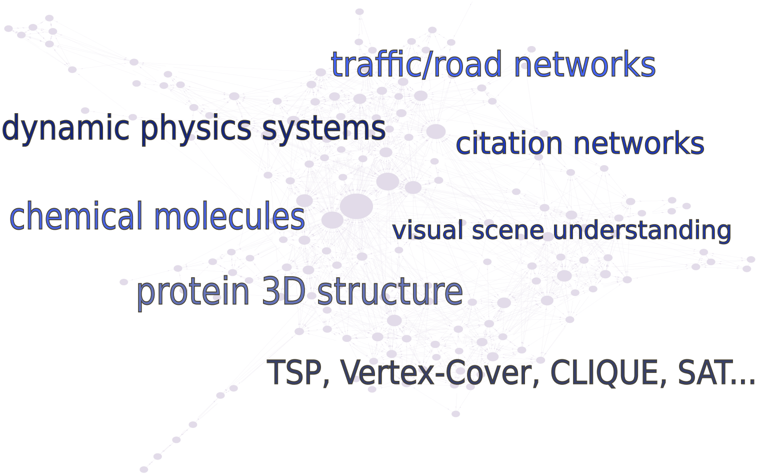
Graph Neural Networks

Felix Becker

University of Greifswald

June 28, 2021

Graphs are everywhere



traffic/road networks

dynamic physics systems

citation networks

chemical molecules

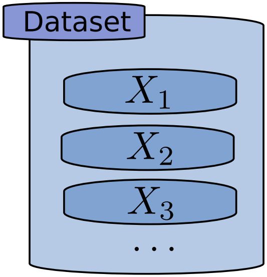
visual scene understanding

protein 3D structure

TSP, Vertex-Cover, CLIQUE, SAT...

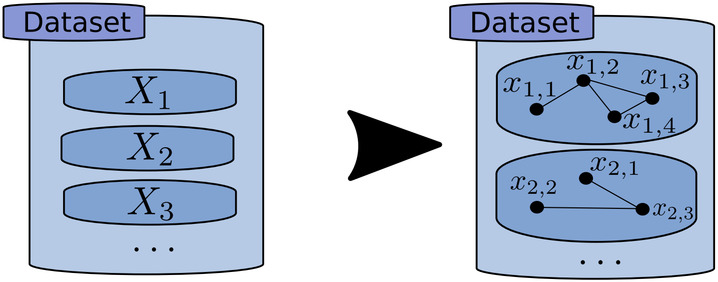
Inductive bias

- Often, data does not come as individual objects...



Inductive bias

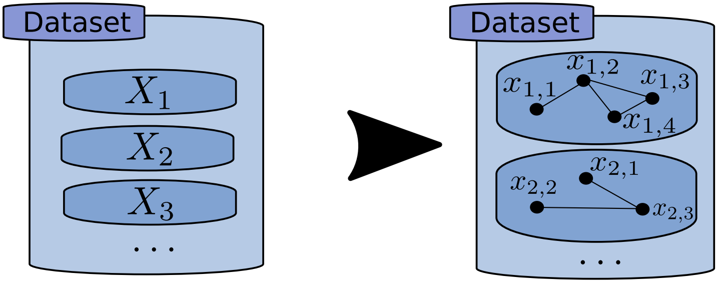
- Often, data does not come as individual objects...



- ... but rather in sets of objects and rules on how they interact.

Inductive bias

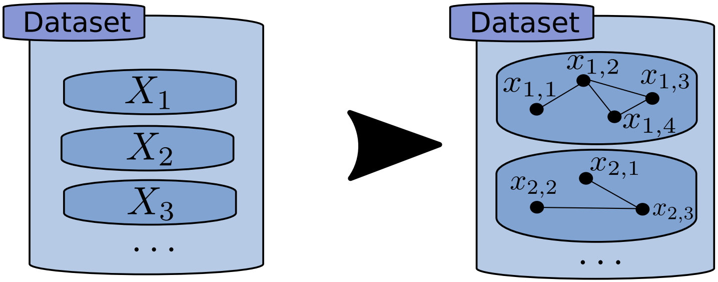
- Often, data does not come as individual objects...



- ... but rather in sets of objects and rules on how they interact.
- Inductive bias: constraints imposed on the set of possible pairwise interactions (represented as a graph).

Inductive bias

- Often, data does not come as individual objects...



- ... but rather in sets of objects and rules on how they interact.
- Inductive bias: constraints imposed on the set of possible pairwise interactions (represented as a graph).
- Making predictions requires 'relational reasoning' based on the graph structure.

Inductive bias

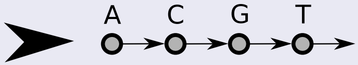
Inductive biases can be well defined independent of the data examples:

Inductive bias

Inductive biases can be well defined independent of the data examples:

Sequences

>1j46_A
ACGTAAGTGTAAG (...)

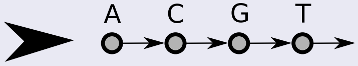


Inductive bias

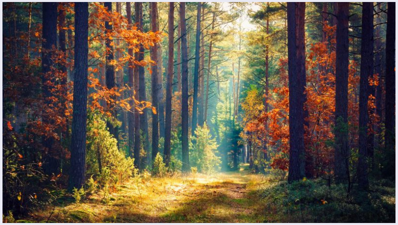
Inductive biases can be well defined independent of the data examples:

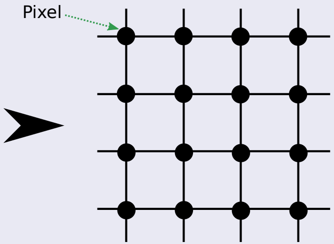
Sequences

>1j46_A
ACGTAAGTGTAAG (...)



Images





Inductive bias

- We have dedicated models for some cases:

Inductive bias

- We have dedicated models for some cases:
    - Recurrent architectures for sequences.

Inductive bias

- We have dedicated models for some cases:
    - Recurrent architectures for sequences.
    - Convolutional neural networks for images.

Inductive bias

- We have dedicated models for some cases:
  - Recurrent architectures for sequences.
  - Convolutional neural networks for images.
- But how to handle data with less well defined inductive biases? (e.g. chemical molecules, road networks, citation networks...)

Graph Neural Networks (GNNs)

Definition: Feature graph

A (directed) feature graph is a 3-tuple $G = (u, V, E)$ with a global attribute u, nodes $V = \{ v_i \}_{i=1,\dots,n}$ where v_i are the attributes of the node at index i and edges $E = \{ (e_j, s_j, r_j) \}_{j=1,\dots,m}$ with edge attributes e_j, a sender node index s_j and a receiver node index r_j.

Graph Neural Networks (GNNs)

Definition: Feature graph

A (directed) feature graph is a 3-tuple $G = (u, V, E)$ with a global attribute u, nodes $V = \{ v_i \}_{i=1,\dots,n}$ where v_i are the attributes of the node at index i and edges $E = \{ (e_j, s_j, r_j) \}_{j=1,\dots,m}$ with edge attributes e_j, a sender node index s_j and a receiver node index r_j.

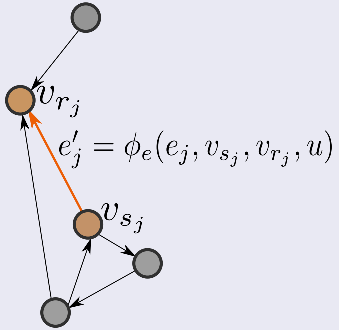
Definition: Graph neural network

A graph neural network (GNN) is a mapping $\omega : G \mapsto G'$ that maps a feature graph $G = (u, V, E)$ to another feature graph $G' = (u', V', E')$ with $V' = \{ v'_i \}_{i=1,\dots,n}$ and $E' = \{ (e'_j, s_j, r_j) \}_{j=1,\dots,m}$.

An implementation of ω

Let ϕ_v, ϕ_e, ϕ_u be learnable non-linear functions (e.g. multilayer perceptrons).

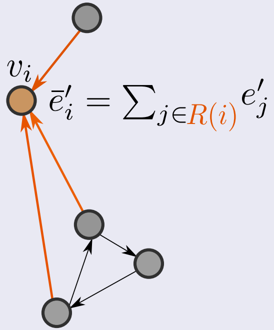
1. Update all edges



An implementation of ω

Let ϕ_v, ϕ_e, ϕ_u be learnable non-linear functions (e.g. multilayer perceptrons).

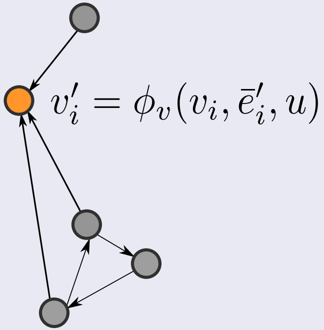
1. Update all edges
2. Aggregate neighborhoods



An implementation of ω

Let ϕ_v, ϕ_e, ϕ_u be learnable non-linear functions (e.g. multilayer perceptrons).

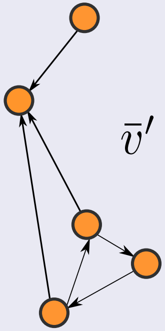
1. Update all edges
2. Aggregate neighborhoods
3. Update all nodes



An implementation of ω

Let ϕ_v, ϕ_e, ϕ_u be learnable non-linear functions (e.g. multilayer perceptrons).

1. Update all edges
2. Aggregate neighborhoods
3. Update all nodes
4. Aggregate nodes

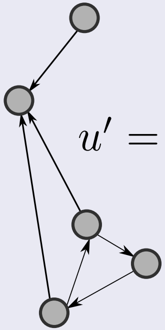


$$\bar{v}' = \sum_i v_i'$$

An implementation of ω

Let ϕ_v, ϕ_e, ϕ_u be learnable non-linear functions (e.g. multilayer perceptrons).

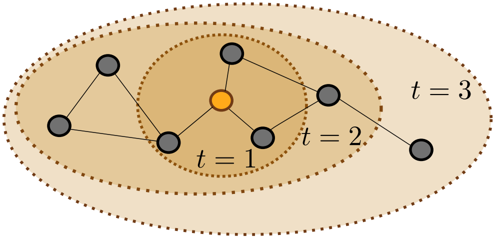
1. Update all edges
2. Aggregate neighborhoods
3. Update all nodes
4. Aggregate nodes
5. Update global attribute



$$u' = \phi_u(u, \bar{v}')$$

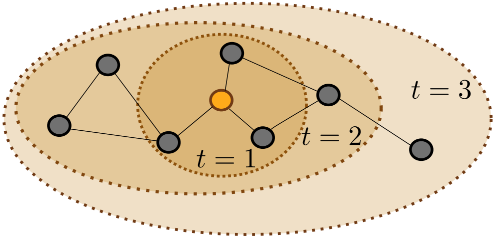
Message passing

Message passing: a composition of a GNN ω with itself for a fixed number of iterations: $\omega(\omega(\ldots\omega(G)))$



Message passing

Message passing: a composition of a GNN ω with itself for a fixed number of iterations: $\omega(\omega(\ldots\omega(G)))$



- If the global attribute u is excluded, the output of a node v after N iterations is conditioned on all nodes with a distance of at most N to v.

Representation learning

What do the learned representations v_i, e_j and u mean?

Representation learning

What do the learned representations v_i, e_j and u mean?
Short answer: We do not know.

Representation learning

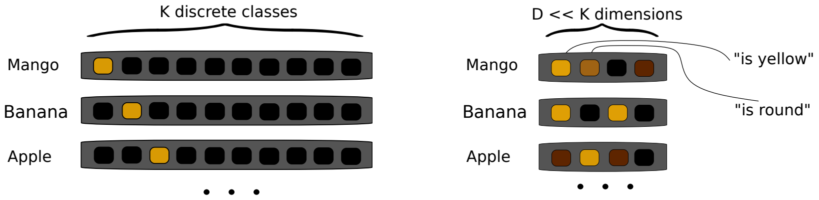
What do the learned representations v_i, e_j and u mean?

Short answer: We do not know.

But we can have an idea:

Representation learning

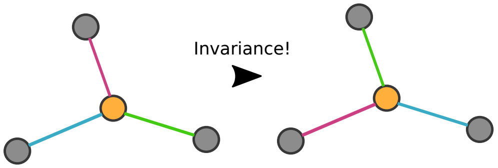
What do the learned representations v_i, e_j and u mean?
Short answer: We do not know.
But we can have an idea:



We use a D dimensional latent space where each neuron could represent a rather simple, independent property. Some of these properties, we can try to interpret as a human.
$\Longrightarrow$ Empirical: A shallow model on top (e.g. a linear combination) could make accurate predictions.

Remarks

A GNN is invariant to graph isomorphism, if the aggregation operations are symmetric functions (sum, average...)



Remarks

- A GNN is differentiable, if ϕ_v, ϕ_e, ϕ_u are (w.r.t. their weights θ).

Remarks

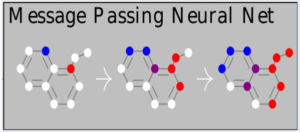
- A GNN is differentiable, if ϕ_v, ϕ_e, ϕ_u are (w.r.t. their weights θ).
- Therefore, we can backpropagate a loss signal in order to update θ.

Remarks

- A GNN is differentiable, if ϕ_v, ϕ_e, ϕ_u are (w.r.t. their weights θ).
- Therefore, we can backpropagate a loss signal in order to update θ.
- The loss may depend on u' (graph focused), V' (node focused) or E' (edge focused) or all of these.

Some GNN applications

Predict properties of chemical molecules



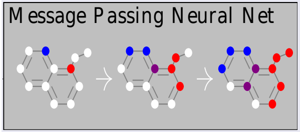
Neural Message Passing for Quantum Chemistry
– Gilmer et al., 2017

Input

Molecule as a graph: Type of atom for each node, type of bond for each edge.

Some GNN applications

Predict properties of chemical molecules



Neural Message Passing for Quantum Chemistry
– Gilmer et al., 2017

Input

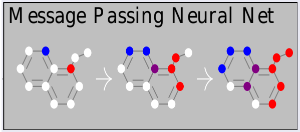
Molecule as a graph: Type of atom for each node, type of bond for each edge.

Output

A global property of the molecule e.g. energy

Some GNN applications

Predict properties of chemical molecules



Neural Message Passing for Quantum Chemistry
– Gilmer et al., 2017

Input

Molecule as a graph: Type of atom for each node, type of bond for each edge.

Output

A global property of the molecule e.g. energy

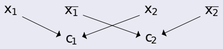
Loss

MSE on the global output u'

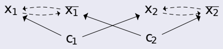
Some GNN applications

Solve SAT

Learning a SAT solver from single-bit supervision – Selsam et al., 2019



(a)



(b)

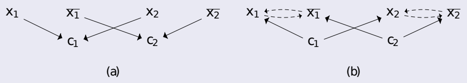
Input

SAT instance I encoded as an unlabeled graph G

Some GNN applications

Solve SAT

Learning a SAT solver from single-bit supervision – Selsam et al., 2019



Input

SAT instance I encoded as an unlabeled graph G

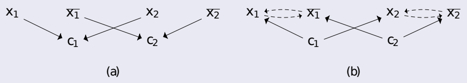
Output

$P(I \text{ is satisfiable} \mid G)$

Some GNN applications

Solve SAT

Learning a SAT solver from single-bit supervision – Selsam et al., 2019



Input

SAT instance I encoded as an unlabeled graph G

Output

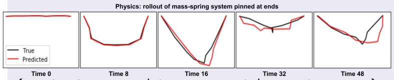
$P(I \text{ is satisfiable} \mid G)$

Loss

Binary cross entropy on the global output u'

Some GNN applications

Timesteps in a dynamic physics system



(github.com/deepmind/graph_nets)

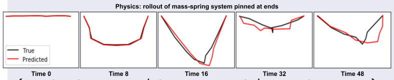
Relational inductive biases, deep learning, and graph networks
– Battaglia et al., 2018

Input

Initial state of the rope as a graph: Masses and positions as node attributes. Only add edges for adjacent masses on the rope.
Possible global attribute: Gravity

Some GNN applications

Timesteps in a dynamic physics system



(github.com/deepmind/graph_nets)

Relational inductive biases, deep learning, and graph networks
– Battaglia et al., 2018

Input

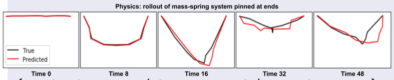
Initial state of the rope as a graph: Masses and positions as node attributes. Only add edges for adjacent masses on the rope.
Possible global attribute: Gravity

Output

State of the rope (i.e. updated node positions) after N timesteps.

Some GNN applications

Timesteps in a dynamic physics system



(github.com/deepmind/graph_nets)

Relational inductive biases, deep learning, and graph networks
– Battaglia et al., 2018

Input

Initial state of the rope as a graph: Masses and positions as node attributes. Only add edges for adjacent masses on the rope.
Possible global attribute: Gravity

Output

State of the rope (i.e. updated node positions) after N timesteps.

Loss

MSA on the node outputs v_i'

A practical example: Sorting numbers

Input

A list of pairwise distinct numbers $x_1, \ldots, x_k$

- WLOG $x_i \in [0, 1]$
- k is variable

Output

A sorted list of the same numbers

A practical example: Sorting numbers

Input

A list of pairwise distinct numbers $x_1, \ldots, x_k$

- WLOG $x_i \in [0, 1]$
- k is variable

Output

A sorted list of the same numbers

Let π be a sorting permutation of the indices, i.e. $\pi(i) = j \Leftrightarrow x_i$ is the jth smallest element

A naive approach without GNNs

We could try to solve the problem by using a simple neural network with an input vector of fixed length L:

$$(x_1, x_2, \ldots, x_k, P, P, \ldots, P)$$

where L is large enough for all reasonable inputs and P is some *padding* added to input lists shorter than L.

A naive approach without GNNs

We could try to solve the problem by using a simple neural network with an input vector of fixed length L:

$$(x_1, x_2, \ldots, x_k, P, P, \ldots, P)$$

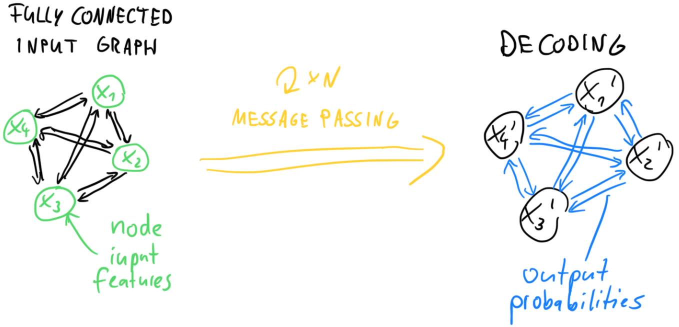
where L is large enough for all reasonable inputs and P is some *padding* added to input lists shorter than L.

Why **NOT** do it this way.

- maximum list length L is not intuitive
- overhead for $k << L$
- no generalization to longer lists than seen during training

Idea

1. Construct a fully connected graph with numbers as nodes
2. Refine nodes/edge embeddings with message passing
3. Decode $P(\pi(j) = \pi(i) + 1 | x_1, x_2, \dots, x_k)$ for all $i, j = 1, \dots, k$



Loss and Training

For details see notebook "Sort.ipynb".