

Multicriteria Scalable Graph Drawing via Stochastic Gradient Descent, (SGD)²

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- Introduction
- Related Work
- The (GD)² Framework
- Properties and Measures
- Conclusions

Drawing Properties

This talk:

- Stress
- Neighborhood Preservation

More in the paper:

- Vertex Resolution
- Ideal Edge Length
- Crossing Number
- Crossing Angle Maximization
- Angular Resolution
- Aspect Ratio
- Gabriel Graph Property

Stress

Quality measure & loss function:

$$L_{ST} = \sum_{i < j} w_{ij} (|X_i - X_j|_2 - d_{ij})^2$$

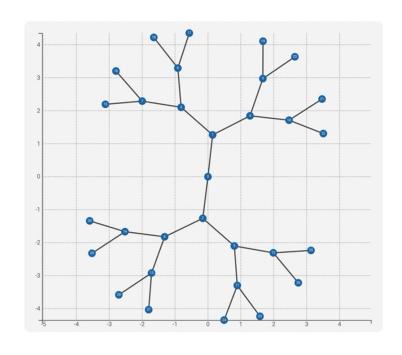
ullet w_{ij} - Normalizing term, we take $w_{ij}=d_{ij}^{-2}$

 $d_{i\,i}$ - Graph theoretical distance

 X_i - coordinate of ith node in the layout

Observation:

 L_{ST} is a <u>differentiable</u> function of the layout X



Stress

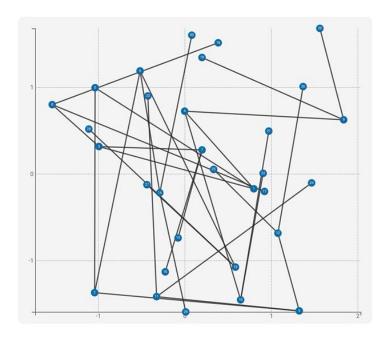
Observation:

 L_{ST} is a <u>differentiable</u> function of the layout X

=> Optimizable via gradient descent

for k in range(max_iter):
$$L_{ST} = \sum_{i < j} w_{ij} (|X_i - X_j|_2 - d_{ij})^2$$

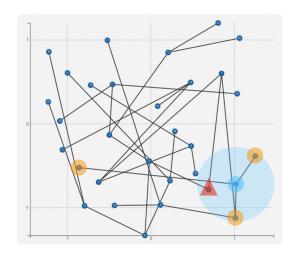
$$X = X - \epsilon \cdot \nabla_X L_{ST}$$



In general:

- We find a loss function that is <u>differentiable</u> with respect to the layout *X*.
 - If the original criterion is *not* differentiable, we find a <u>surrogate function</u>.

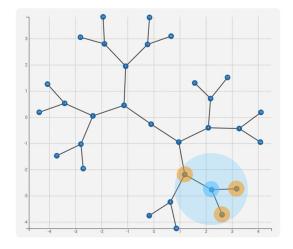
(Intuition)



Bad Neighborhood Preservation

Neighbors in layout ≠ Neighbors in graph

{ ▲ , ● , ● } ≠ { ● , ● , ● }



Good Neighborhood Preservation

Neighbors in layout = Neighbors in graph

{ •, •, • } = { •, •, • }

(Goal & Quality measure)

• Quality Measure (the hither, the better):

$$Q_{NP} := \text{Jaccard Index } (K, Adj)$$

$$= \frac{|\{(i,j):K_{ij}=1an, |d_{jij}=1\}|}{|\{(i,j):K_{ij}=10rAd_{jij}=1\}|}$$

K - k-NN Matrix

 k_i - (Chosen to be) the degree of node i

Adj - Adjacency Matrix

Goal:

k-NN Matrix (K) \approx Adjacency Matrix (Adj)

(Goal & Quality measure)

Quality Measure (the hither, the better):

$$Q_{NP} := \text{Jaccard Index } (K, Adj)$$

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Goal:

k-NN Matrix (K) \approx Adjacency Matrix (Adj)

(Goal & Quality measure)

Goal / Intuition

k-NN Matrix (K) \approx Adjacency Matrix (Adj)

• Quality Measure (the higher, the better):

$$Q_{NP}:= \text{Jaccard Index }(K, Adj) = \frac{|\{(i,j):K_{ij}=1 \text{ and } Adj_{ij}=1\}|}{|\{(i,j):K_{ij}=1 \text{ or } Adj_{ij}=1\}|}$$

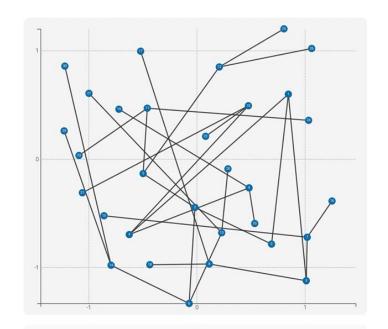
► Notation:



 k_i - chosen to be the degree of node i

Adj - ground truth, constant

K - layout-dependent, but *not* (yet) differentiable



(Making K differentiable)

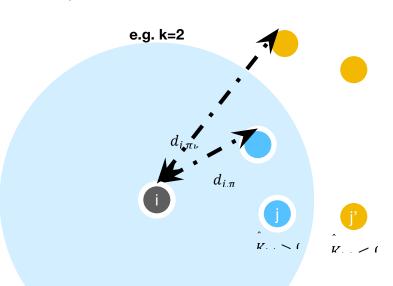
k-NN Matrix (K) ≈ Adjacency Matrix (Adj)



distance to the kth nearest neighbor of node i

$$\hat{K}_{i,j} = \begin{cases} -(||X_i - X_j|| - \frac{d_{i,\pi_k} + d_{i,\pi_{k+1}}}{2}) & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

- ullet $K_{i,j}$ is differentiable function of X_i and X_j
- $ullet K_{i,j} \geq 0$ if node j is one of the k nearest neighbors of node i
- $K_{i,j} < 0$ otherwise



Kruiger et al.: Graph layouts by t-SNE. Comput. Graph. Forum36(3), 283–294 (2017)

(Making K differentiable)

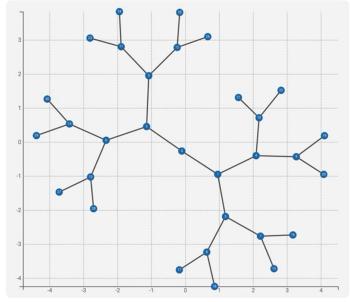


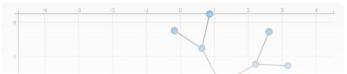
 $Q_{NP} := \text{Jaccard Index } (K, Adj)$

distance to the kth nearest neighbor of node i

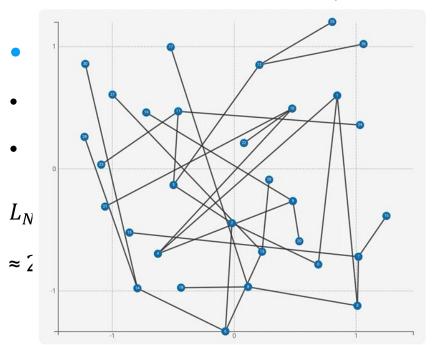
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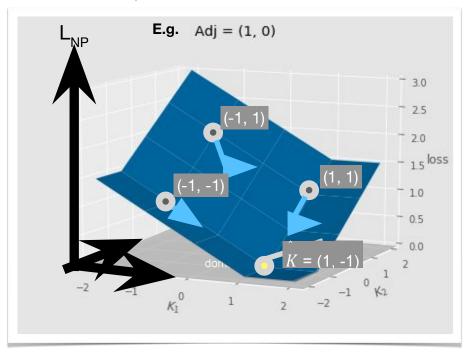
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- $\hat{K}_{i,j} \leq 0$ otherwise





(Relax Jaccard Index)





Berman et al.: The Lovász-softmax loss: a tractable surrogate for the optimization of the intersection-over-union measure in neural networks. In: Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition. pp. 4413–4421 (2018)

In general:

- We find a loss function that is <u>differentiable</u> with respect to the layout
 X.
- If the original criterion is *not* differentiable, we find a <u>surrogate</u> <u>function</u>.

Vertex Resolution

• Goal / Intuition:

Distribute nodes evenly

• Quality measure (higher the better):

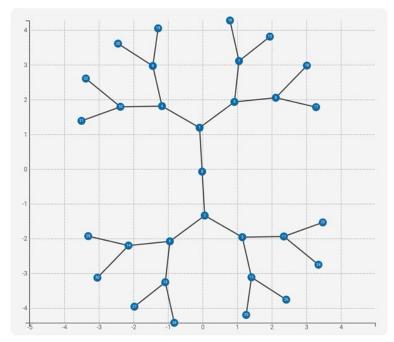
$$Q_{VR} = \frac{\min_{i \neq j} ||X_i - X_j||}{\max_{k \neq l} ||X_k - X_l||}$$

Loss function:

For any target resolution $r \in [0,1]$

$$L_{VR} = \sum_{i,j \in V, i \neq j} \left[ReLU \left(1 - \frac{||X_i - X_j||}{r \cdot d_{max}} \right) \right]^2$$

• We take $r := \frac{1}{\sqrt{|V|}}$





Vertex Resolution (cont.)

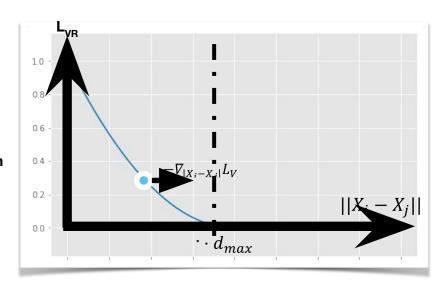
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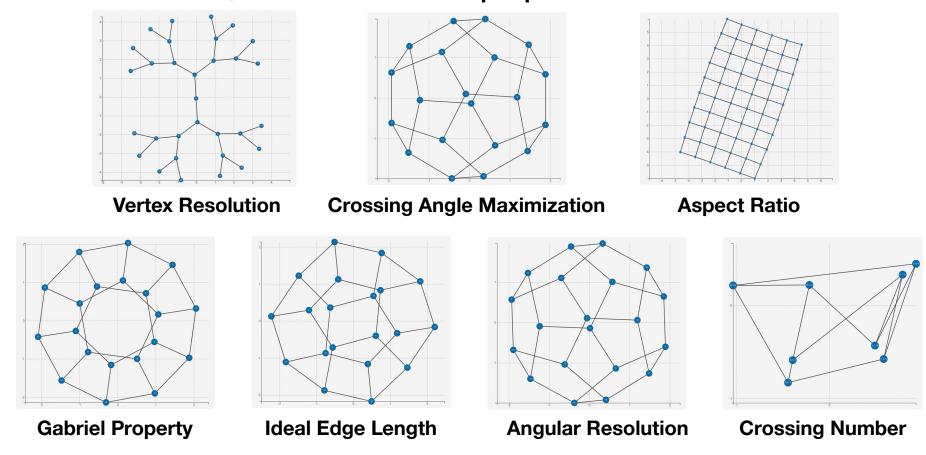
For any target resolution $r \in [0,1]$

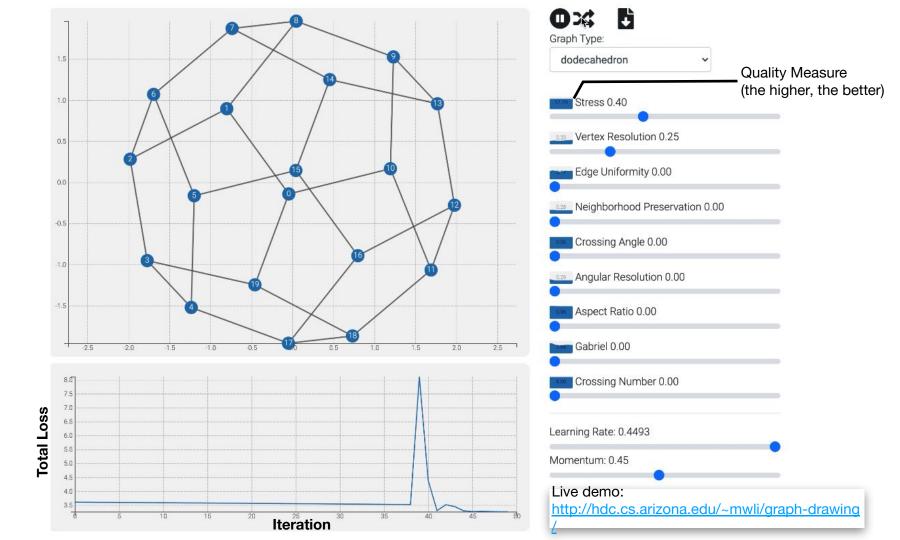
$$L_{VR} = \sum_{i,j \in V, i \neq j} \left[ReLU \left(1 - \frac{||X_i - X_j||}{r \cdot d_{max}} \right) \right]^2$$
Target Resolution

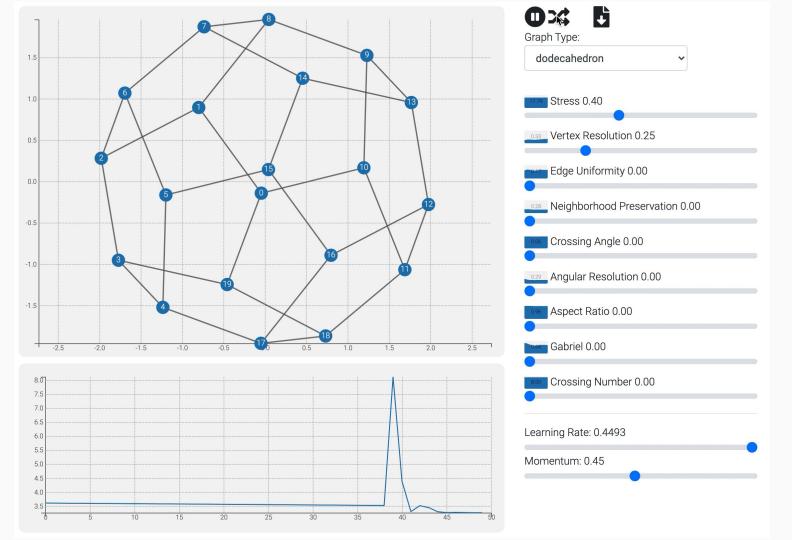
• We take $r := \frac{1}{\sqrt{|V|}}$



Seven more, details in the paper





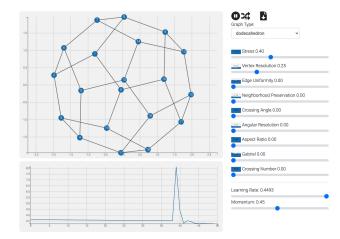


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Discussion?

Conclusion

- We proposed a general framework, (GD)², that optimizes multiple drawing criteria for graph layouts.
- To optimize multiple criteria jointly, we take a weighted sum of individual loss functions.
- For each criterion, we either optimize it directly or find a **surrogate** loss function if the criterion is not differentiable.



Live demo:

http://hdc.cs.arizona.edu/~mwli/graph-drawing/

Paper (arXiv): https://arxiv.org/abs/2008.05584
Graph Drawing via Gradient Descent, (GD)²
by Reyan Ahmed (abureyanahmed@email.arizona.edu),
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