Graph Neural Networks
Efficient Tensor Operations In CUDA/GPU
Custom Deep Learning Framework In C++
Applications In Quantum Chemistry

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Table of Contents

Our publication

Covariant Compositional Networks For Learning Graphs (ICLR 2018)

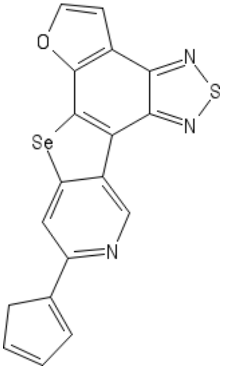
What are Graph Neural Networks?

What are Tensor Operations?

What is a Deep Learning framework?

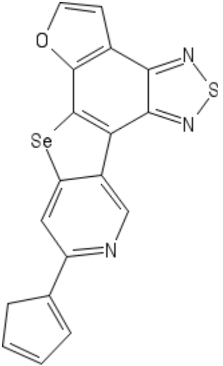
Molecular Chemical Representation

Harvard Clean Energy Project (HCEP) Dataset [2]

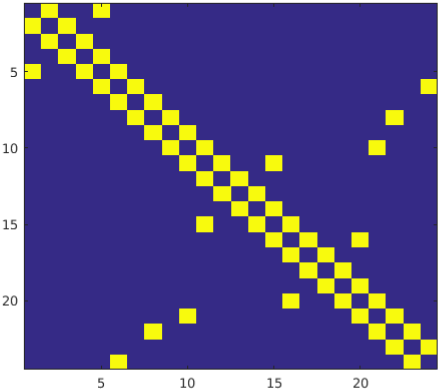


Compound: C18H9N3OSSe
SMILES: C1C=CC=C1c1cc2[Se]c3c4occc4c4nsnc4c3c2cn1
Power Conversion Efficiency (PCE, range 0 - 11): 5.16195

Molecular Graph Representation



C18H9N3OSSe



Adjacency matrix

Covariant Neural Networks

Tensor Contractions

Virtual Indexing System

GPU Multi-threading

CPU Multi-threading

Performance Test: GPU Matrix Multiplication

Performance Test: GPU Tensor Contractions

Synthetic Graph Dataset

Small-scale Molecular Test

Real-world Dataset

Conclusion and Future Research

We implemented the state-of-the-art generalized convolution operation for Graph Neural Networks in order to approximate Density Functional Theory. We obtained very promising results on the Harvard Clean Energy Project dataset.

We are developing our custom Deep Learning framework in CUDA/C++ named GraphFlow which supports symbolic differentitation and dynamic computation graph. We expect that this framework will enable us to design more flexible, efficient Graph Neural Networks at a large scale in the future.

Acknowledgements

We would like to acknowledge my advisor Professor Risi Kondor for his valuable instructions and especially for his great ideas in generalizing convolution operations in graphs. We also want to thank other members of Machine Learning group at the University of Chicago for their dedicated support.

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N. Shervashidze, P. Schweitzer, E. J. van Leeuwen, K. Mehlhorn, K. M. Borgwardt, "Weisfeiler-Lehman Graph Kernels", *Journal of Machine Learning Research*, vol. 12, 2011.

J. Hachmann, R. O. Amaya, S. A. Evrenk, C. A. Bedolla, R. S. S. Carrera, A. G. Parker, L. Vogt, A. M. Brockway, and A. A. Guzik, "The Harvard Clean Energy Project: Large-Scale Computational Screening and Design of Organic Photovoltaics on the World Community Grid", *The Journal of Physical Chemistry Letters*, pp. 2241–2251, 2011.

R. I. Kondor, and J. Lafferty, "Diffusion Kernels on Graphs and Other Discrete Structures", *International Conference on Machine Learning (ICML)*, 2002.

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Reference

N. M. Kriege, P. L. Giscard, R. C. Wilson, "On Valid Optimal Assignment Kernels and Applications to Graph Classification", *Neural Information Processing Systems (NIPS)*, 2016.

S. Kearnes, K. McCloskey, M. Berndl, V. Pande, P. Riley, "Molecular Graph Convolutions: Moving Beyond Fingerprints", *Journal of Computer-Aided Molecular Design*, vol. 30, pp. 595–608, 2016.

D. Duvenaud, D. Maclaurin, J. A. Iparraguirre, R. G. Bombarelli, T. Hirzel, A. A. Guzik, R. P. Adams, "Convolutional Networks on Graphs for Learning Molecular Fingerprints", *Neural Information Processing Systems (NIPS)*, 2015.

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Reference

T. N. Kipf, M. Welling, "Semi-Supervised Classification with Graph Convolutional Networks", *International Conference on Learning Representations (ICLR)*, 2017.

L. V. D. Maaten, G. Hinton, "Visualizing Data using t-SNE", *Journal of Machine Learning Research*, vol. 9, pp. 2579–2605, 2008.

Thank you very much for your attention!