GNN LST

An introduction to GNNs and an exploratory roadmap

February 21st, 2023

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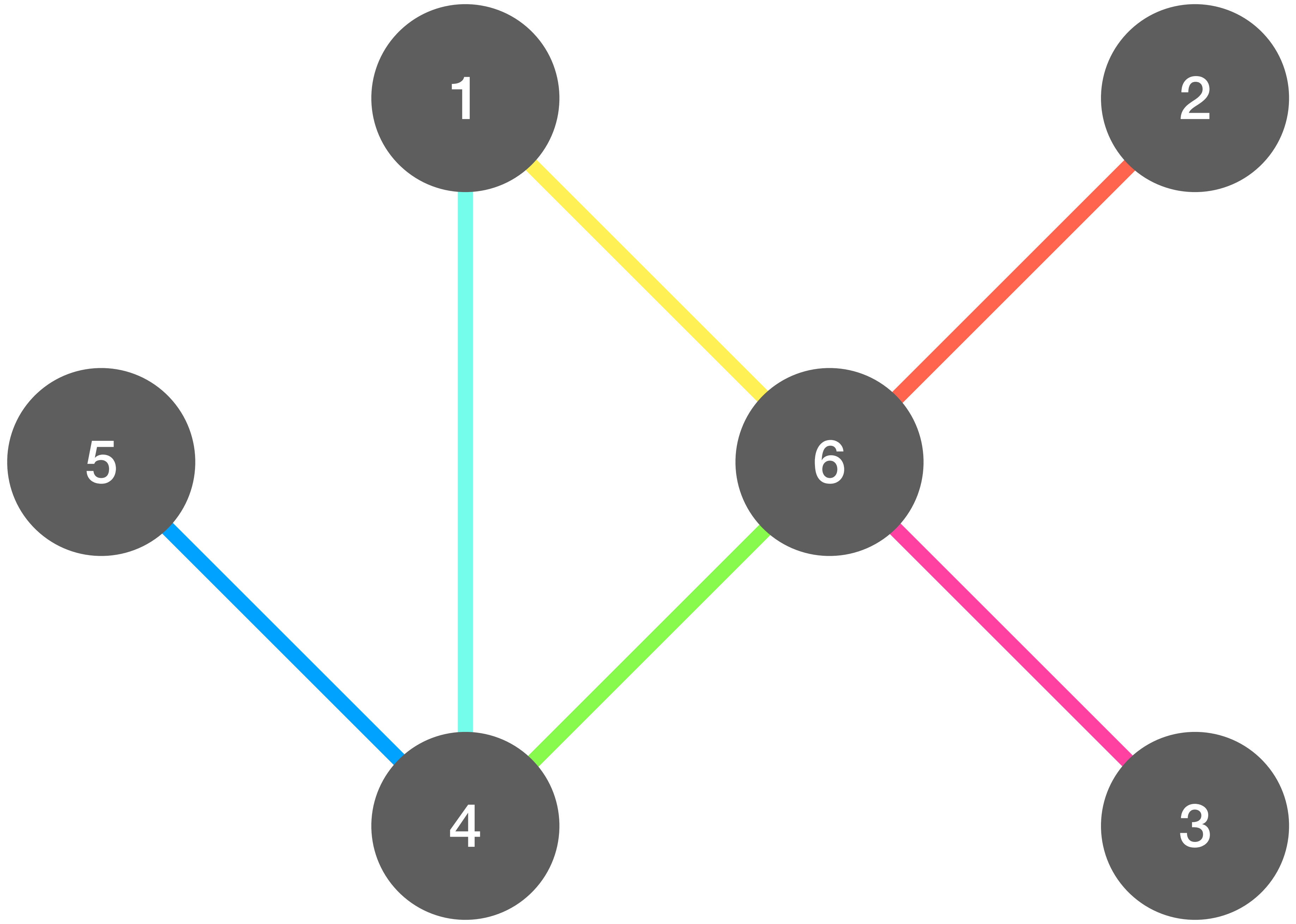
GNN Fundamentals

The GNN Algorithm: Notation

Connectivity of a graph can be represented as a matrix



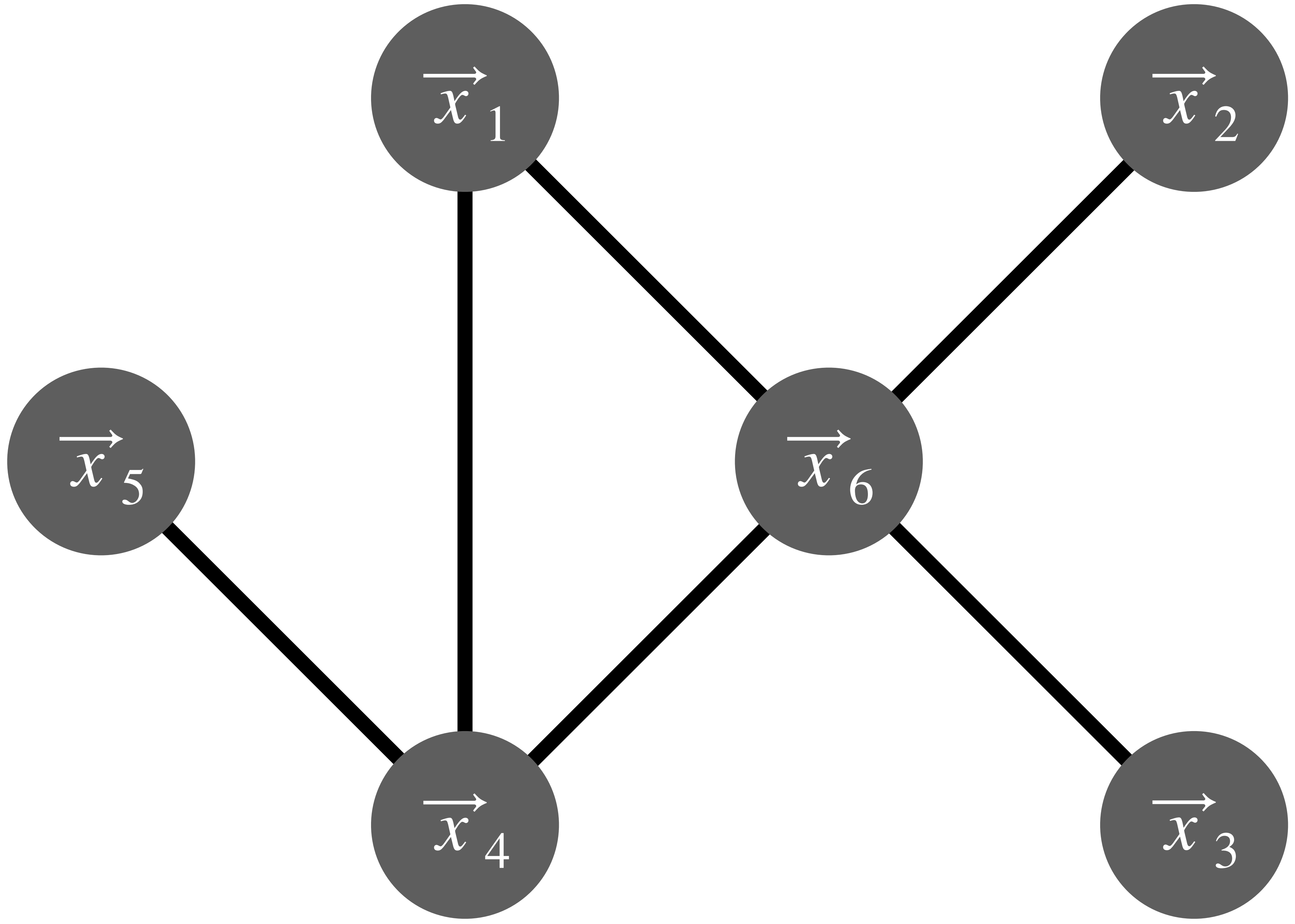
Graph

$$A = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \end{pmatrix}$$

Adjacency matrix

The GNN Algorithm: Notation

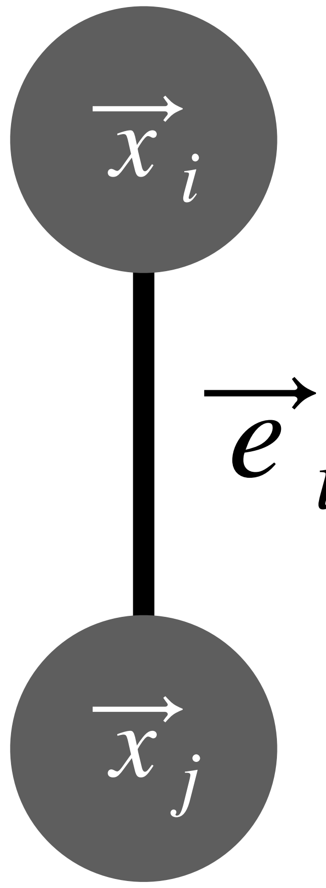
For GNNs, nodes and edges correspond to vectors of information



Input graph

$$\vec{x}_i = \begin{pmatrix} x_i^1 \\ x_i^2 \\ x_i^3 \\ \vdots \\ x_i^m \end{pmatrix}$$

Node i



$$\vec{e}_{ij} = \begin{pmatrix} e_{ij}^1 \\ e_{ij}^2 \\ e_{ij}^3 \\ \vdots \\ e_{ij}^m \end{pmatrix}$$

Edge ij

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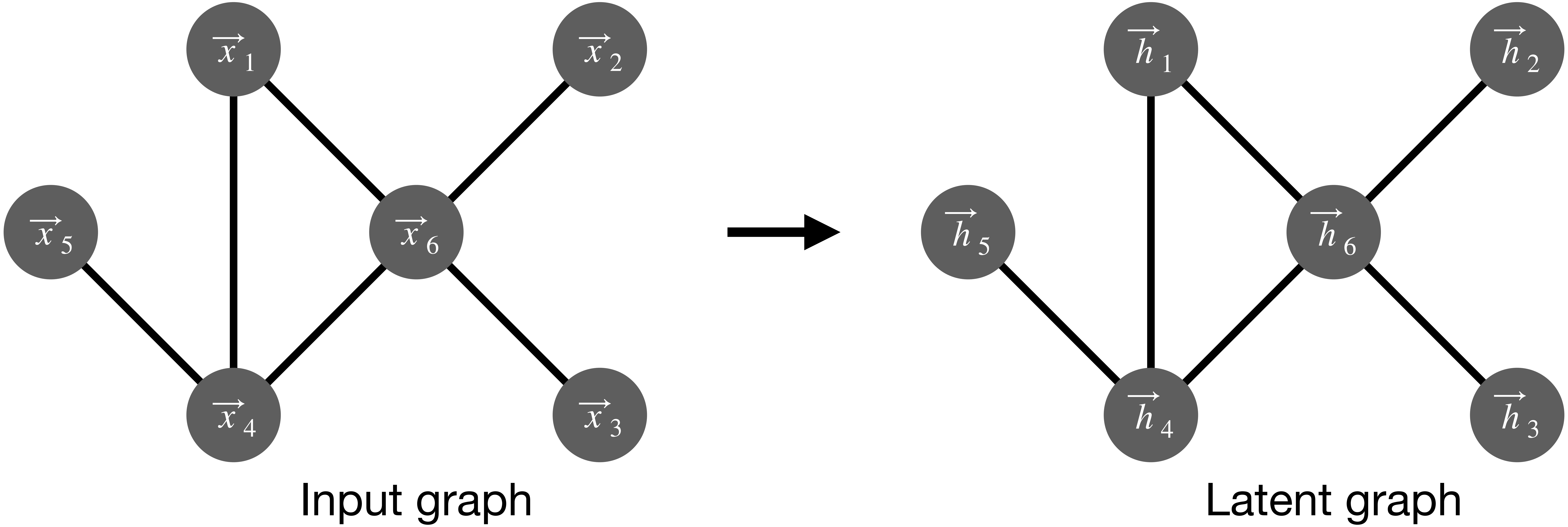
The GNN Algorithm: Notation

GNN input is necessarily a graph (of course)



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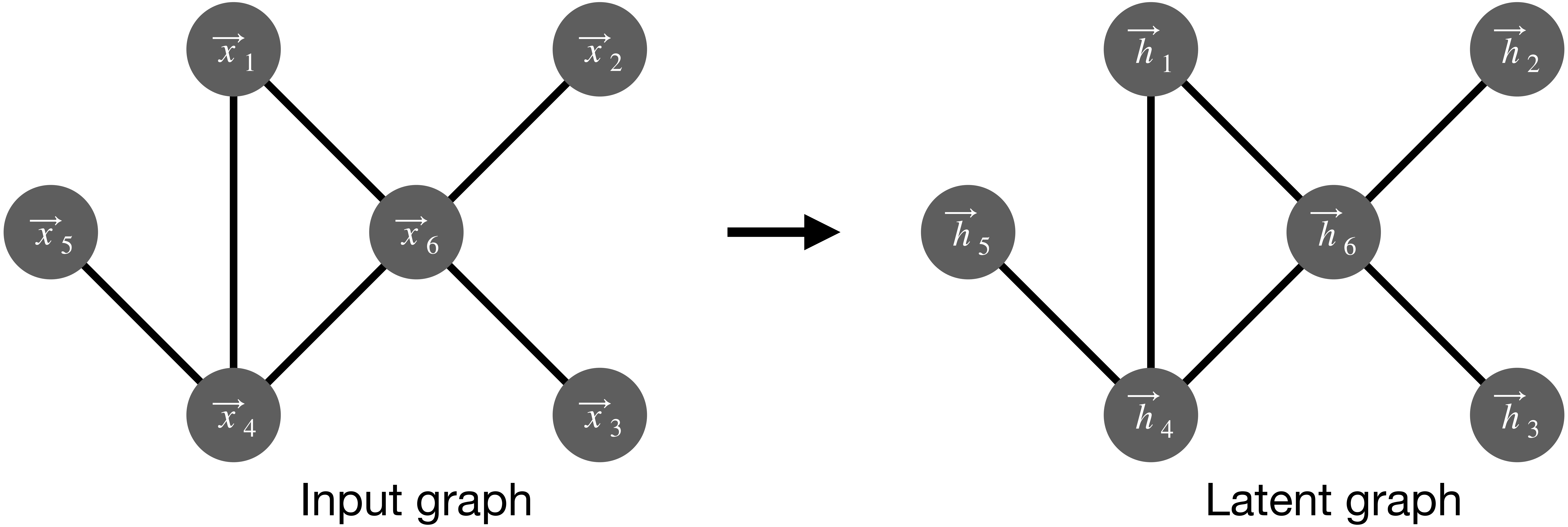
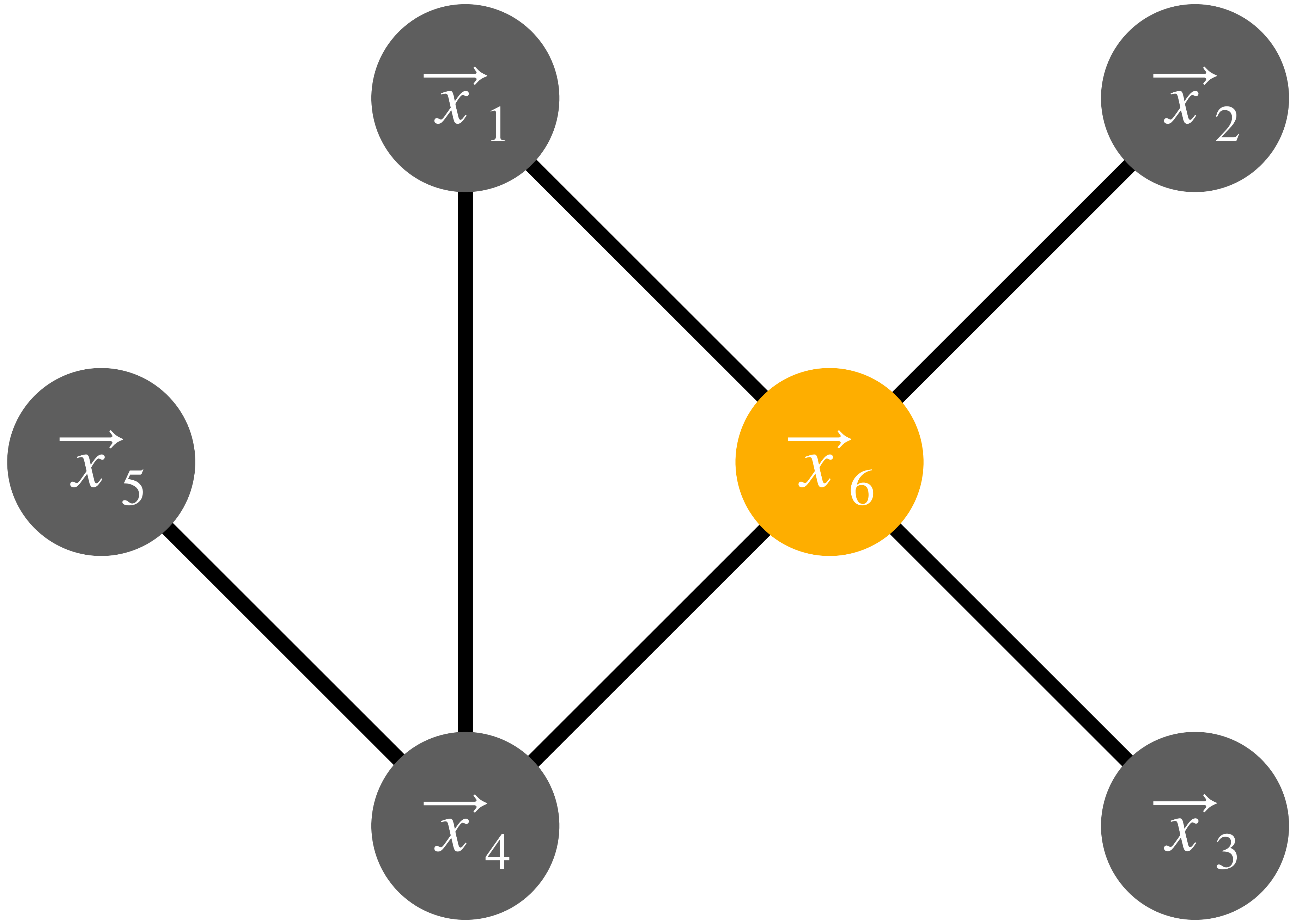
The GNN Algorithm

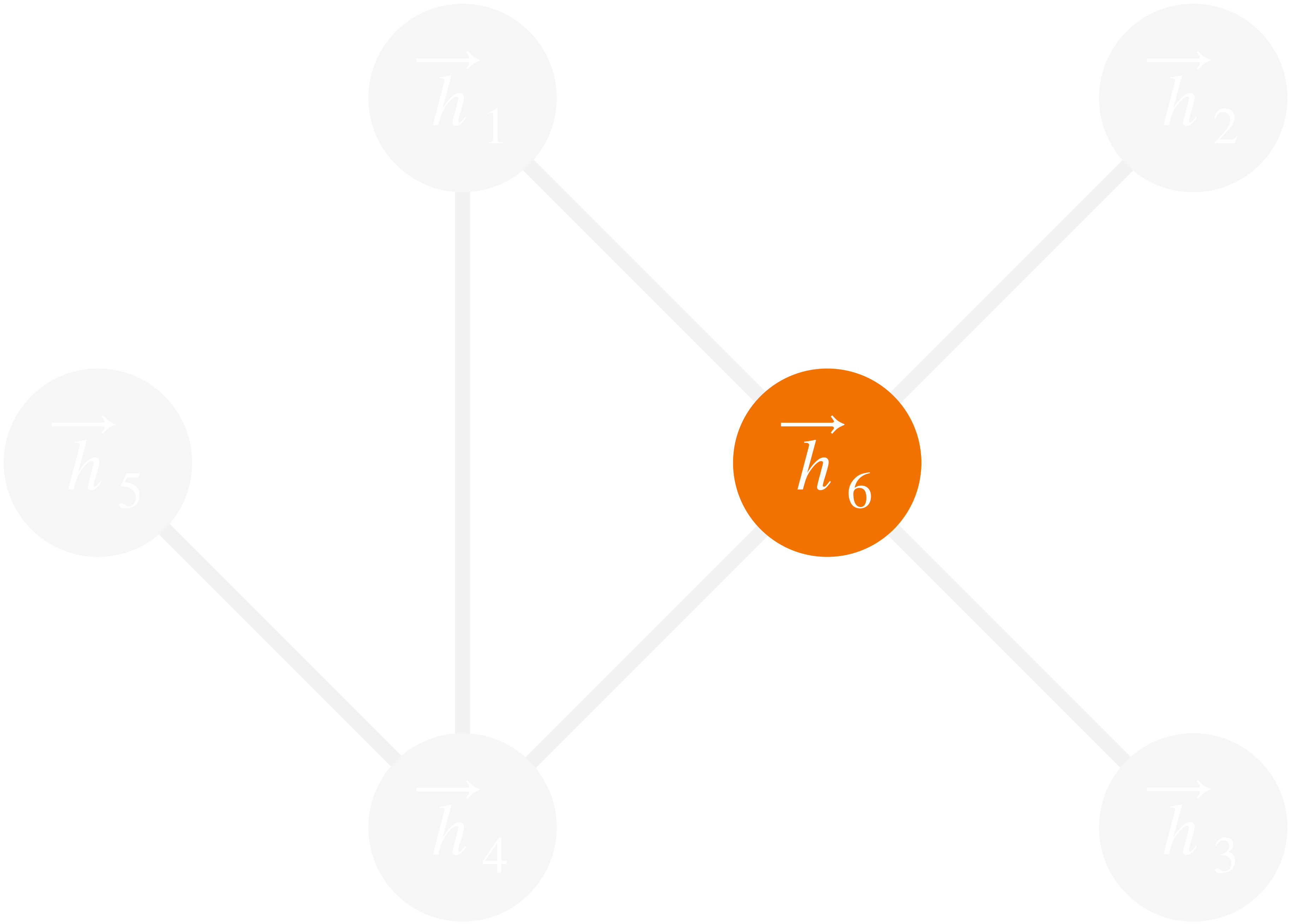
Goal: transform input graph to latent representation
(and bias transformation to encode information)



The GNN Algorithm

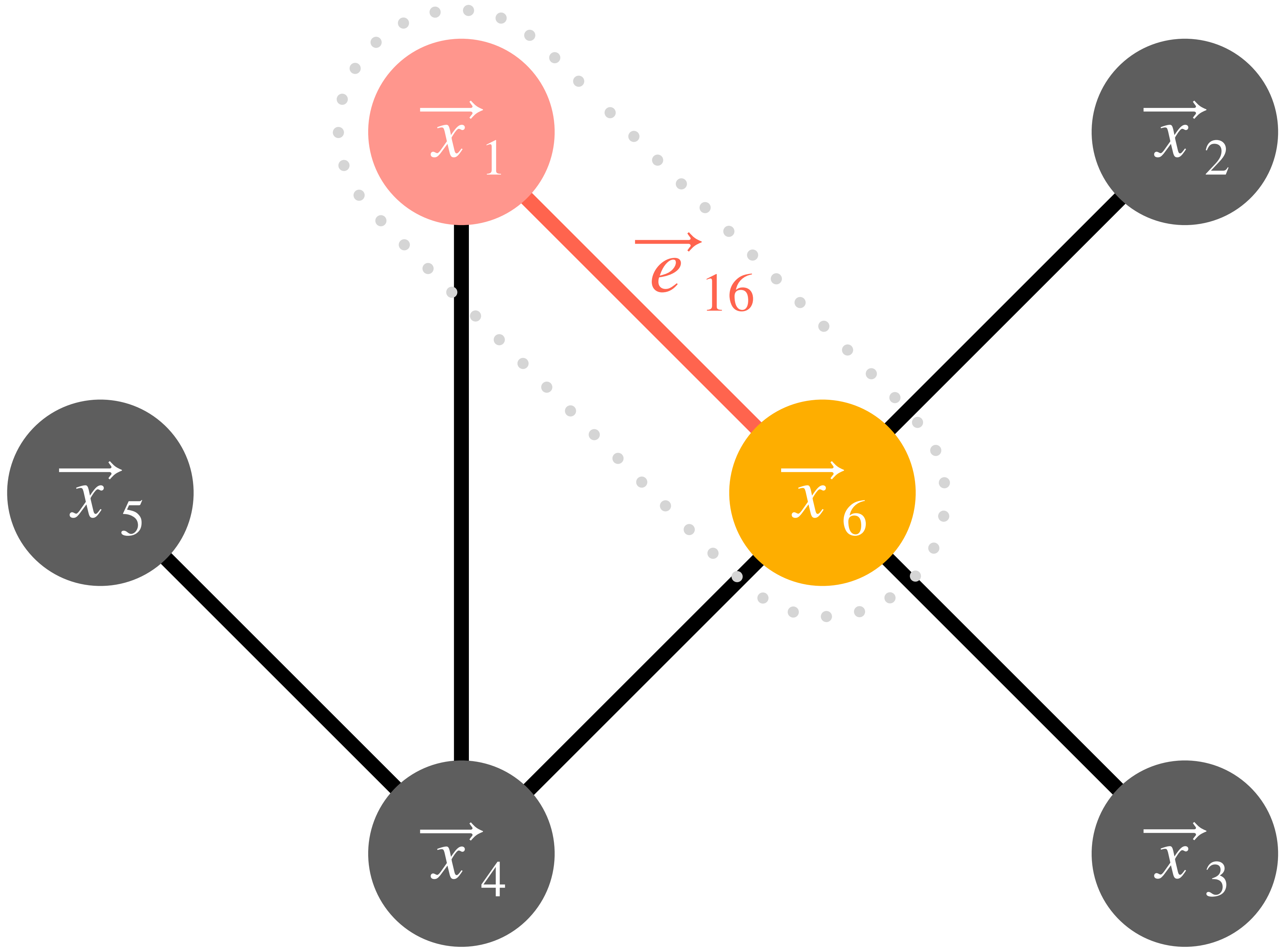
Transformation is done node-wise, let's start with Node 6

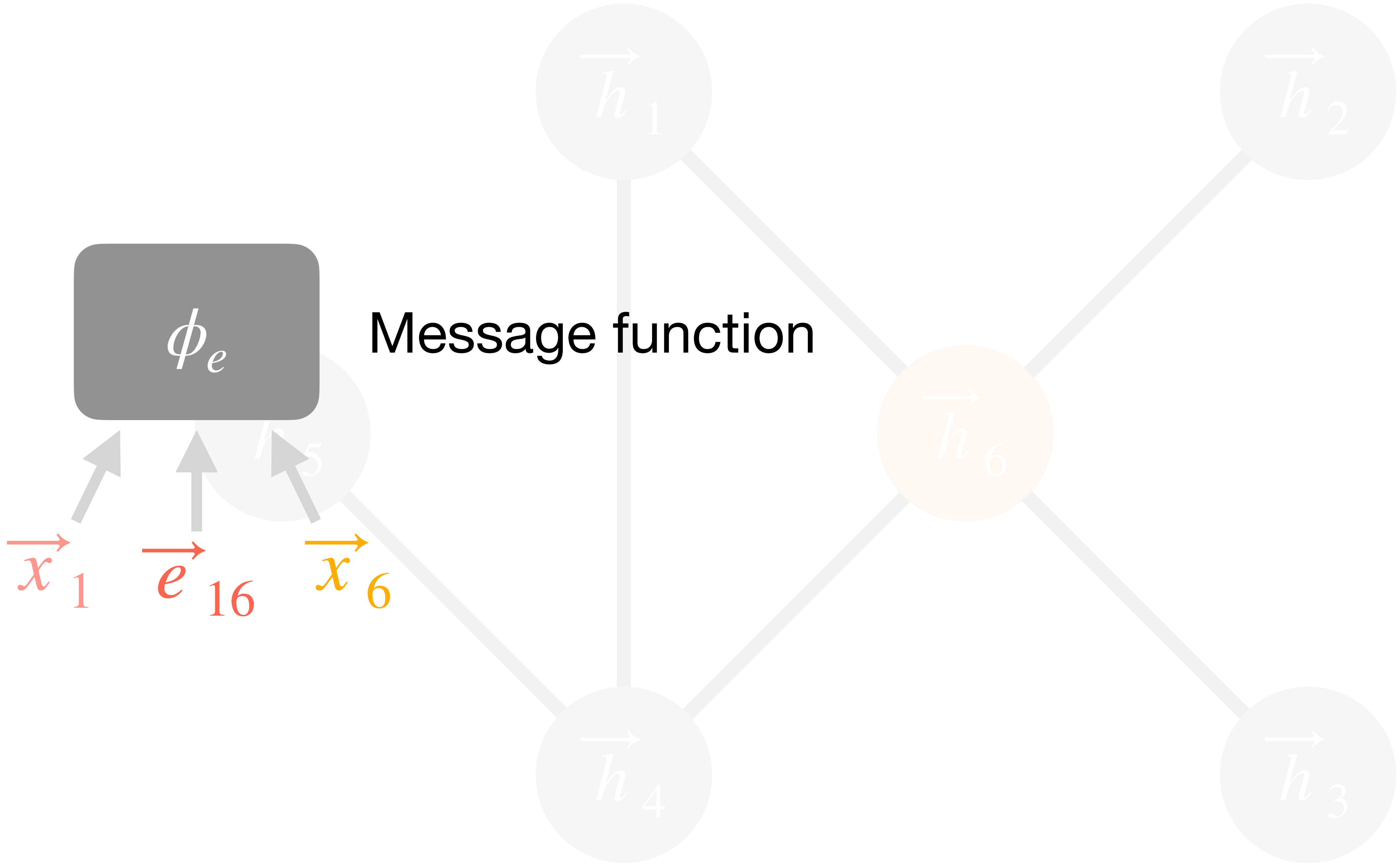




The GNN Algorithm

For each neighbor of Node 6 pass link information into **message function***

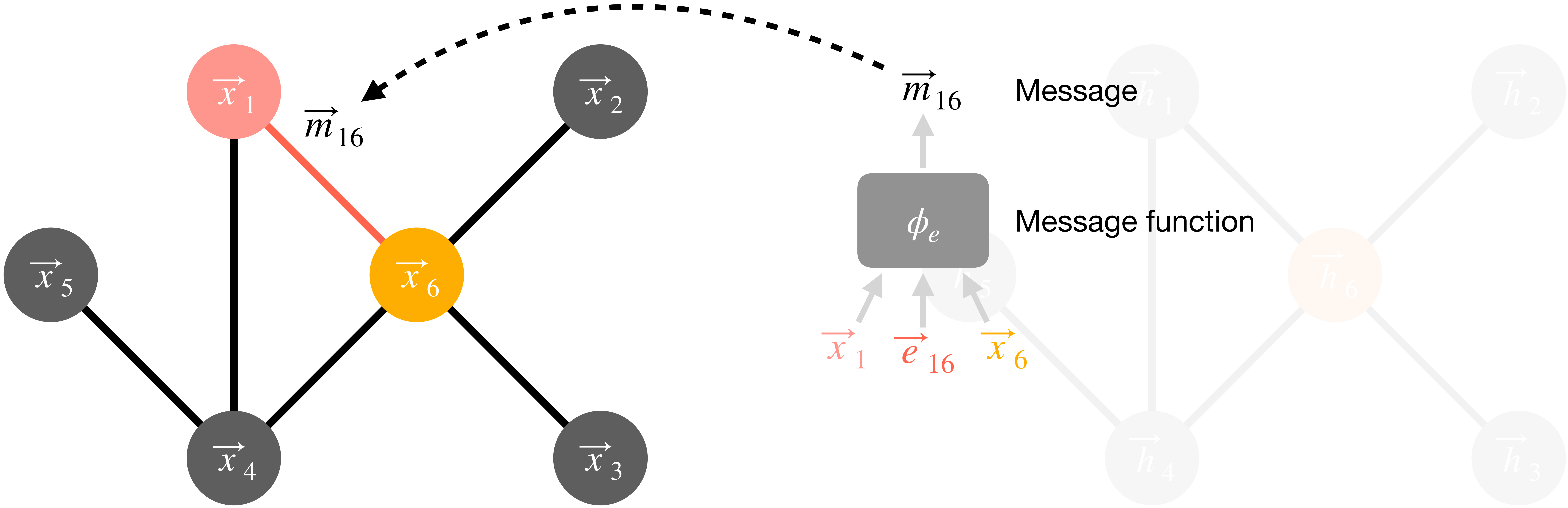




*The “e” subscript in ϕ_e stands for “edge,” per the edge-like dimension of the function

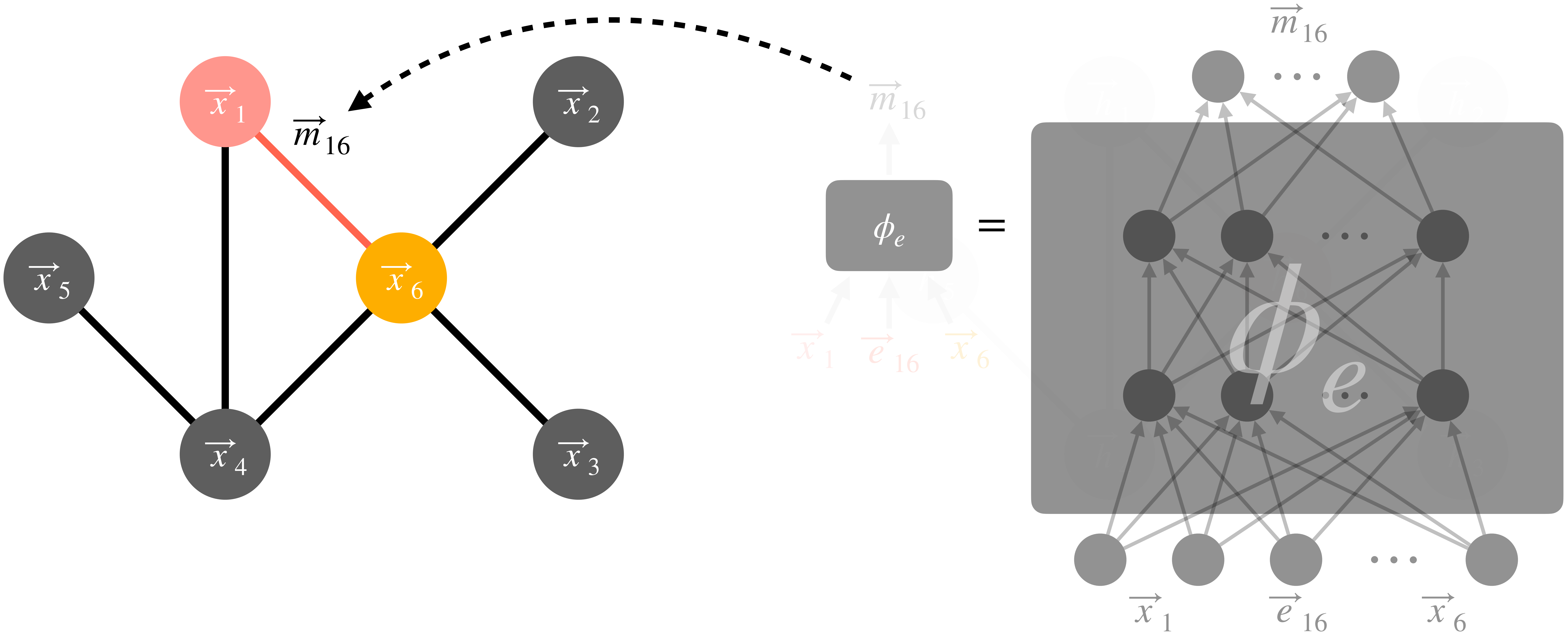
The GNN Algorithm

Message function produces a **message** conditioned by edge features



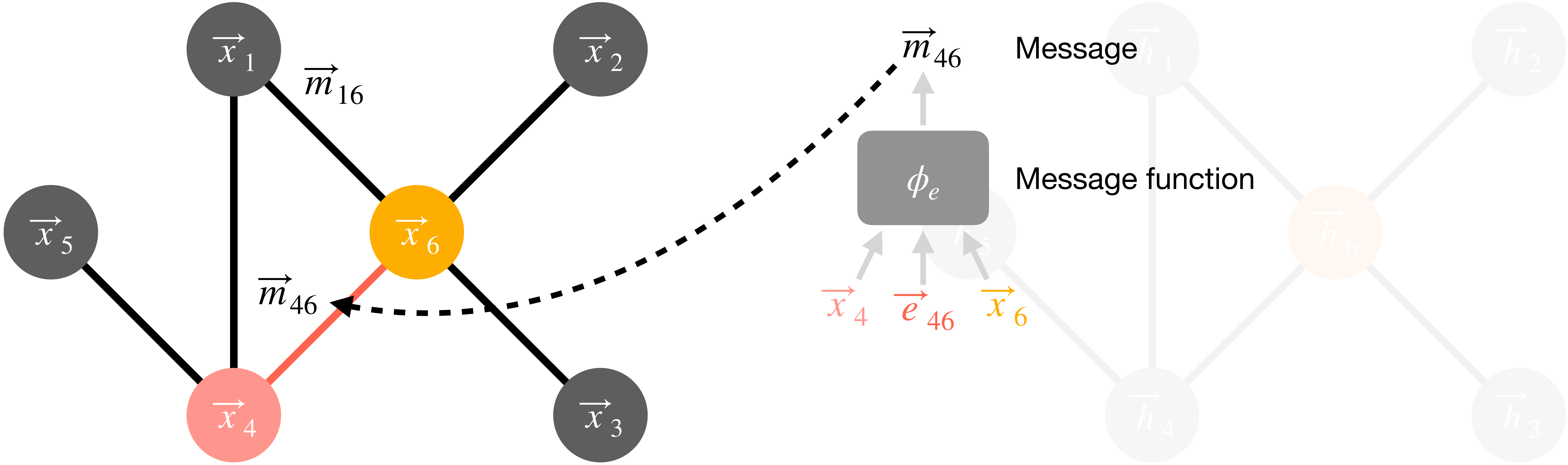
The GNN Algorithm

The message function is usually Multilayer Perceptron (MLP)



The GNN Algorithm

Compute a message for every neighbor of Node 6



The GNN Algorithm

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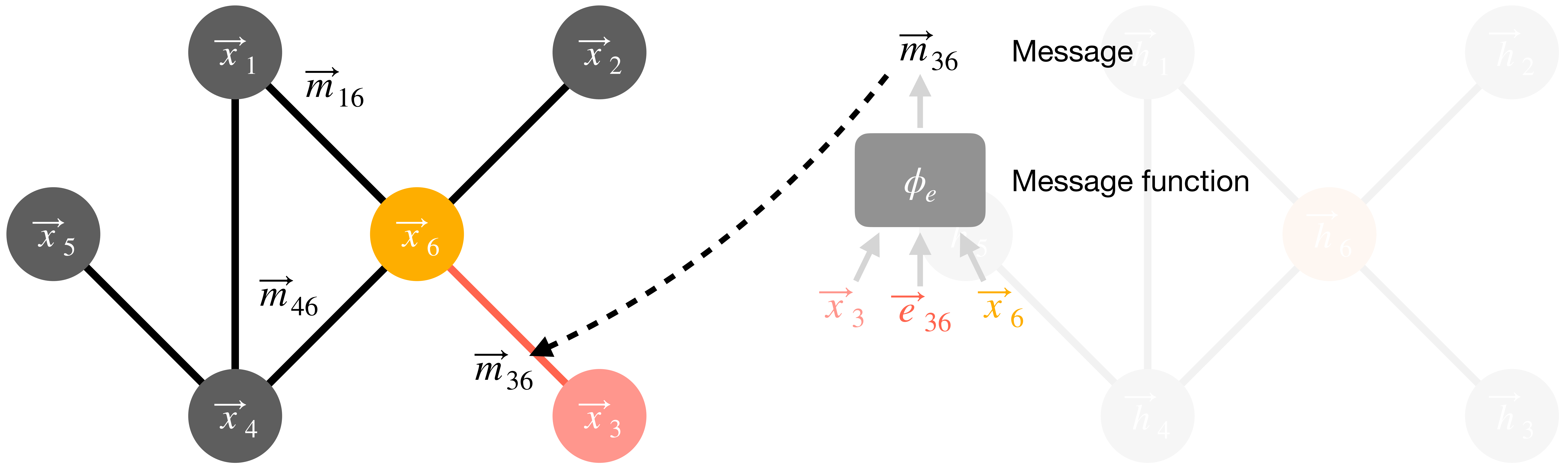

The GNN Algorithm

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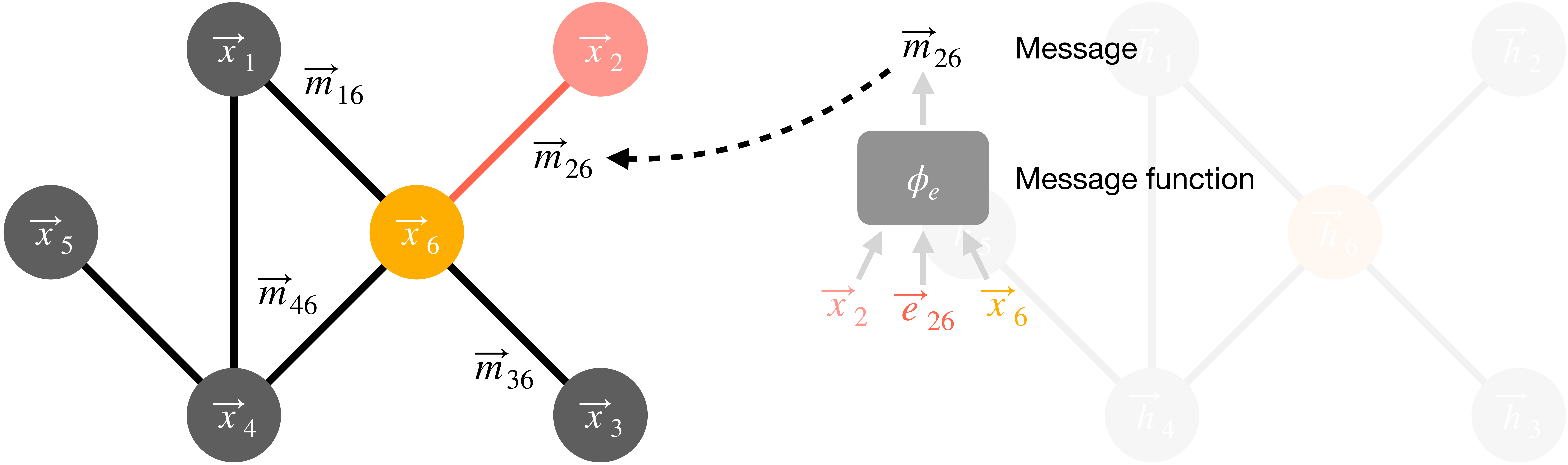

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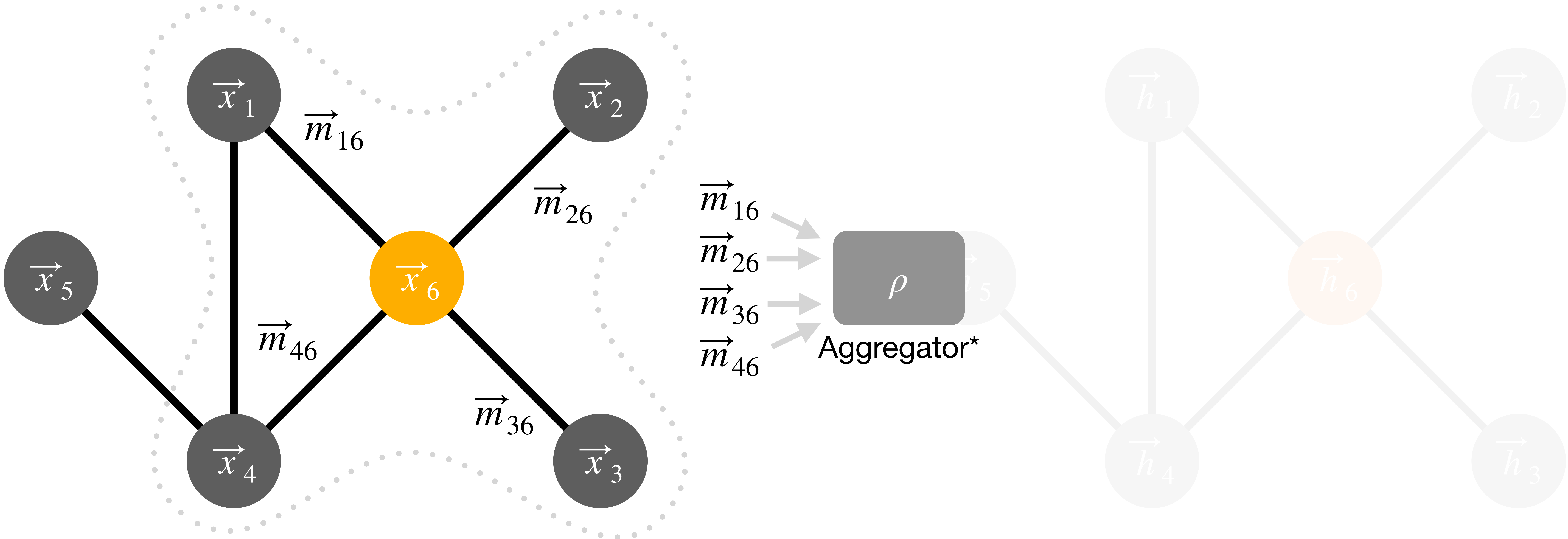
The GNN Algorithm

Next, we **aggregate** all messages together



*Must be permutation invariant, e.g. a simple sum: $\vec{m}_{16} + \vec{m}_{26} + \vec{m}_{36} + \vec{m}_{46}$

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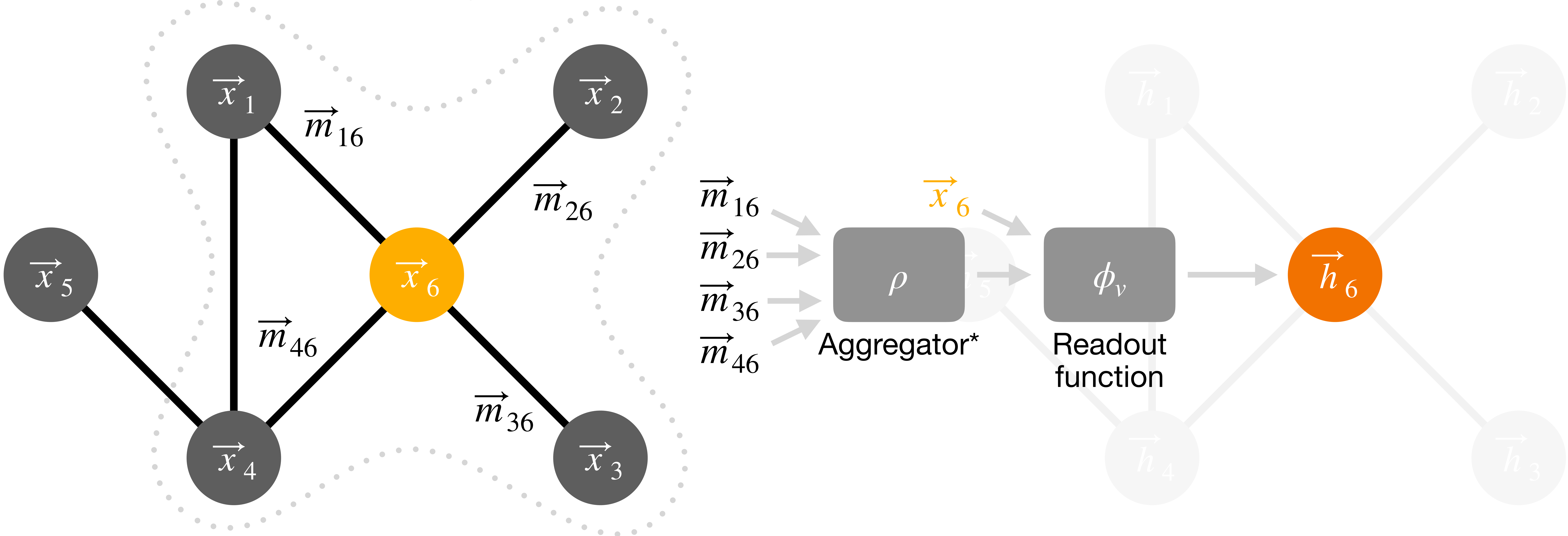
The GNN Algorithm

Pass aggregation and Node 6 itself through **readout function***
to get latent representation of Node 6



*The “v” subscript in ϕ_v stands for “vertex” (i.e. node), per the vertex-like dimension of the function

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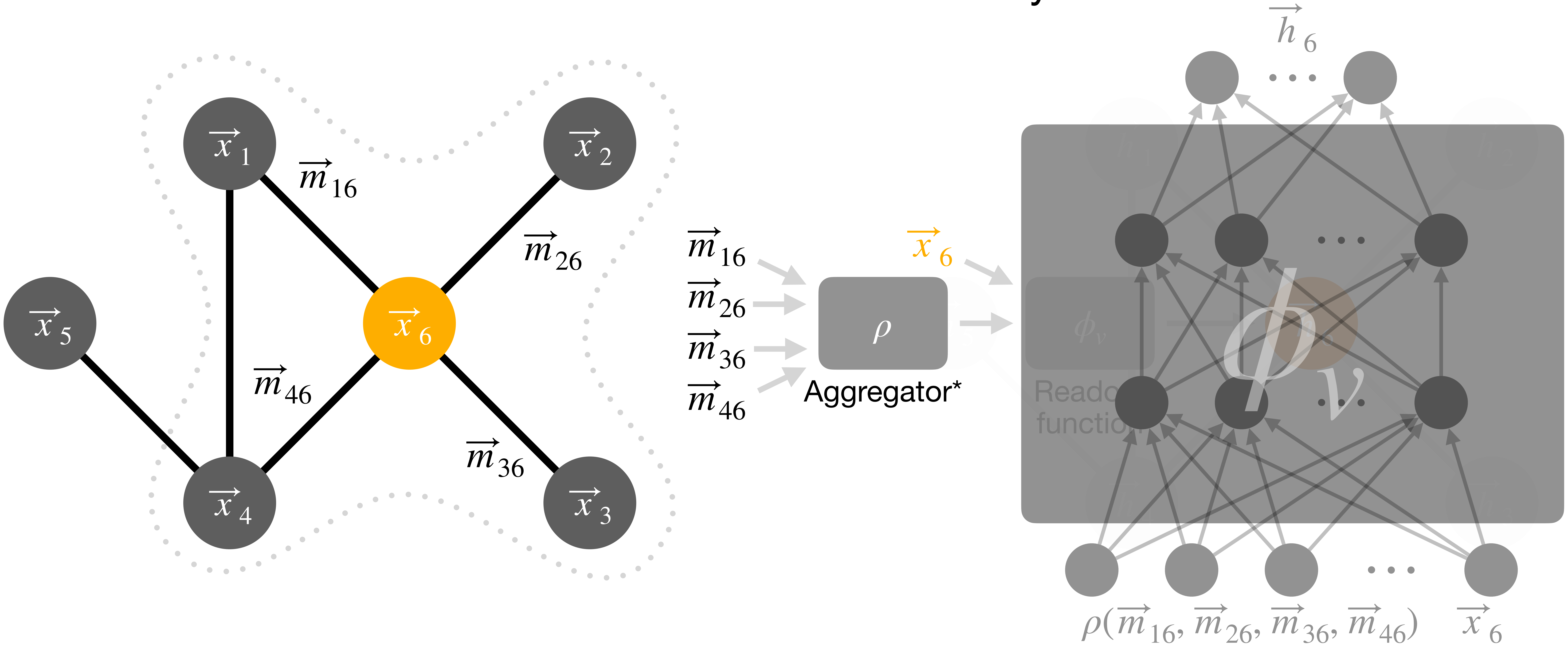
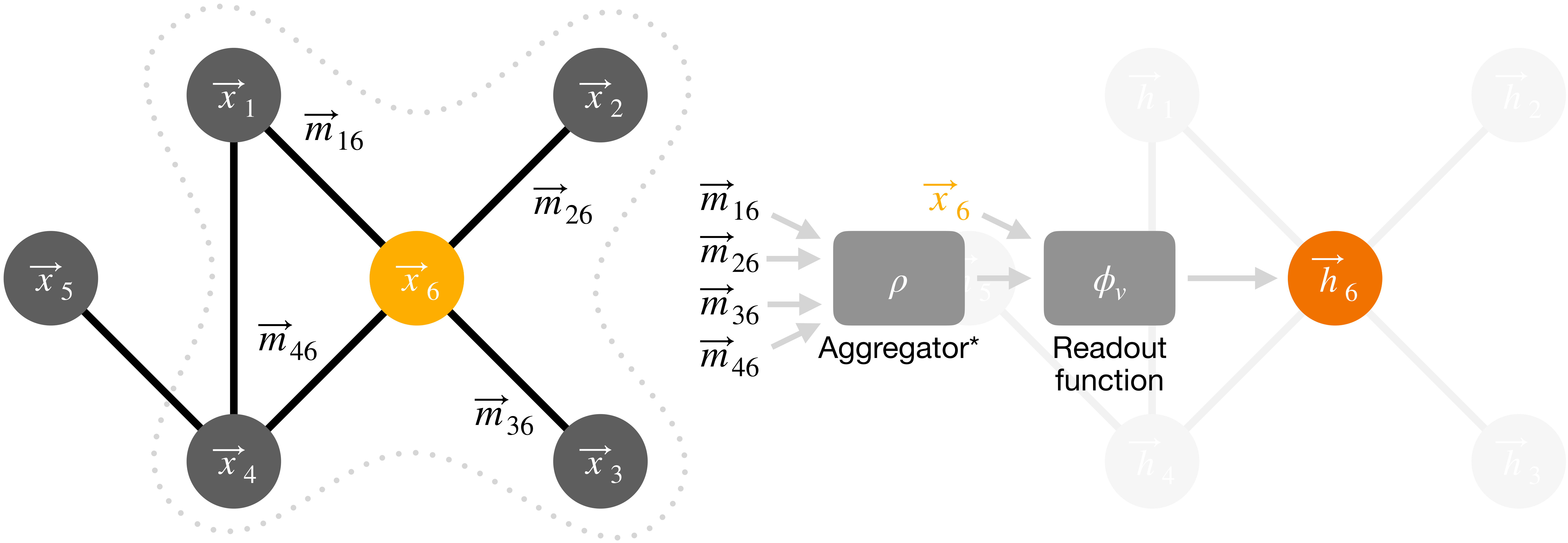
The GNN Algorithm

The readout function is also usually a MLP



The GNN Algorithm

Finally, repeat process for all nodes in the graph



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The GNN Algorithm

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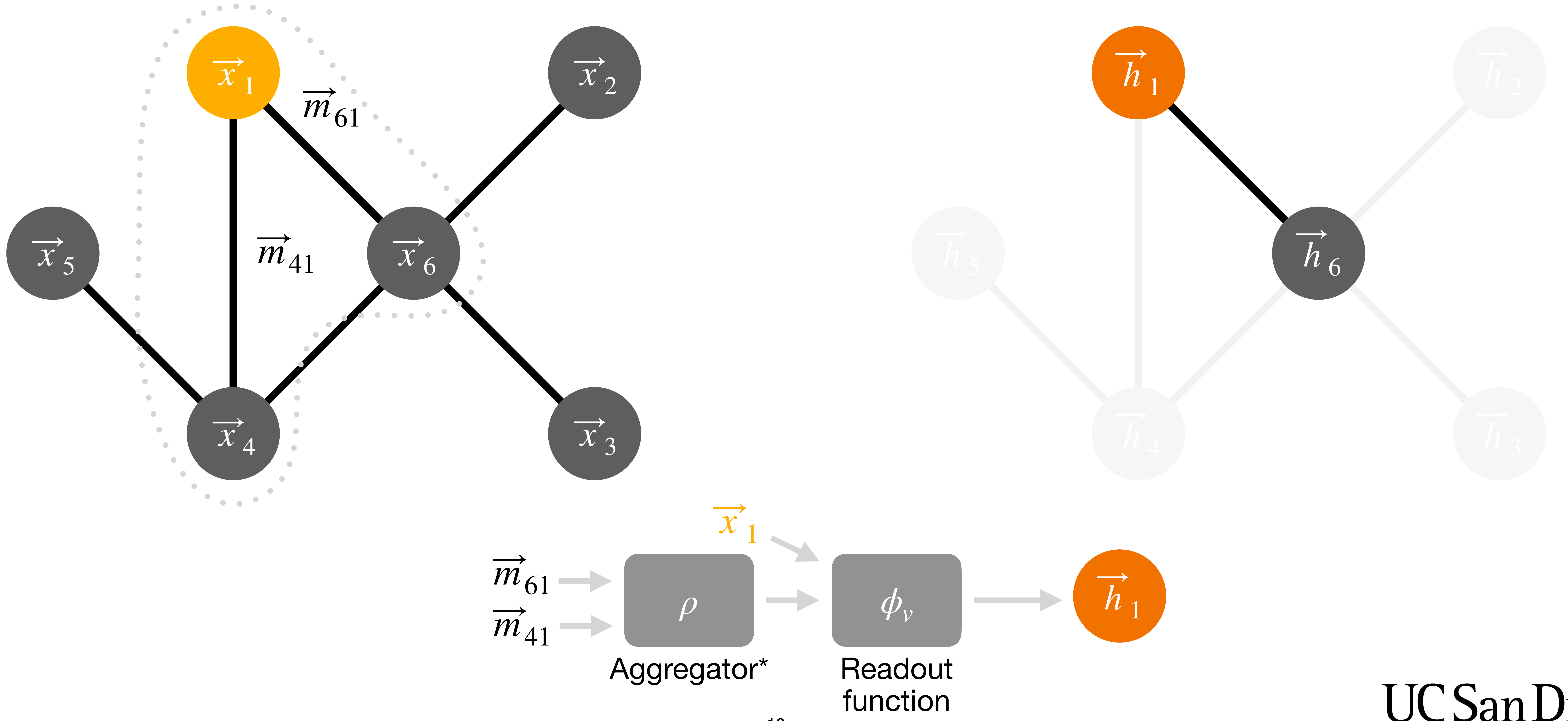

The GNN Algorithm

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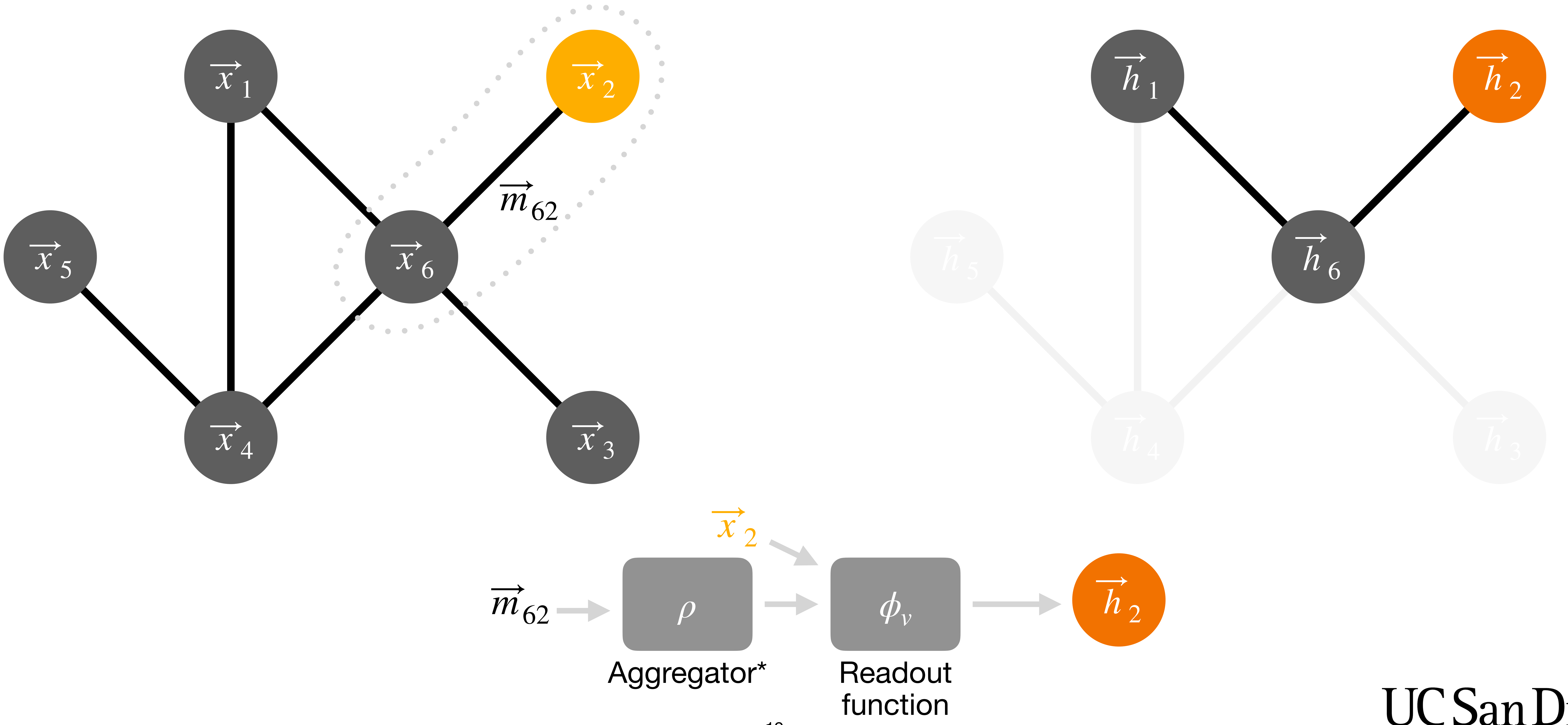

The GNN Algorithm

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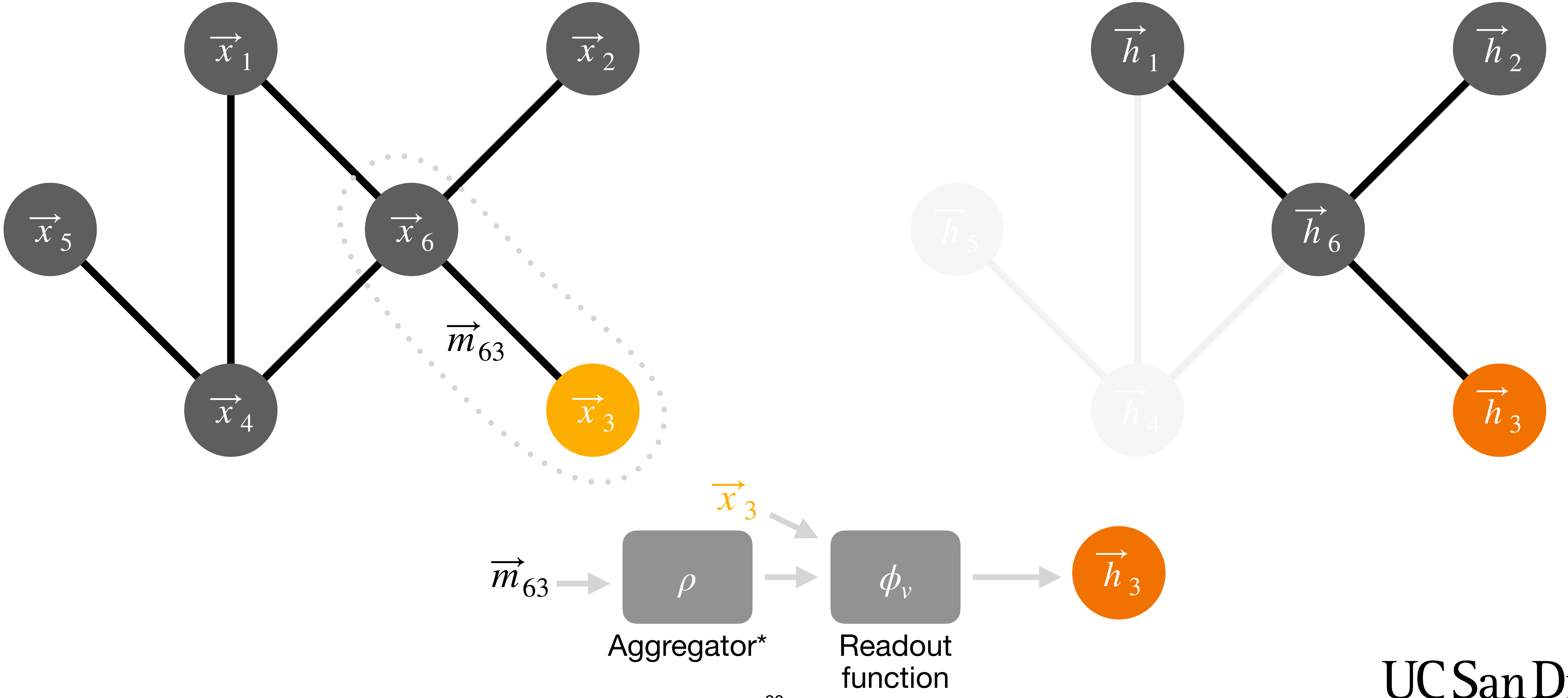

The GNN Algorithm

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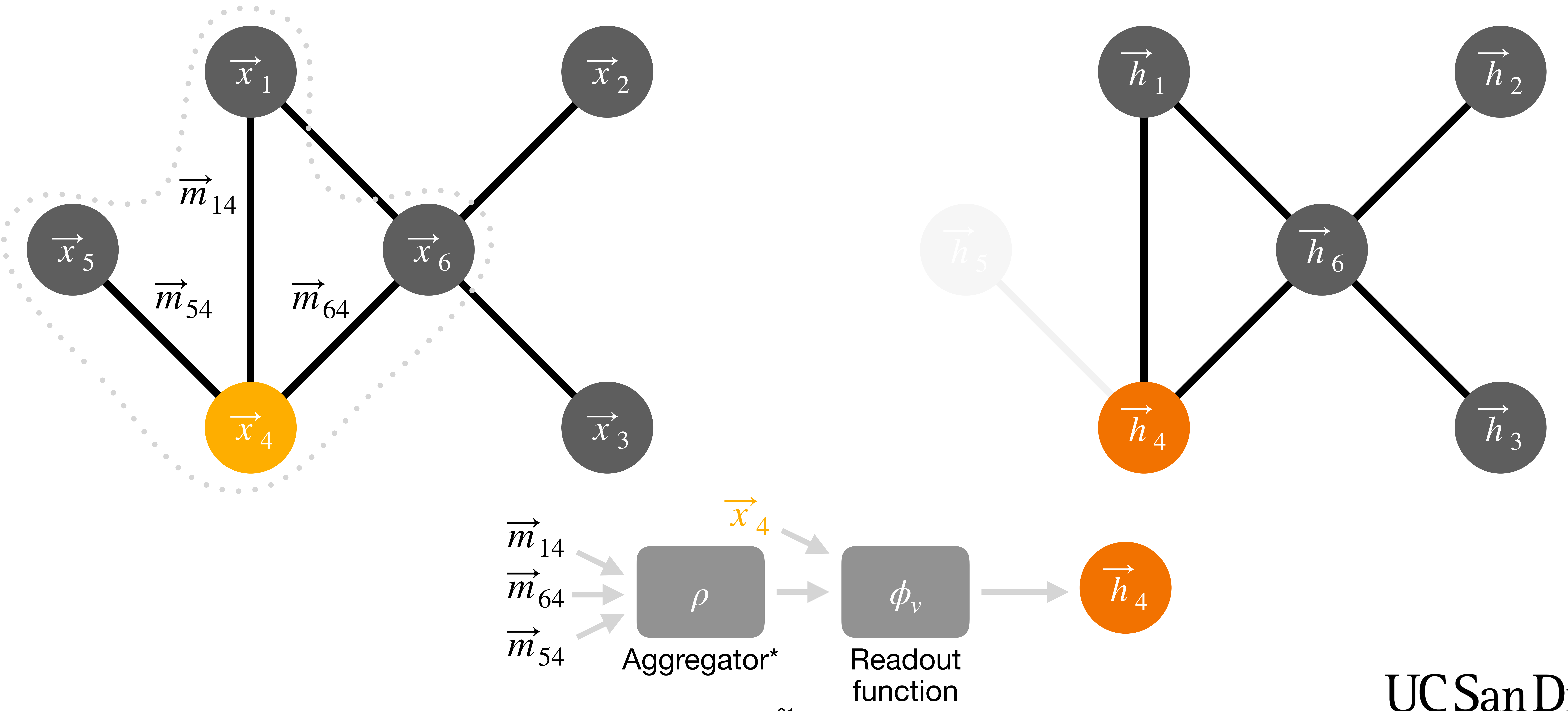

The GNN Algorithm

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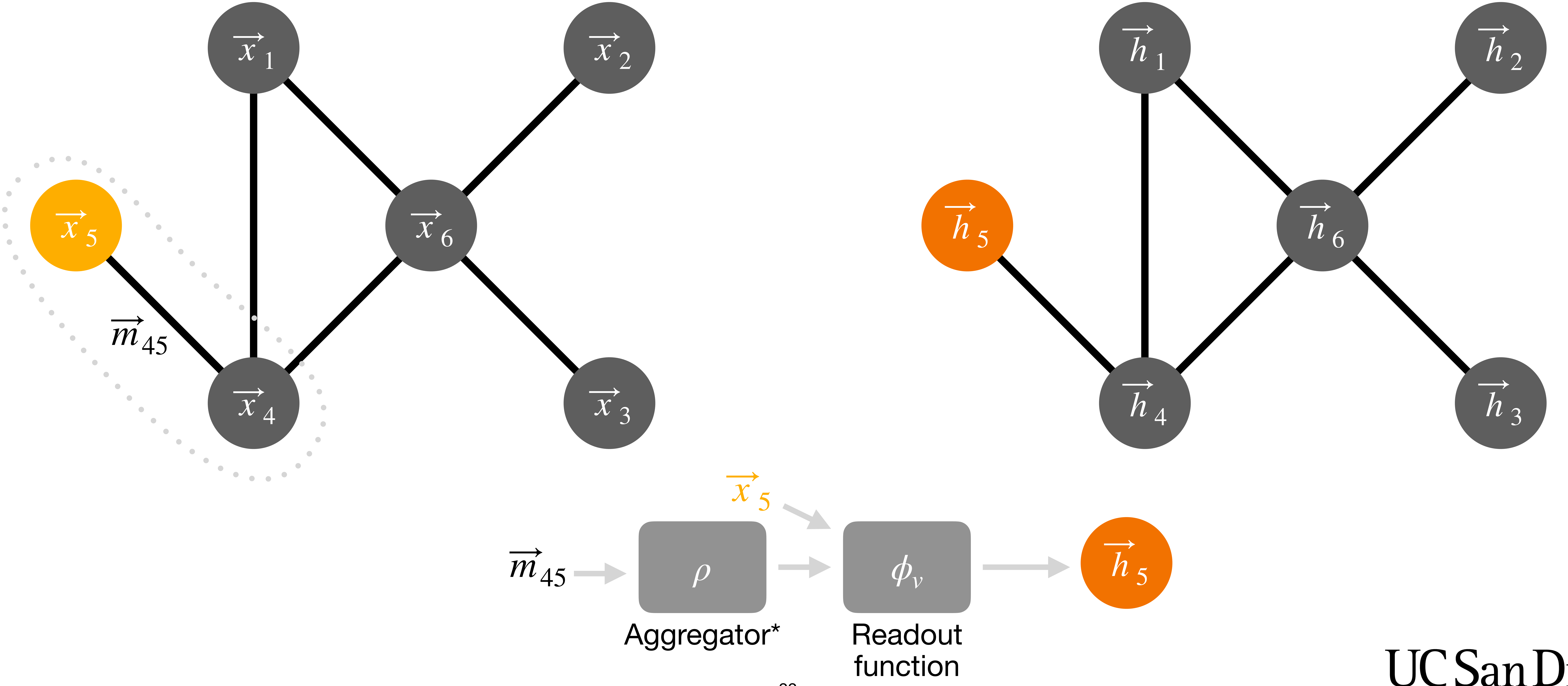
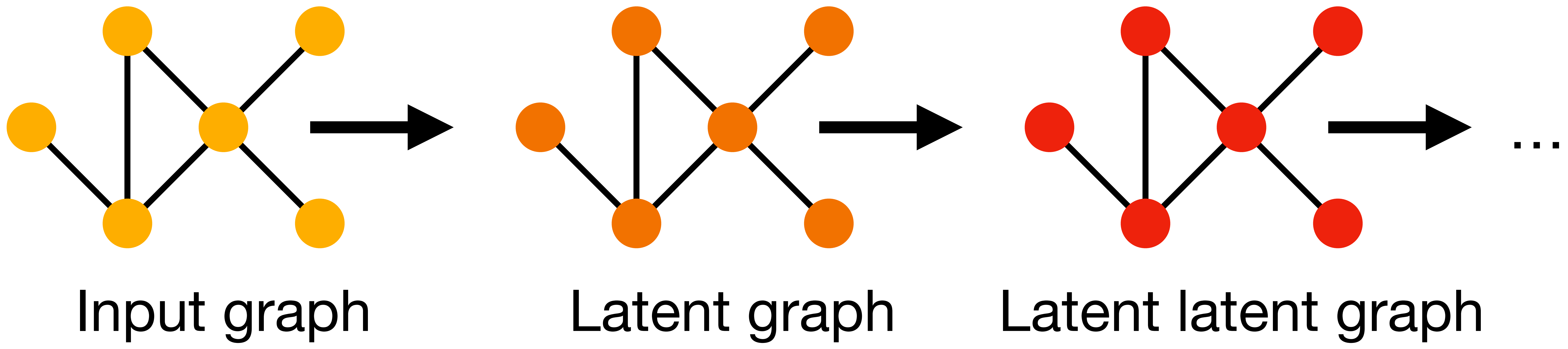


The GNN Algorithm

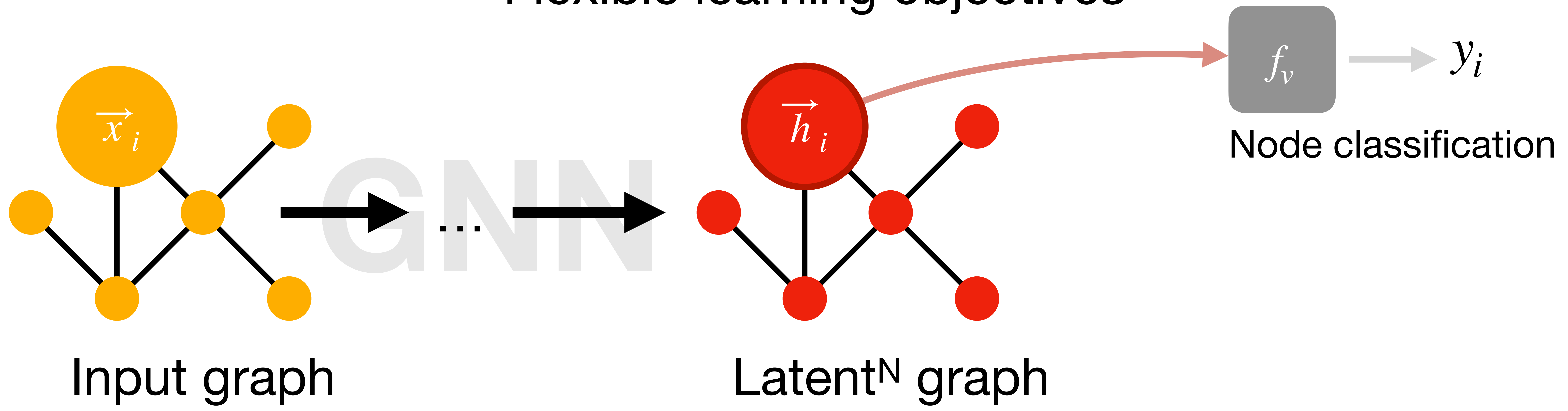
Can perform multiple rounds of message passing to diffuse graph information



- Each round of message passing aggregates info from neighbors of Node i to latent Node i
- Doing this multiple times effectively diffuses information across graph
  - Only takes a few rounds to “saturate” this process

The GNN Algorithm

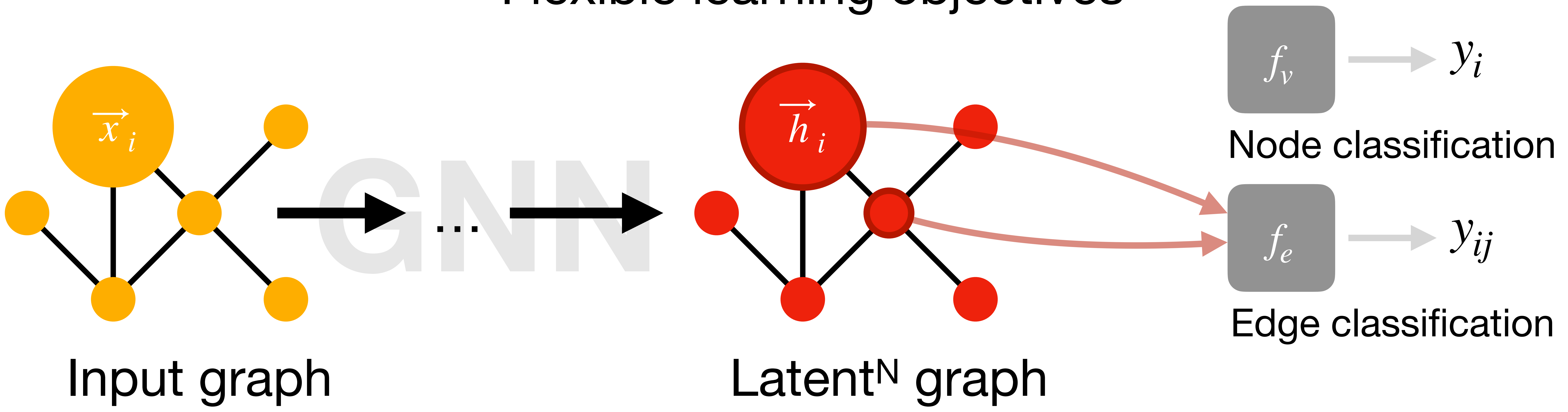
Flexible learning objectives



- The power of the latent graph is leveraged by another classifier
  - e.g. attach a MLP to the end of the GNN "pipeline" and train it to infer data about your input graph from the latent representation
- Can be done in three dimensions: node

The GNN Algorithm

Flexible learning objectives



- The power of the latent graph is leveraged by another classifier
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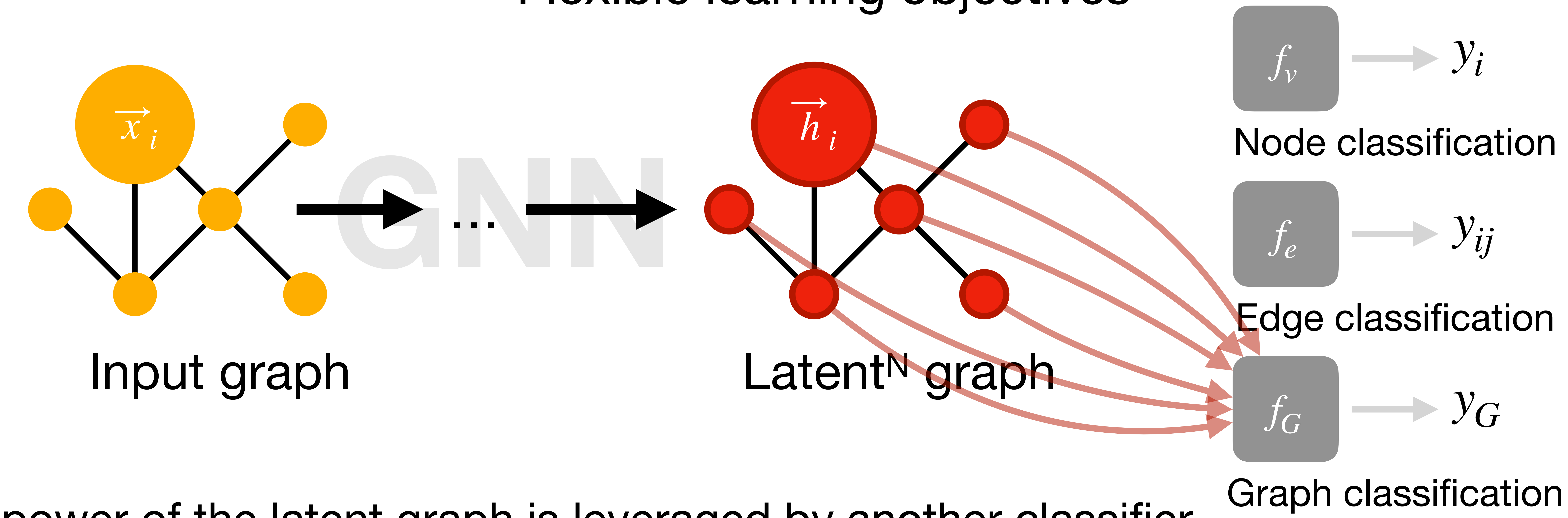
- Can be done in three dimensions: node, edge

The GNN Algorithm

Flexible learning objectives

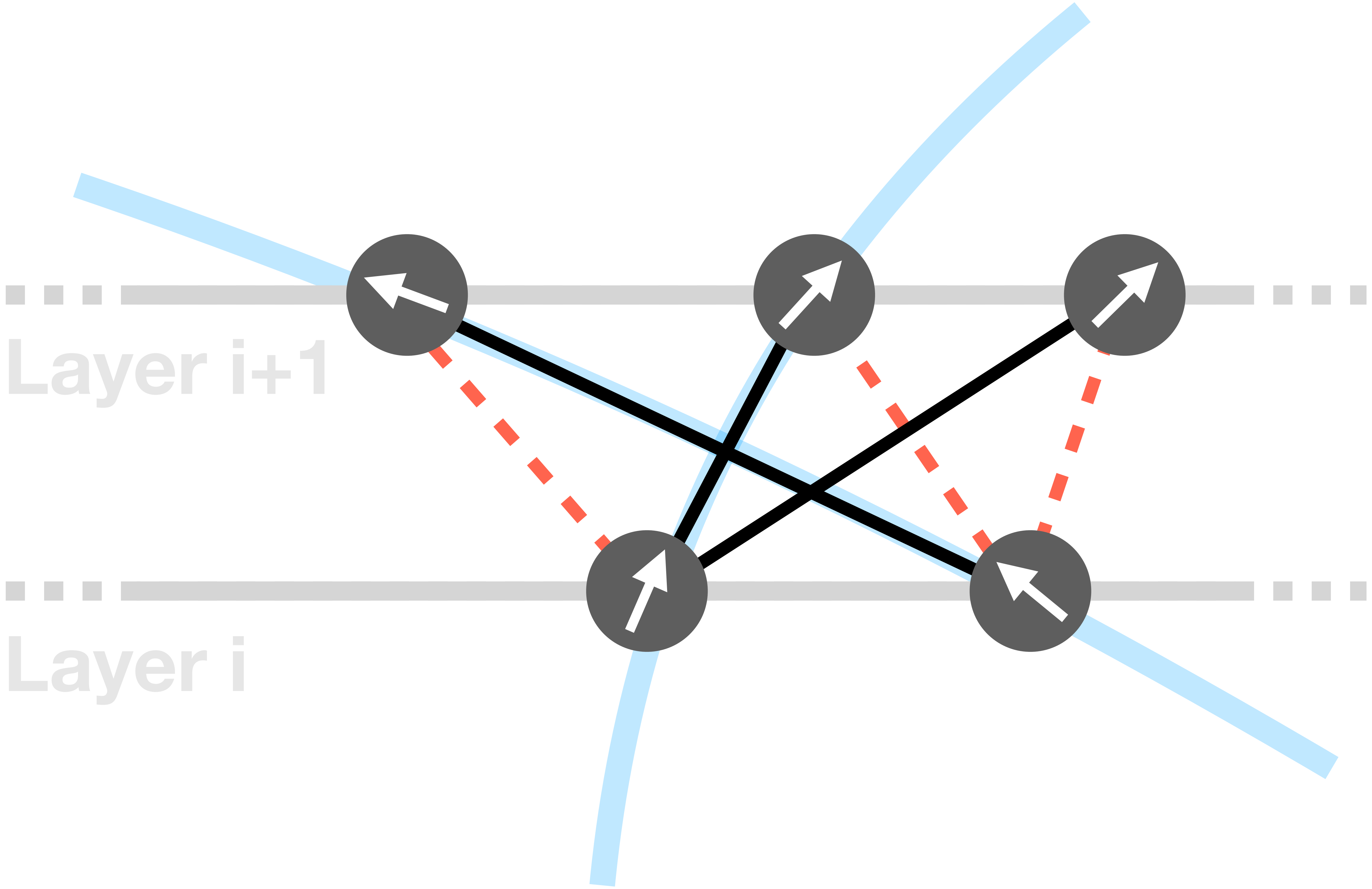


- The power of the latent graph is leveraged by another classifier
    - e.g. attach a MLP to the end of the GNN “pipeline” and train it to infer data about your input graph from the latent representation
- Can be done in three dimensions: node, edge, graph

GNNs and LST

GNN LST: Line Segments

- Currently form all line segments and check for (rough) p_T consistency
- Because these are low level objects, make very loose cuts
  - Large # of true segments
  - Very large # of fake segments
- **First exploration:** can the GNN select the same # of true, but a smaller # of fake segments?



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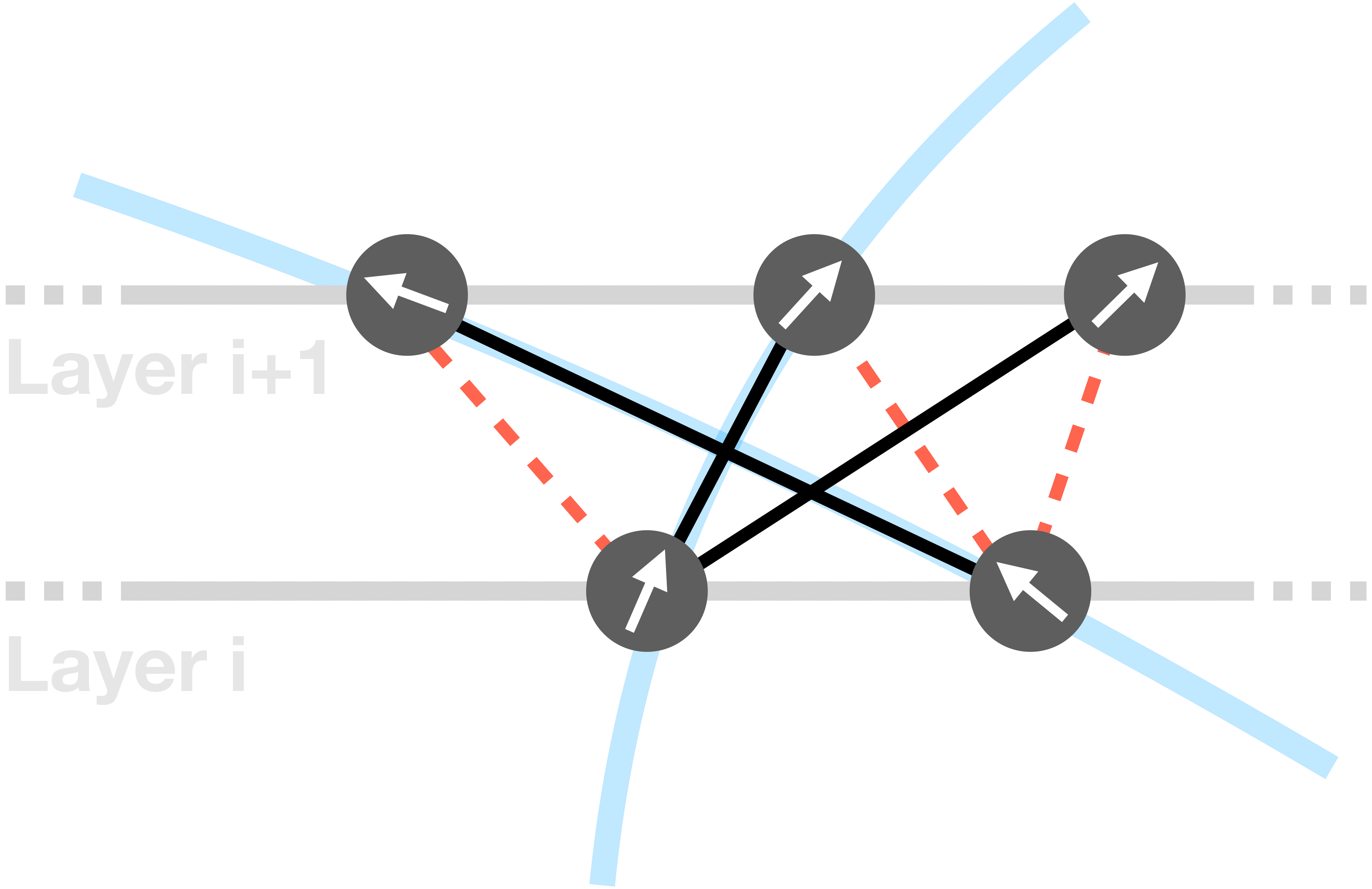
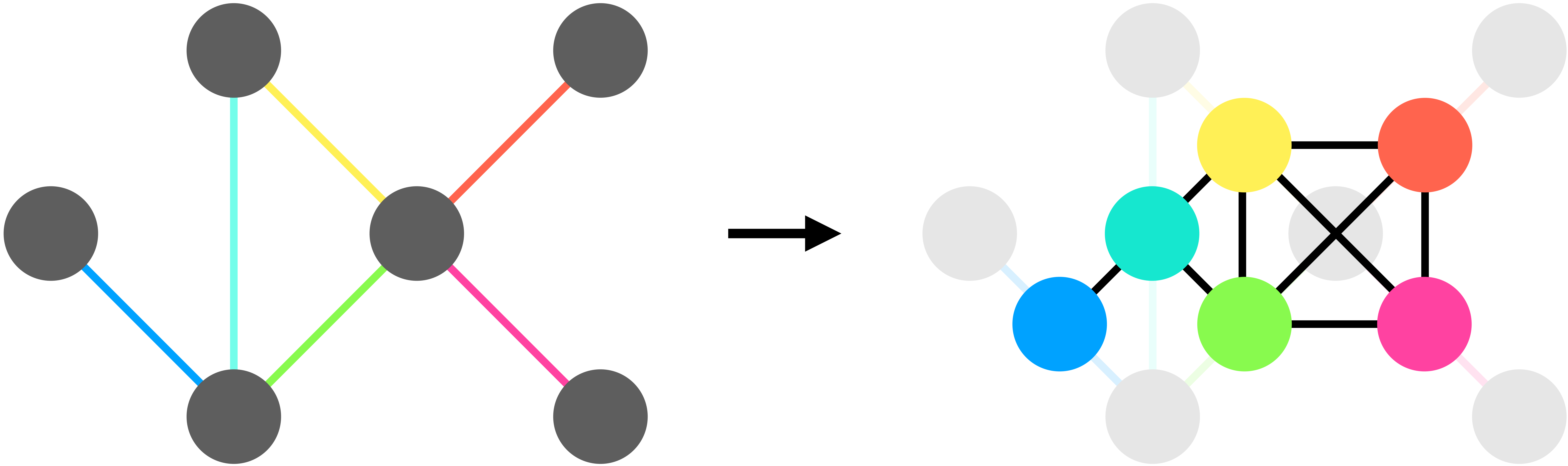
GNN LST: Line Segments

- **First exploration:** can the GNN select the same # of true, but a smaller # of fake segments?
- Run GNN on segments from LST LS step
- Philip has already done this, but only ran the simplest model
  - e.g. only 1 round of message passing
- Maybe also loosen p_T consistency cuts
  - We suspect this will only give more fakes and not much more true tracks



GNN LST: High-level Inferences



- For making high-level objects, can “pool” graph together in various ways
- e.g. Make every segment a node in a new graph
    - Then, connections between these nodes are triplet candidates

GNN LST: Stepwise Explorations

- **Second exploration:** can the GNN select the same # of true, but a smaller # of fake triplets?
- **Third exploration:** can the GNN select the same # of true, but a smaller # of fake quintuplets?
- …
- **Nth exploration:** can the GNN select the same # of true, but smaller # of fake track candidates?
- At each step, compare efficiency metrics with current LST algorithm

Summary

- GNNs leverage interconnectivity of data to better use multiple MLPs towards a diverse set of classification problems
- We propose a step-wise exploration of incorporating GNNs into LST
  - Try to reconstruct different objects and compare efficiency/performance
  - i.e. walk our way from line segments to entire track candidates
- Next steps:
  - ~~Run Philip's existing GNN pipeline~~
  - Modify Philip's GNN
  - Compare # true and # fake LS (i.e. the "first exploration")

Backup

GNN Information Diffusion

- Each round of message passing aggregates info from neighbors of Node i to latent Node i
- Doing this multiple times effectively diffuses information across graph
- Only takes a few rounds to “saturate” this process

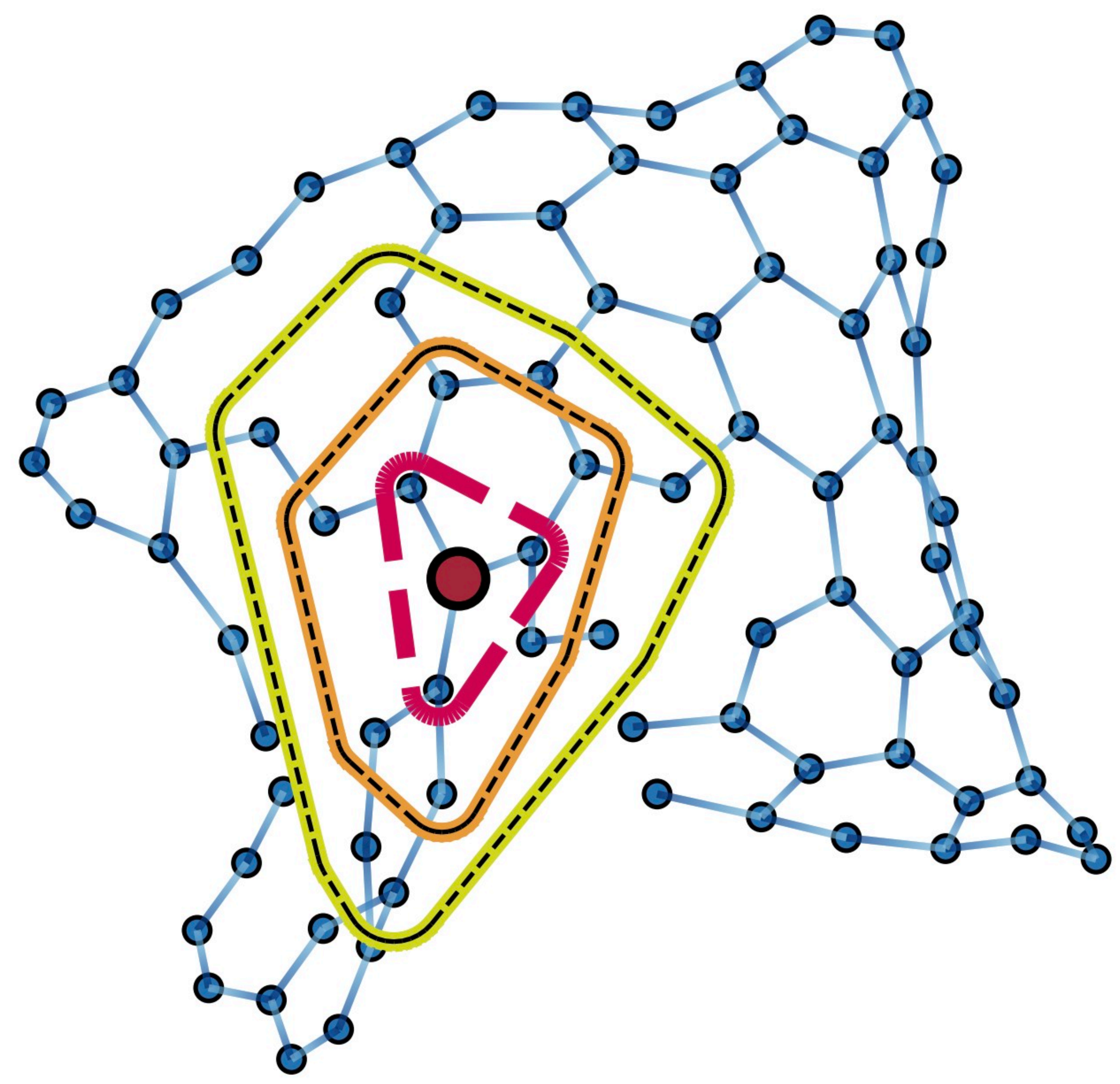


Fig. 10. The red, orange-highlighted, and yellow-highlighted dotted lines represent the enlarging neighborhood of nodes that may communicate with the red node after one, two, and three iterations of message passing, respectively [41]. Those nodes outside of the yellow-highlighted dotted boundary do not influence the red node after three iterations.

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