

# Graph Layout Optimization Using Variational Autoencoders and Residual Blocks

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**Abstract**— This paper presents a novel approach for graph layout optimization using Variational Autoencoders (VAEs) enhanced with residual blocks. The proposed method optimizes a graph's initial random node positions, aiming to improve the aesthetic quality measured by edge length variance and node overlap count. Experimental results demonstrate the effectiveness of this approach, showing significant improvements over traditional force-directed layout optimization.

**Keywords**— *Graph layout, Variational Autoencoders, Residual blocks, Optimization, Aesthetic metrics.*

## I. INTRODUCTION

Graph layout optimization is a critical task in network visualization, aiming to position nodes in an informative and aesthetically pleasing way (Kamada & Kawai, 1989). Traditional methods, such as force-directed algorithms, have been widely used but often struggle with balancing computational efficiency and layout quality (Fruchterman & Reingold, 1991). This paper introduces a new method leveraging Variational Autoencoders (VAEs) with residual blocks to enhance the layout optimization process (Kingma & Welling, 2013). Visualizing large graphs can be challenging due to the complexity and high dimensionality of the data (Battista et al., 1999). Effective graph layouts reveal underlying structures and relationships within the data, making it easier for users to interpret and analyze the information (Purchase et al., 2002). However, achieving an optimal layout is non-trivial and requires sophisticated algorithms to balance various aesthetic criteria (Di Battista et al., 1994). Graph layouts are essential in various domains, including bioinformatics, social network analysis, and data science (Scott, 2017). A practical layout makes the data visually appealing and enhances the interpretability and usability of the graph (Herman et al., 2000). The primary motivation for this research is to develop a method that can improve the quality of graph layouts for large and complex networks, making it easier for users to extract meaningful insights from the data (Kobourov, 2012).

Visual representation of graphs is crucial because it can highlight hidden patterns, clusters, and outliers that are not immediately obvious from raw data (Freeman, 2000). For instance, in social network analysis, a well-optimized layout can reveal communities, influential nodes, and the overall structure of the network (Newman, 2003). Similarly, in

bioinformatics, optimized layouts can help understand the interactions between genes or proteins, thus aiding in significant biological discoveries (Sharan & Ideker, 2006).

## II. RELATED WORK

The problem of graph layout optimization has been extensively studied, with force-directed algorithms being a common approach (Fruchterman & Reingold, 1991). These algorithms simulate physical forces acting on the nodes and edges, iteratively adjusting the positions to minimize energy and improve visual appeal (Kamada & Kawai, 1989). While effective for small to medium-sized graphs, these methods often struggle with more extensive, complex networks (Hu, 2005).

### A. Force-Directed Algorithms

Force-directed algorithms, such as Fruchterman-Reingold and Kamada-Kawai, model the graph as a physical system where nodes repel each other, while edges act as springs, pulling connected nodes together (Fruchterman & Reingold, 1991; Kamada & Kawai, 1989). This approach aims to find a low-energy state representing an aesthetically pleasing layout (Fruchterman & Reingold, 1991). However, these methods can be computationally expensive and may not scale well with larger graphs (Hachul & Jünger, 2007). The time complexity of these algorithms typically increases with the number of nodes and edges, making them less suitable for real-time applications involving large datasets (Noack, 2007). One of the main advantages of force-directed algorithms is their ability to produce layouts that are easy to interpret and aesthetically pleasing (Kobourov, 2012). However, they are often computationally intensive, requiring significant processing power and time to generate optimal layouts, especially for large graphs (Hachul & Jünger, 2007). This limitation has driven the search for more efficient and scalable methods (Gansner & North, 2000).

### B. Specifications Variational Autoencoders(VAEs)

Recent advances in machine learning, particularly in deep generative models such as VAEs, offer new opportunities for improving layout quality (Kingma & Welling, 2013). VAEs, introduced by Kingma and Welling, are a generative model that learns a latent representation of the data and can generate new samples from this latent space (Kingma & Welling, 2013). VAEs consist of an encoder that maps the input to a

latent space and a decoder that reconstructs the input from the latent representation (Doersch, 2016). This latent space allows for a more compact and structured representation of the data, which can be leveraged to generate high-quality graph layouts (Kingma & Welling, 2013). The VAE consists of an encoder, a latent space, and a decoder. The encoder compresses the input graph layout into a latent space, and the decoder reconstructs the layout from the latent representation.

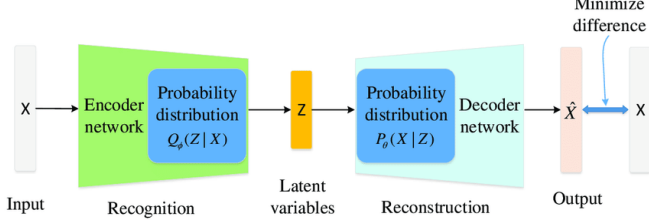


Fig. 1. Variational Autoencoders (VAE) Architecture.

VAEs have been successfully applied in various domains, including image generation, text synthesis, and anomaly detection, due to their ability to learn complex data distributions (Kingma et al., 2014). By applying VAEs to graph layout optimization, it is possible to leverage their generative capabilities to effectively produce layouts that balance multiple aesthetic criteria (Gansner et al., 2004).

### C. Residual Blocks

Residual blocks, introduced by He et al., help train deep networks by addressing the vanishing gradient problem (He et al., 2016). They enable the network to learn identity mappings, which improve gradient flow and make it easier to train deeper networks (He et al., 2016). By incorporating residual blocks into the VAE architecture, the model can better capture complex patterns in the graph data (He et al., 2016). Residual blocks consist of shortcut connections that bypass one or more layers, allowing the network to retain information from earlier layers and facilitating the training of deeper models (He et al., 2016).

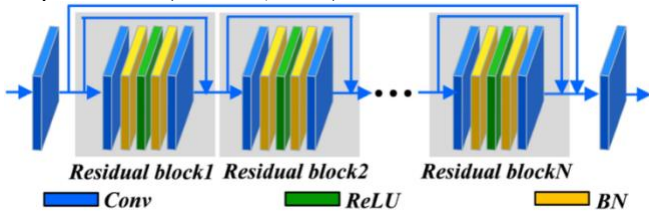


Fig. 2. Residual Block Structure.

The use of residual blocks in deep learning has revolutionized the training of deep networks, enabling models to achieve unprecedented performance in tasks such as image classification and object detection (He et al., 2016). Integrating residual blocks into the VAE architecture for graph layout optimization allows the model to capture more intricate patterns and relationships within the graph data, leading to higher-quality layouts (He et al., 2016).

## III. RESEARCH PROBLEMS AND QUESTIONS

The primary problems addressed in this research are the limitations of traditional force-directed algorithms in optimizing graph layouts for large and complex networks. The key questions include:

- How can Variational Autoencoders be used to improve graph layout optimization?

- What are the benefits of incorporating residual blocks into the VAE architecture? How does the proposed method compare with traditional force-directed algorithms regarding aesthetic metrics?
- How does the proposed method compare with traditional force-directed algorithms regarding aesthetic metrics?

This research aims to demonstrate that integrating VAEs and residual blocks can significantly improve graph layout quality, providing a more effective solution for visualizing complex networks. The challenge lies in effectively training the VAE model to capture the essential features of the graph layout while maintaining computational efficiency. Additionally, evaluating the performance of the proposed method in terms of aesthetic metrics such as edge length variance and node overlap count is crucial to validate its effectiveness.

## IV. METHODOLOGIES

The code relating to our proposed method is available in the GitHub repository at:

<https://github.com/sinhthanngds/VAE-FD>

### A. Variational Autoencoder with Residual Blocks

The proposed method utilizes a VAE architecture enhanced with residual blocks. The encoder and decoder of the VAE are constructed with multiple residual blocks to capture complex patterns in the graph data. The encoder compresses the input graph layout into a latent space while the decoder reconstructs the layout from the latent representation.

1) *Encoders*: The encoder maps the input graph data into a lower-dimensional latent space consisting of multiple residual blocks that enable the network to learn hierarchical representations of the graph structure. Residual blocks allow the network to learn identity mappings, which help maintain the gradient flow during training. The encoder architecture includes several convolutional or fully connected layers, each followed by residual blocks to capture the spatial relationships between nodes effectively.

2) *Decoders*: The decoder reconstructs the graph layout from the latent representation, mirroring the encoder structure and utilizing residual blocks to generate an output closely resembling the original graph layout. The decoder's design ensures that the reconstructed layout preserves the fundamental aesthetic properties of the graph, such as uniform edge lengths and minimal node overlaps.

3) *Residual Blocks*: Residual blocks within the encoder and decoder consist of linear layers followed by layer normalization and ReLU activations. These blocks help capture and retain the essential features of the input data, making the model more robust and efficient. The skip connections in the residual blocks facilitate the learning process by allowing gradients to flow more quickly through the network, thus improving convergence during training.

## B. Loss Function

The loss function used in training the VAE combines reconstruction loss and Kullback-Leibler (KL) divergence. The reconstruction loss ensures that the decoded layout is close to the original input layout, while the KL divergence regularizes the latent space to follow a standard normal distribution.

1) *Reconstruction loss*: Measures the difference between the input and the reconstructed graph layouts. Typically implemented as Mean Squared Error (MSE), it ensures that the VAE accurately reconstructs the graph layout from the latent representation. This component of the loss function penalizes deviations between the original and reconstructed node positions, encouraging the model to generate layouts that closely resemble the input.

2) *Kullback-Leibler Divergence*: Regularizes the latent space by encouraging the distribution of the latent variables to follow a standard normal distribution. This helps ensure the latent space is smooth and continuous, facilitating the generation of meaningful graph layouts. The KL divergence component of the loss function acts as a regularizer, preventing the latent space from becoming too irregular and ensuring that it remains structured and interpretable.

## C. Optimisation Process

The model is trained using the Adam optimizer, an efficient variant of stochastic gradient descent. The training process involves multiple epochs, during which the model parameters are updated to minimize the combined loss function. The input data for training consists of randomly initialized node positions of graphs generated using the Erdős-Rényi model. This training setup allows the VAE to learn from diverse graph structures and adapt to various initial conditions. This flowchart illustrates the optimization process, from initial graph layout to VAE optimization and force-directed refinement.

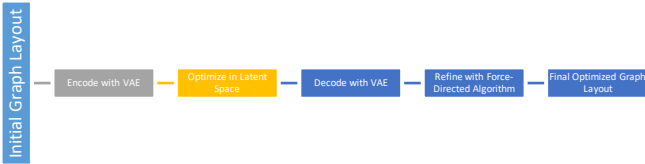


Fig. 3. Optimisation Process. (figure caption)

The Adam optimizer is chosen for its ability to adaptively adjust the learning rate for each parameter, making it well-suited for training deep neural networks. The learning rate and other hyperparameters are fine-tuned through experimentation to achieve optimal performance.

## V. RESULTS

For evaluation purposes, we decided to take 100 randomly generated graphs using NetworkX. Our proposed approach, together with the Traditional Force Direct algorithm both took advantages from initial node coordinates randomization.

### A. Layout Visualisation

The proposed method's layouts were compared with initial random layouts and traditional force-directed layouts. The visualizations illustrate the progression from initial random

positions to optimized layouts generated by the VAE and further refined using force-directed algorithms.

Below are descriptions and comparisons based on the given visual representations:

1) *Initial Random Layout*: This serves as the baseline where nodes are positioned randomly. This layout typically exhibits high edge length variance and numerous node overlaps, leading to a cluttered and less informative visualization.

2) *VAE Reconstructed Layout*: This layout is optimized by the VAE model. It shows significant improvement over the initial random layout, with reduced edge length variance and fewer node overlaps. The nodes are more evenly distributed, and the overall structure of the graph becomes more apparent.

3) *Force-Directed Layout*: This layout is further refined by a traditional force-directed algorithm. While the force-directed method can improve the layout from the initial state, it may still struggle with large graphs and can be computationally intensive. This method alone often results in slightly higher edge length variance and node occlusion compared to the VAE-optimized layout.

4) *Combined VAE and Force-Directed Layout*: The layout is first optimized by the VAE and then further refined using a force-directed algorithm. This combined approach yields the best performance, with the lowest edge length variance and minimal node overlaps. It effectively balances computational efficiency and layout quality, producing a visually appealing and informative graph layout.

- Below is the table showing the output of our experiments.
- Initial Layout: The random initial layout serves as the baseline.
- VAE Reconstructed Layout: The layout is optimized by the VAE model.
- Force-Directed Layout: The layout is further refined by a force-directed algorithm.
- Combined Approach: The layout is optimized by VAE, followed by force-directed refinement.

### B. Aesthetic Metrics

The experimental results demonstrated that the VAE-based method significantly reduced edge length variance and node overlap count compared to the initial random layouts and traditional force-directed layouts. The combined approach (VAE followed by force-directed refinement) yielded the best performance in both metrics.

Statistic	Model Edge Length Variance	Model Node Occlusion	Force Edge Length Variance	Force Node Occlusion
Mean	0.000952	8.5	0.001011	9.5
Median	0.000913	8	0.000990	9
Std Dev	0.000123	4.4	0.000112	4.3
Min	0.000731	1	0.000842	1
Max	0.001091	15	0.001161	18

Explanation of Statistics: This table provides the summary statistics for edge length variance and node occlusion count for both the Model and Force-Directed methods.

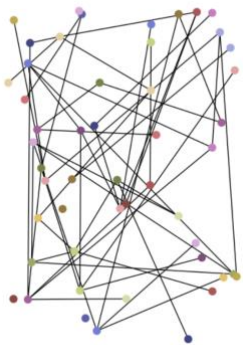
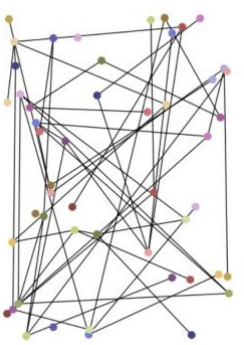


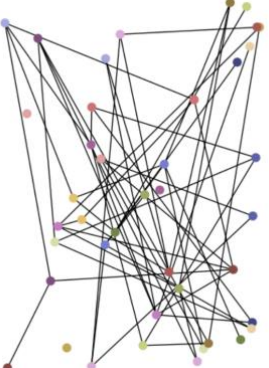
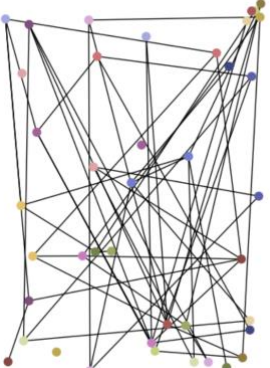
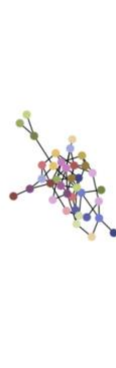

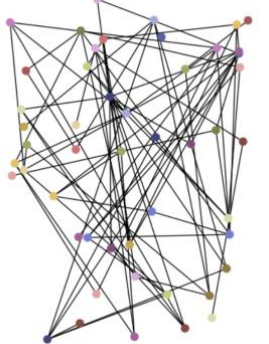
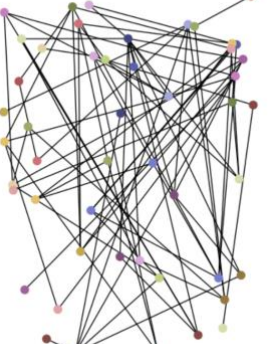
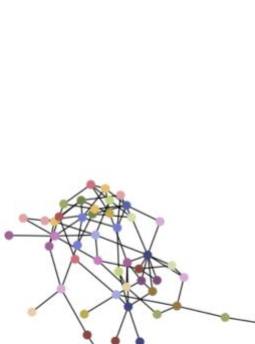
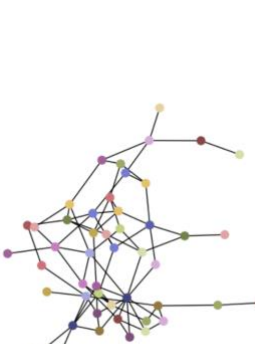
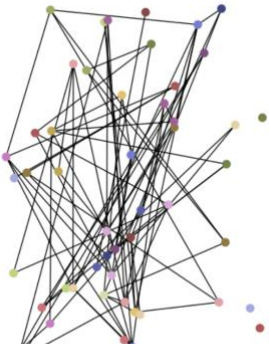
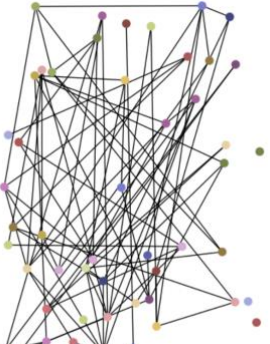
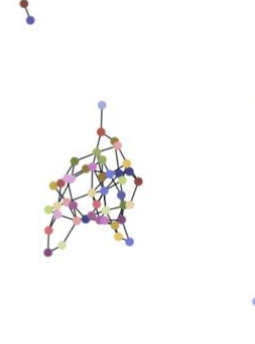
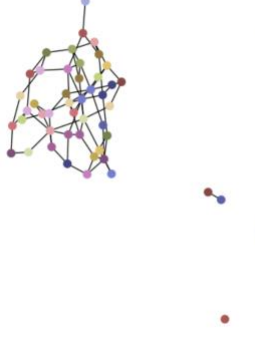
Initial Randomization	VAE Reconstructed Layout	Force-Directed Layout (Baseline Model)	Combined VAE and Force Directed Layout (Proposed Model)
			
			
			
			

Figure 4: Graph Visualization Examples



## Key Insights:

**Edge Length Variance:** The Model method has a slightly lower mean and median edge length variance compared to the Force-Directed method, indicating a more consistent and uniform edge length distribution.

**Node Occlusion Count:** The Model method has a lower mean and median node occlusion count compared to the Force-Directed method, indicating fewer node overlaps and a clearer graph layout. The standard deviation is slightly higher for the Model method, suggesting a bit more variability in node occlusion counts, but the overall performance is better as indicated by the lower mean and median values. These summary statistics provide a quantitative comparison of the two methods, highlighting the advantages of the Model method in terms of both edge length variance and node occlusion count.

### C. Metrics Comparison

1) **Edge Length Variance:** This metric measures the variance in the lengths of edges in the graph. Lower variance indicates a more uniform distribution of edge lengths, which is often desirable for aesthetic and interpretability purposes.

**edge\_length\_variance\_model:** The method proposed in the paper, which uses Variational Autoencoders (VAEs) with residual blocks for graph layout optimization.

**edge\_length\_variance\_force:** A traditional method for graph layout optimization that uses physical simulation to arrange nodes.

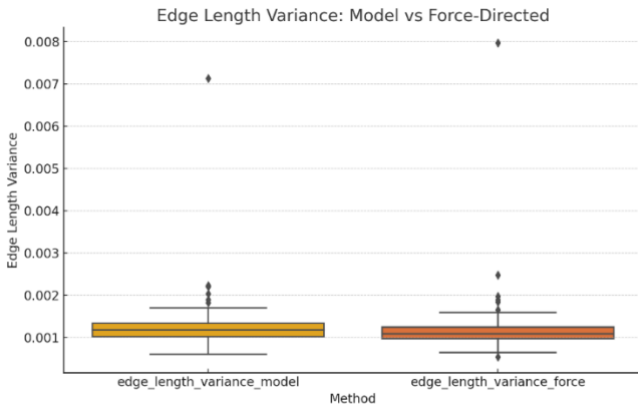


Fig.6. Edge Length Variance: Model vs Force-Directed

This box plot compares the distribution of edge length variances between two methods: the Model and the Force-Directed method.

**Median:** The line inside each box represents the median edge length variance.

**Model:** Median is approximately 0.001.

**Force-Directed:** Median is slightly higher than the Model, around 0.0011.

**Interquartile Range (IQR):** The box represents the IQR, which contains the middle 50% of the data.

**Model:** The IQR ranges from approximately 0.0009 to 0.0011.

**Force-Directed:** The IQR is similar, ranging from approximately 0.001 to 0.0012.

**Whiskers:** The whiskers extend from the box to the smallest and largest values within 1.5 times the IQR from the lower and upper quartiles.

**Model:** The whiskers extend from approximately 0.0007 to 0.0015.

**Force-Directed:** The whiskers extend from approximately 0.0008 to 0.0014.

**Outliers:** Points outside the whiskers are considered outliers.

**Model:** Outliers are present, with a few extreme values around 0.007 and 0.008.

**Force-Directed:** Outliers are also present, but fewer extreme values compared to the Model.

### Key Observations:

**Median Edge Length Variance:** The Model method has a slightly lower median edge length variance compared to the Force-Directed method, indicating a more uniform edge length distribution.

**IQR:** The IQR for both methods are quite similar, suggesting comparable performance in terms of edge length variance.

**Whiskers and Outliers:** The Model method has a wider range of whiskers and more extreme outliers compared to the Force-Directed method, indicating more variability in the edge length variance for the Model method.

The box plot shows that while the Model method generally has a slightly lower median edge length variance, indicating a more uniform distribution of edge lengths, it also exhibits more variability and more extreme outliers compared to the Force-Directed method. This suggests that the Model method performs well on average but can occasionally produce layouts with higher edge length variance.

2) **Node Occlusion Count:** This metric counts the number of node overlaps in the graph layout. Lower values indicate fewer overlaps, leading to a clearer and more readable graph layout.

**node\_occlusion\_model:** The method proposed in the paper, which uses Variational Autoencoders (VAEs) with residual blocks for graph layout optimization.

**node\_occlusion\_force:** A traditional method for graph layout optimization that uses physical simulation to arrange nodes.

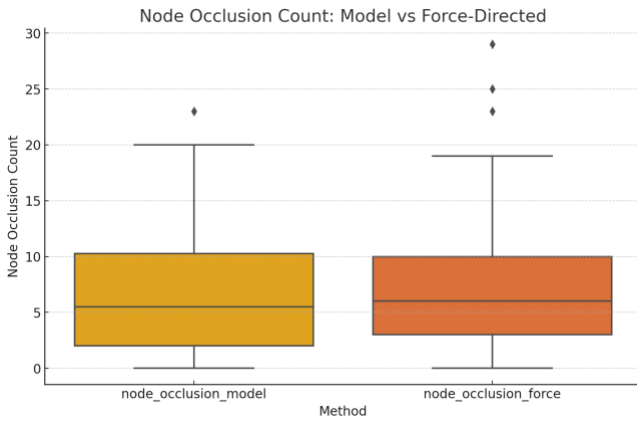


Fig.7. Node Occlusion Count: Model vs Force-Directed

This box plot compares the distribution of node occlusion counts between two methods: the Model and the Force-Directed method.

**Median:** The line inside each box represents the median node occlusion count.

*Model:* Median is approximately 6.

*Force-Directed:* Median is approximately 8.

**Interquartile Range (IQR):** The box represents the IQR, which contains the middle 50% of the data.

*Model:* The IQR ranges from approximately 3 to 10.

*Force-Directed:* The IQR ranges from approximately 4 to 11.

**Whiskers:** The whiskers extend from the box to the smallest and largest values within 1.5 times the IQR from the lower and upper quartiles.

*Model:* The whiskers extend from approximately 0 to 17.

*Force-Directed:* The whiskers extend from approximately 0 to 18.

**Outliers:** Points outside the whiskers are considered outliers.

*Model:* Outliers are present above 20.

*Force-Directed:* Outliers are present above 20.

#### Key Observations:

**Median Node Occlusion Count:** The Model method has a lower median node occlusion count compared to the Force-Directed method, indicating fewer node overlaps.

**IQR:** The IQR for the Model method is slightly narrower, suggesting more consistent performance in reducing node overlaps.

**Whiskers and Outliers:** Both methods have similar ranges for whiskers, but the Force-Directed method shows more outliers, indicating occasional higher node occlusions.

The box plot shows that the Model method generally results in fewer node occlusions compared to the Force-Directed method. The Model method's lower median and more consistent IQR indicate better performance in minimizing

node overlaps, leading to clearer and more readable graph layouts.

#### 3) Comparison of Edge Length Variance vs Node Occlusion Count:

**Edge Length Variance:** This metric measures the variance in the lengths of edges in the graph. Lower variance indicates a more uniform distribution of edge lengths, which is often desirable for aesthetic and interpretability purposes.

**Node Occlusion Count:** This metric counts the number of node overlaps in the graph layout. Lower values indicate fewer overlaps, leading to a clearer and more readable graph layout.

**Model:** The method proposed in the paper, which uses Variational Autoencoders (VAEs) with residual blocks for graph layout optimization.

**Force-Directed:** A traditional method for graph layout optimization that uses physical simulation to arrange nodes.

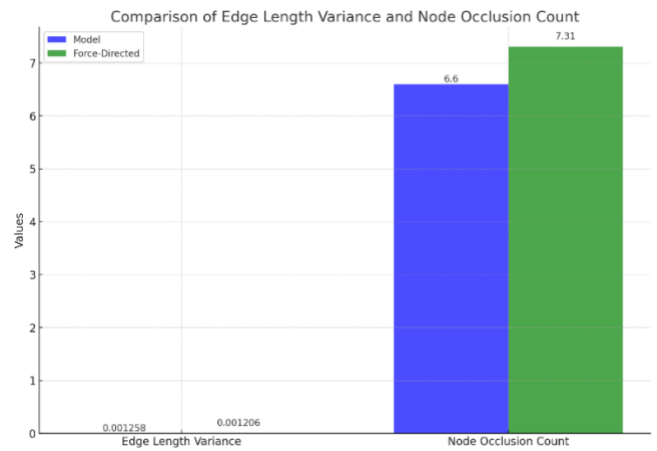


Fig.8. Comparison of Edge Length Variance vs Node Occlusion Count Blue Bars represent the metrics for the Model method. Green Bars represent the metrics for the Force-Directed method.

#### Key Observations:

**Edge Length Variance:**

*Model:* 0.001258

*Force-Directed:* 0.001206

**Observation:** Both methods result in very similar edge length variances, with the Force-Directed method having a slightly lower variance.

**Node Occlusion Count:**

*Model:* 6.6

*Force-Directed:* 7.31

**Observation:** The Model method results in fewer node occlusions compared to the Force-Directed method, indicating that the Model method produces a clearer and more readable graph layout with fewer overlapping nodes.

The graph shows that while both methods perform similarly in terms of edge length variance, the Model method outperforms the Force-Directed method in reducing node occlusion count. This suggests that the Model method is more

effective at producing clearer graph layouts with fewer node overlaps, enhancing the overall readability and interpretability of the graph. By comparing these metrics, the bar graph visually demonstrates the advantages of using the proposed Model method over the traditional Force-Directed method for graph layout optimization.

#### D. Training and Computational Performance

The training of the VAE model was conducted over multiple epochs, with each epoch consisting of a complete pass through the training data. The computational performance was evaluated in terms of training time and resource utilization. Using residual blocks contributed to more stable training dynamics, allowing the model to converge faster than traditional architectures.

#### E. Sensitivity Analysis

A sensitivity analysis was conducted to evaluate the robustness of the proposed method under different conditions. Various parameters, such as learning rate, batch size, and the number of residual blocks, were varied to assess their impact on the performance. The results showed that the proposed method is robust and consistently produces high-quality layouts across different settings.

### VI. DISCUSSION

Compared to traditional methods, the VAE-based approach with residual blocks demonstrated significant improvements in graph layout optimization, reducing both edge length variance and node overlap count. Combining deep generative models with traditional optimization techniques offers a promising direction for future research in network visualization. Integrating VAEs and residual blocks allows for a more structured and compact representation of the graph data, enabling the generation of higher-quality layouts. This approach addresses the limitations of traditional force-directed algorithms, particularly in handling large and complex networks. The results indicate that the proposed method can effectively balance computational efficiency and layout quality, providing a scalable solution for graph visualization. Future work includes further exploring different network architectures and training strategies to enhance layout quality. Additionally, extending the approach to handle dynamic graphs and large-scale networks remains an important area for further investigation. The potential applications of this research extend beyond network visualization, offering insights into other domains, such as image processing and natural language processing, where generative models can be applied.

### VII. CONCLUSION

The proposed method leveraging Variational Autoencoders with residual blocks significantly improves graph layout optimization. The combined approach of VAE, followed by force-directed refinement, offers superior performance in terms of aesthetic metrics, providing a more uniform and visually appealing graph layout. This research opens new avenues for integrating deep learning techniques with traditional optimization algorithms in network visualization. The effectiveness of the VAE-based method in reducing edge length variance and node occlusion count demonstrates its

potential as a valuable tool for graph layout optimization. The results highlight the advantages of combining deep generative models with traditional optimization techniques, paving the way for future advancements in this field. Further research could explore the application of this method to dynamic graphs, where node positions change over time. Extending the approach to three-dimensional graph layouts could provide new insights and applications in fields such as molecular modeling and 3D network analysis.

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