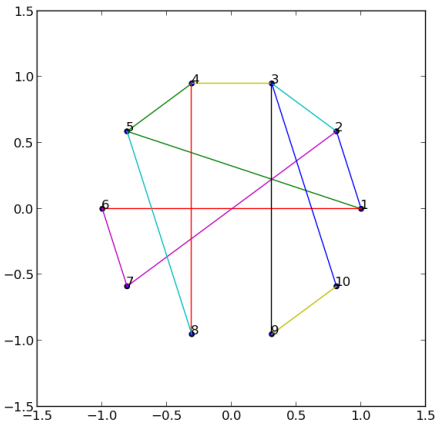


(a) Initial State

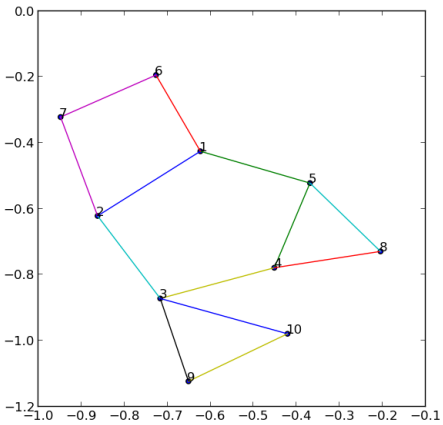


(b) State after 46 steps

Figure 3: Pyramid graph (compare fig.3*b* in [5])

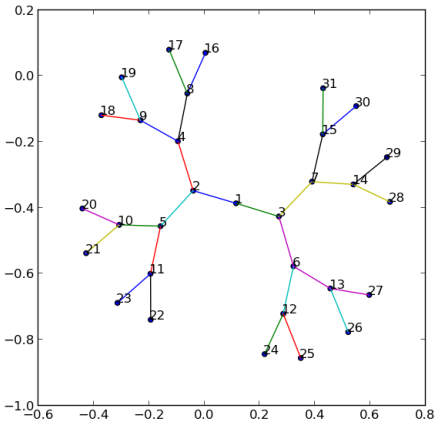


(a) Initial State

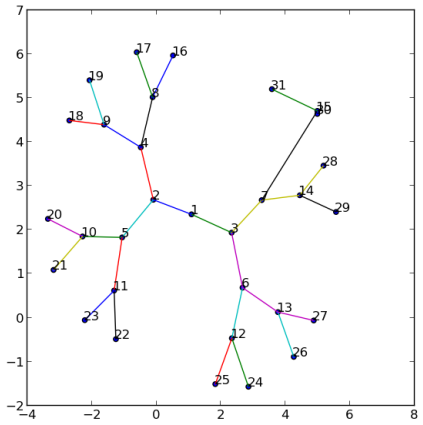


(b) State after $maxit = 1000$ steps

Figure 4: Non symmetric graph (compare fig.5 in [5])



(a) Result with KKA



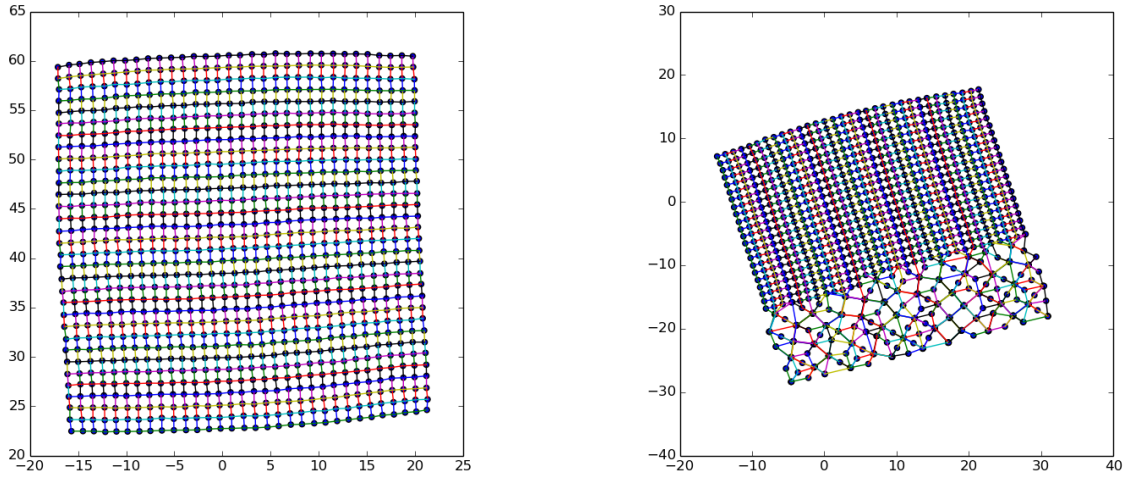
(b) Result with HKA

Figure 5: Full Binary tree of depth 5 for both algorithms

Algorithm of Harel and Koren

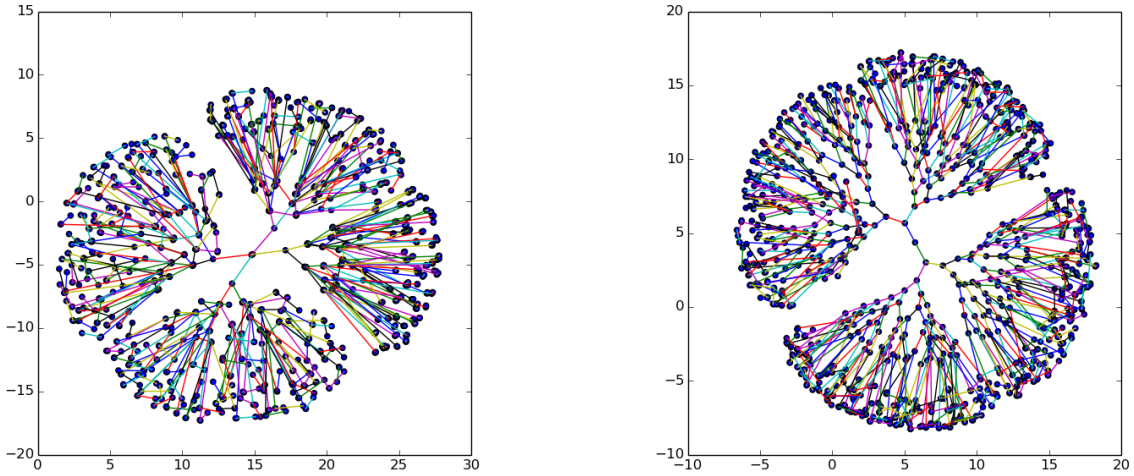
Compared with the KKA the algorithm of Harel and Koren includes 4 parameters: minimal size of the coarsest graph ($MinSize$), ratio between number of vertices in two consecutive levels ($Ratio$), number of iterations of local beautification ($Iterations$), size of the neighbourhood (Rad). As a further parameter one can consider the desired length of graph edges (l), but the authors do not mention it specially. The authors claim, that for all examples in their paper they used the following parameters: $MinSize = 10$, $Ratio = 3$, $Iterations = 4$, $Rad = 7$ (for the complete binary tree Rad was set to 16 or 17) and achieved reasonable results.

Unfortunately, that was not always the case in our evaluation. So on figure 6 one can see that in case of square grid graphs some vertices stay clustered after the final iteration of the algorithm with the default settings. On the other hand, in case of complete binary tree default settings deliver better drawing results (see 7).



(a) $MinSize = 2$, $Ratio = 2$ (b) $MinSize = 10$, $Ratio = 3$

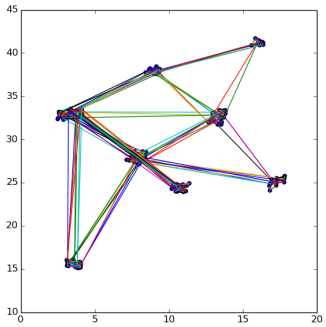
Figure 6: Square grid graph 32×32 (compare fig.1 in [3])



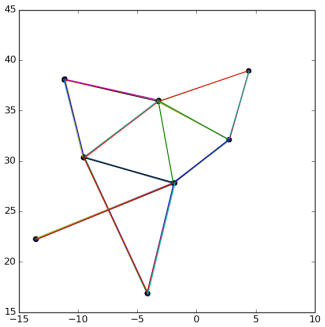
(a) $MinSize = 2$, $Ratio = 2$, $Rad = 18$ (b) $MinSize = 10$, $Ratio = 3$, $Rad = 18$

Figure 7: Complete binary tree with 1023 vertices (compare fig.6 in [3])

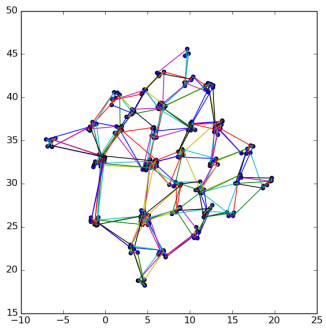
We also found out, that a random noise added to vertex coordinates (see line 10 in algorithm 4) has some impact on the end result. On fig. 8 one can see that adding smaller noise (for example from $(0, 0)$ to $(0.1, 0.1)$) leads to better drawing result in our implementation. Convinced by this result, we added factor 0.1 to *rand* in original algorithm.



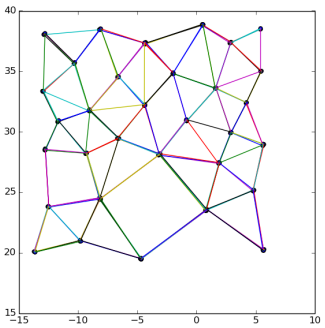
(a) Step 3



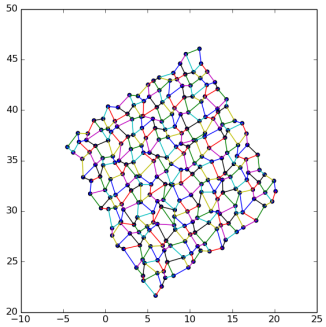
(b) Step 3



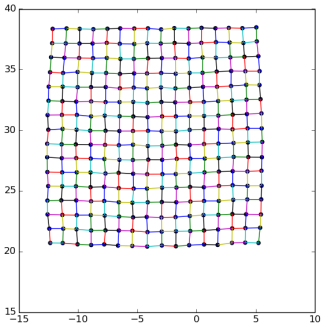
(c) Step 5



(d) Step 5



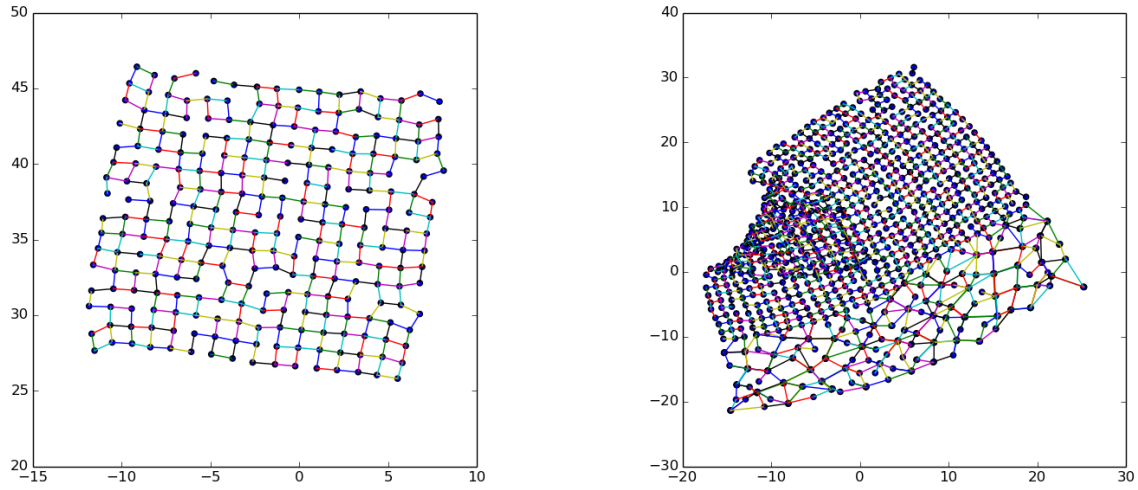
(e) Step 8



(f) Step 8

Figure 8: Influence of the random noise HKA on the example of grid graph 16×16. Left column : $(0, 0) < rand < (1, 1)$, right column - $(0, 0) < rand < (0.1, 0.1)$

In figure 9 we show the result of applying the HKA to the sparse grid graphs (1/3 of edges were omitted). Unfortunately, the images do not look so spectacular as in the original paper (see fig.4 in [3]).



(a) Sparse square grid graph 16×16 (256 vertices), $MinSize = 2$, $Ratio = 2$

(b) Sparse square grid graph 32×32 (1024 vertices), $MinSize = 10$, $Ratio = 3$

Figure 9: Sparse square grid graphs (compare fig.4 in [3]

The performance of our implementation of HKA can be seen in table 2. Computations were made on an Intel Core i7-3520M CPU @ 2.90GHz×4.

Algorithm HKA	$\|V\|$	Parameters	HKA	
Complete Binary Graph	255	$MinSize = 10$, $Ratio = 3$, $Rad = 18$	0.626503s	3
Complete Binary Graph	1023	$MinSize = 10$, $Ratio = 3$,$Rad = 18$	1402.674150s	5
Complete Binary Graph	1023	$MinSize = 2$, $Ratio = 2$, $Rad = 18$	261.274154s	9
Square Grid Graph	256	$MinSize = 2$, $Ratio = 2$	20.029714s	8
Square Grid Graph	256	$MinSize = 10$, $Ratio = 3$	0.615102s	3
Square Grid Graph	1024	$MinSize = 2$, $Ratio = 2$	3854.181407s	10
Square Grid Graph	1024	$MinSize = 10$, $Ratio = 3$	1403.437832s	5
Sparse Square Grid Graph	256	$MinSize = 2$, $Ratio = 2$	20.168194s	8
Sparse Square Grid Graph	1024	$MinSize = 10$, $Ratio = 3$	1439.099359s	5

Table 2: Results of HKA (optimized version) for large graphs

As we have alredy mentioned, our first implementation consisted of many loops. For example, before using verctorization the time needed to draw the complete binary three with 1023 vertices counted 30527.096519s comparing to 1402.674150s or 261.274154s after optimization.

6 Conclusions

We successfully implemented the algorithms described in [5] and [3] and were able to reproduce most of their results.

We found out that KKA is a good choice for drawing small graphs but takes too long for a high number of vertices.

HKA is much better suited for handling larger graphs. Unfortunately, in our implementation the HKA is not so fast, as it is mentioned in the paper. So we were not able to test it on the graphs with more then 1024 vertices in reasonable time. Also, using the same parameters for all graph types, as it was made in the paper [3], did not lead in our case to the equally good

results for all graphs. On the other hand, changing the parameters to get better results led to increased running time.
As we already have mentioned, our implementation could be better optimized. If we were to keep working on the graph drawing problem we see two possibilities. We could try to further optimize our implementation of HKA. However we might need to port it in $C++$ to achieve the same speed described in [3]. There the algorithm was initially implemeted in $C++$ using an additional library for efficient graph algorithms.

The more interesting thing to do would be to follow another idea by Harel and Koren and take a look at [4]. Here the authors propose a new approach where they first embed the graph in a high dimensional space and then project it into 2D using principal component analysis. This would lead us back to the theory we encountered in our Machine Learning lecture.

The impact on the implementation was divided uniquelly between the authors. The KKA was implemented and tested by Mr. Roeger, the HKA as well as the GUI by Mrs.Tikhoncheva. Additional functions such as reading the adjacency matrix and coordinates of the vertices from a file, generating of complete binary trees, floyd algorithm were implemented by Mr. Roeger.

After the first performance tests we encountered that the performance was rather poor. Therefore after discussion on the possible improvement the matrix approach suggested by Mr. Roeger was implemented by Mrs. Tikhoncheva.

References

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