From Theory to Practice: Rethinking Green and Martin Kernels for Unleashing Graph Transformers

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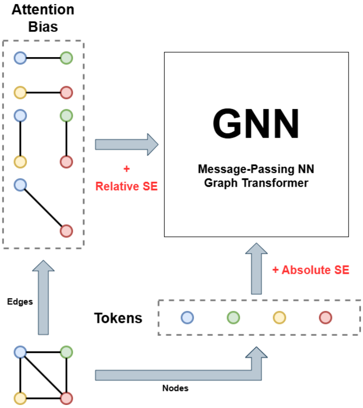
- **Structural Encoding (SE)**: injects graph structure into GNN.
  - Absolute SE: $\mathcal{V} \to \mathbb{R}^K$
  - Relative SE: $\mathcal{V} \times \mathcal{V} \to \mathbb{R}^K$
- **Kernel-based SE**: uses integral kernel as SE.
  - Kernel is a function of two variables, $\mathcal{K} : \mathcal{V} \times \mathcal{V} \to \mathbb{R}^K$
  - Absolute SE at $x = \mathcal{K}(x, x)$
  - Relative SE at $(x, y) = \mathcal{K}(x, y)$
- What kernels do we use?
  - Heat kernel, Poisson kernel, Fourier kernel, etc



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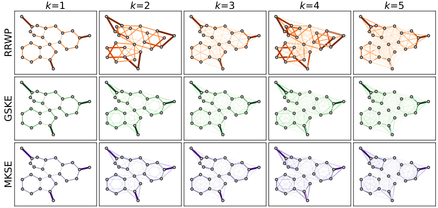
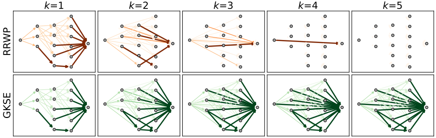
- Random walk related kernels
  - **Green Kernel**
    - Expected number of visits via random walk
    - $\mathbf{G}(x, y) = \mathbb{E}_{\omega \in \Omega(x)} \left[L_y^{\infty} \right]$
  - **Martin Kernel**
    - Probability of passing via random walk
    - $\mathbf{M}(x, y) = \mathbb{P}_{\omega \in \Omega(x)} [\tau_y < \infty]$
- Technical issues
  - Green and Martin kernels cannot be defined on recurrent graphs
  - Diagonal entries of Martin kernel are always 1
- Adaptation strategies
  - Use random walk within a limited number of steps
  - Use first return time τ_y^+ for $\mathbf{M}$





- Modified kernels
  - **finite-step Green kernel** $\mathbf{G}^{(k)}(x,y) = \mathbb{E}_{\omega \in \Omega(x)}\left[L_y^k\right]$
  - **finite-step Martin kernel** $\mathbf{M}^{(k)}(x,y) = \mathbb{P}_{\omega \in \Omega(x)}\left[\tau_y^+ \leq k\right]$
- Our proposed SEs
  - **Green Kernel Structural Encoding (GKSE)**
    - GKSE $(x,y) = [\mathbf{G}^{(0)}(x,y), \ldots, \mathbf{G}^{(K-1)}(x,y)] \in \mathbb{R}^K$
  - **Martin Kernel Structural Encoding (MKSE)**
    - MKSE $(x,y) = [\mathbf{M}^{(0)}(x,y), \ldots, \mathbf{M}^{(K-1)}(x,y)] \in \mathbb{R}^K$

Test performance on **PCQM4Mv2**

Model	MAE ↓	# Param
GCN	0.1379	2.0M
GCN-virtual	0.1153	4.9M
GIN	0.1195	3.8M
GIN-virtual	0.1083	6.7M
TokenGT (ORF)	0.0962	48.6M
TokenGT (Lap)	0.0910	48.5M
GRPE	0.0890	46.2M
EGT	0.0869	89.3M
Graphormer	0.0864	48.3M
Specformer-medium	0.0916	4.1M
GPS-small	0.0938	6.2M
GPS-medium	0.0858	19.4M
GRIT+RRWP	0.0859	16.6M
GRIT+GKSE (ours)	0.0837 ± 0.0002	11.8M
GRIT+MKSE (ours)	0.0839 ± 0.0002	11.8M

Test performance on **OCB**

Model	Ckt-Bench101	Ckt-Bench301
	MAE↓	MAE↓
GCN	0.0801 ± 0.0017	0.0584 ± 0.0006
GAT	0.0719 ± 0.0012	0.0583 ± 0.0016
GIN	0.0691 ± 0.0011	0.0528 ± 0.0004
GraphSAGE	0.0662 ± 0.0004	0.0545 ± 0.0005
GatedGCN	0.0668 ± 0.0006	0.0527 ± 0.0004
GPS+LapPE	0.0440 ± 0.0011	0.0199 ± 0.0004
GRIT+DAGPE	0.0444 ± 0.0011	0.0240 ± 0.0004
GRIT+RRWP	0.0418 ± 0.0021	0.0190 ± 0.0005
GRIT+GKSE (ours)	0.0395 ± 0.0033	0.0188 ± 0.0004
GRIT+MKSE (ours)	0.0409 ± 0.0016	0.0192 ± 0.0004

Thank you!