Initial Placement for Fruchterman–Reingold Force Model with Coordinate Newton Direction

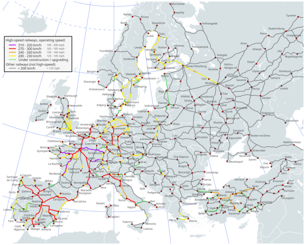
Hiroki Hamaguchi
5th lab
Supervisor: Prof. Akiko Takeda

2024/11/29

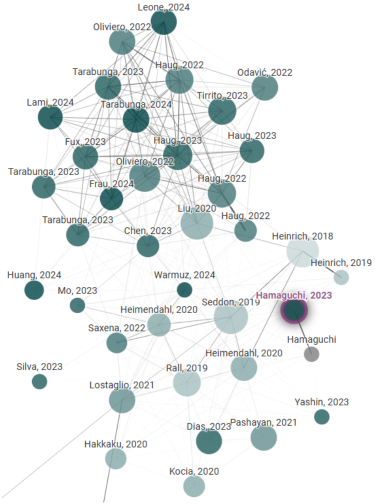
Introduction of Graph Drawing

Graph $G = (V, E)$ (vertices V / edges E)
Graph Drawing is an fundamental task.
Force-directed graph drawing is a popular method.

Social Network Graph
Designed by Freepik



Railroad Graph
By Bernese media, CC BY-SA 3.0



By CONNECTED PAPERS (Link)

Graph Drawing by NetworkX

Fruchterman–Reingold (FR) force model is prominent; flexible, intuitive, and simple.

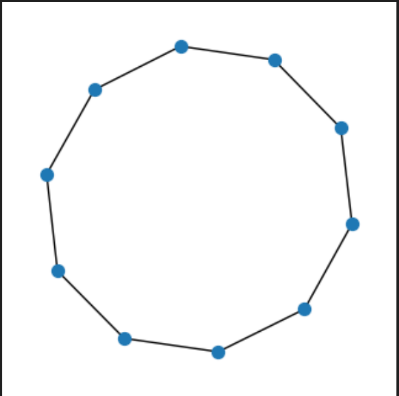
NetworkX [1] is a popular Python library.
`nx.draw`: **FR algorithm** works with 50 iterations.

$|V| = \ 10\text{:} \quad 0.2 \text{ sec } / \text{ Well Visualized}$

```python
import networkx as nx

G = nx.cycle_graph(10)
nx.draw(G, node_size=50)
```

✓ 0.2s



Graph Drawing by NetworkX

Fruchterman–Reingold (FR) force model is prominent; flexible, intuitive, and simple.

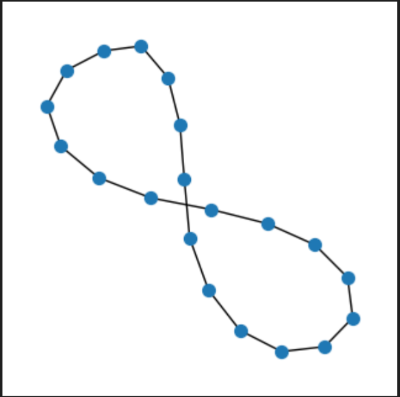
NetworkX [1] is a popular Python library.
`nx.draw`: **FR algorithm** works with 50 iterations.

$|V| = $ 10: 0.2 sec / Well Visualized
$|V| = $ 20: 0.2 sec / Tangled?

```python
import networkx as nx

G = nx.cycle_graph(20)
nx.draw(G, node_size=50)
```

✓ 0.2s

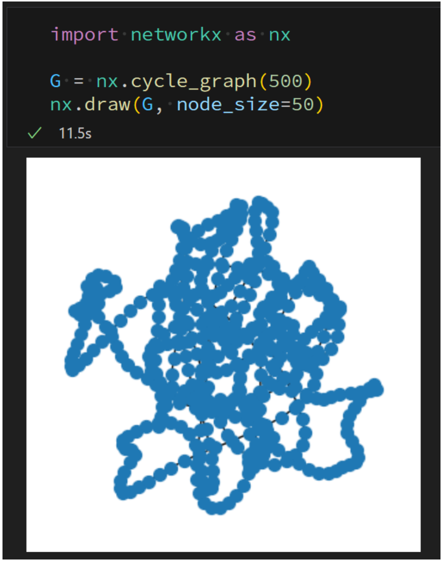


Graph Drawing by NetworkX

Fruchterman–Reingold (FR) force model is prominent; flexible, intuitive, and simple.

NetworkX [1] is a popular Python library.
`nx.draw`: **FR algorithm** works with 50 iterations.

$|V| = 10$: 0.2 sec / Well Visualized
$|V| = 20$: 0.2 sec / Tangled?
$|V| = 500$: 11.5 sec / WHAT IS THIS???

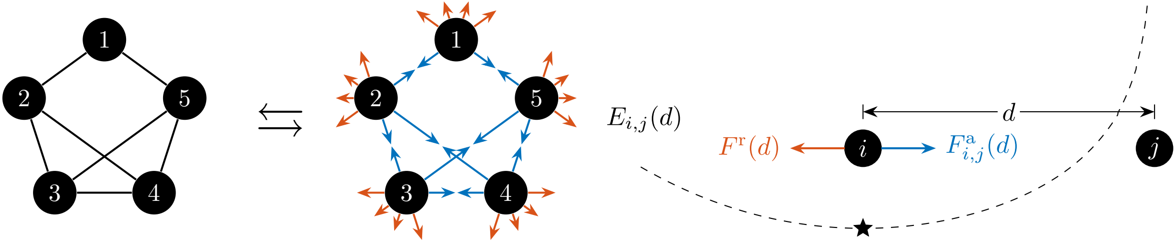


Fruchterman–Reingold Force Model

The **FR force model** uses a force model [2] with **a**ttractive force and **r**epulsive force:

$$F^{\mathrm{a}}_{i,j}(d) := \frac{w_{i,j} d^2}{k}, \quad F^{\mathrm{r}}(d) := -\frac{k^2}{d}.$$

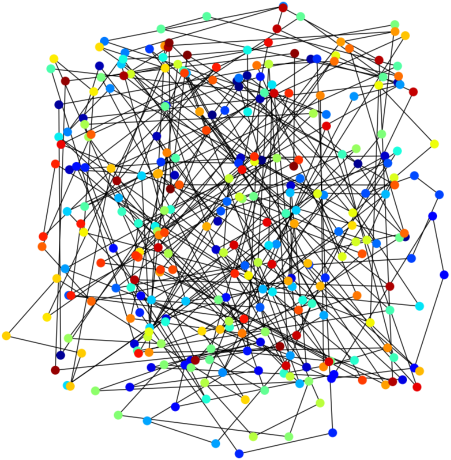
The **FR algorithm** seeks an **equilibrium** of two kind forces:



$$w_{i,j} > 0 \iff \{i,j\} \in E \qquad d = \|x_i - x_j\|$$

"Twist" Causes Stagnation

Twist: unnecessary folded and tangled structures [3, 4].
$\rightarrow$ Causing stagnation of the simulation process.
Slow for large-scale graphs. $\mathcal{O}\left(|V|^2\right)$ per iteration.



Previous Works (1/2) - L-BFGS

L-BFGS (Quasi-Newton Method) [5]

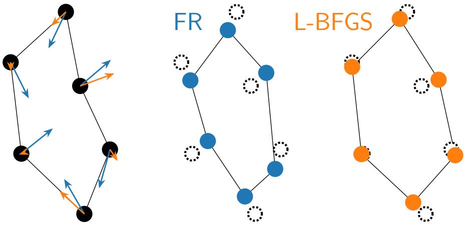
Numerical optimization approach.
Overcome "twist" issues to some extent.
Effective for reducing stress.

Limitations

May fail to achieve the optimal visualization.
Treats just as a general optimization problem.
Start from **a random initial placement**.

Our Aim

Accelerate by improving initial placement.



$$n := |V|, \quad X = (x_1, x_2, \ldots, x_n),$$

$$\min_{X \in \mathbb{R}^{2 \times n}} f(X) \to \min_{\overline{X} \in \mathbb{R}^{2n}} \overline{f}(\overline{X})$$

Previous Works (2/2) - Simulated Annealing

Simulated Annealing (SA) [6]

- Providing an initial placement
- Effective for addressing "twist" issues.

Limitations

- Restricted to unweighted graphs.
- Limited to circle placement.
- Inefficient due to random swapping.
- Ignored sparsity of graphs.

Our Aim

- Improve the strategy.
- Extend the applicability.

$$
\begin{aligned}
\underset{X \in \mathbb{R}^{2\times n}}{\text{minimize}} \quad & \sum_{\{i,j\} \in E \cup E_2} |\angle(x_i, x_j)|, \\
\text{subject to} \quad & x_i \in Q^{\text{circle}} \quad \text{for } 1 \le i \le n, \\
& x_i \ne x_j \quad \text{for } 1 \le i < j \le n.
\end{aligned}
$$

$Q^{\text{circle}} := \{(\cos(2\pi i/n), \sin(2\pi i/n)) \mid 1 \le i \le n\}$
E_2: a set of vertex pairs with a shortest path distance equal to 2. $|E_2|$ **could be** $\Theta(n^2)$.

$\angle(a, b)$: the angle between the lines from the origin to the points a and b.

Our Contribution

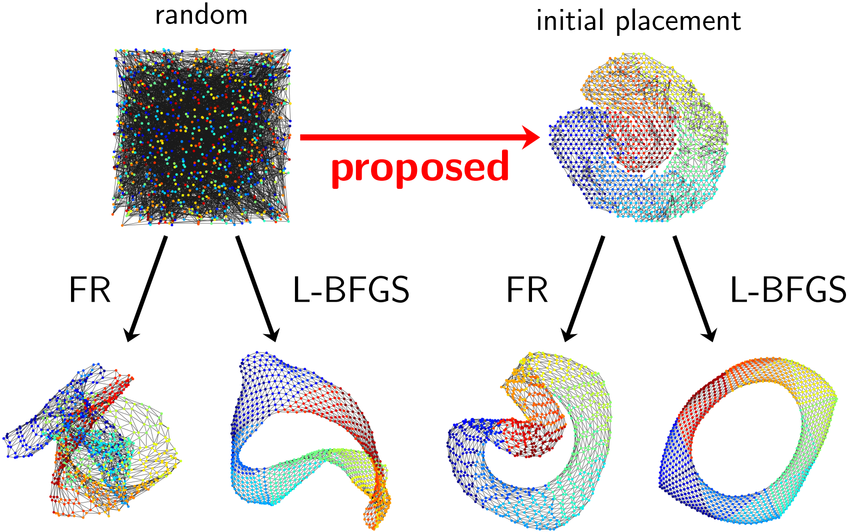
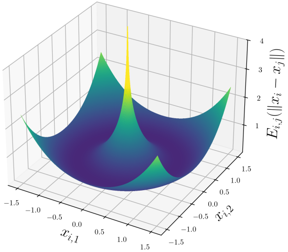


Figure: `jagmesh1` dataset after 50 iterations.

Formulation of the Problem



The two forces in the FR force model:

$$F^{\mathrm{a}}_{i,j}(d) := \frac{w_{i,j} d^2}{k}, \quad F^{\mathrm{r}}(d) := -\frac{k^2}{d}.$$

Its scalar potential, energy, is defined as

$$E^{\mathrm{a}}_{i,j}(d) := \int_0^d F^{\mathrm{a}}_{i,j}(r)\,\mathrm{d}r = \frac{w_{i,j} d^3}{3k}, \quad E^{\mathrm{r}}(d) := \int_\infty^d F^{\mathrm{r}}(r)\,\mathrm{d}r = -k^2 \log d,$$

$$E_{i,j}(d) := E^{\mathrm{a}}_{i,j}(d) + E^{\mathrm{r}}(d).$$

Seek equilibrium $\Leftrightarrow$ **find local minimum of** $f(X)$ (**non**-convex):

$$\underset{X \in \mathbb{R}^{2 \times n}}{\text{minimize}} \quad f(X) := \sum_{i<j} E_{i,j}(\|x_i - x_j\|). \tag{1}$$

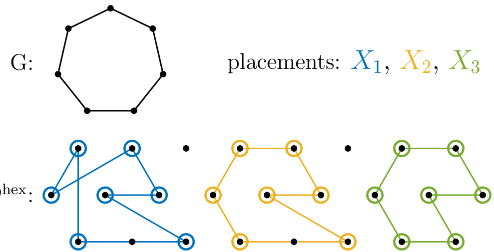
Simplify the Problem (1/2)

Obtain approximated solution quickly. Instead of the problem (1), we solve:

$$\begin{aligned} \underset{X \in \mathbb{R}^{2\times n}}{\text{minimize}} \quad & \sum_{\{i,j\}\in E} \frac{w_{i,j}\|x_i - x_j\|^3}{3k}, \\ \text{subject to} \quad & x_i \in Q^{\text{hex}} \quad \text{for } 1 \le i \le n, \\ & x_i \ne x_j \quad \text{for } 1 \le i < j \le n. \end{aligned} \tag{2}$$

where

$$Q^{\text{hex}} := \left\{ \left(q + \tfrac{1}{2} r, \tfrac{\sqrt{3}}{2} r \right) \,\middle|\, q \in \mathbb{Z}, r \in \mathbb{Z} \right\}.$$



We explain the reason. We simplify the problem (1). Separate $f(X)$ into $E^{\text{a}}_{i,j}$ and E^{r}.

$$\underset{X \in \mathbb{R}^{2\times n}}{\text{minimize}} \quad \sum_{\{i,j\}\in E} \frac{w_{i,j}\|x_i - x_j\|^3}{3k} - \sum_{i<j} k^2 \log \|x_i - x_j\|.$$

Simplify the Problem (2/2)

Following previous research, fix the possible positions x_i to a discrete points set Q:

$$\begin{aligned}\underset{X\in\mathbb{R}^{2\times n}}{\text{minimize}} \quad & \sum_{\{i,j\}\in E}\frac{w_{i,j}\|x_i-x_j\|^3}{3k}-\sum_{i<j}k^2\log\|x_i-x_j\|,\\ \text{subject to} \quad & x_i\in Q \quad \text{for } 1\le i\le n,\\ & x_i\ne x_j \quad \text{for } 1\le i<j\le n.\end{aligned}$$

$|\{\{i,j\} \text{ s.t. } \{i,j\}\in E\}| \ll |\{\{i,j\} \text{ s.t. } i<j\}|$. We want to drop the second term.
Take Q such that $\|q_i-q_j\|\ge\epsilon$ for all $q_i,q_j\in Q (q_i\ne q_j)$. Then, the second term is negligible.

$$\begin{aligned}\underset{X\in\mathbb{R}^{2\times n}}{\text{minimize}} \quad & f^{\mathrm{a}}(X):=\sum_{\{i,j\}\in E}\frac{w_{i,j}\|x_i-x_j\|^3}{3k},\\ \text{subject to} \quad & x_i\in Q \quad \text{for } 1\le i\le n,\\ & x_i\ne x_j \quad \text{for } 1\le i<j\le n.\end{aligned}$$

Only treat **a**ttractive force. Thus, the points set Q should be as dense as possible.
$\rightarrow$ **closet packing** (hexagonal lattice Q^{hex}).

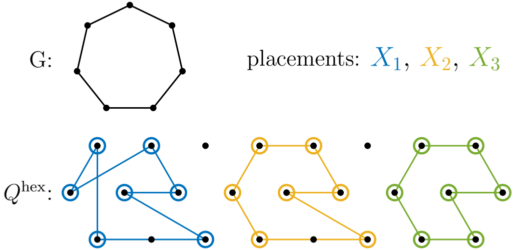
Summary of the First Half

The problem is

$$\underset{X \in \mathbb{R}^{2\times n}}{\text{minimize}} \quad f(X) := \sum_{i<j} E_{i,j}(\|x_i - x_j\|) = \sum_{\{i,j\}\in E} \frac{w_{i,j}\|x_i - x_j\|^3}{3k} - \sum_{i<j} k^2 \log \|x_i - x_j\|. \quad (1)$$

We simplify the problem as

$$\begin{aligned} \underset{X \in \mathbb{R}^{2\times n}}{\text{minimize}} \quad & f^{\mathrm{a}}(X) := \sum_{\{i,j\}\in E} \frac{w_{i,j}\|x_i - x_j\|^3}{3k}, \quad (2) \\ \text{subject to} \quad & x_i \in Q^{\mathrm{hex}} \quad \text{for } 1 \le i \le n, \\ & x_i \neq x_j \quad \text{for } 1 \le i < j \le n. \end{aligned}$$



We will explain how to solve in the second half.

Base of Proposed Algorithm - Stochastic Coordinate Descent

Let $f : \mathbb{R}^n \to \mathbb{R}$ be strictly convex. The second order approximation at x_0 is

$$f(x) \approx f(x_0) + \nabla f(x_0)^\top (x - x_0) + \frac{1}{2}(x - x_0)^\top \nabla^2 f(x_0)(x - x_0).$$

The minimum x^* satisfies

$$\begin{aligned} &\nabla f(x_0) + \nabla^2 f(x_0)(x^* - x_0) = 0 \\ \iff &x^* = x_0 - \nabla^2 f(x_0)^{-1} \nabla f(x_0). \qquad \textbf{(Newton direction)} \end{aligned}$$

Although it is effective, computing the Newton direction is **too expensive**...

We use the **stochastic coordinate descent** with the **coordinate Newton direction**.
Let $f_i(x_i)$ be the limitation to the i-th coordinate (randomly selected).
The coordinate Newton direction: $d_i = -\nabla^2 f_i(x_i)^{-1} \nabla f_i(x_i)$. $\leftarrow$ **Cheap! Computable!**

Proposed Algorithm (1/3) - Coordinate Newton Direction

We solve the problem (2) using **the coordinate Newton direction.**
Let $f_i^{\mathrm{a}}(x_i)$ corresponding to a vertex v_i be

$$f_i^{\mathrm{a}}(x_i) := \sum_{j \neq i} \frac{w_{i,j} \|x_i - x_j\|^3}{3k}.$$

Its gradient and Hessian matrix are

$$\nabla f_i^{\mathrm{a}}(x_i) = \sum_{j \neq i} \frac{w_{i,j} \|x_i - x_j\|}{k} (x_i - x_j),$$

$$\nabla^2 f_i^{\mathrm{a}}(x_i) = \sum_{j \neq i} \frac{w_{i,j} \|x_i - x_j\|}{k} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sum_{j \neq i} \frac{w_{i,j}}{k \|x_i - x_j\|} (x_i - x_j)(x_i - x_j)^\top.$$

f_i^{a} is **strictly convex**. Different from $E_{i,j}(\|\cdot - x_j\|)$ in (1) and $f^{\mathrm{a}}(\cdot)$ in (2) (non-convex).

Proposed Algorithm (2/3) - Update Rule

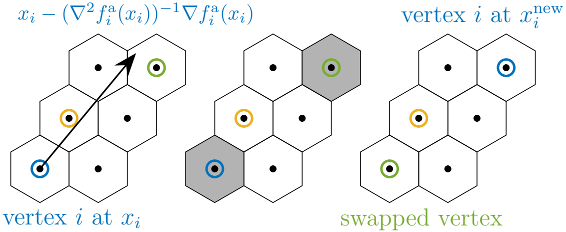
Ordinary updated rule:

$$x_i^{\mathrm{new}} \leftarrow x_i - \nabla^2 f_i^{\mathrm{a}}(x_i)^{-1} \nabla f_i^{\mathrm{a}}(x_i).$$

x_i^{new} may not be in the hexagonal lattice Q^{hex}. Need rounding to the nearest point in Q^{hex}.
We empirically found that adding a random noise is effective.

$$x_i^{\mathrm{new}} \leftarrow \mathrm{round}\left(x_i - \nabla^2 f_i^{\mathrm{a}}(x_i)^{-1} \nabla f_i^{\mathrm{a}}(x_i) + t \cdot \mathsf{rand}\right),$$

($\mathrm{round}(\hat{x})$: the operation assigning $\hat{x}$ to the nearest point in Q^{hex},
rand is a random vector with a unit norm, and t is a parameter controlling the randomness.)



Proposed Algorithm (3/3) - Optimal Scaling

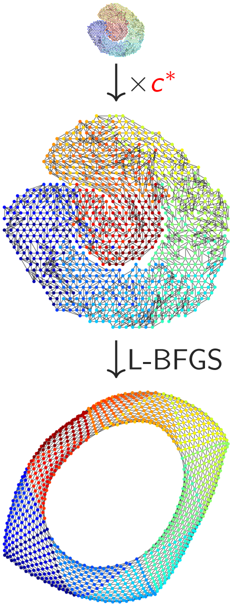
We can find optimal scaling factor c^*. We scale $X = (x_1, \ldots, x_n)$ as $x_i \leftarrow cx_i$ for all i. This problem is to minimize $\phi(c)$:

$$\phi(c) := \left(\sum_{\{i,j\} \in E} \frac{w_{i,j}(c\|x_i - x_j\|)^3}{3k} \right) - k^2 \sum_{i<j} \log(c\|x_i - x_j\|)$$

$\phi(c)$ is convex, and the optimal scaling factor c^* by

$$c^* = \left(\frac{k^2 n(n-1)}{2 \sum_{\{i,j\} \in E} \frac{w_{i,j}\|x_i - x_j\|^3}{k}} \right)^{1/3}. \tag{3}$$

This value can be computed in the $\mathcal{O}(|E|)$ complexity.
As far as we rescale the placement by c^*,
we can select any ϵ to define the hexagonal lattice Q^{hex}.



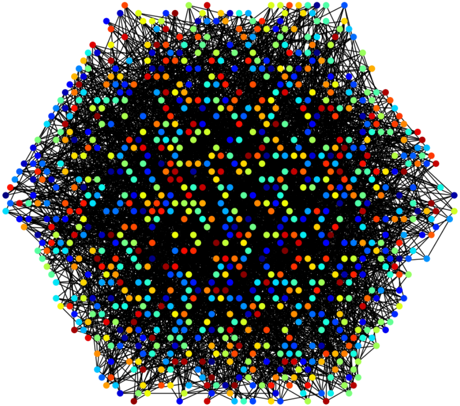
Pseudo Code

Algorithm 1: Proposed algorithm as initial placement

Input: Graph $G = (V, E)$, Weight $(w_{i,j})_{\{i,j\}\in E}$, Parameters $N_{\mathrm{iter}}^{\mathrm{CN}} \in \mathbb{N}$, $t_0 > 0$
Output: Initial placement $X = (x_1, \ldots, x_n)$

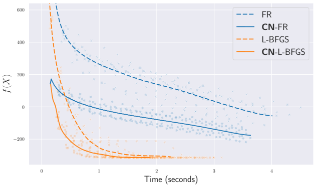
```
t ← t_0;
Sample x_i ∈ Q for all i ∈ V without replacement;
for m ← 0 to N_iter^CN do
    Select vertex i ∈ V randomly;
    x_i^new ← round(x_i − ∇²f_i(x_i)^{-1} ∇f_i(x_i) + t · rand);
    if ∃j ∈ V s.t. x_j = x_i^new then
        Swap x_i and x_j;
    else
        x_i ← x_i^new;
    t ← t − t_0 / N_iter^CN;
x_i ← c* x_i for all i ∈ V with c* by Eq.(3);
return X
```

Experiments Result (gif)

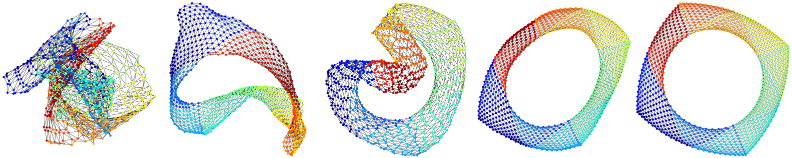


Experiments Result (individual 1)

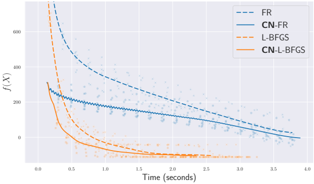
`jagmesh1` $(|V| = 936, |E| = 2664, \text{sparsity} = 0.609\%)$ Figures are at 50 iterations.



FR L-BFGS **CN**-FR **CN**-L-BFGS BEST



`dwt_1005` $(|V| = 1005, |E| = 3808, \text{sparsity} = 0.755\%)$ Figures are at 100 iterations.



FR L-BFGS **CN**-FR **CN**-L-BFGS BEST

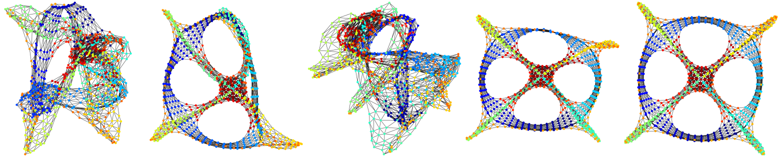
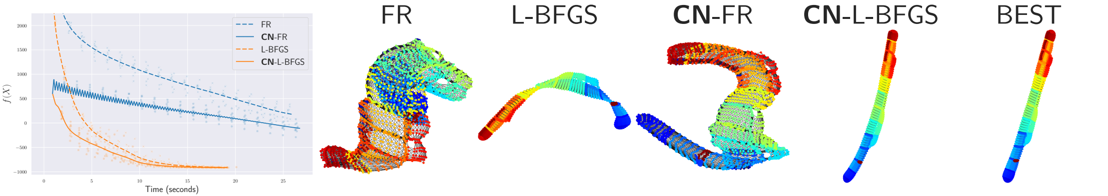


Figure: "BEST" is the 500th iteration of the proposed algorithm.

Experiments Result (individual 2)

`dwt_2680` $(|V| = 2680, |E| = 11173, \text{sparsity} = 0.311\%)$ Figures are at 150 iterations.



`3elt` $(|V| = 4720, |E| = 13722, \text{sparsity} = 0.123\%)$ Figures are at 150 iterations.

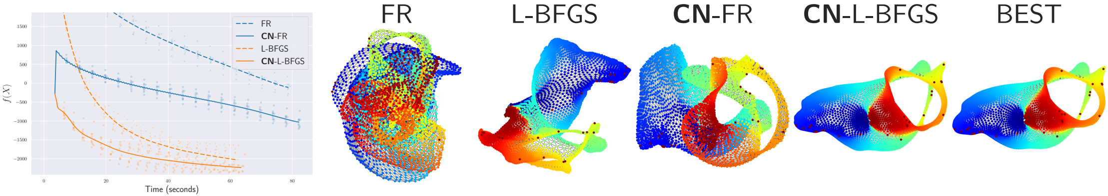


Figure: "BEST" is the 500th iteration of the proposed algorithm.

Experiments Result (overall)

As a dataset, we used matrices from Sparse Matrix Collection [7], in total 124 graphs.

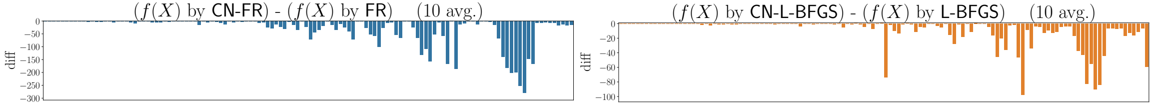


Figure: Comparison of the proposed initialization (CN) with random initialization (no prefix).

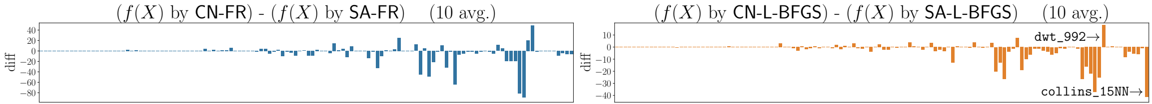


Figure: Comparison of the proposed initialization (CN) with circle initialization (SA) in Ref. [6].

Comparision with SA method

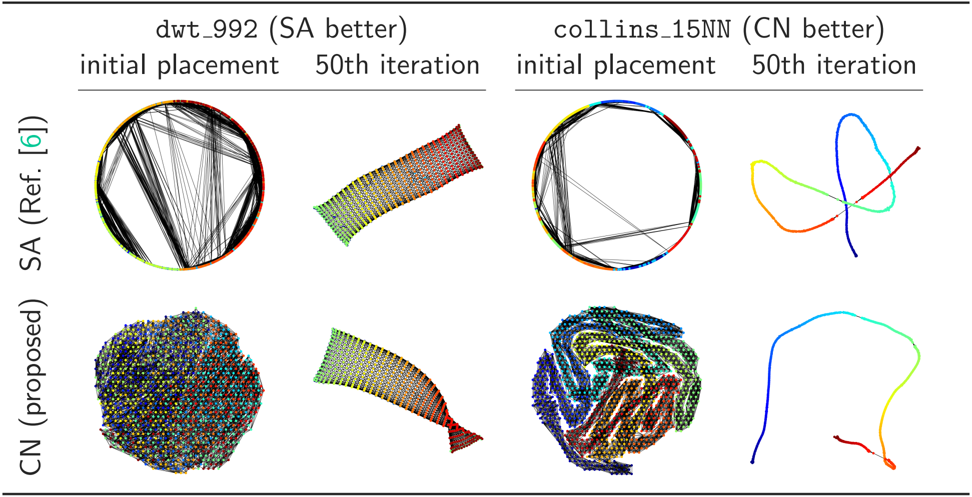


Figure: Visualization results showing initial and 50th iteration placements for `dwt_992` and `collins_15NN`.

Rationale of the Proposed Method

Q: Why we cannot directly apply coordinate descent to the problem?
A: The ignorance of other vertex movements.

Discrete optimization problem
→ **At least** ϵ movement
→ **More efficient** than direct application.

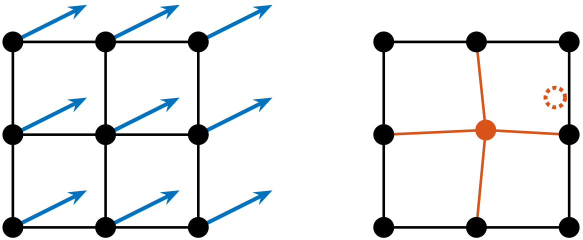


Figure: The ignorance of other vertex movements. Although the blue arrows show the forces in this situation, the red vertex barely moves by the coordinate Newton direction.

Future Work (1/2) - Combine with `sfdp`

`sfdp` **in Graphviz**  **[8]**

- **S**calable **F**orce-**D**irected **P**lacement.
- This is a **Multilevel** approach.
- Barnes–Hut algorithm (Q-tree)[9, 10].
- These methods are compatible with the proposed method.

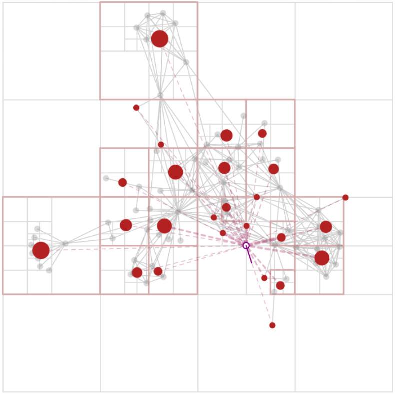


Figure: link

Future Work (2/2) - Broader Applications

"objective functions arising from graphs" [11]

$$f(X) = \sum_{\{i,j\}\in E} f_{i,j}(x_i, x_j) + \lambda \sum_{i=1}^{n} \Omega_i(x_i)$$

General optimization problem arising from graphs.

stochastic coordinate descent [11] only with the gradient is a popular.

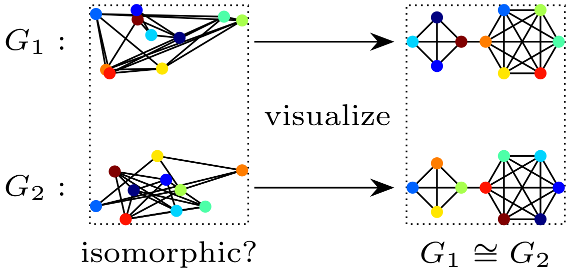
Can we use coordinate Newton direction?

Graph Isomorphism Problem

Drawing graph symmetry is at least as difficult as the graph isomorphism problem [12].

Continuous relaxation → optimization on Riemannian manifolds [13]

Can we utilize coordinate Newton direction to Riemannian optimization?



End of the Presentation

Summary

Fruchterman–Reingold layout is a tough problem
Hexagonal Lattice + coordinate Newton direction
initialization + L-BFGS gives the best result

Acknowledgement

I would like to express my sincere gratitude to **Pierre-Louis Poirion**, **Andi Han**, and **Naoki Marumo**.

Reference I

[1] A. Hagberg, P. J. Swart, and D. A. Schult, “Exploring network structure, dynamics, and function using NetworkX,” Los Alamos National Laboratory (LANL), Los Alamos, NM (United States), Tech. Rep., 2008.

[2] T. M. J. Fruchterman and E. M. Reingold, “Graph drawing by force-directed placement,” *Software: Practice and Experience*, vol. 21, no. 11, pp. 1129–1164, 1991. [Online]. Available: https://onlinelibrary.wiley.com/doi/abs/10.1002/spe.4380211102

[3] T. L. Veldhuizen, “Dynamic Multilevel Graph Visualization,” 2007. [Online]. Available: http://arxiv.org/abs/0712.1549

[4] S.-H. Cheong and Y.-W. Si, “Snapshot Visualization of Complex Graphs with Force-Directed Algorithms,” in *2018 IEEE International Conference on Big Knowledge (ICBK)*, 2018, pp. 139–145. [Online]. Available: https://ieeexplore.ieee.org/document/8588785/?arnumber=8588785

[5] H. Hosobe, “Numerical optimization-based graph drawing revisited,” in *2012 IEEE Pacific Visualization Symposium*, 2012, pp. 81–88.

[6] F. Ghassemi Toosi, N. S. Nikolov, and M. Eaton, “Simulated Annealing as a Pre-Processing Step for Force-Directed Graph Drawing,” in *Proceedings of the 2016 on Genetic and Evolutionary Computation Conference Companion*, ser. GECCO '16 Companion. Association for Computing Machinery, 2016, pp. 997–1000. [Online]. Available: https://dl.acm.org/doi/10.1145/2908961.2931660

Reference II

[7] T. A. Davis and Y. Hu, "The University of Florida sparse matrix collection," *ACM Transactions on Mathematical Software (TOMS)*, vol. 38, no. 1, pp. 1–25, 2011.

[8] J. Ellson, E. Gansner, L. Koutsofios, S. C. North, and G. Woodhull, "Graphviz— Open Source Graph Drawing Tools," in *Graph Drawing*, P. Mutzel, M. Jünger, and S. Leipert, Eds. Springer, 2002, pp. 483–484.

[9] Y. Hu, "Efficient, high-quality force-directed graph drawing," *The Mathematica journal*, vol. 10, pp. 37–71, 2006. [Online]. Available: https://api.semanticscholar.org/CorpusID:14599587

[10] J. Barnes and P. Hut, "A hierarchical O(N log N) force-calculation algorithm," *Nature*, vol. 324, no. 6096, pp. 446–449, 1986. [Online]. Available: https://www.nature.com/articles/324446a0

[11] B. Recht and S. J. Wright, "Optimization for modern data analysis," 2019. [Online]. Available: https://people.eecs.berkeley.edu/~brecht/opt4ml_book/

[12] P. Eades, "A heuristic for graph drawing," *Congressus numerantium*, vol. 42, no. 11, pp. 149–160, 1984.

[13] S. Klus and P. Gelß, "Continuous optimization methods for the graph isomorphism problem," 2023. [Online]. Available: http://arxiv.org/abs/2311.16912