Thoughts About ALIGNN

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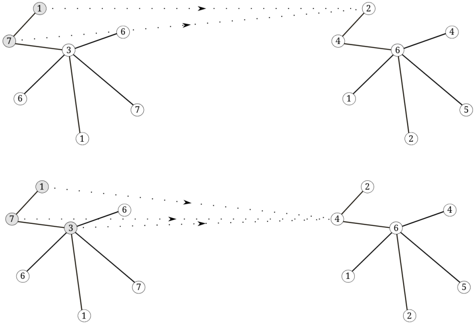
Outline

Graphs Networks are General

- framework accepts complicated data structures
  - process arbitrary dependencies between elements of input set
- can relate features of nodes and features of connections in many ways
  - local convolution
  - attention
  - sampling and aggregation (SAGE)
  - isomorphism



graph convolution illustrated[a]

[a]Daigavane, Ravindran, and Aggarwal

My Reading of GNN Implementations

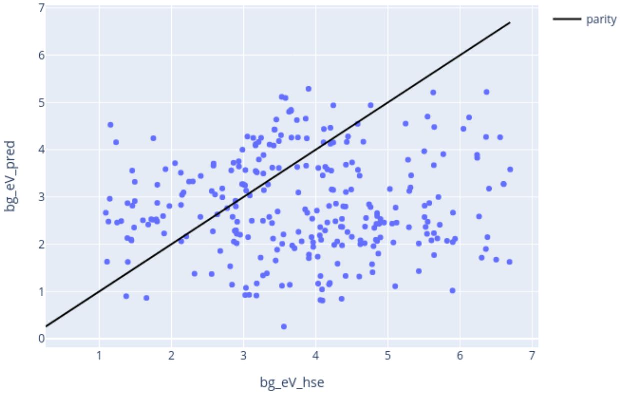
MEGnet

- leverages Materials Project infrastructure
  - suite of structure manipulation algorithms
  - flexible IO
- integrates well with high-throughput simulation workflows
- data structure enables global feature definitions
- graph in $\rightarrow$ graph out?

ALIGNN

- very nice piece of software
- easy to use and distribute
- much more accessible code-base
  - more familiar core dependencies
  - more extensible
- graph in $\rightarrow$ anything out?

Test Band Gap Predictions



JARVIS b88vdw band gap model on Perovskite HSE calculations

Training Status

GPU resources

- start using Gilbreth cluster to perform training

Perovskites data

- WIP NoSQL database for managing workflows and results

Questions

Prediction Validity v Experiment

- input features easy to obtain for experimental measurements?

ALIGNN Scalability

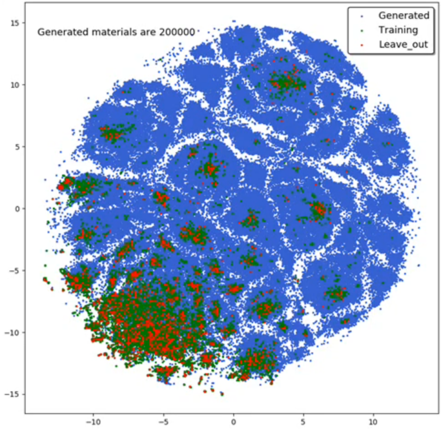
- crystal graph edge count increases exponentially with crystal size?
- how is periodicity encoded in graph?

Bench marking

- ALIGNN Competes mostly with MODNet in matbench suite, not MEGnet, anymore.
- I don't know much about MODNet

Generative Adversarial Neural Networks

Design of Perovskites attempted by MATGANIP[a]



Reinforcement Learning Applications

- one neural network is the reward function of another
  - in pure GANs, both networks learn from each other
- many correct answers

[a]Hu, Li, and Gao

ALIGNN for Materials Design I

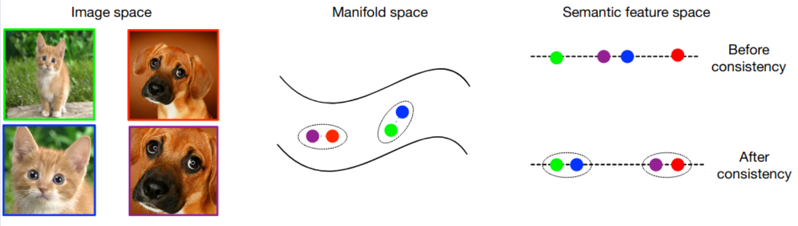
ALIGNN Design Generator

create adversary to generate materials for ALIGNN predictions

- creating a complimentary generator
    - ALIGNN as a discriminator?
- encoder/generator paradigm with ALIGNN as encoder
- "BiGAN" encoder-generator may extend adversary to consider additional constraints in material generation.
    - a type of auto-encoder

ALIGNN for Materials Design II

Training Considerations

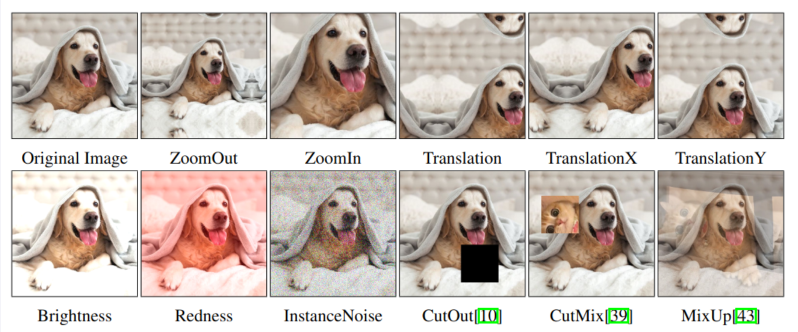


consistency regularization to promote clustering in latent space[a]

[a]Zhang et al.

ALIGNN for Materials Design III

Training Considerations



Data Augmentation (DA) via structure mutation[a]

[a] Zhao et al.

Daigavane, Ameya, Balaraman Ravindran, and Gaurav Aggarwal. "Understanding Convolutions on Graphs". In: *Distill* 6.8 (Aug. 2021). ISSN: 2476-0757. DOI: 10.23915/distill.00032. URL: http://dx.doi.org/10.23915/distill.00032 (cit. on p. 3).

Hu, Junjie, Mu Li, and Peng Gao. "Matganip: Learning To Discover the Structure-Property Relationship in Perovskites With Generative Adversarial Networks". In: *CoRR* (2019). arXiv: 1910.09003v1 [cond-mat.dis-nn]. URL: http://arxiv.org/abs/1910.09003v1 (cit. on p. 8).

Zhang, Han et al. "Consistency Regularization for Generative Adversarial Networks". In: *CoRR* (2019). arXiv: 1910.12027v2 [cs.LG]. URL: http://arxiv.org/abs/1910.12027v2 (cit. on p. 10).

Zhao, Zhengli et al. "Image Augmentations for Gan Training". In: *CoRR* (2020). arXiv: 2006.02595v1 [cs.LG]. URL: http://arxiv.org/abs/2006.02595v1 (cit. on p. 11).