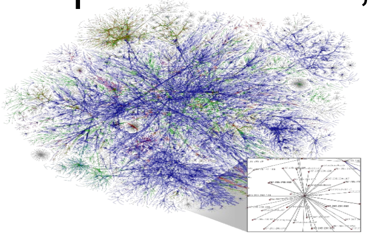
Graph Representation Learning and Generation

Jian Tang
Assistant Professor
Montréal Institute for Learning Algorithms (MILA)
HEC Montréal
tangjianpku@gmail.com

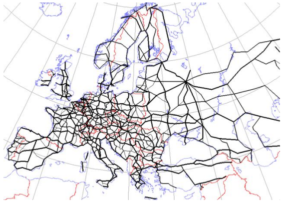
Graphs: general and flexible data structures

- Ubiquitous in real-world, arises in multiple disciplines
  - computer science, social science, healthcare, bioinformatics, ...

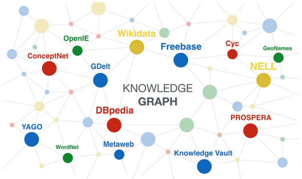


World Wide Web

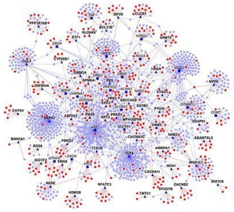
Social Network



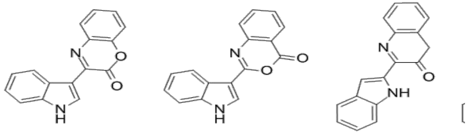
Road Network



Knowledge Graph



Protein-protein Interaction Graph



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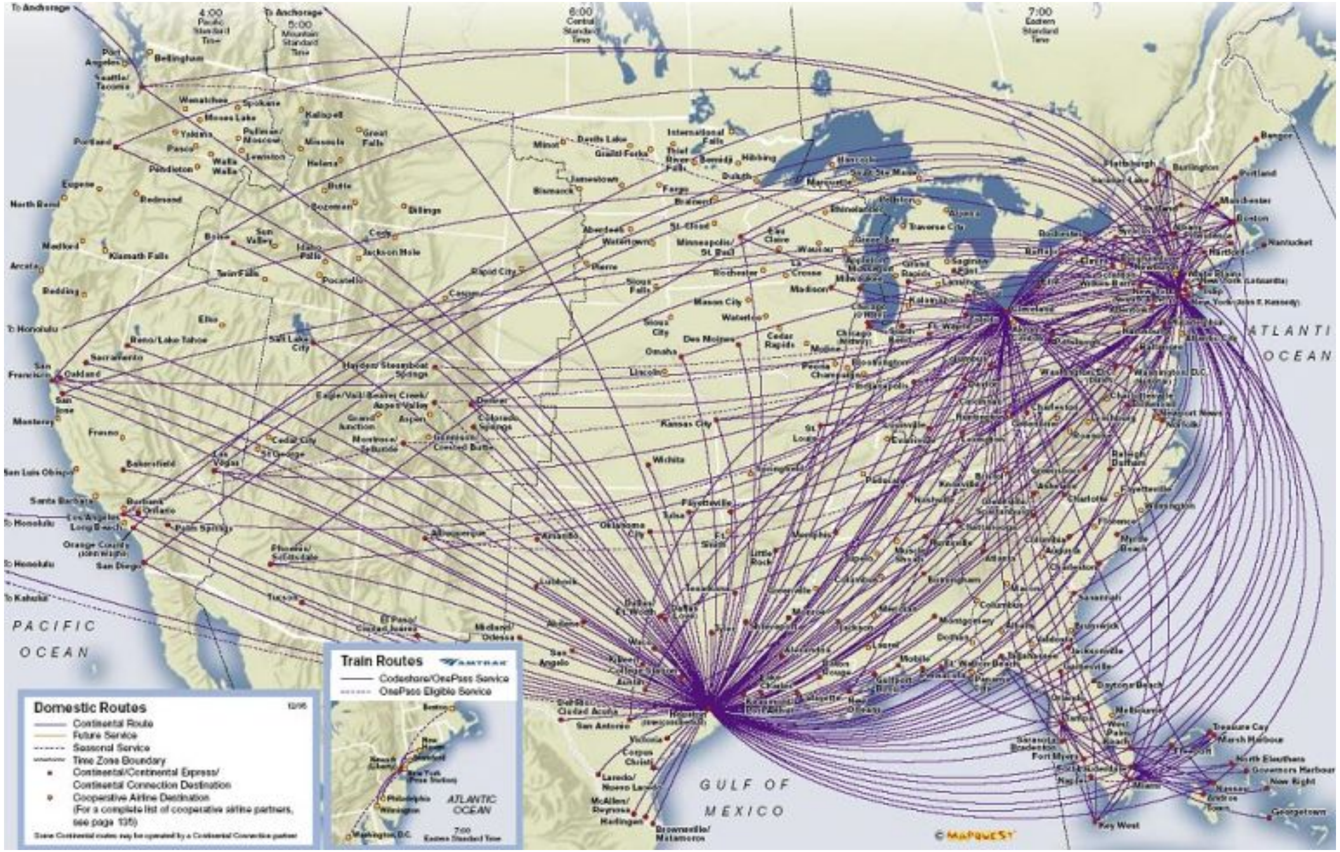
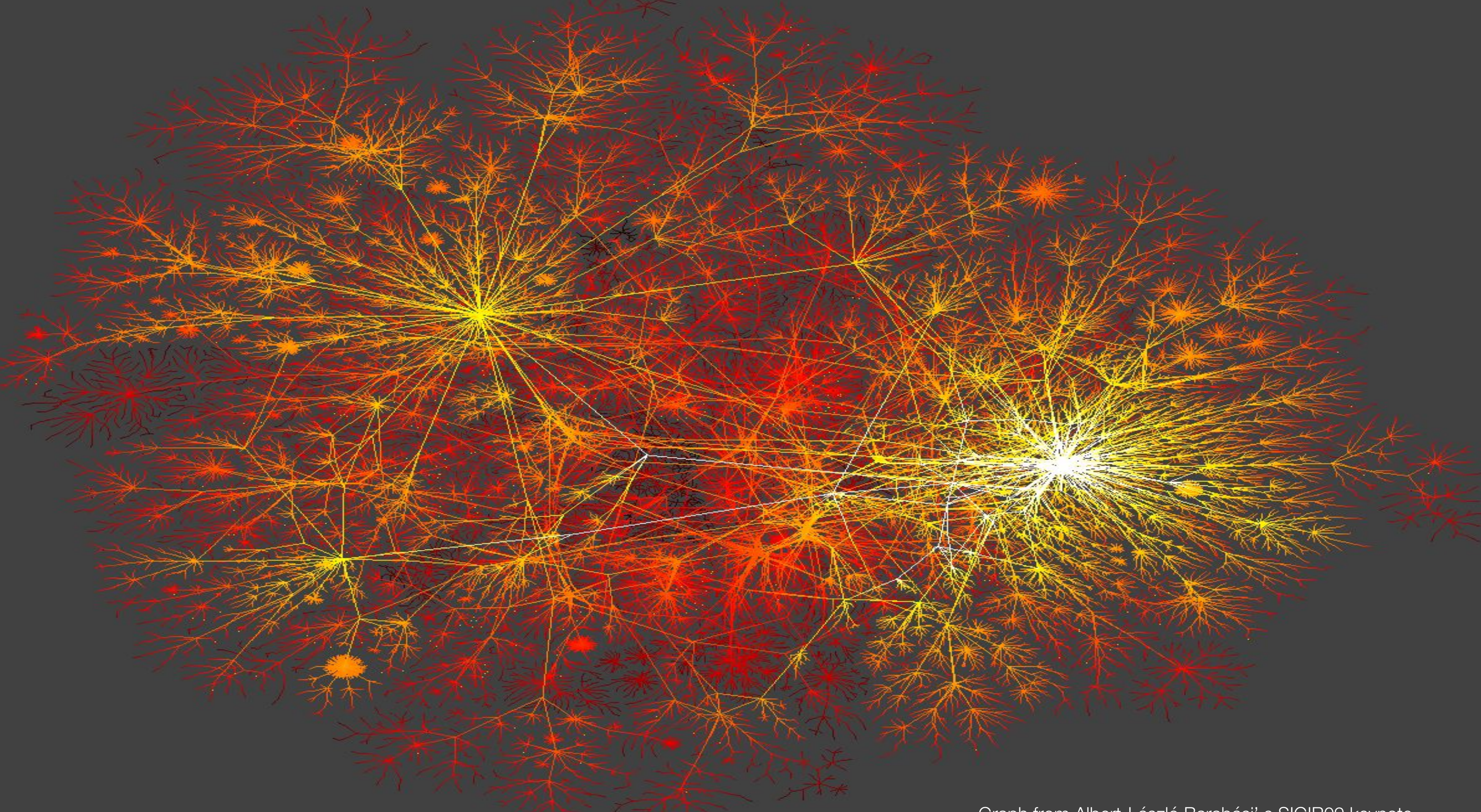
Molecular structures

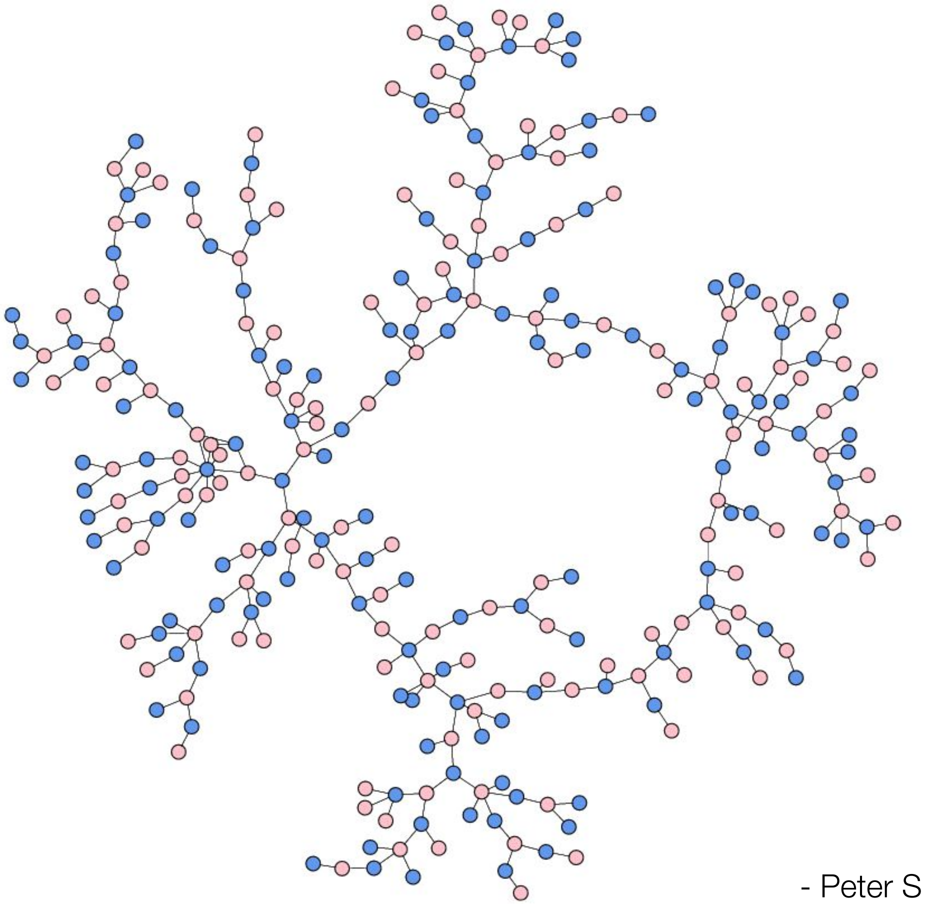
- Many data can be formulated as graphs
  - Images as graphs with two-dimensional grid structures



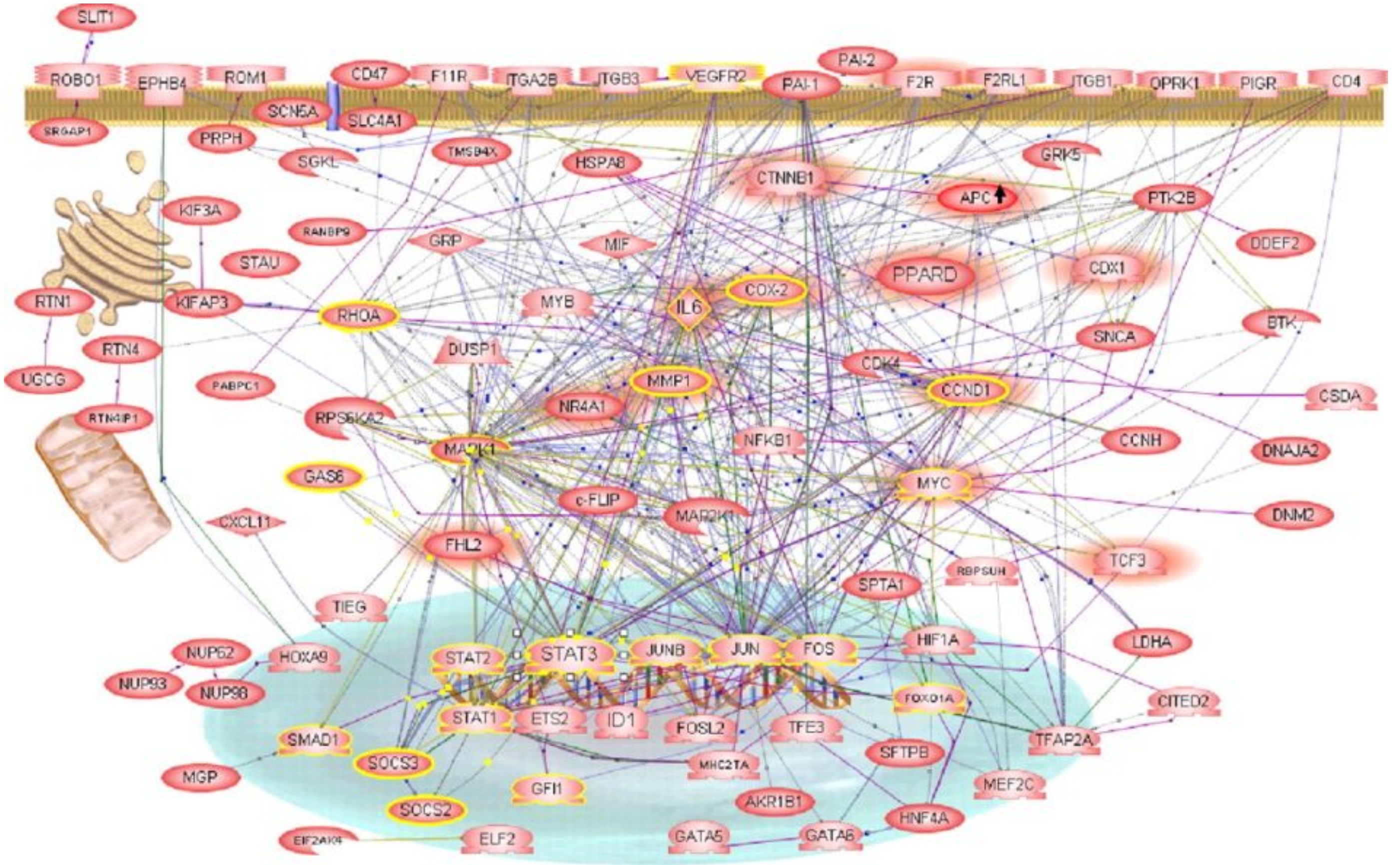
Continental Airline: Source: http://www.airlineroutemaps.com/



Graph from Albert-László Barabási’ s SIGIR09 keynote



- Peter S. Bearman, James Moody and Katherine Stovel
Chains of affection: The structure of adolescent romantic and sexual networks , *American Journal of Sociology* 110 44-91 (2004)



- Abdollahi et al. Transcriptional network governing the angiogenic switch in human pancreatic cancer. PNAS vol. 104 no. 31,2007

Gene-Regulatory Network

Various Applications on Graphs

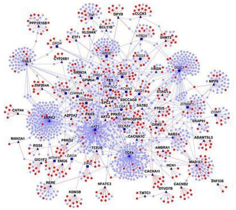
- Applications
  - Predicting political bias of people in social networks
  - Recommending friends in social networks
  - Recommending coauthors/papers in coauthor/author-paper graphs
  - Predict the roles of proteins in a protein-protein interaction graphs
  - Predict the properties of molecules
  - Generating new molecules for drug discovery
  - …

Most applications are essentially making predictions on graphs!

Research Problem (1) : Learning Node Representations of Graphs

- Learning **node representations** for large-scale graphs
  - e.g., social graphs, protein-protein interaction graphs

Social Network

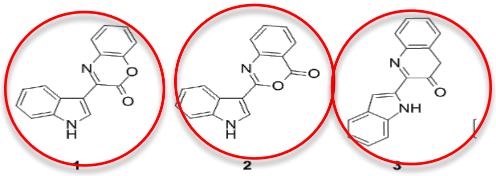


Protein-protein Interaction Graph

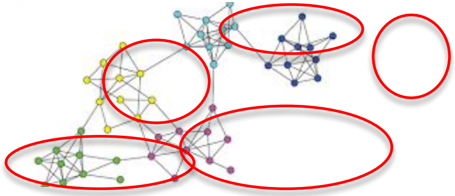
- Challenges:
  - Large-scale: >millions of nodes and billions of edges
  - Heterogeneous: multiple types of nodes and edges
  - Dynamic: structures evolve over time

Research Problem (2): Learning Representations of Entire Graphs

- Learning **representations** for entire graphs (subgraphs)
  - i.e., representing entire graphs (subgraphs) with a vector
  - E.g., molecular structures, community structures in social networks



Molecular structures

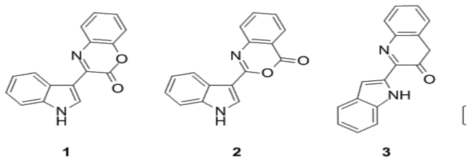


Communities in social networks

- Challenges:
  - The structures of different graphs are different
  - Existing models (e.g., CNN and RNN) are mainly developed for images and sequences.

Research Problem (3): Graph Generation

- How to generate graphs
    - E.g., for drug discovery



- Challenges:
    - Discrete
    - Arbitrary graph structure

Neural Message Passing Algorithms

...

Shagun Sodhani

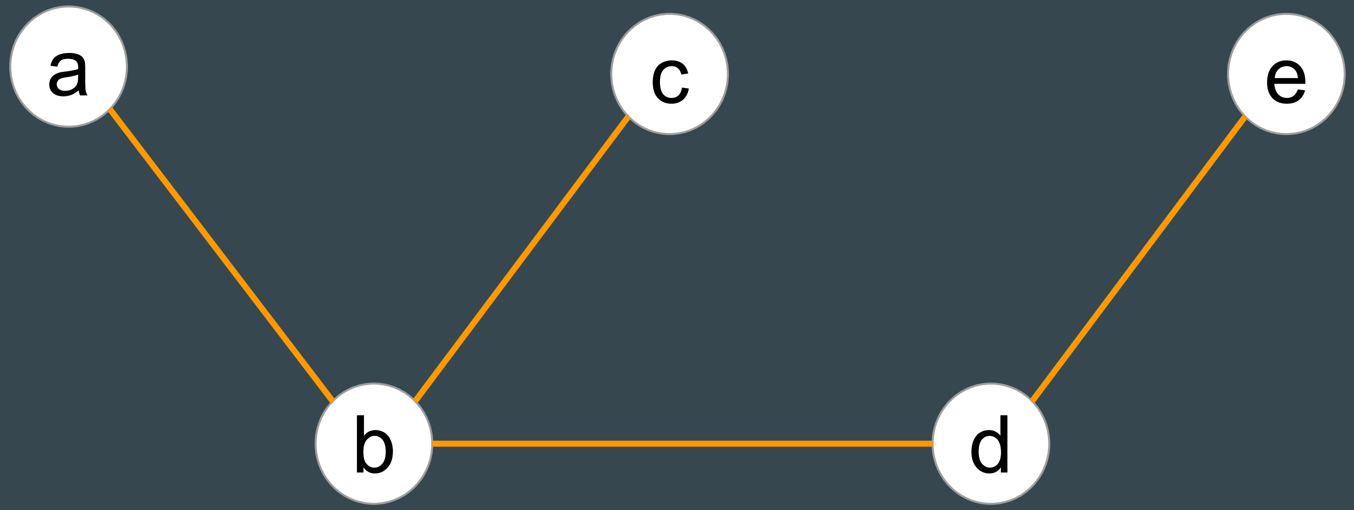
Preliminaries

- G - Undirected Graph
- x_v - Node Features
- $e_{v,w}$ - Edge Features
- h^t_v - Node Representation at time t

Message Passing Neural Network

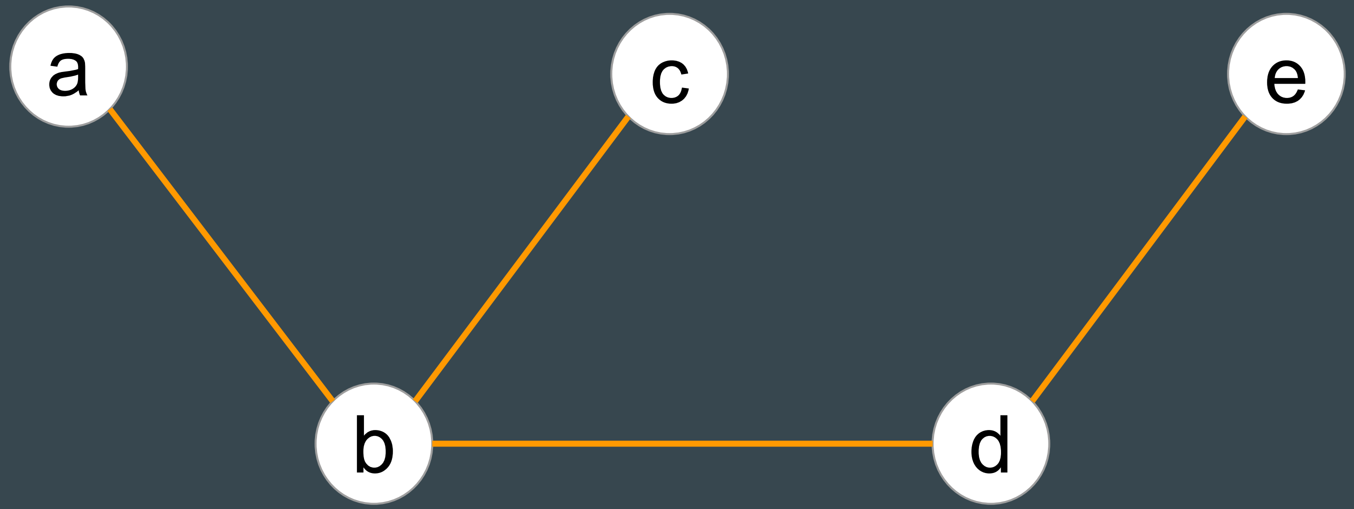
Message Passing Neural Network

Given an undirected graph



Message Passing Neural Network

Every node receives a message from its neighbour



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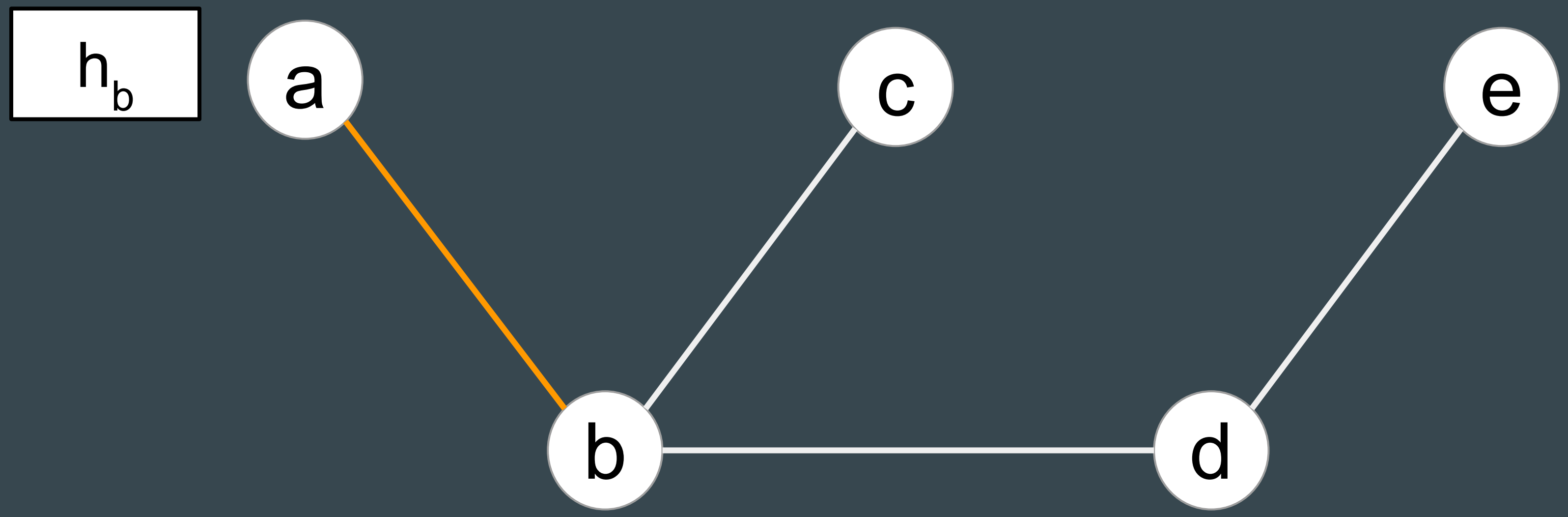

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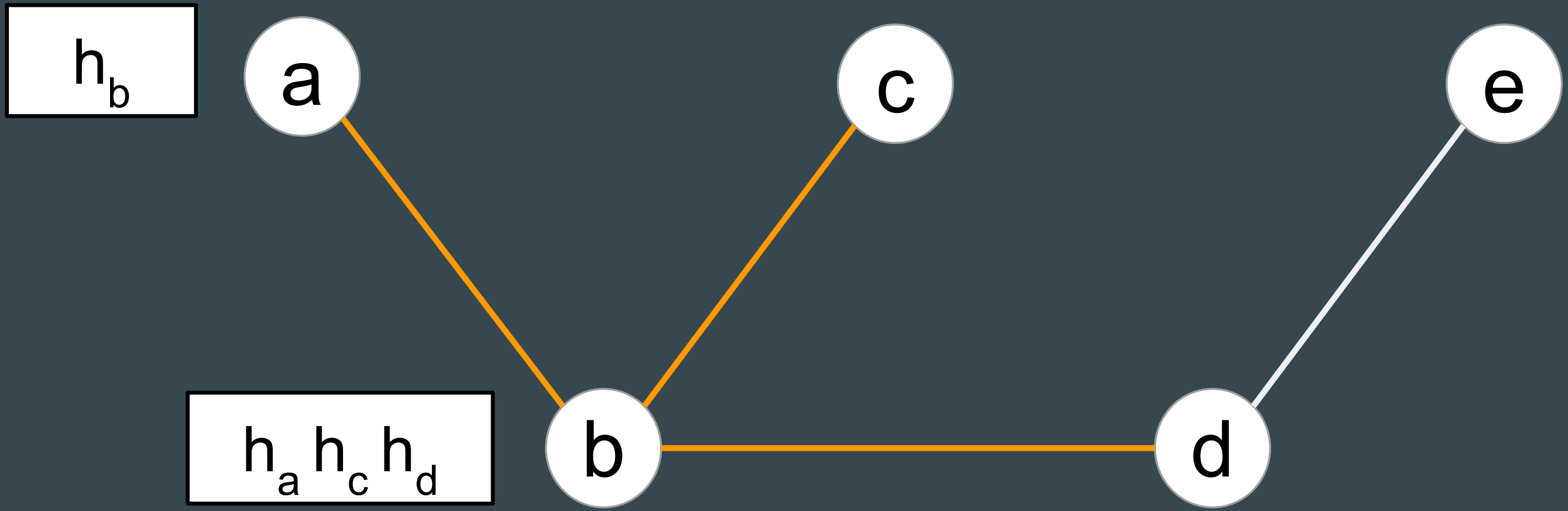

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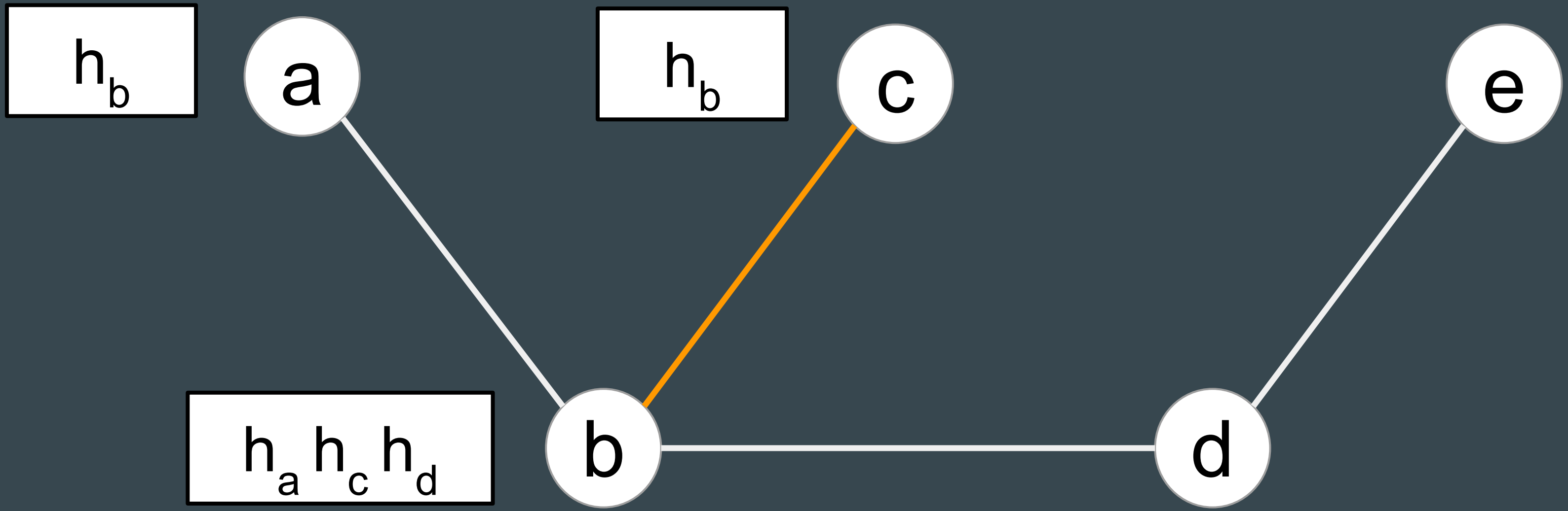

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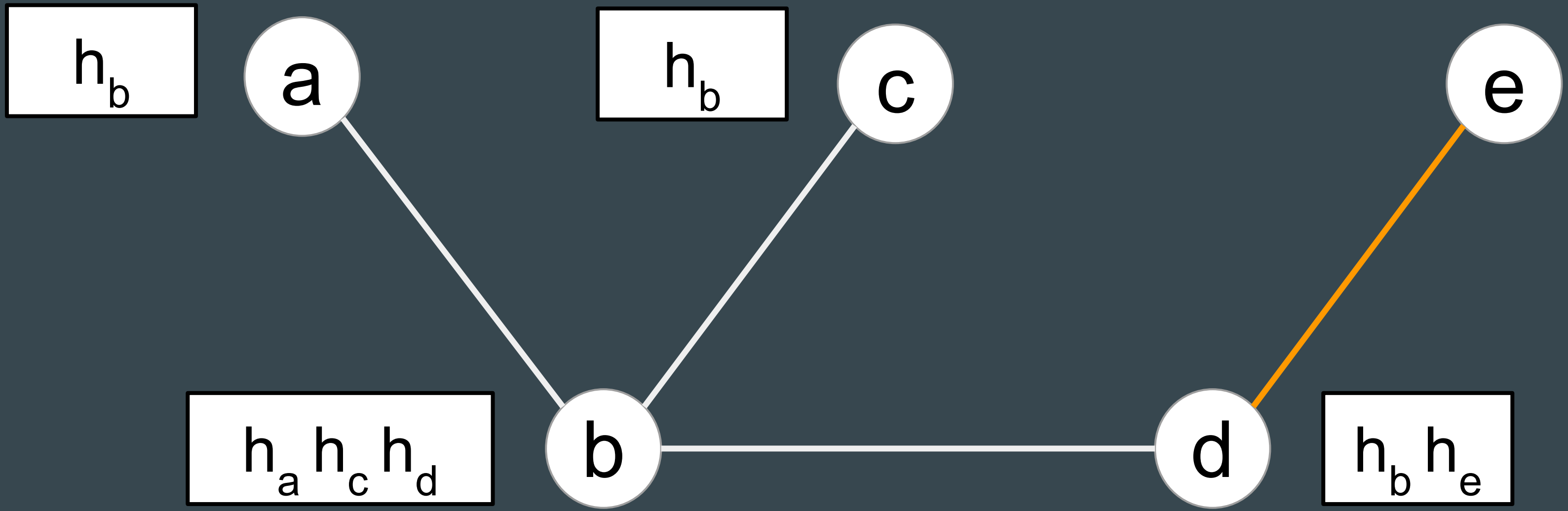

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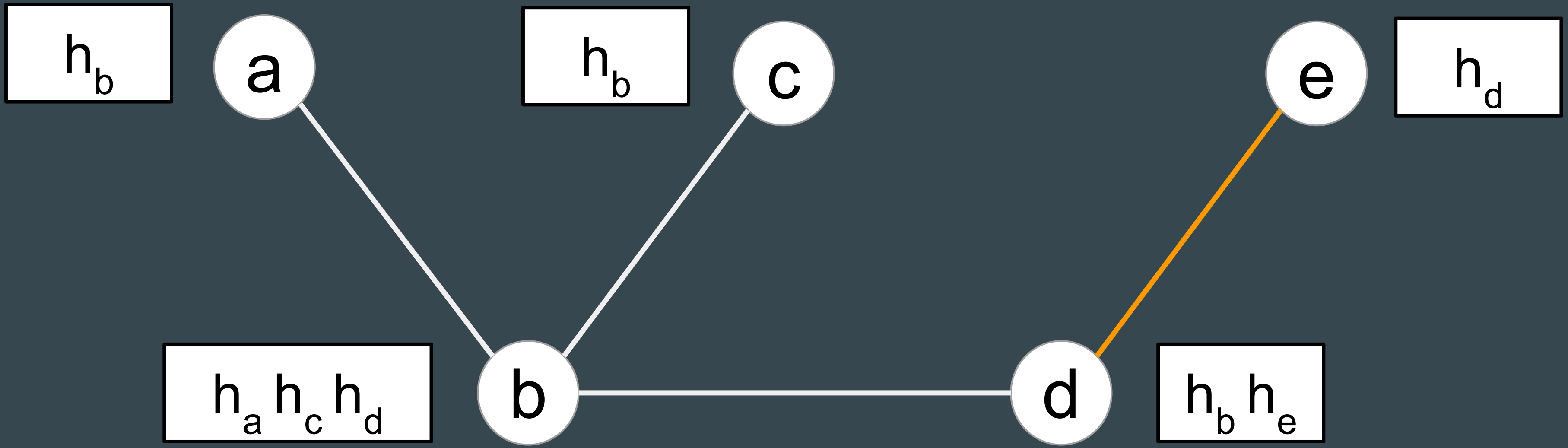
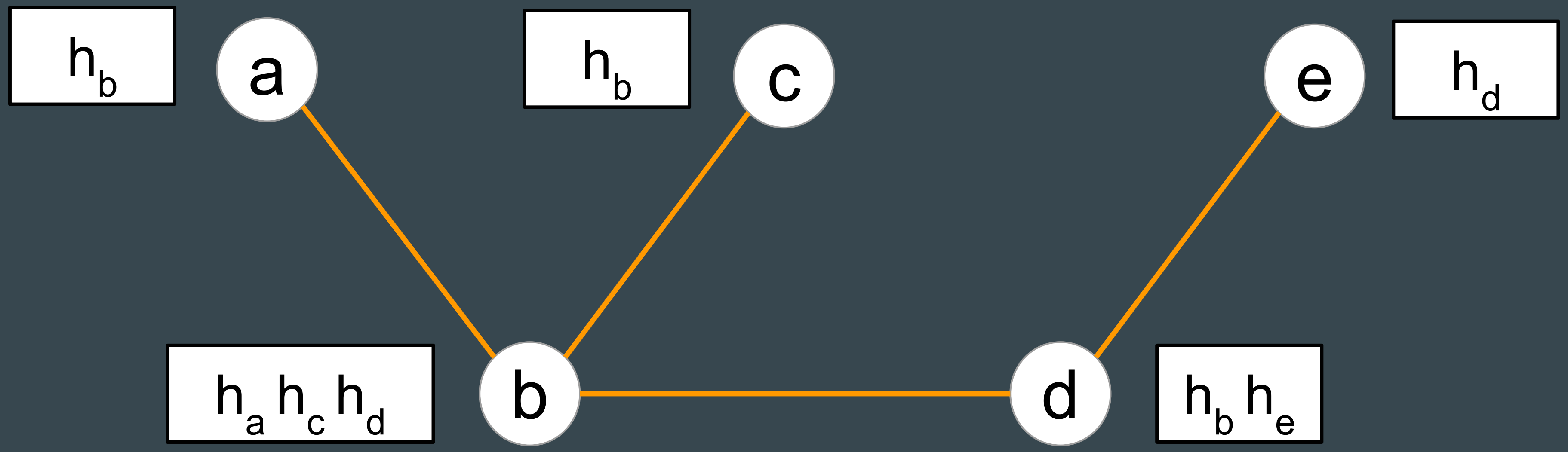


Message Passing Neural Network

Nodes updated their embedding using the messages



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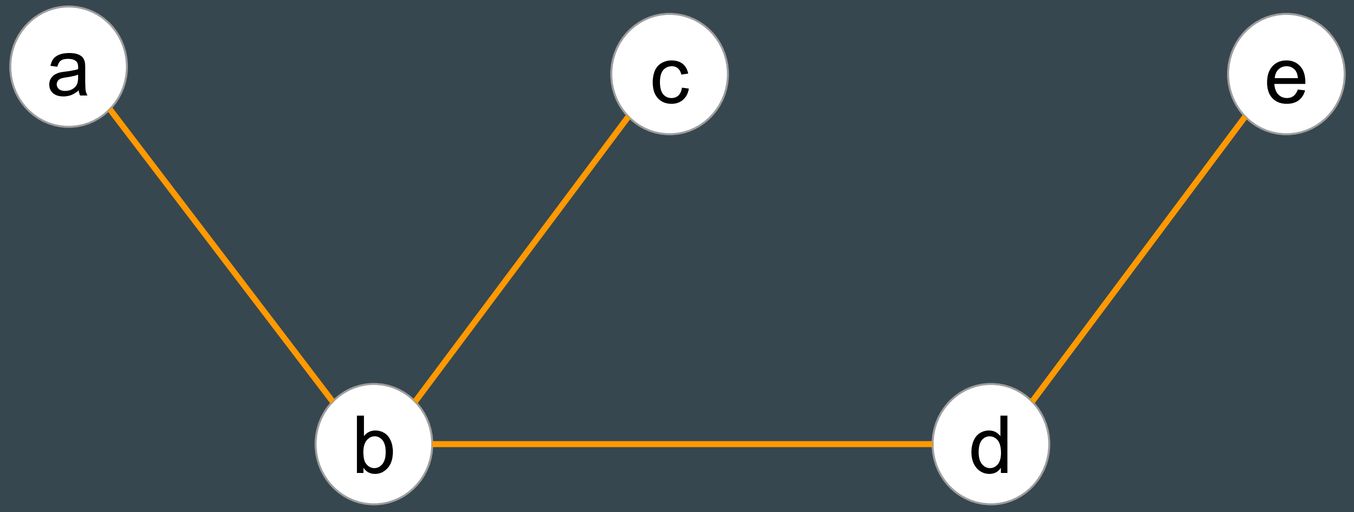

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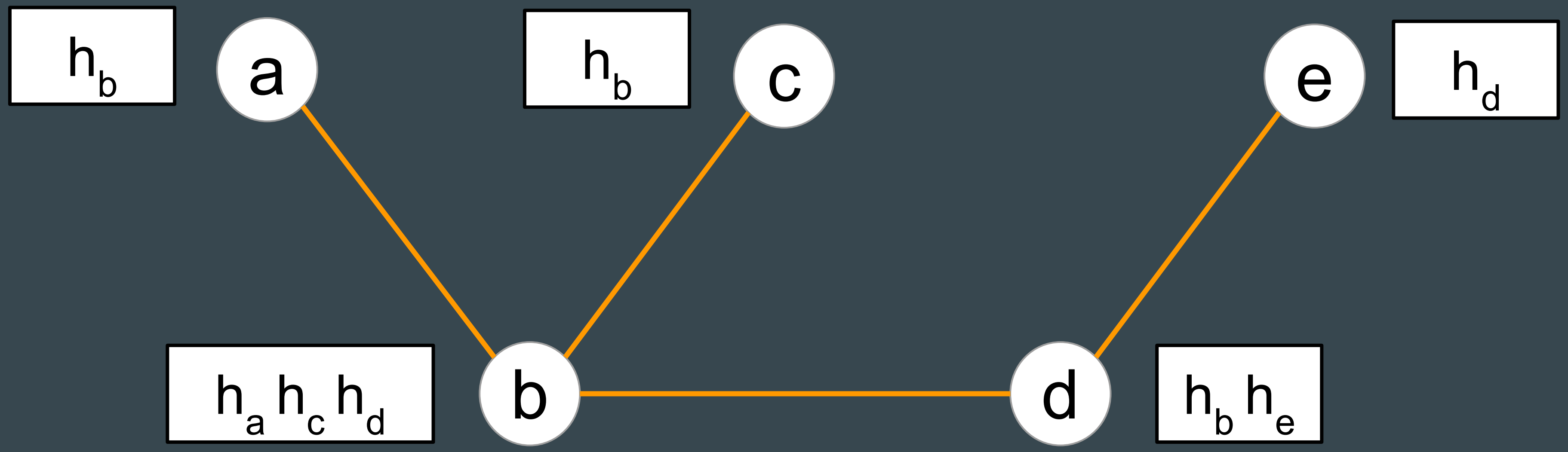

Message Passing Phase

Every node receives a message from its neighbour

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$$m_v^{t+1} = \sum_{w \in N(v)} M_t(h_v^t, h_w^t, e_{vw})$$

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$$m_v^{t+1} = \sum_{w \in N(v)} M_t(h_v^t, h_w^t, e_{vw})$$

M could be *concatenation*, *element-wise product*, NN, etc

Message Passing Phase

Nodes updated their embedding using the messages

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$$h_v^{t+1} = U_t(h_v^t, m_v^{t+1})$$

Message Passing Phase

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$$h_v^{t+1} = U_t(h_v^t, m_v^{t+1})$$

U could be *element-wise product*, NN, etc

Message Passing Phase

$$m_v^{t+1} = \sum_{w \in N(v)} M_t(h_v^t, h_w^t, e_{vw})$$

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Message Passing Neural Network

Message Passing Phase

Read Phase

$$m_v^{t+1} = \sum_{w \in N(v)} M_t(h_v^t, h_w^t, e_{vw})$$

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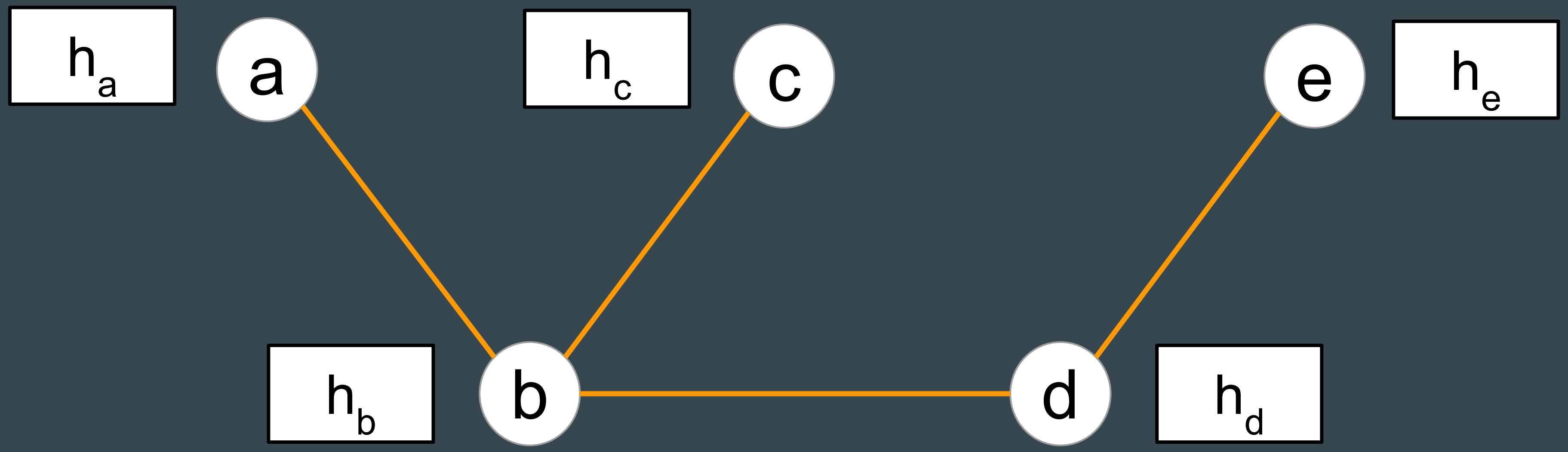
Read Phase

Combine embedding for all the nodes



Read Phase

Combine embedding for all the nodes

$\boxed{h_a}$ $\boxed{h_b}$ $\boxed{h_c}$ $\boxed{h_d}$ $\boxed{h_e}$

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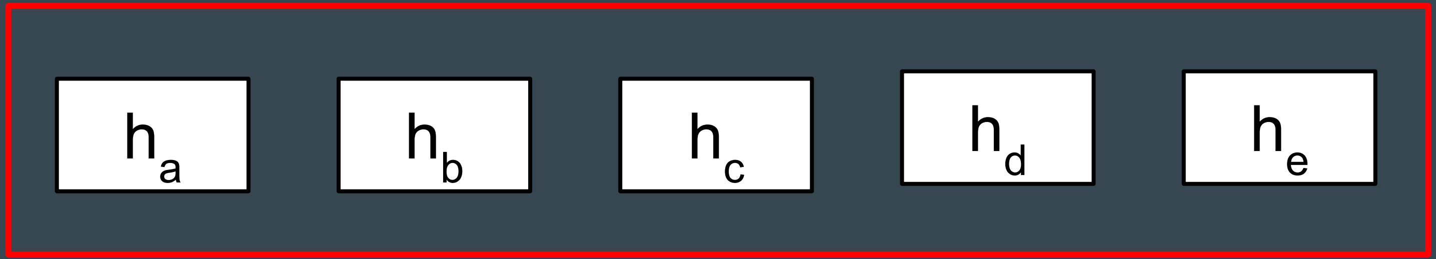

Read Phase

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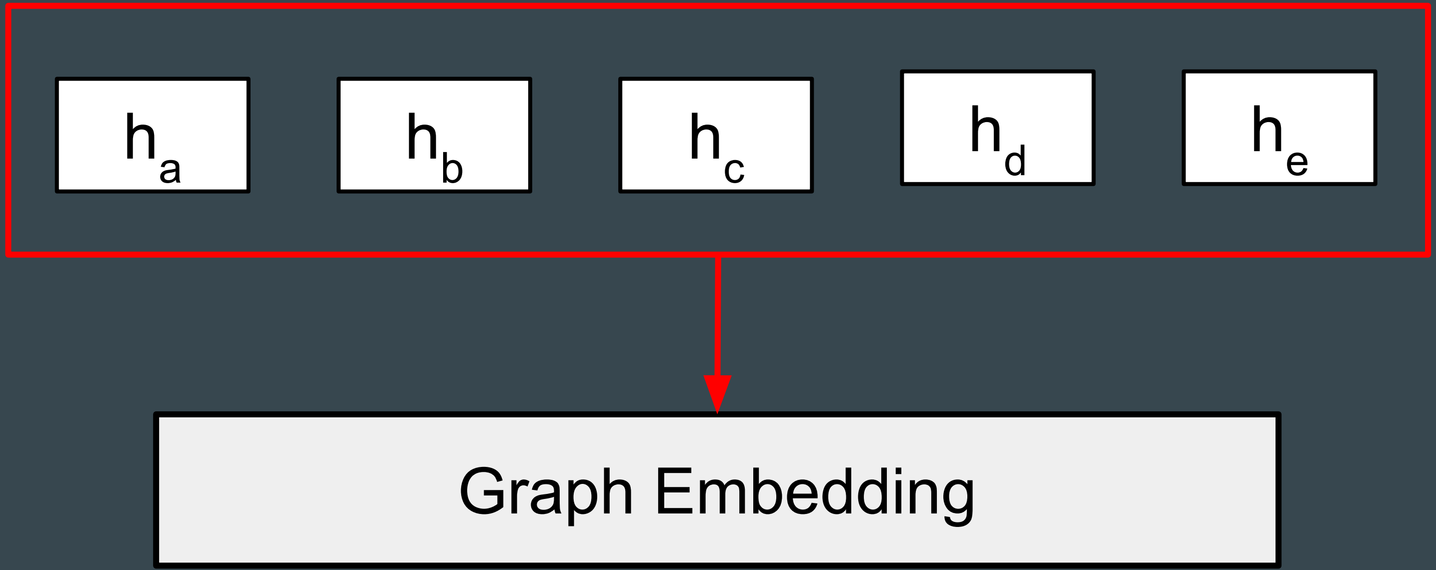

Read Phase

$$\hat{y} = R(\{h_v^T \mid v \in G\})$$

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R could be any operation which is invariant to node permutation.

Message Passing Neural Network

Message Passing Phase

$$m_v^{t+1} = \sum_{w \in N(v)} M_t(h_v^t, h_w^t, e_{vw})$$

$$h_v^{t+1} = U_t(h_v^t, m_v^{t+1})$$

Read Phase

$$\hat{y} = R(\{h_v^T \mid v \in G\}).$$

Message Passing Neural Network

- M - Message Function
- U - (Vertex) Update Function
- R - Readout Function
- All are learnt differentiable functions

Convolutional Networks for Learning Molecular Fingerprints

Variants of Message Passing Neural Network

$$M(h_v, h_w, e_{vw}) = (h_w, e_{vw})$$

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$$M(h_v, h_w, e_{vw}) = (h_w, e_{vw})$$

$$U_t(h_v^t, m_v^{t+1}) = \sigma(H_t^{\deg(v)} m_v^{t+1})$$

Convolutional Networks for Learning Molecular Fingerprints

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Convolutional Networks for Learning Molecular Fingerprints

Variants of Message Passing Neural Network

$$M(h_v, h_w, e_{vw}) = (h_w, e_{vw})$$

$$U_t(h_v^t, m_v^{t+1}) = \sigma(H_t^{\deg(v)} m_v^{t+1})$$

$$R = f\left(\sum_{v,t} \mathrm{softmax}(W_t h_v^t)\right)$$

Gated Graph Neural Networks

Variants of Message Passing Neural Network

$$M_t(h_v^t, h_w^t, e_{vw}) = A_{e_{vw}} h_w$$

Gated Graph Neural Networks
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$$M_t(h_v^t, h_w^t, e_{vw}) = A_{e_{vw}} h_w$$

$$U_t = \mathrm{GRU}(h_v^t, m_v^{t+1})$$

Gated Graph Neural Networks

Variants of Message Passing Neural Network

$$M_t(h_v^t, h_w^t, e_{vw}) = A_{e_{vw}} h_w$$

$$U_t = \mathrm{GRU}(h_v^t, m_v^{t+1})$$

$$R = \sum_{v \in V} \sigma\left(i(h_v^{(T)}, h_v^0)\right) \odot \left(j(h_v^{(T)})\right)$$

Interaction Networks

Variants of Message Passing Neural Network

$$M(h_v, h_w, e_{vw}) = f(h_v, h_w, e_{vw}))$$

$$U(h_v, x_v, m_v = g(h_v, x_v, m_v))$$

$$R = f(\sum_{v \in G} h_v^T)$$

Molecular Graph Convolutions

Variants of Message Passing Neural Network

$$\mathrm{M}(\mathrm{h}_v^t, h_w^t, e_{vw}^t) = e_{vw}^t$$

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Molecular Graph Convolutions

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$$\mathrm{M}(\mathrm{h}_v^t, h_w^t, e_{vw}^t) = e_{vw}^t$$

$$\mathrm{U}_t(h_v^t, m_v^{t+1}) = \alpha(W_1(\alpha(W_0 h_v^t), m_v^{t+1}))$$

$$\mathrm{e}_{vw}^{t+1} = \alpha(W_4(\alpha(W_2, e_{vw}^t), \alpha(W_3(h_v^t, h_w^t))))$$

Deep Tensor Neural Networks

Variants of Message Passing Neural Network

$$M_t = \tanh\left(W^{fc}((W^{cf}h_w^t + b_1) \odot (W^{df}e_{vw} + b_2))\right)$$

$$U_t(h_v^t, m_v^{t+1}) = h_v^t + m_v^{t+1}$$

$$R = \sum_v \mathrm{NN}(h_v^T)$$

Graph Convolutional Network

Variants of Message Passing Neural Network

$$M_t(h_v^t, h_w^t) = C_{vw}^t h_w^t$$

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Variants of Message Passing Neural Network

$$M_t(h_v^t, h_w^t) = C_{vw}^t h_w^t$$

$$U_t(h_v^t, m_v^{t+1}) = \sigma(m_v^{t+1})$$

Graph Convolutional Network

Variants of Message Passing Neural Network

$$M_t(h_v^t, h_w^t) = c_{vw} h_w^t$$

Graph Convolutional Network

Variants of Message Passing Neural Network

$$M_t(h_v^t, h_w^t) = c_{vw} h_w^t$$

$$U_v^t(h_v^t, m_v^{t+1}) = \mathrm{ReLU}(W^t m_v^{t+1})$$

Graph Convolutional Network

Variants of Message Passing Neural Network

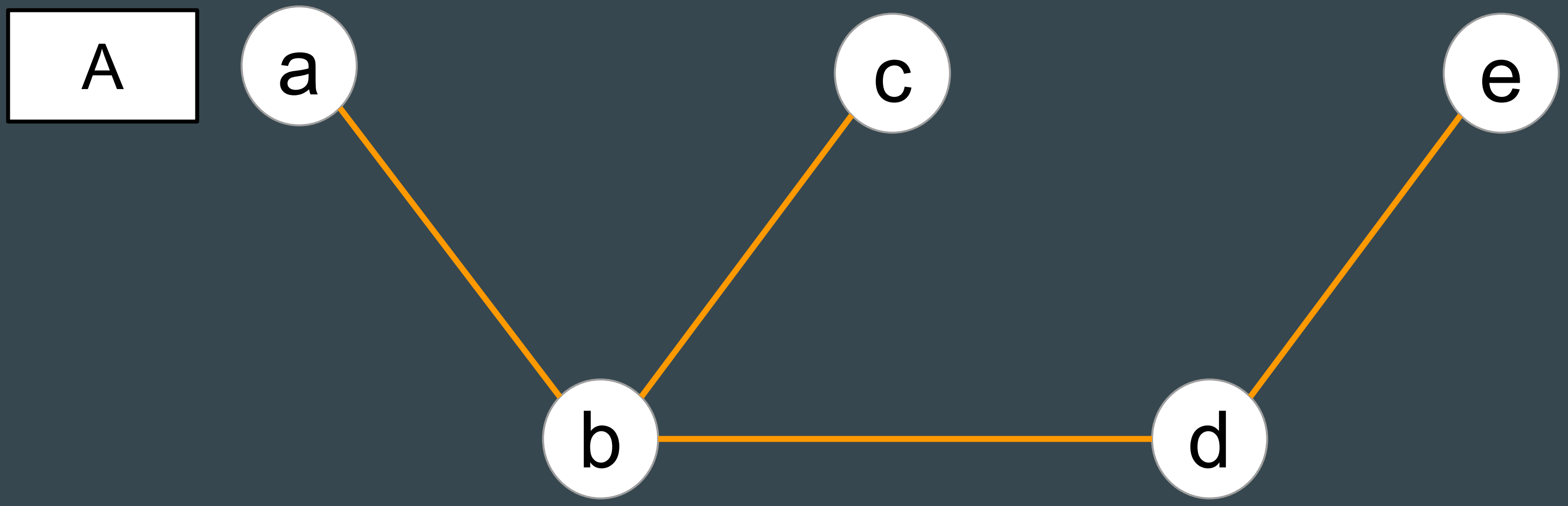
$$M_t(h_v^t, h_w^t) = c_{vw} h_w^t$$

$$U_v^t(h_v^t, m_v^{t+1}) = \mathrm{ReLU}(W^t m_v^{t+1})$$

$$c_{vw} = \left(\deg(v)\deg(w)\right)^{-1/2} A_{vw}$$

Message Passing Neural Network

Trajectory of a Message



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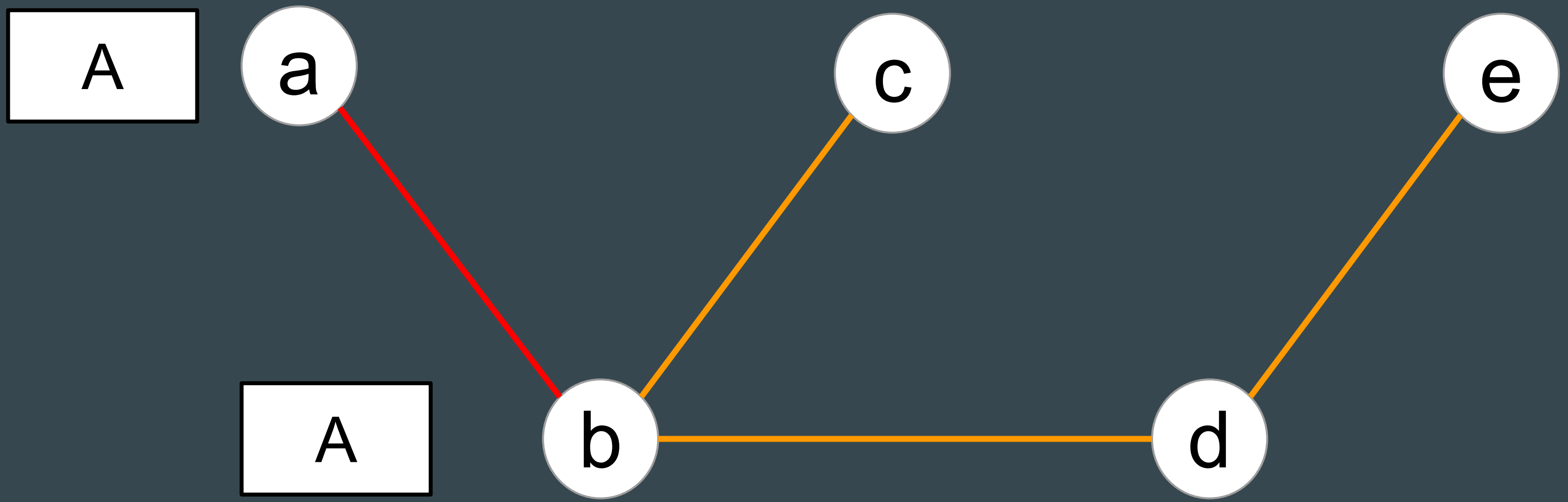

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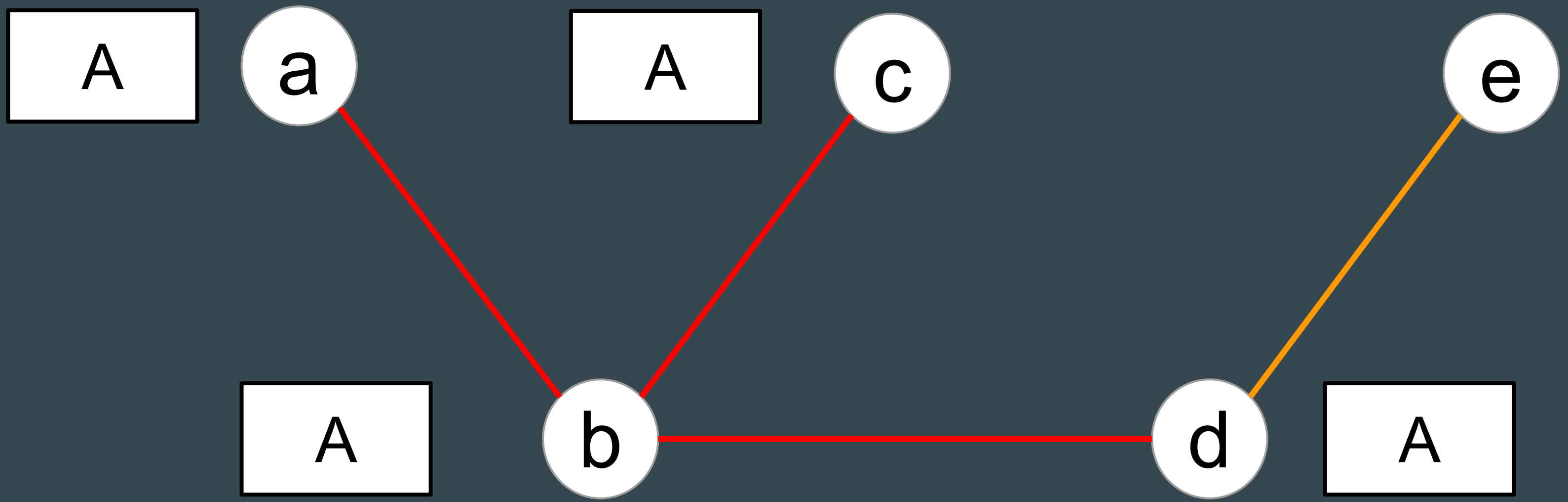

Message Passing Neural Network

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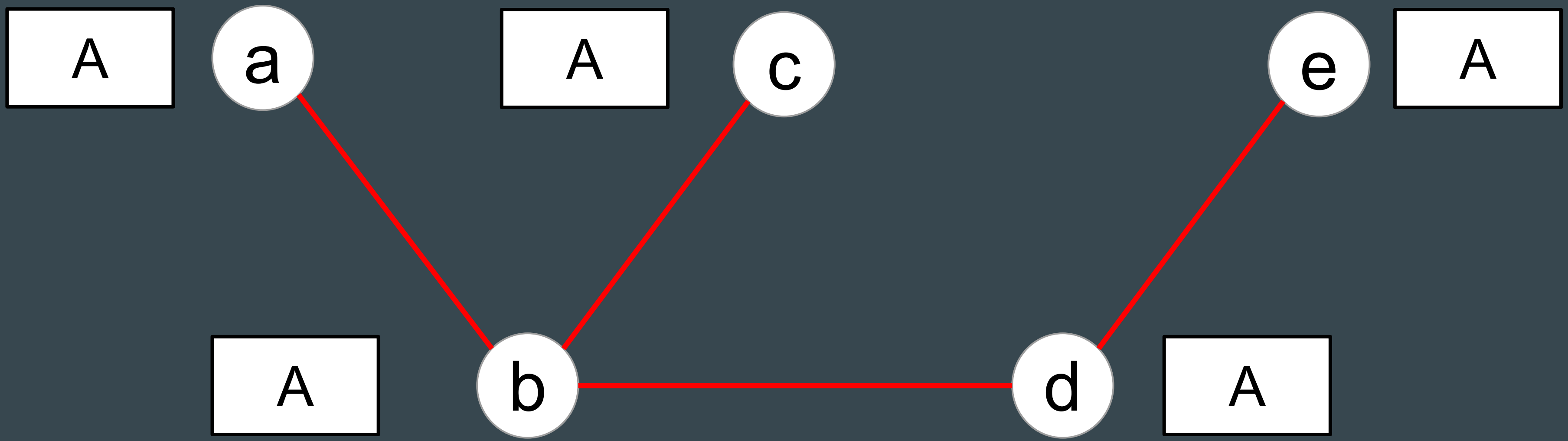
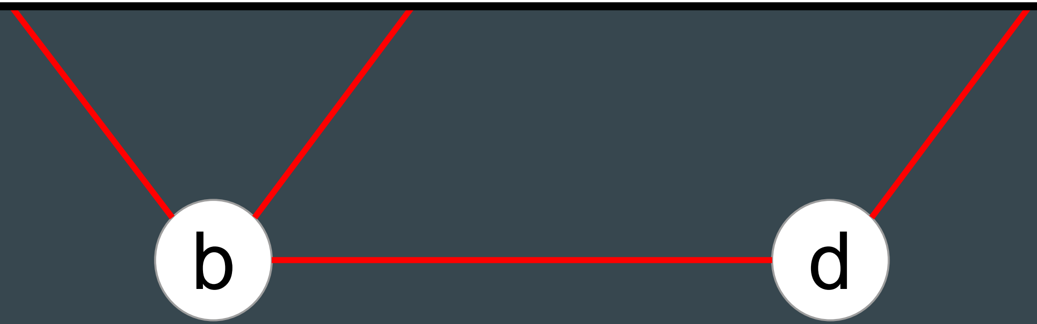


Message Passing Neural Network

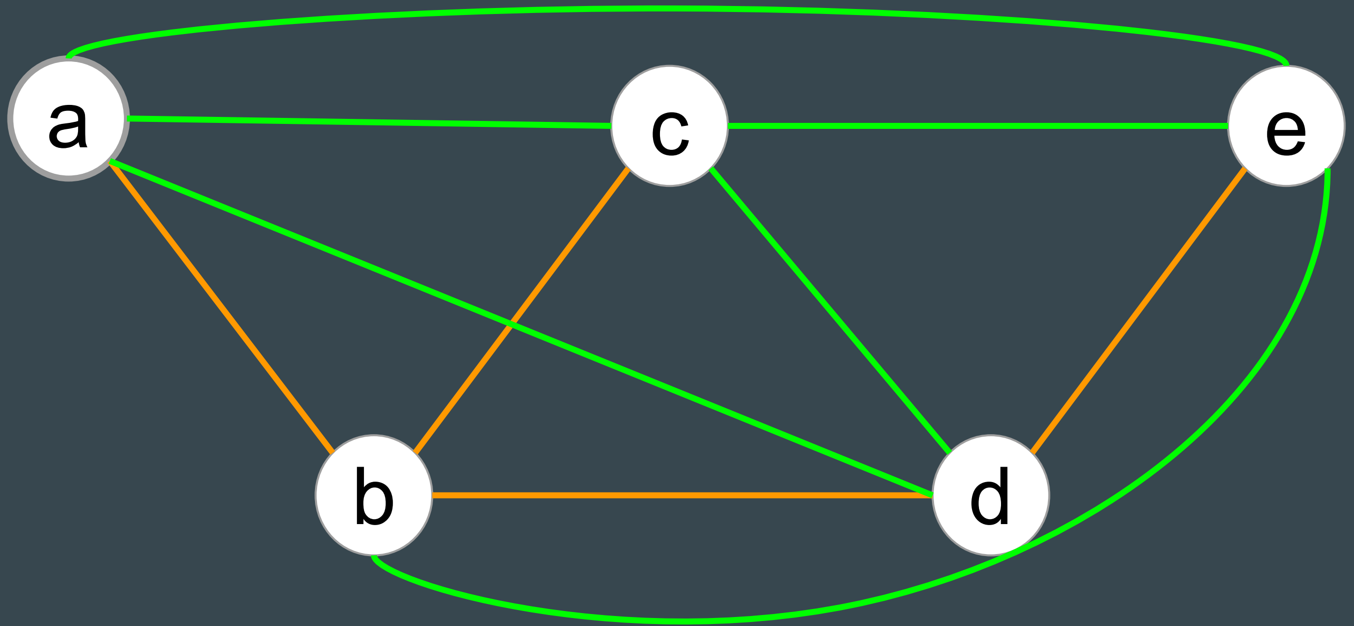
Trajectory of a Message

Message could take a while to reach other nodes!



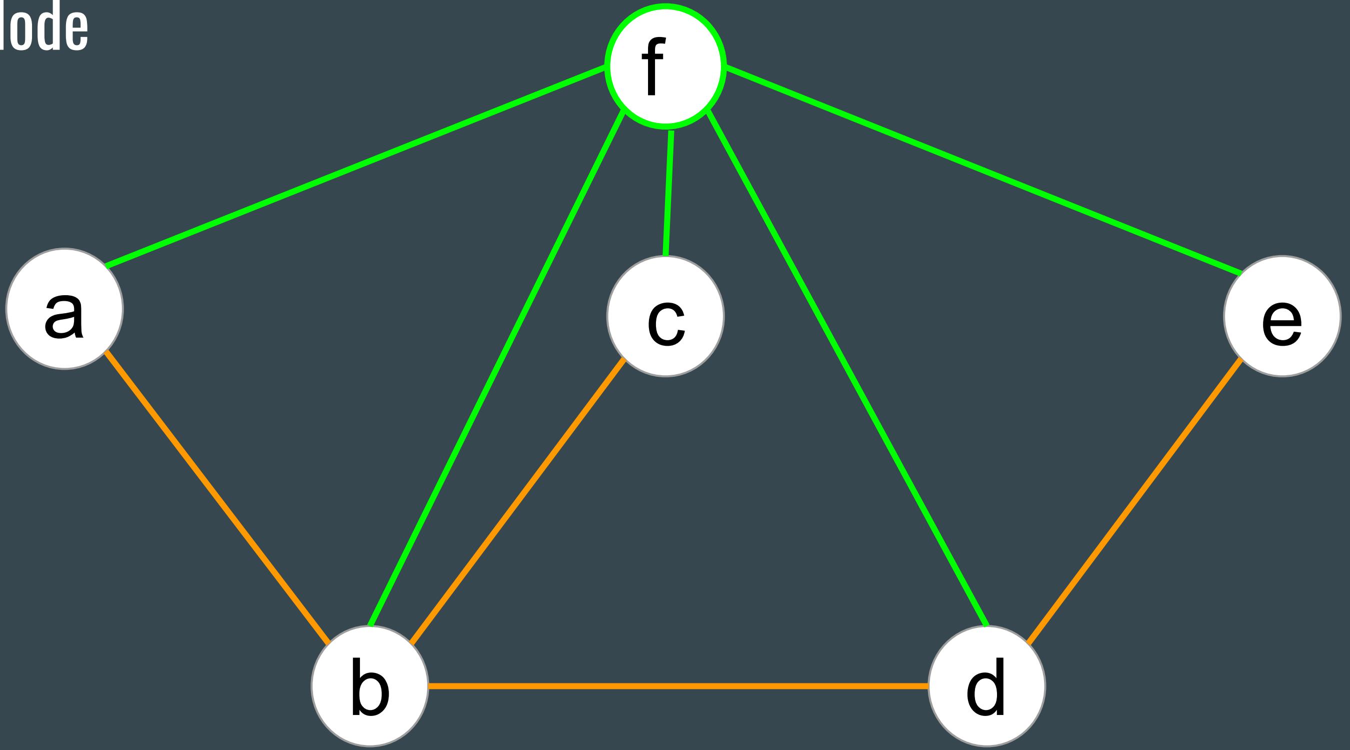
Message Passing Neural Network

Virtual Edges



Message Passing Neural Network

Virtual Node



References

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2. Convolutional Networks for Learning Molecular Fingerprints, Duvenaud et al. (2015)
3. Gated Graph Neural Networks (GG-NN), Li et al. (2016)
4. Interaction Networks, Battaglia et al. (2016)
5. Molecular Graph Convolutions, Kearnes et al. (2016)
6. Deep Tensor Neural Networks, Schutt et al. ¨ (2017)
7. Semi-Supervised Classification with Graph Convolutional Networks. Kipf et al. (2016)

Thank You