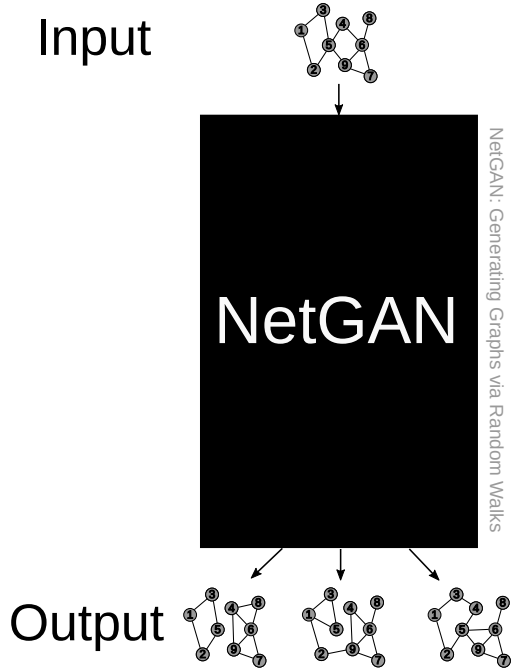
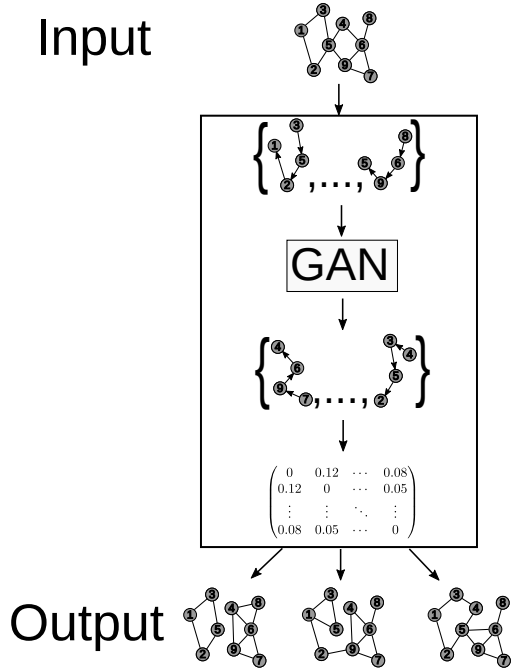
NetGAN without GAN: From Random Walks to Low-Rank Approximations

Luca Rendsburg, Holger Heidrich, Ulrike von Luxburg

ICML 2020


Input
NetGAN
Output
NetGAN: Generating Graphs via Random Walks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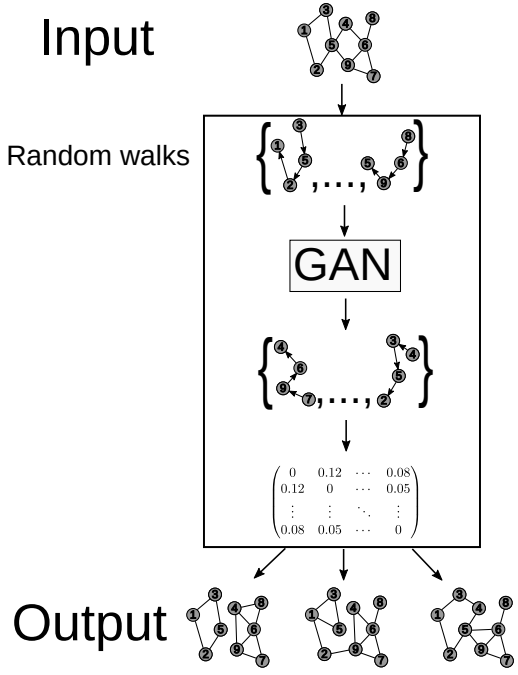
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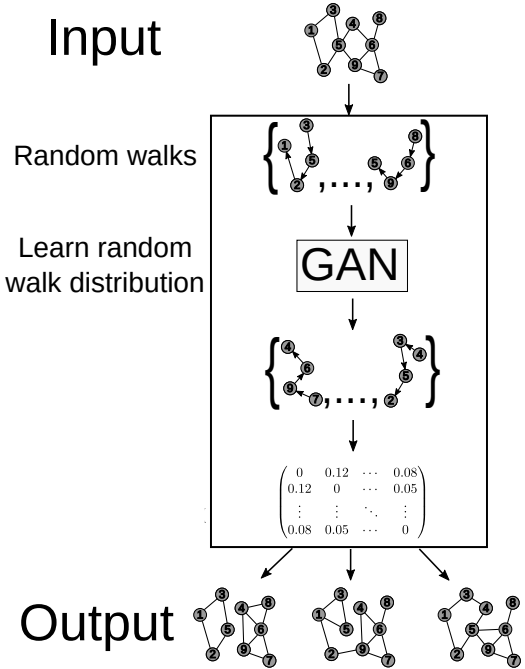
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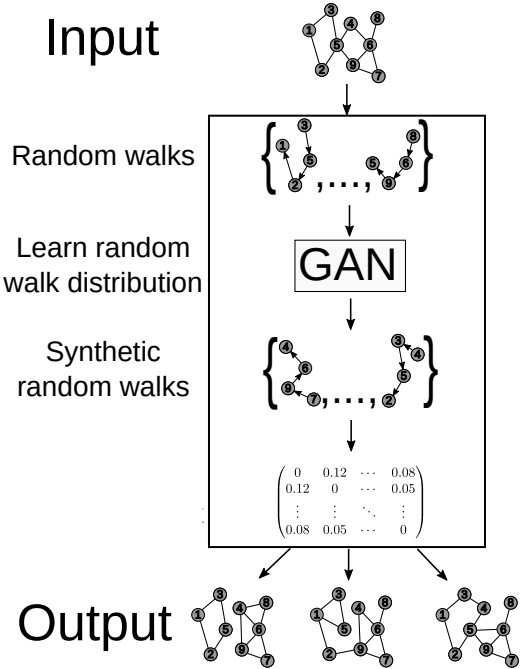
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Synthetic random walks
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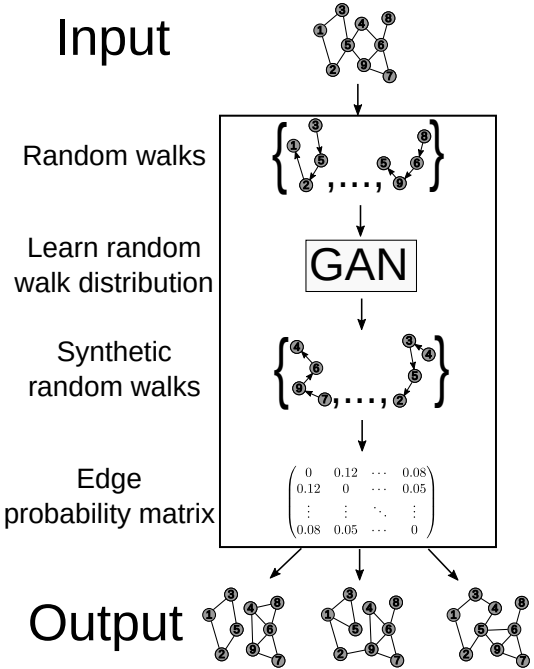
Input
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Learn random walk distribution
GAN
Synthetic random walks
Edge probability matrix
Output

Our contribution

Conceptual analysis

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Conceptual analysis

- Inductive bias of NetGAN

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Simplified version (no GAN, no sampling): "Cross-Entropy Low-rank Logits (CELL)"

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- Comparable generalization performance
- Huge speedup

NetGAN: learning step

- **Goal:** learn random walk distribution

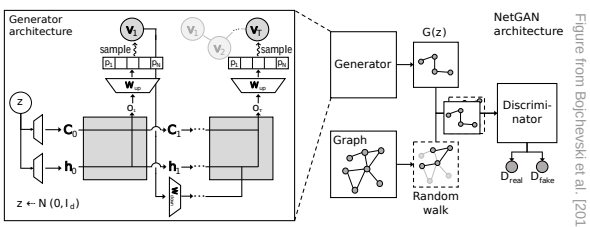

Figure from Bojchevski et al. [2018]

NetGAN: learning step

- **Goal:** learn random walk distribution
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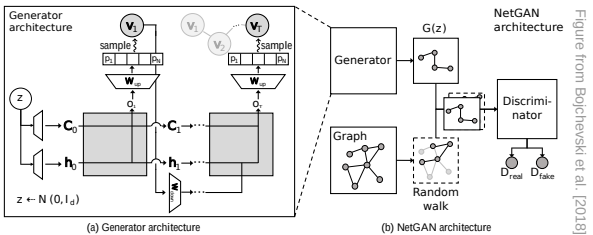

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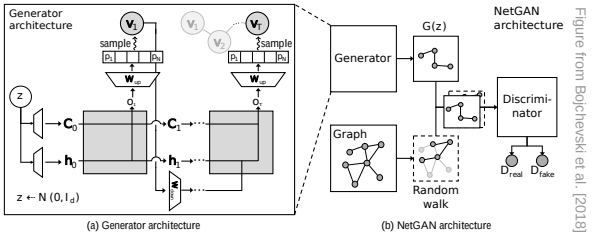

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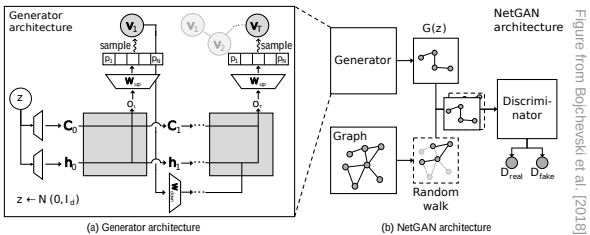

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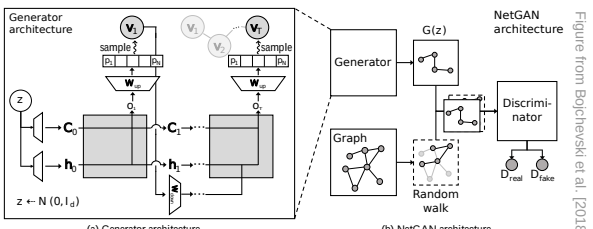
- **Architecture:** LSTMs with Wasserstein loss



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NetGAN: reconstruction step

Generator

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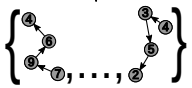
Generate *many* synthetic random walks



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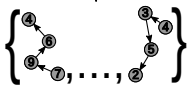

Count transitions in *score matrix S*

$$\begin{pmatrix} 0 & 360 & \cdots & 212 \\ 307 & 0 & \cdots & 150 \\ \vdots & \vdots & \ddots & \vdots \\ 240 & 143 & \cdots & 0 \end{pmatrix}$$

$S_{i,j} = \#$ transitions from i to j

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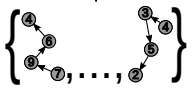

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Transform *S* into edge probability matrix $A^\dagger$

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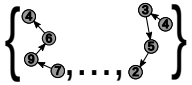

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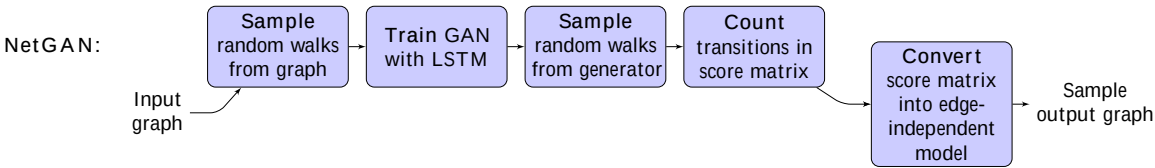
Sample edges without replacement

Overview of simplifications



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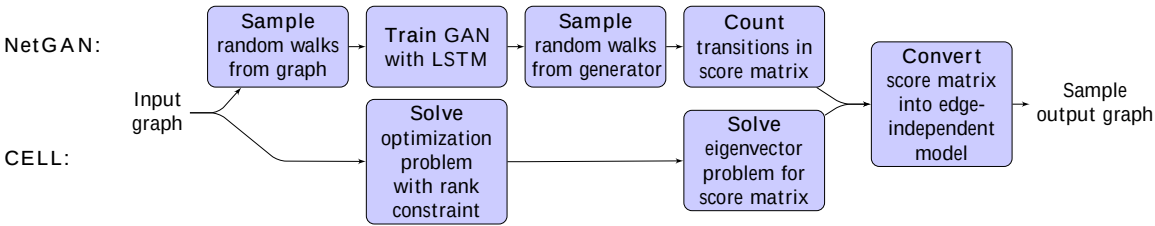

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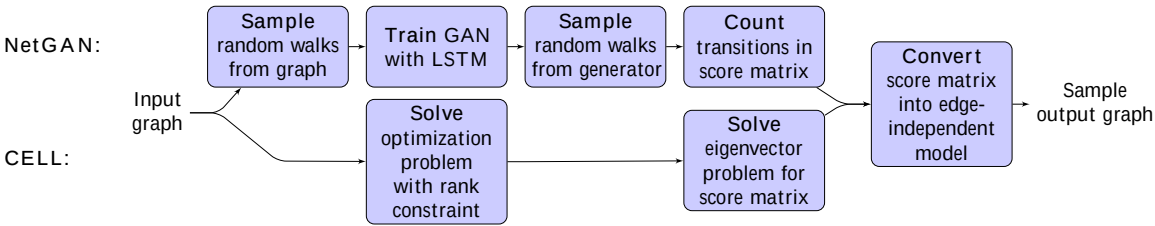

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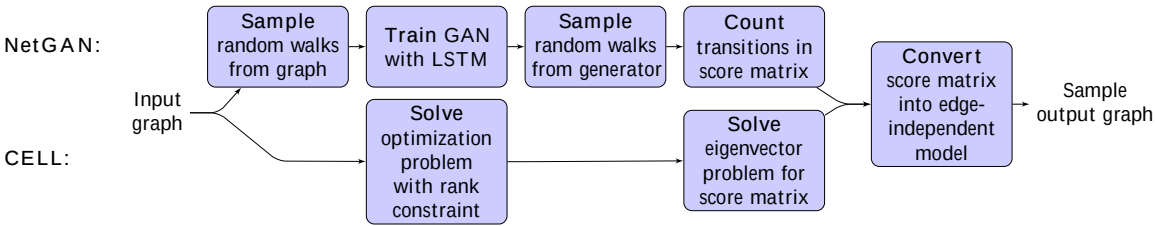
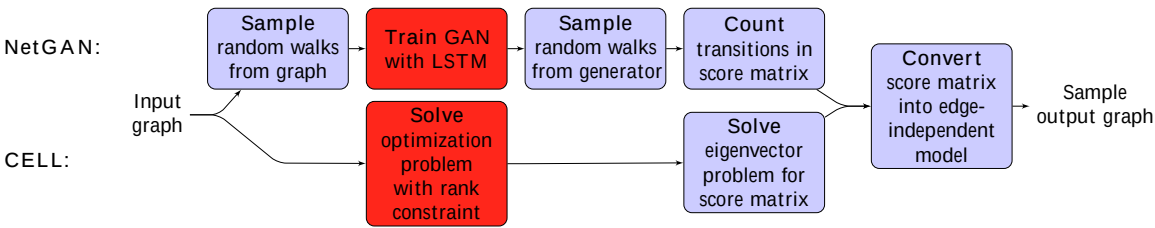


1. Replace GAN with rank-constrained optimization problem
2. Bypass random walk sampling

Replacing the GAN (1)



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What causes the generalization of NetGAN?

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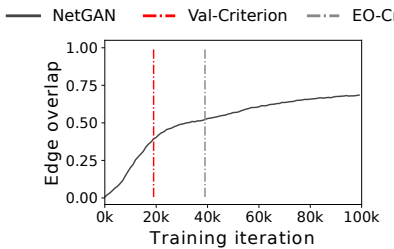

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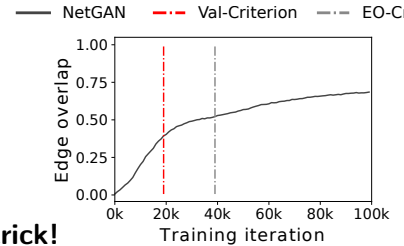

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Computational trick!

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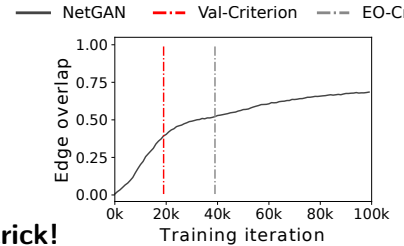

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3 Low-dimensional bottleneck

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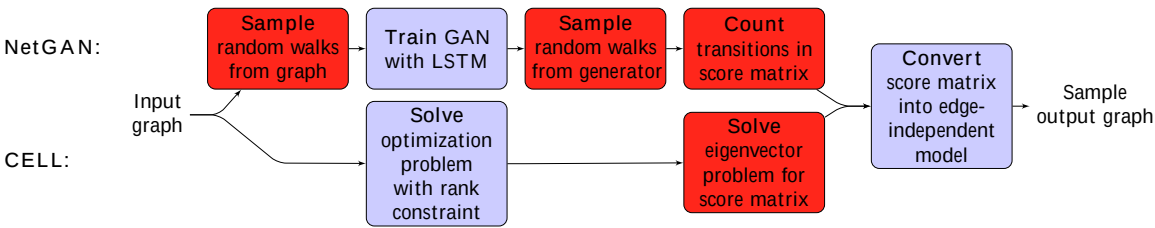
$$P \quad \{\sigma_{\text{rows}}(W) \in \mathbb{R}^{N \times N} : W \in \mathbb{R}^{N \times N}, \operatorname{rank}(W) \leq H\}.$$

- Do this directly with **maximum likelihood estimation**

$$\min_{W \in \mathbb{R}^{N \times N}} \sum_{(i,j) \in R} \log \sigma_{\text{rows}}(W)_{i,j}, \quad \text{s.t.} \quad \operatorname{rank}(W) \leq H.$$

Bypassing sampling (1)



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$$\frac{S}{nT} \xrightarrow[n,T \to \infty]{} \mathrm{diag}(\pi) P,$$

where P is corresponding random walk transition matrix and π its stationary distribution.

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Replace normalized score matrix with its limit

Bypassing sampling (3)

1. Learning step (with adjacency matrix A)

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Bypass sampling in both steps

Experiments (1)

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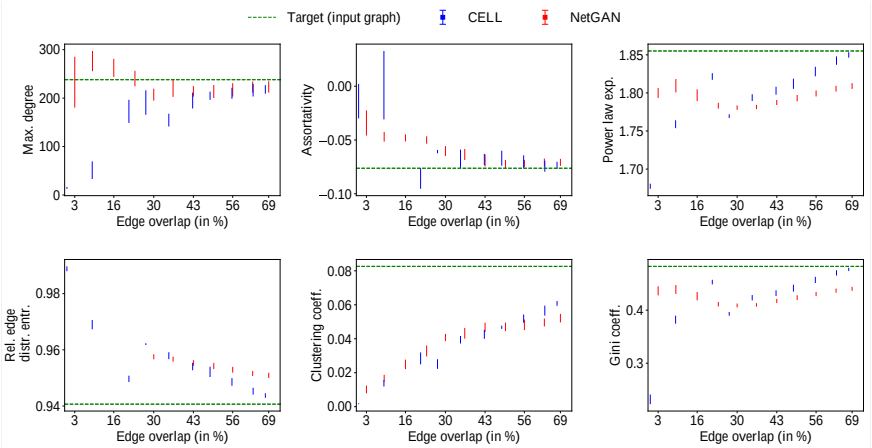
Graph: CORA-ML citation network (2,810/ 7,981)



Experiments (2)

CELL is significantly faster

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Table: Training time (in seconds) for NetGAN and CELL on a variety of networks. NetGAN requires a GPU, while CELL runs on a CPU.

Data set (Nodes/ Edges)	NetGAN	CELL
CORA-ML (2,810/ 7,981)	7,478	21
Citeseer (2,110/ 3,668)	4,654	10
PolBlogs (1,222/ 16,779)	55,276	15
RT-GOP (4,687/ 5,529)	14,800	23
Web-EDU (3,031/ 6,474)	11,000	16

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