Generating Graphs with Specified Properties

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Context

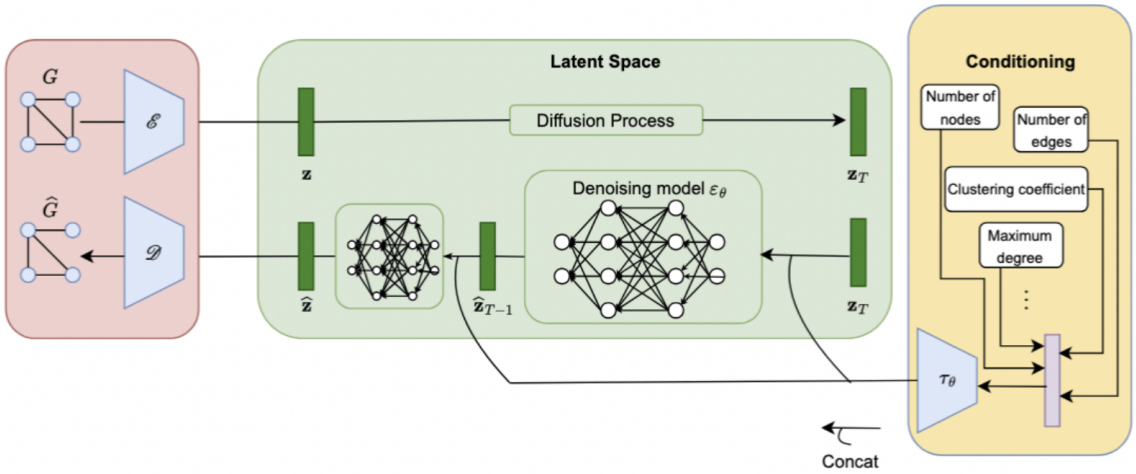

Figure – NGG pipeline

Variational Autoencoder (VAE) + diffusion process in the latent vector space

Our approach

- NGG is already state-of-art
- Didn't try other structure like GAN's and AutoRegressive Model which are more unstable to train
- Focused on improving the already existing architecture without increasing the computational cost

Encoder

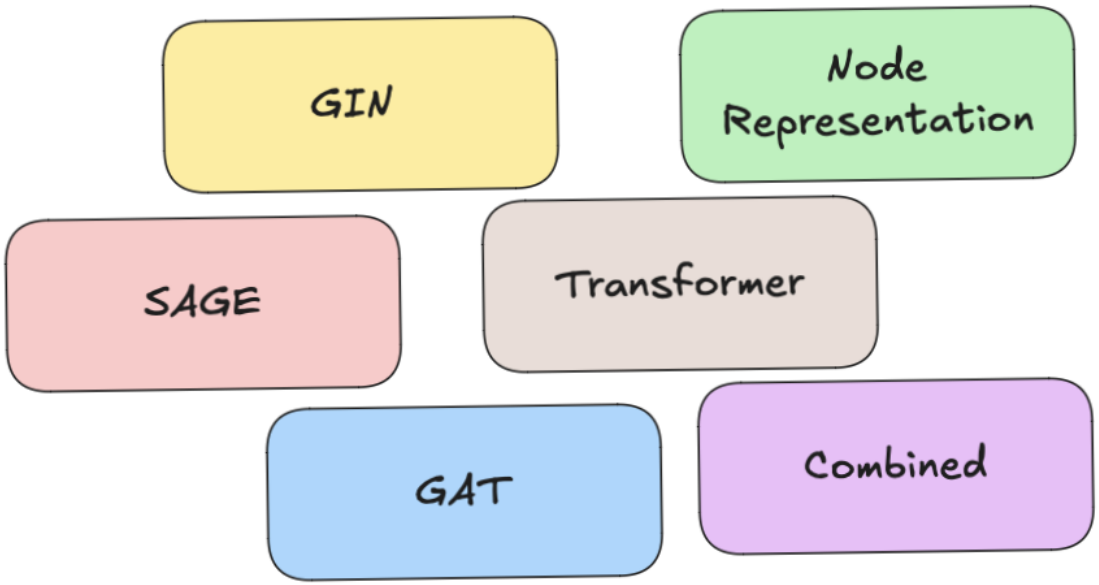

Figure – Tried Encoder Structures

Decoder

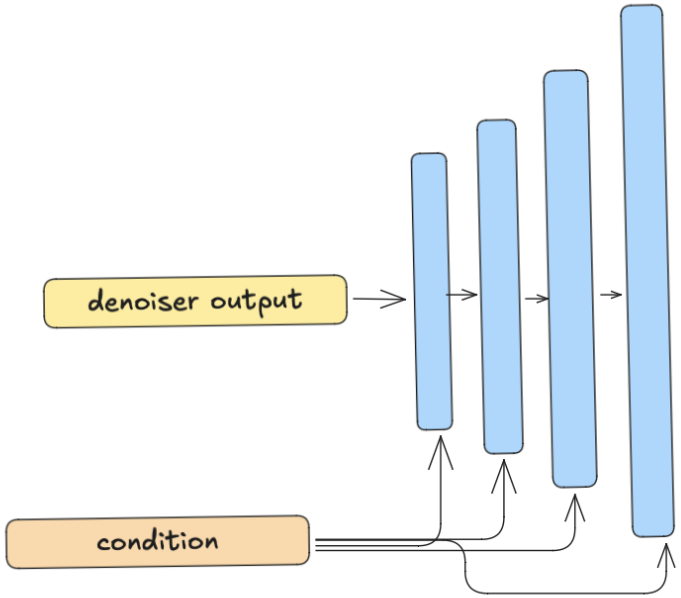

Figure – Decoder Structure

- Introduced a temperature parameter in order to draw more certain predictions

Denoiser

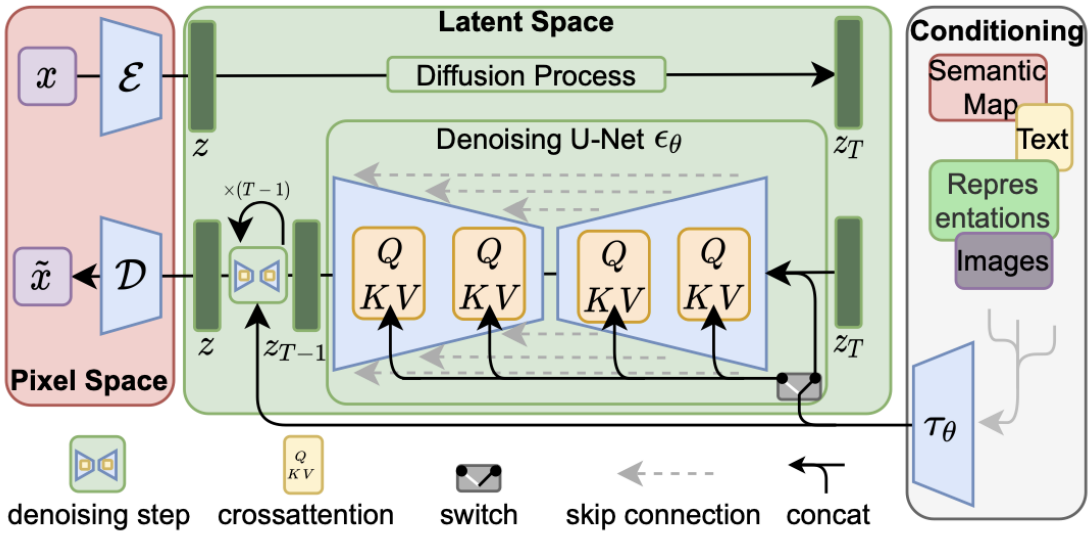

Figure – Stable diffusion Pipeline

- Used the 1D-Unet module with 2 input channels : one for the latent generation and one for the condition
- Worked really well but too computationally expensive

Conditioning

- Tried to use a Language Model to process the text condition
- RoBERTa : (60-75) x 768
- Didn't keep it since graph features could be extracted by a deterministic way
- Need for a better extractor for generalization to other sentence structures

Inference

- Not proportional link between the VAE and Denoiser loss and the final MAE
- Wanted to find a way to find another loss to obtained more coherent results
- Didn't find sustainable way to use differentiable function to approximate feature score
- Instead, implemented a Rejection Mechanism that generated multiple graphs and choose the one closer to features
- Thought we recognize it is not scalable

Final Model

- Our main goal was to keep computational effectiveness

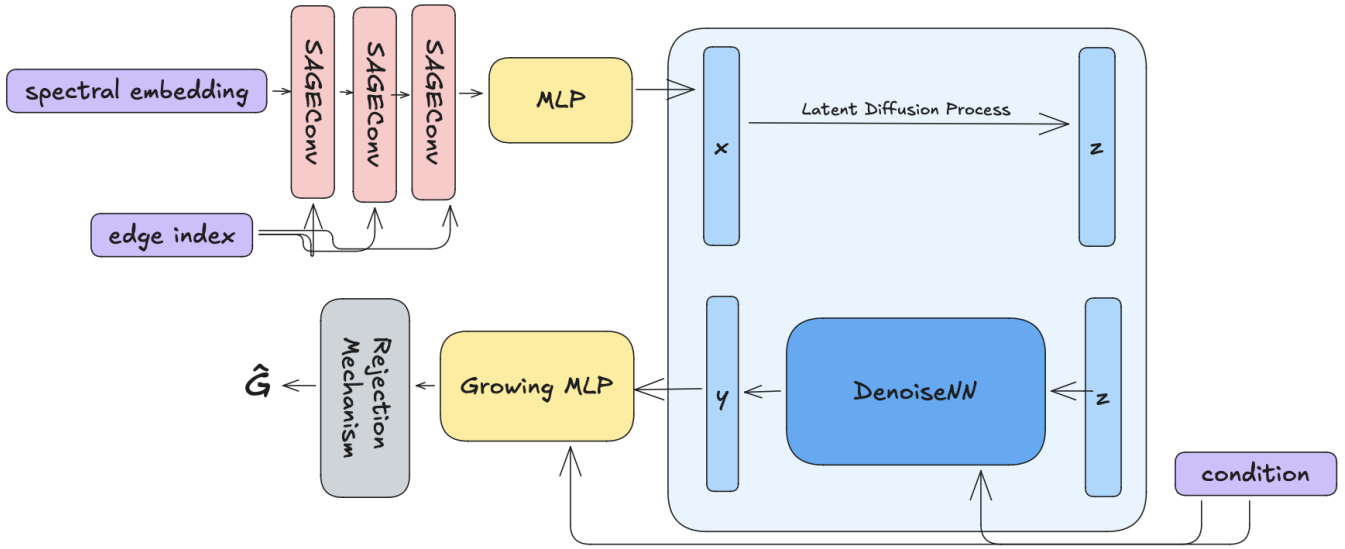

Figure – Our Final Pipeline

Fine-tuning

Epochs AutoEncoder	Epochs Denoiser	Modification	Nb of Graphs	MAE Score
200	200	Base - 4 layers Decoder	1	0.029
200	200	Base - 4 layers Decoder	10	0.014
200	200	Denoiser (5 layers)	10	0.021
200	200	Denoiser (3 layers)	10	0.014
400	400	Denoiser (4 layers), scheduler after 200 epochs, added epochs	10	0.015
500	400	LR = 1e-4, Denoiser (4 layers), added epochs	10	0.017

Table – Results of fine-tuning the AutoEncoder

Critics and Results

- As we said, hard to find a convenient loss to properly improve the weights of our model
- Doesn't generalize to other sentences structures
- Final Score based on MAE close to 0.05 - Top 8 at the Kaggle Challenge

References

[1] Rombach, R., Blattmann, A., Lorenz, D., Esser, P., & Ommer, B. (2021). *High-Resolution Image Synthesis with Latent Diffusion Models*. In Proceedings of the Conference on Computer Vision and Pattern Recognition (CVPR), Ludwig Maximilian University of Munich & IWR, Heidelberg University, Germany, Runway ML.

[2] Evdaimon, I., Nikolentzos, G., Xypolopoulos, C., Kammoun, A., Chatzianastasis, M., Abdine, H., & Vazirgiannis, M. (2024). *Neural Graph Generator : Feature-Conditioned Graph Generation using Latent Diffusion Models*.