DEEP SETS ARE VIABLE GRAPH LEARNERS

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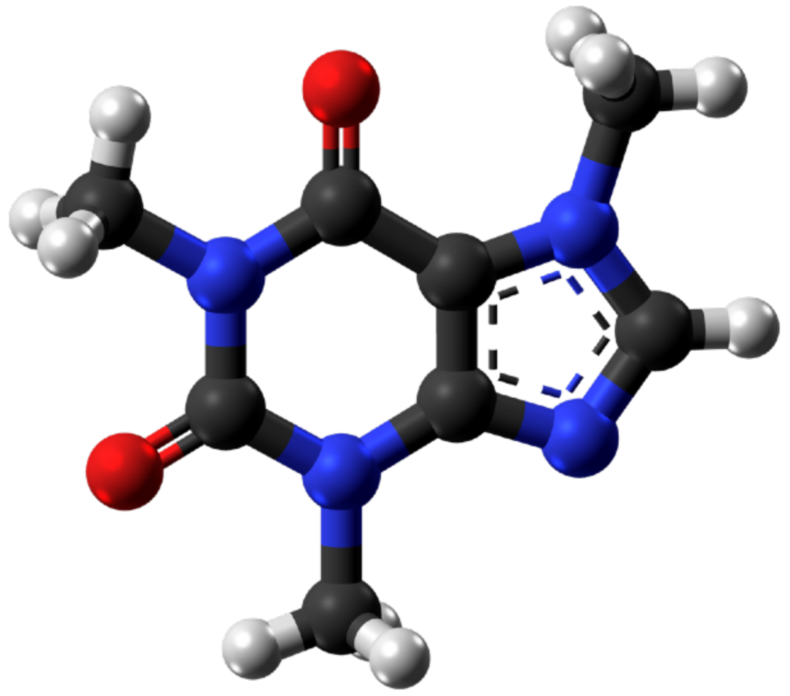
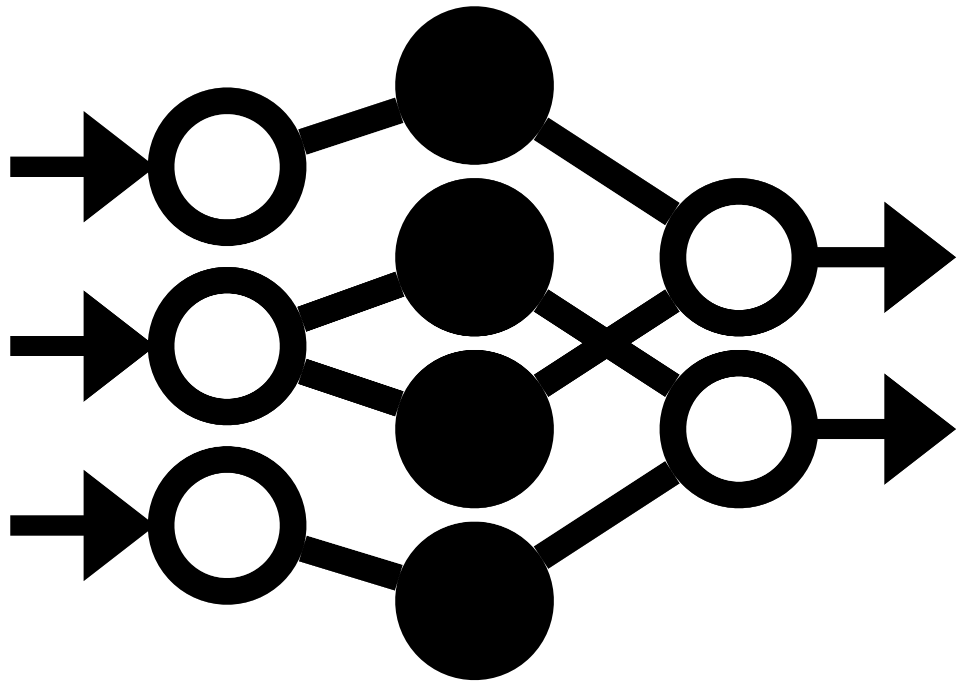
COMPLEX NETWORKS

dfki ai
Deutsches Forschungszentrum für Künstliche Intelligenz
German Research Center for Artificial Intelligence

Predictions on Graphs



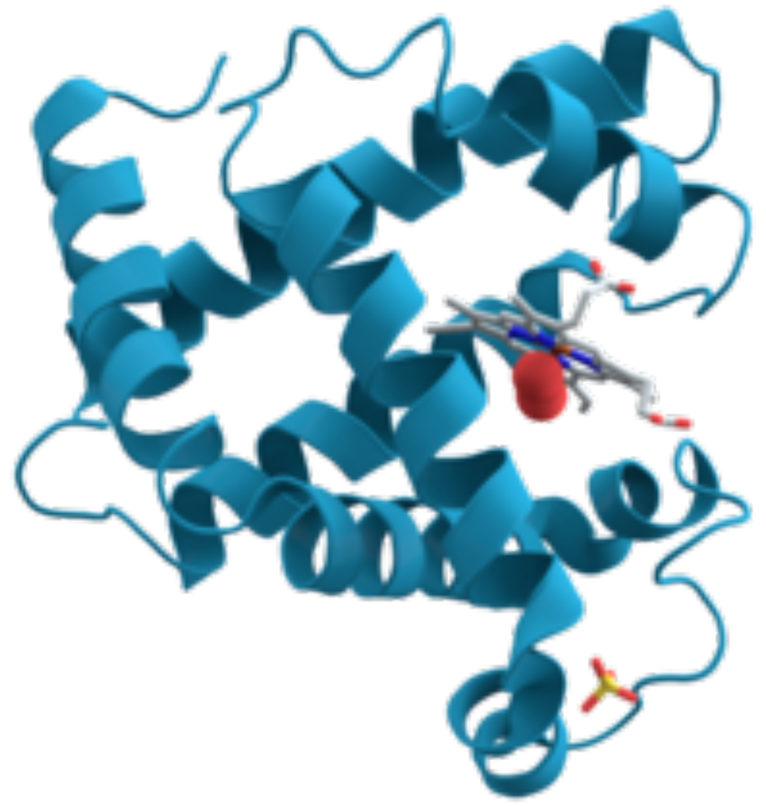


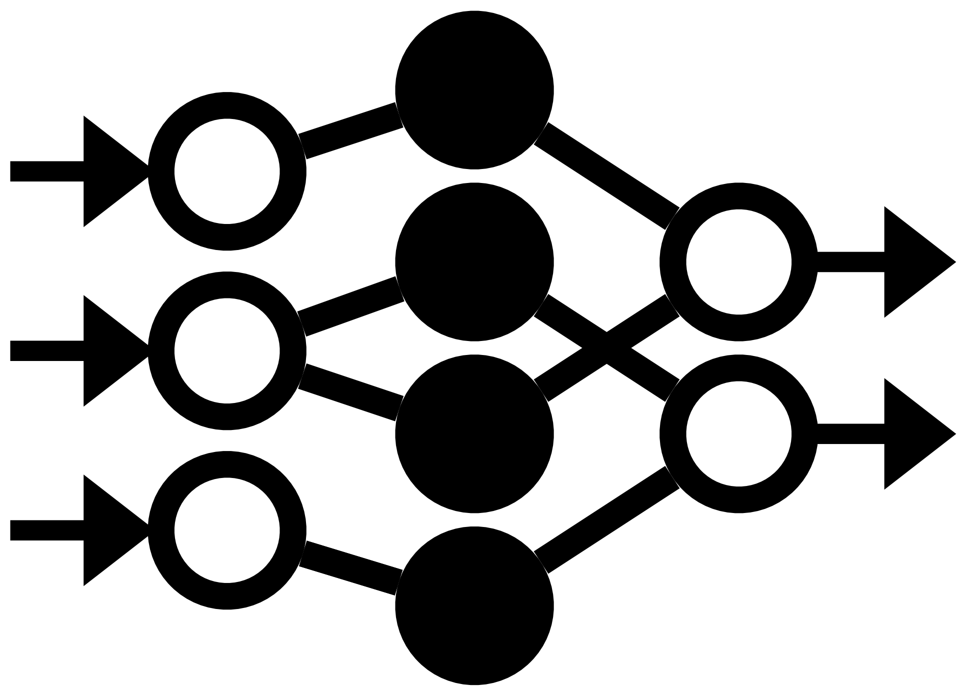
Toxic vs Non-Toxic

In many ways, graphs are the main modality
of data we receive from nature.

- Petar Veličković

Predictions on Graphs



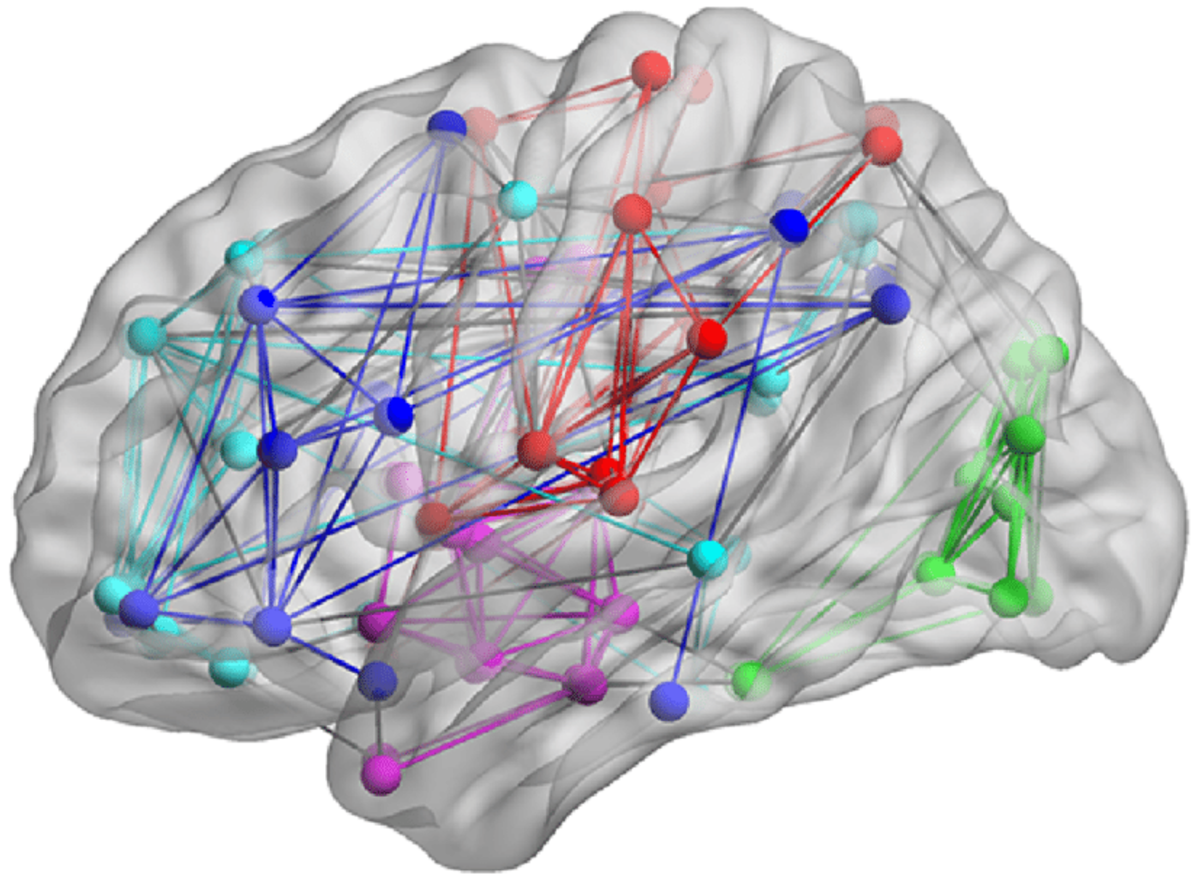


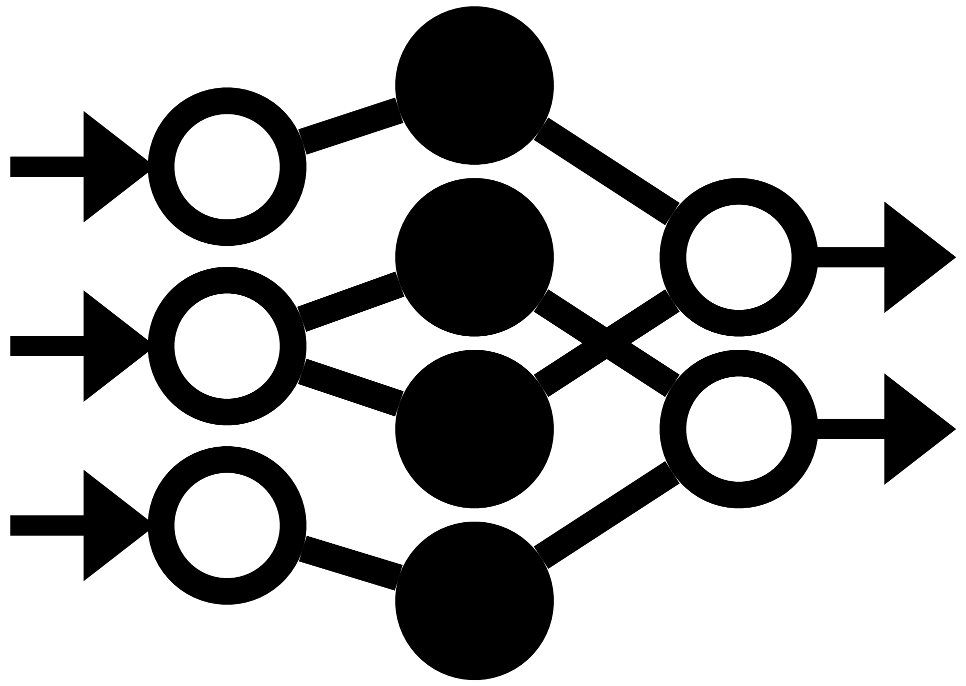
Kinase vs Phosphatase

In many ways, graphs are the main modality
of data we receive from nature.

- Petar Veličković

Predictions on Graphs





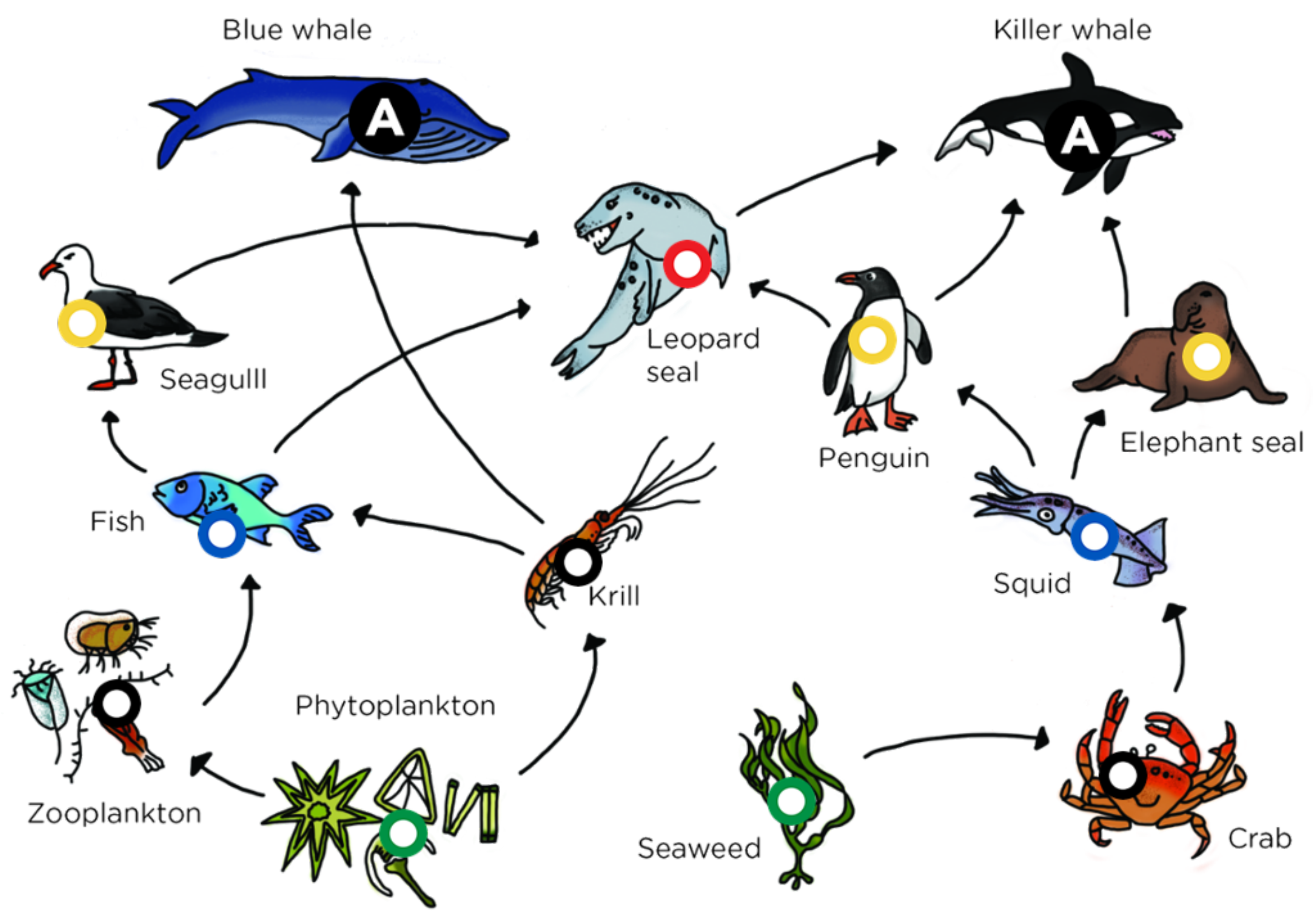
Attentive vs Distracted

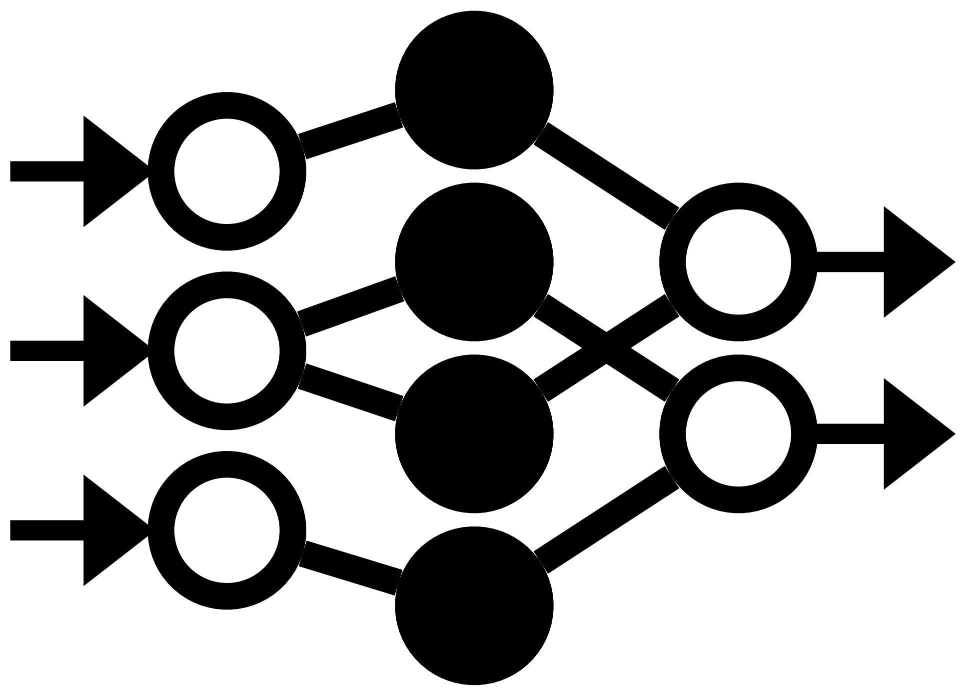
In many ways, graphs are the main modality of data we receive from nature.

- Petar Veličković

https://www.researchgate.net/publication/348379922_A_Novel_Word_Sense_Disambiguation_Approach_Using_WordNet_Knowledge_Graph/figures?lo=1

Predictions on Graphs



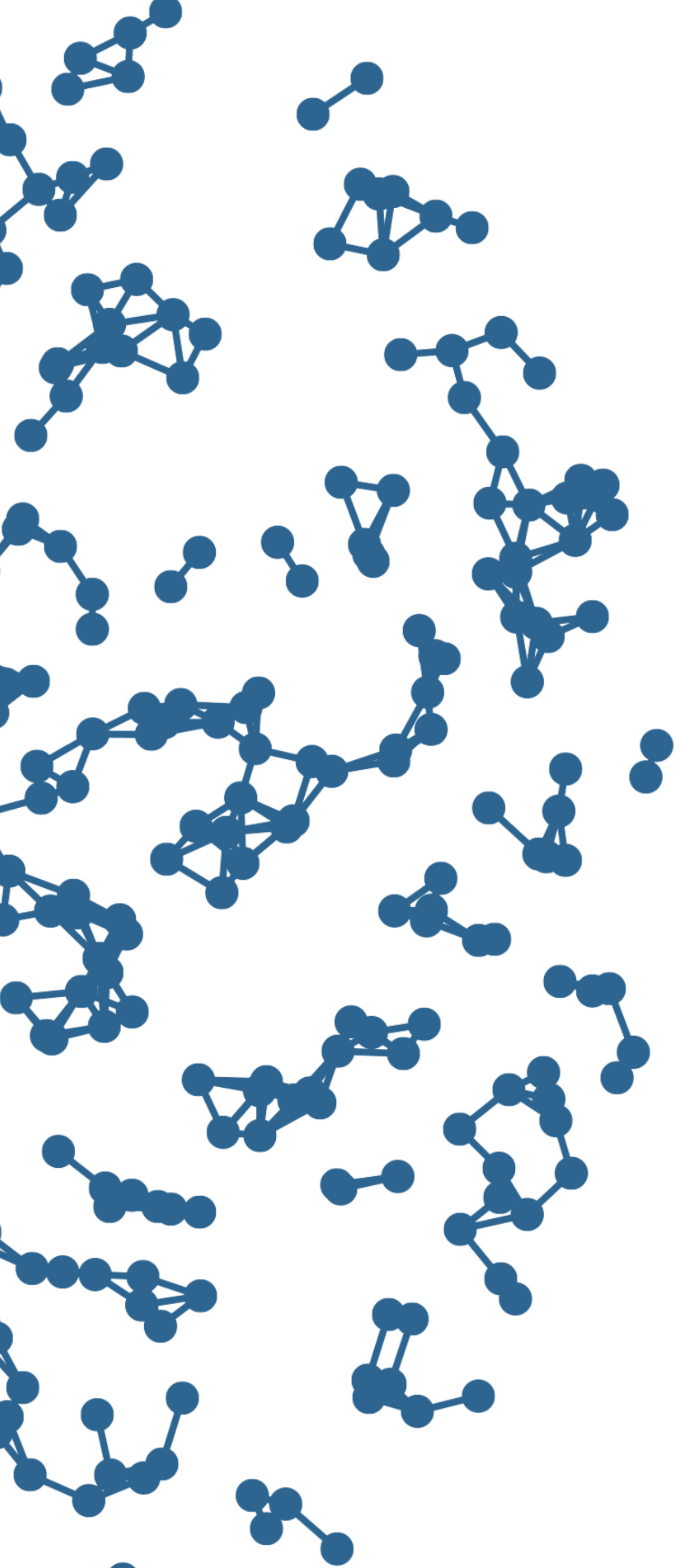


Stable vs Endangered

In many ways, graphs are the main modality of data we receive from nature.

- Petar Veličković

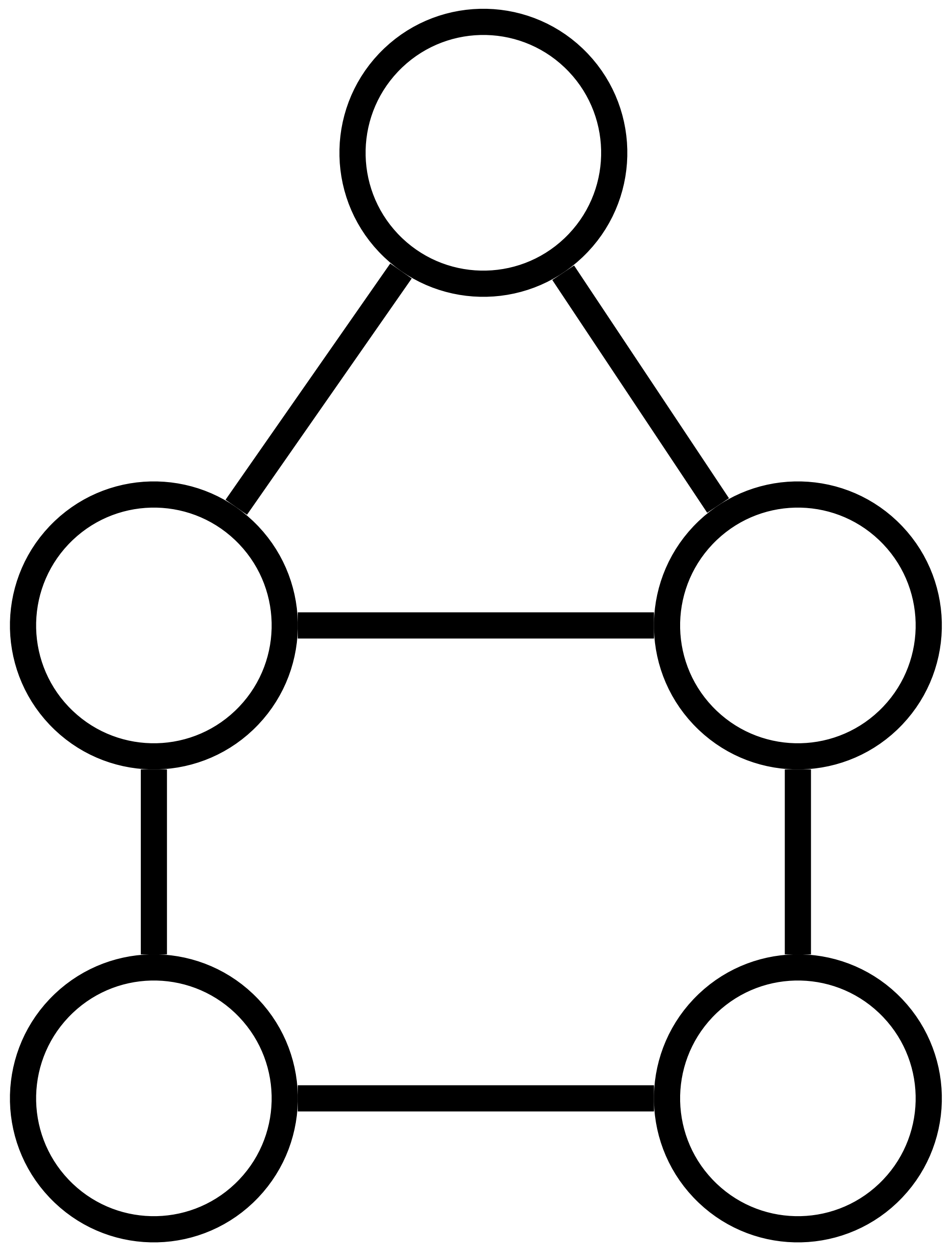
https://mlurgi.github.io/networks_for_r/



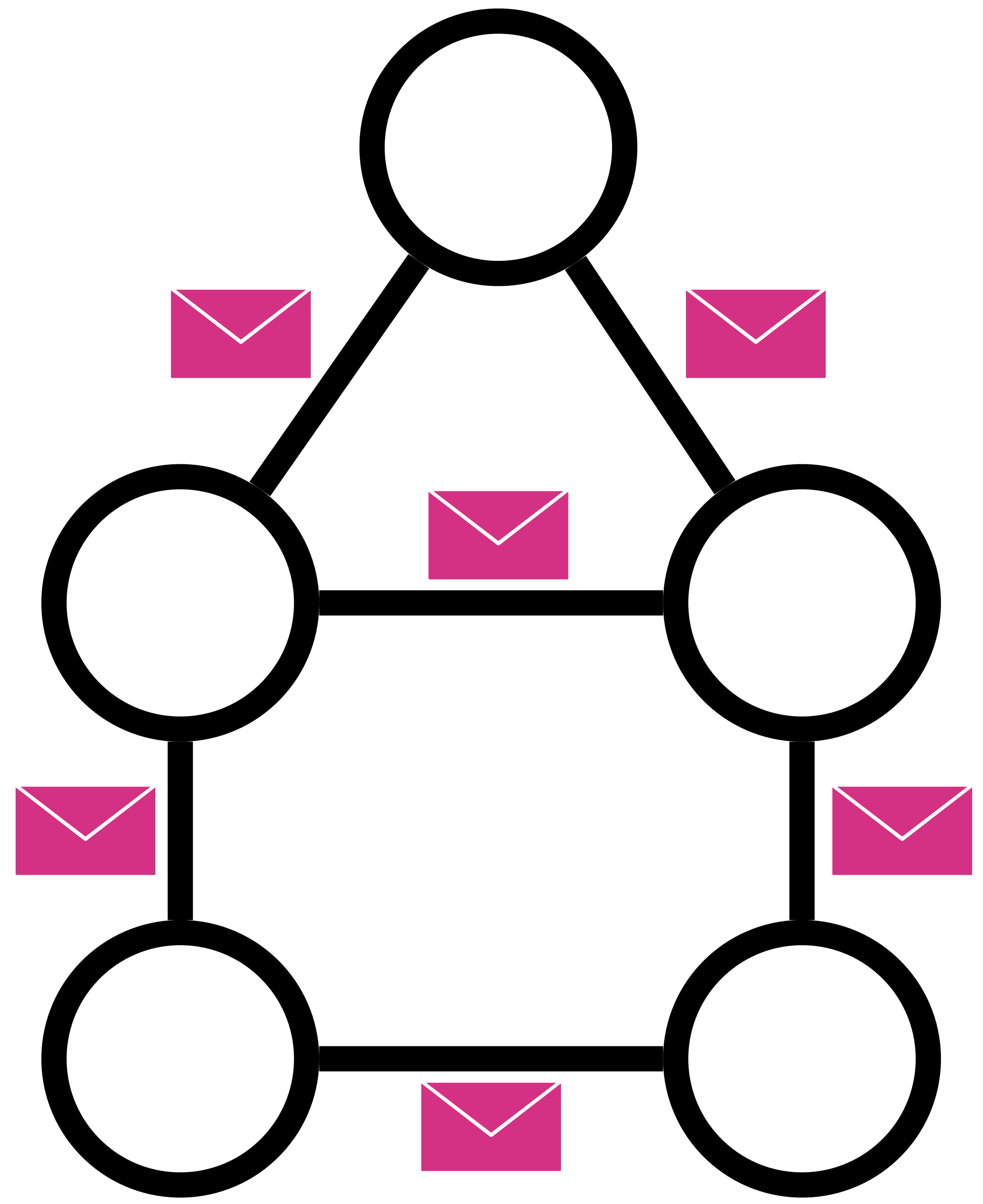
Part I

MESSAGE PASSING

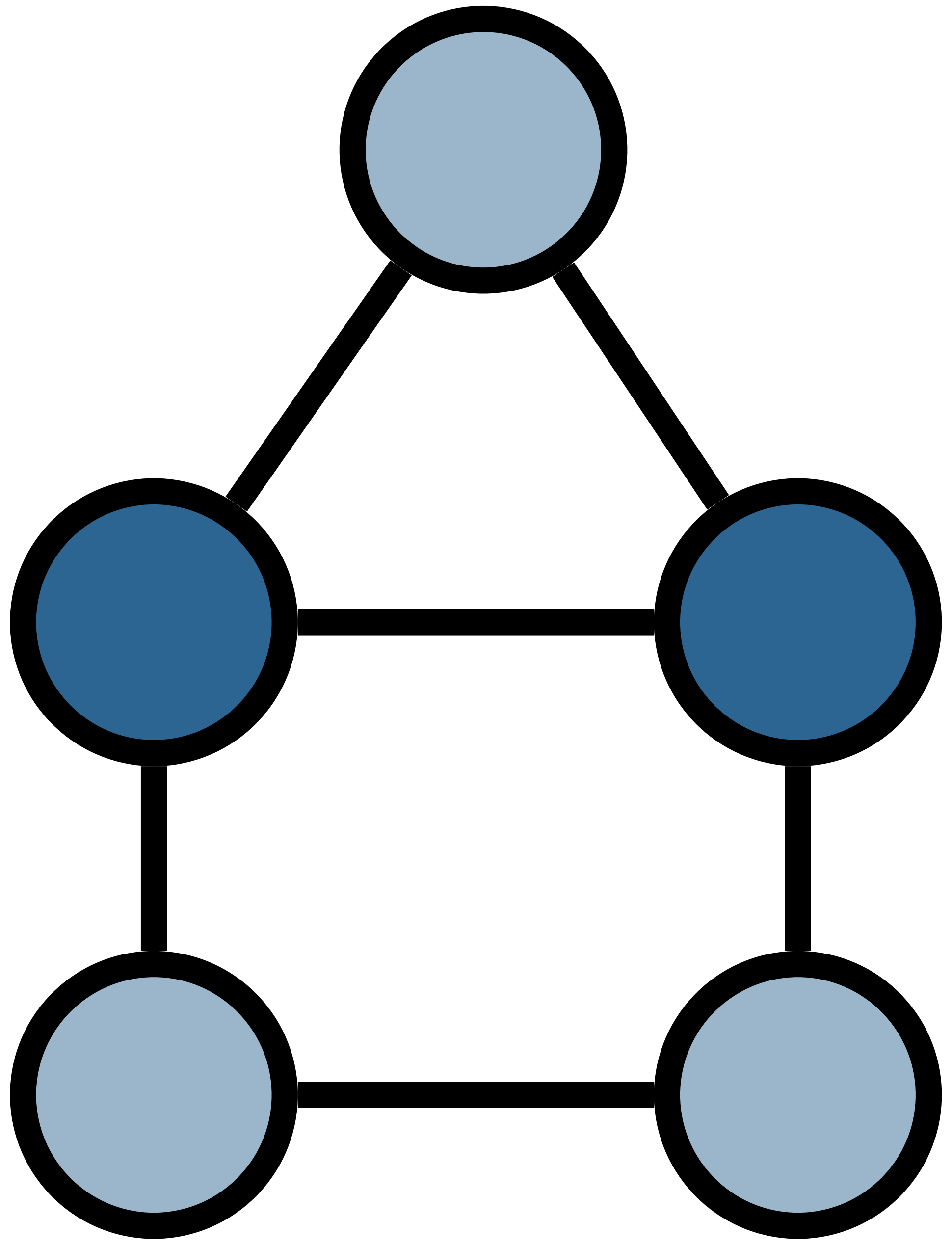
Message Passing



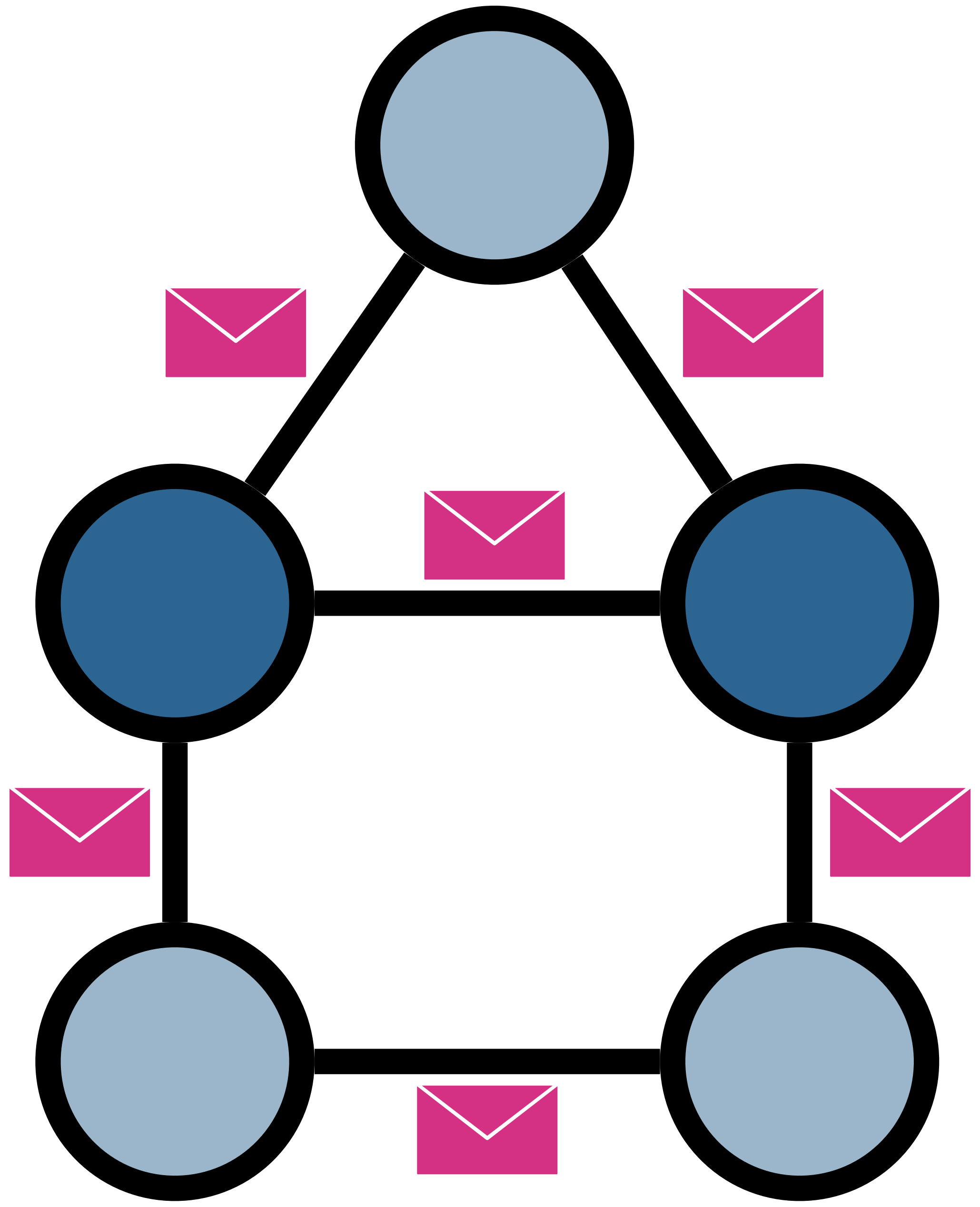
Message Passing



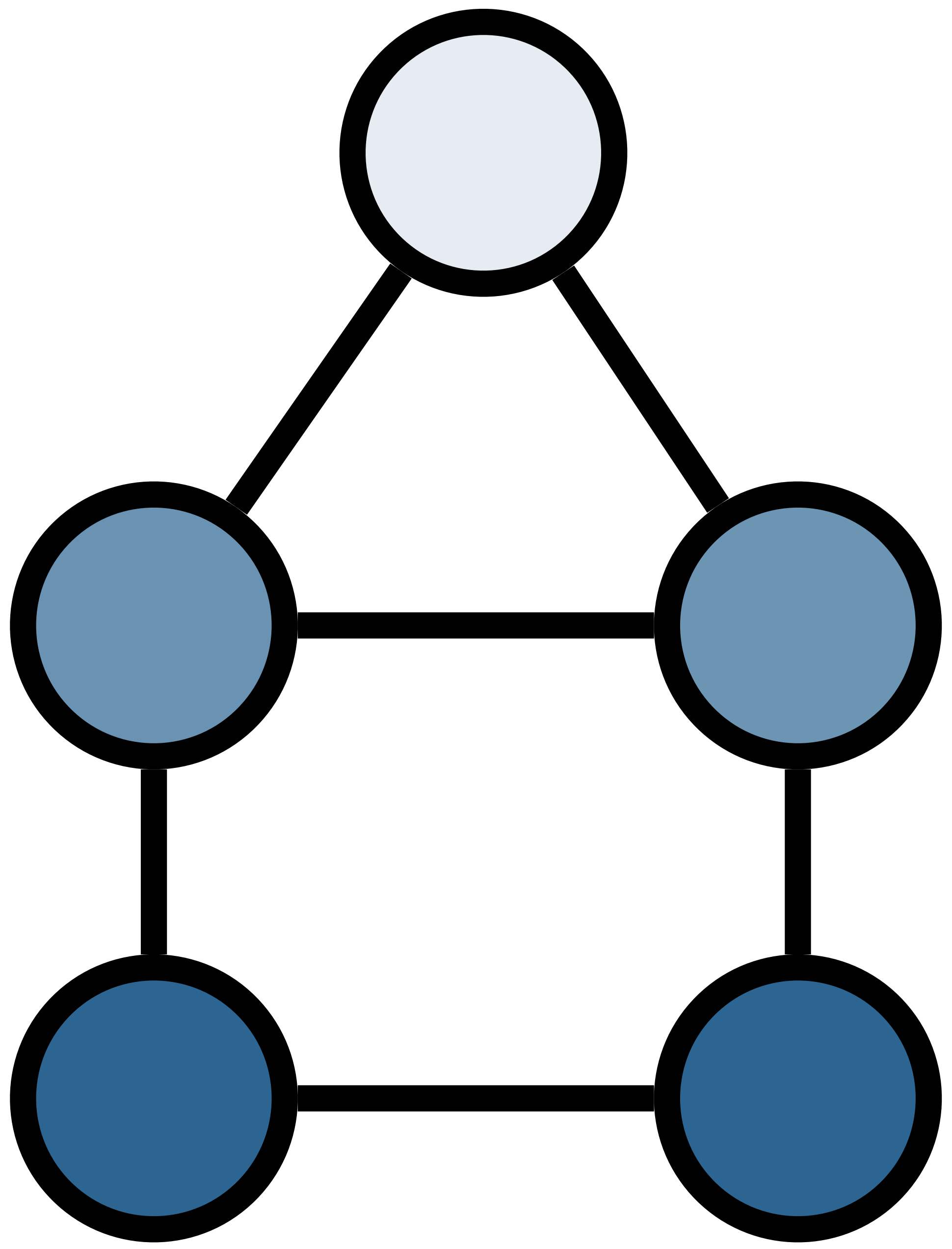
Message Passing



Message Passing



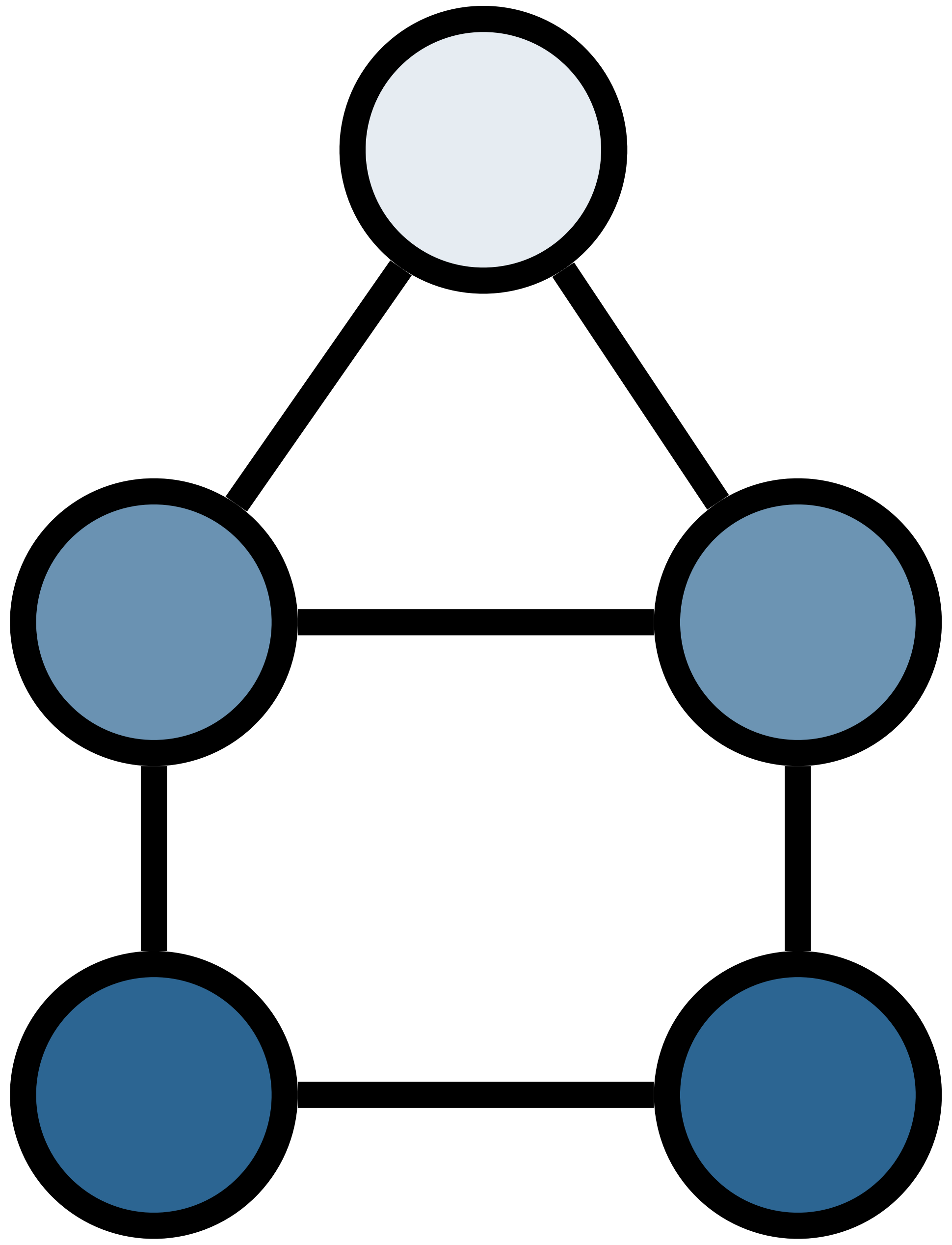
Message Passing



- Input graphs of arbitrary size.
- Isomorphic graphs are guaranteed to produce the same results.

- Pair-wise relations expensive.
- Not very powerful (in their vanilla form)

Message Passing



?

Do we really need *message passing* to capture the topology of a graph?

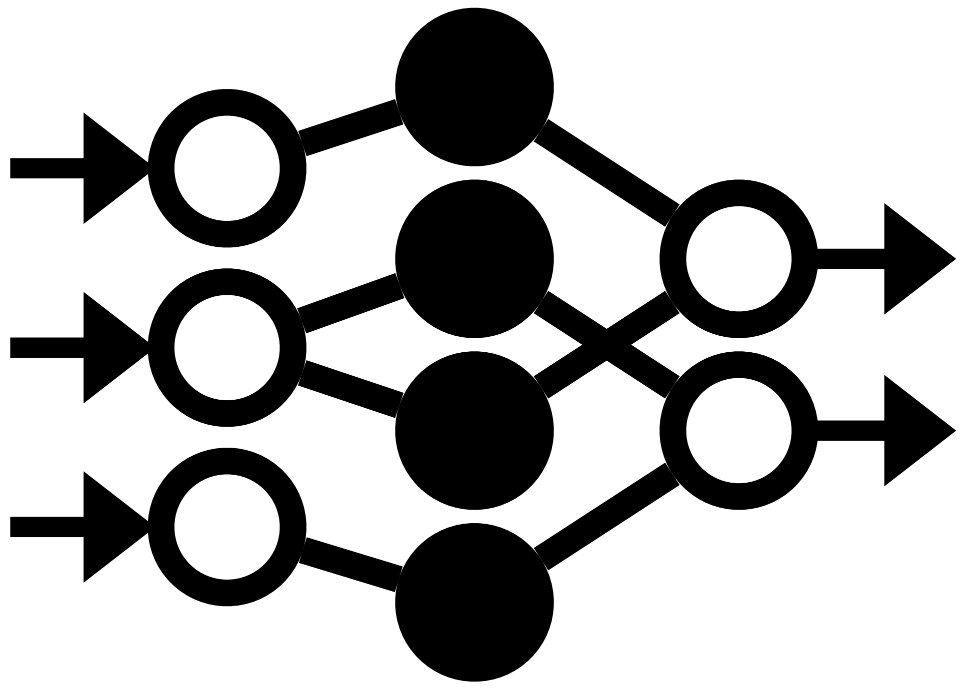
Part II

DEEP SETS

Deep Sets

Deep Sets are neural networks that operate on (multi)sets.

$\{1,2,3,4\}$

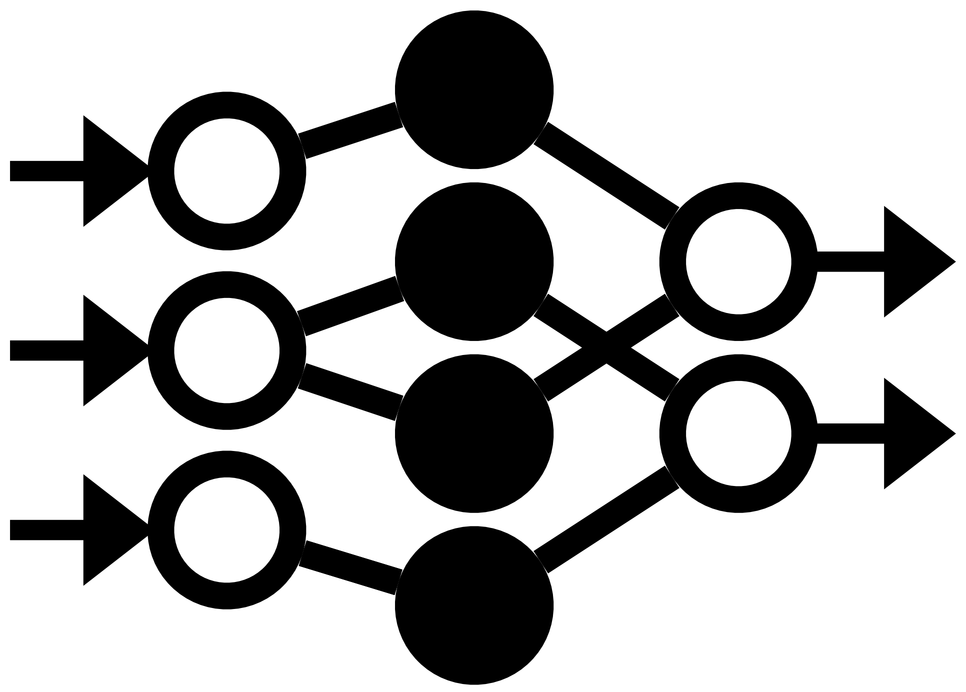


Contains the Number 5

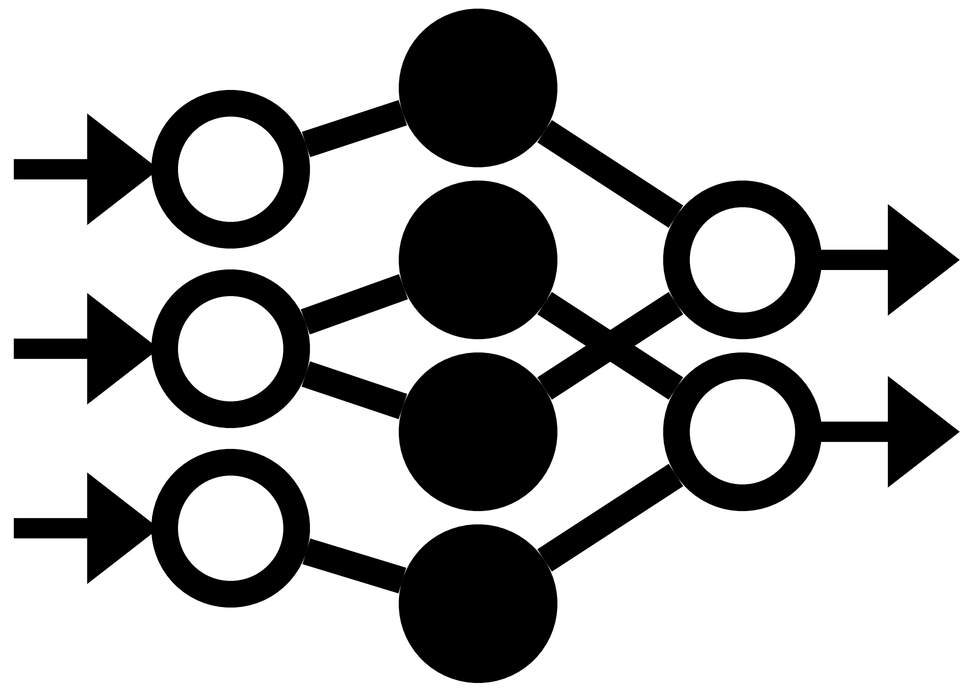
Deep Sets

Deep Sets are neural networks that operate on (multi)sets.

[1,2,3,4]

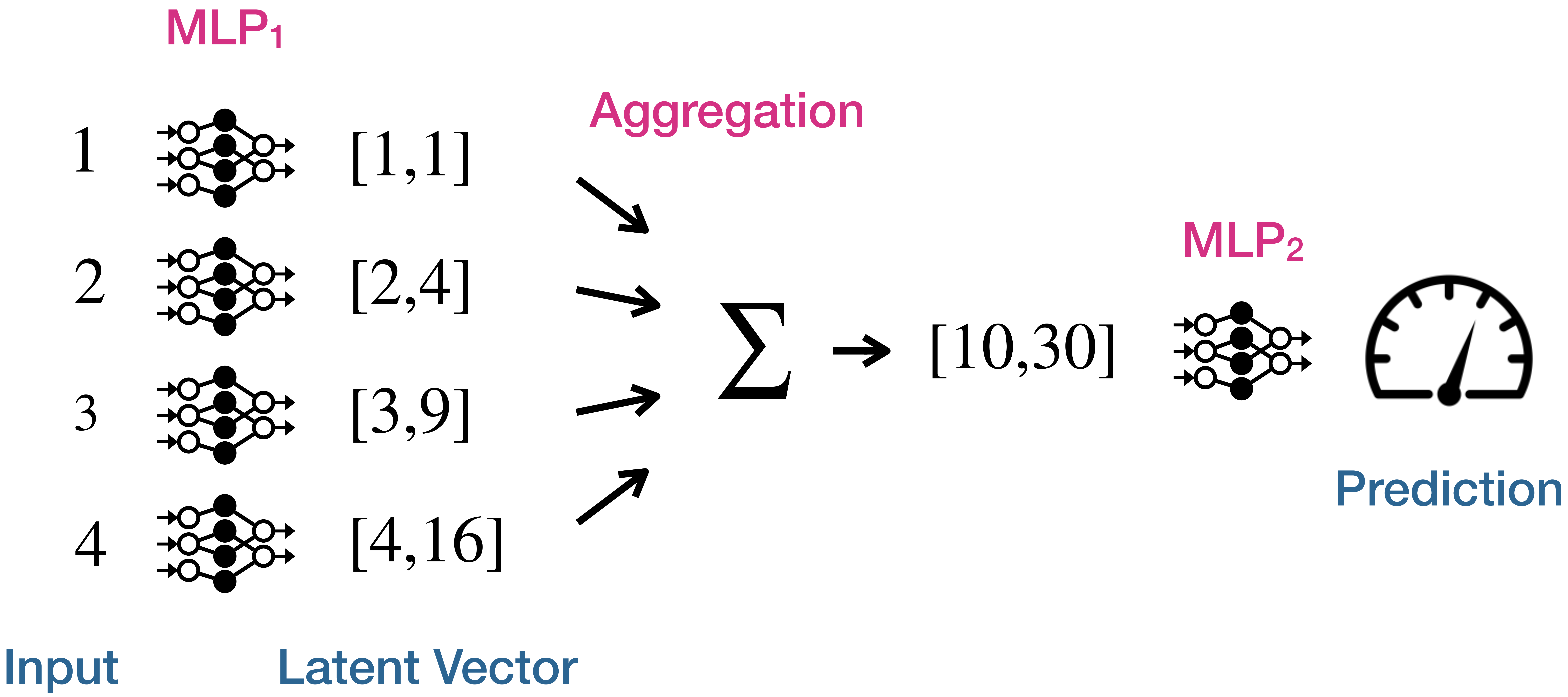


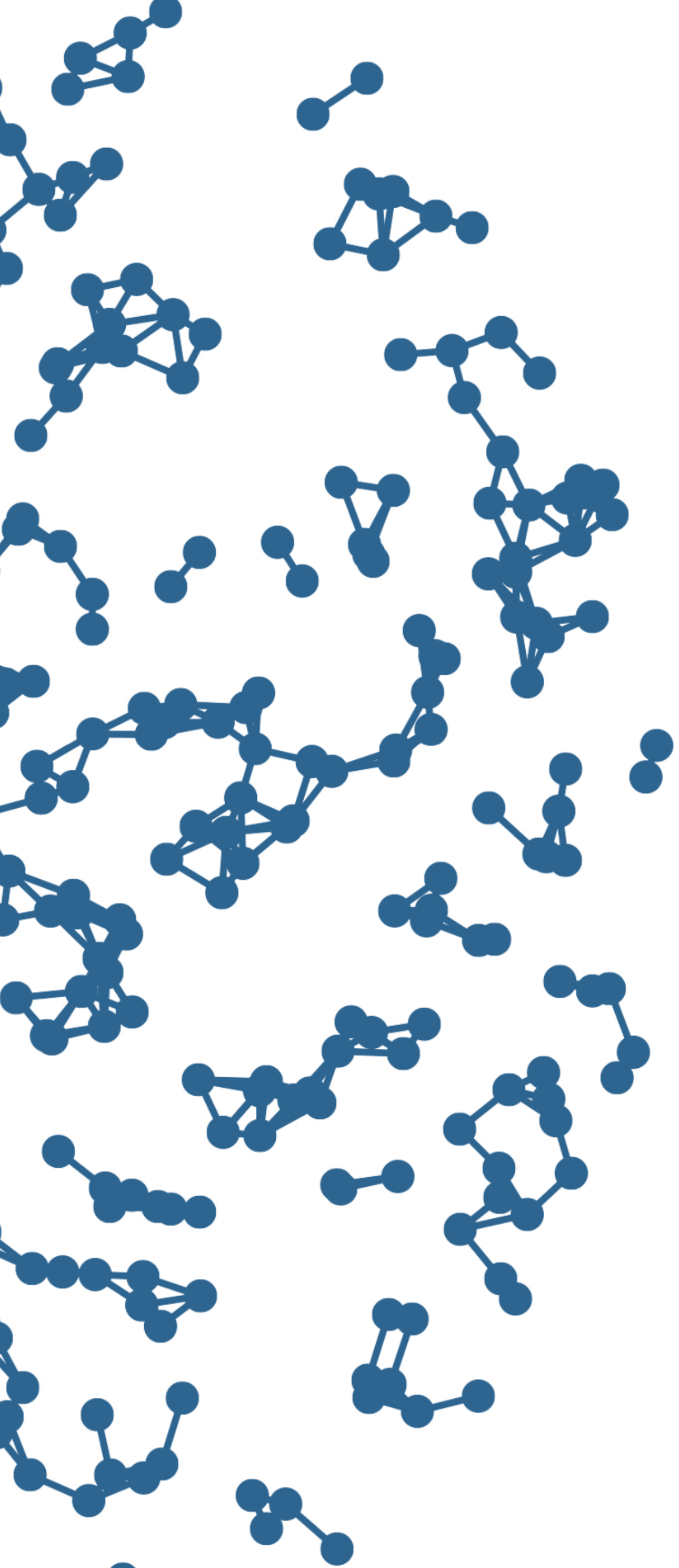
[4,3,1,2]



Guaranteed to produce the same results.

Deep Sets

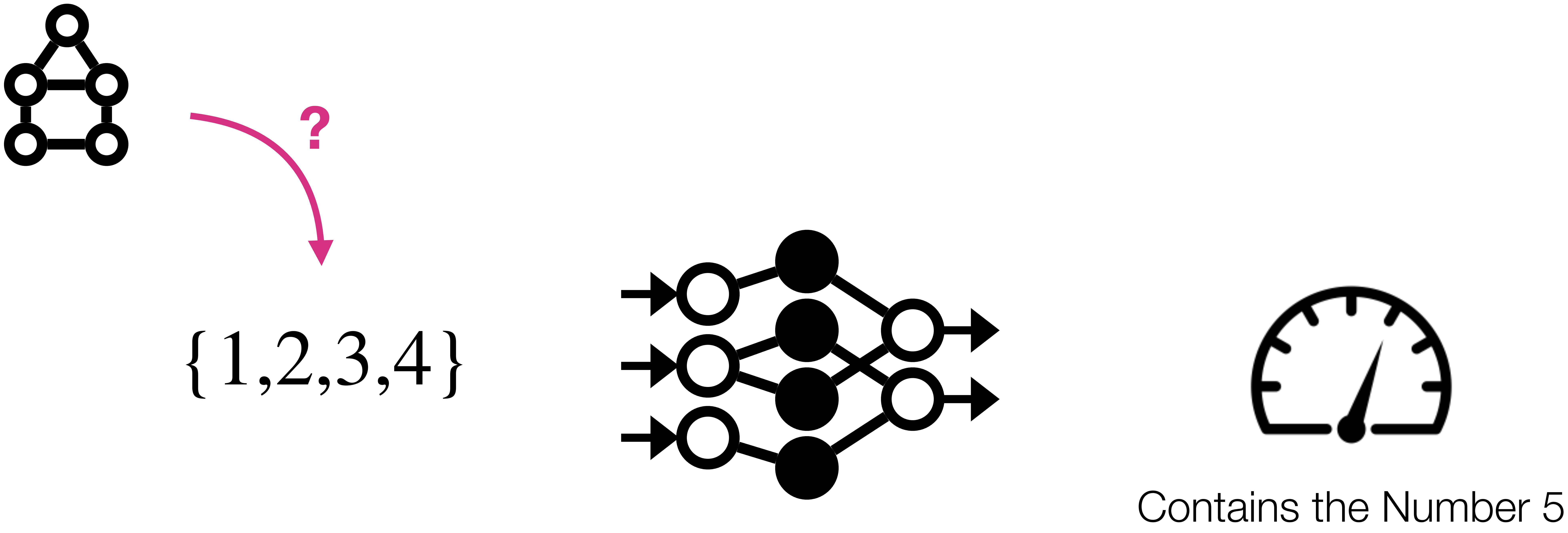

MLP$_1$
Aggregation
1
2
3
4
[1,1]
[2,4]
[3,9]
[4,16]
$\sum$
[10,30]
MLP$_2$
Prediction
Input
Latent Vector



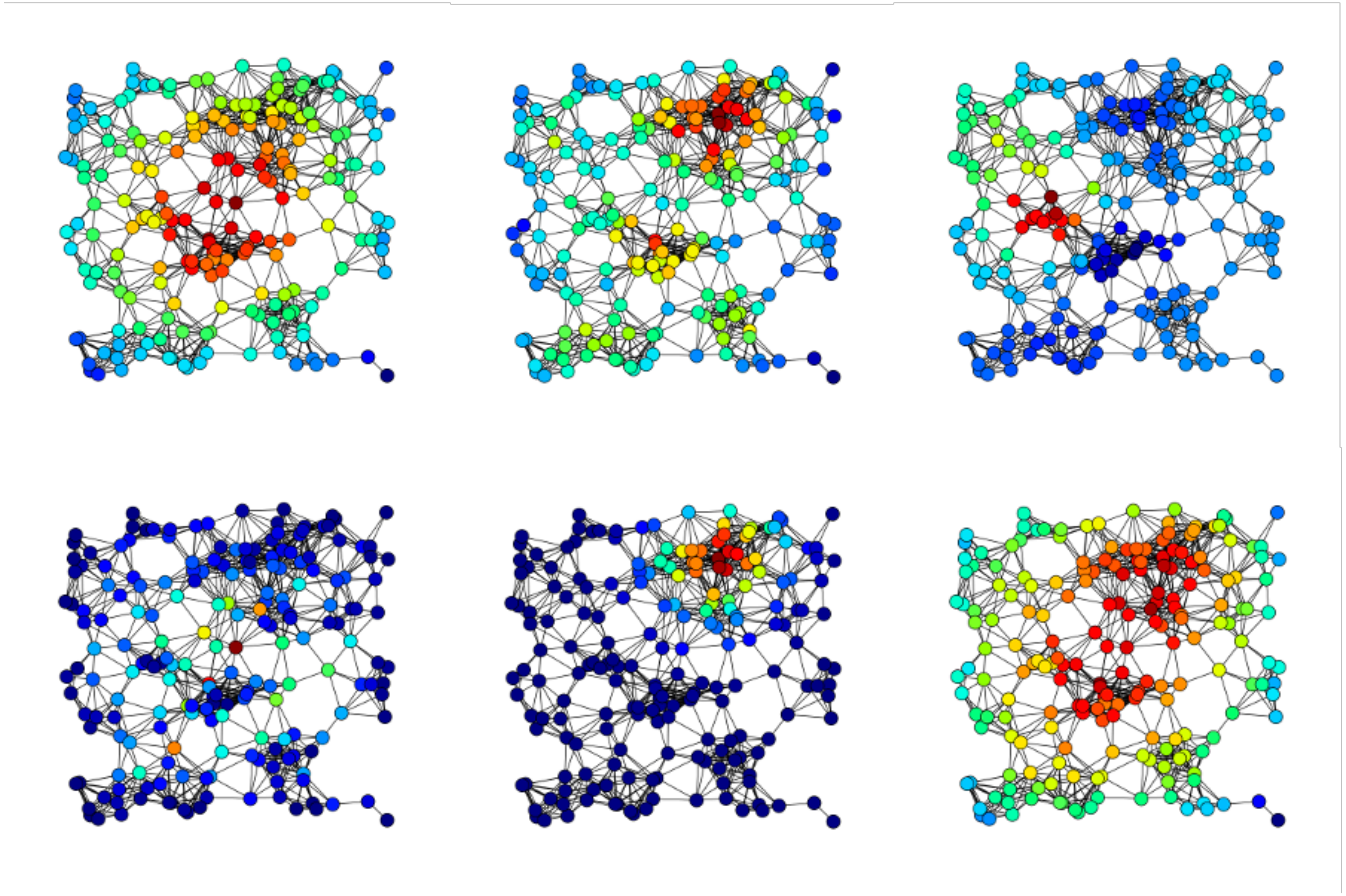
Part III

DEEP SETS ON GRAPHS

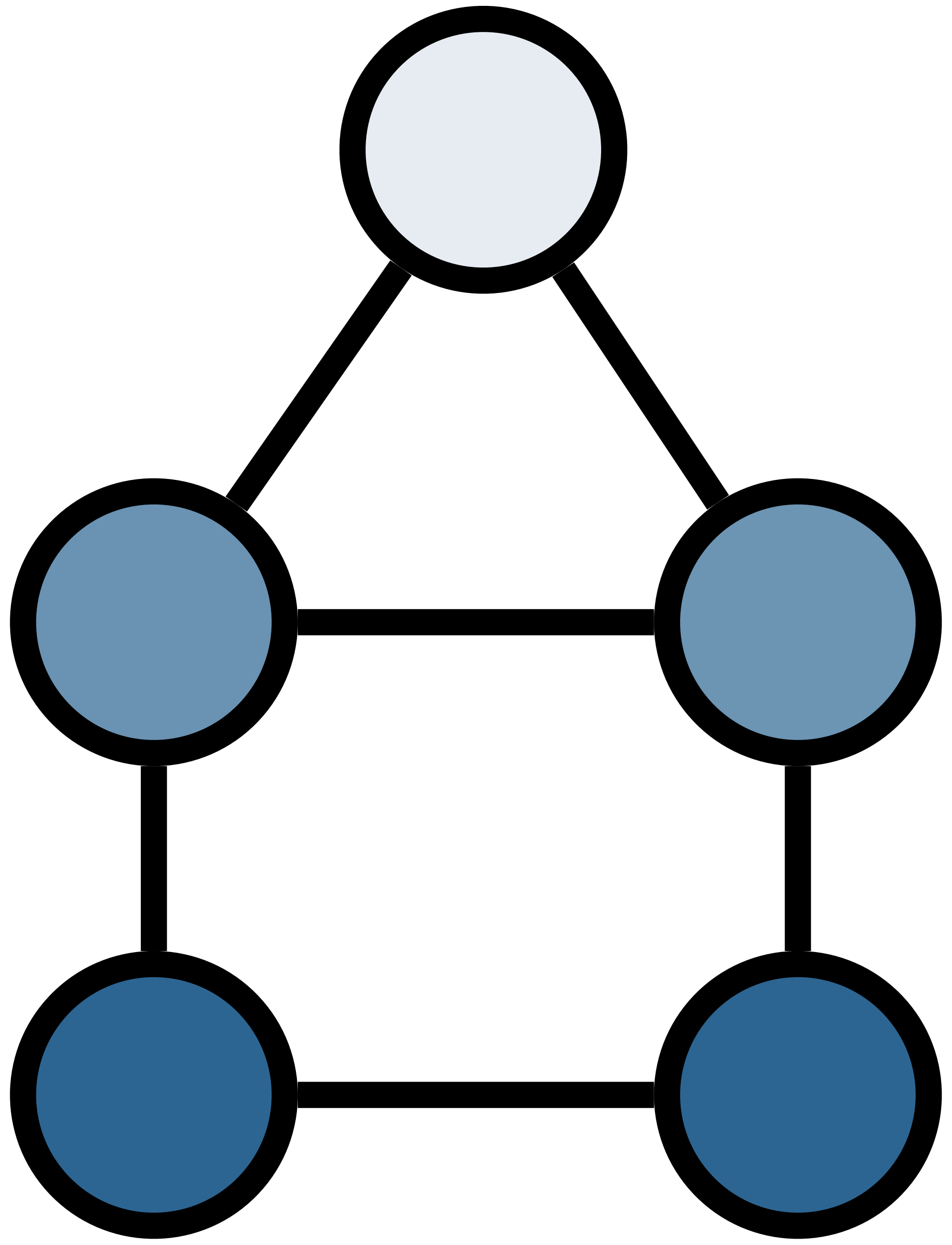
Deep Sets on Graphs



Centrality



Message Passing

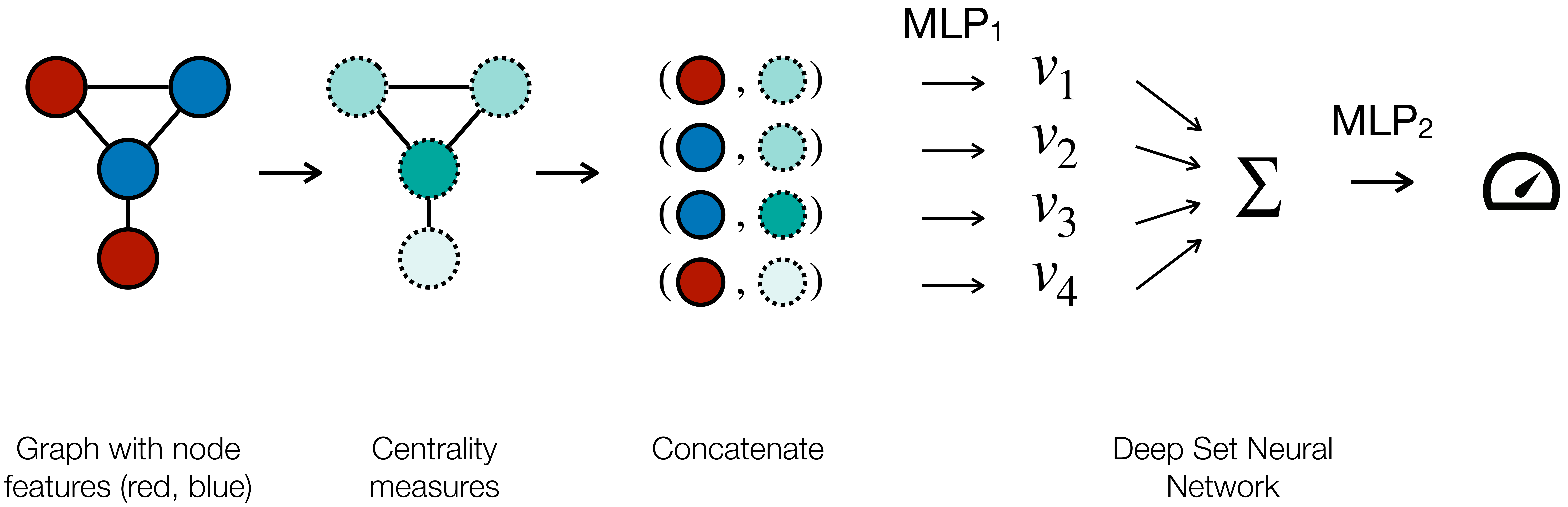


?

Do we really need *message passing* to capture the topology of a graph?

Maybe *centrality measures* are enough?

Deep Sets



MLP1
v_1
v_2
v_3
v_4
Σ
MLP2
Graph with node features (red, blue)
Centrality measures
Concatenate
Deep Set Neural Network

Part IV

EXPRESSIVENESS

Expressiveness

Expressiveness of GNNs is measured by their ability to distinguish non-isomorphic graphs

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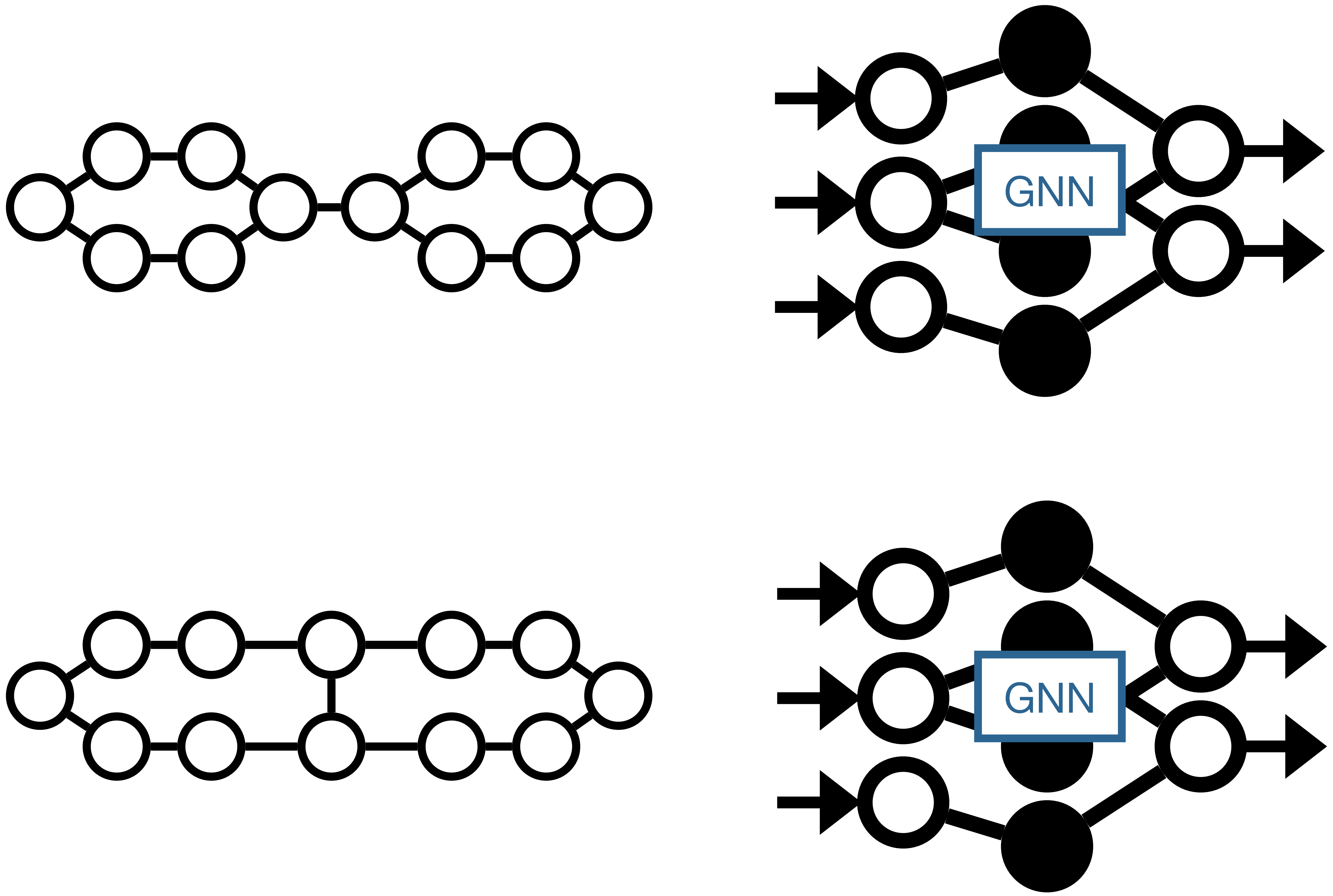
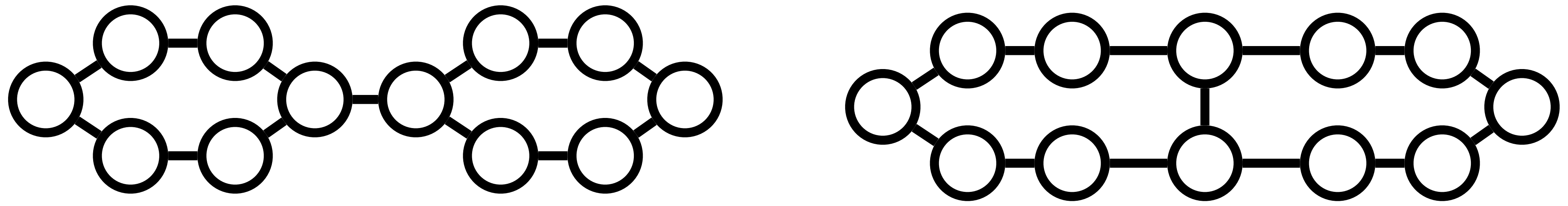


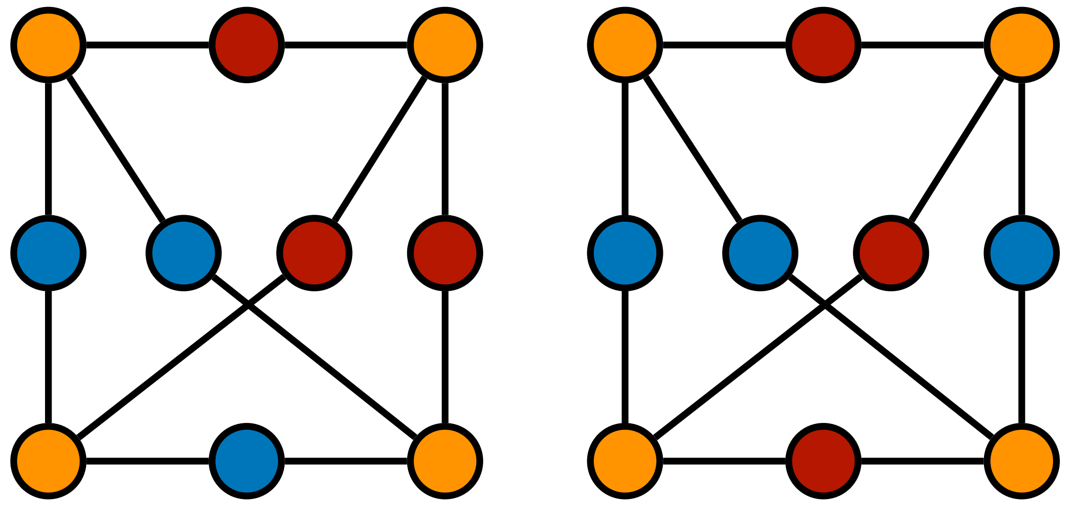
Guaranteed to produce the same results.

Expressiveness

Deep Sets can distinguish graphs that GNNs cannot:



GNNs can distinguish graphs that Deep Sets cannot:



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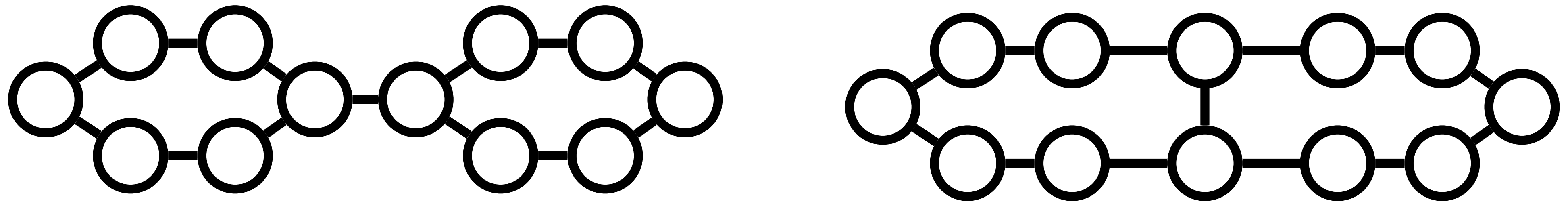

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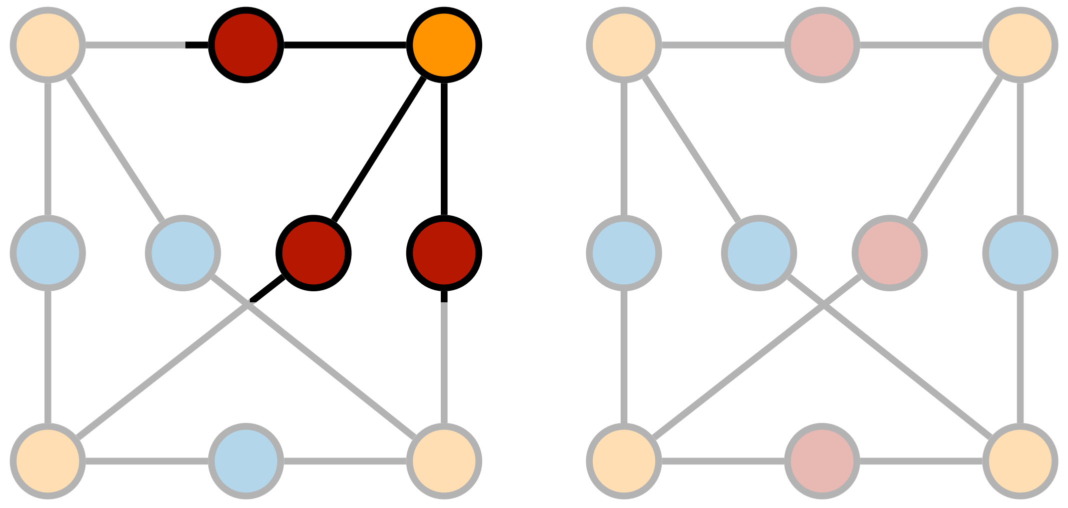

Yellow node with three **red** neighbors
exists only in one of them.

Expressiveness

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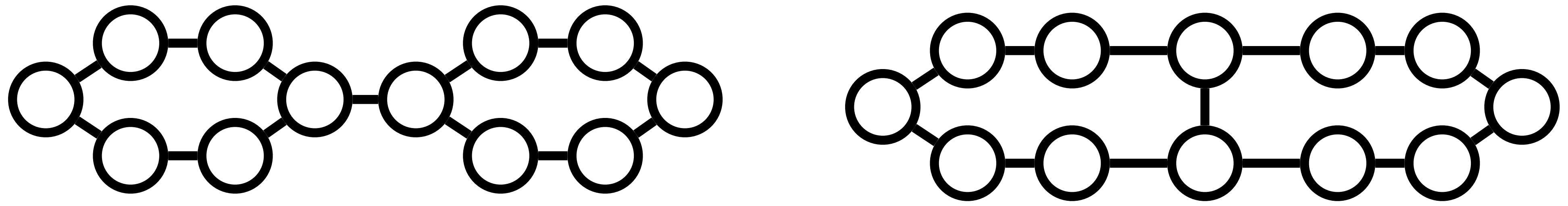

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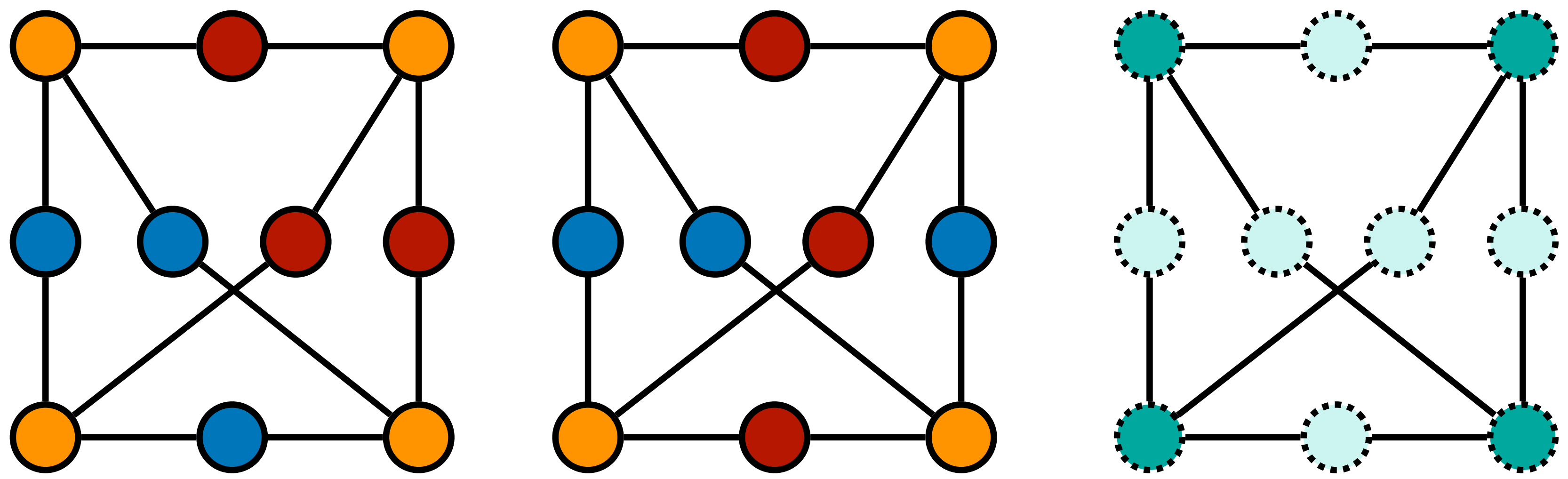

Same centralities
for both graphs

Expressiveness

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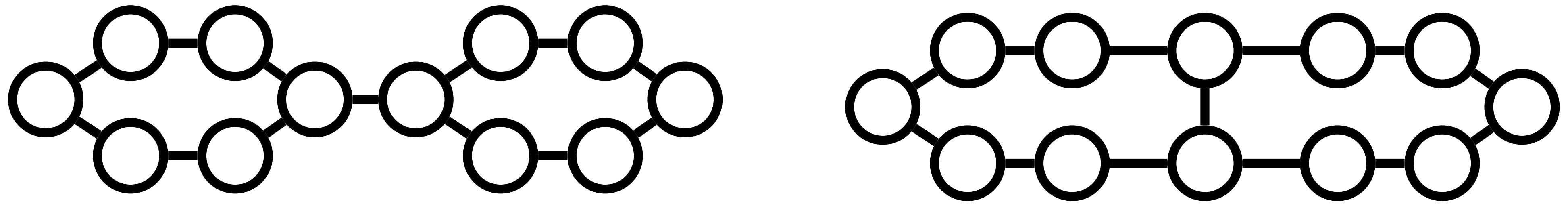

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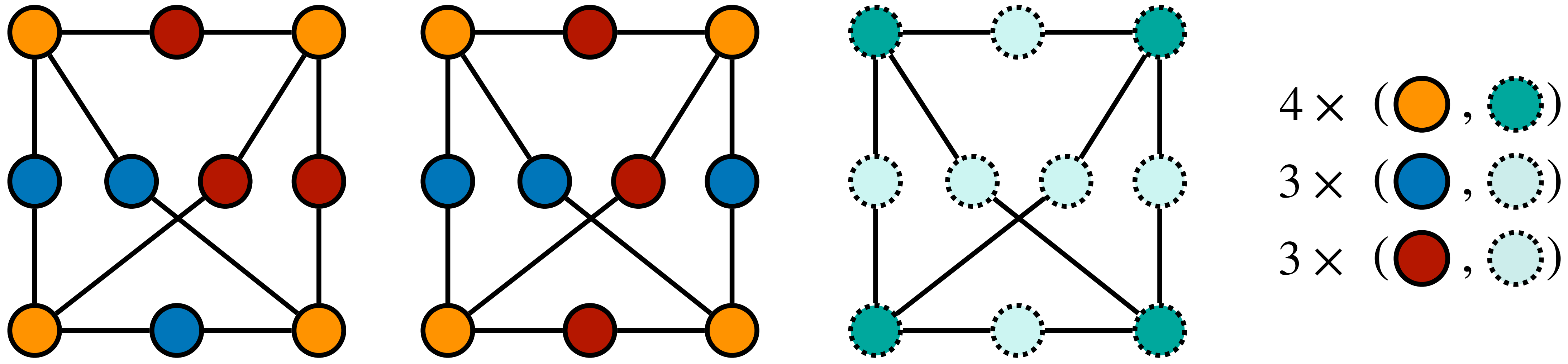

Same multiset
for both graph

Expressiveness

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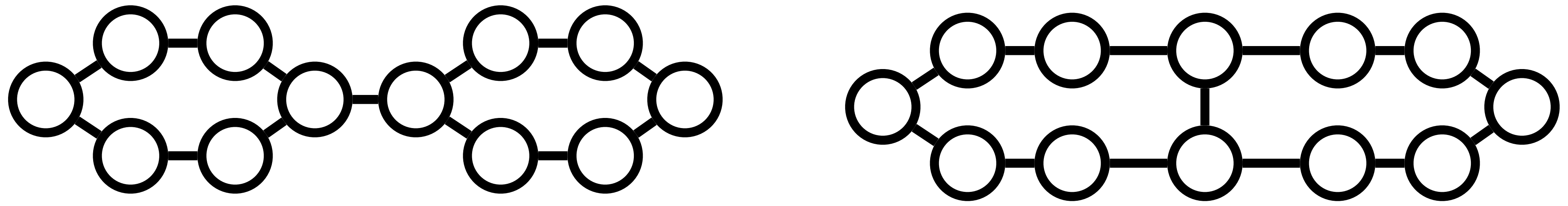
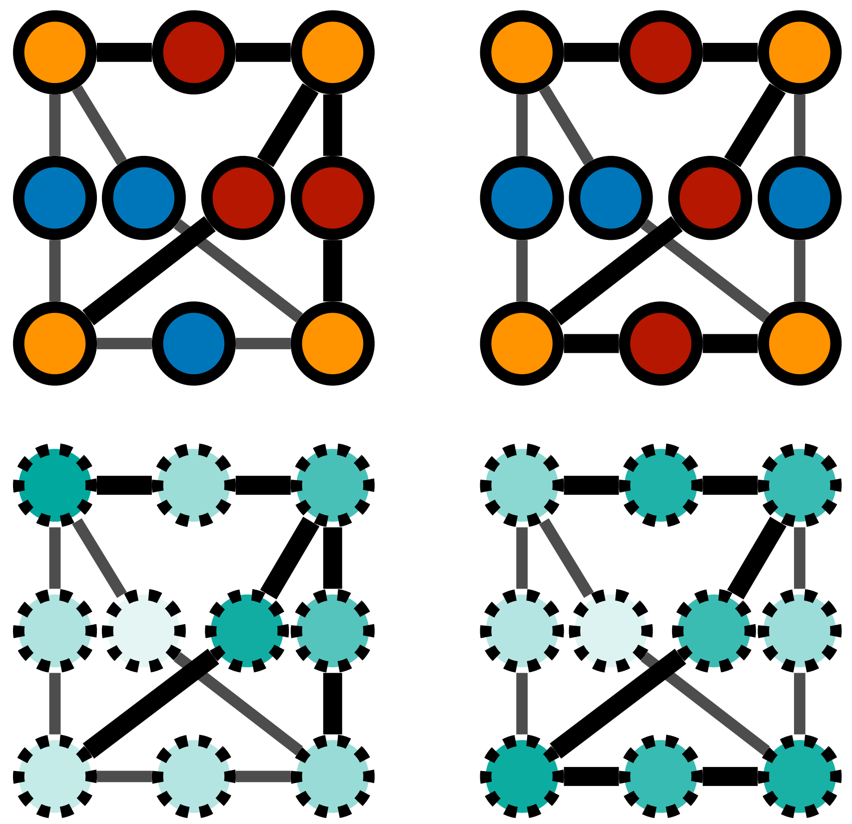


GNNs can distinguish graphs that Deep Sets cannot:

Potential solution:
Make centrality aware of
node-features



Expressiveness

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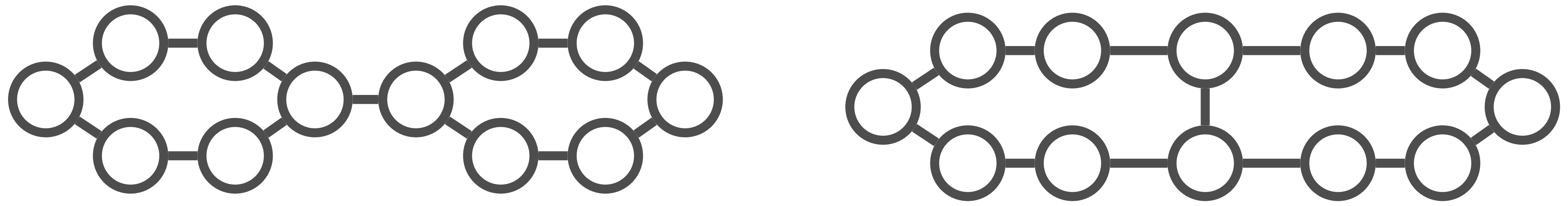

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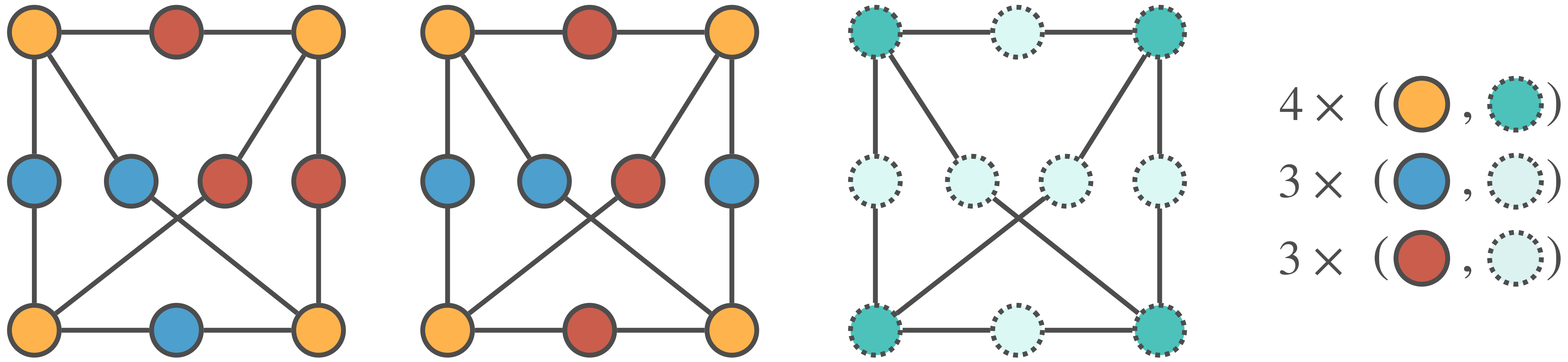


Open Problem: Exact position in the Weisfeiler-Lehman hierarchy

Part V

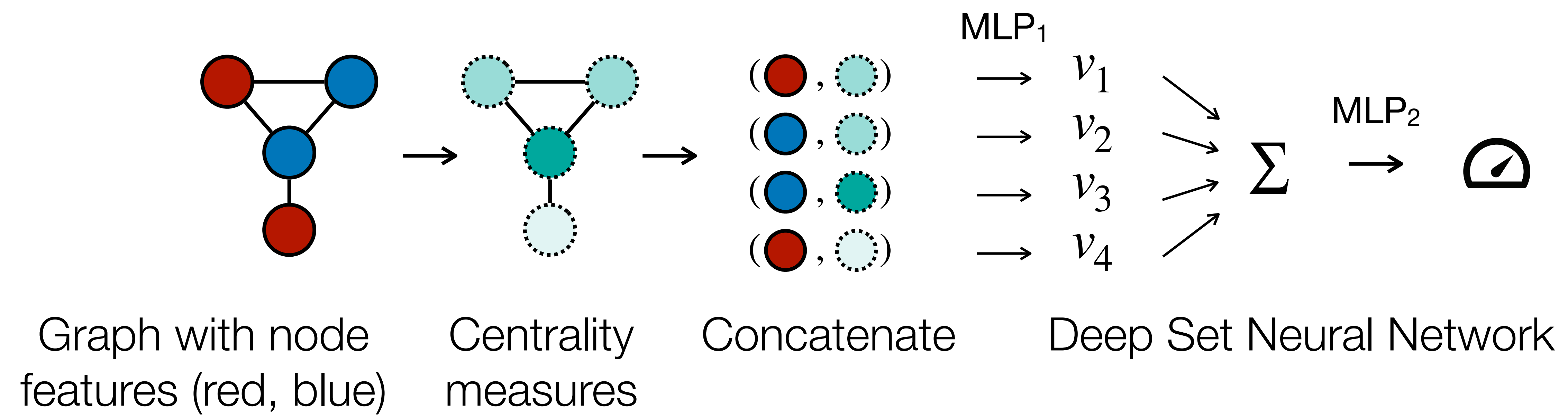
RESULTS

Results

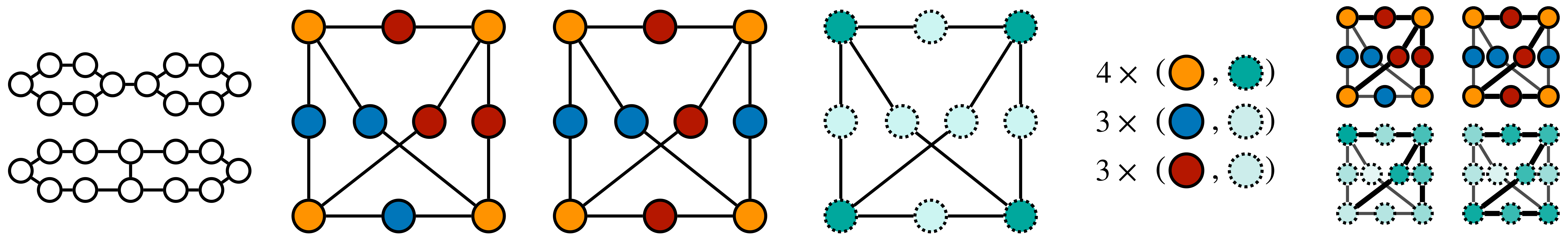
Dataset	DSNN	GCN	GIN	PNA	SOTA	$\oslash$ # N	$\oslash$ # E	# G
PROTEIN	0.74 ± 0.01	0.65 ± 0.01	0.61 ± 0.02	0.59 ± 0.04	0.85	39.1	145.6	1113
MUTAG	0.80 ± 0.06	0.55 ± 0.06	0.79 ± 0.04	0.52 ± 0.00	1.0	17.9	39.6	188
ENZYMES	0.40 ± 0.10	0.25 ± 0.01	0.34 ± 0.04	0.28 ± 0.04	0.78	32.6	124.2	600
IMBD-BINARY	0.72 ± 0.02	0.49 ± 0.44	0.52 ± 0.08	0.63 ± 0.02	0.96	19.8	193.1	1000

Concluding Remarks

Method:



Expressiveness:



Different graphs with same multiset representation

Open Problems:

- Expressive power of centralities?
- Which centrality measures work best and why?
- Use set of edges instead?