Graph Neural Networks
1. Know what to use to implement a Graph Neural Network
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2. Intuition for the kinds of problems in which GNNs will provide an advantage
1. Know what to use to implement a Graph Neural Network

2. Intuition for the kinds of problems in which GNNs will provide an advantage

3. Understand why structure is crucial in determining the behavior of interacting systems
1. Know what to use to implement a Graph Neural Network

2. Intuition for the kinds of problems in which GNNs will provide an advantage

3. Understand why structure is crucial in determining the behavior of interacting systems

4. Understand why relational inductive biases are critical for learning about interacting systems
This talk

- Motivation
- Mechanisms
- Survey
- Challenges
Motivation

Mechanisms

Survey

Challenges

Structure

Programs

Drug Interactions

GNN

Relevance

https://www.semanticscholar.org/paper/Learning-to-Represent-Programs

Motivation

Structure

GNN

Relevance

Mechanisms

Programs

https://www.semanticscholar.org/paper/Learning-to-Represent-Programs

Physical Systems

\[ \sim 10^3 \text{ seconds} \]

\[ \sim 10^{-2} \text{ seconds} \]

Survey

Drug Interactions


Challenges


https://www.semanticscholar.org/paper/Learning-to-Represent-Programs
**Mechanisms**

<table>
<thead>
<tr>
<th>Structure</th>
<th>GNN</th>
<th>Relevance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Programs</td>
<td>Drug Interactions</td>
<td>Physical Systems</td>
</tr>
</tbody>
</table>

**Survey**

<table>
<thead>
<tr>
<th>Programs</th>
</tr>
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<tbody>
<tr>
<td>DFT</td>
</tr>
<tr>
<td>(E, \omega_0, \ldots)</td>
</tr>
<tr>
<td>Message Passing Neural Net</td>
</tr>
<tr>
<td>(\sim 10^{-2}) seconds</td>
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**Challenges**

<table>
<thead>
<tr>
<th>Economic Networks</th>
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<tbody>
<tr>
<td>Polypharmacy side effects</td>
</tr>
<tr>
<td>Simvastatin</td>
</tr>
<tr>
<td>Doxycycline</td>
</tr>
<tr>
<td>Ciprofloxacin</td>
</tr>
<tr>
<td>Mupirocin</td>
</tr>
<tr>
<td>(f_1) Gastrointestinal bleed side effect</td>
</tr>
<tr>
<td>(f_2) Bradycardia side effect</td>
</tr>
</tbody>
</table>

https://science.sciencemag.org/content/325/5939/422
<table>
<thead>
<tr>
<th>Motivation</th>
<th>Mechanisms</th>
<th>Survey</th>
<th>Challenges</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brief foray into Cognitive Science...</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Brief foray into Cognitive Science...

Cognitive Representation

Brief foray into Cognitive Science...

Cognitive Representation

A graph $G_1 = (V_1, E_1)$ is isomorphic to a subgraph of a graph $G_2 = (V_2, E_2)$ if there exists a subgraph of $G_2$, say $G'_2$, such that $G_1 \cong G'_2$.


GNN as meta-architecture for imparting relational inductive biases
Recurrent units + MLPs + Convolutional units projected onto a graph structure

GNN as meta-architecture for imparting **relational inductive biases**
GNN as meta-architecture for imparting **relational inductive biases**

Recurrent units + MLPs + Convolutional units projected onto a graph structure

Node Embedding:
GNN as meta-architecture for imparting **relational inductive biases**

- Recurrent units + MLPs + Convolutional units projected onto a graph structure

**Node Embedding:**

![Diagram of GNN structure]
GNN as meta-architecture for imparting **relational inductive biases**

Recurrent units + MLPs + Convolutional units projected onto a graph structure

Node Embedding:

Link Prediction:
GNN as meta-architecture for imparting **relational inductive biases**

Recurrent units + MLPs + Convolutional units projected onto a graph structure

Node Embedding:

Link Prediction:
GNN as meta-architecture for imparting relational inductive biases

Recurrent units + MLPs + Convolutional units projected onto a graph structure

Node Embedding:

Link Prediction:

Graph Embedding:
GNN as meta-architecture for imparting **relational inductive biases**

**Recurrence units + MLPs + Convolutional units projected onto a graph structure**

**Node Embedding:**

**Link Prediction:**

**Graph Embedding:**

\[ \sum = \text{Molecule } X \]
GNN as meta-architecture for imparting *relational inductive biases*

Recurrent units + MLPs + Convolutional units projected onto a graph structure

**Node Embedding:**

**Link Prediction:**

**Graph Embedding:**

\[ \Sigma = \text{Molecule } X \]

<table>
<thead>
<tr>
<th>Component</th>
<th>Entities</th>
<th>Relations</th>
<th>Rel. inductive bias</th>
<th>Invariance</th>
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<tr>
<td>Fully connected</td>
<td>Units</td>
<td>All-to-all</td>
<td>Weak</td>
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<tr>
<td>Convolutional</td>
<td>Grid elements</td>
<td>Local</td>
<td>Locality</td>
<td>Spatial translation</td>
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<tr>
<td>Recurrent</td>
<td>Timesteps</td>
<td>Sequential</td>
<td>Sequentiality</td>
<td>Time translation</td>
</tr>
<tr>
<td>Graph network</td>
<td>Nodes</td>
<td>Edges</td>
<td>Arbitrary</td>
<td>Node, edge permutations</td>
</tr>
</tbody>
</table>

State of the art in:

- Quantum/Computational Chemistry (chemical synthesis)
- Citation Prediction
- 3D vision
- Recommender systems
- Visual Question Answering
State of the art in:

- Quantum/Computational Chemistry (chemical synthesis)
- Citation Prediction
- 3D vision
- Recommender systems
- Visual Question Answering

2019 NeurIPS opened a new session called "Graph Representation Learning"
2019 NeurIPS opened a new session called "Graph Representation Learning"

Graph-based methods are gaining prominence...
<table>
<thead>
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<th>Motivation</th>
<th>Mechanisms</th>
<th>Survey</th>
<th>Challenges</th>
</tr>
</thead>
<tbody>
<tr>
<td>Message Passing Neural Network</td>
<td>Most fundamental kind of GNN</td>
<td>More recent work, applying principles from CNN architectures in GNNs</td>
<td>Network</td>
</tr>
<tr>
<td>Motivation</td>
<td>Mechanisms</td>
<td>Survey</td>
<td>Challenges</td>
</tr>
<tr>
<td>------------</td>
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<td>--------</td>
<td>------------</td>
</tr>
<tr>
<td>Message Passing Neural Network</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Graph Conv. Network</td>
<td></td>
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</tr>
</tbody>
</table>
Motivation

Mechanisms

Survey

Challenges

Message

Passing

Neural Network

Graph Conv. Network

H₃C

CH₃

CH₃

O

O

N
Message Passing Neural Network

Graph Conv. Network

Motivation

Mechanisms

Survey

Challenges
**Mechanisms**

- Node Embedding
- Neural Network (MLP)

**Message Passing Neural Network**

**Graph Conv. Network**

**Motivation**

**Survey**

**Challenges**
**Message Passing Neural Network**

- **Node Embedding**
- **Neural Network (MLP)**
- **Recurrent Unit**

**Mechanisms**

**Graph Conv. Network**

**Survey**

**Challenges**

**Motivation**
Mechanisms

- Node Embedding
- Neural Network (MLP)
- Recurrent Unit

Message Passing Neural Network

Graph Conv. Network
Mechanisms

- Node Embedding
- Neural Network (MLP)
- Recurrent Unit
Message Passing Neural Network

Node Embedding -> Classification

Nitrogen: 0.79
Oxygen: 0.11
Hydrogen: 0.01
...
Mechanisms

- Node Embedding
- Neural Network (MLP)
- Recurrent Unit

Message Passing Neural Network

Graph Conv. Network

CH₃

H₃C
Mechanisms

Motivation

Message Passing

Neural Network (MLP)

Node Embedding

Recurrent Unit

Survey

Challenges

Graph Conv. Network

- CH₃
- H₃C
- CONE
Motivation

Mechanisms

Survey

Challenges

Message Passing Neural Network

Node Embedding

Neural Network (MLP)

Recurrent Unit

Graph Conv. Network

Edge Classification/Clustering
Mechanisms

- Node Embedding
- Neural Network (MLP)
- Recurrent Unit
Motivation

Mechanisms

- Node Embedding
- Neural Network (MLP)
- Recurrent Unit

Survey

Challenges

Message Passing Neural Network

Graph Conv. Network

Graph Embedding -> Classification

Caffeine: 0.85
Dopamine: 0.03
Serotonin: 0.01
...
...
\[ H^{(l+1)} = \sigma \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right) \]
$H^{(l+1)} = \sigma \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right)$

$A = \text{np.matrix}([[0, 1, 0, 0], [0, 0, 1, 1], [0, 1, 0, 0], [1, 0, 1, 0]], \text{dtype}=\text{float})$
Hierarchical equation:

\[ H^{(l+1)} = \sigma \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right) \]

Features:

\[ X = \text{matrix}([[0., 0.], [1., -1.], [2., -2.], [3., -3.]]) \]

\[ A = \text{np.matrix}([[0, 1, 0, 0], [0, 0, 1, 1], [0, 1, 0, 0], [1, 0, 1, 0]], \text{dtype}=\text{float}) \]
Mechanisms

Motivation

Survey

Challenges

Message Passing Neural Network

Graph Conv. Network

Features:

\[
A = \text{np.matrix}([[0, 1, 0, 0],
[0, 0, 1, 1],
[0, 1, 0, 0],
[1, 0, 1, 0]],
dtype=float)
\]

\[
X = \text{matrix}([[0., 0.],
[1., -1.],
[2., -2.],
[3., -3.]])
\]

\[
A*X = \text{matrix}([[1., -1.],
[5., -5.],
[1., -1.],
[2., -2.]])
\]

\[
H^{(l+1)} = \sigma\left(\tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} H^{(l)} W^{(l)}\right)
\]
$H^{(l+1)} = \sigma \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right)$
<table>
<thead>
<tr>
<th>Motivation</th>
<th>Mechanisms</th>
<th>Survey</th>
</tr>
</thead>
<tbody>
<tr>
<td>NRI</td>
<td>Neural Relational Inference</td>
<td>Polypharmacy prediction</td>
</tr>
<tr>
<td>Decagon</td>
<td></td>
<td>Review graph-based approaches</td>
</tr>
<tr>
<td>Relational Reasoning</td>
<td></td>
<td>Popular frameworks + datasets</td>
</tr>
<tr>
<td>Implementation</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Goals:
1) learn to infer the latent interaction graph
2) learn dynamics of the interacting system using 1)
3) complete 1) and 2) using only object trajectories as input
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1) learn to infer the latent interaction graph
2) learn dynamics of the interacting system using 1)
3) complete 1) and 2) using only object trajectories as input

Data:
1) Simulated object trajectories (masses on springs, charged particles, phase coupled oscillators)
Goals:
1) learn to infer the latent interaction graph
2) learn dynamics of the interacting system using 1)
3) complete 1) and 2) using only object trajectories as input

Data:
1) Simulated object trajectories (masses on springs, charged particles, phase coupled oscillators)

Model:
1) Encoder which predicts interactions/types given trajectories
2) Decoder that learns the dynamical model given the interaction graph
NRI

Decagon

Relational Reasoning

Implementation

Survey

Legend:  
: Node emb.  
: Edge emb.  
: MLP  
: Concrete distribution  
: Sampling

Learned Regularizer

66
NRI
Decagon
Relational Reasoning
Implementation
Motivation

Mechanisms

Survey

Challenges

Legend:  
- Node emb.  
- Edge emb.  
- MLP  
- : Concrete distribution  
- : Sampling

NRI

Decagon

Relational Reasoning

Implementation

Learned Regularizer

Training Signal:

Δx
**Table 1.** Accuracy (in %) of unsupervised interaction recovery.

<table>
<thead>
<tr>
<th>Model</th>
<th>Springs</th>
<th>Charged</th>
<th>Kuramoto</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corr. (path)</td>
<td>52.4±0.0</td>
<td>55.8±0.0</td>
<td>62.8±0.0</td>
</tr>
<tr>
<td>Corr. (LSTM)</td>
<td>52.7±0.9</td>
<td>54.2±2.0</td>
<td>54.4±0.5</td>
</tr>
<tr>
<td>NRI (sim.)</td>
<td>99.8±0.0</td>
<td>59.6±0.8</td>
<td>–</td>
</tr>
<tr>
<td>NRI (learned)</td>
<td>99.9±0.0</td>
<td>82.1±0.6</td>
<td>96.0±0.1</td>
</tr>
</tbody>
</table>
Goal:
1) learn to predict polypharmacy side effects
2) flag and prioritize polypharmacy side effects for follow-up analysis via formal pharmacological studies.
**Goal:**

1) learn to predict polypharmacy side effects
2) flag and prioritize polypharmacy side effects for follow-up analysis via formal pharmacological studies.

**Data:**

1) multimodal graph of protein-protein interactions, drug-protein target interactions, and the polypharmacy side effects, which are represented as **drug-drug interactions, where each side effect is an edge of a different type.**
**Motivation**

**NRI**

**Decagon**

**Relational Reasoning**

**Implementation**

**Survey**

**Goal:**

1) learn to predict polypharmacy side effects
2) flag and prioritize polypharmacy side effects for follow-up analysis via formal pharmacological studies.

**Data:**

1) multimodal graph of protein-protein interactions, drug-protein target interactions, and the polypharmacy side effects, which are represented as drug-drug interactions, where each side effect is an edge of a different type.

**Model:**

1) (Encoder) Graph Convolutional Network for multi-relational link prediction in multimodal networks
2) (Decoder) Tensor Factorization to reconstruct edges between drugs
Motivation

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NRI

Decagon

Relational Reasoning

Implementation

\[
\mathbf{h}_i^{(k+1)} = \phi \left( \sum_r \sum_{j \in \mathcal{N}_r^i} c_{ij} \mathbf{W}_r^{(k)} \mathbf{h}_j^{(k)} + c_i \mathbf{h}_i^{(k)} \right)
\]
\[ h^{(k+1)}_i = \phi \left( \sum_r \sum_{j \in \mathcal{N}_r^i} c^{ij}_r W^{(k)}_r h^{(k)}_j + c^i_r h^{(k)}_i \right) \]
Table 2. Area under ROC curve (AUROC), area under precision-recall curve (AUPRC), and average precision at 50 (AP@50) for polypharmacy side effect prediction. Reported are average performance values for 964 side effect types.

<table>
<thead>
<tr>
<th>Approach</th>
<th>AUROC</th>
<th>AUPRC</th>
<th>AP@50</th>
</tr>
</thead>
<tbody>
<tr>
<td>Decagon</td>
<td>0.872</td>
<td>0.832</td>
<td>0.803</td>
</tr>
<tr>
<td>RESCAL tensor factorization</td>
<td>0.693</td>
<td>0.613</td>
<td>0.476</td>
</tr>
<tr>
<td>DEDICOM tensor factorization</td>
<td>0.705</td>
<td>0.637</td>
<td>0.567</td>
</tr>
<tr>
<td>DeepWalk neural embeddings</td>
<td>0.761</td>
<td>0.737</td>
<td>0.658</td>
</tr>
<tr>
<td>Concatenated drug features</td>
<td>0.793</td>
<td>0.764</td>
<td>0.712</td>
</tr>
</tbody>
</table>
Goal:

1) answer questions about objects in visual scenes
Goal:
1) answer questions about objects in visual scenes

Data:
1) curated images of entities of different sizes/types
Goal:
1) answer questions about objects in visual scenes

Data:
1) curated images of entities of different sizes/types

Model:
1) Varied - CNN + graph structured representations
Q: Are there an **equal number** of large things and metal spheres?
Q: What size is the cylinder that is left of the brown metal thing that is left of the big sphere?
Q: There is a **sphere** with the same size as the metal cube; is it made of the same material as the small red sphere?
Q: How many objects are either small cylinders or red things?
Motivation

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!=
Q: Are there an equal number of large things and metal spheres?
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Motivation

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What size is the cylinder that is left of the brown metal thing that is left of the big sphere?

[Diagram of a CNN feature map with connections labeled as 'Conv.', 'object', 'RN', 'gθ-MLP', 'f∅-MLP', 'Element-wise sum', 'small', 'what size is ... sphere', 'LSTM', 'https://arxiv.org/pdf/1706.01427.pdf']
<table>
<thead>
<tr>
<th>Model</th>
<th>Overall</th>
<th>Count</th>
<th>Exist</th>
<th>Compare Numbers</th>
<th>Query Attribute</th>
<th>Compare Attribute</th>
</tr>
</thead>
<tbody>
<tr>
<td>Human</td>
<td>92.6</td>
<td>86.7</td>
<td>96.6</td>
<td>86.5</td>
<td>95.0</td>
<td>96.0</td>
</tr>
<tr>
<td>Q-type baseline</td>
<td>41.8</td>
<td>34.6</td>
<td>50.2</td>
<td>51.0</td>
<td>36.0</td>
<td>51.3</td>
</tr>
<tr>
<td>LSTM</td>
<td>46.8</td>
<td>41.7</td>
<td>61.1</td>
<td>69.8</td>
<td>36.8</td>
<td>51.8</td>
</tr>
<tr>
<td>CNN+LSTM</td>
<td>52.3</td>
<td>43.7</td>
<td>65.2</td>
<td>67.1</td>
<td>49.3</td>
<td>53.0</td>
</tr>
<tr>
<td>CNN+LSTM+SA</td>
<td>68.5</td>
<td>52.2</td>
<td>71.1</td>
<td>73.5</td>
<td>85.3</td>
<td>52.3</td>
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<tr>
<td>CNN+LSTM+SA*</td>
<td>76.6</td>
<td>64.4</td>
<td>82.7</td>
<td>77.4</td>
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<td>75.4</td>
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<tr>
<td>CNN+LSTM+RN</td>
<td><strong>95.5</strong></td>
<td><strong>90.1</strong></td>
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<td><strong>93.6</strong></td>
<td><strong>97.9</strong></td>
<td><strong>97.1</strong></td>
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</table>
DeepMind GraphNets
https://github.com/deepmind/graph_nets
Motivation

Decagon

Relational Reasoning

Implementation

NRI

DeepMind GraphNets
https://github.com/deepmind/graph_nets

PyTorch Geometric
https://pytorch-geometric.readthedocs.io

Open Graph Benchmark
http://ogb.stanford.edu
# Open Graph Benchmark

[http://ogb.stanford.edu](http://ogb.stanford.edu)

## Survey

### NRI

<table>
<thead>
<tr>
<th>Name</th>
<th>Size</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ogbn-proteins</td>
<td>100 K</td>
<td>Protein-protein association network linked across species</td>
</tr>
<tr>
<td>ogbn-wiki</td>
<td>1 M</td>
<td>Wikipedia hyperlinks</td>
</tr>
<tr>
<td>ogbn-products</td>
<td>2 M</td>
<td>Amazon co-purchasing network</td>
</tr>
</tbody>
</table>

### Decagon

<table>
<thead>
<tr>
<th>Name</th>
<th>Size</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ogbl-ddi</td>
<td>15 K</td>
<td>Drug-drug interaction network</td>
</tr>
<tr>
<td>ogbl-biomed</td>
<td>100 K</td>
<td>Human biomedical knowledge graph</td>
</tr>
<tr>
<td>ogbl-ppa</td>
<td>500 K</td>
<td>Protein-protein association network</td>
</tr>
<tr>
<td>ogbl-reviews</td>
<td>10 M</td>
<td>Amazon user-item review dataset</td>
</tr>
<tr>
<td>ogbl-citations</td>
<td>200 M</td>
<td>Microsoft Academic Graph citation network</td>
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### Relational Reasoning

<table>
<thead>
<tr>
<th>Name</th>
<th>Size</th>
<th>Description</th>
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<tbody>
<tr>
<td>ogbg-mol</td>
<td>500 K</td>
<td>Molecular property prediction datasets from MoleculeNet</td>
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<tr>
<td>ogbg-code</td>
<td>1 M</td>
<td>Abstract Syntax Trees of code snippets</td>
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<tr>
<td>ogbg-ppi</td>
<td>10 M</td>
<td>Protein-protein interaction network</td>
</tr>
</tbody>
</table>
Depth | Cannot currently make “deep” GNNs
---|---
Scaling | Computational concerns
Generation | Converting sensory data into structured representations
Problem 1: eventually we run out of nodes
Problem 1: eventually we run out of nodes
Problem 1: eventually we run out of nodes

Problem 2: smoothing
Problem 1: eventually we run out of nodes

Depth

Problem 2: smoothing

Scaling

Generation

neighbor aggregation
Problem 1: Current GCN formulation relies on adjacency matrix
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Problem 2: Models with a single network per node
Problem 1: Huge amounts of sensory data, all “1-dimensional”
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1. Know what to use to implement a Graph Neural Network
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2. Intuition for the kinds of problems in which GNNs will provide an advantage
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2. Intuition for the kinds of problems in which GNNs will provide an advantage

3. Understand why structure is crucial in determining the behavior of interacting systems
1. Know what to use to implement a Graph Neural Network

2. Intuition for the kinds of problems in which GNNs will provide an advantage

3. Understand why structure is crucial in determining the behavior of interacting systems

4. Understand why \textit{relational inductive biases} are critical for learning about interacting systems
Resources


- Non-comprehensive but substantial list of geometric DL papers: https://github.com/thunlp/GNNPapers

- Graph Representation Learning @NeurIPS: https://grlearning.github.io/papers/