THE UNIVERSITY OF BRITISH COLUMBIA

Topics in AI (CPSC 532S):
Multimodal Learning with Vision, Language and Sound

Lecture 19: Generative Models [part 4]

Logistics

Research Paper Presentations:

— Papers are assigned last week (do not need to do one if you’re auditing)

— Presentations by Friday, **November 25th**

Research Paper Readings:

— Paper 2 is posted due Thursday

— Paper 3 & 4 of your choosing one per week

Logistics

Grading

— Assignment 3 & 4 being graded this week

— Project proposal documents will not be graded until later (do not wait for these)

Plans for the rest of term

— **Option 1**: Project presentations in Class (Dec 1 & 6), alt Dec 12 or 13

— **Option 2**: Discussion of research papers

— **Option 3**: I continue to lecture on additional topics

Generative Models — Overview

Pixel CNN/RNN — An explicit tractable density model. Accurate, easy to train but no latent variables.

VAE — An intractable density model with latent variables. Marginalizes the latent variables, but can only optimize the lower bound.

GANs — No explicit density model, just focused on sampling.

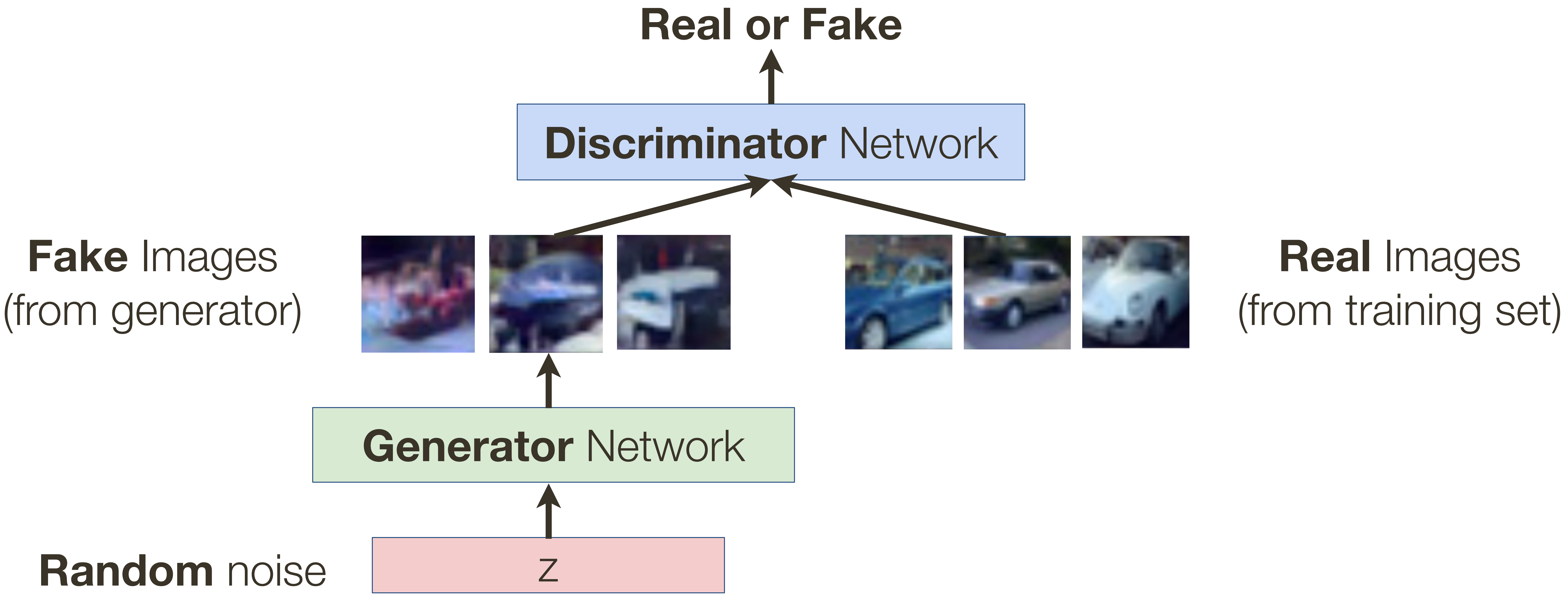
Diffusion Models — No explicit density model, similar to GANs in many ways.

Generative Adversarial Networks (GANs)

Training GANs: Two-player Game

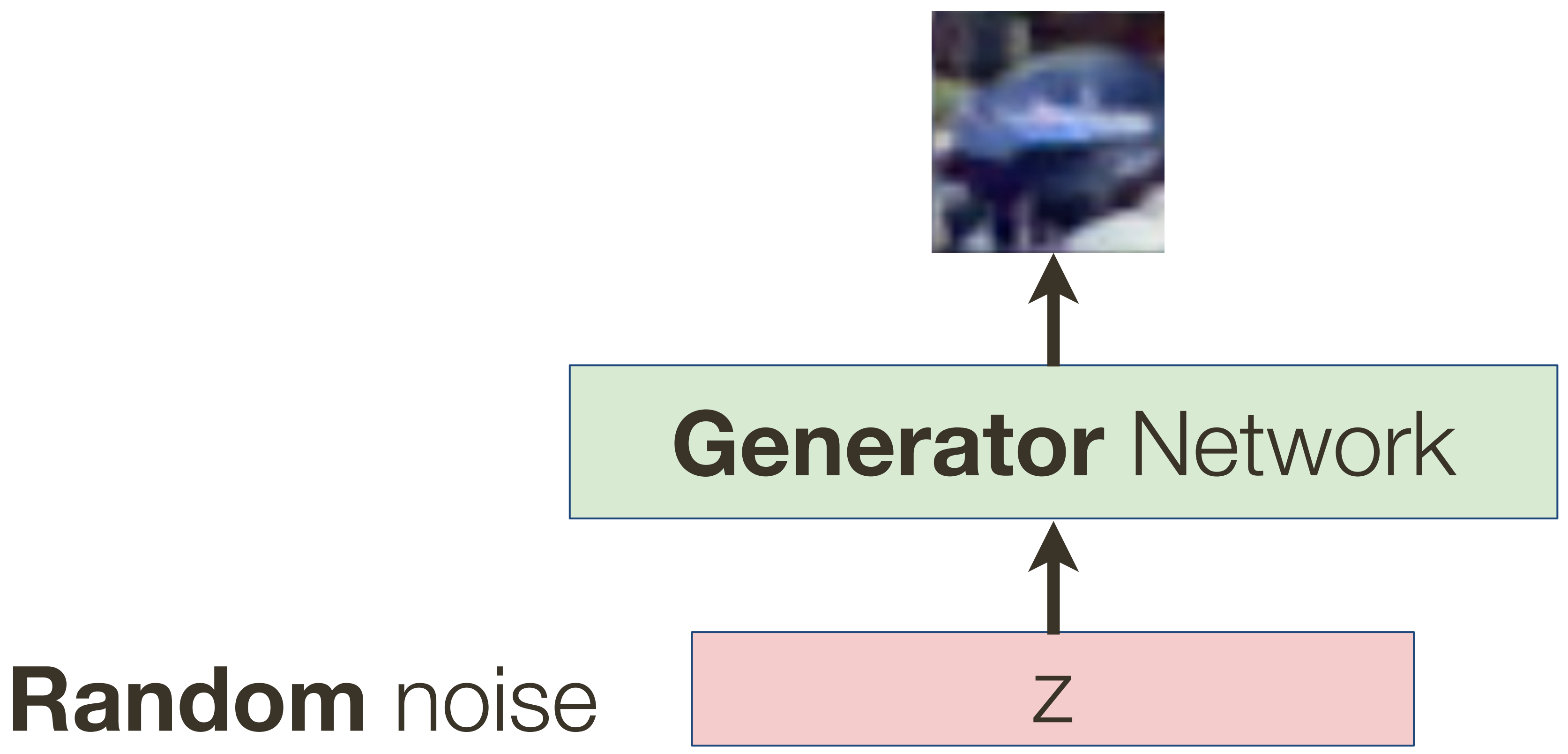
[Goodfellow et al., 2014]

Generator network: try to fool the discriminator by generating real-looking images
Discriminator network: try to distinguish between real and fake images



* slide from Fei-Dei Li, Justin Johnson, Serena Yeung, **cs231n Stanford**

Sampling **GAN**s



* slide from Fei-Dei Li, Justin Johnson, Serena Yeung, **cs231n Stanford**

Conditional GAN: Text-to-Image Synthesis

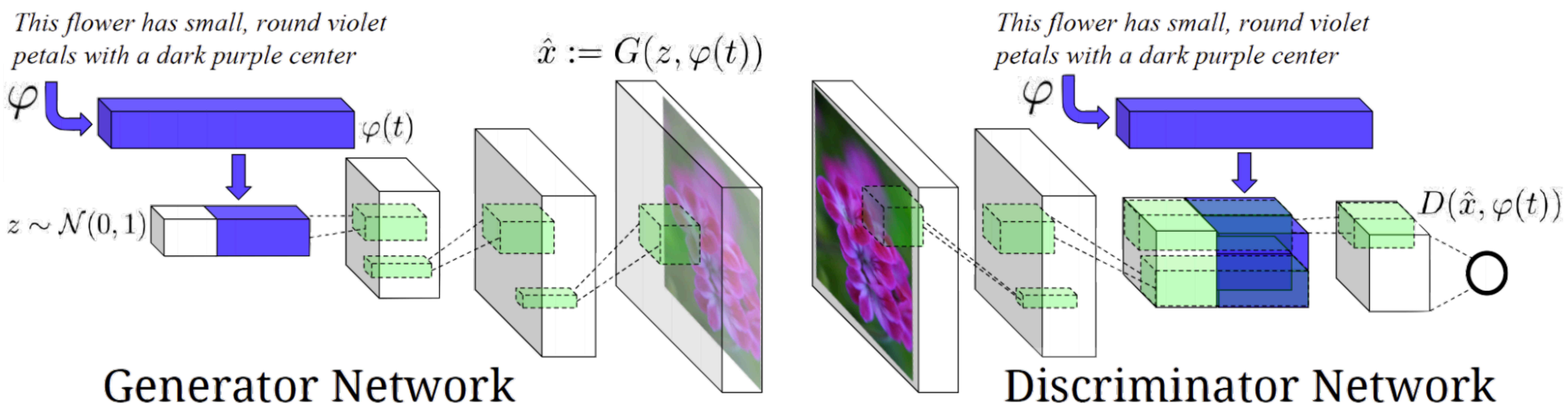


Figure 2 in the original paper.

Positive Example:

Real Image, Right Text

Negative Examples:

Real Image, Wrong Text

Fake Image, Right Text

[Reed et al., ICML 2016]

Conditional GAN: Image-to-Image translation

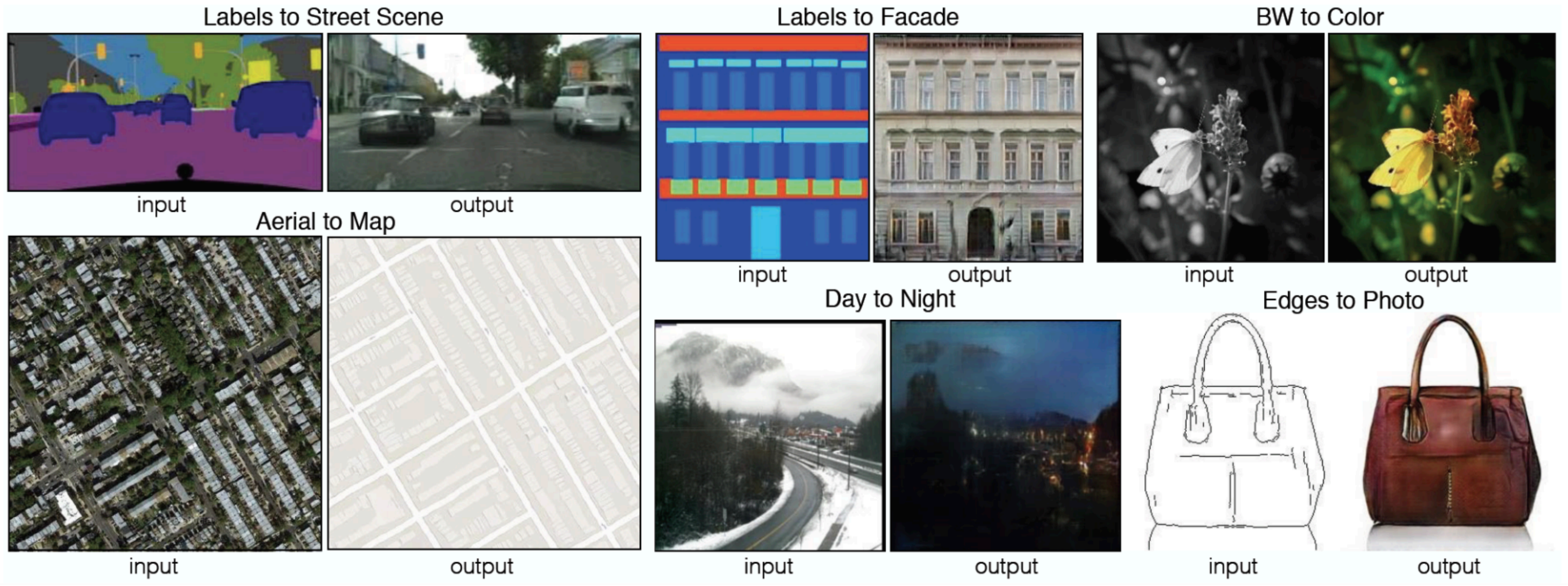


Figure 1 in the original paper.

[Isola et al., 2016]

Conditional GAN: Image-to-Image translation

Architecture: DCGAN-based

Training is conditioned on the **images from the source domain**

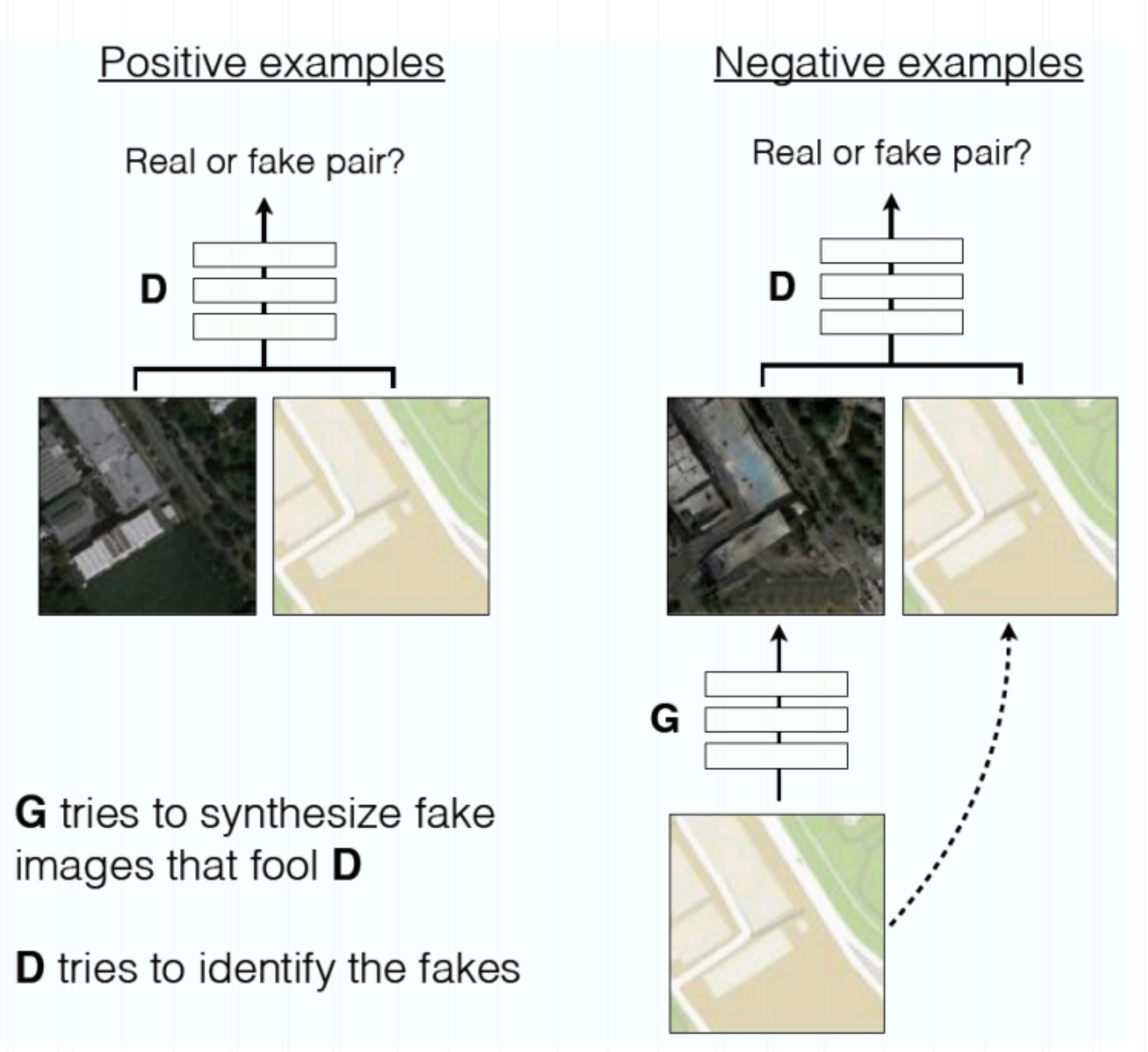
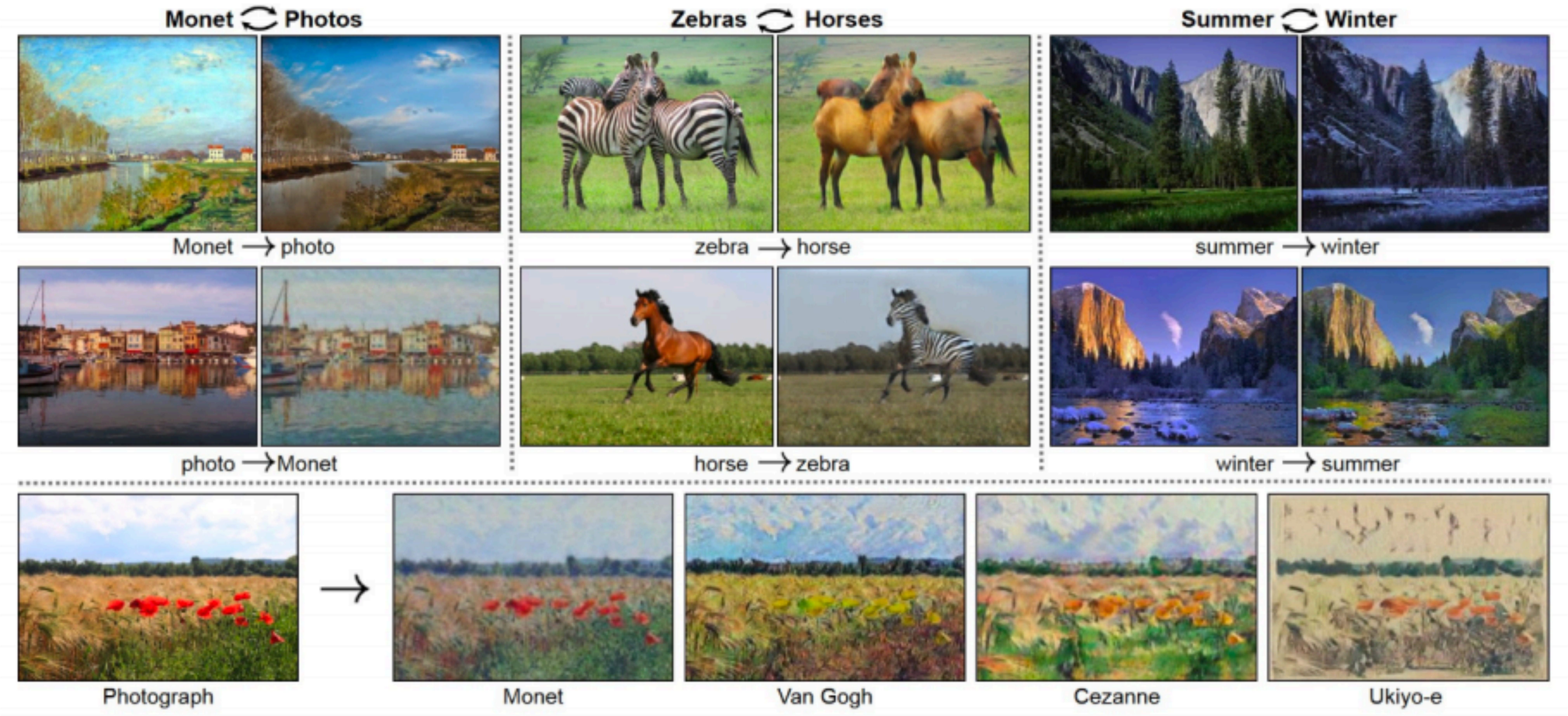


Figure 2 in the original paper.

[Isola et al., 2016]

CycleGAN: Unpaired Image-to-Image translation

Style transfer: change the style of an image while preserving the content



Data: two unrelated collections of image, one for each style

[Zhu et al., 2017]

CycleGAN: Unpaired Image-to-Image translation

Style transfer: change the style of an image while preserving the content

— Train **two different generator networks** to go from Style 1 to Style 2 and vice versa

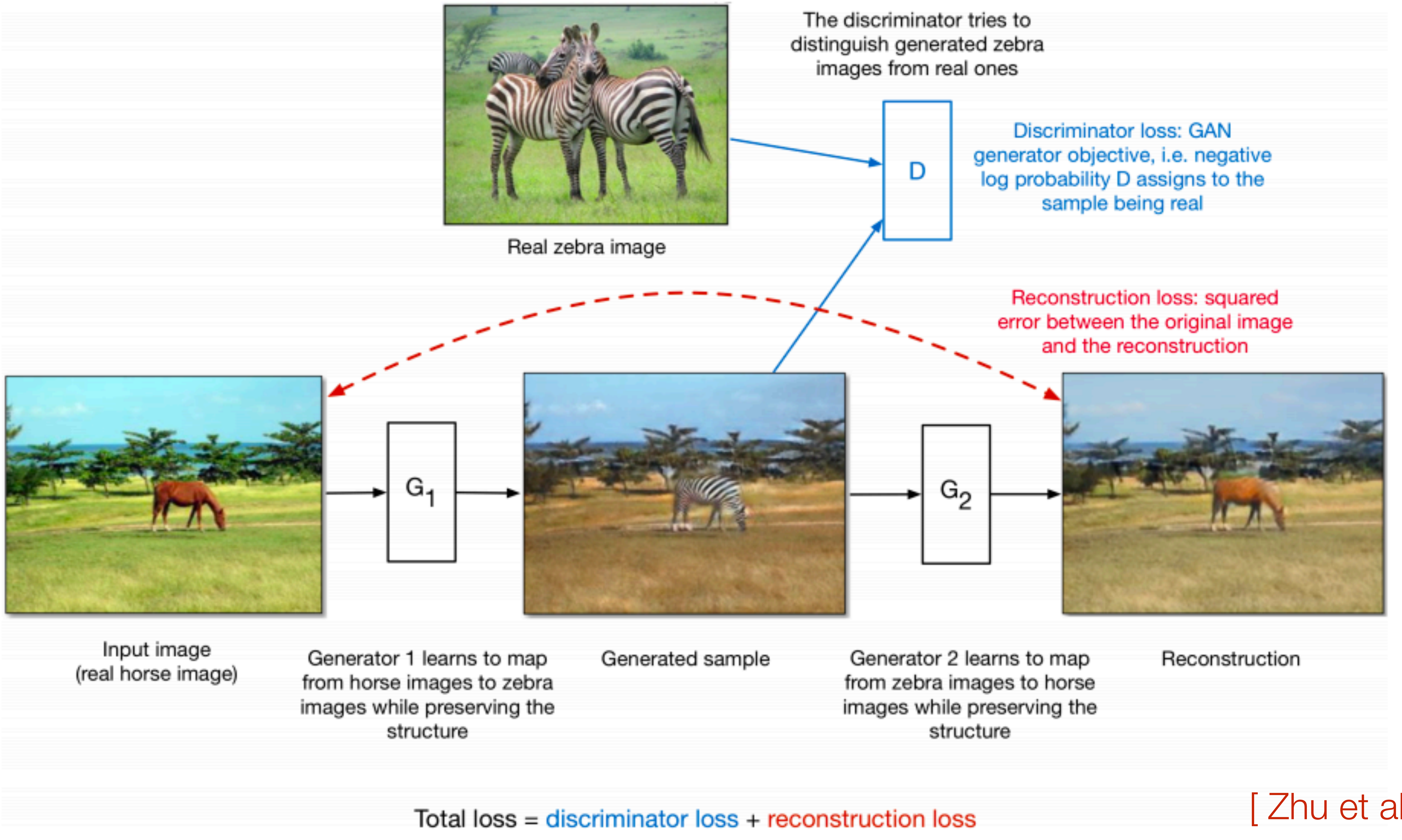
— Make sure the generated (translated) samples of Style 2 are indistinguishable from real images of Style 2 by a discriminator network

— Make sure the generated (translated) samples of Style 1 are indistinguishable from real images of Style 1 by a discriminator network

— Make sure the generators are **cycle-consistent**: mapping Style1 -> Style 2 -> Style 1 should give close to the original image

[Zhu et al., 2017]

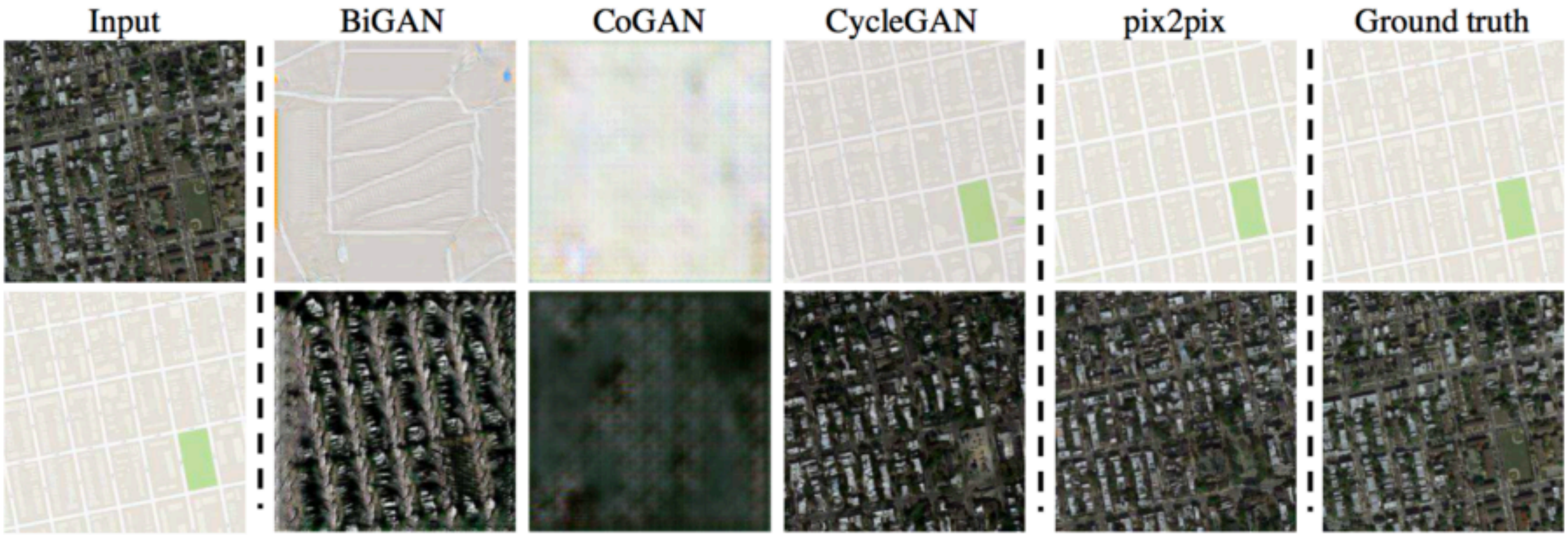
CycleGAN: Unpaired Image-to-Image translation



[Zhu et al., 2017]

CycleGAN: Unpaired Image-to-Image translation

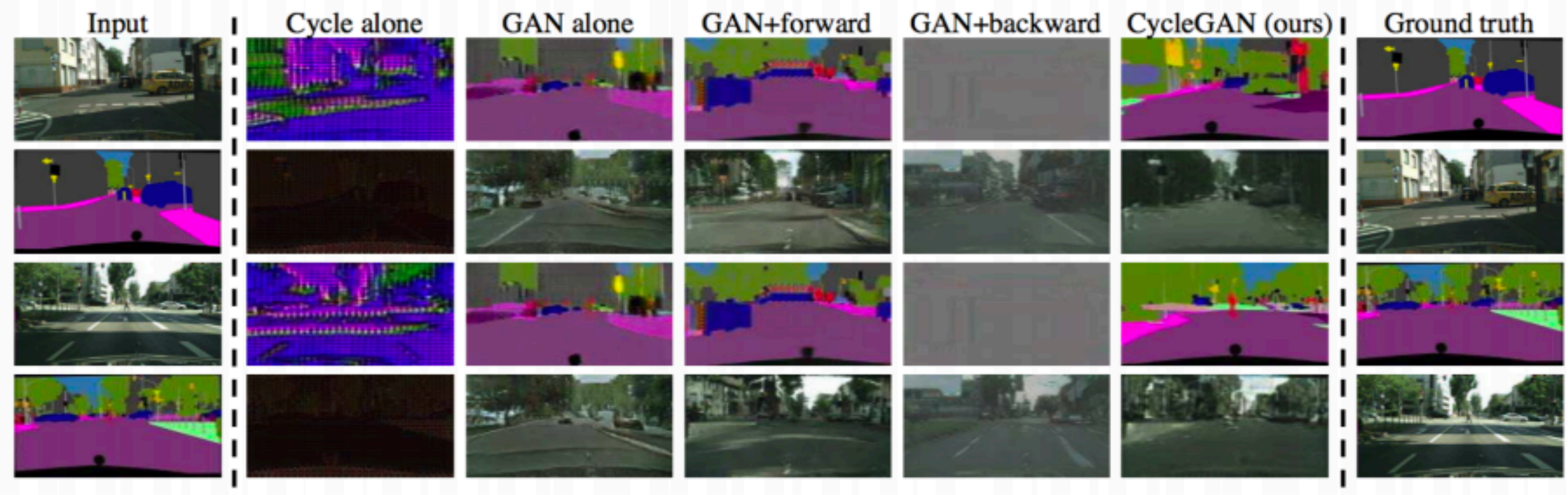
Ariel photos to **maps:**



[Zhu et al., 2017]

CycleGAN: Unpaired Image-to-Image translation

Images to **semantic segmentation:**



[Zhu et al., 2017]

Laplacian Pyramid GAN

Building a **Laplacian Pyramid** — a loss-less hierarchical representation of image

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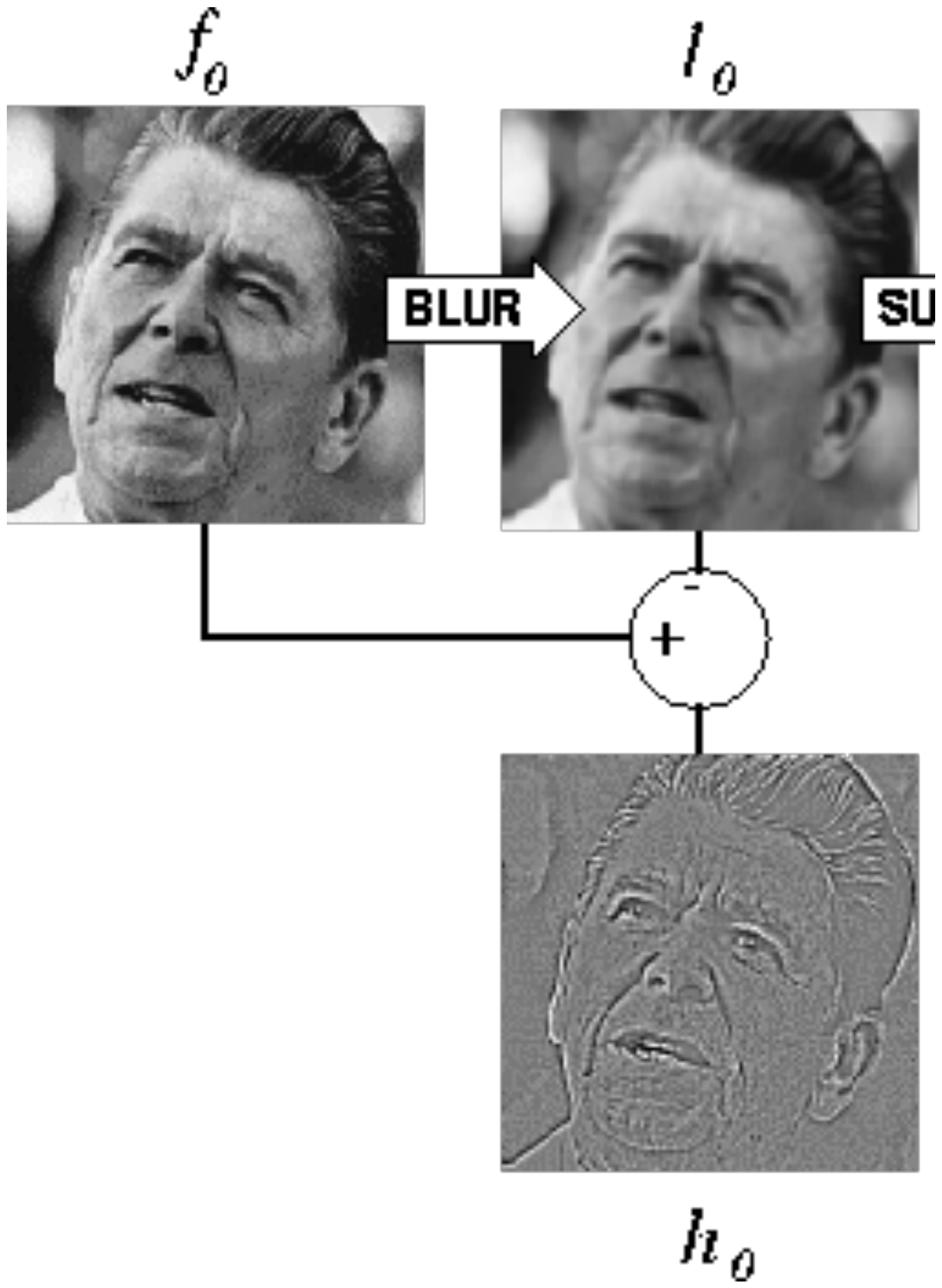
Laplacian Pyramid GAN

Building a **Laplacian Pyramid** — a loss-less hierarchical representation of image

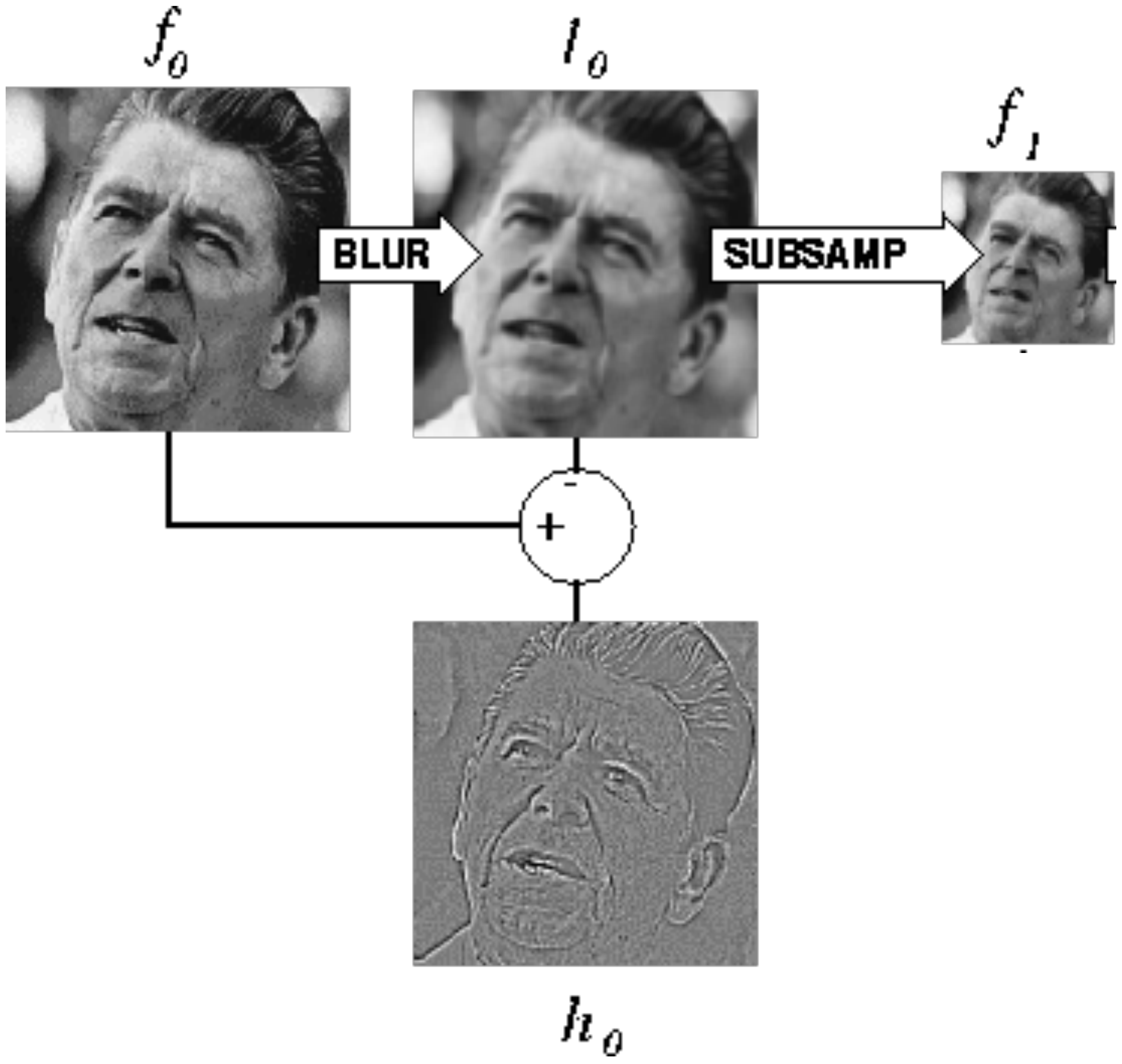
Laplacian Pyramid GAN

Building a **Laplacian Pyramid** — a loss-less hierarchical representation of image



Laplacian Pyramid GAN

Building a **Laplacian Pyramid** — a loss-less hierarchical representation of image



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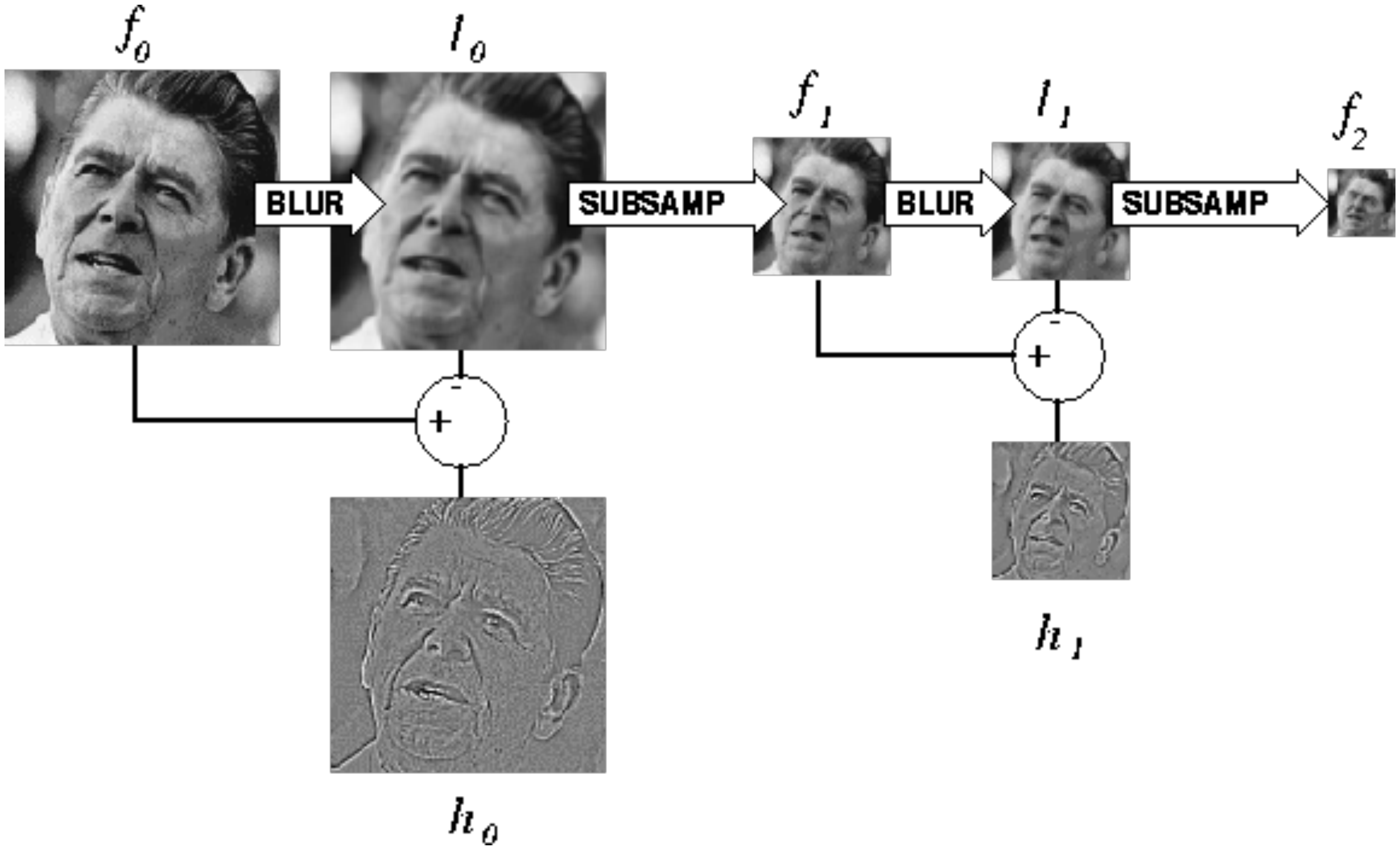

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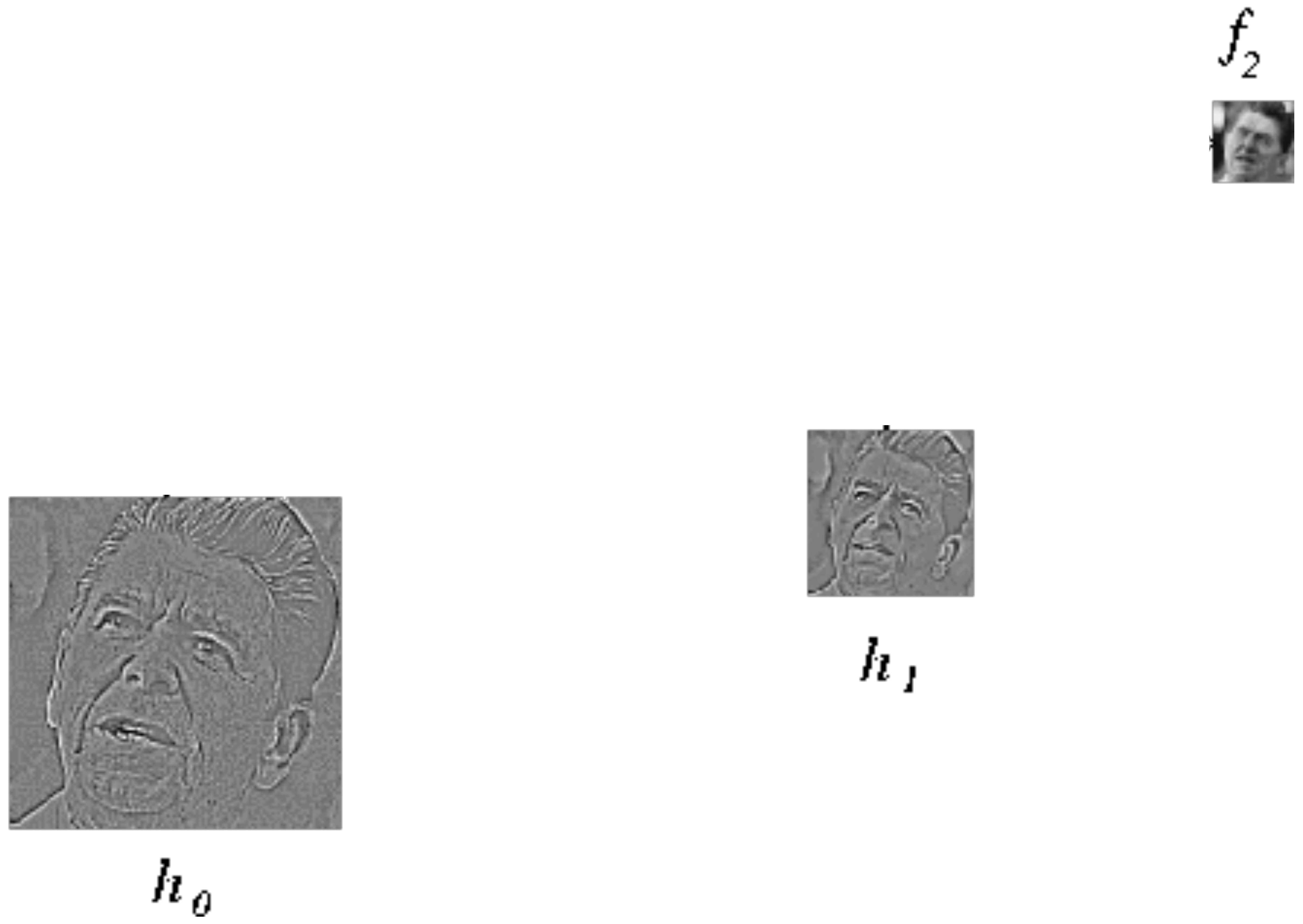
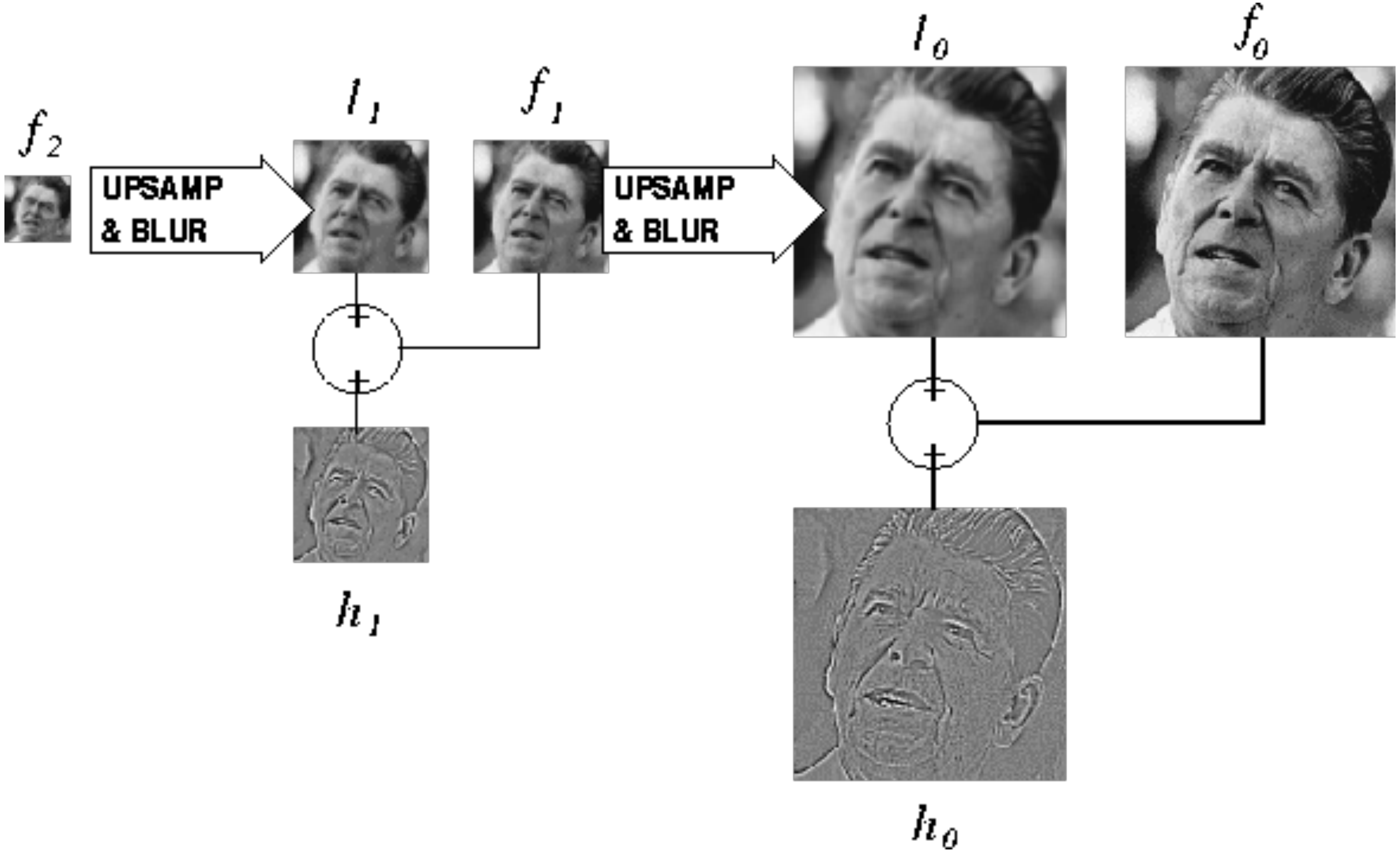


Laplacian Pyramid GAN

Reconstructing a **Laplacian Pyramid**



Laplacian Pyramid GAN

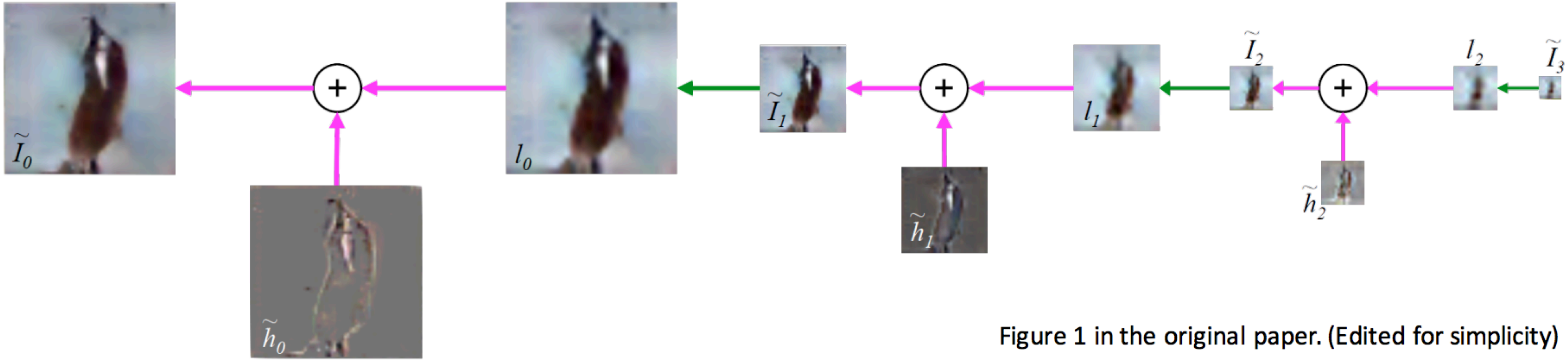


Figure 1 in the original paper. (Edited for simplicity)

— Based on the **Laplacian Pyramid** representation of images

— Generates high resolution images by using **hierarchical set of GANs** by iteratively increasing image resolution and quality

[Denton et al., 2015]

Laplacian Pyramid GAN

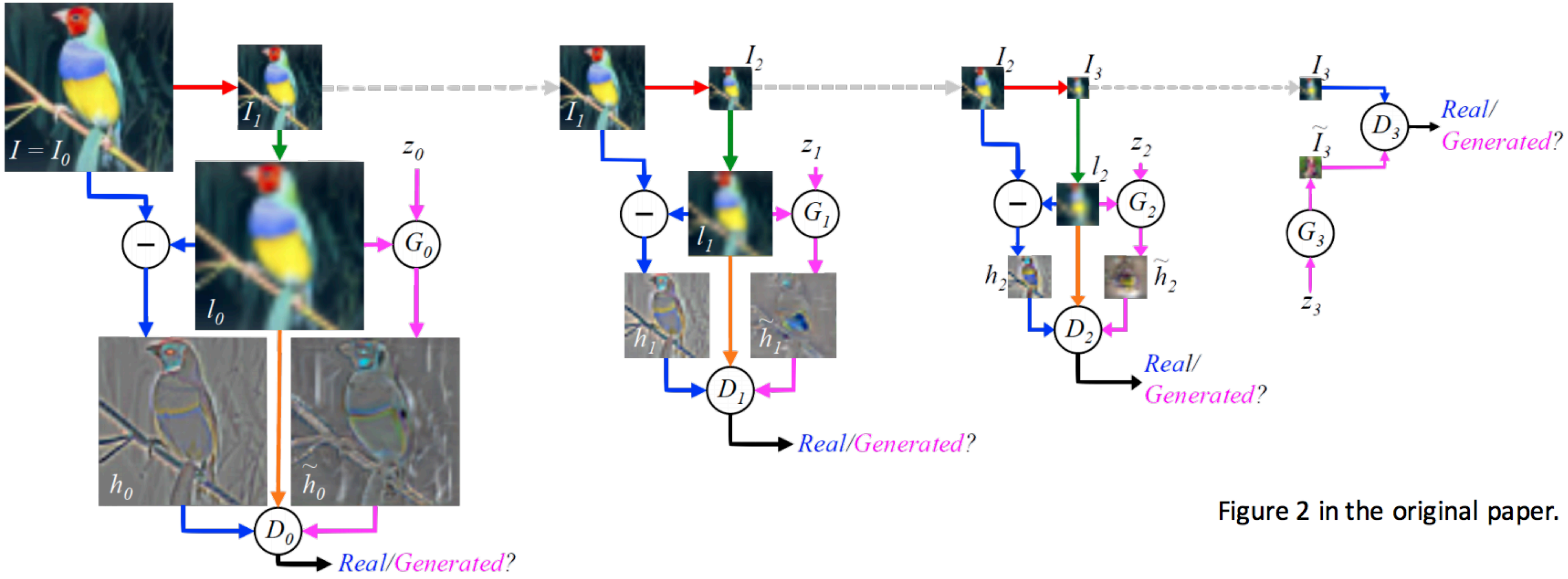


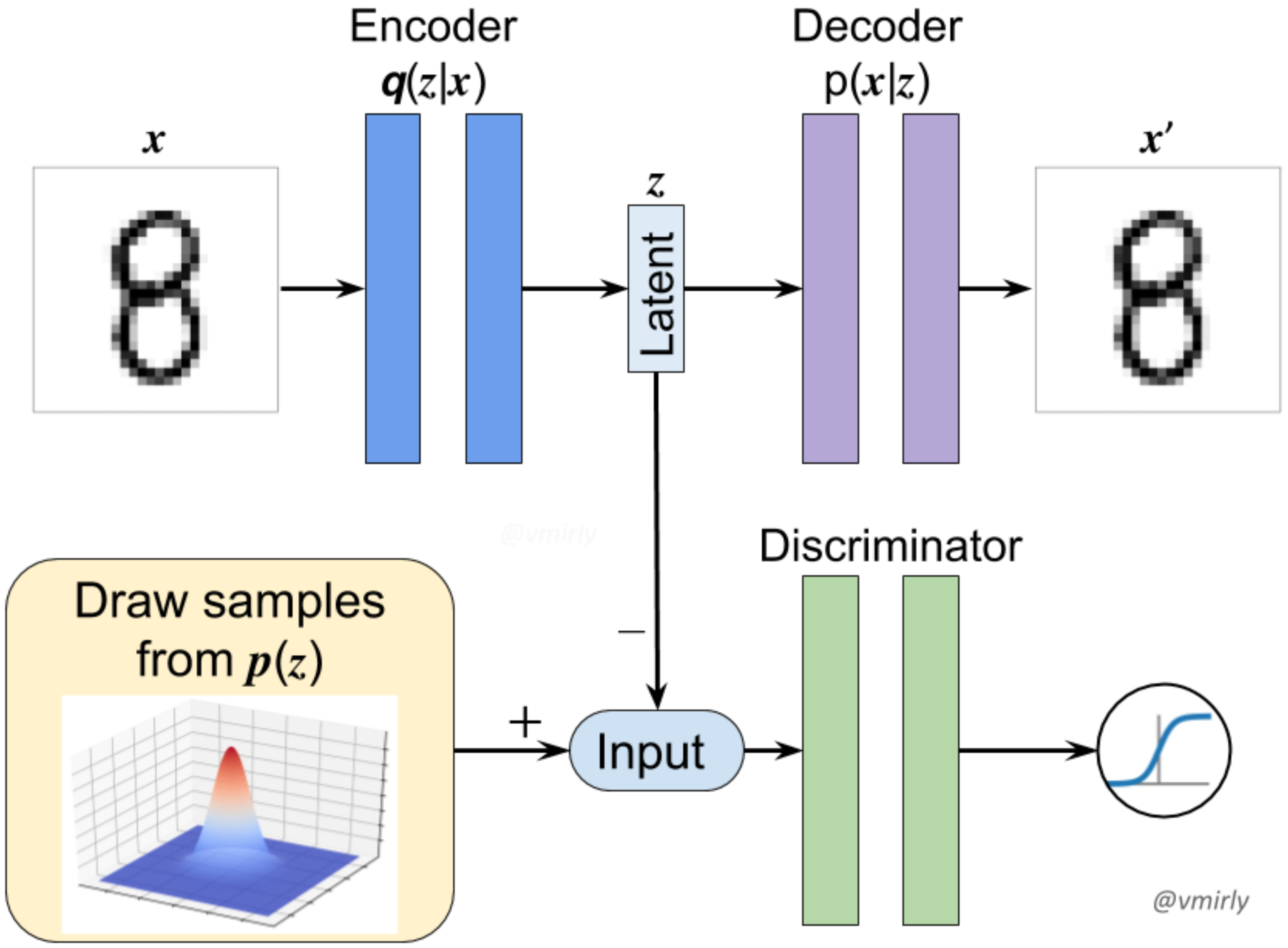
Figure 2 in the original paper.

— Based on the **Laplacian Pyramid** representation of images

— Generates high resolution images by using **hierarchical set of GANs** by iteratively increasing image resolution and quality

[Denton et al., 2015]

Adversarial Autoencoder (GAN + VAE)



[Makhzani et al., 2015]

CVPR LONG BEACH CALIFORNIA
June 16-20, 2019

Image Generation from Layout


Bo Zhao


Lili Meng

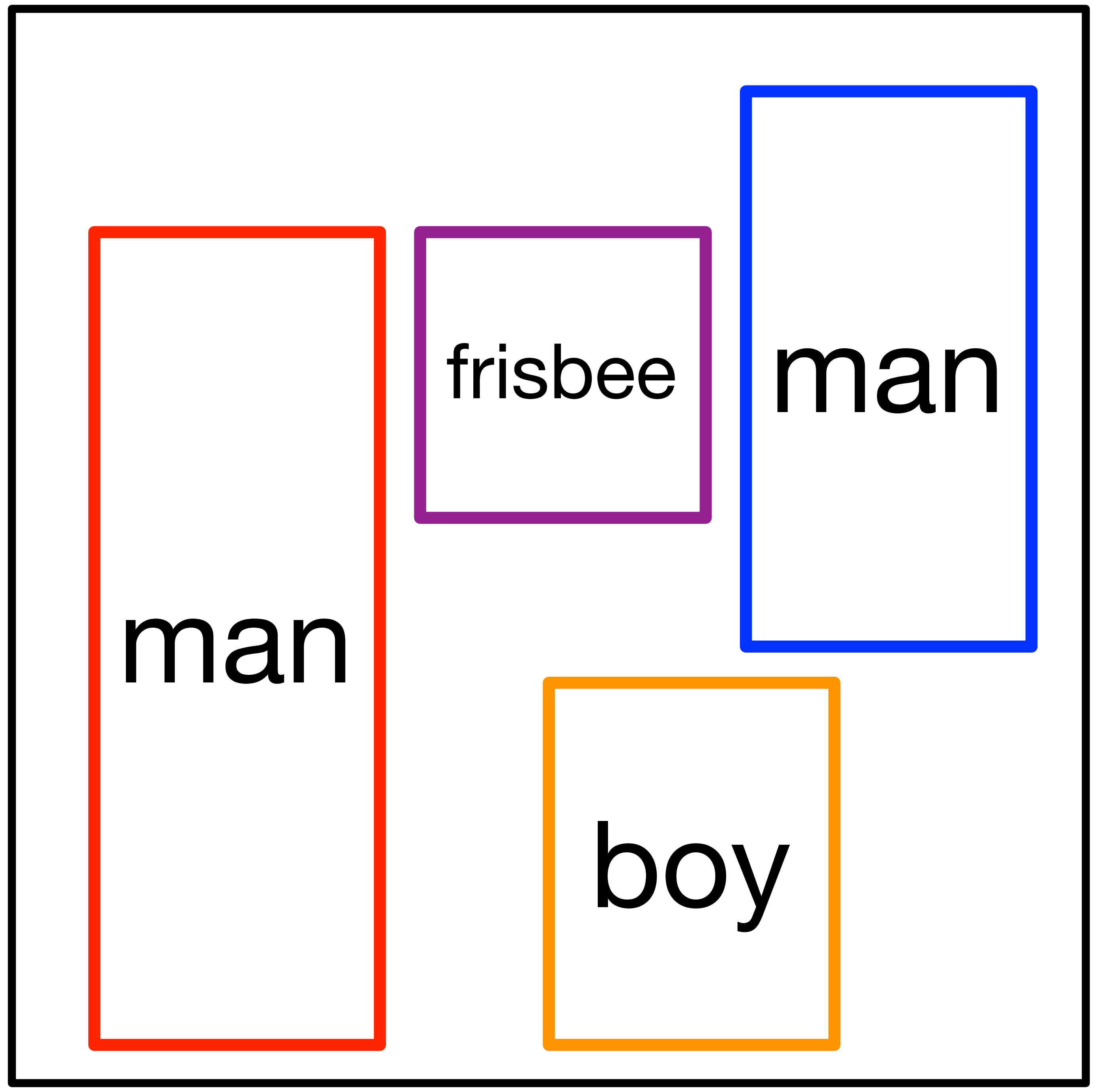

Weidong Yin


Leonid Sigal

UBC

Image Generation from Layout

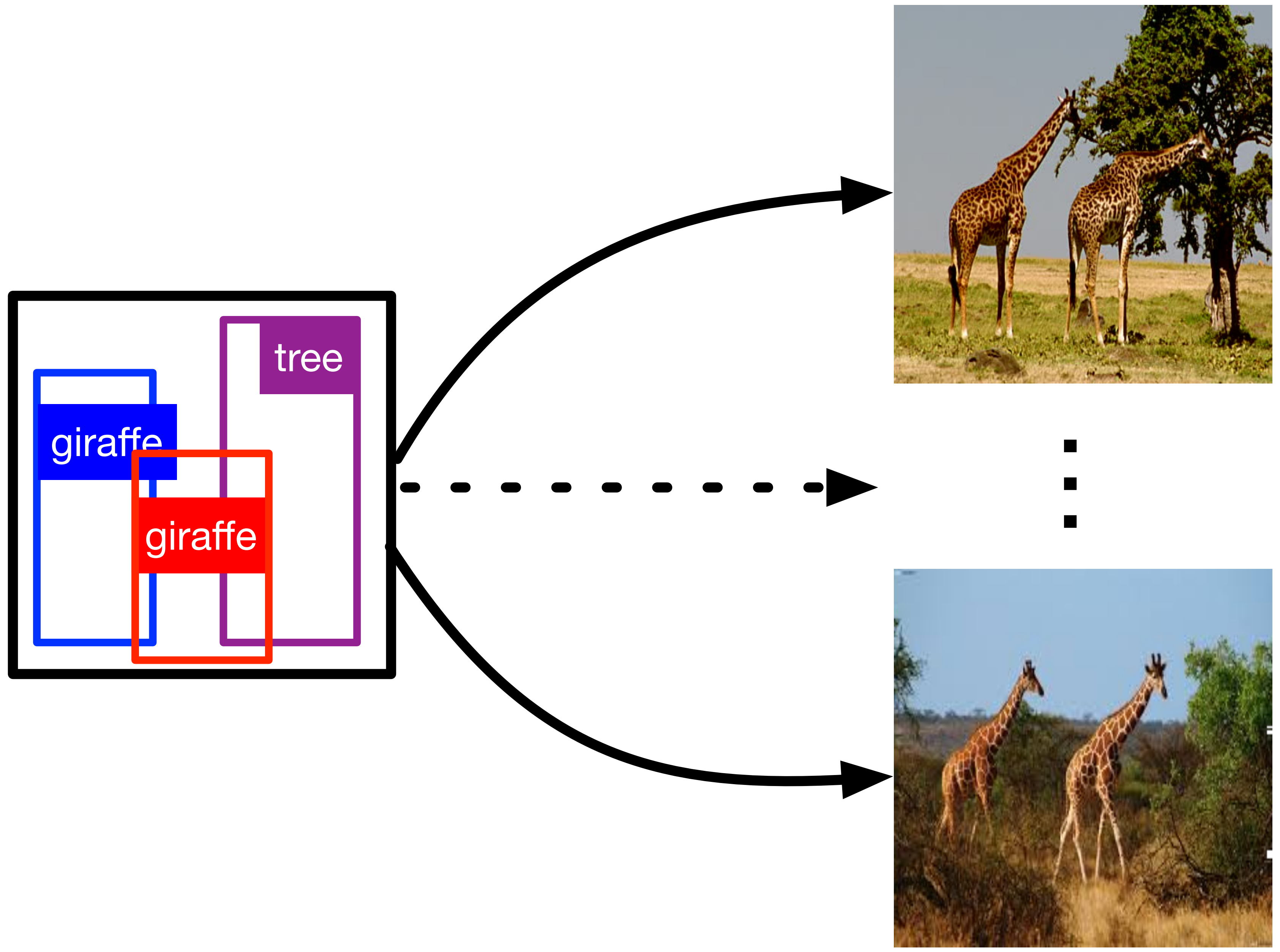
Image Generation from Layout



Layout

Results

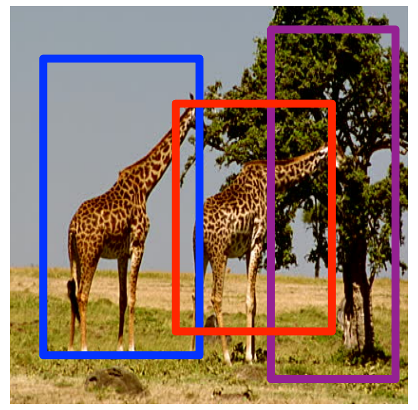
Image Generation from Layout: **Challenges**



- One-to-many mapping
- Information in layout is limited (but important)
- Important interactions between objects in overlap regions and with scene

Model **Architecture**: Training

Model **Architecture**: Training



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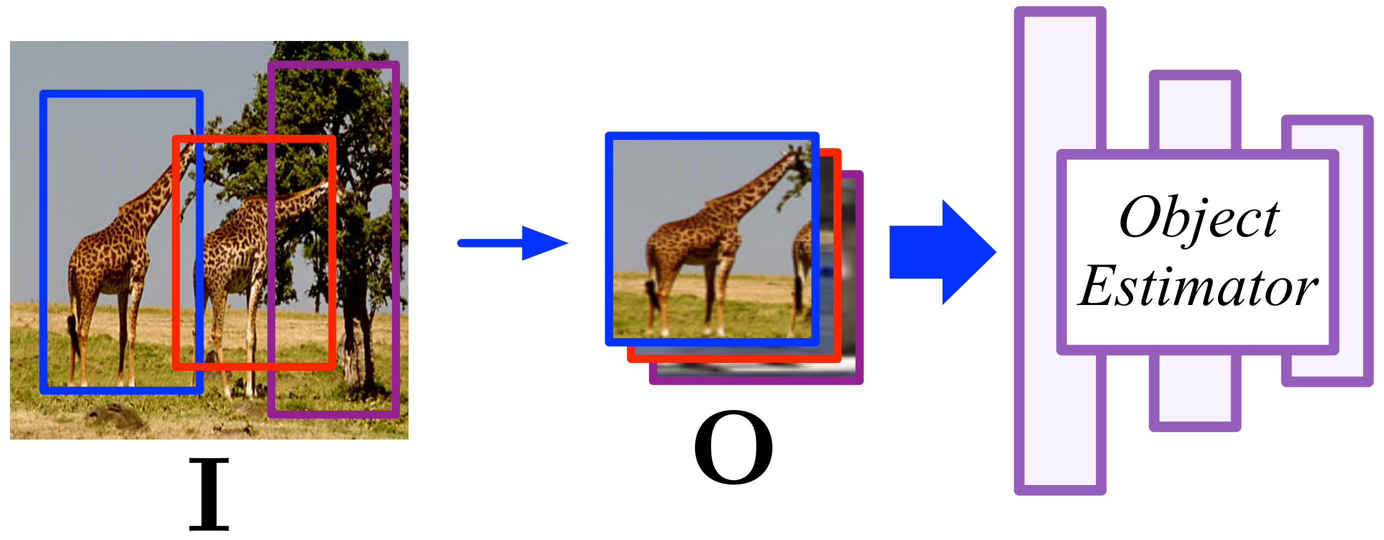
Model **Architecture**: Training



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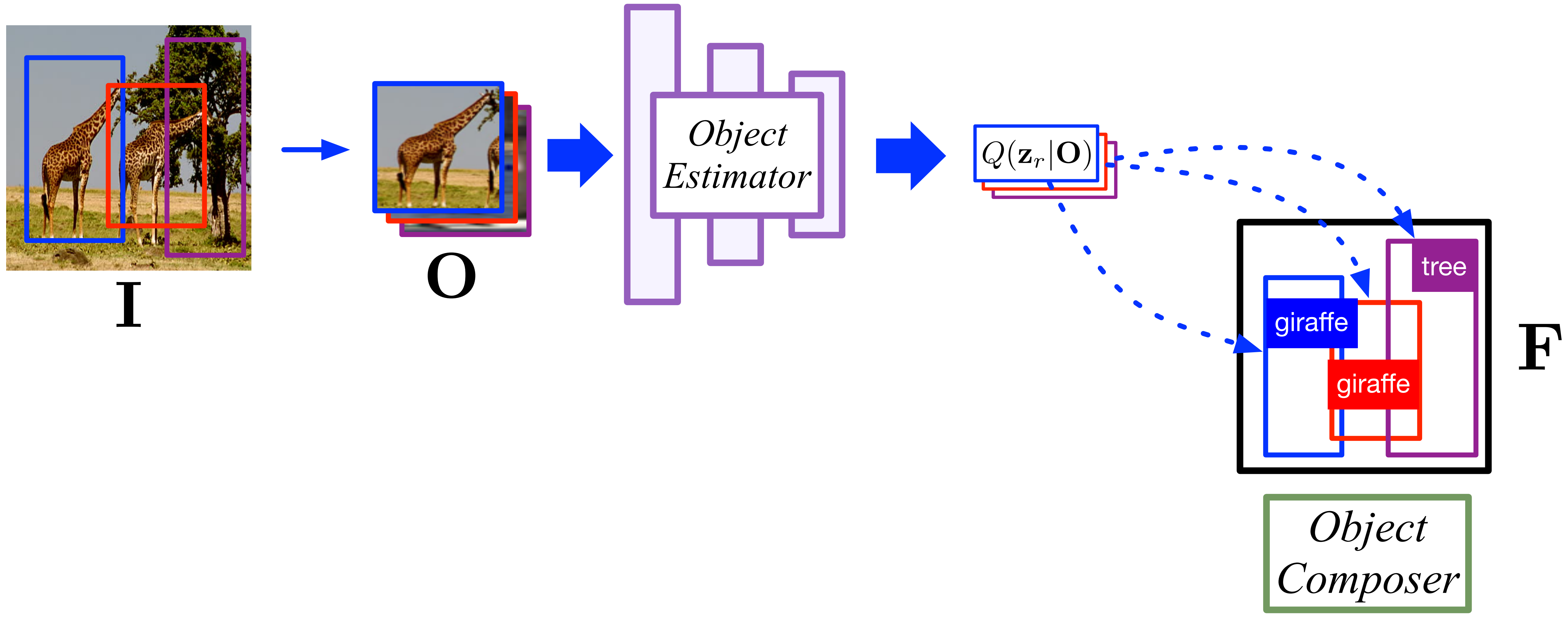

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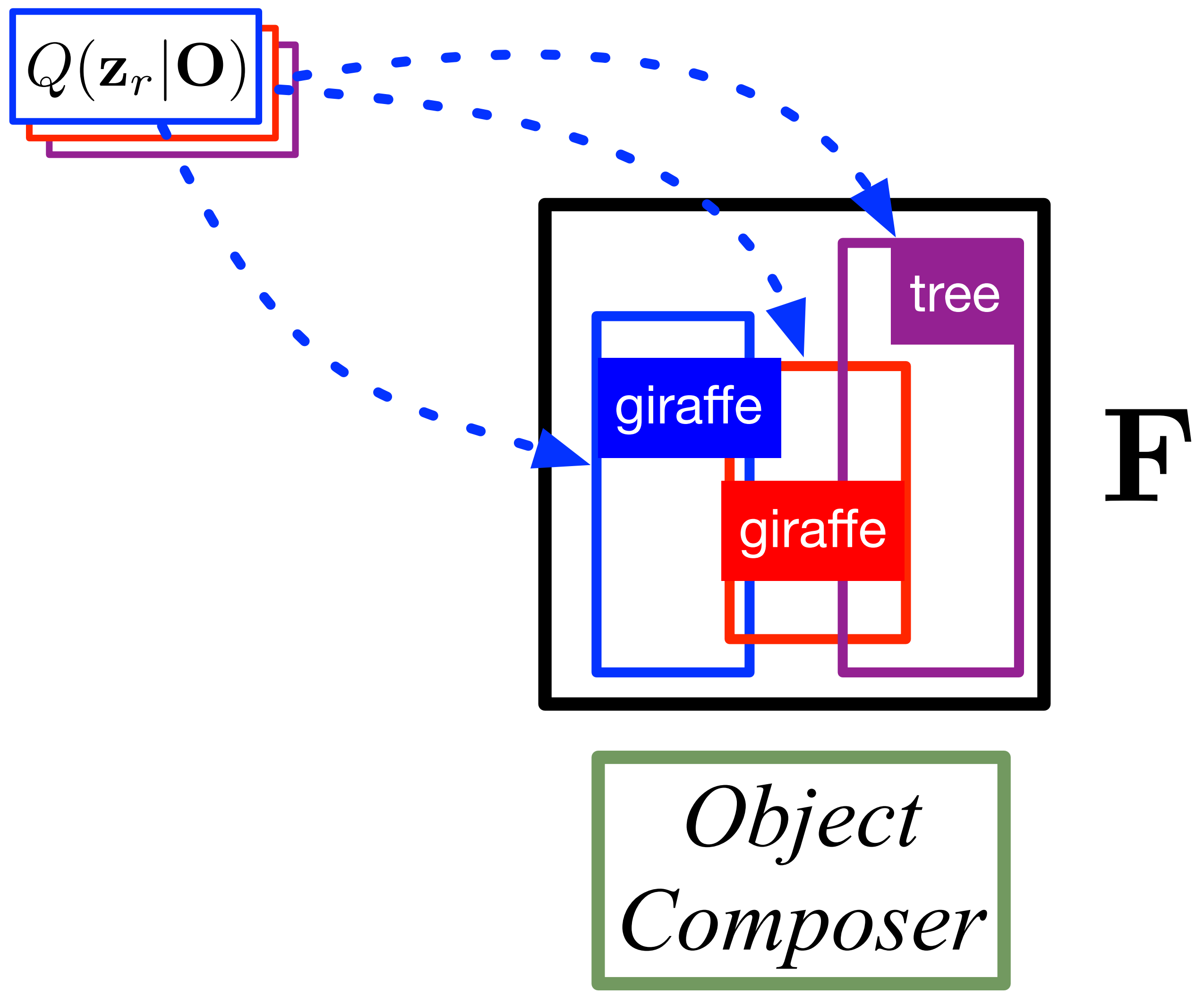

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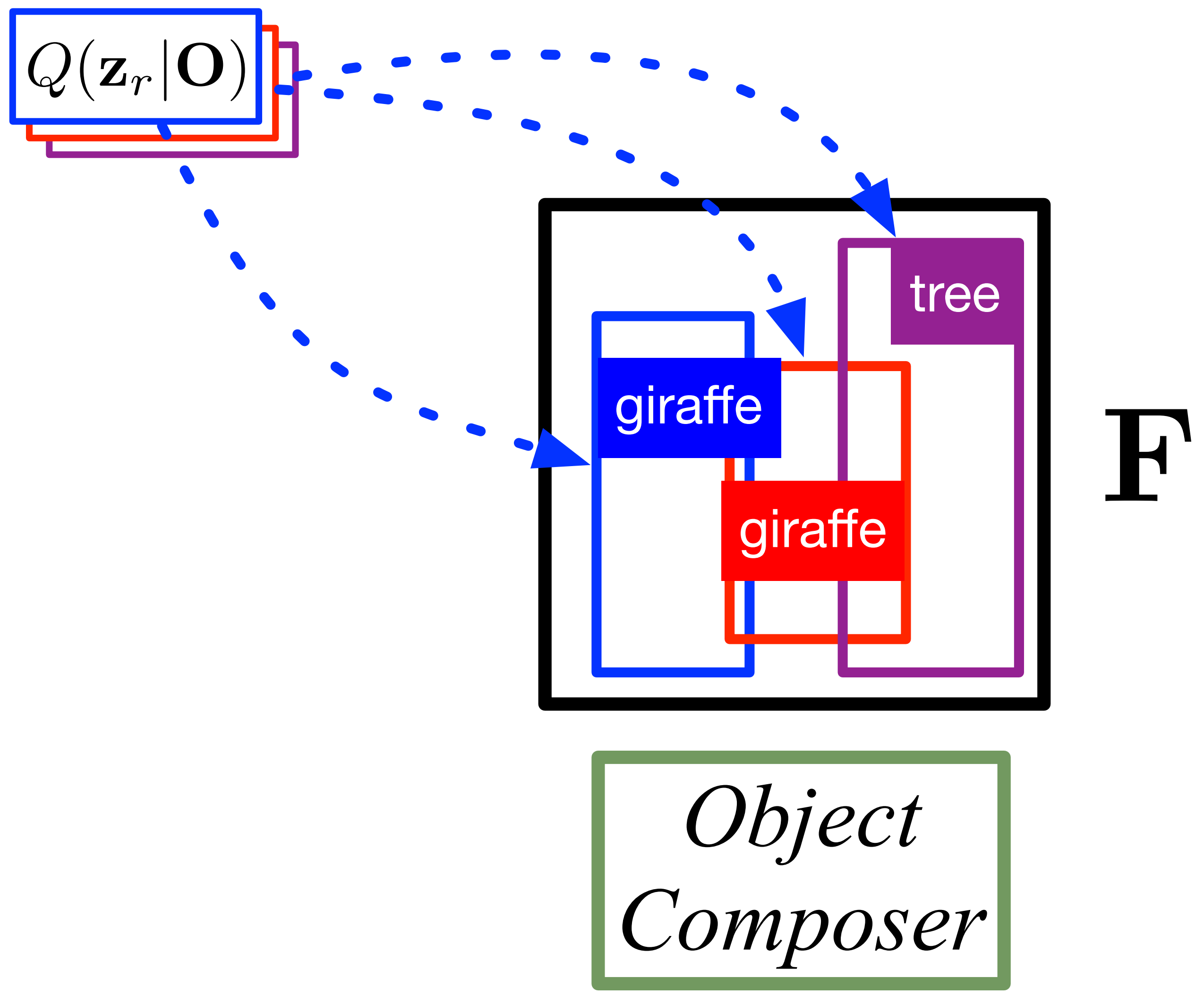

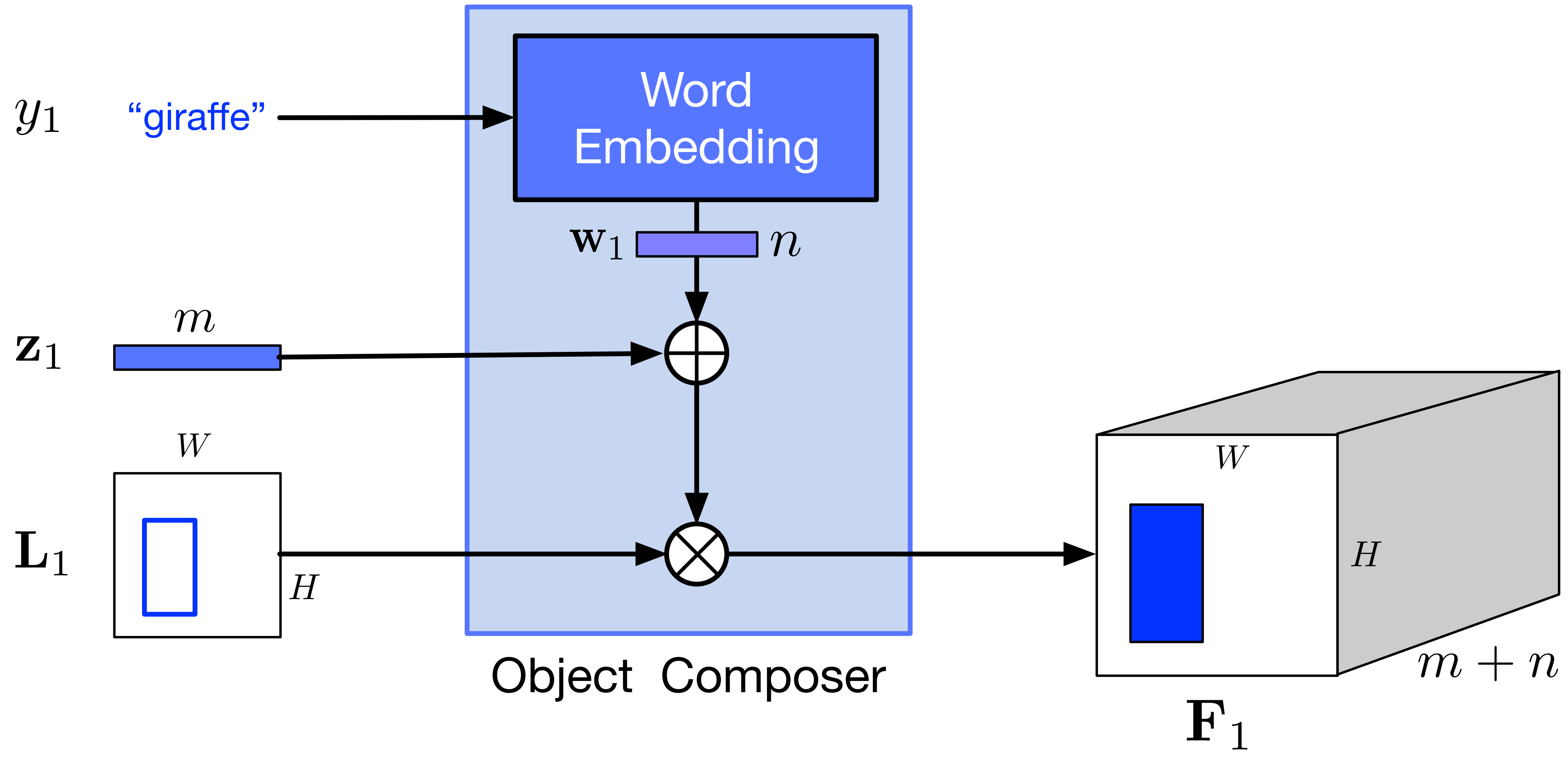

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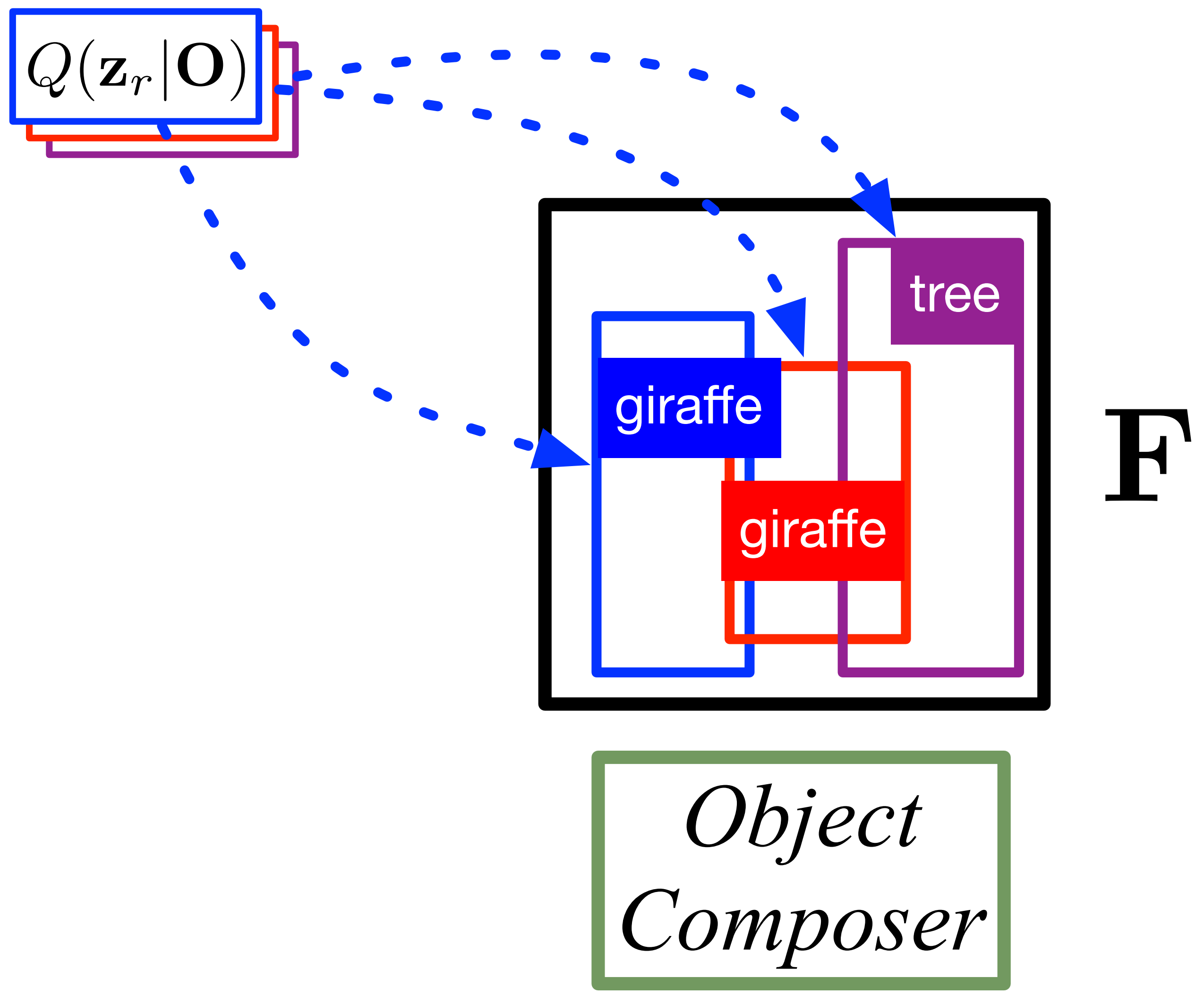

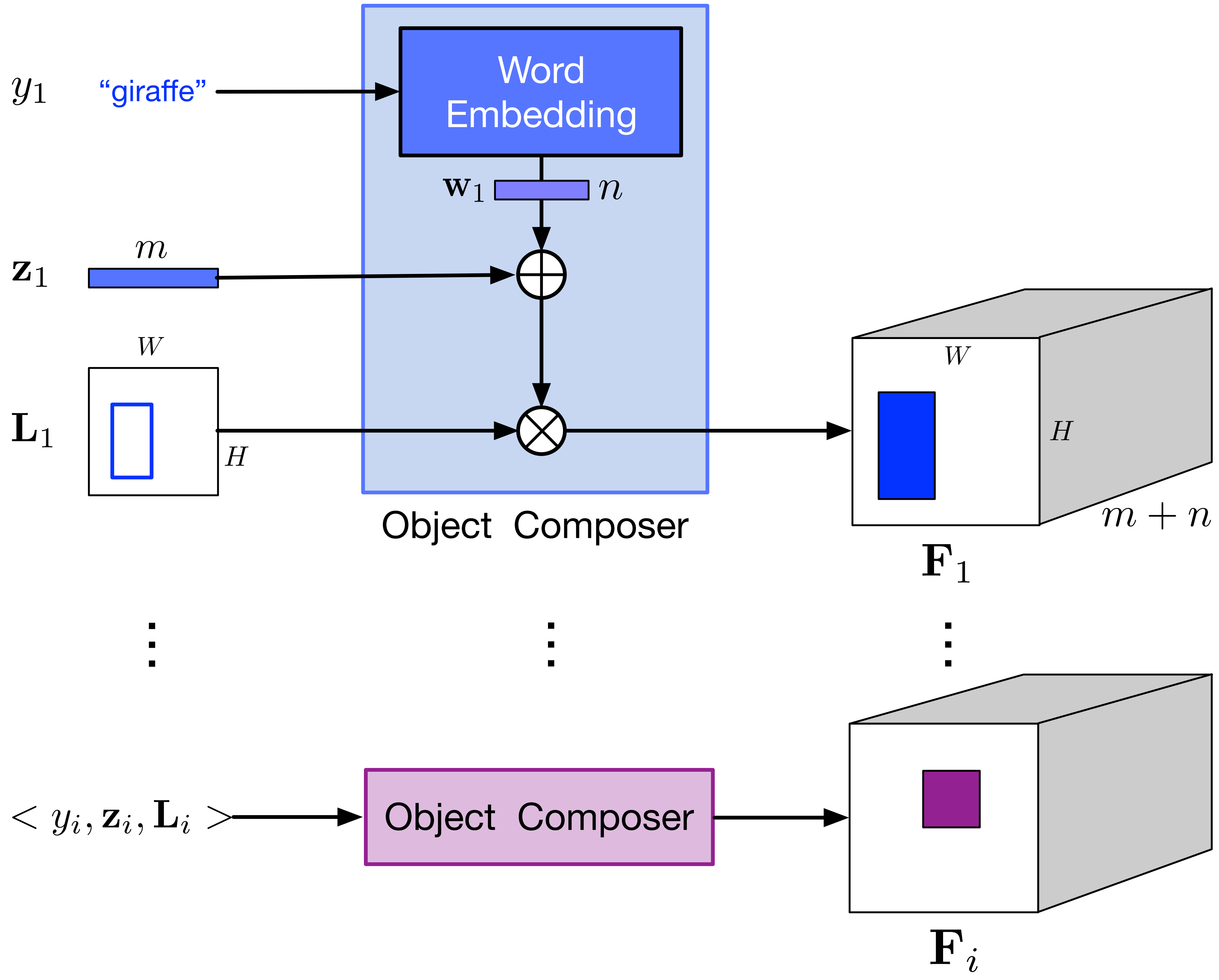

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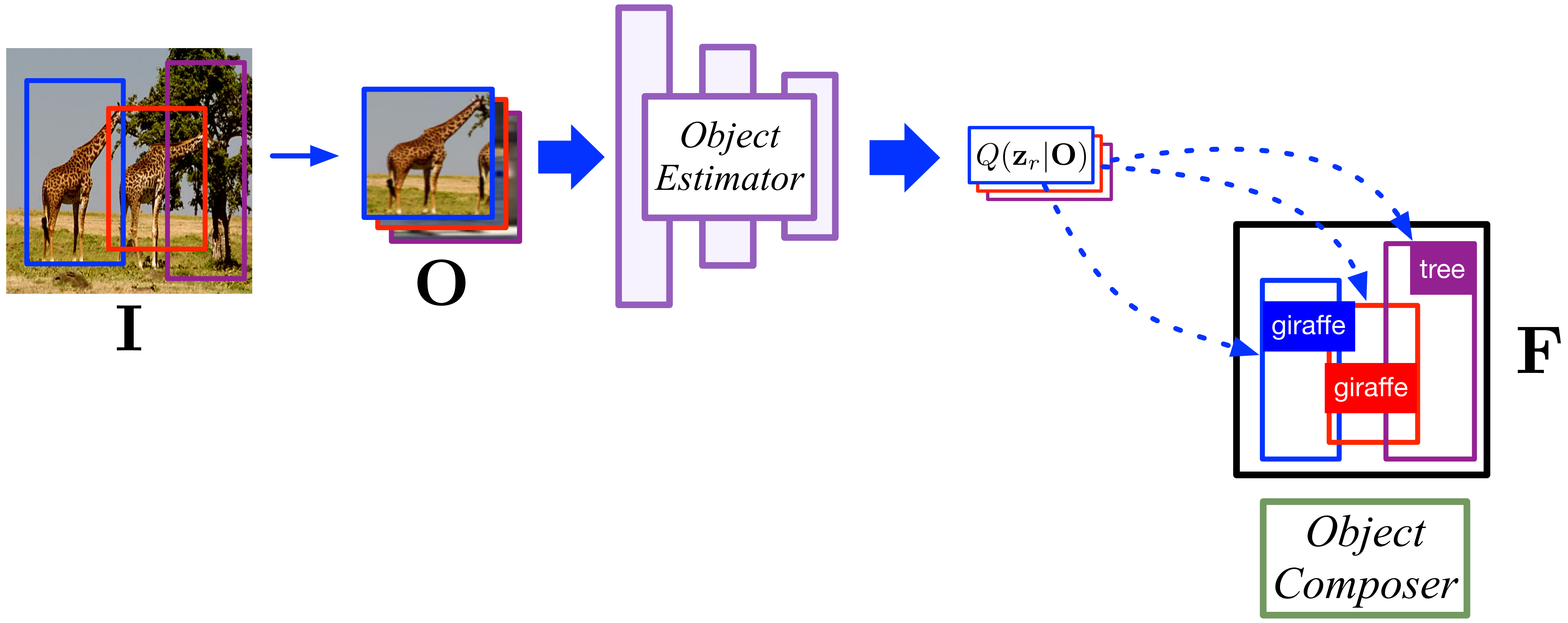

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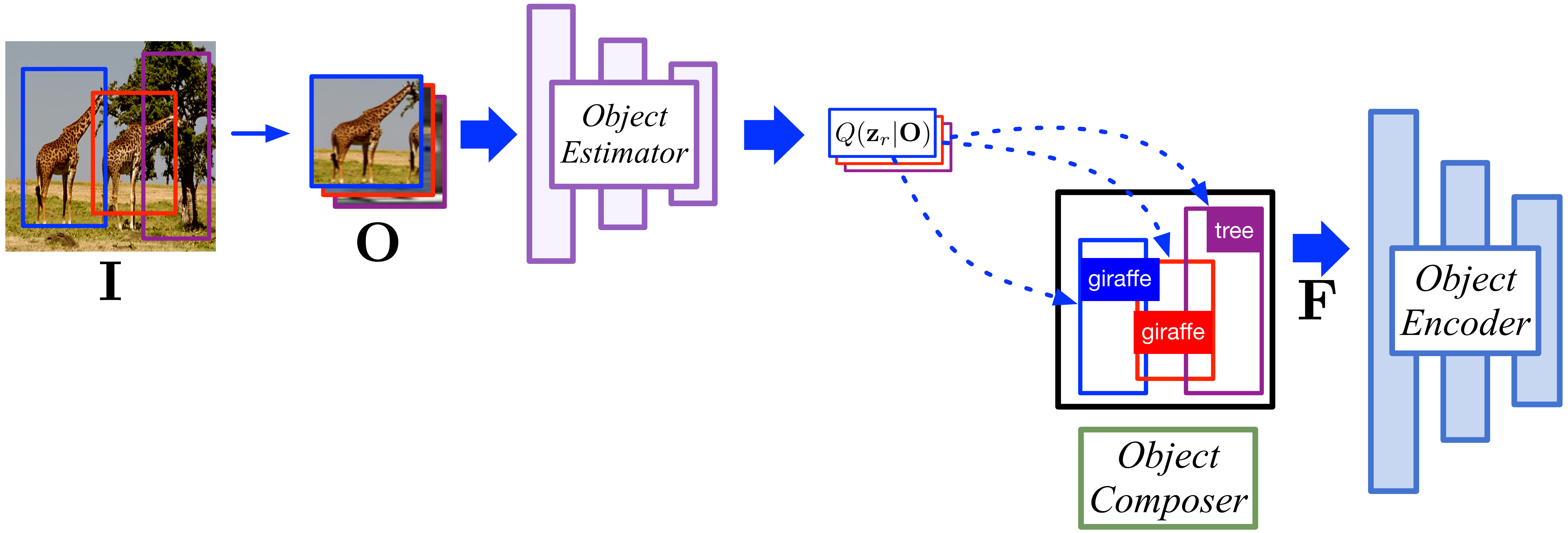

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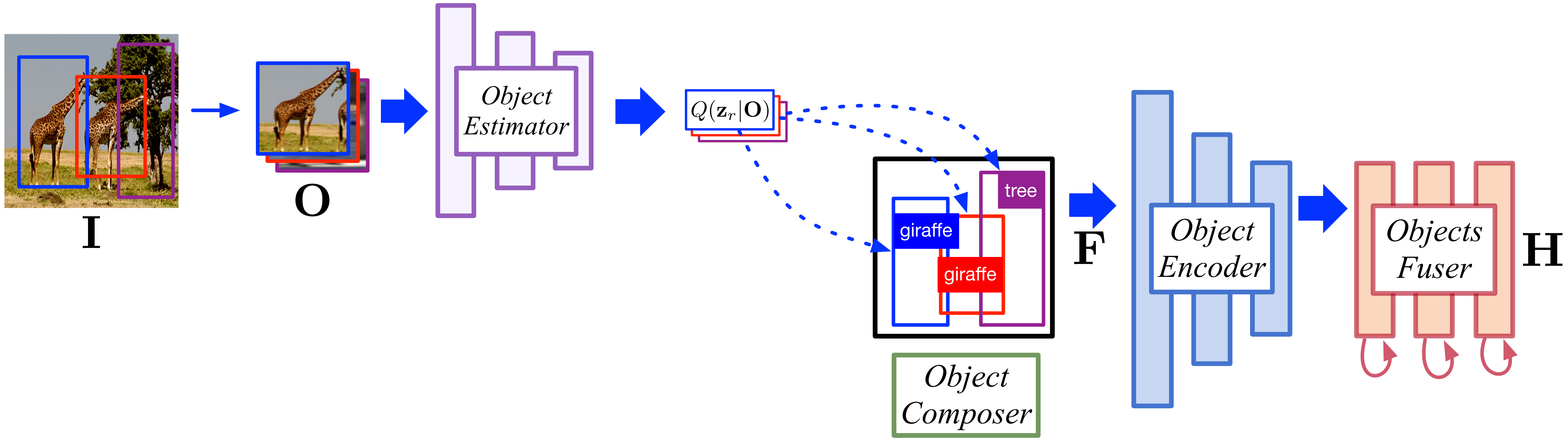

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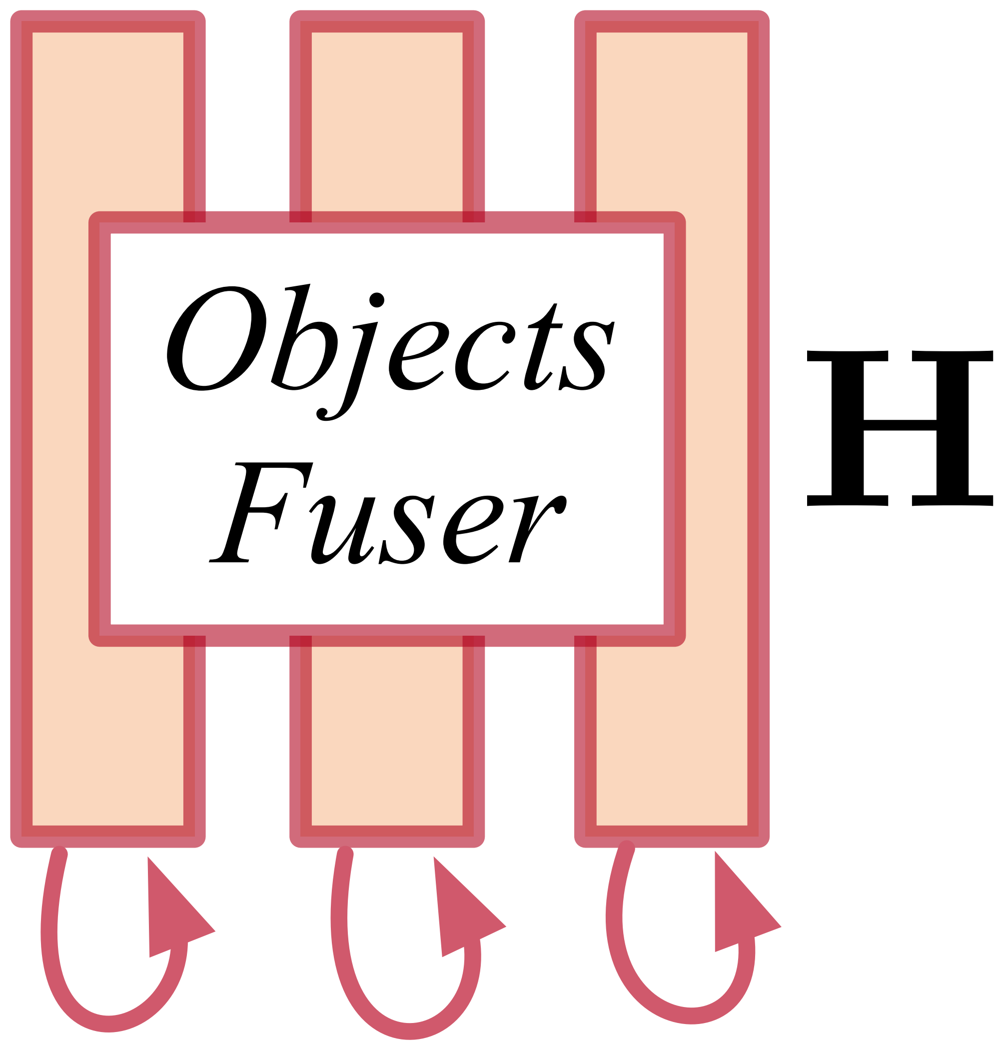

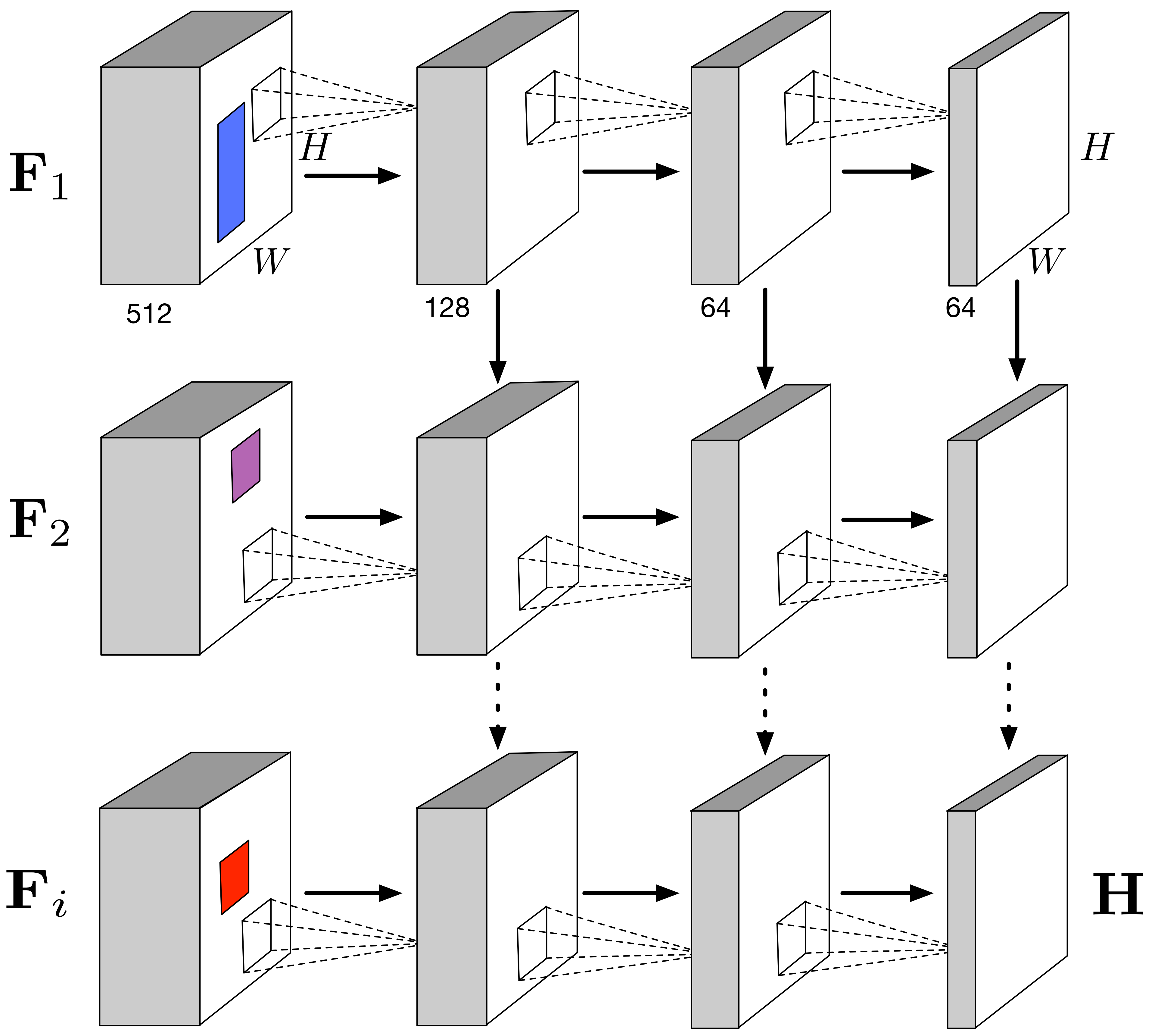

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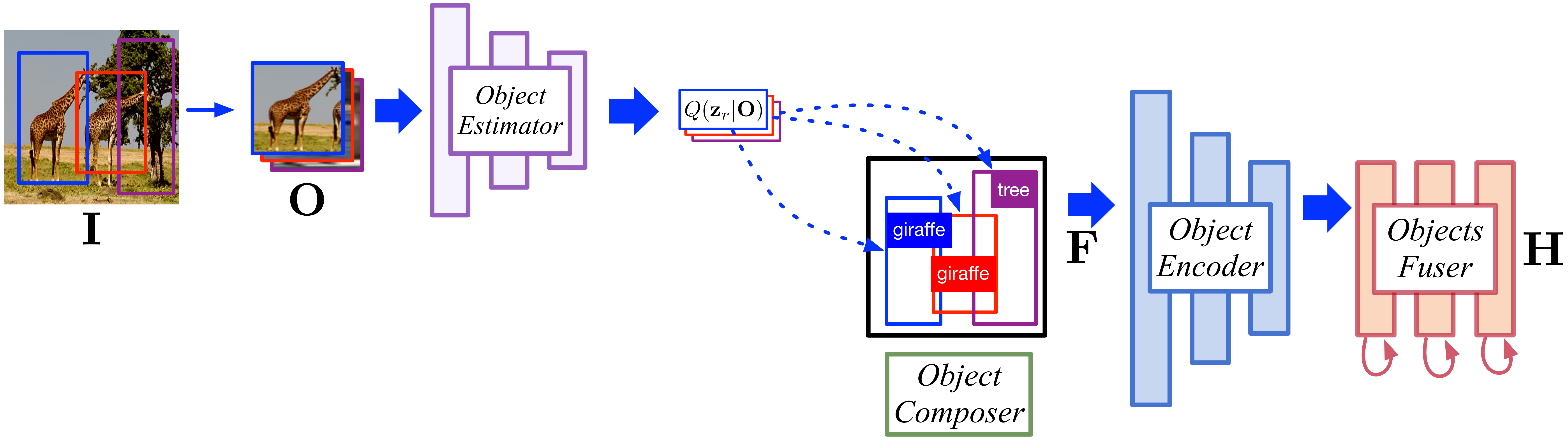

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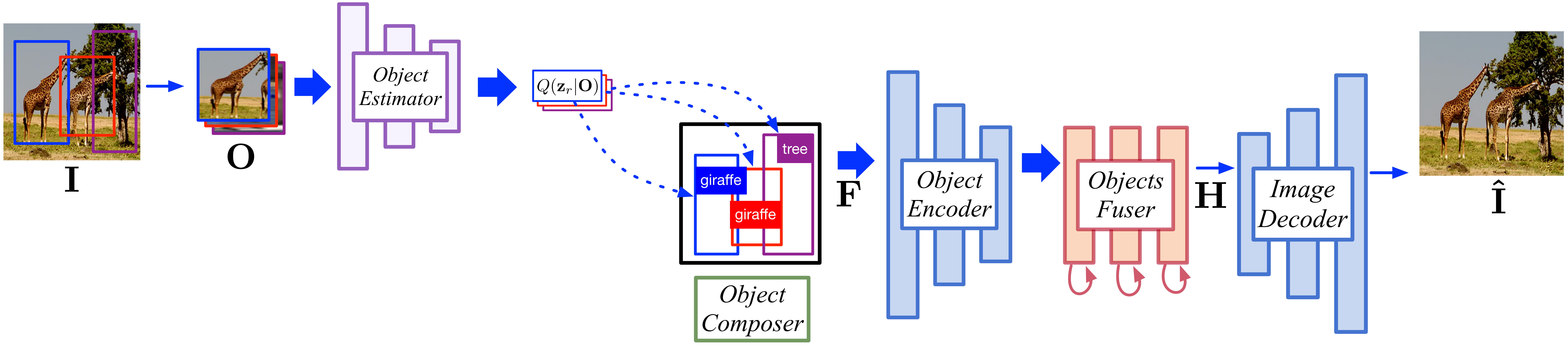

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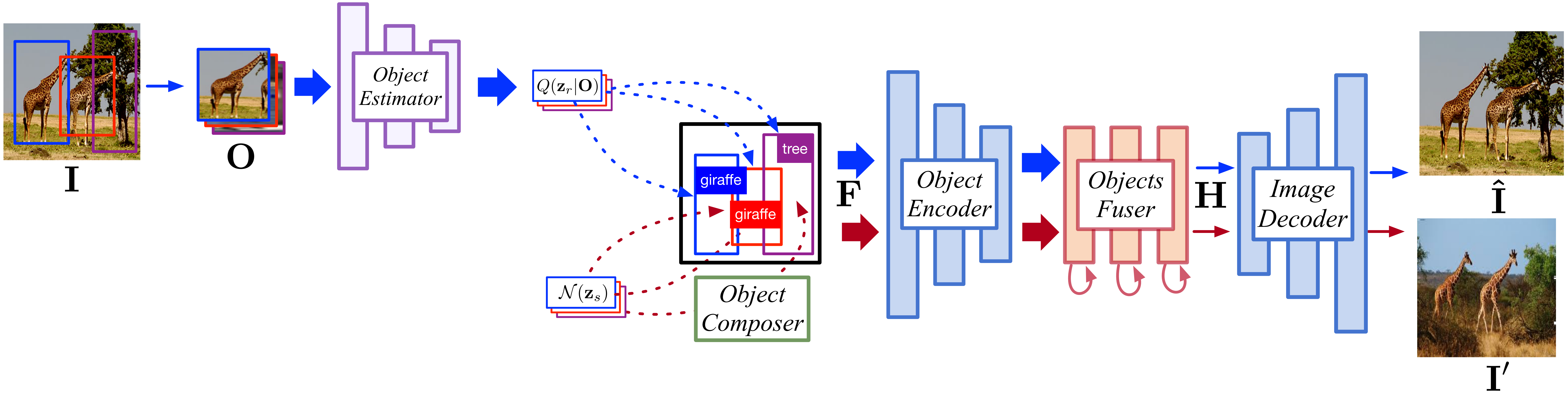

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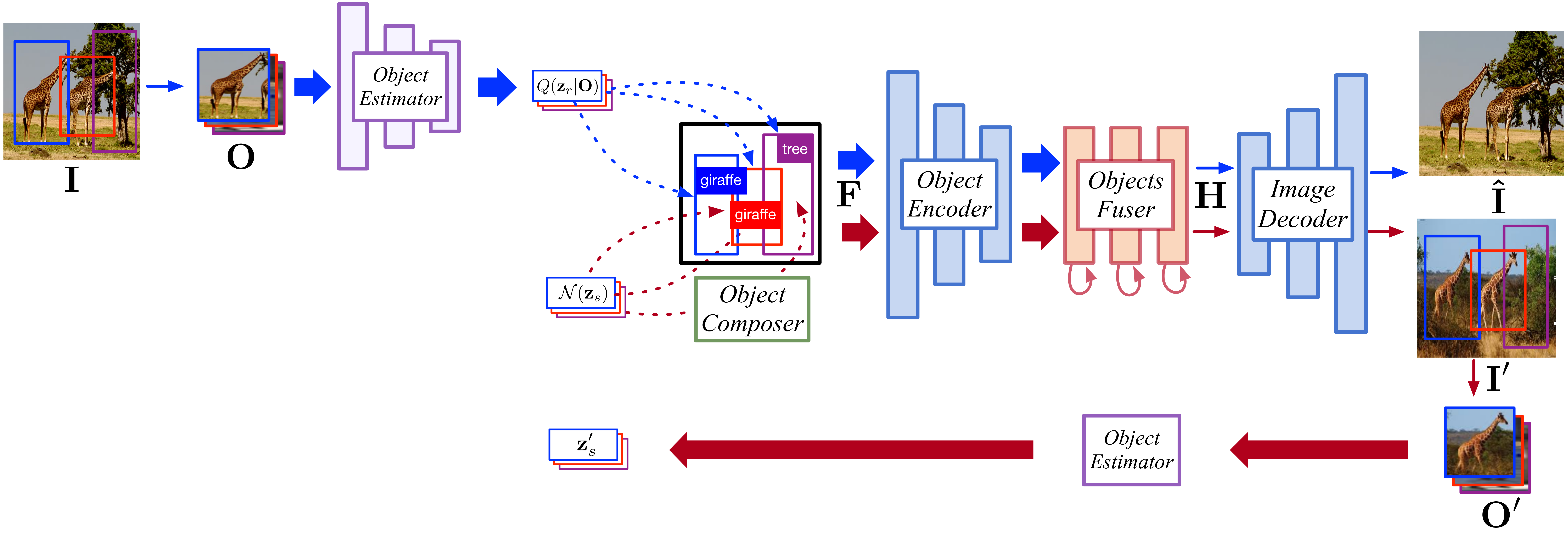
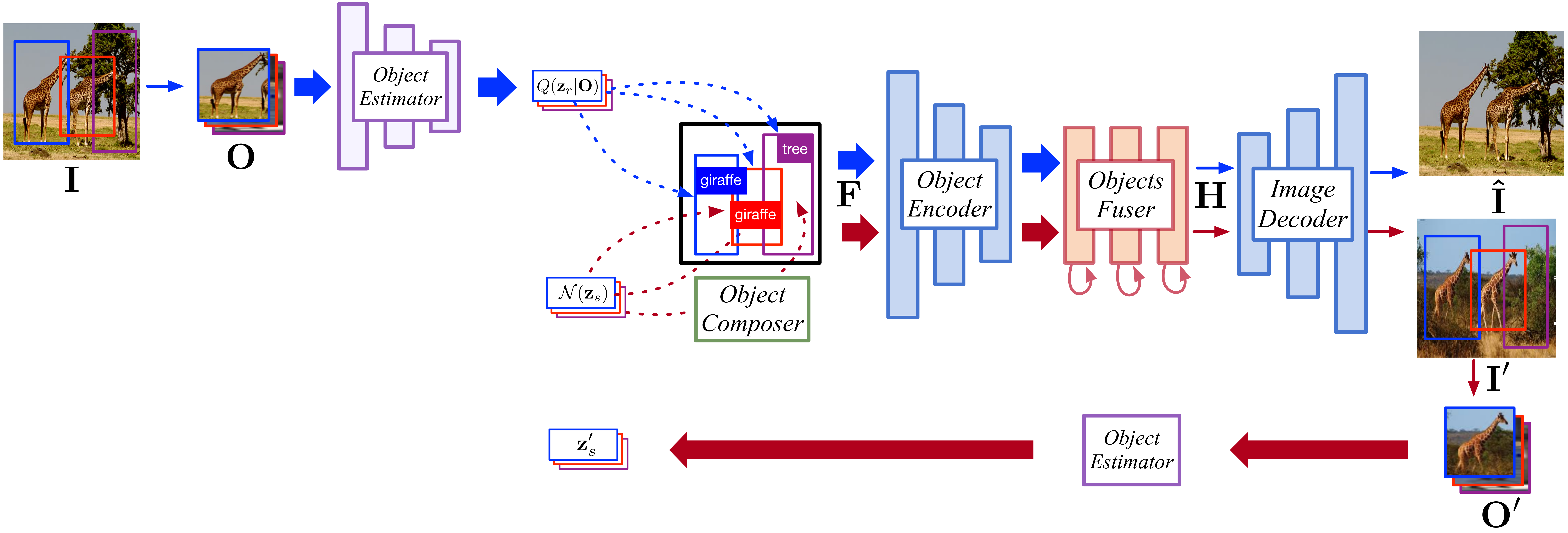


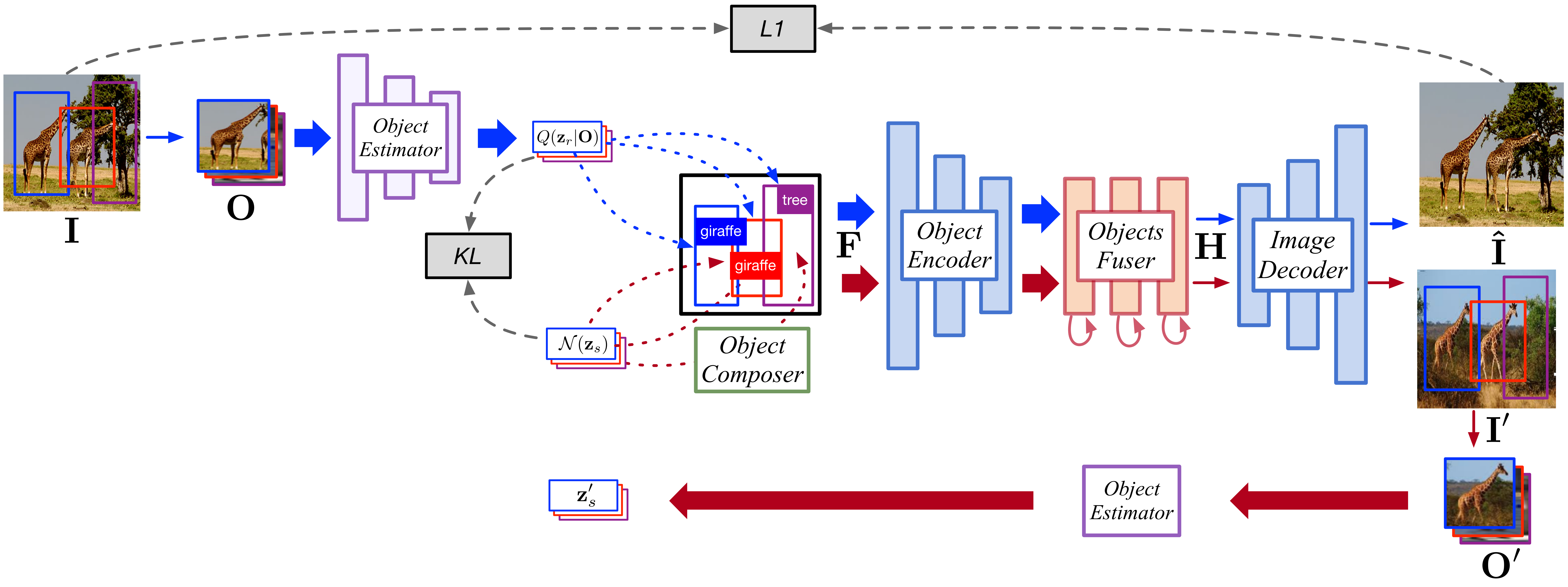
Model **Architecture**: Training

Losses



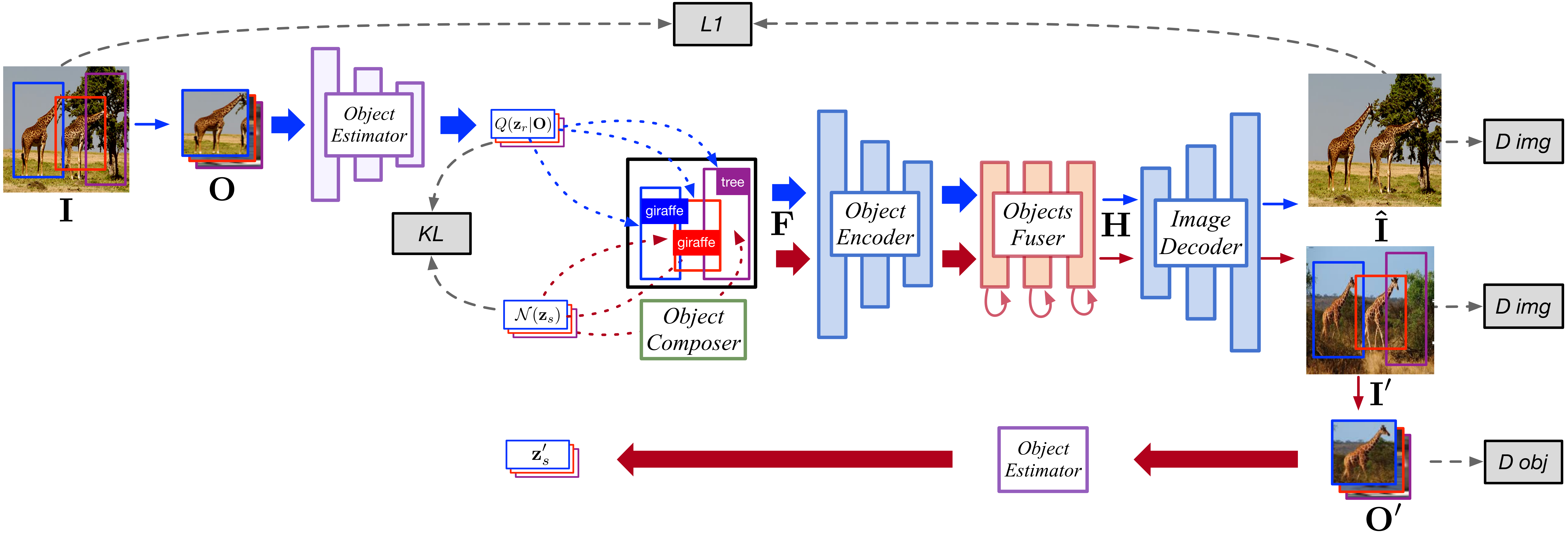
Model **Architecture**: Training

Losses



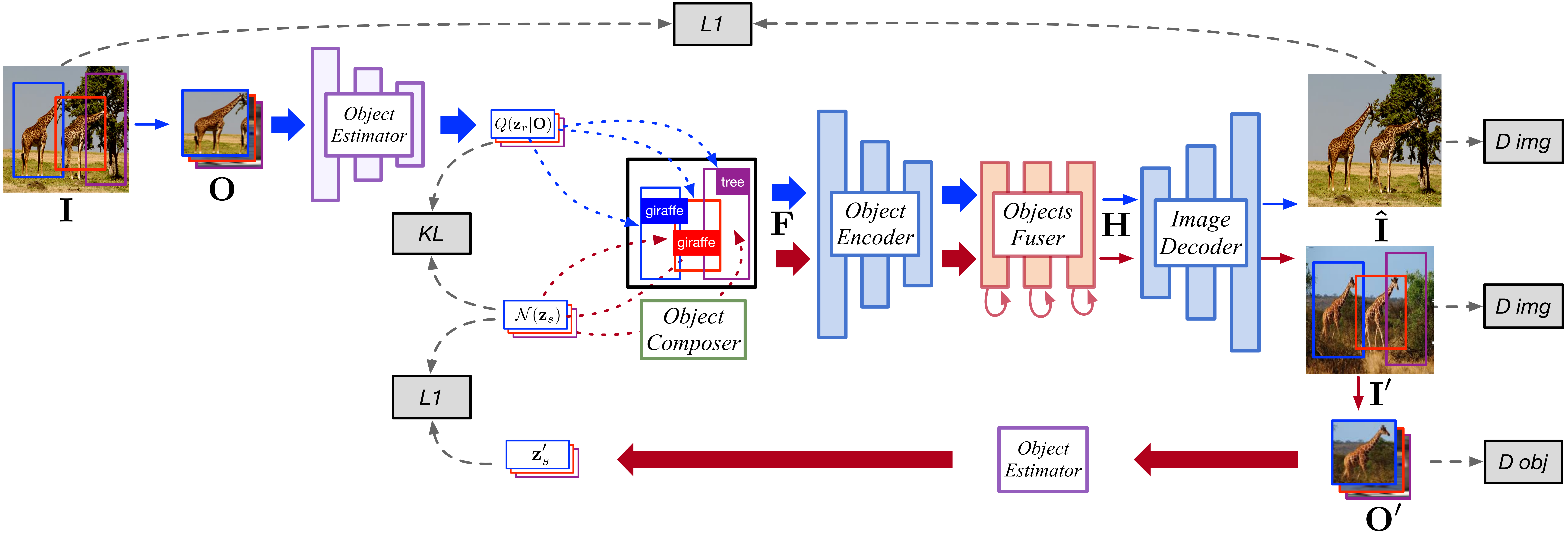
Model **Architecture**: Training

Losses



Model **Architecture**: Training

Losses



Model **Architecture**: Runtime

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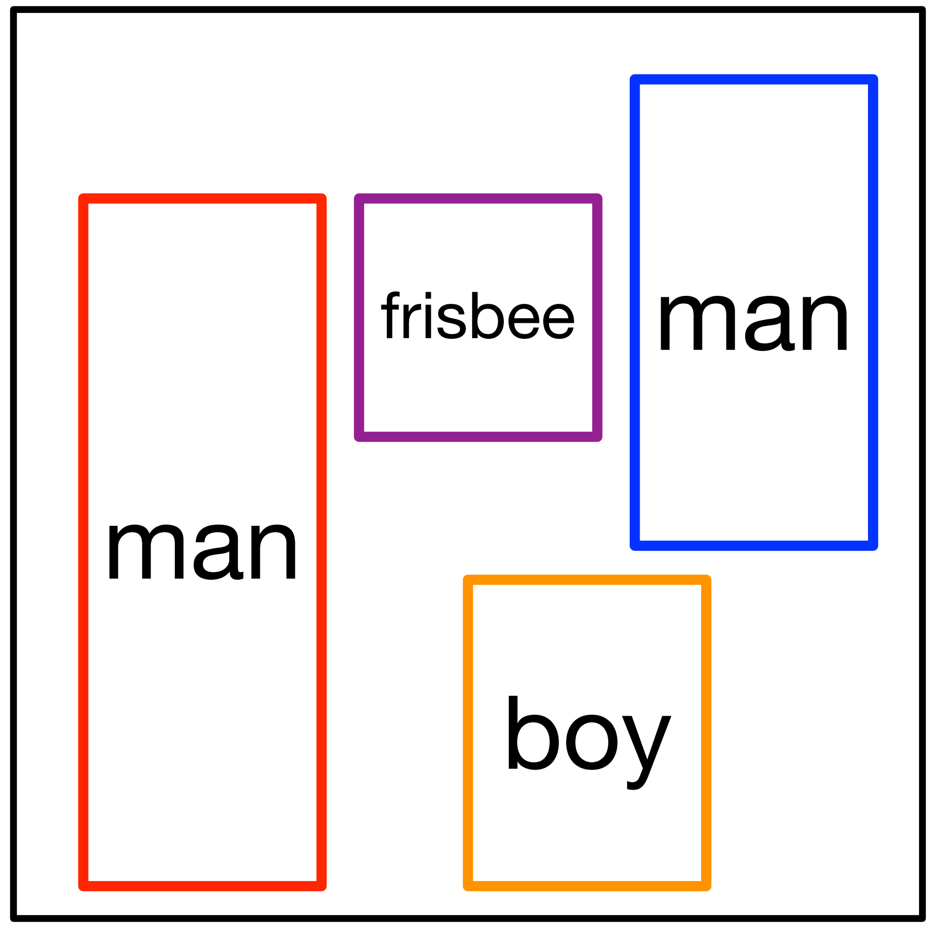

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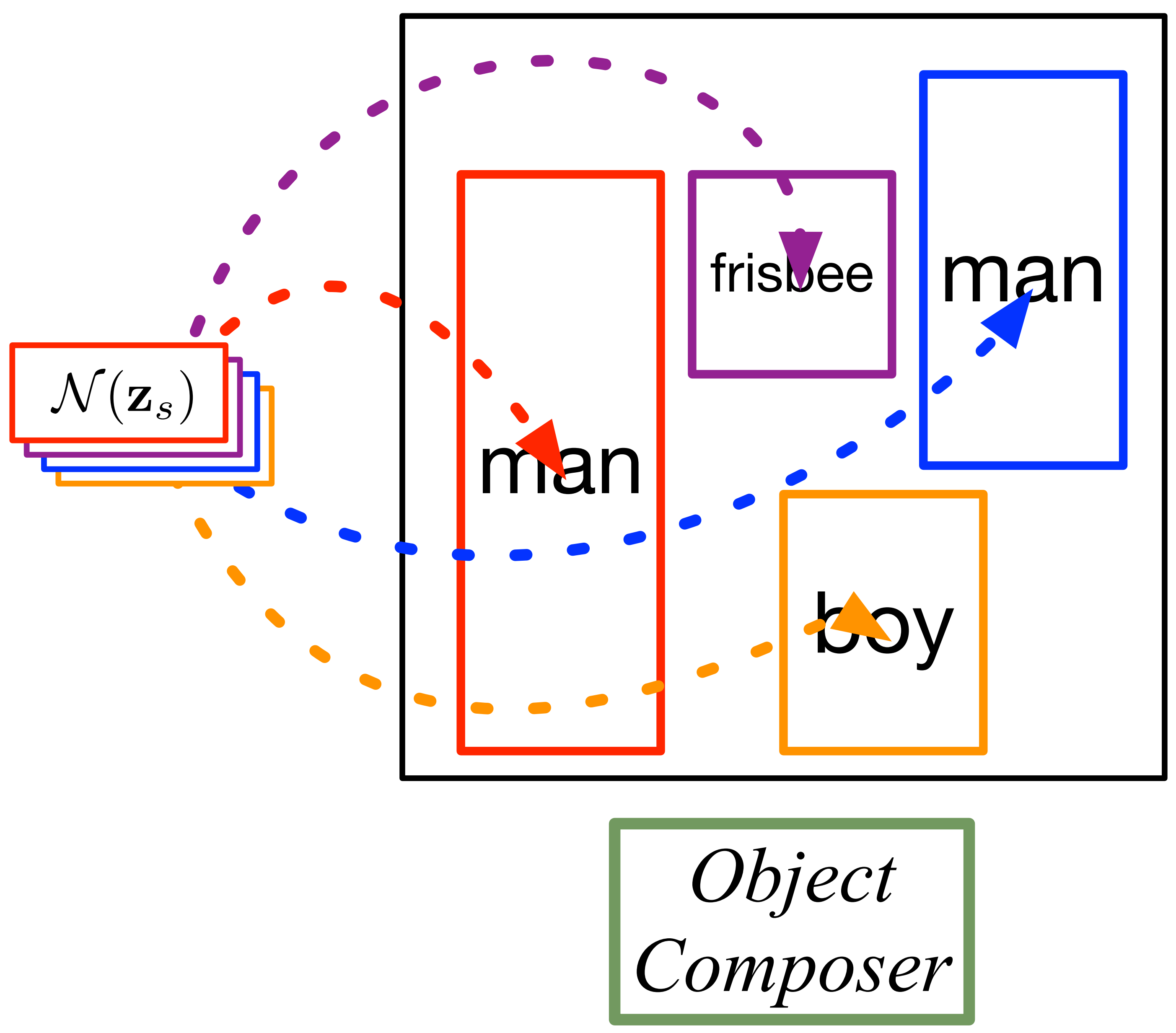

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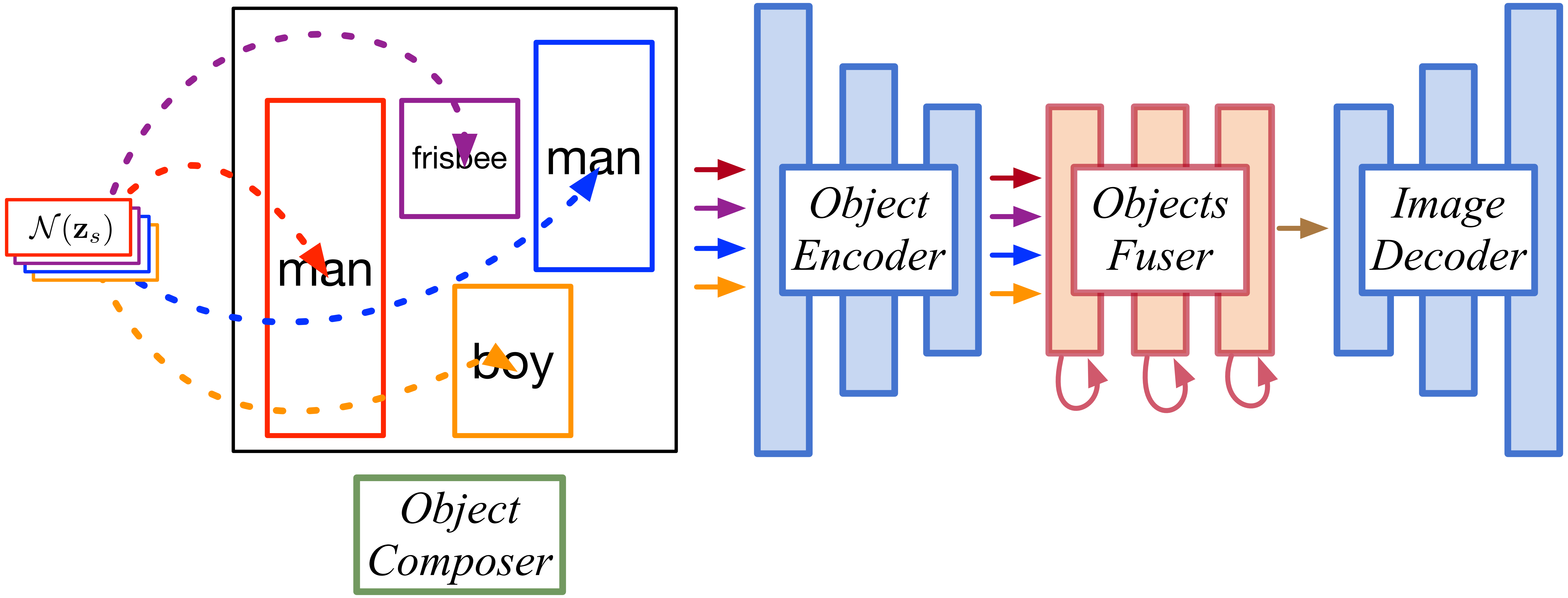
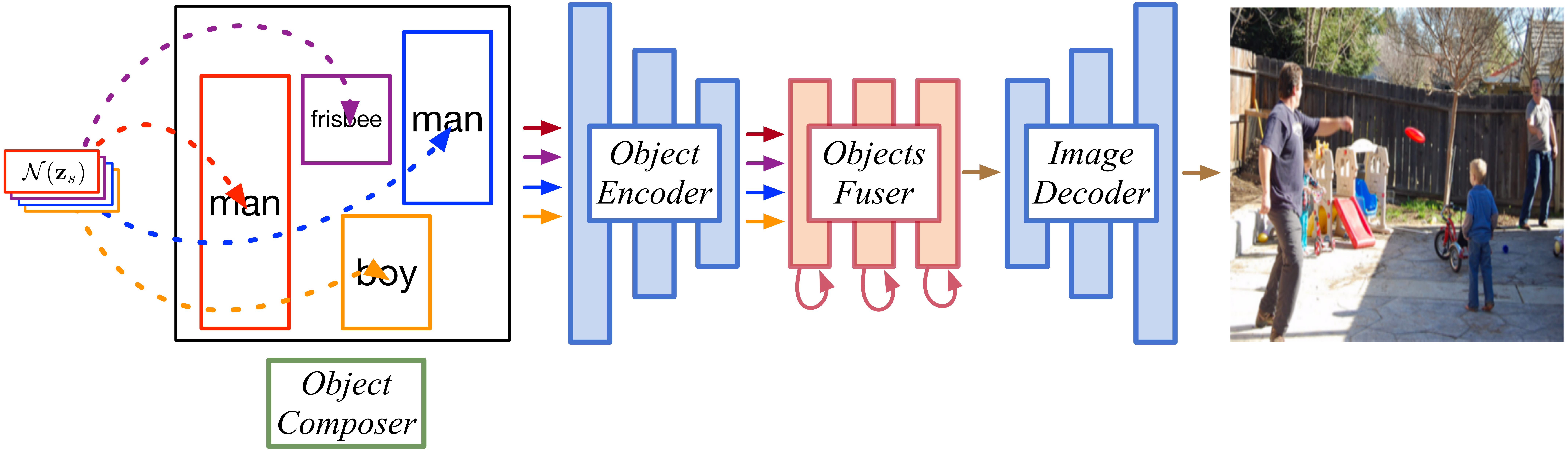


Model **Architecture**: Runtime



Experiments: Quantitative Results

Datasets:

Dataset	Train	Val.	Test	# Obj.	# Obj. in Image
COCO [1]	24,972	1,024	2,048	171	$3 \sim 8$
VG [18]	62,565	5,506	5,088	178	$3 \sim 30$

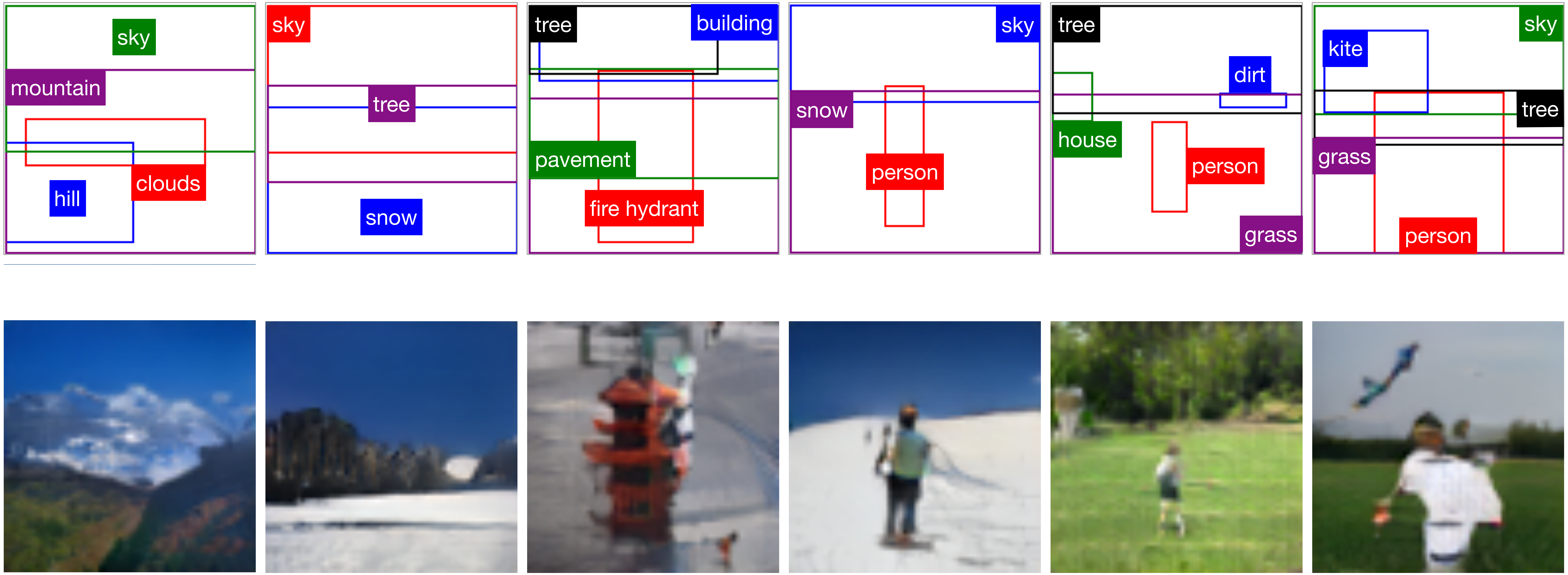
Evaluation:

Method	**Inception** Score		Object **Classification** Score		**Diversity** Score	
	COCO	VG	COCO	VG	COCO	VG
Real Images (64×64)	16.3 ± 0.4	13.9 ± 0.5	55.16	49.13	-	-
pix2pix [12]	3.5 ± 0.1	2.7 ± 0.02	12.06	9.20	0	0
sg2im (GT Layout) [13]	7.3 ± 0.1	6.3 ± 0.2	30.04	40.29	0.02 ± 0.01	0.15 ± 0.12
Ours	$\mathbf{9.1 \pm 0.1}$	$\mathbf{8.1 \pm 0.1}$	**50.84**	**48.09**	$\mathbf{0.15 \pm 0.06}$	$\mathbf{0.17 \pm 0.09}$

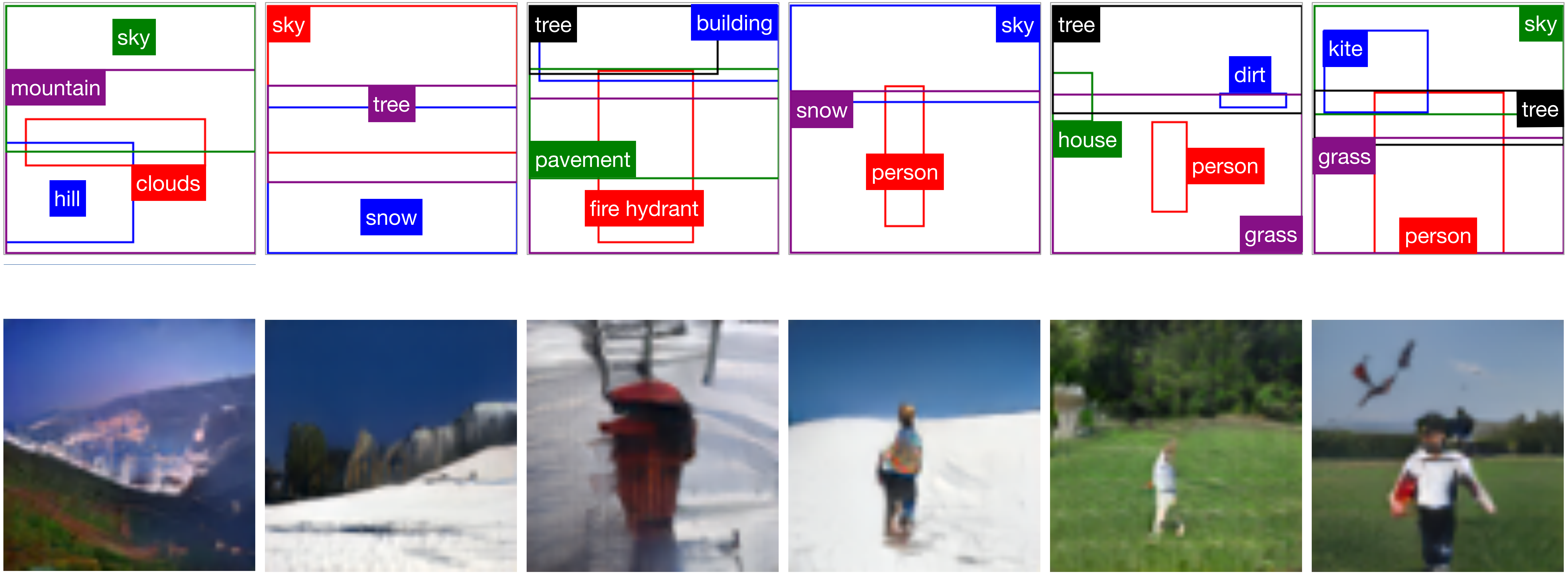
Results on COCO

Results on Visual Genome

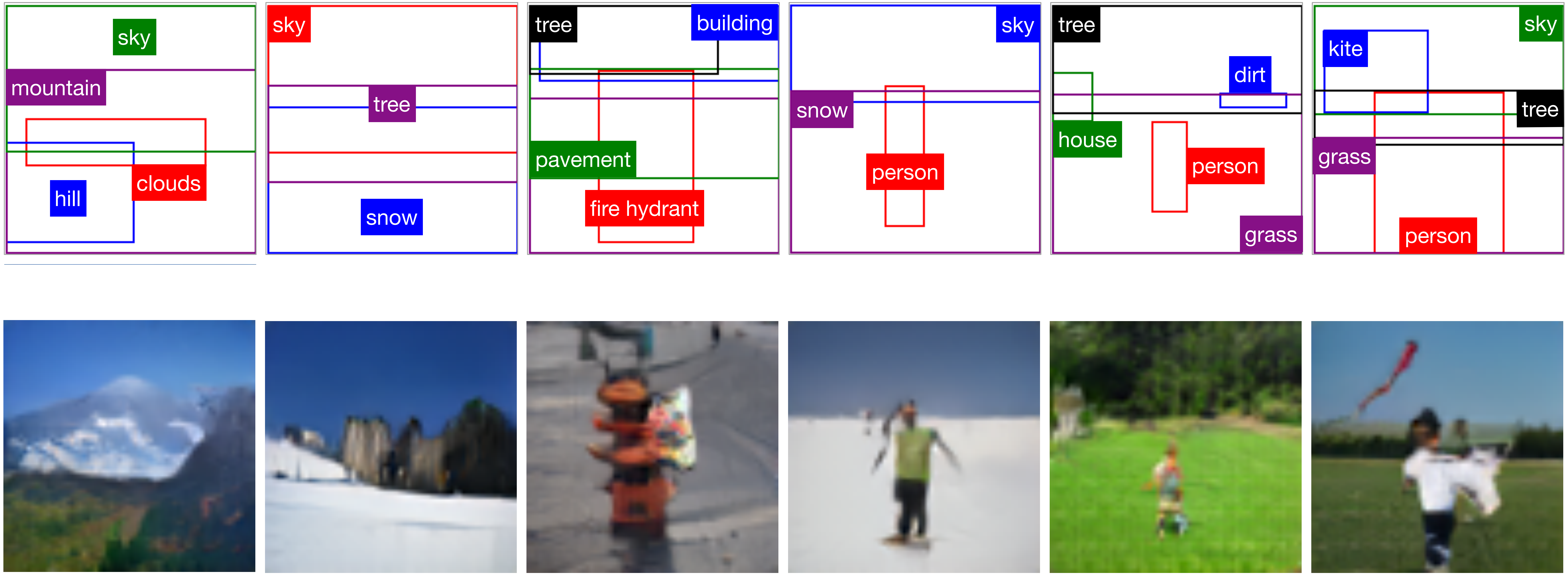
Results: Diversity



Results: Diversity



Results: Diversity



Layout to Image

Drag to draw bounding boxes and assign labels or simply load a pre-defined layout.

PERSON PERSONS INDOOR BEACH FOOD BOAT WINDOW CAR COW MONITOR

Labels

Layout

Images

GENERATE START OVER

Image Generation from Layout, Bo Zhao, Lili Meng, Weidong Yin and Leonid Sigal, CVPR 2019.

Web Application Developed by Mark (Ke) Ma

Layout to Image

Drag to draw bounding boxes and assign labels or simply load a pre-defined layout.

PERSON | PERSONS | INDOOR | BEACH | FOOD | BOAT | WINDOW | CAR | COW | MONITOR

Labels

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Images

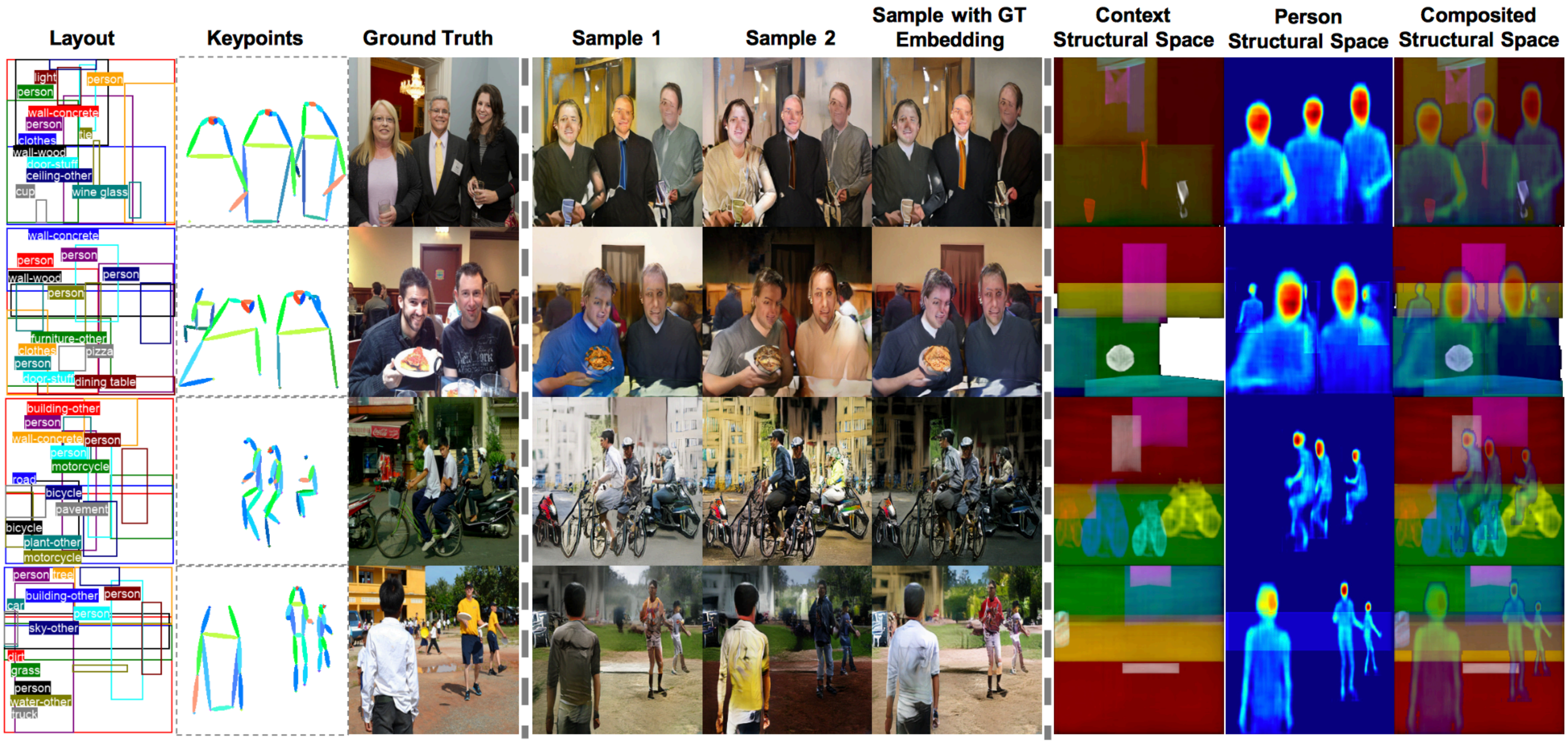
GENERATE | START OVER

Image Generation from Layout, Bo Zhao, Lili Meng, Weidong Yin and Leonid Sigal, CVPR 2019.

Web Application Developed by Mark (Ke) Ma

Extensions

[Yin et al., WACV 2021]



GANs

Don't work with an explicit density function

Take game-theoretic approach: learn to generate from training distribution through 2-player game

Pros:

— Beautiful, state-of-the-art samples!

Cons:

— Trickier / more unstable to train

— Can't solve inference queries such as p(x), p(z|x)

Active area of research:

— Better loss functions, more stable training (Wasserstein GAN, LSGAN, many others)

— Conditional GANs, GANs for all kinds of applications

Non-Convergence

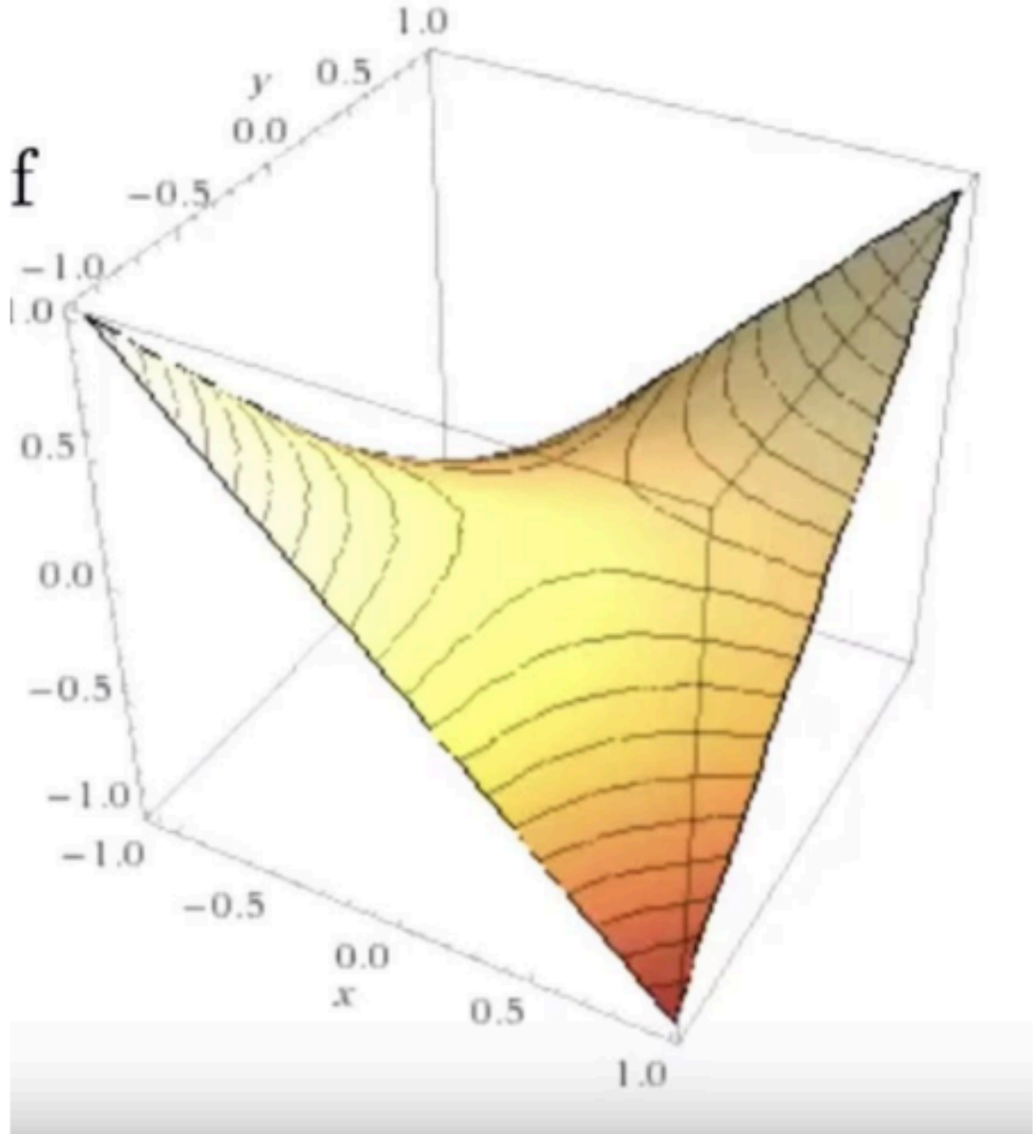
- Differential Equation's solution has sinusoidal terms
- Even with a small learning rate, it will not converge
- Discrete time gradient descent can spiral outward for large step size

D & G nullifies each others learning in every iteration

Train for a long time – without generating good quality samples

$$V(x, y) = xy$$

$$x = 0, \qquad y = 0$$



$$V(x(t), y(t)) = x(t)y(t)$$

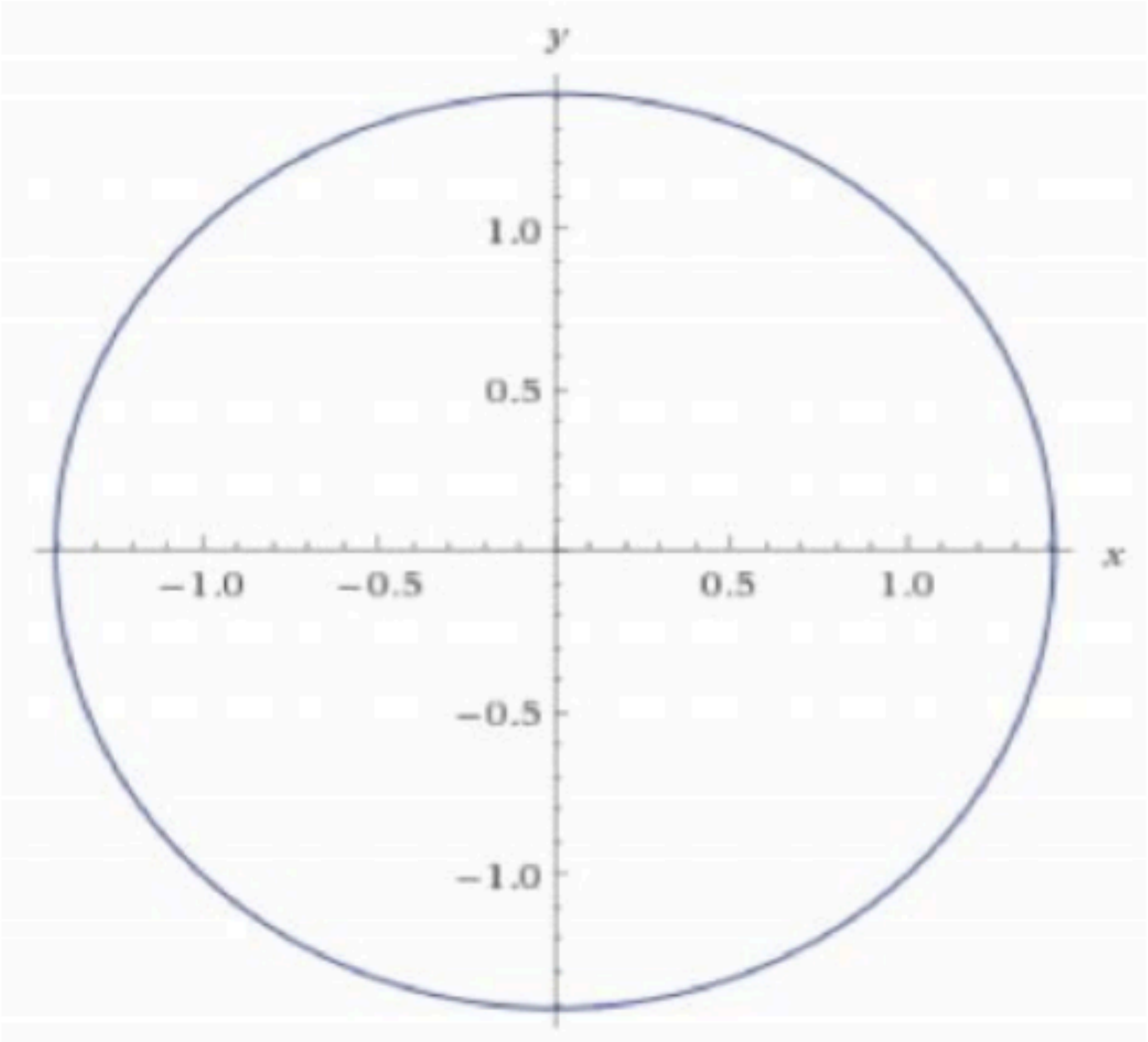
$$\frac{\partial x}{\partial t} = -y(t)$$

$$\frac{\partial y}{\partial t} = x(t)$$

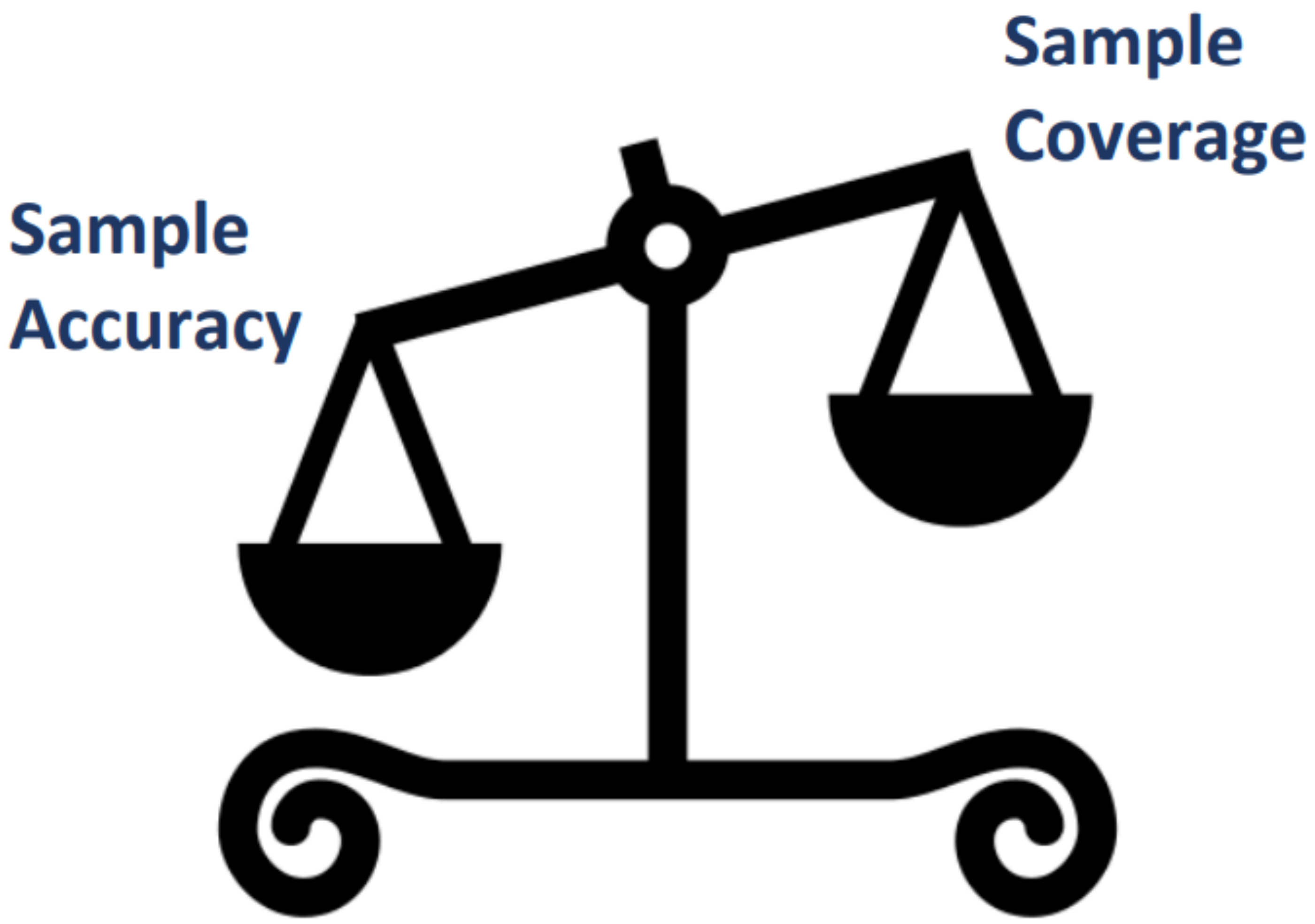
$$\frac{\partial^2 y}{\partial t^2} = \frac{\partial x}{\partial t}. = -y(t)$$

$$x(t) = x(0)cost(t) - y(0)\sin(t)$$

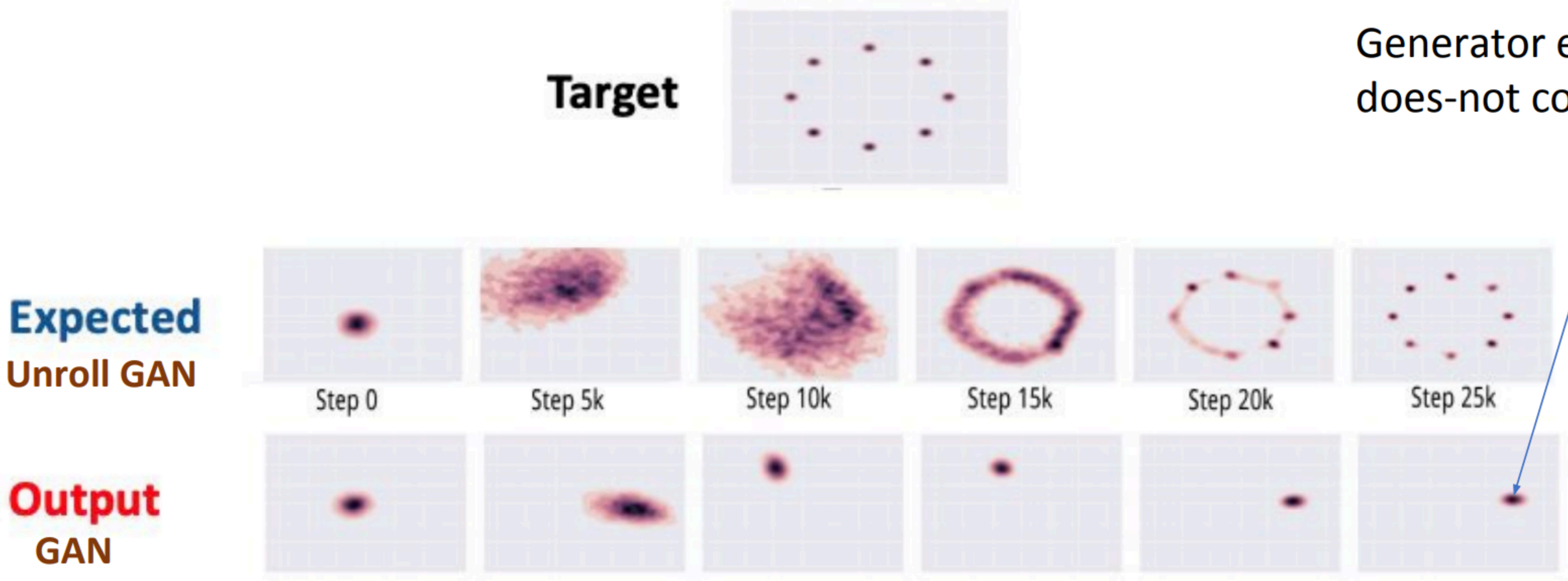
$$y(t) = x(0)cost(t) - y(0)\sin(t)$$



Mode Collapse



Generator excels in a subspace but does-not cover entire real distribution



Luke et al. 2016

Why **GANs** are hard to train?

- — Generator keeps generating similar images — so nothing to learn
- — Maintain trade-off of generating more **accurate** vs. high **coverage** samples
- — Two learning tasks need to have balance to achieve stability
  - — If the **discriminator** is not sufficiently trained — it can worsen generator
  - — If the **discriminator** is too good — will produce no gradients

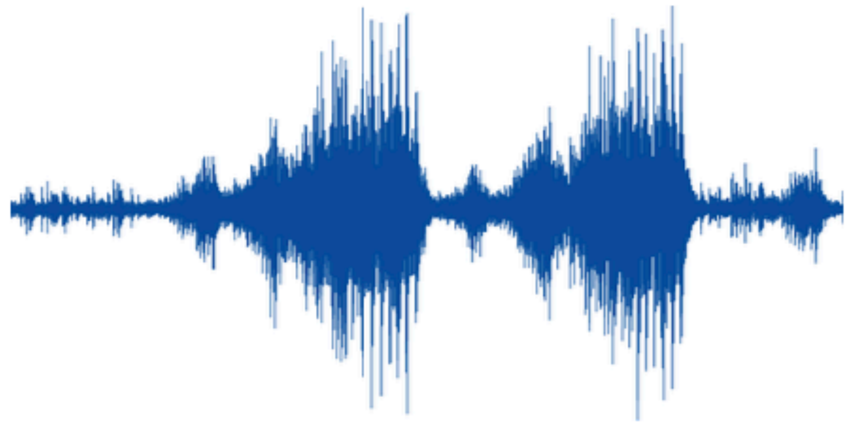
Topics in AI (CPSC 532S):
Multimodal Learning with Vision, Language and Sound

Lecture 19: Graph Neural Networks

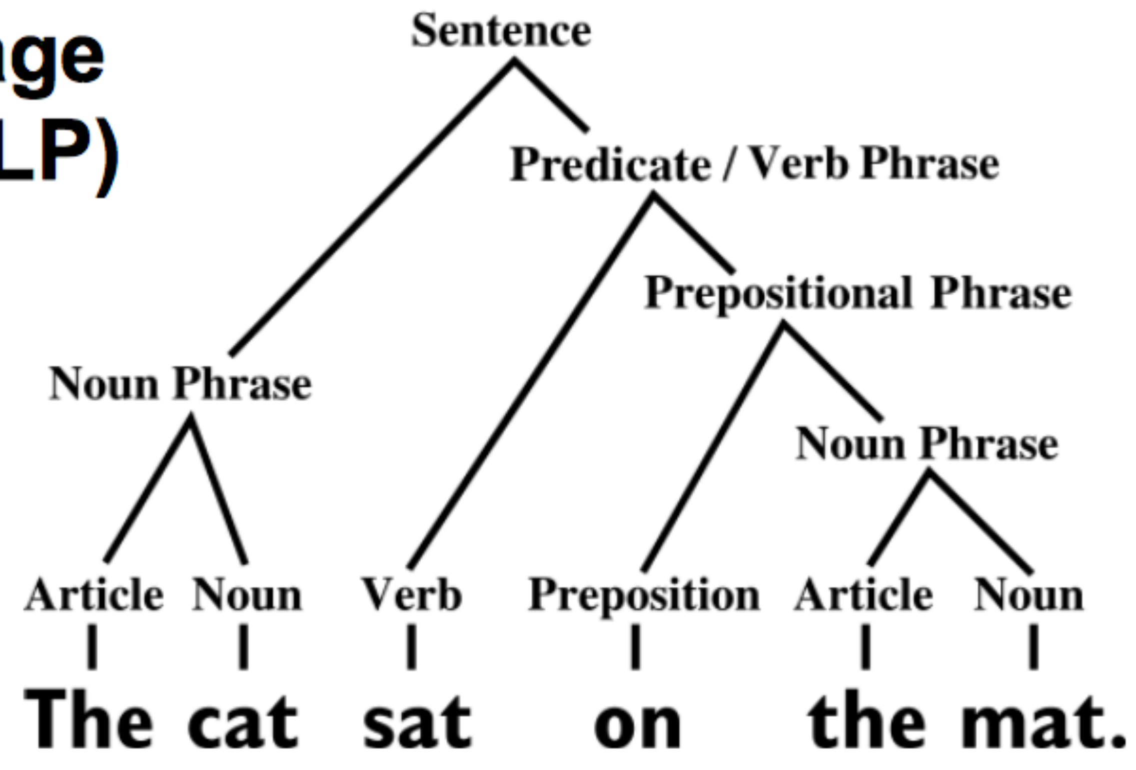
Traditional **Neural Networks**

IMAGENET

Speech data



Natural language processing (NLP)



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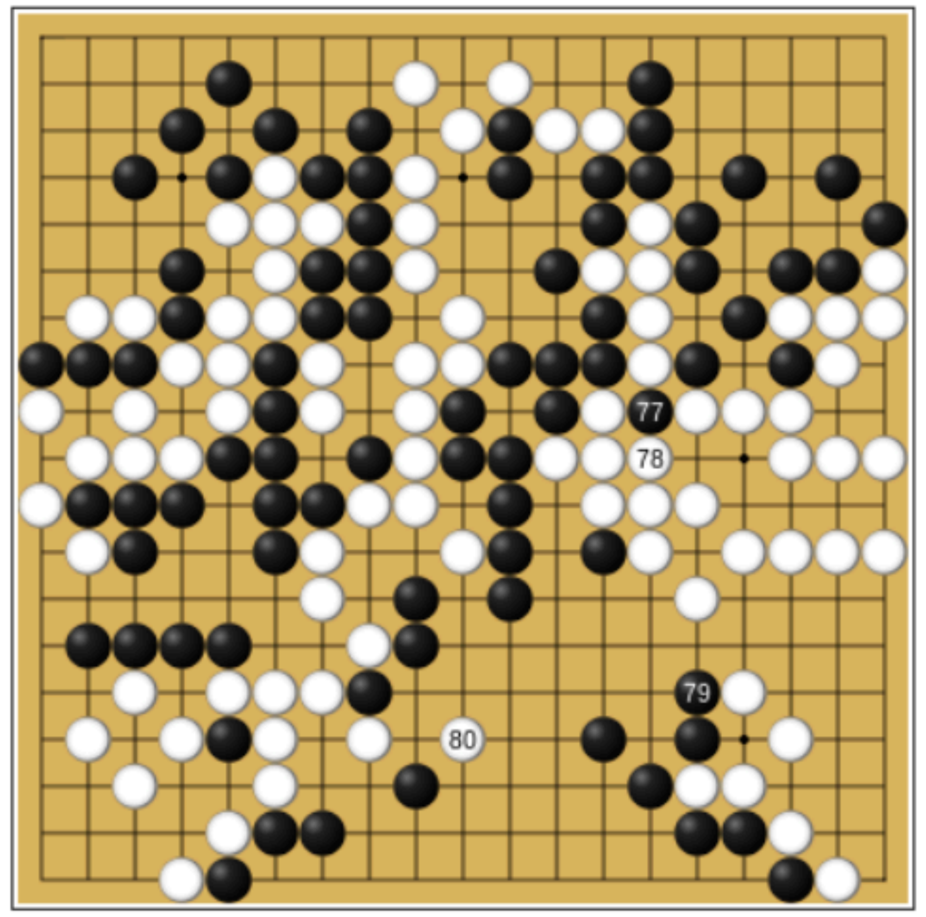
Grid games



Deep neural nets that exploit:

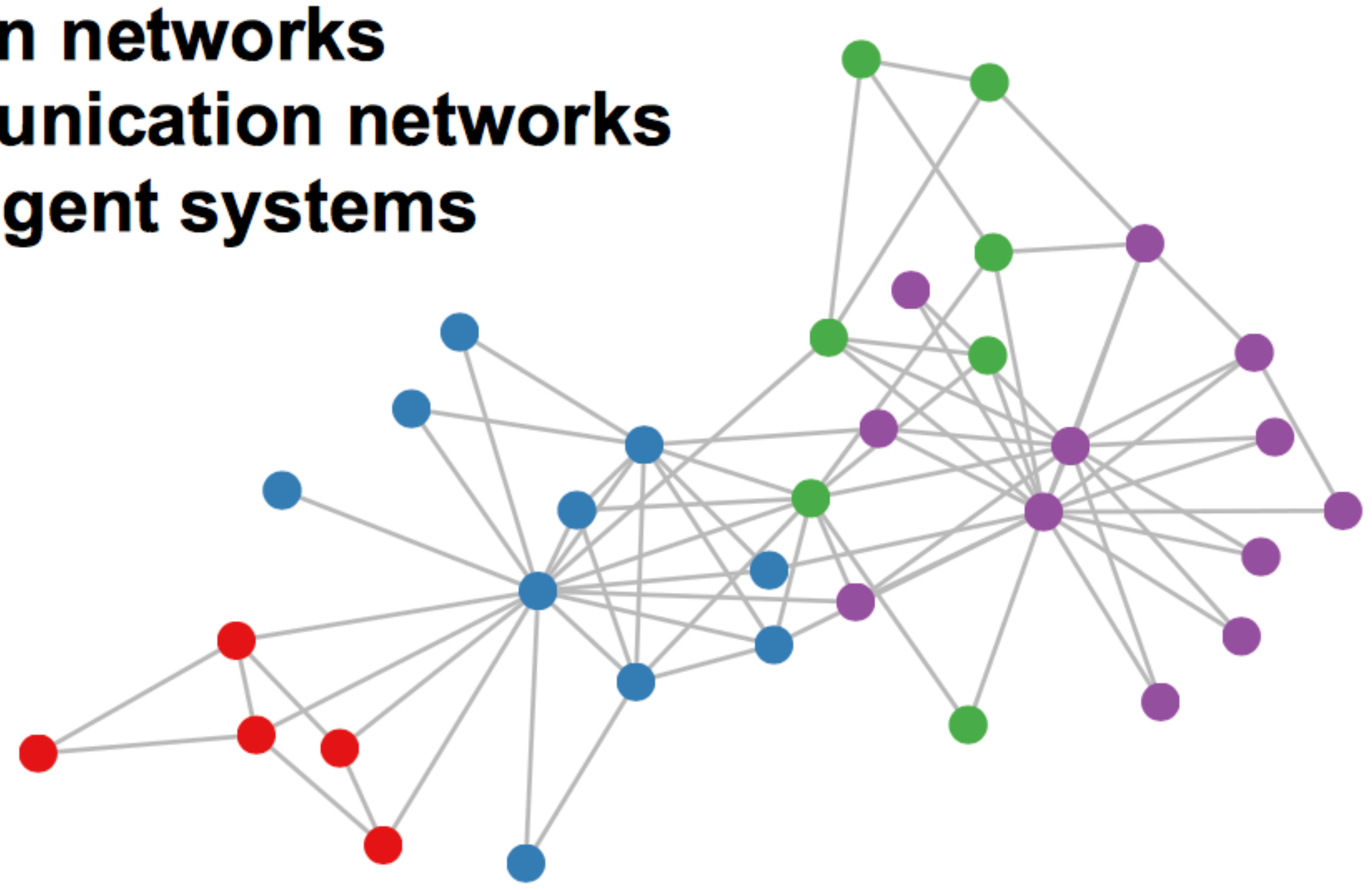
- translation equivariance (weight sharing)
- hierarchical compositionality

* slide from Thomas Kipf, **University of Amsterdam**

Graph-structured Data

A lot of real-world data does not “live” on grids

Social networks
Citation networks
Communication networks
Multi-agent systems



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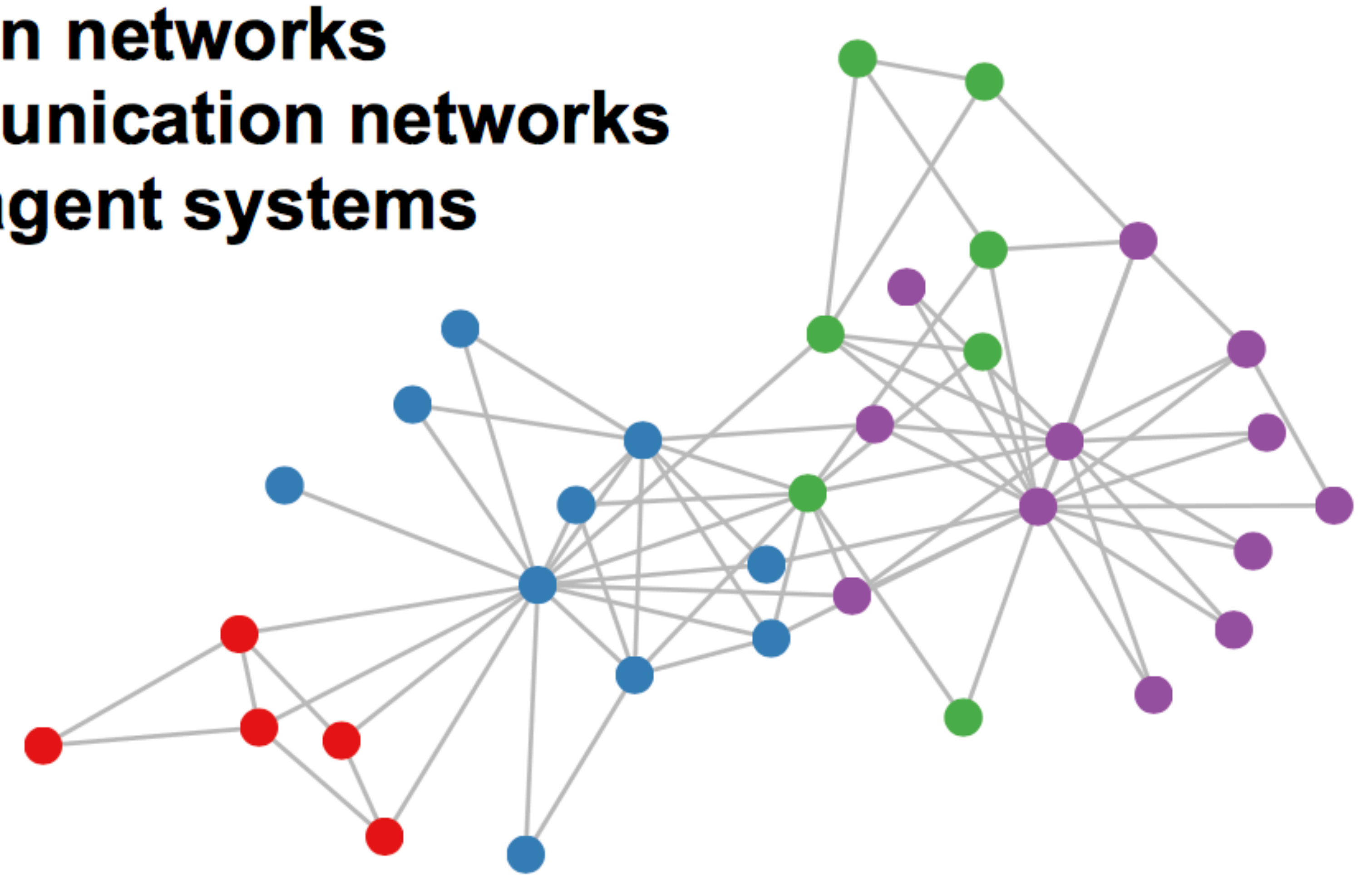
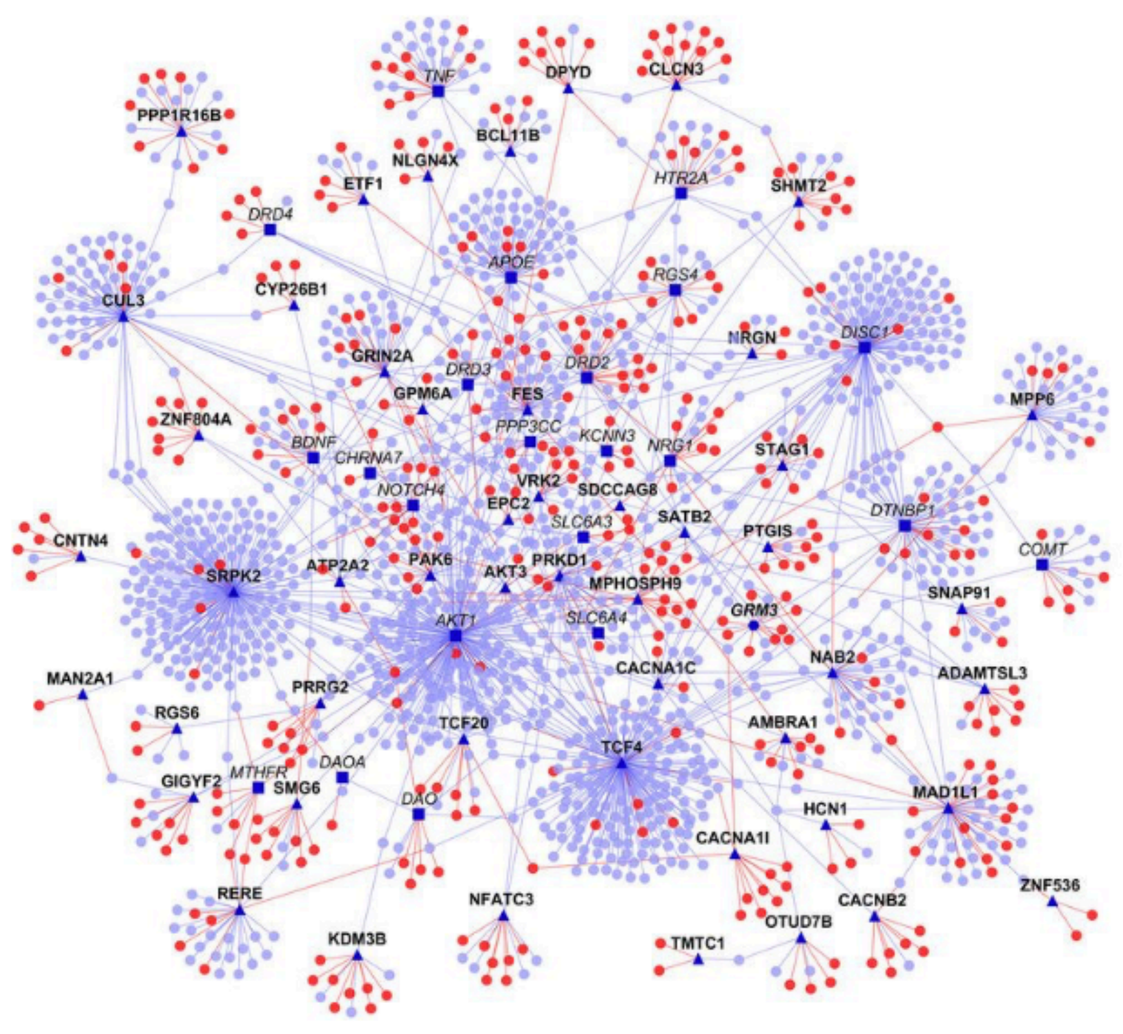


Protein interaction networks



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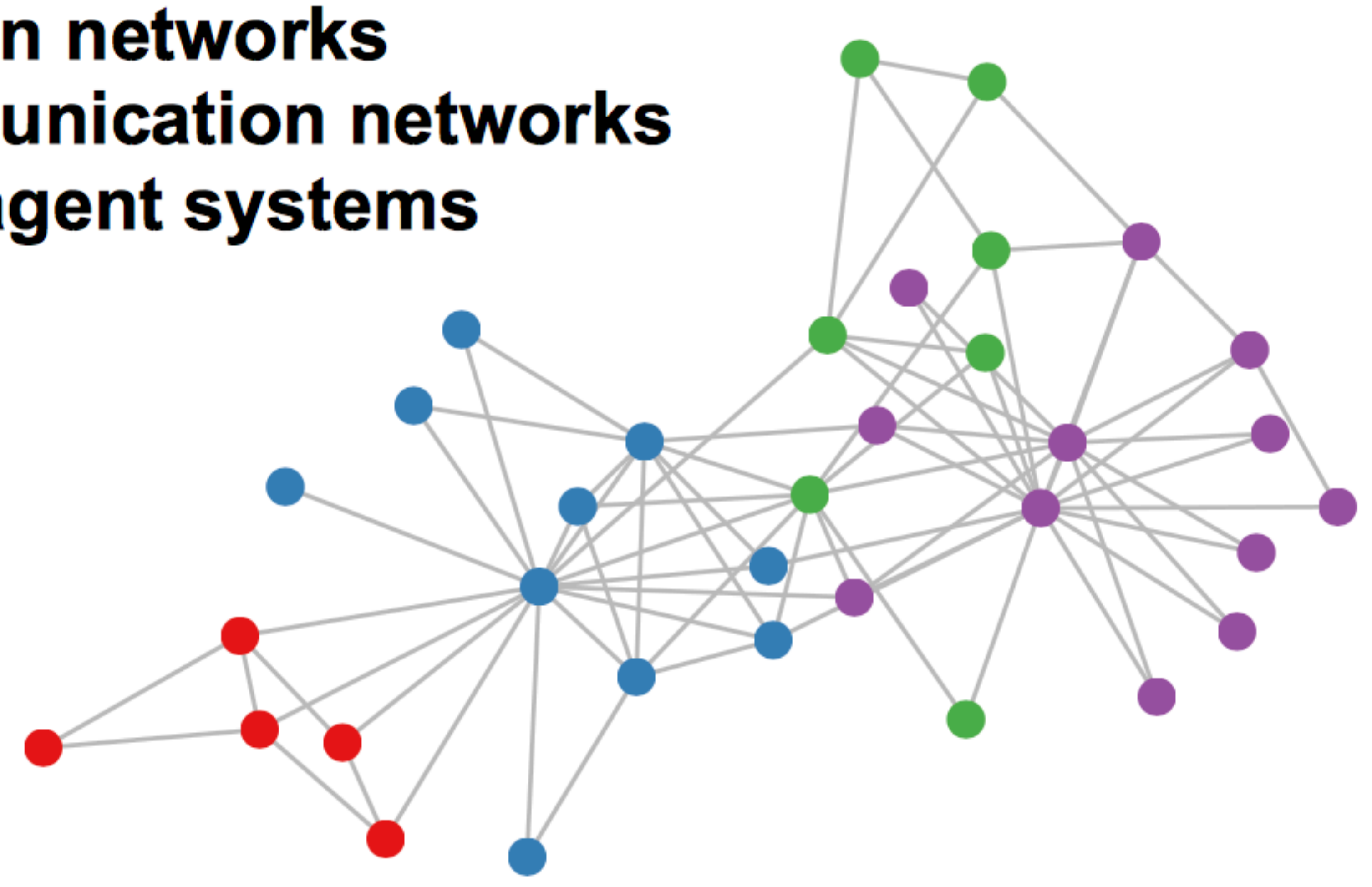
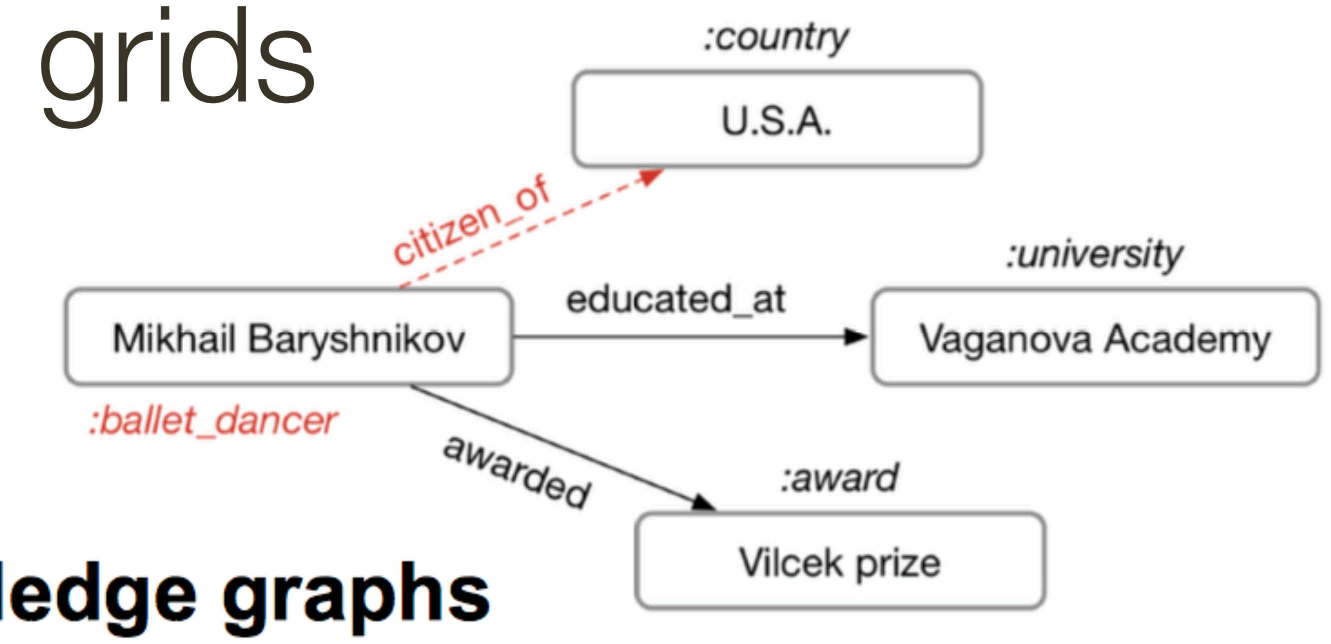
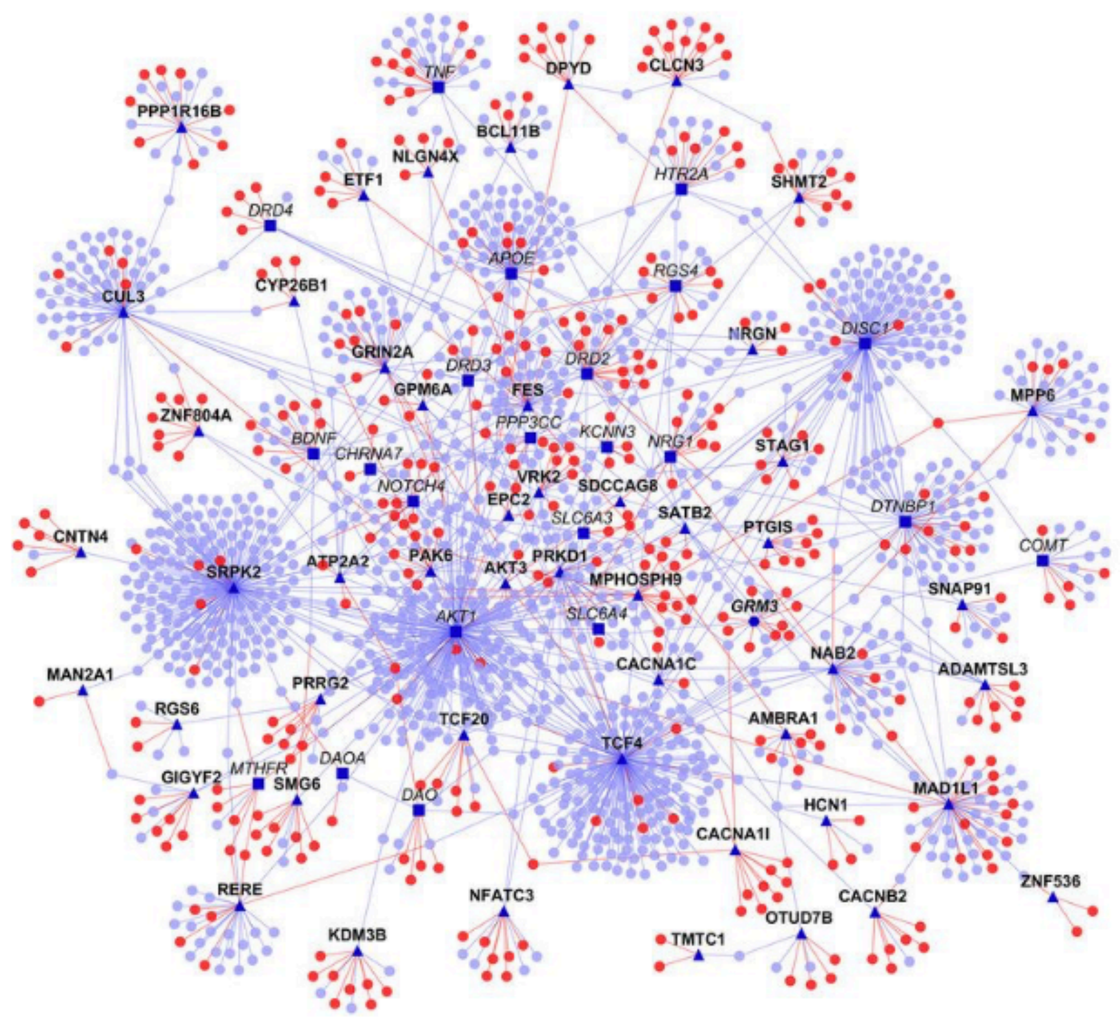




Knowledge graphs



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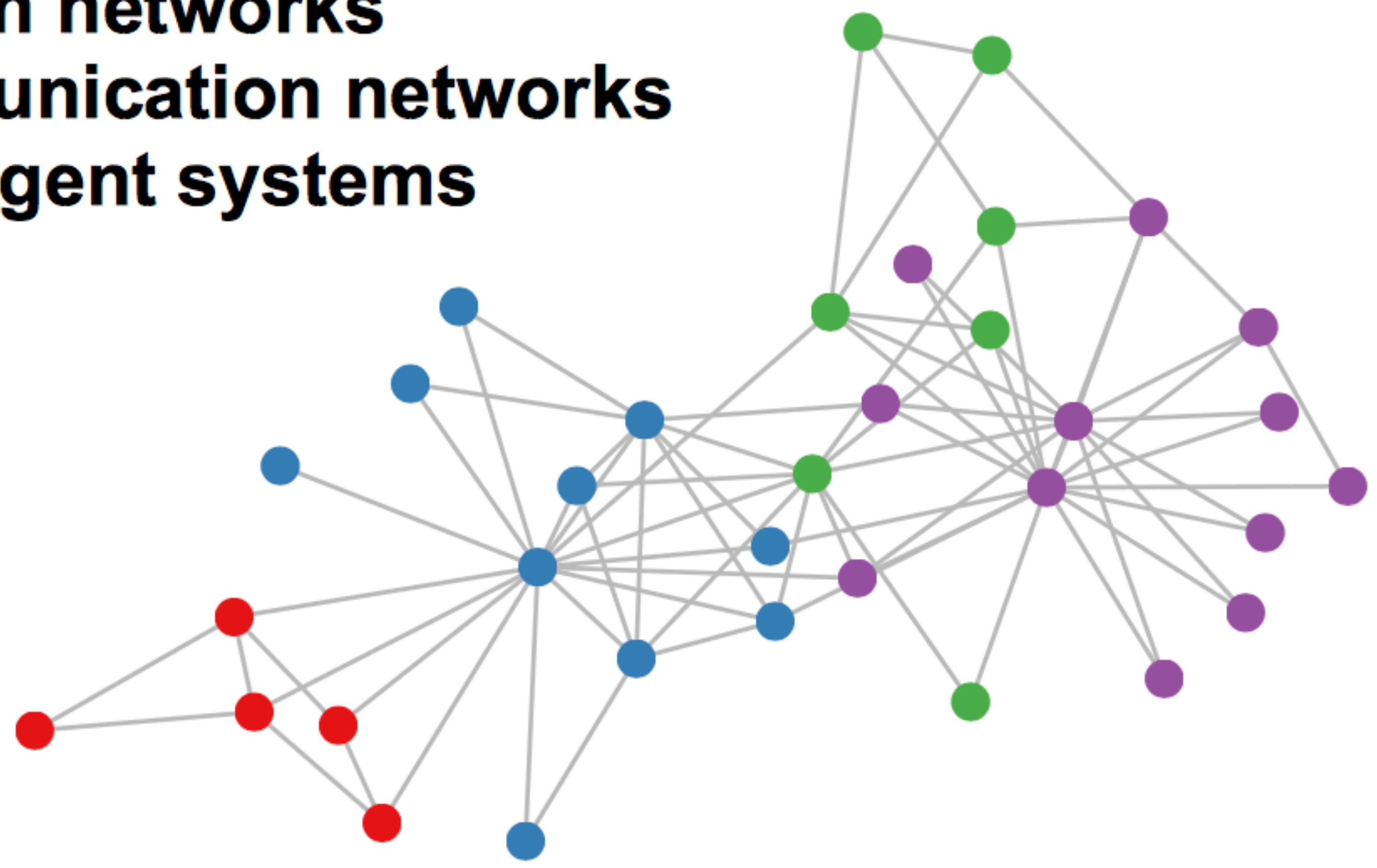

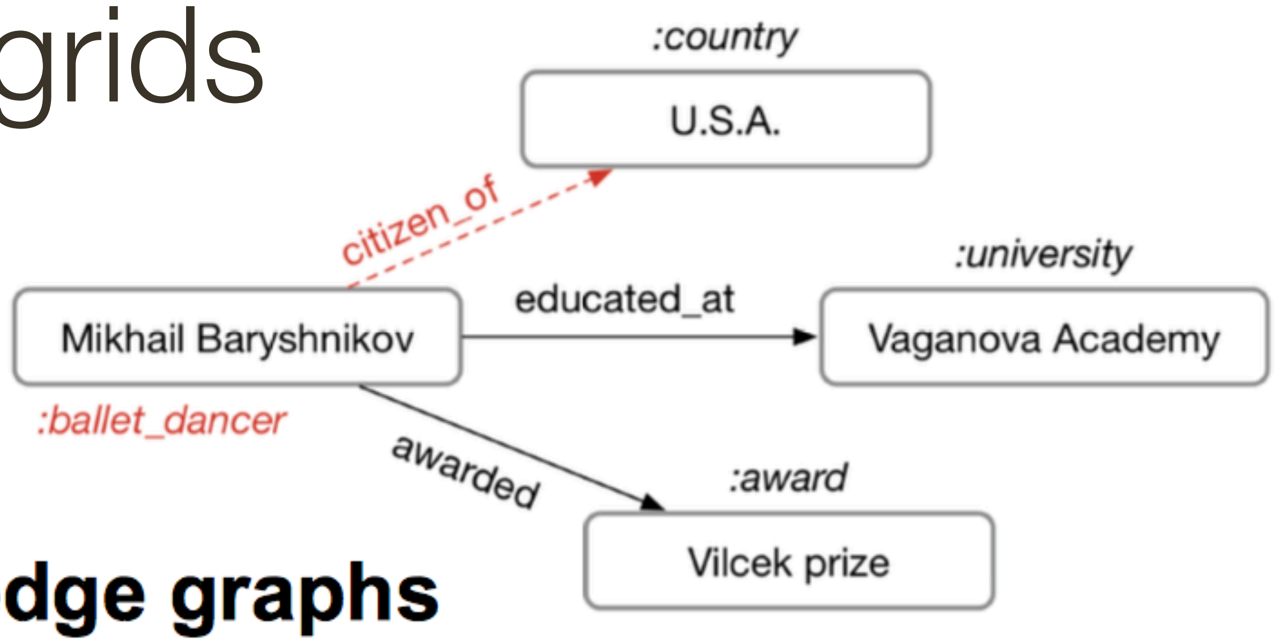

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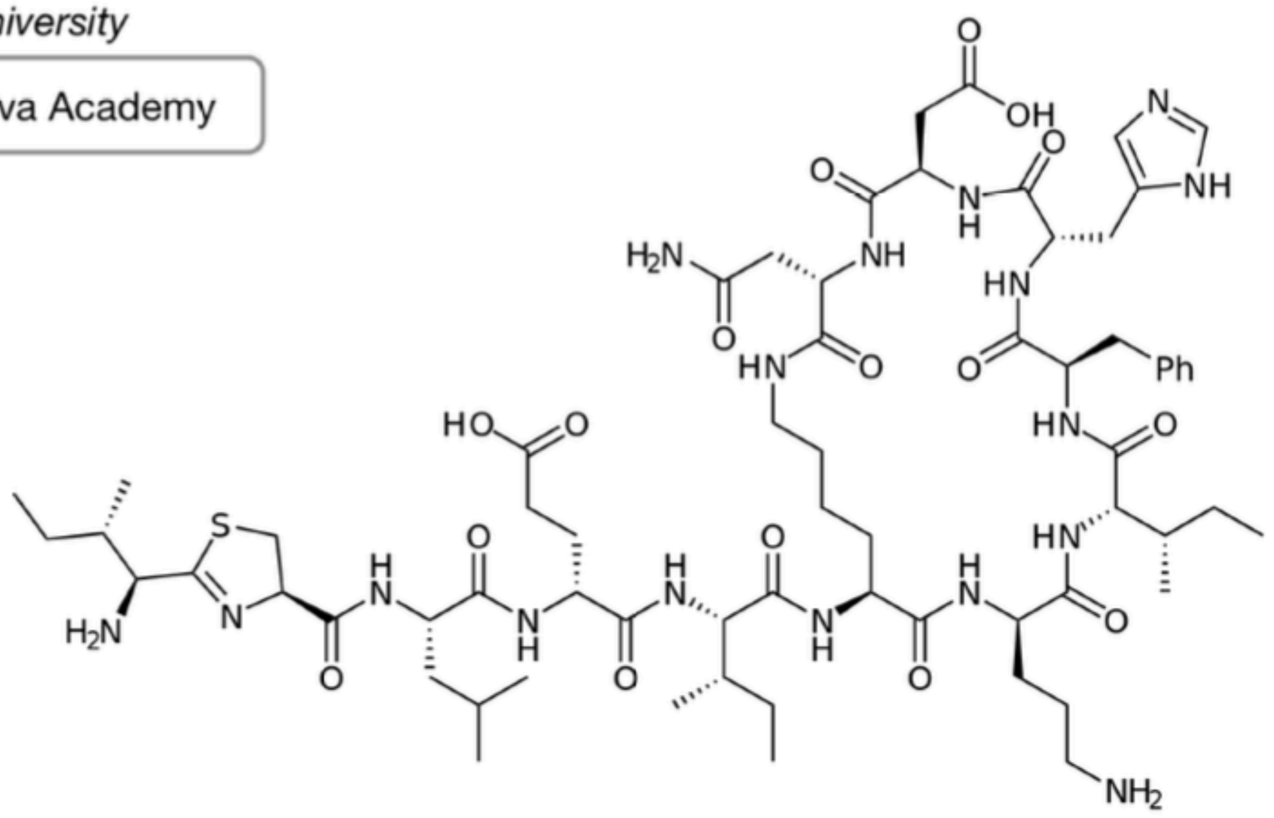
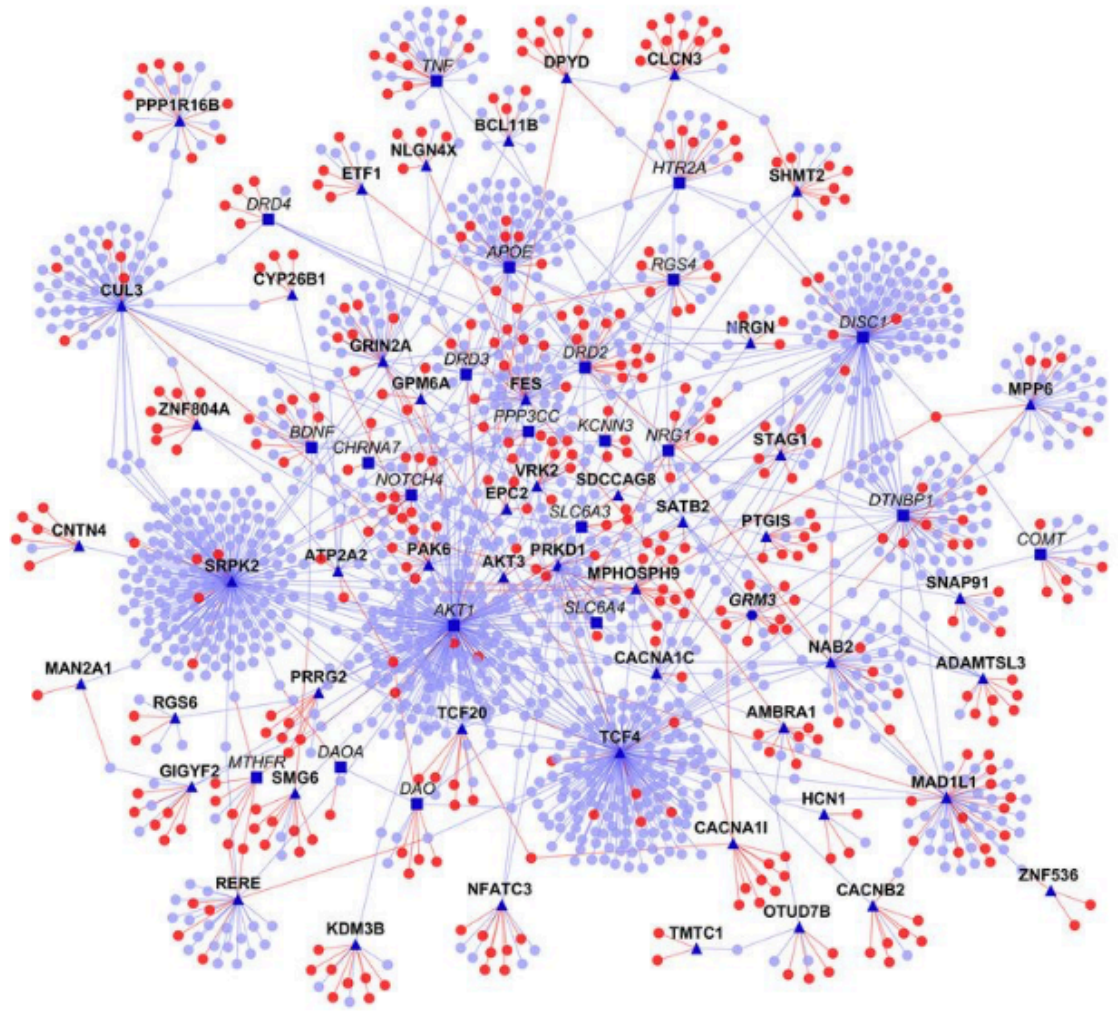
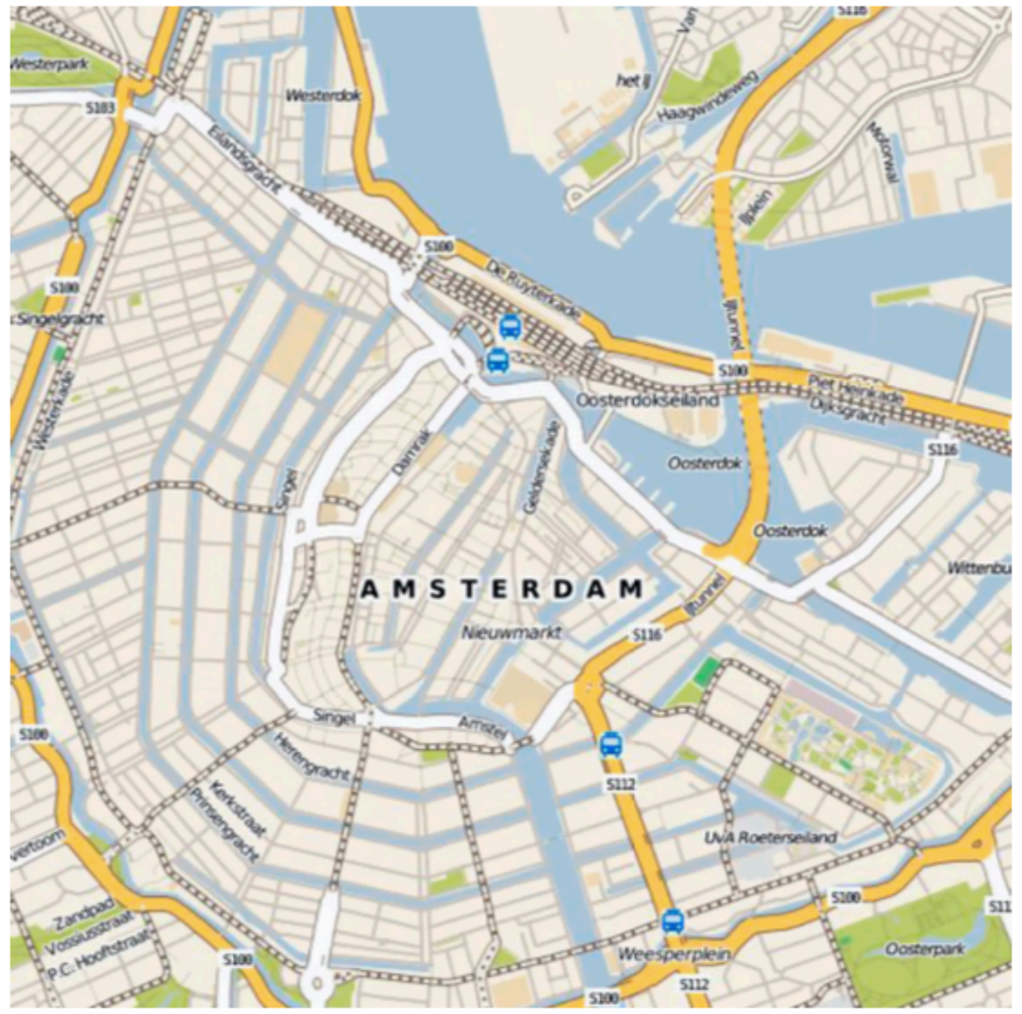


Molecules

Protein interaction networks



Road maps



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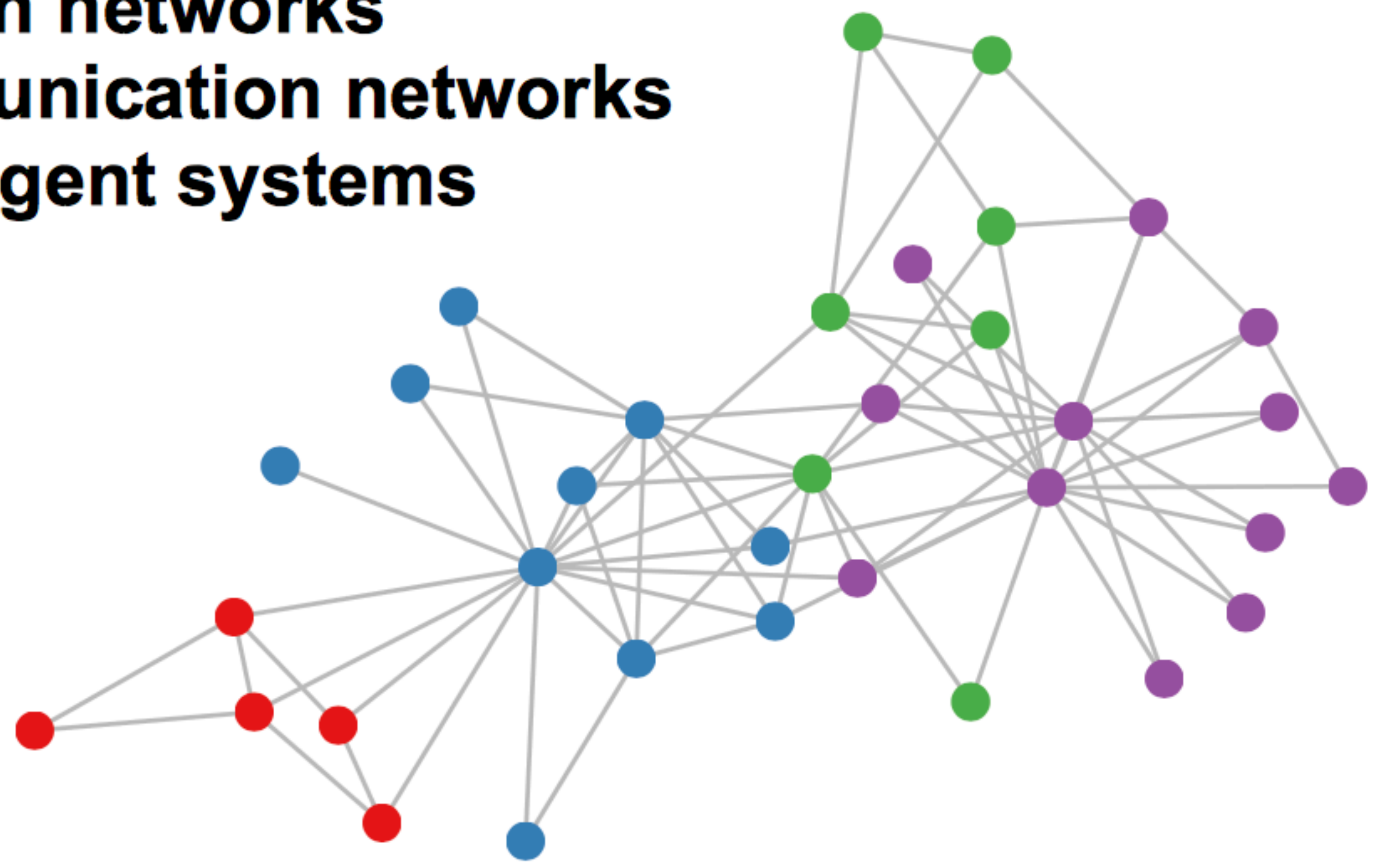

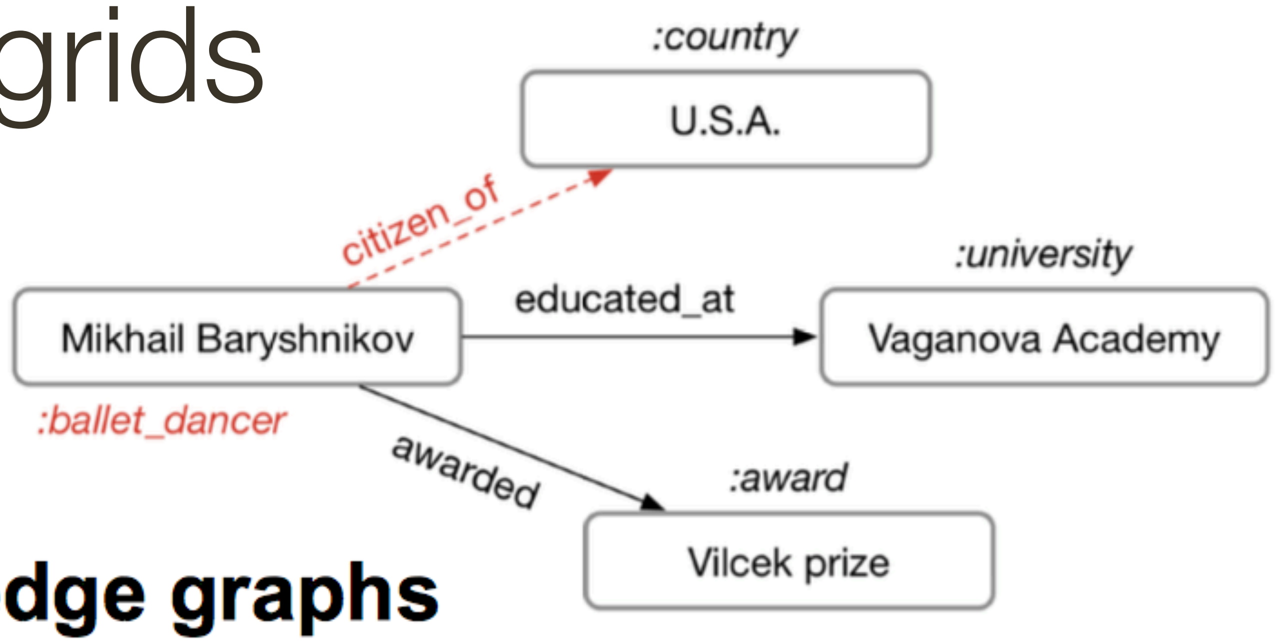

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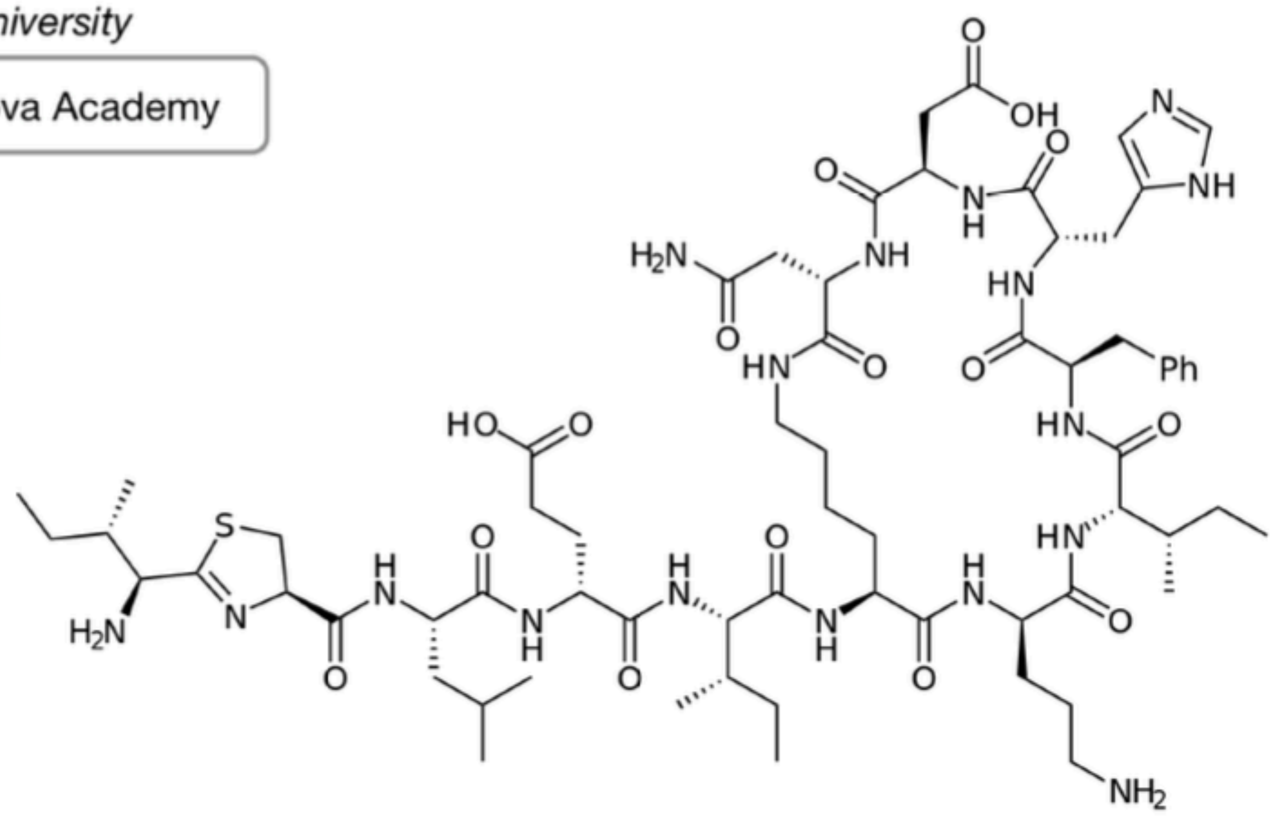

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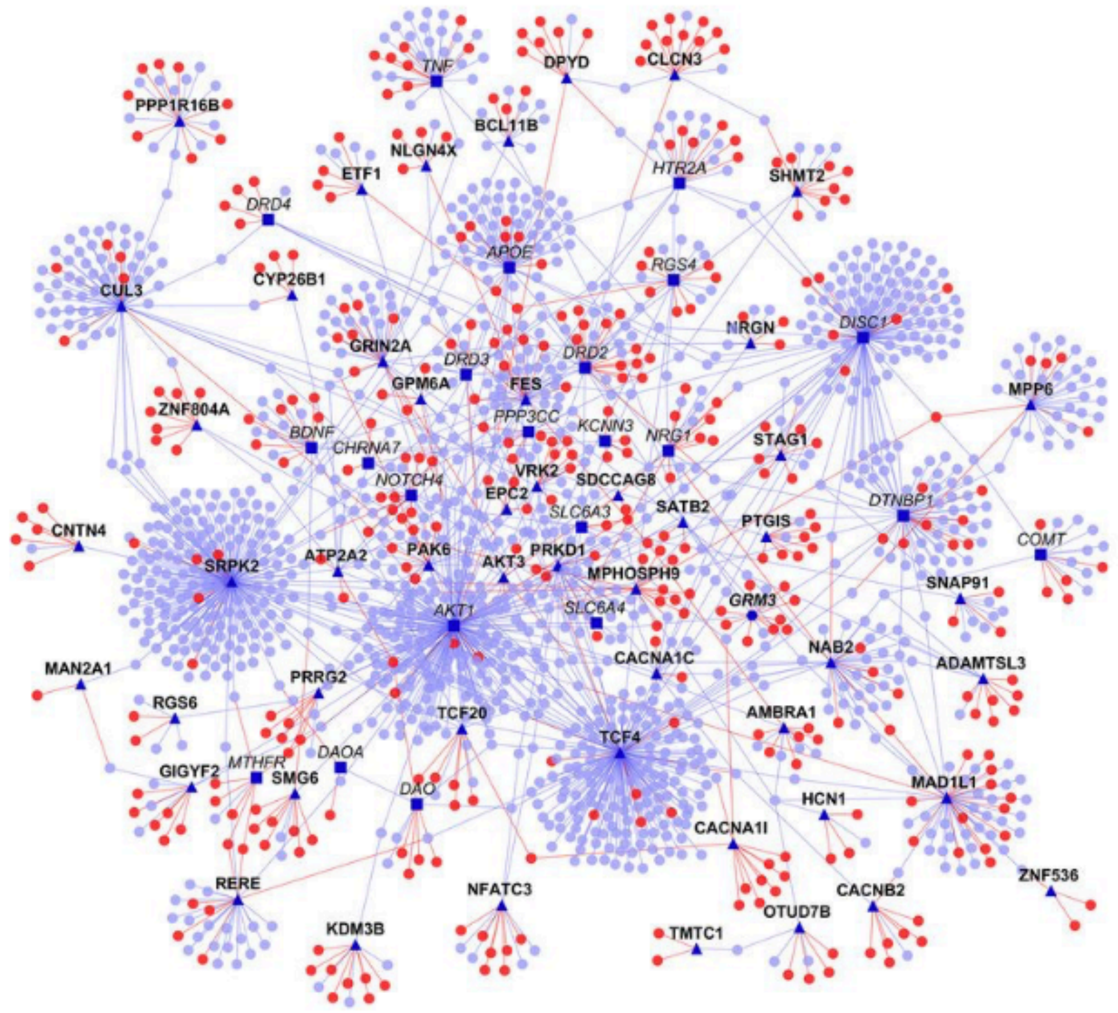
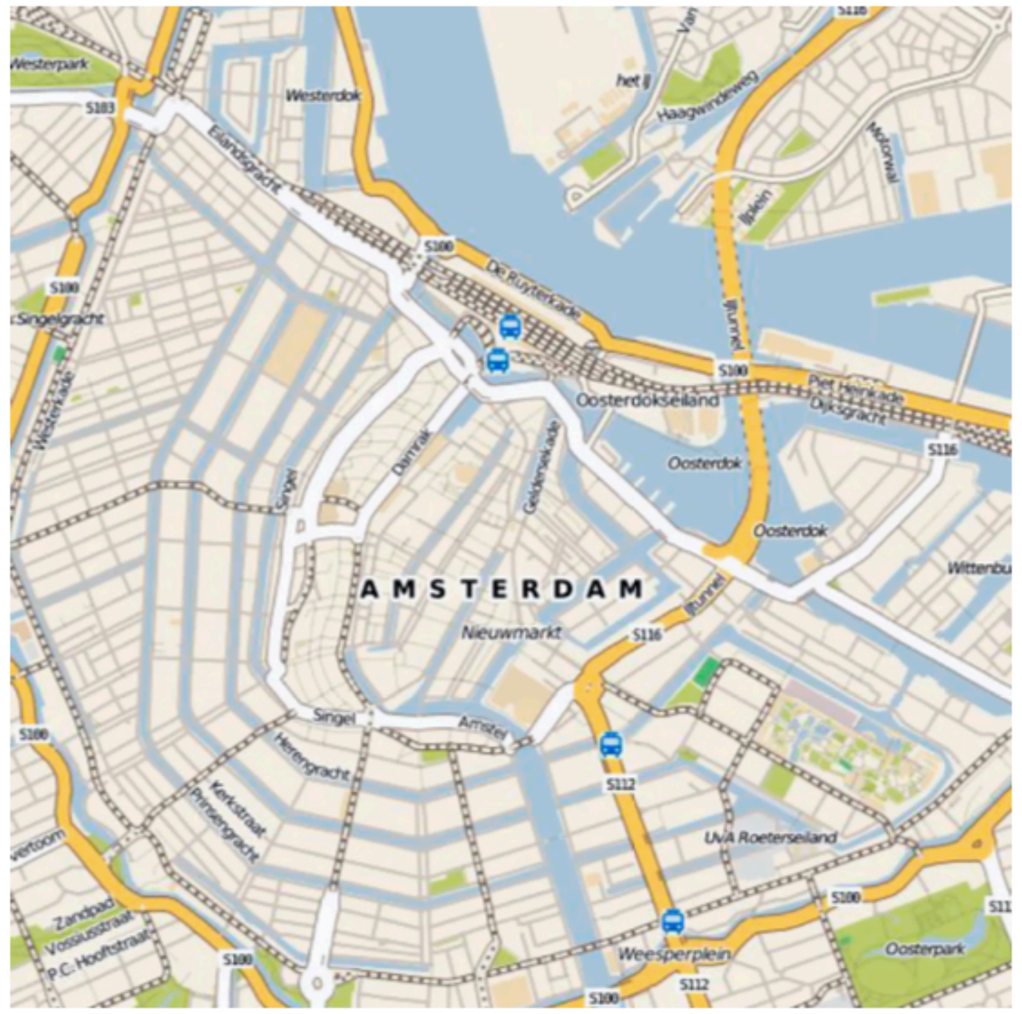


Protein interaction networks



Road maps

Standard **CNN** and **RNN** architectures don’t work on this data

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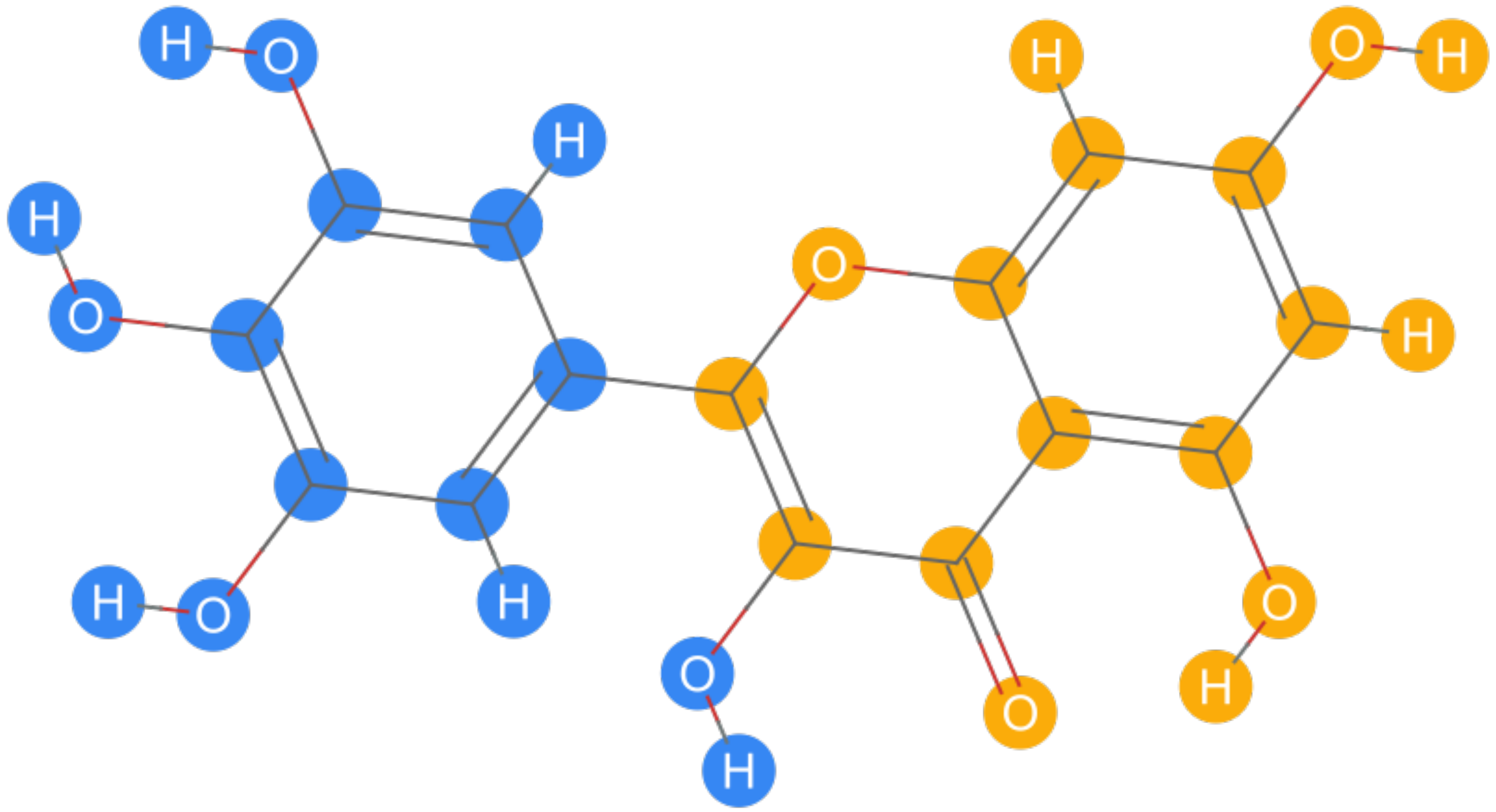
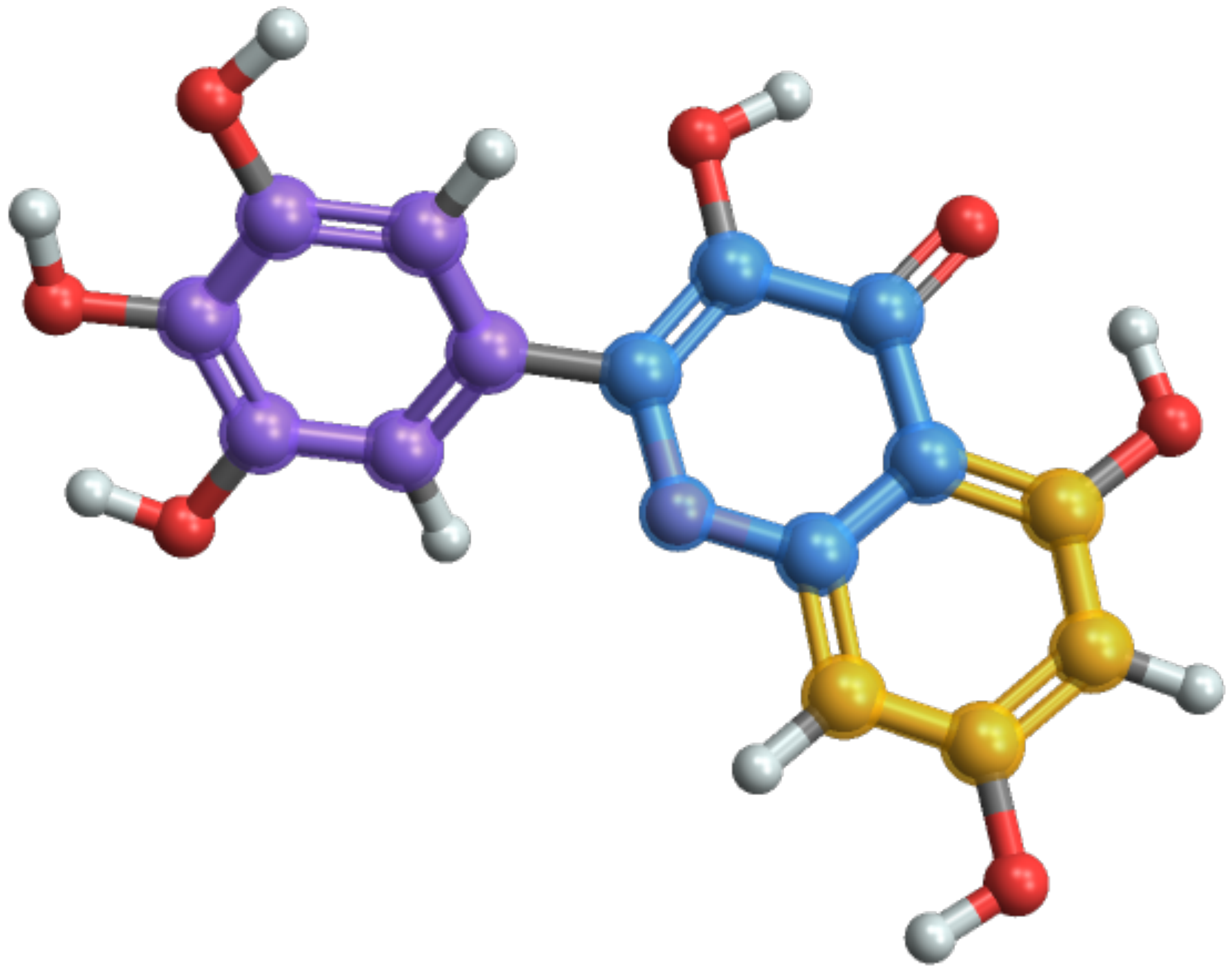
Graph-structured Data — Molecular Data





Characteristics:

— Nodes have different types (atoms)

— Edges have types and there could be multiple edges (types of bonds)

Image Credit: https://www.wolfram.com/language/12/molecular-structure-and-computation/molecule-graphs.html.en?product=mathematica
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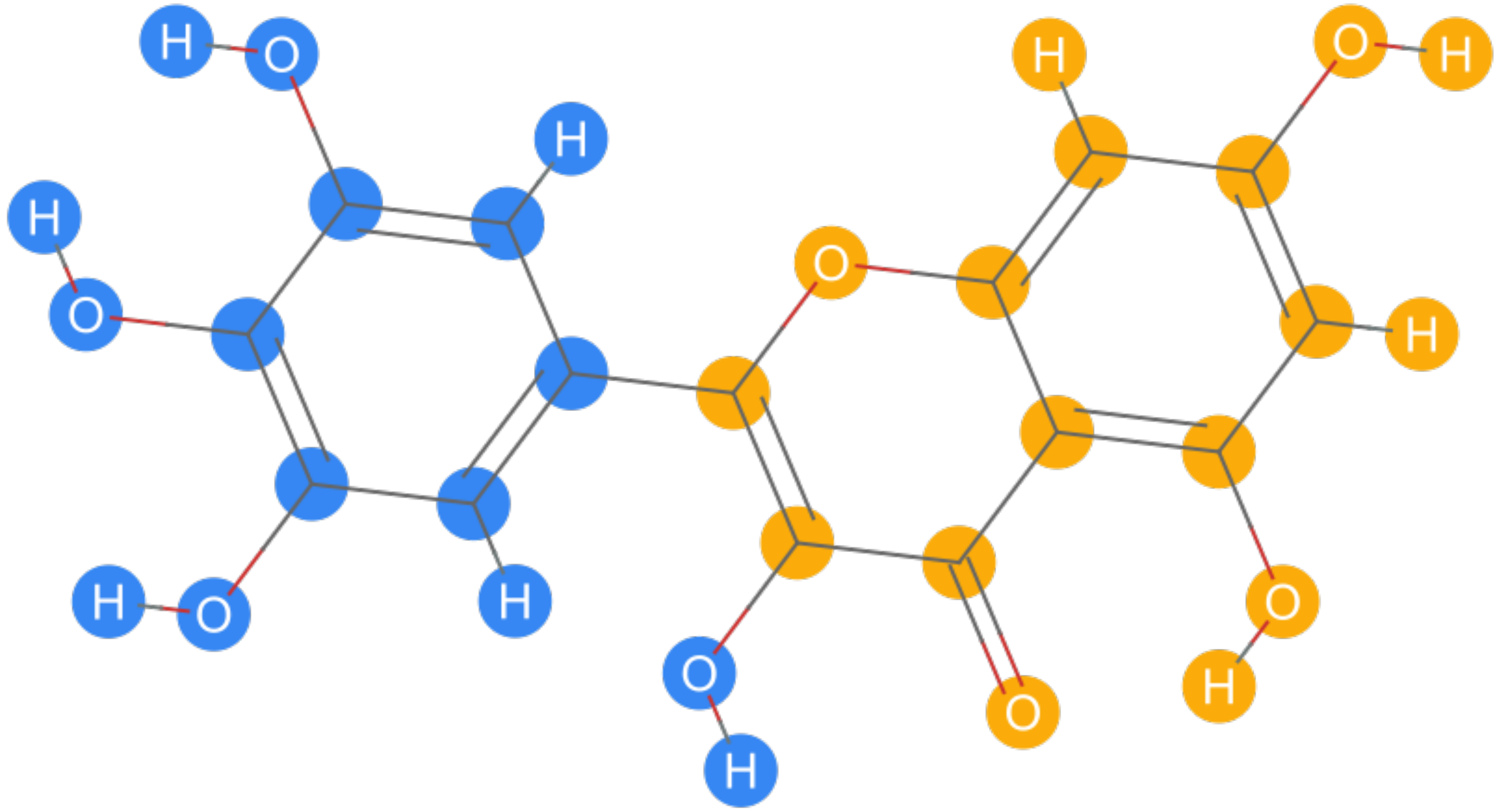

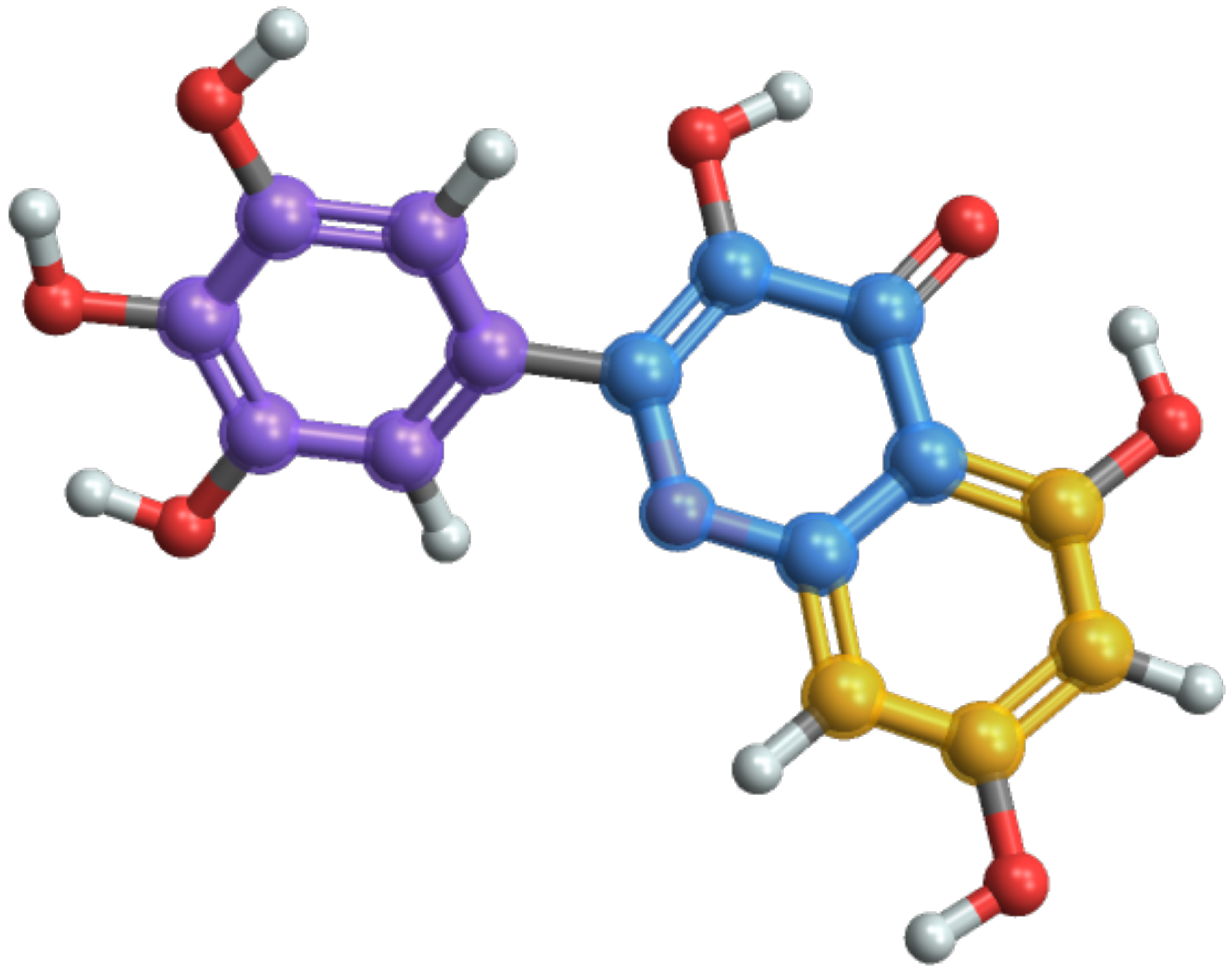

Problems:

- Molecule property prediction (physiology, physical chemistry, quantum mechanics)
- Molecular scoring or docking (pharmacology — screening of drug candidates)
- Molecular dynamics (e.g., position or motion of atoms)

Image Credit: https://www.wolfram.com/language/12/molecular-structure-and-computation/molecule-graphs.html.en?product=mathematica
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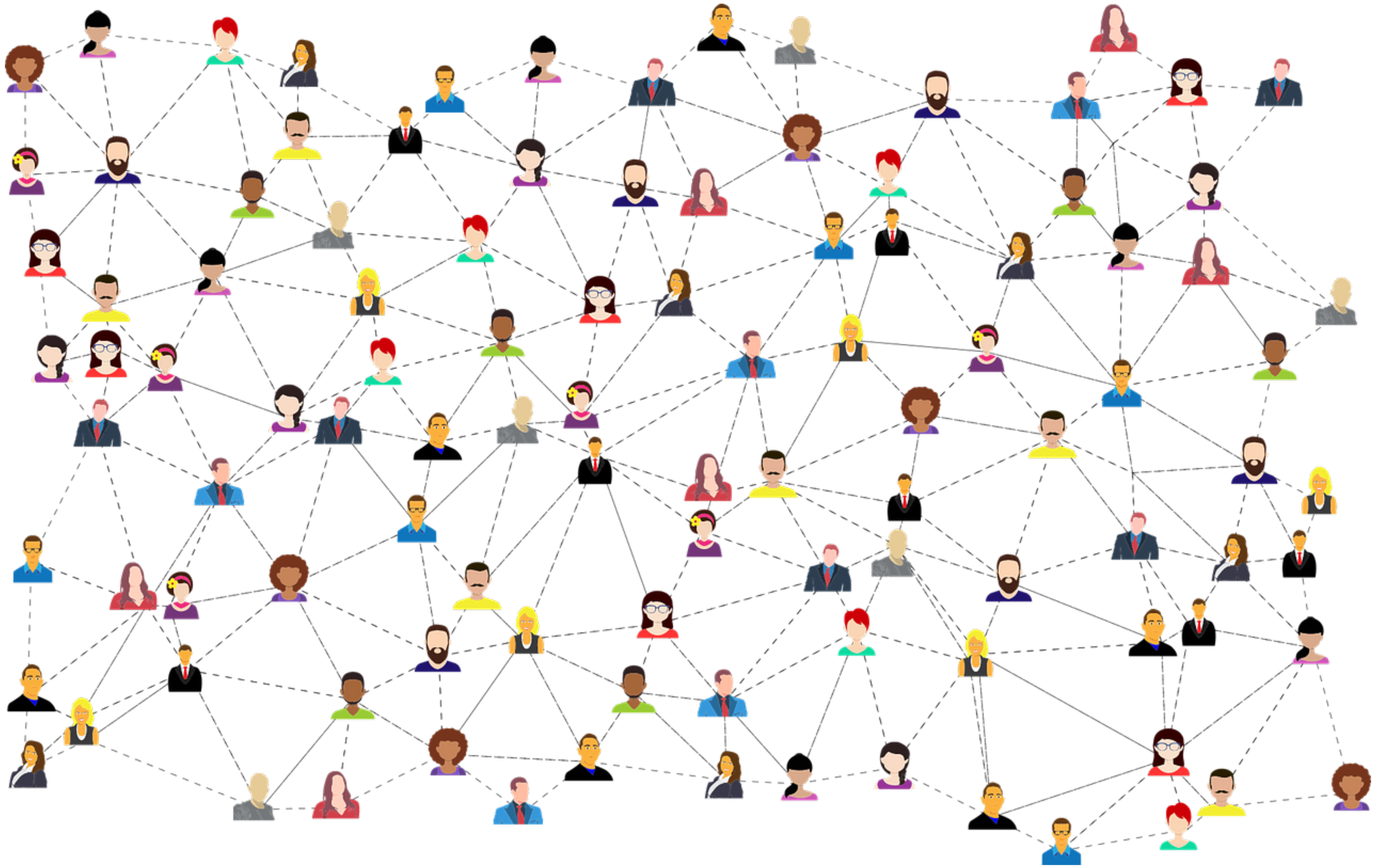
Graph-structured Data — Social Networks



Problems:

Link prediction

Image Credit: http://blog.soton.ac.uk/hive/2012/05/10/recommendation-system-of-hive/

Graph-structured Data — Network Recommendation

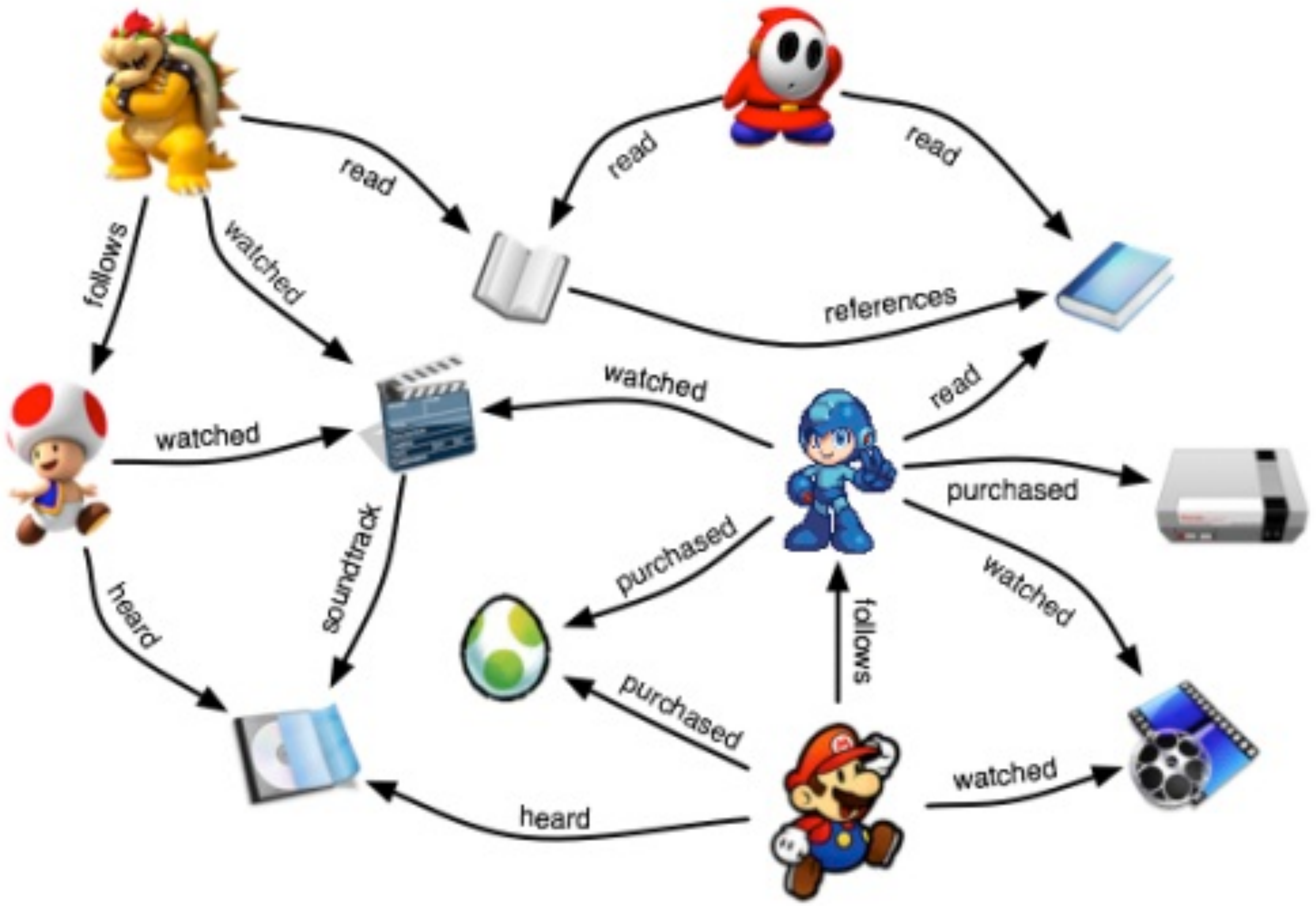


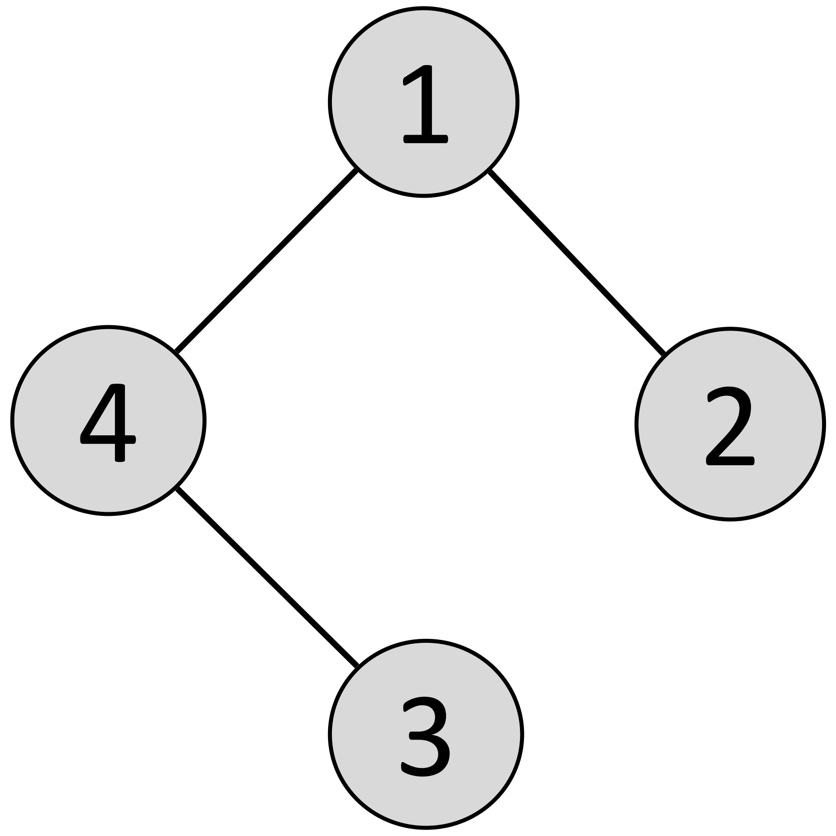
Image Credit: https://www.science.org/doi/10.1126/sciadv.aau4212

Graph **Representations**

Connectivity

— Adjacency List: $\mathcal{G} = (\mathcal{V}, \mathcal{E})$

— Adjacency Matrix: A (sometimes we have weights)



V = {1,2,3,4}, E = {(1,2), (1,4), (4,3)}

	1	2	3	4
1	0	1	0	1
2	1	0	0	0
3	0	0	0	1
4	1	0	1	0

Feature

— Node Feature: X

— Edge Feature

— Graph Feature

Graph Data: (A, X)

- Adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$
- Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times F}$

Slide from Renjie Liao

Graph **Isomorphism**

Permutation

V = [1,2,3,4] => V’ = [2,1,3,4]

E = [(1,2), (1,4), (4,3)] => E’ = [(2,1), (2,4), (4,3)]

Permute Rows

	1	2	3	4
1	0	1	0	0
2	1	0	0	0
3	0	0	1	0
4	0	0	0	1

Permutation Matrix

	1	2	3	4
1	0	1	0	1
2	1	0	0	0
3	0	0	0	1
4	1	0	1	0

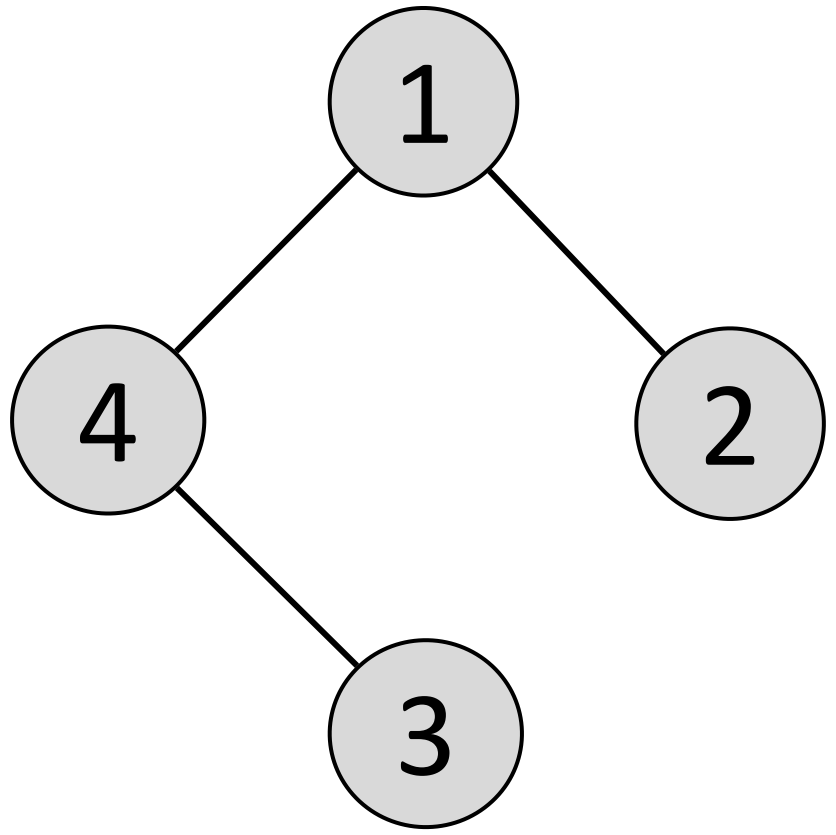
Original Adj Matrix

Permute Columns

	1	2	3	4
1	0	1	0	0
2	1	0	0	0
3	0	0	1	0
4	0	0	0	1

Transposed Permutation Matrix

=



	1	2	3	4
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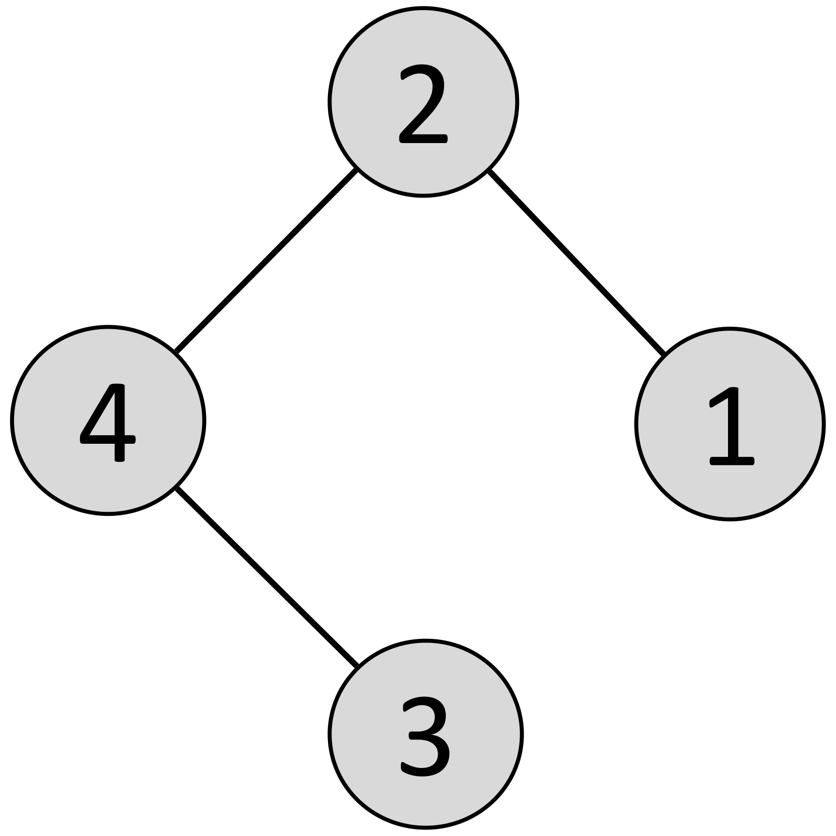
V = {1,2,3,4}, E = {(1,2), (1,4), (4,3)}



	1	2	3	4
1	0	1	0	1
2	1	0	0	0
3	0	0	0	1
4	1	0	1	0

V = {2,1,3,4}, E = {(2,1), (2,4), (4,3)}

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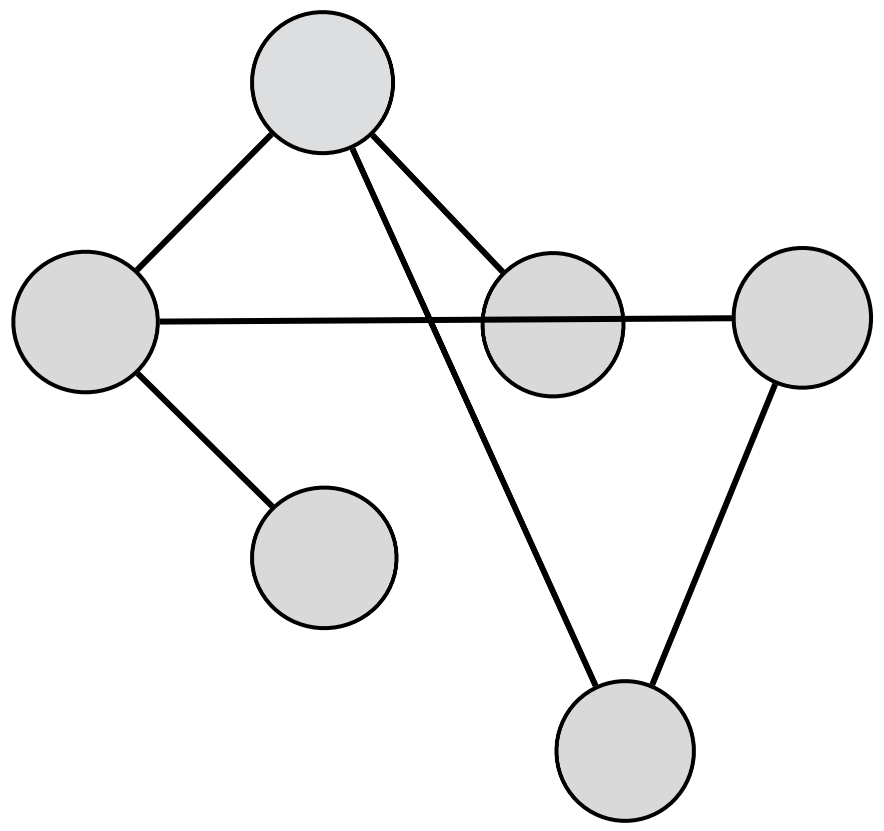
Challenge #1: **Unordered** Neighborhoods



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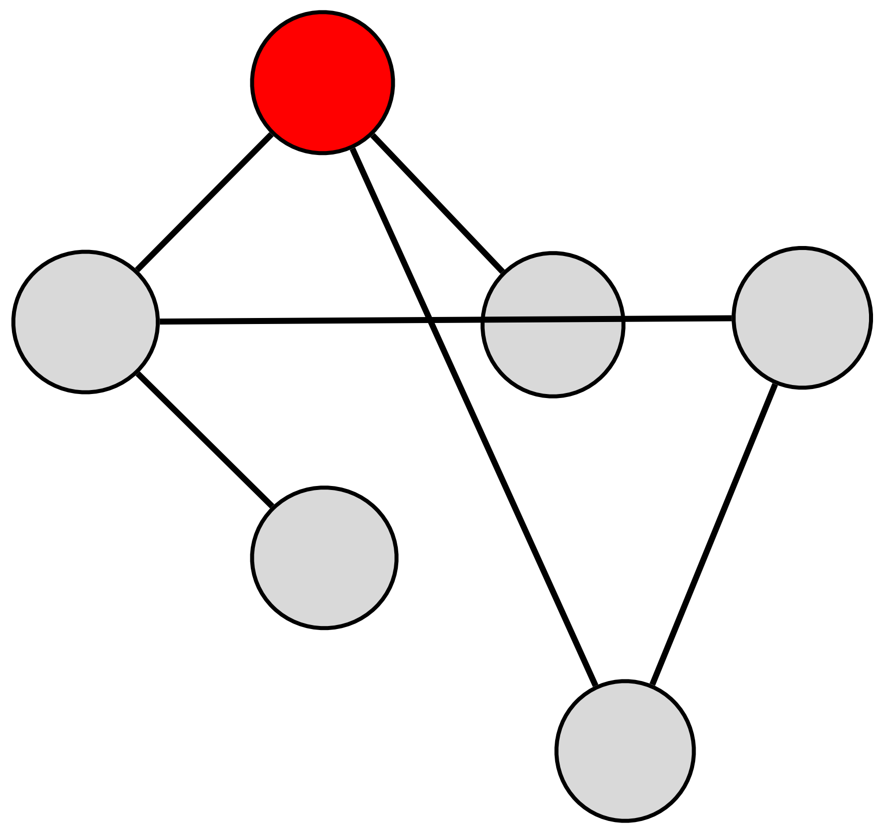

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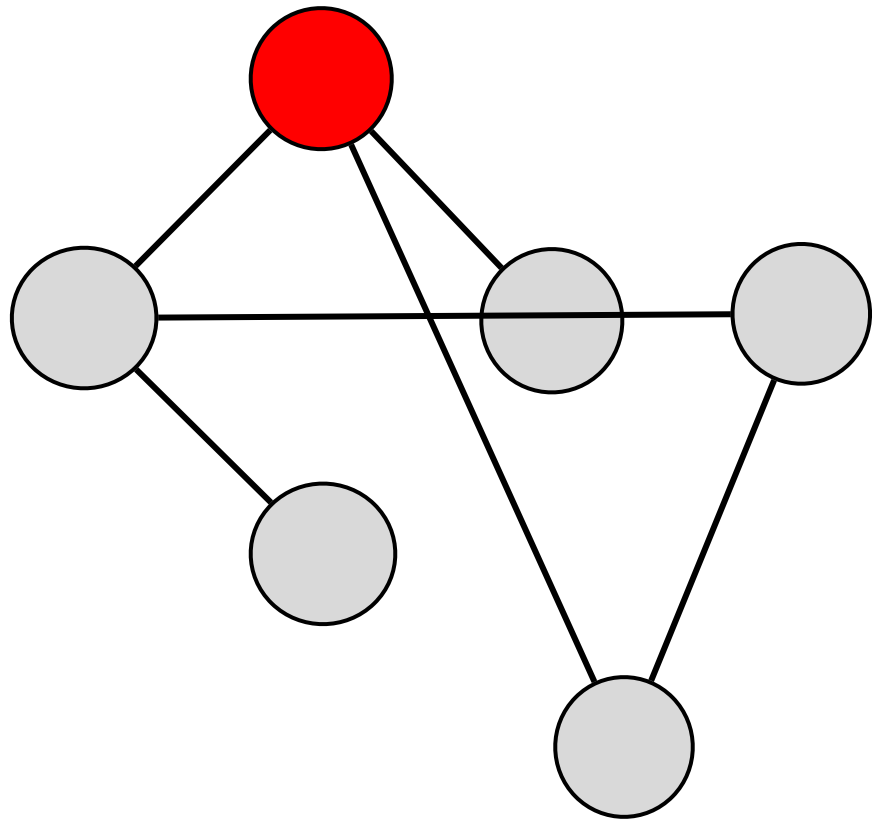

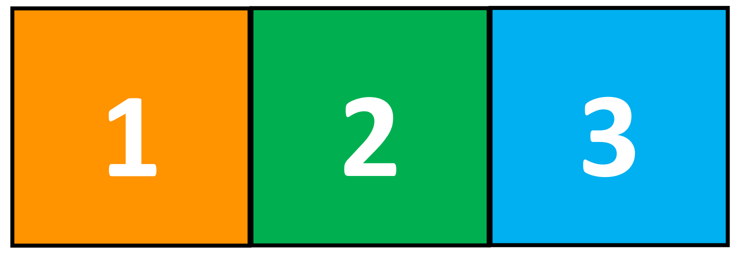

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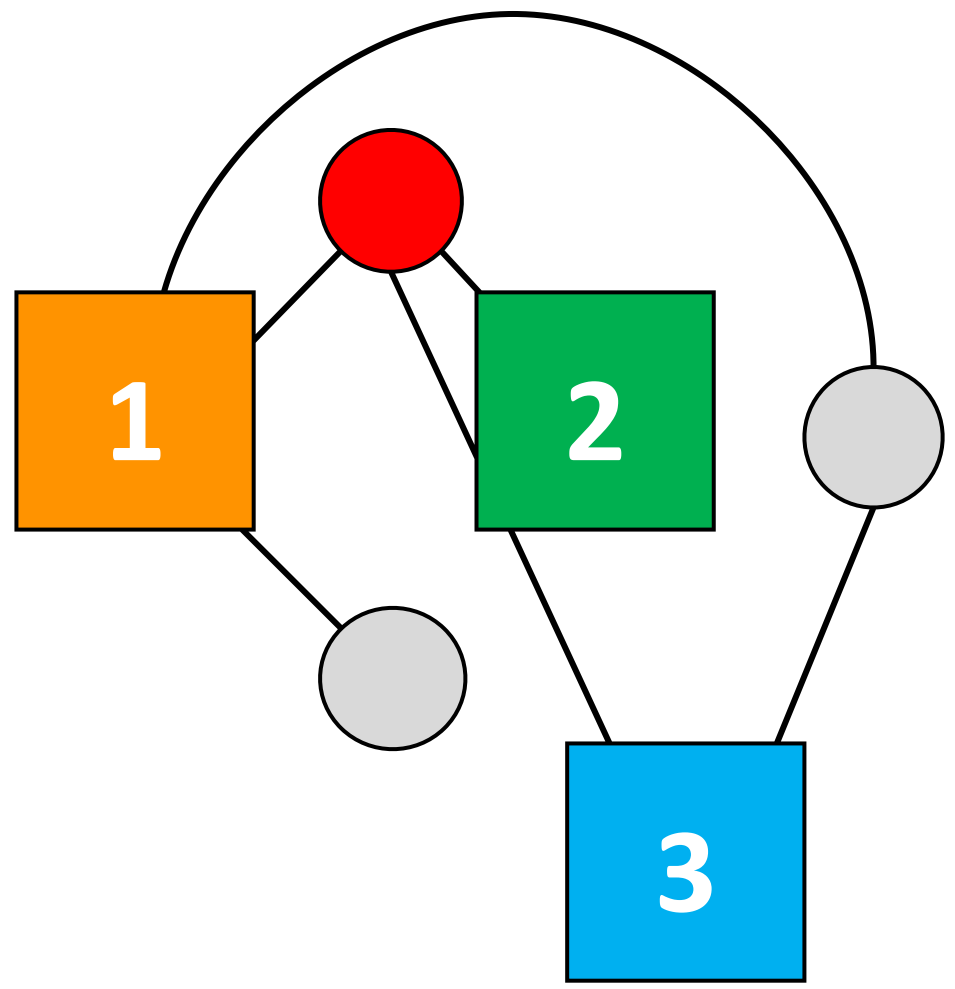

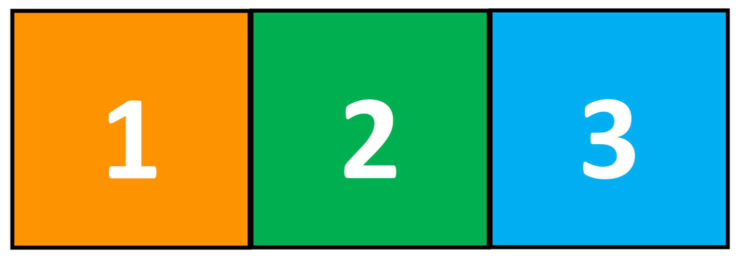

Option 1

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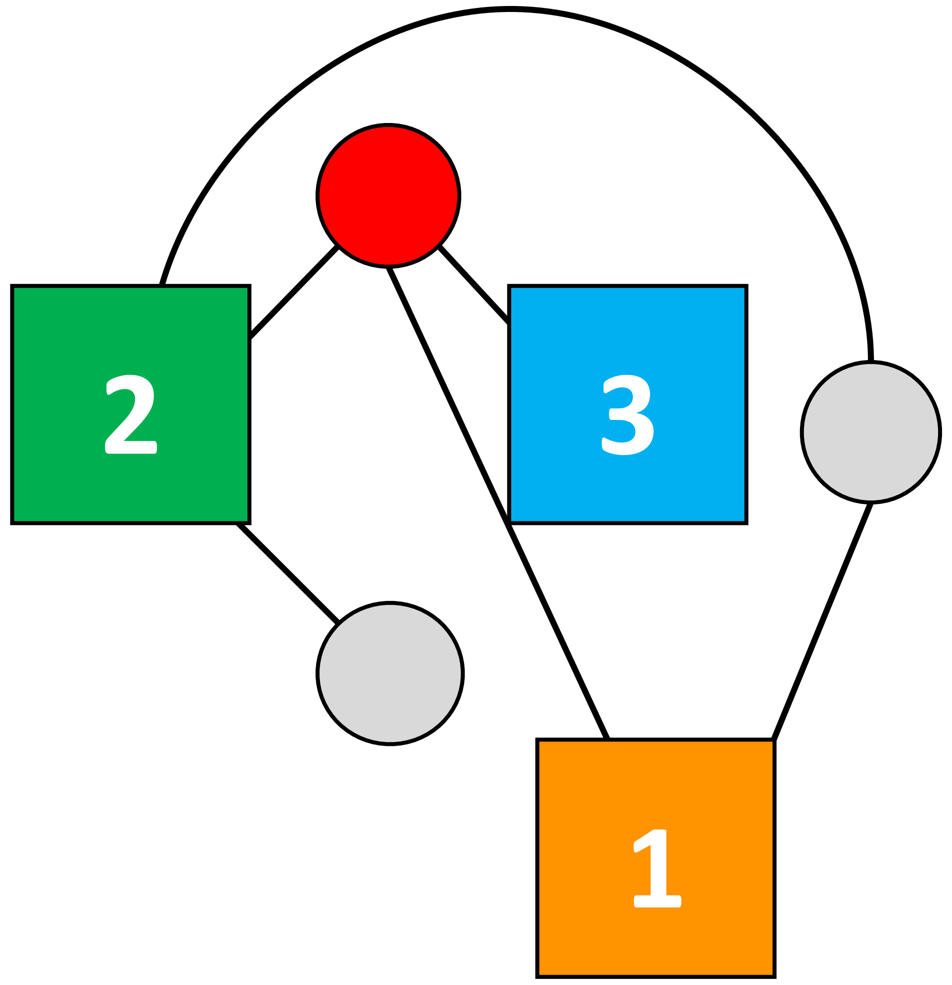
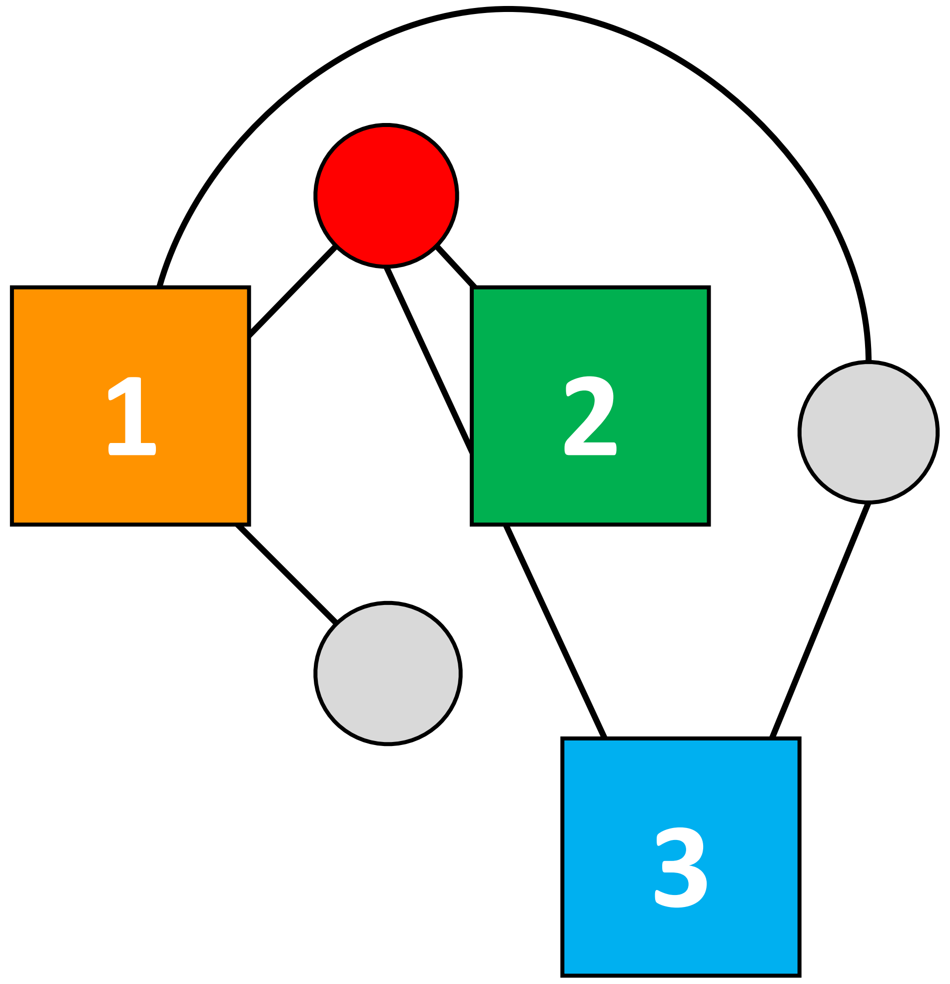


Option 2



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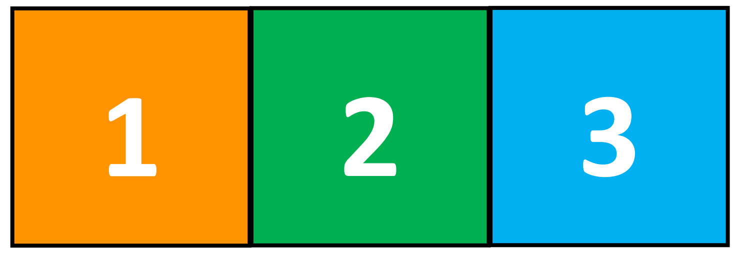

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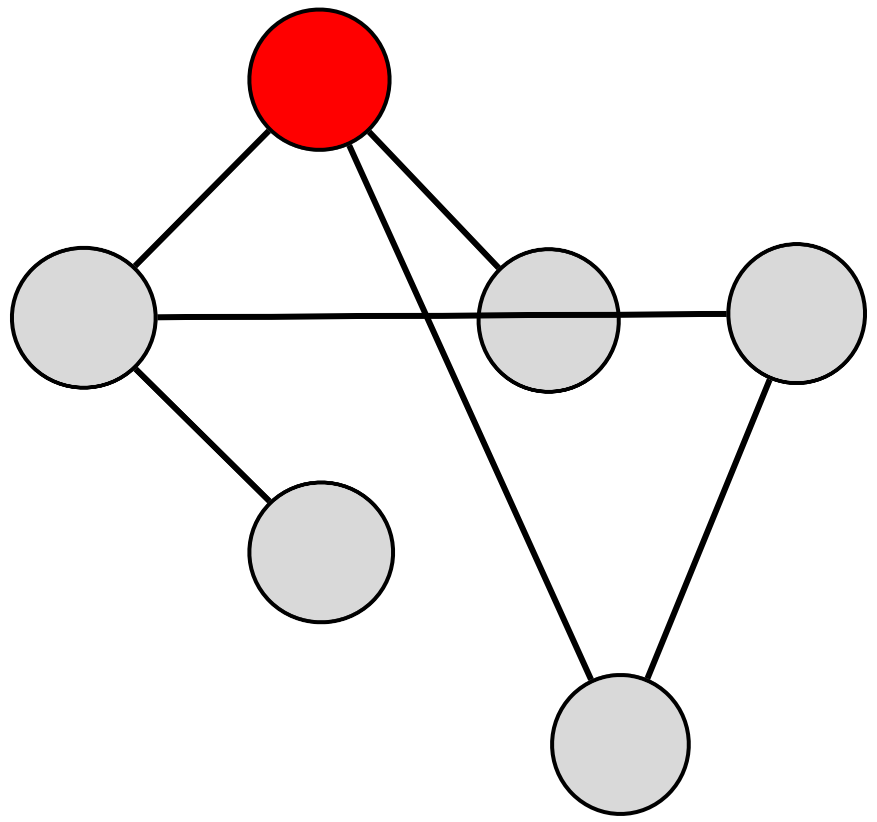
Challenge #2: **Varying** Neighborhood Sizes



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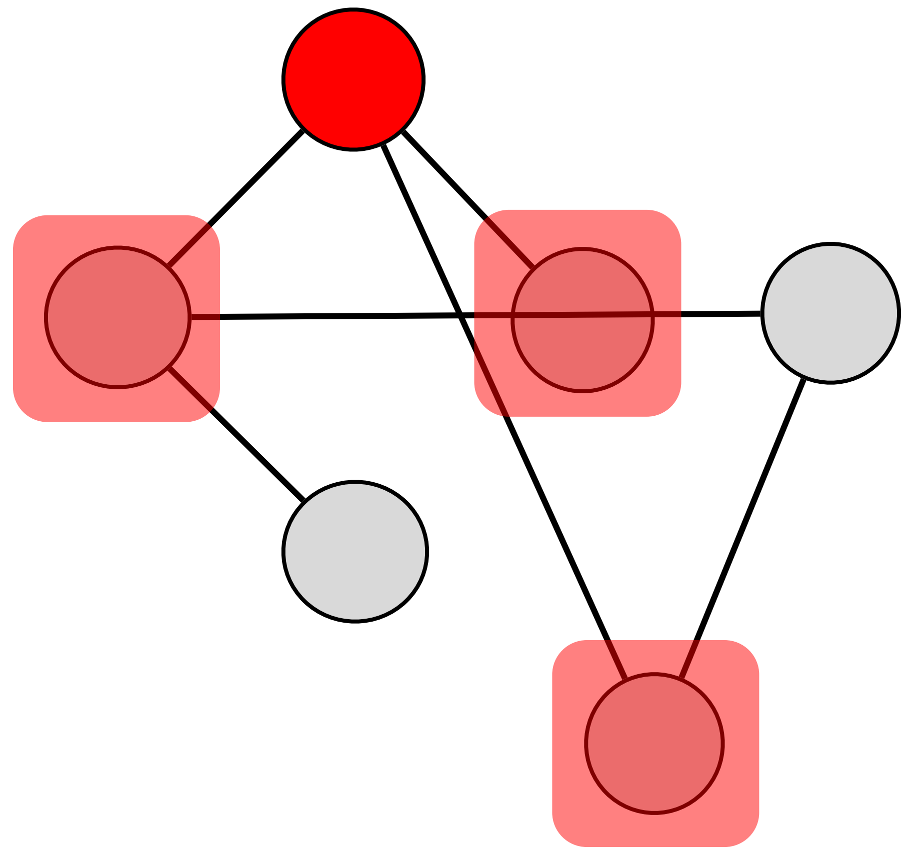

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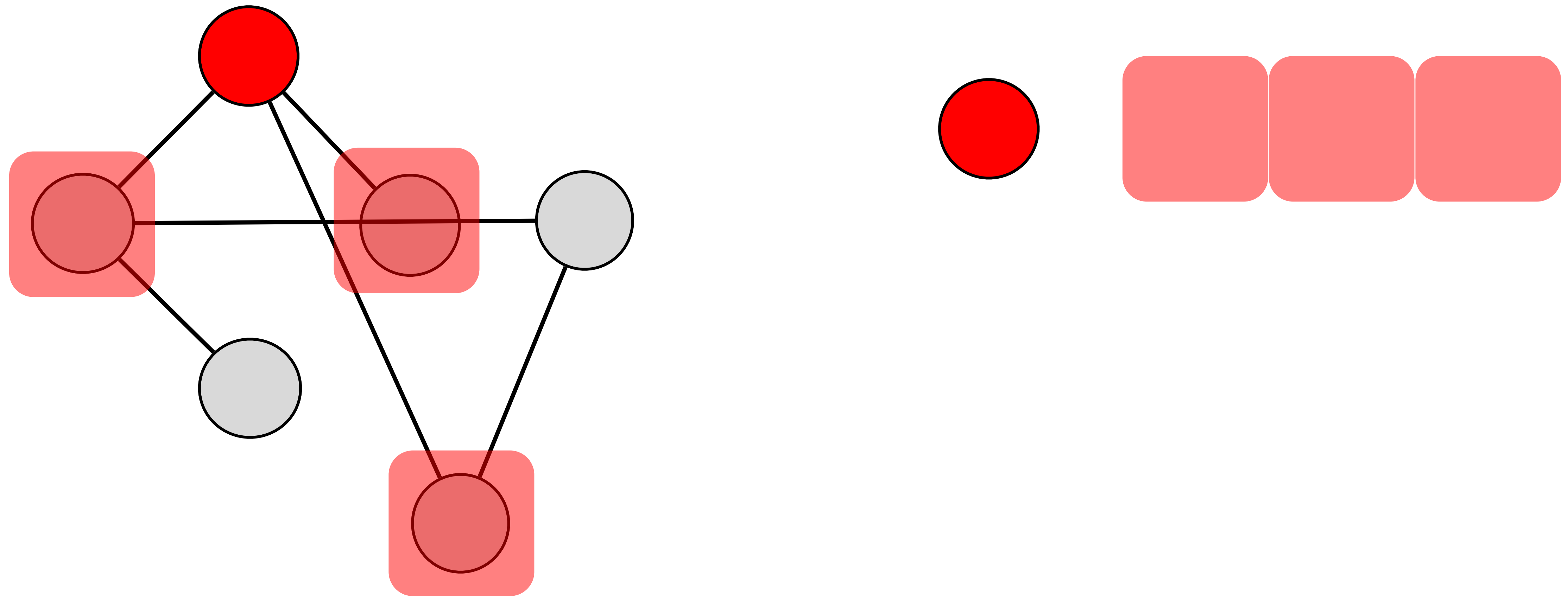

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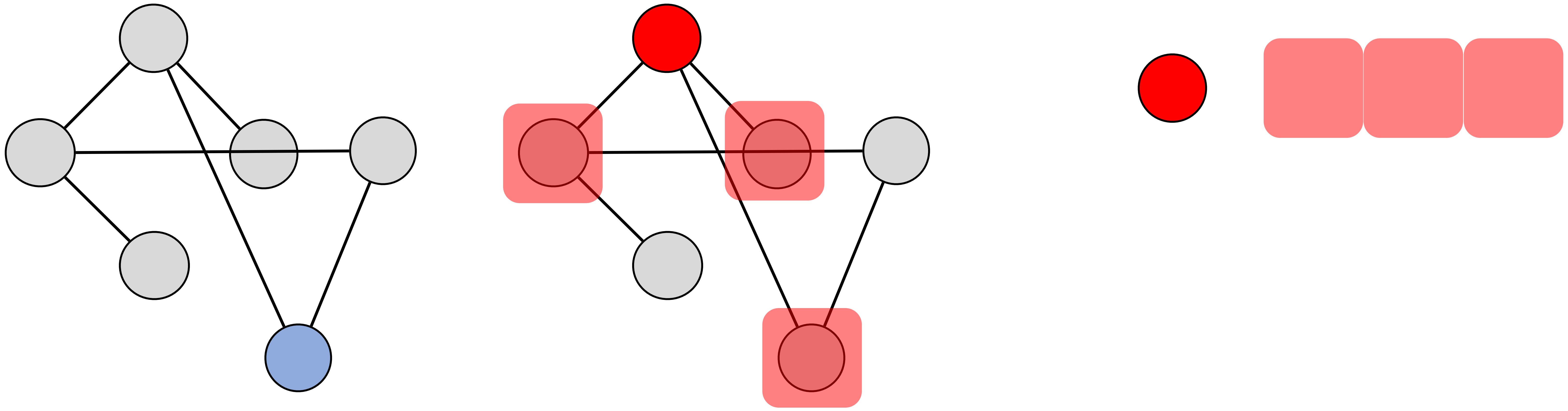

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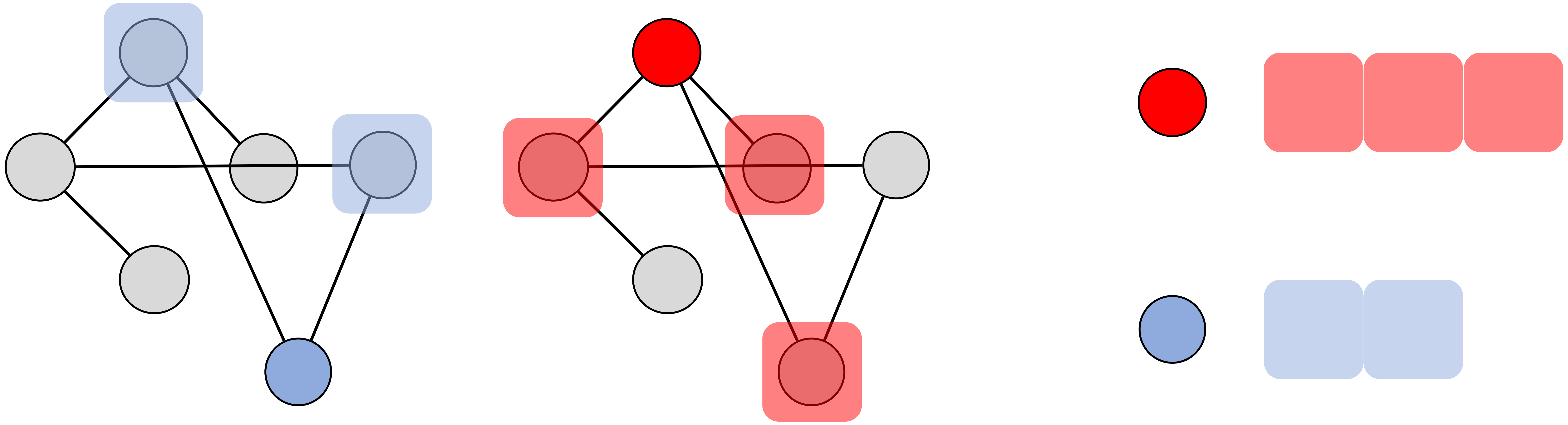
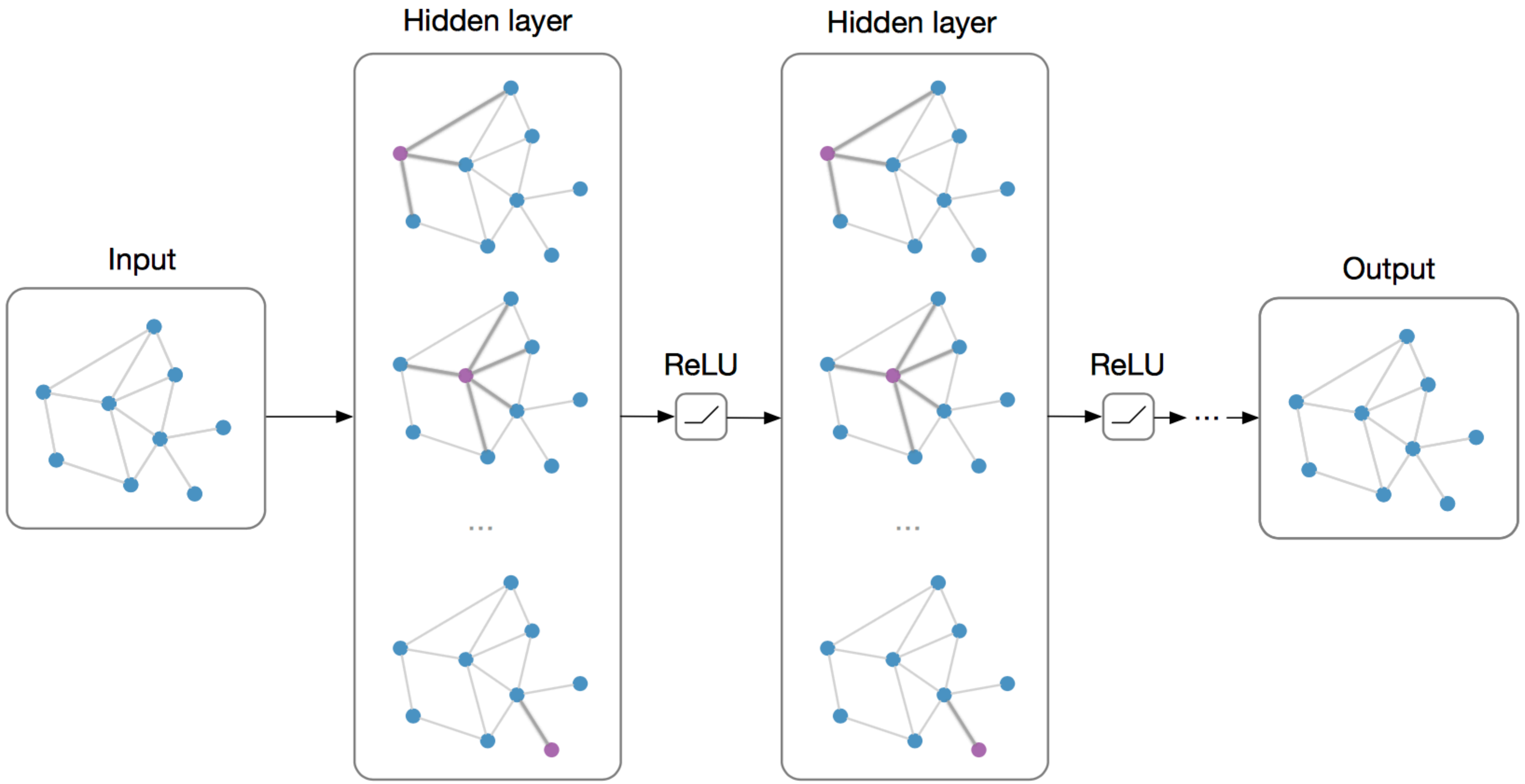


Slide from Renjie Liao

Nearly all (if not all) Graph Neural Networks can be expressed as **Message Passing** paradigms

Graph Neural Networks (GNNs)



Main Idea: Pass massages between pairs of nodes and agglomerate

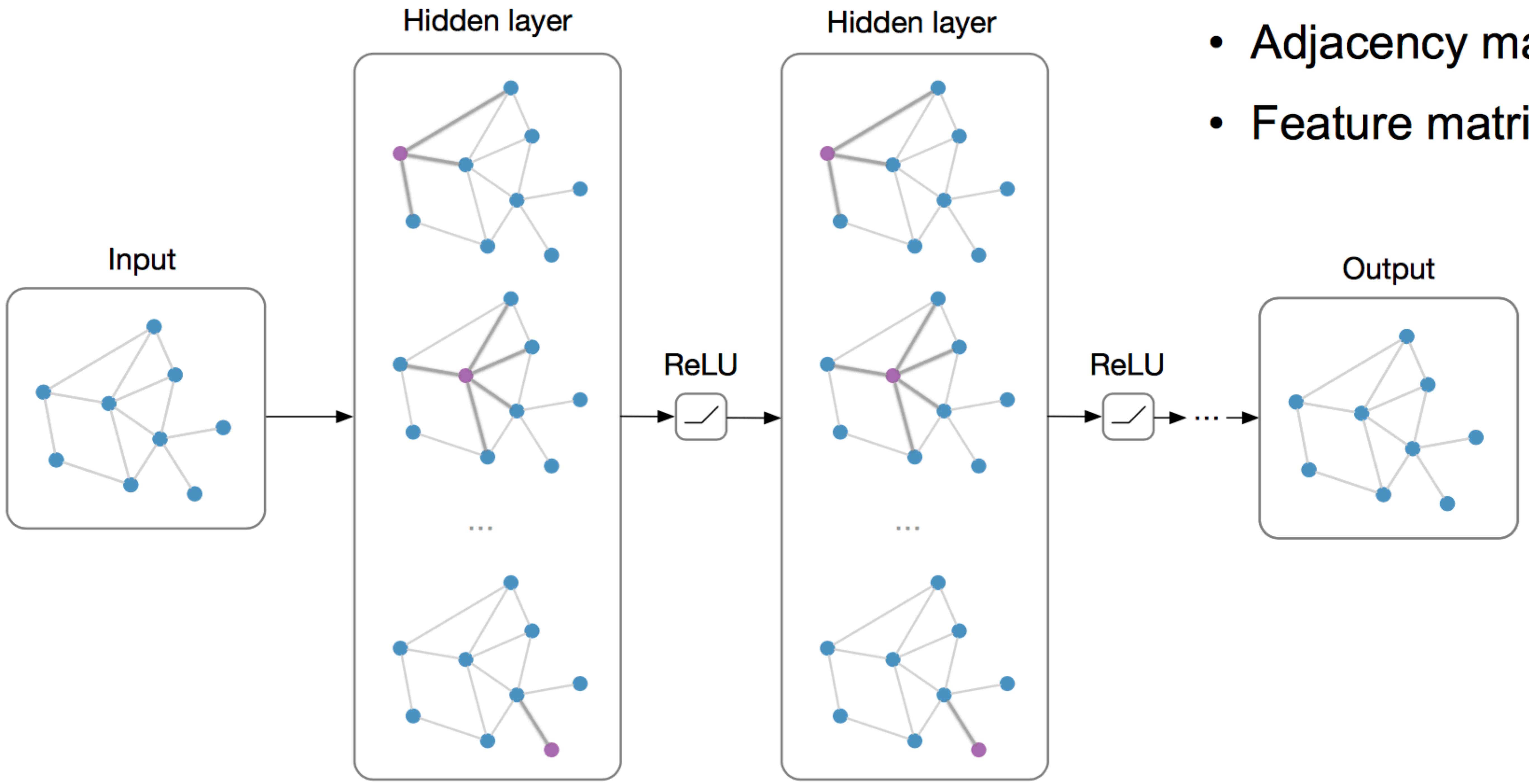
Alternative Interpretation: Pass massages between nodes to refine node (and possibly edge) representations

* slide from Thomas Kipf, **University of Amsterdam**

Graph Neural Networks (GNNs)

Notation: $\mathcal{G} = (\mathbf{A}, \mathbf{X})$

- Adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$
- Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times F}$



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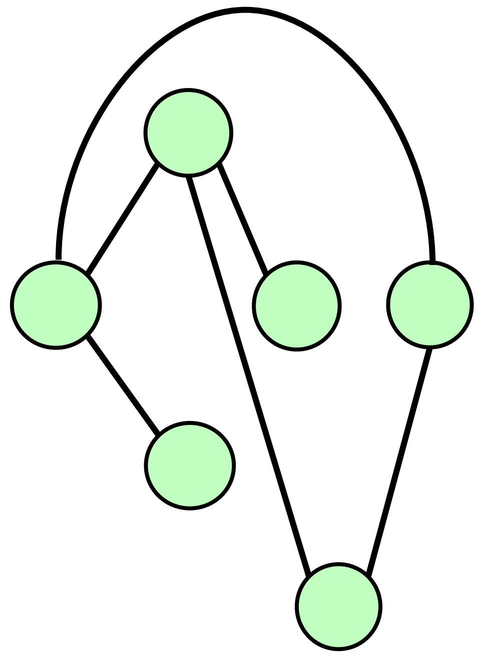

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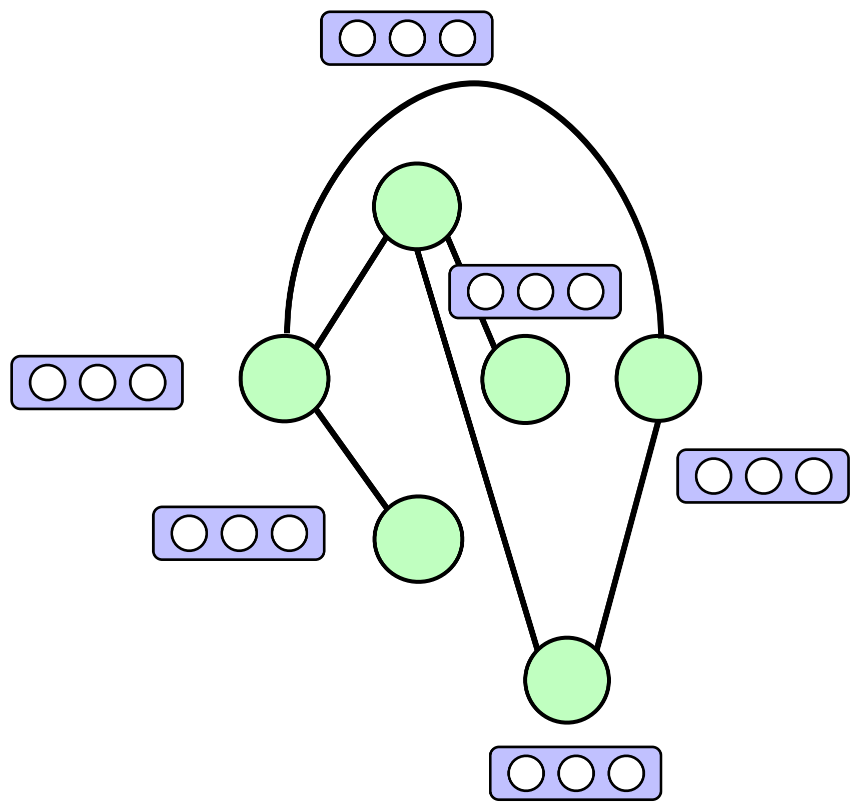

Input Encoding

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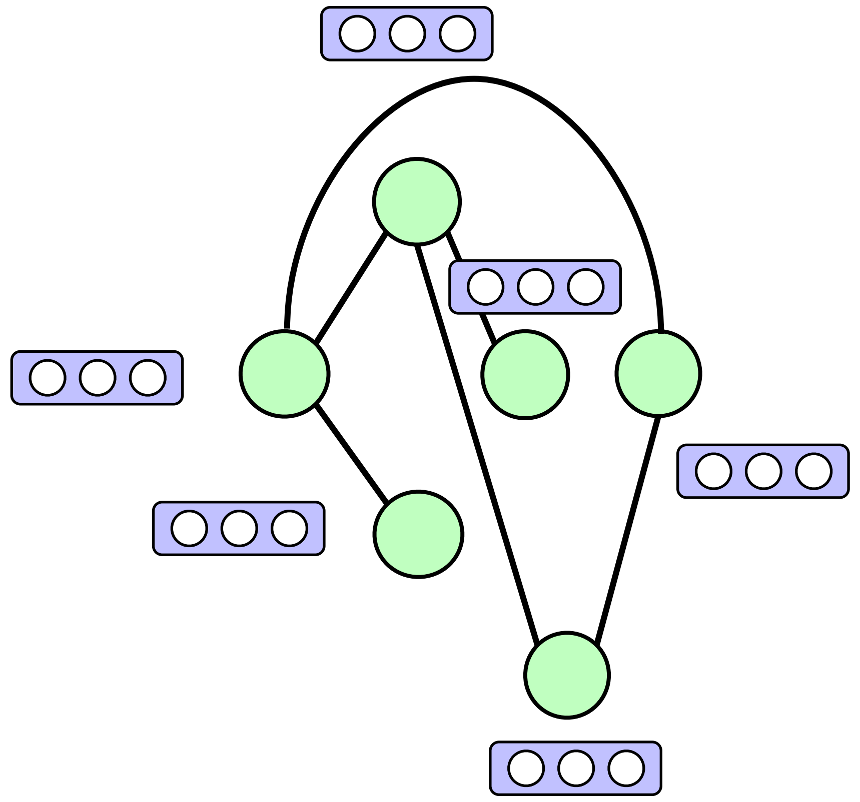


Input Encoding

1. Node Feature

   — *If it is unavailable, use 1-of-K, random, index encoding of node*

2. Edge Feature

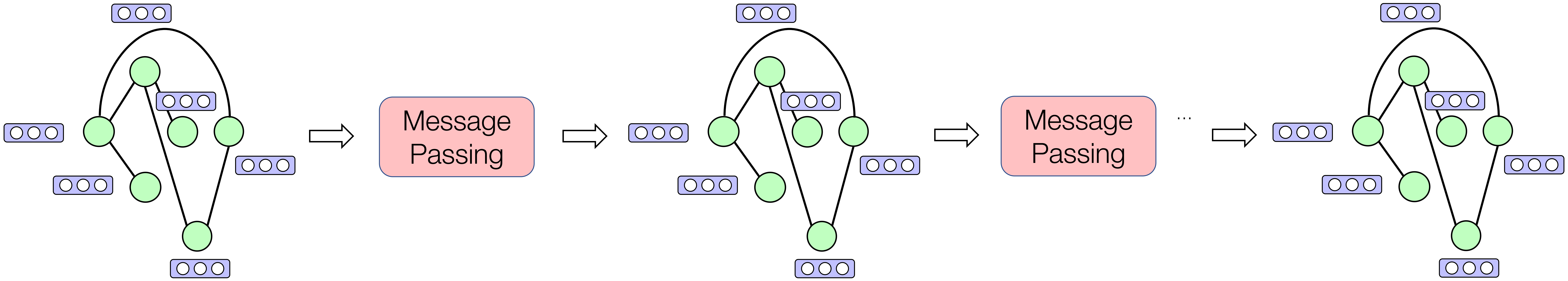
   — *Feed it to message network*

3. Graph Feature

   — *Treat it as a super node in your graph*

   — *Feed graph feature to readout layer*

Graph Neural Networks (GNNs)



Input Encoding

Message Passing Layers/Steps

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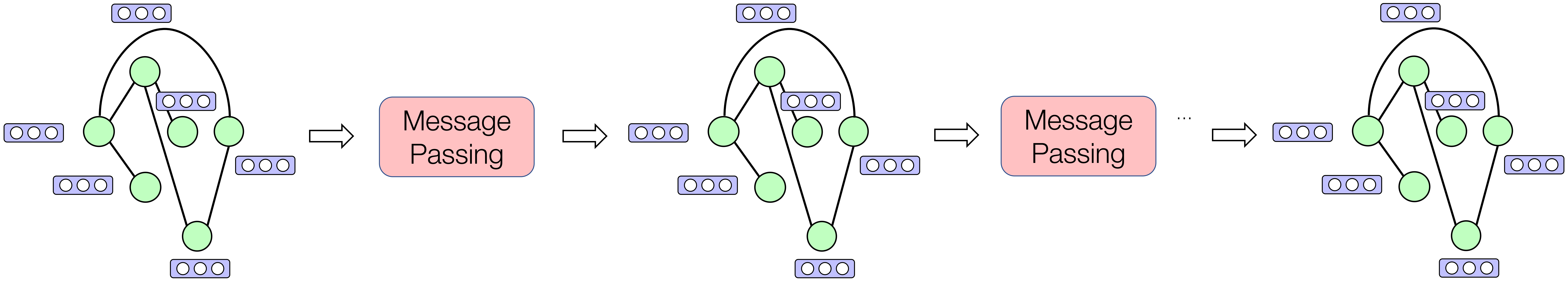
Graph Neural Networks (GNNs)



Input Encoding

Message Passing Layers/Steps

Steps: share message passing module (Recurrent Networks)
Layers: do not share message passing module (Feedforward Networks)

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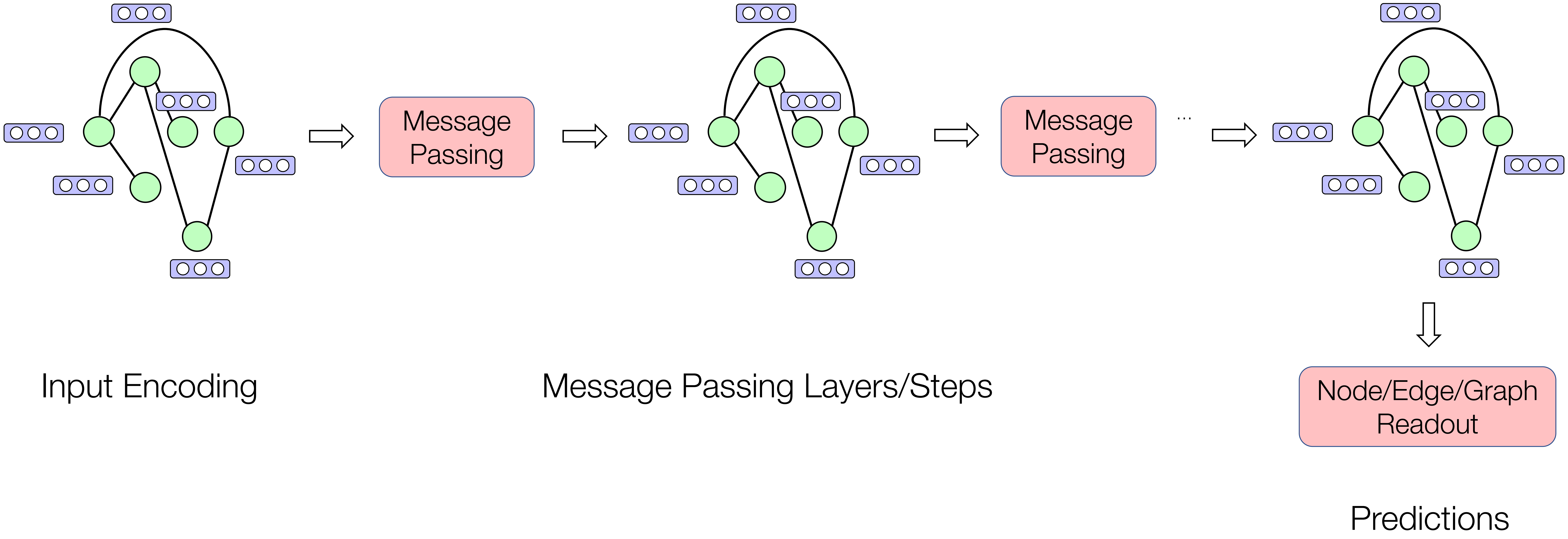
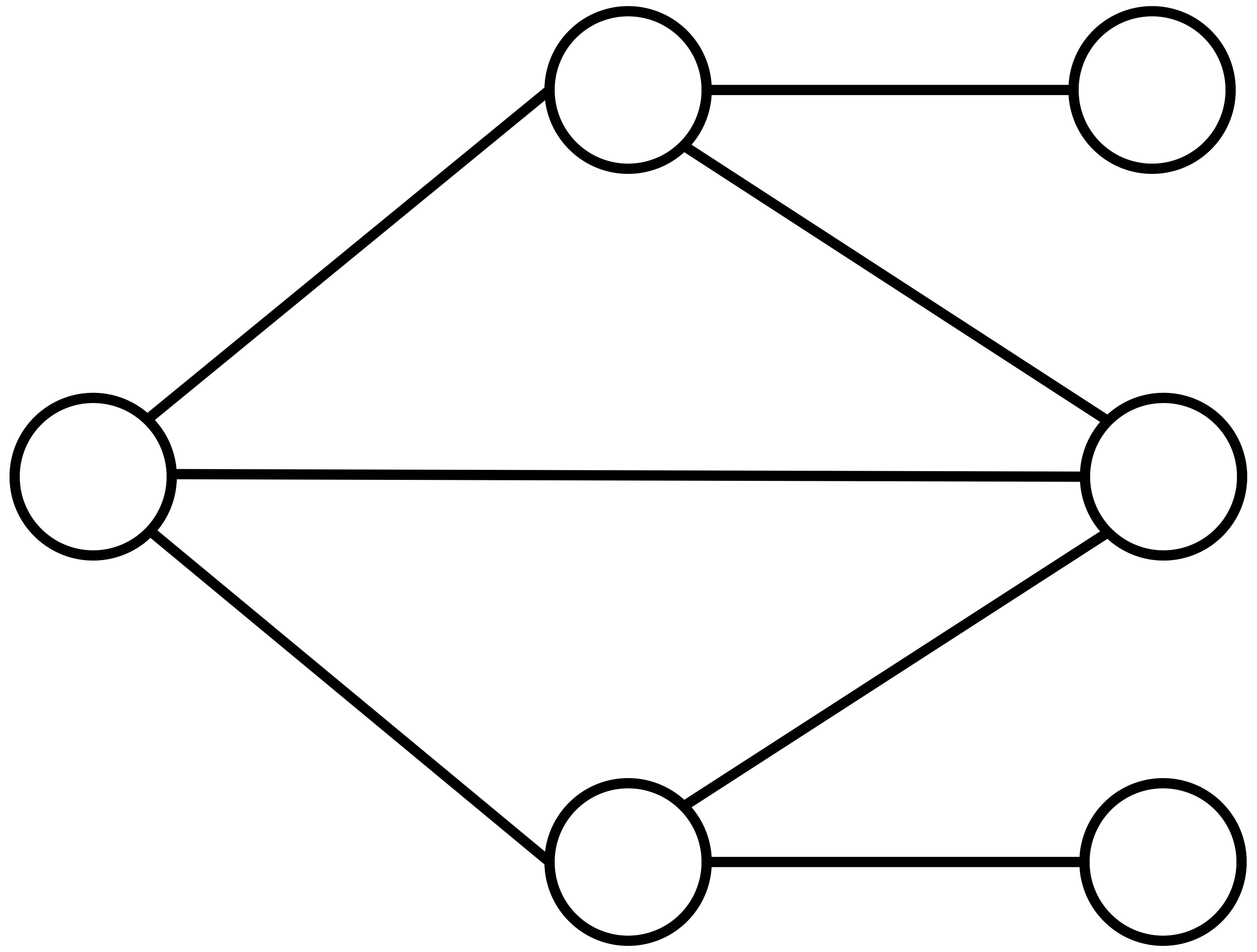
Graph Neural Networks (GNNs)



Message Passing in GNNs

(t+1)-th message passing step/layer



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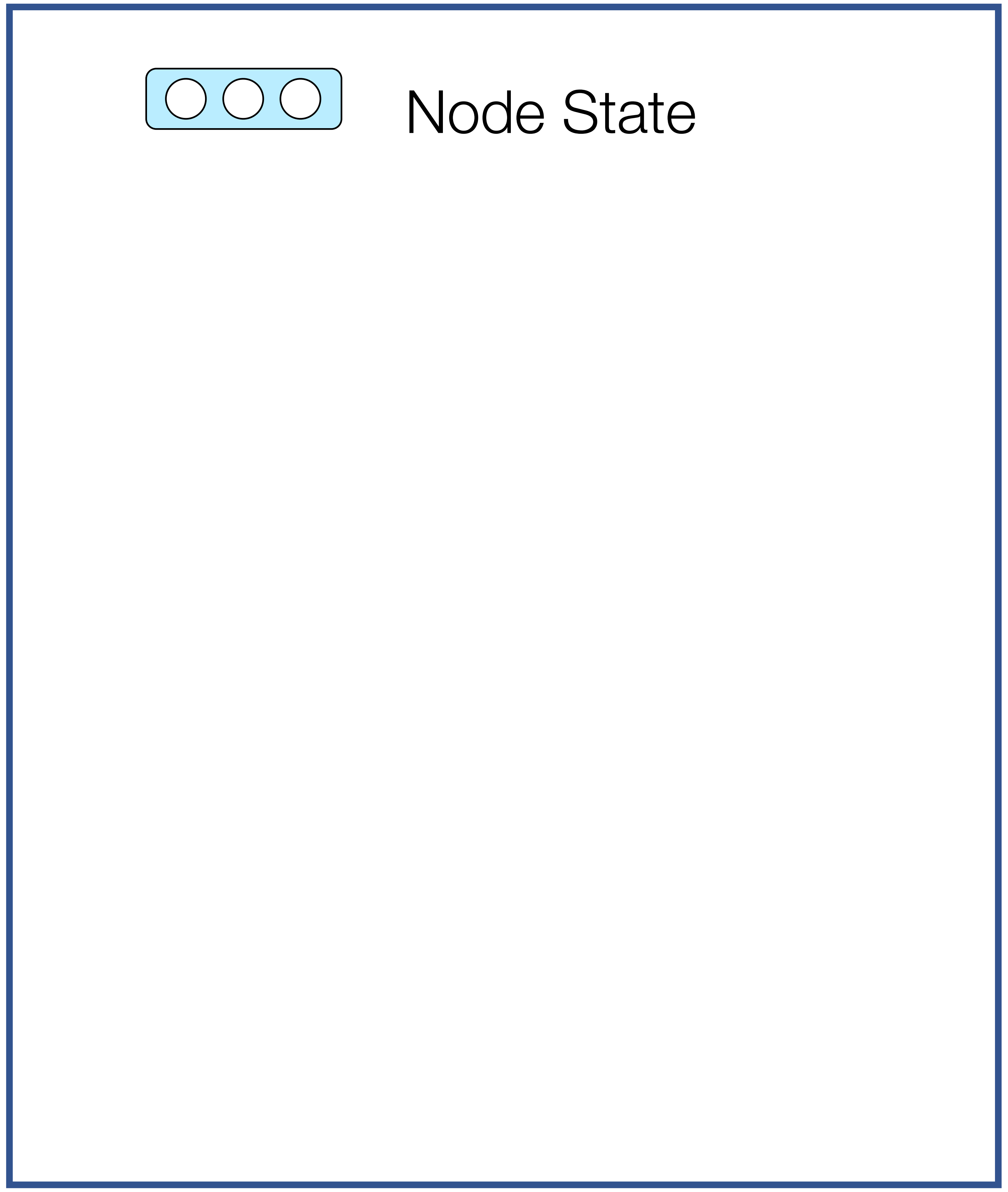
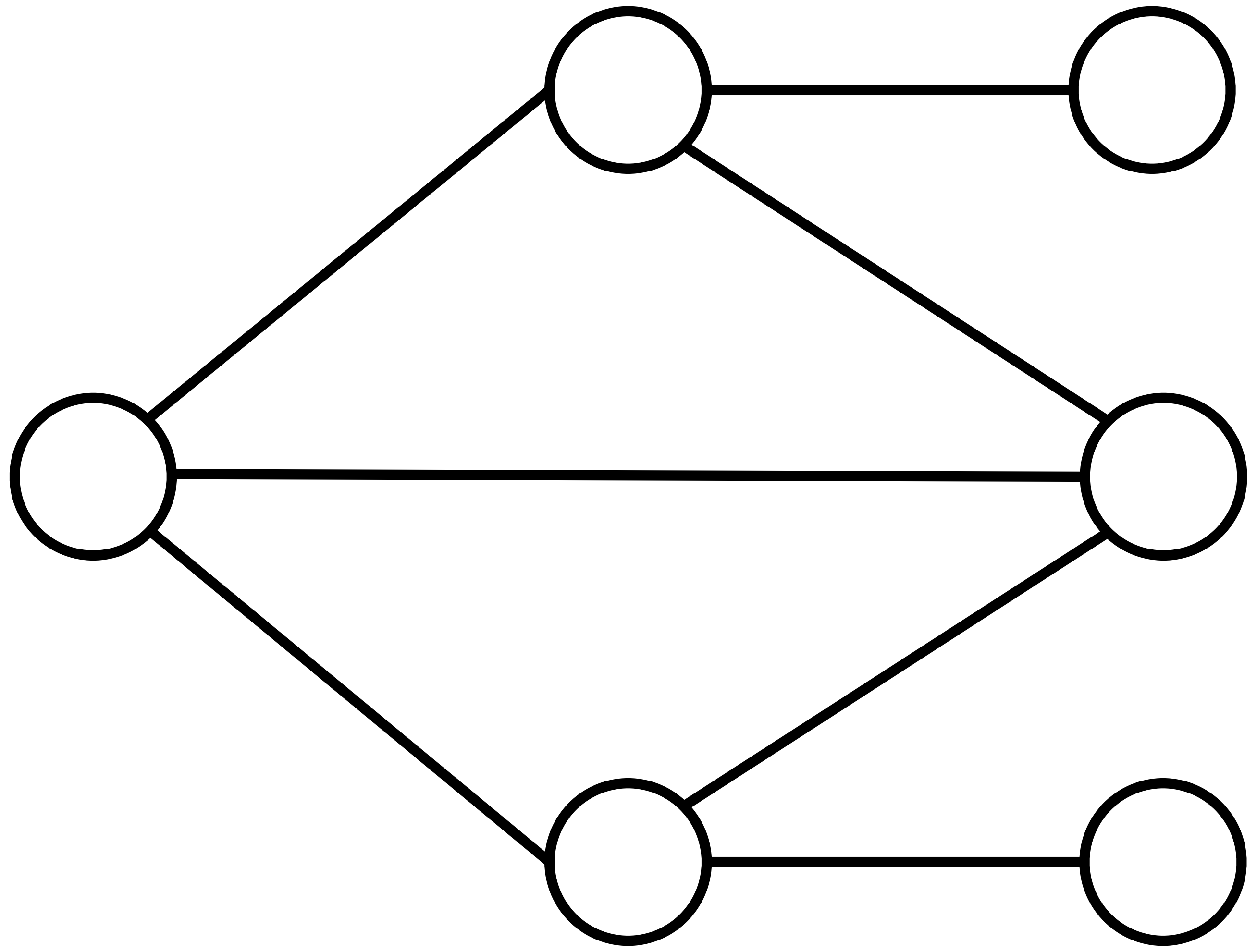
Message Passing in GNNs

(t+1)-th message passing step/layer

$\mathbf{h}_i^t$





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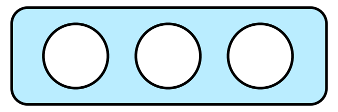
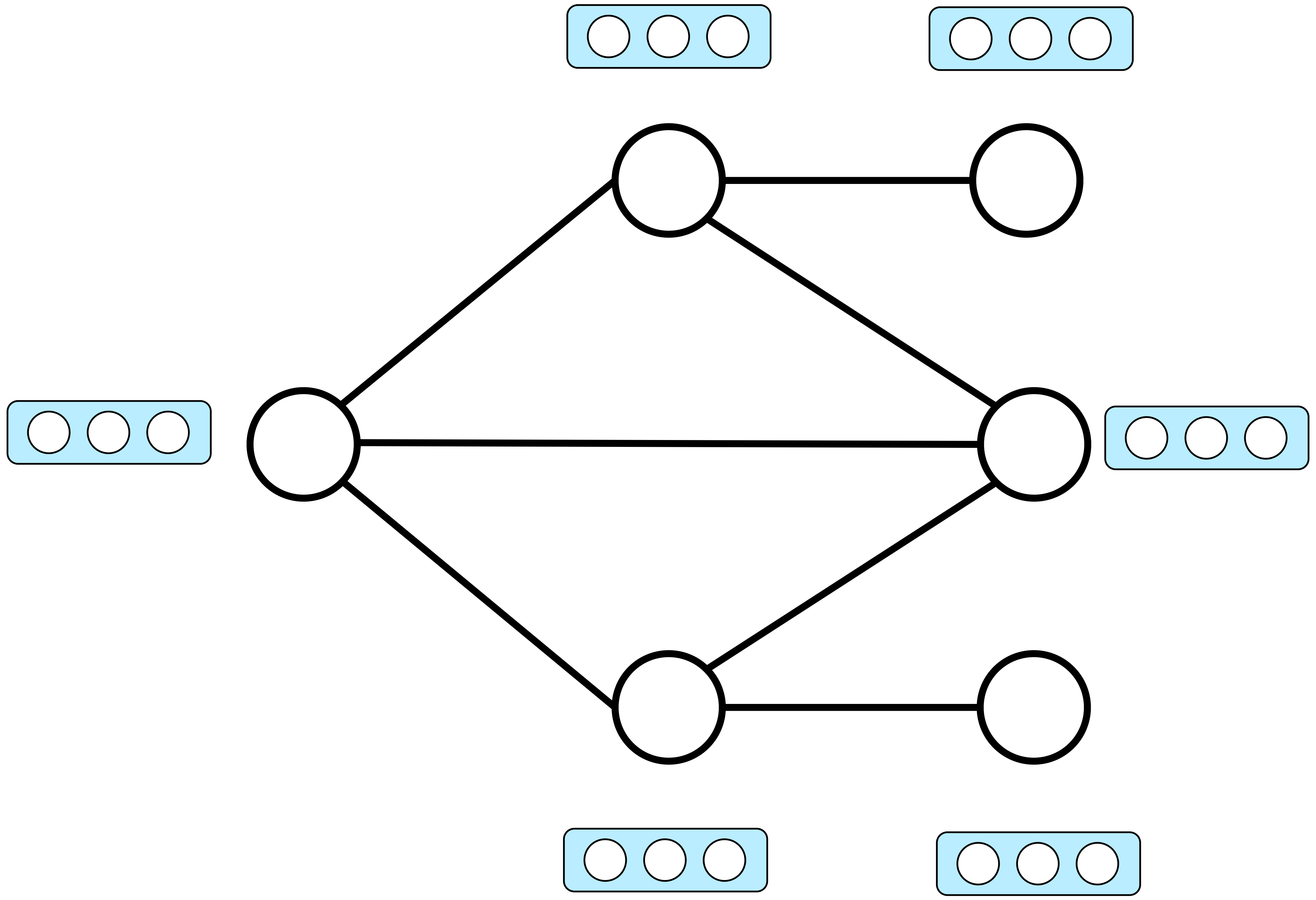


Node State



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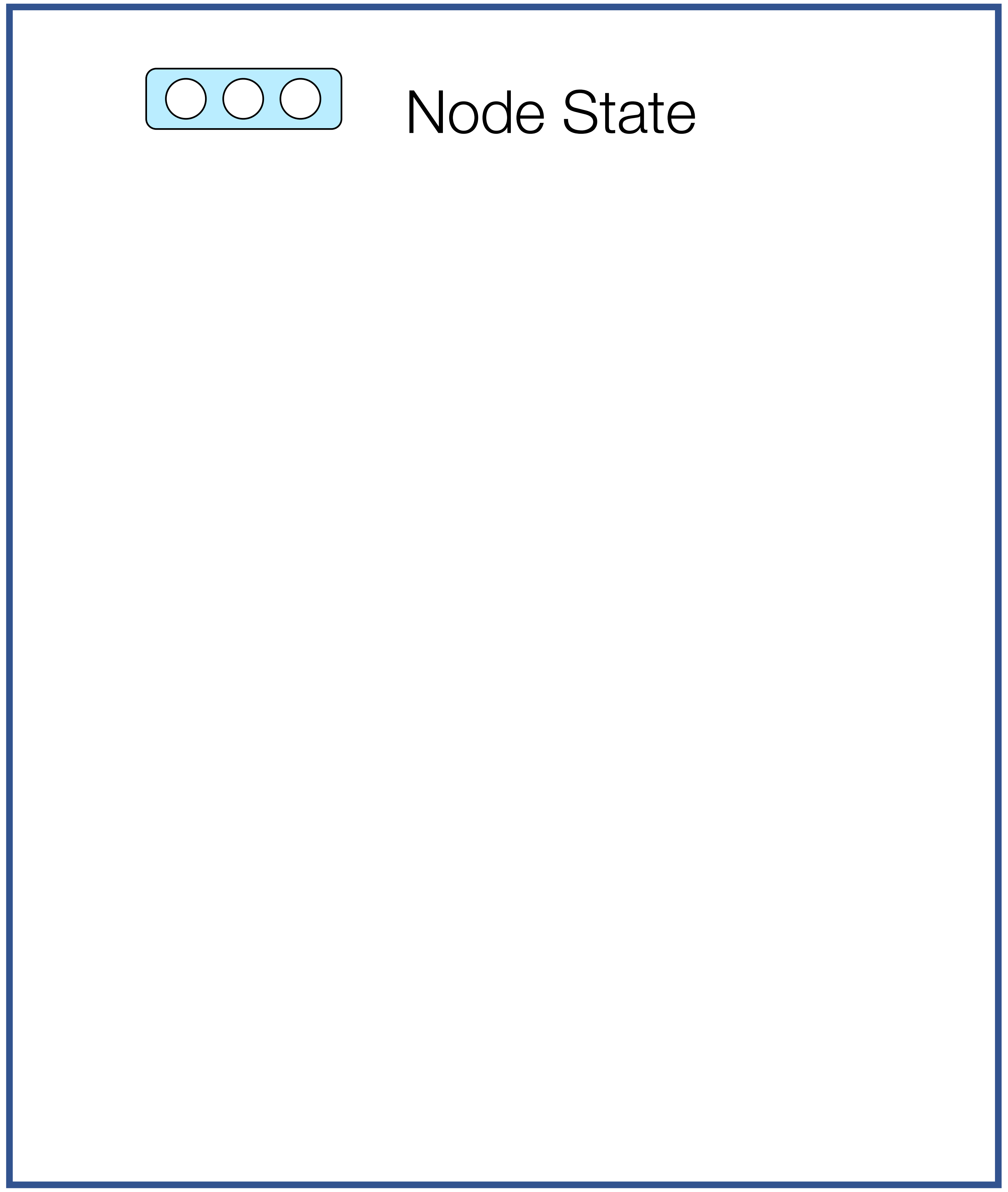
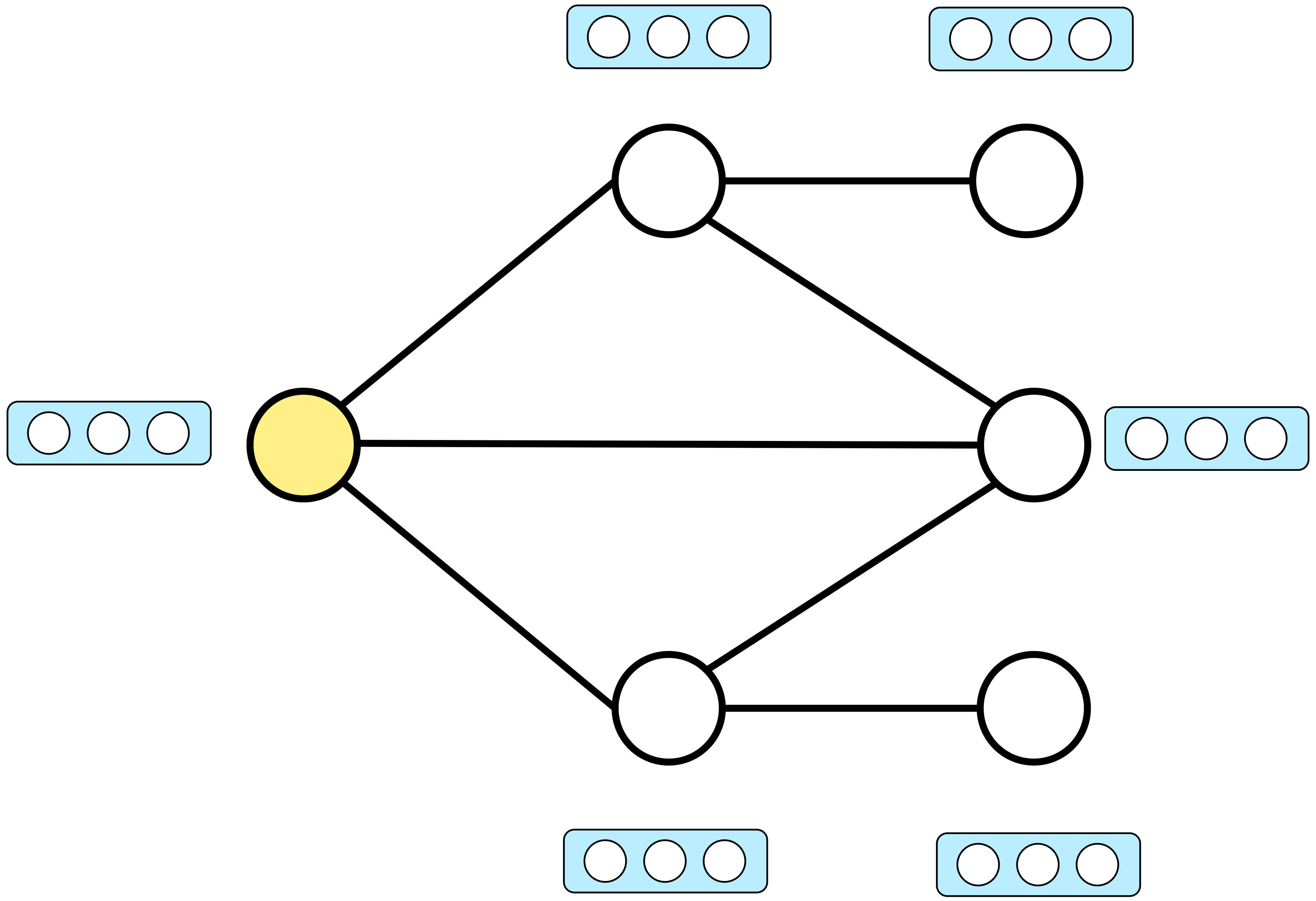
$\mathbf{h}_i^t$



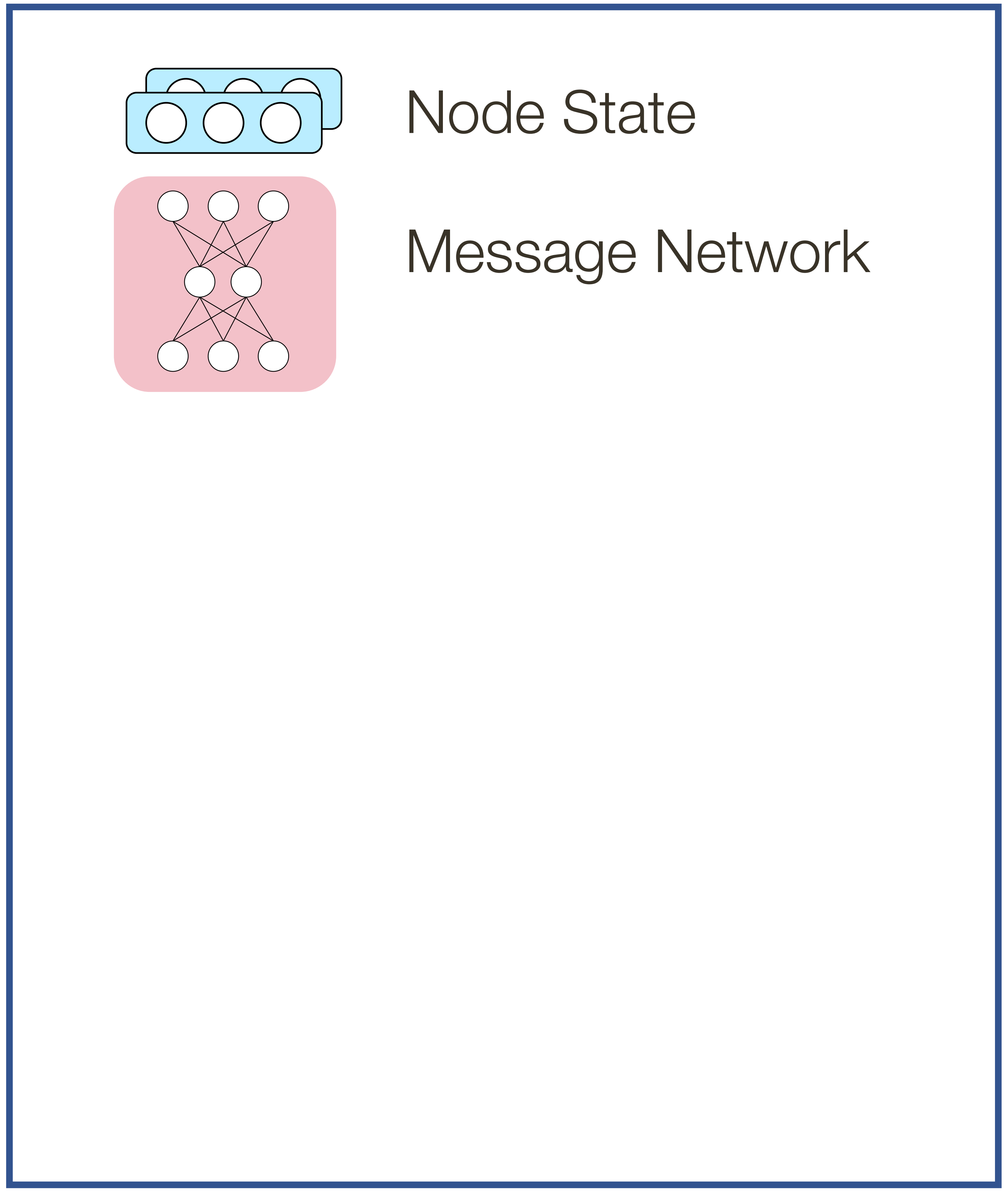


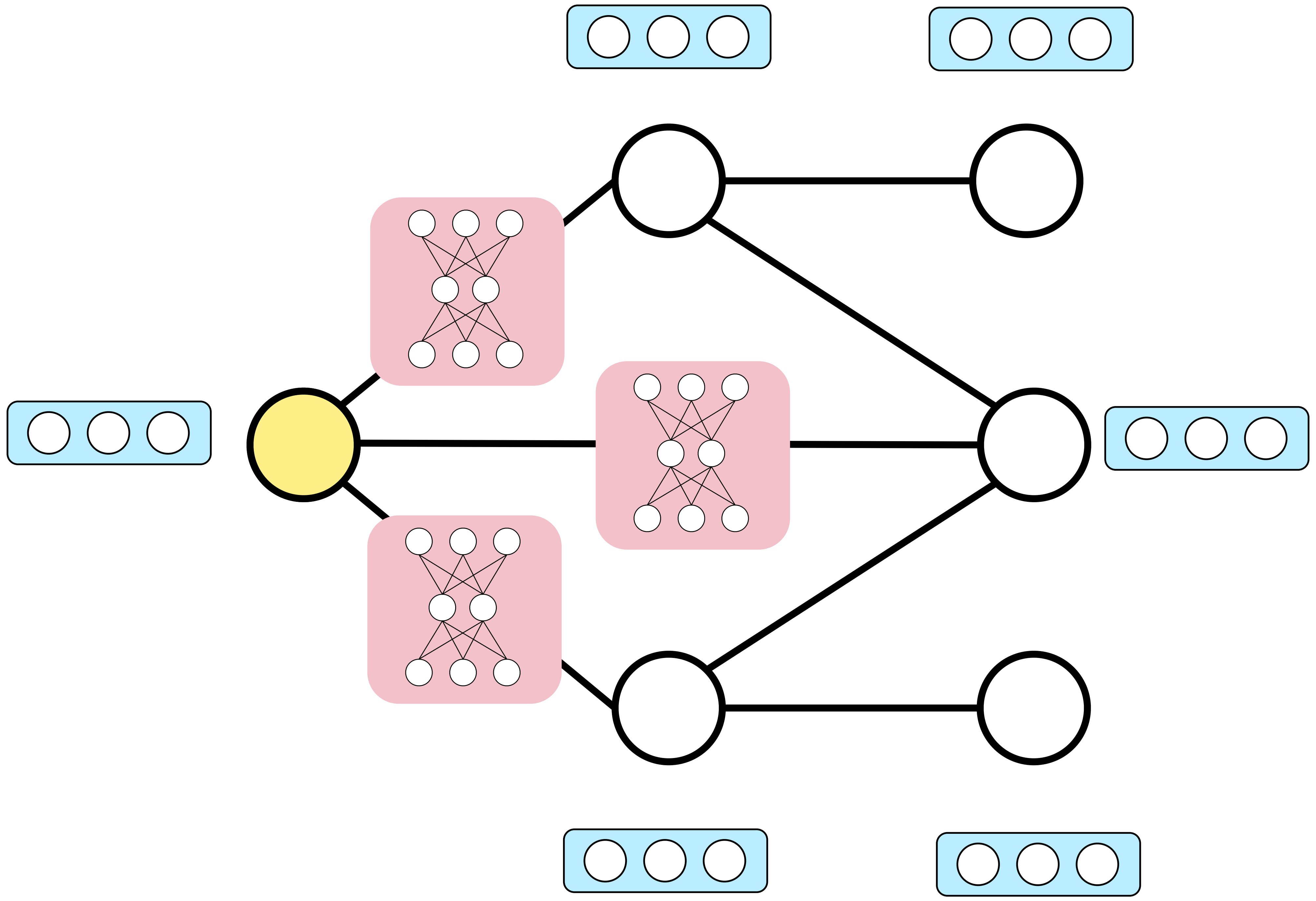
Slide from Renjie Liao

Message Passing in GNNs

(t+1)-th message passing step/layer

$\mathbf{h}_i^t \quad \mathbf{h}_j^t$





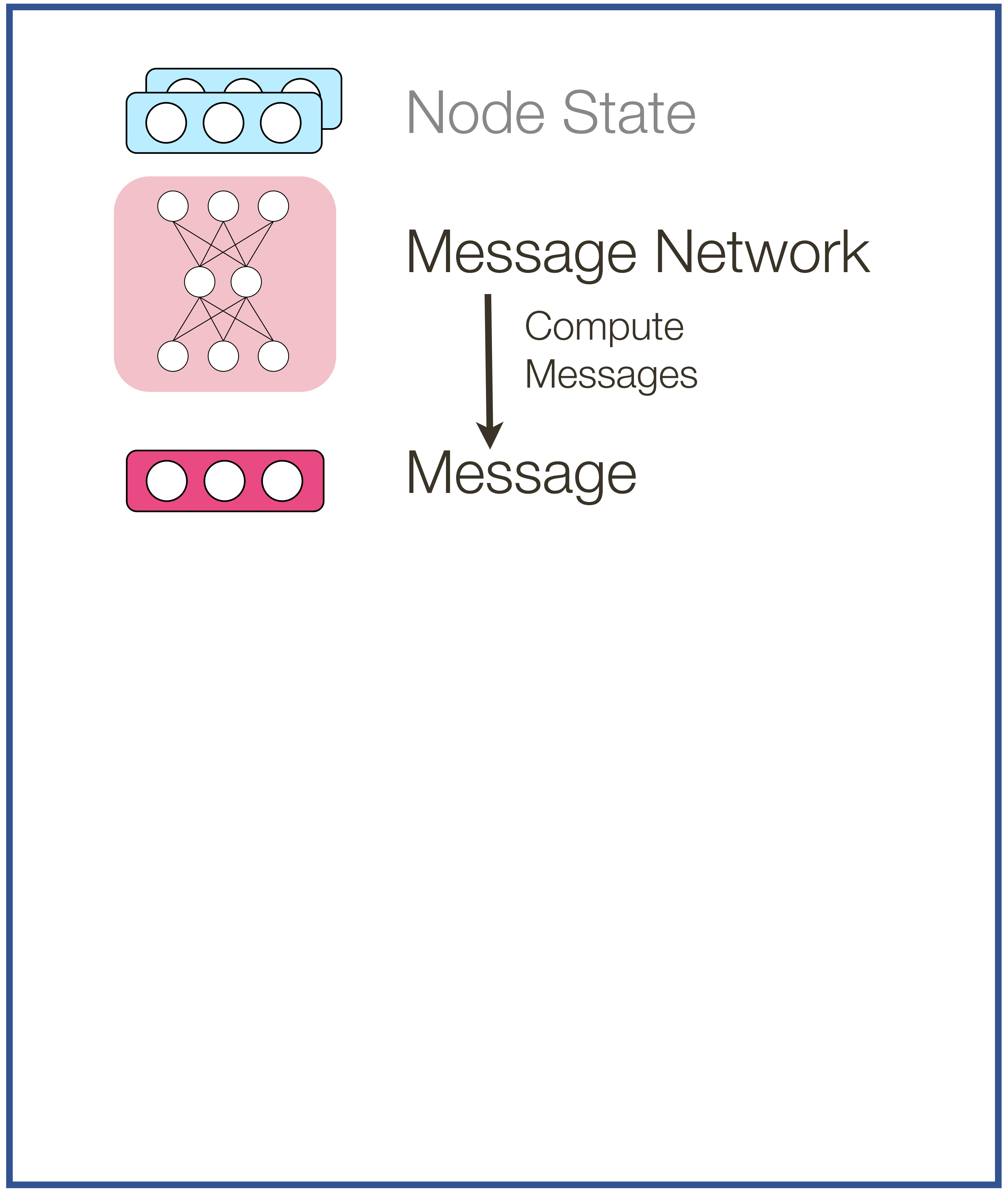
Slide from Renjie Liao

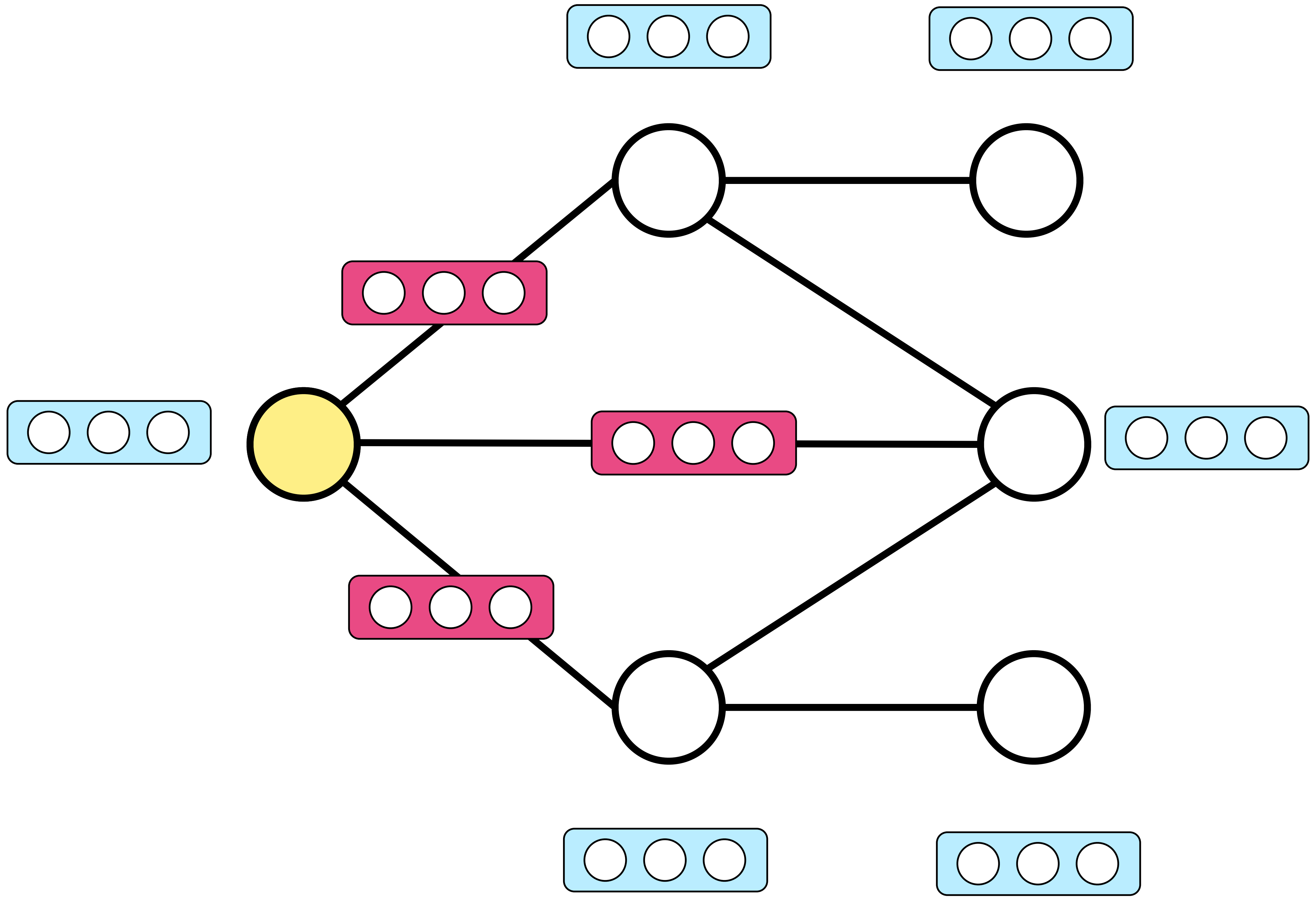
Message Passing in GNNs

(t+1)-th message passing step/layer

$\mathbf{h}_i^t \quad \mathbf{h}_j^t$

$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$





Message Passing in GNNs

(t+1)-th message passing step/layer

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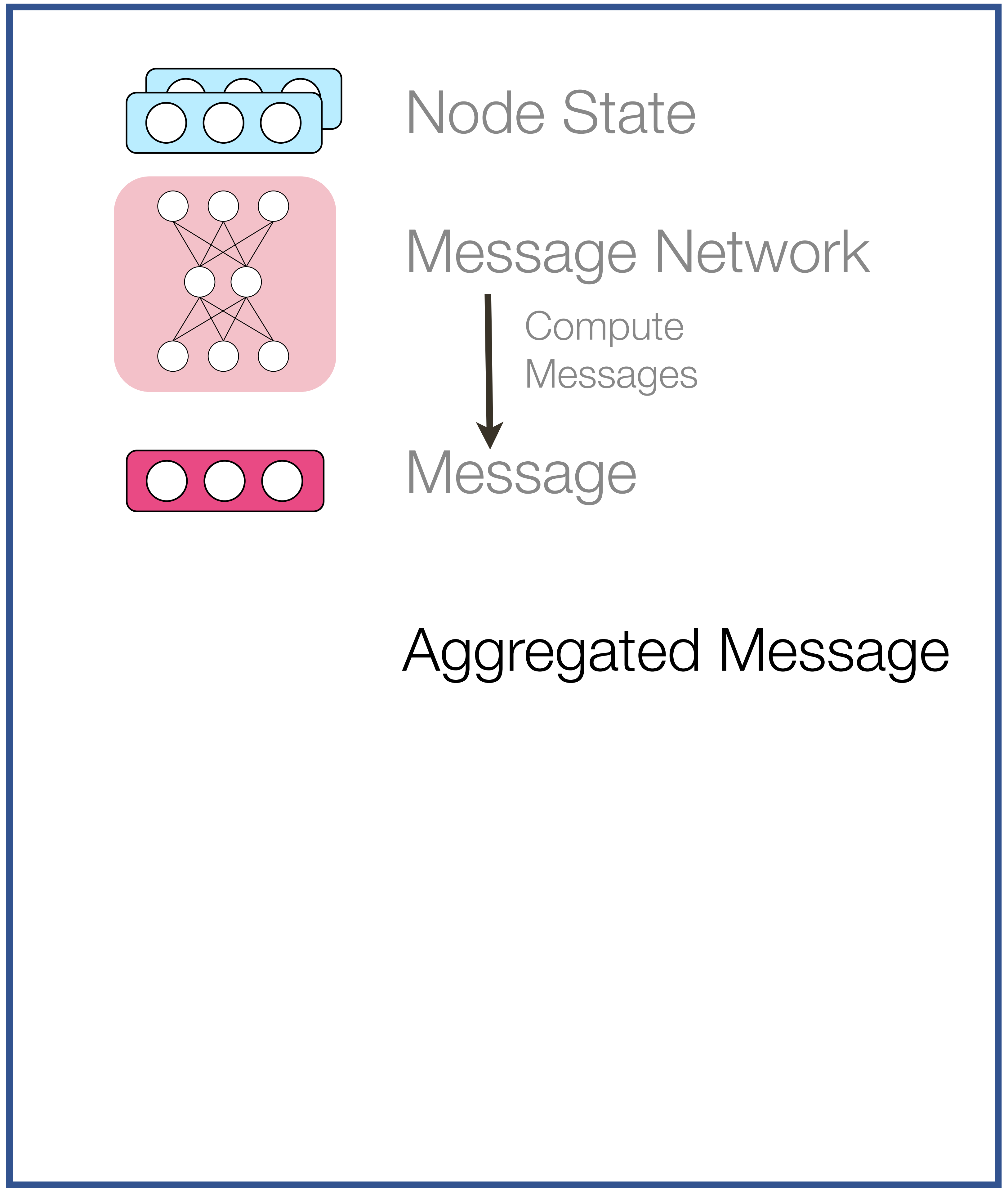

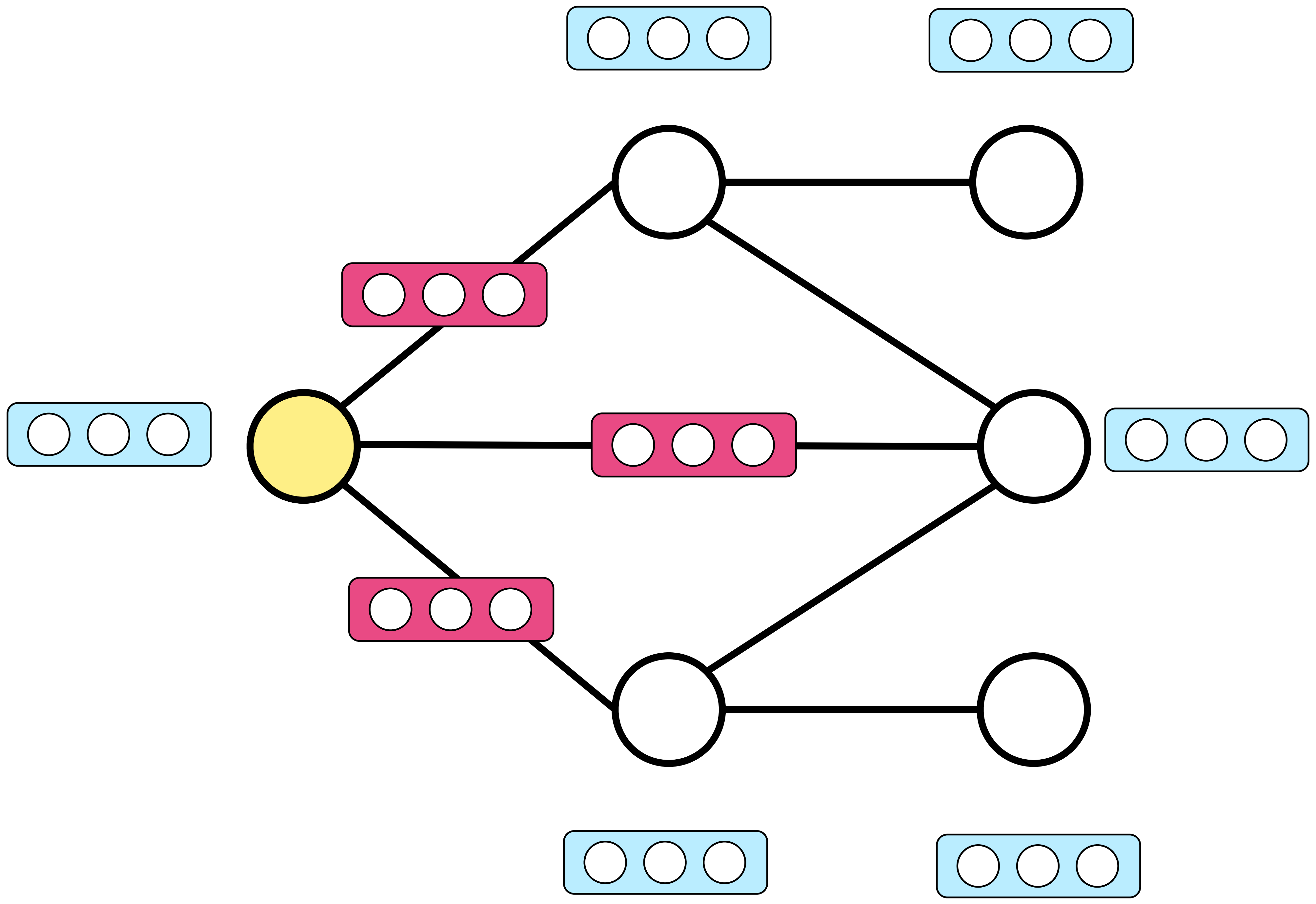

Slide from Renjie Liao

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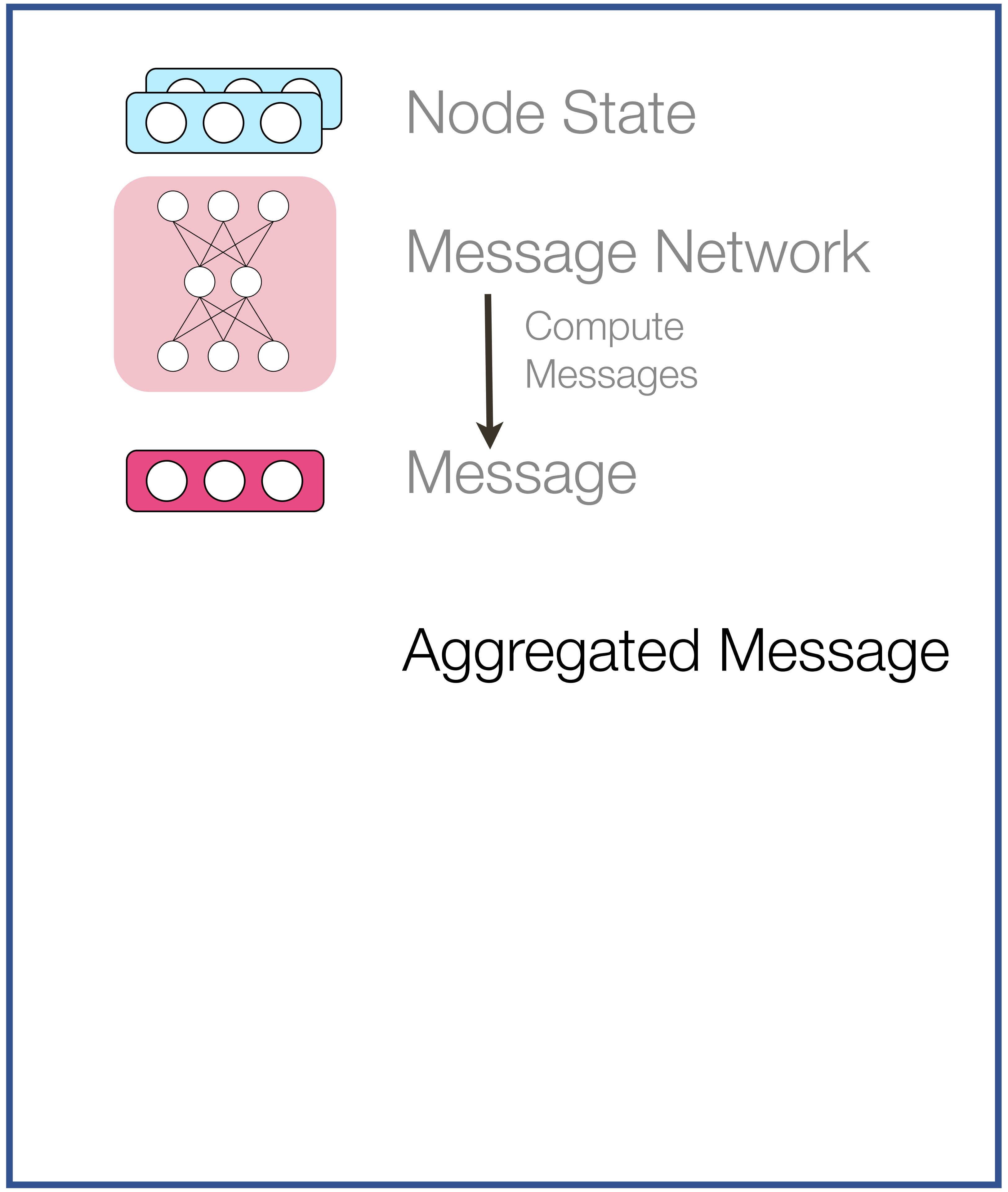
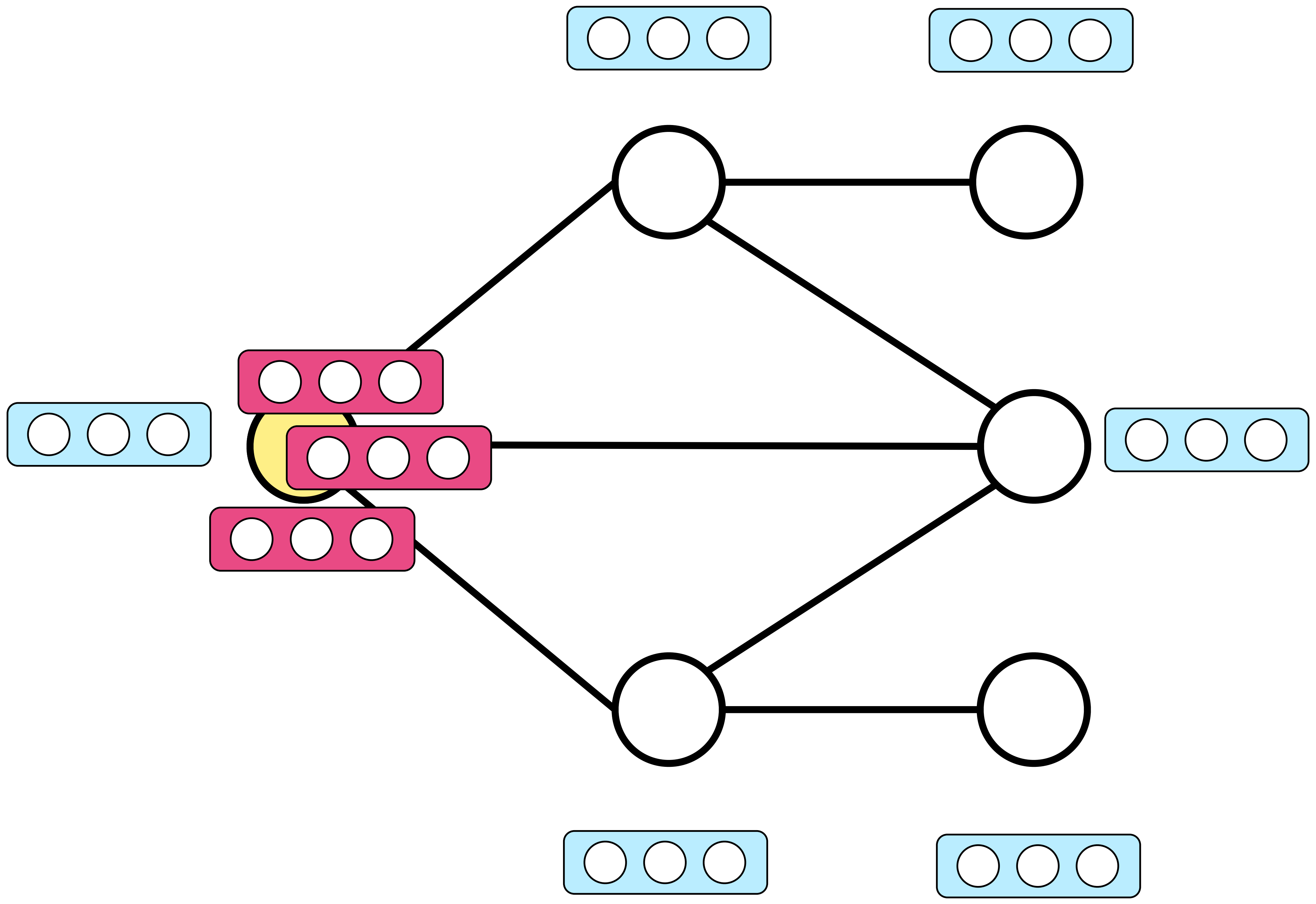


(t+1)-th message passing step/layer



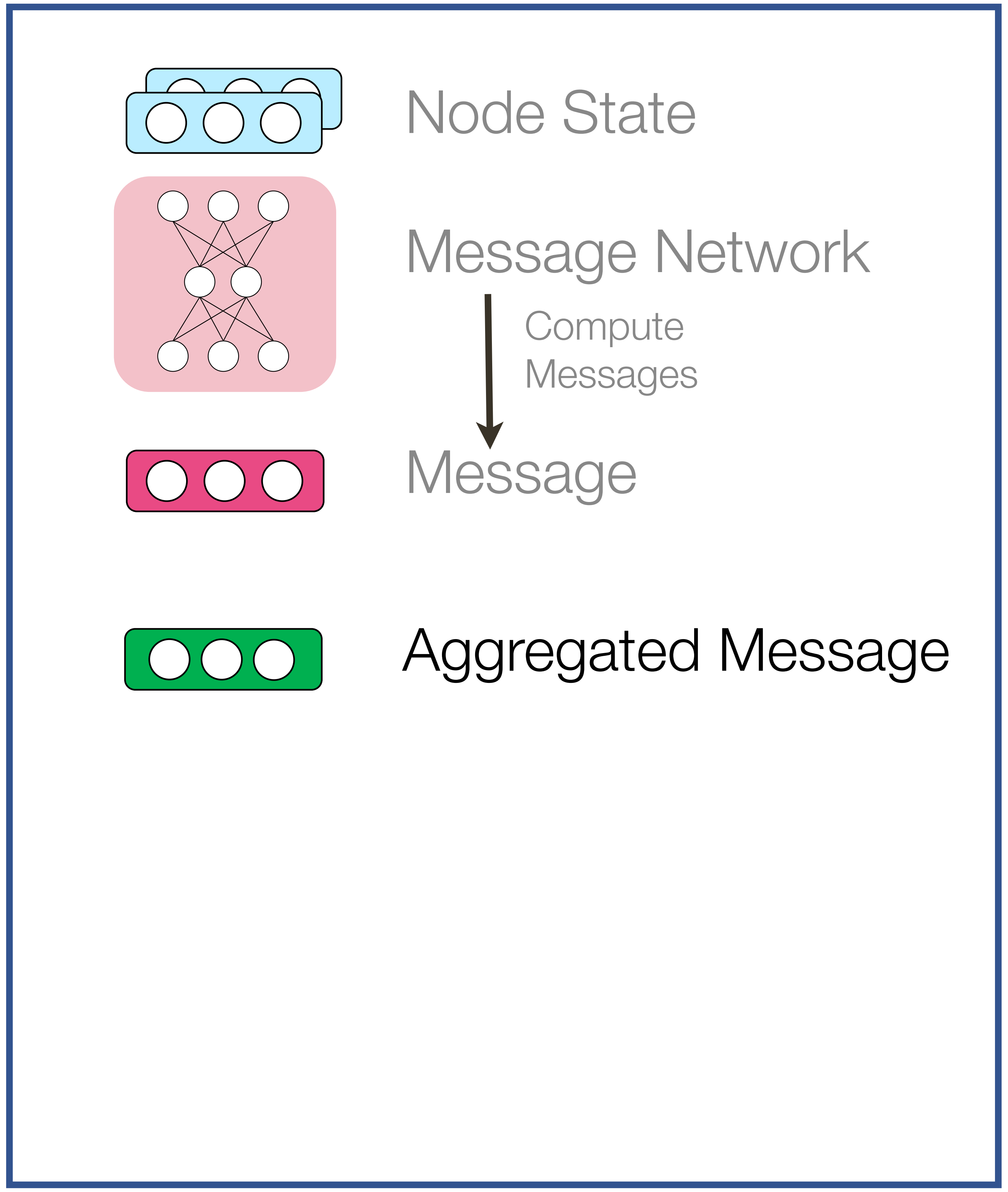
Message Passing in GNNs

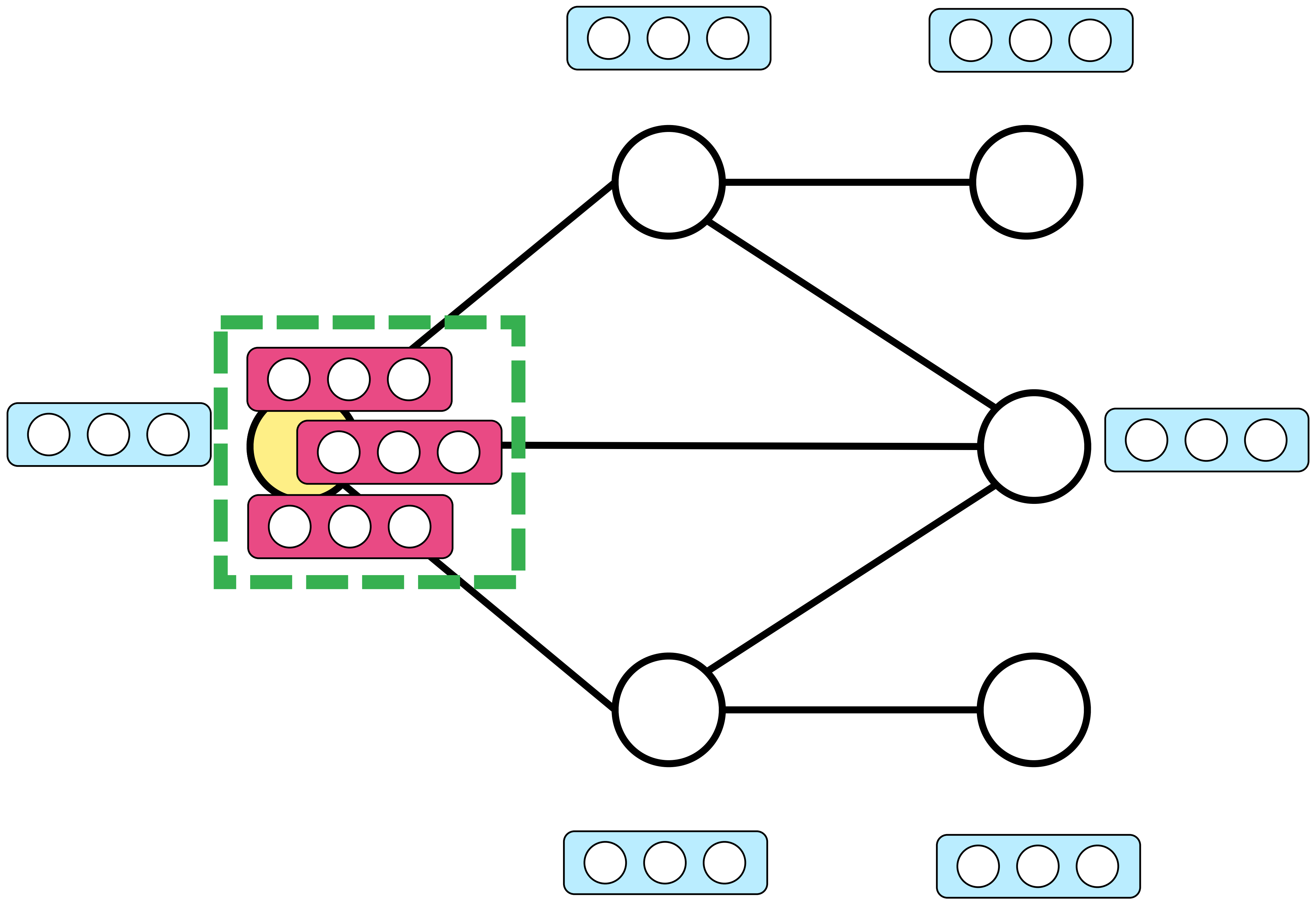
(t+1)-th message passing step/layer

$$\mathbf{h}_i^t \quad \mathbf{h}_j^t$$

$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

$$\bar{\mathbf{m}}_i^t = f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$





Slide from Renjie Liao

Message Passing in GNNs

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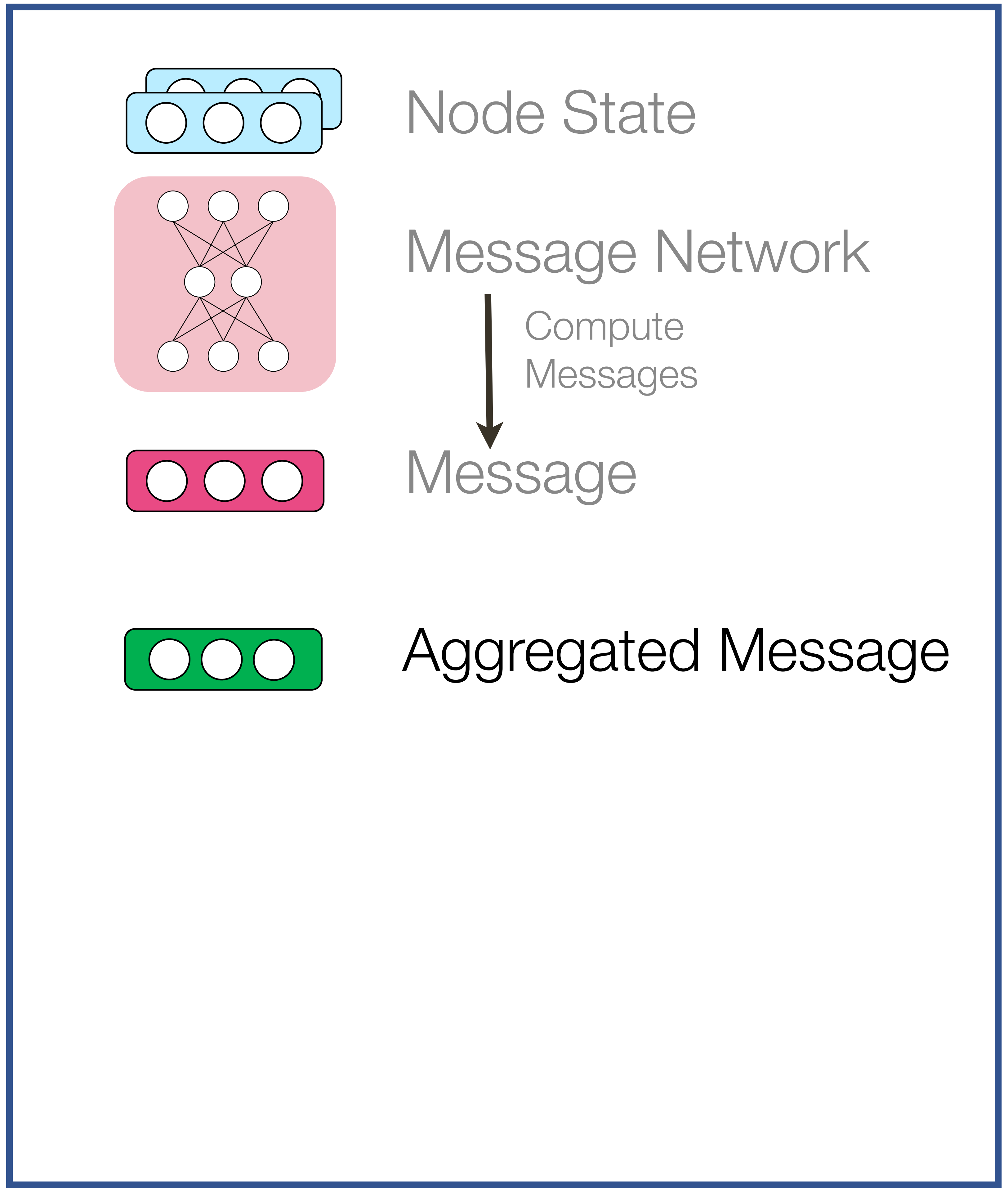

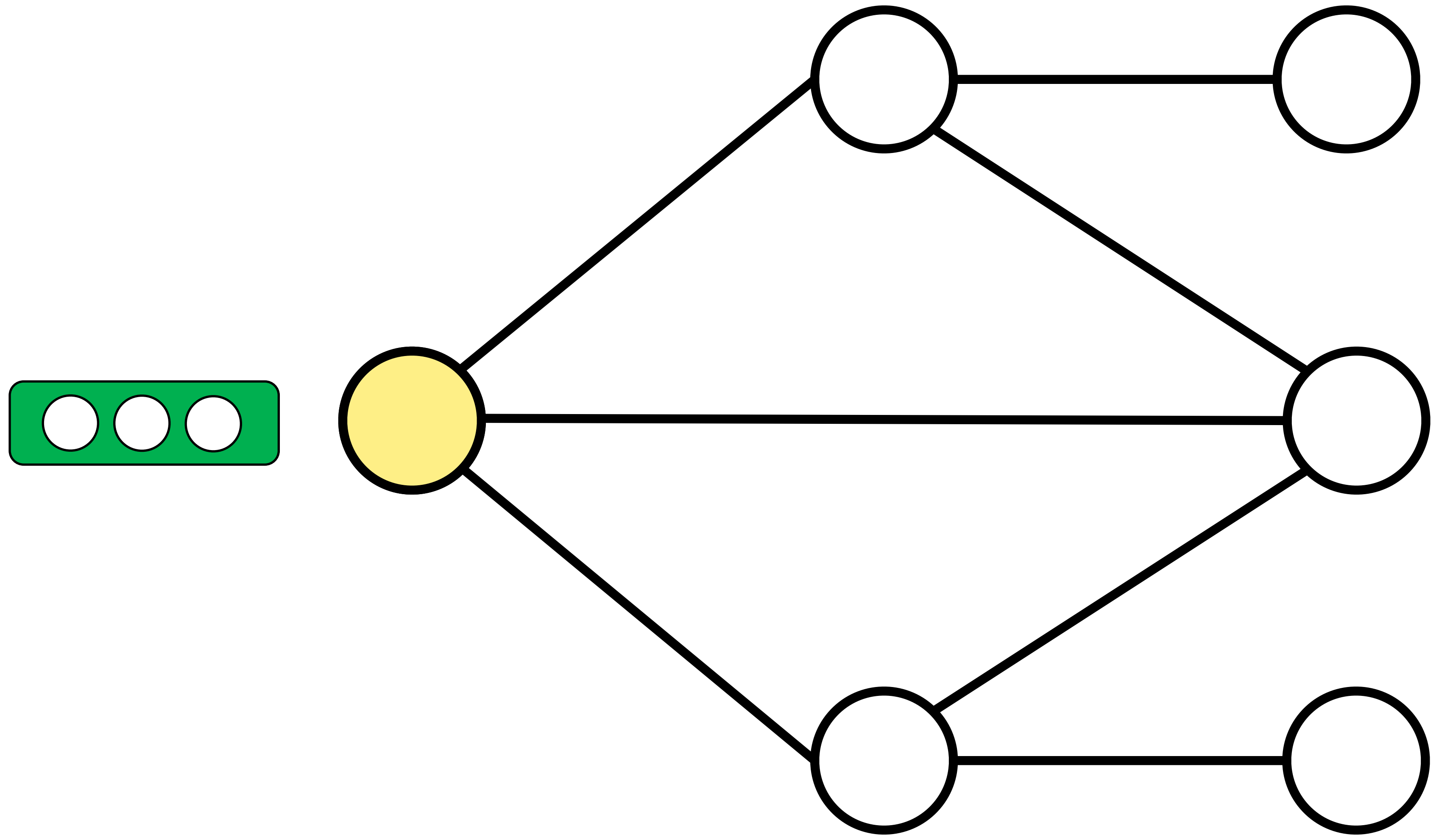

Slide from Renjie Liao

Message Passing in GNNs

(t+1)-th message passing step/layer

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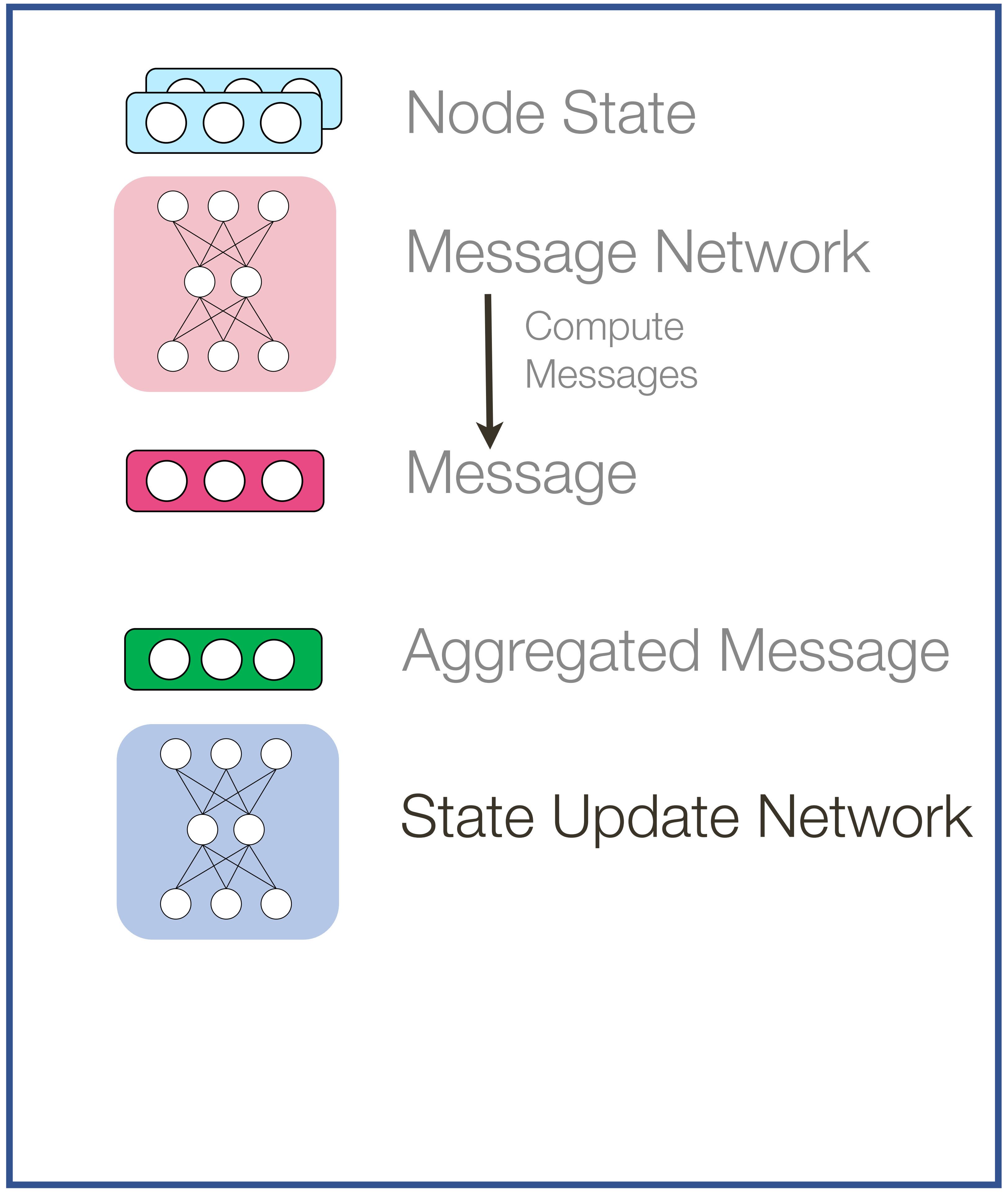
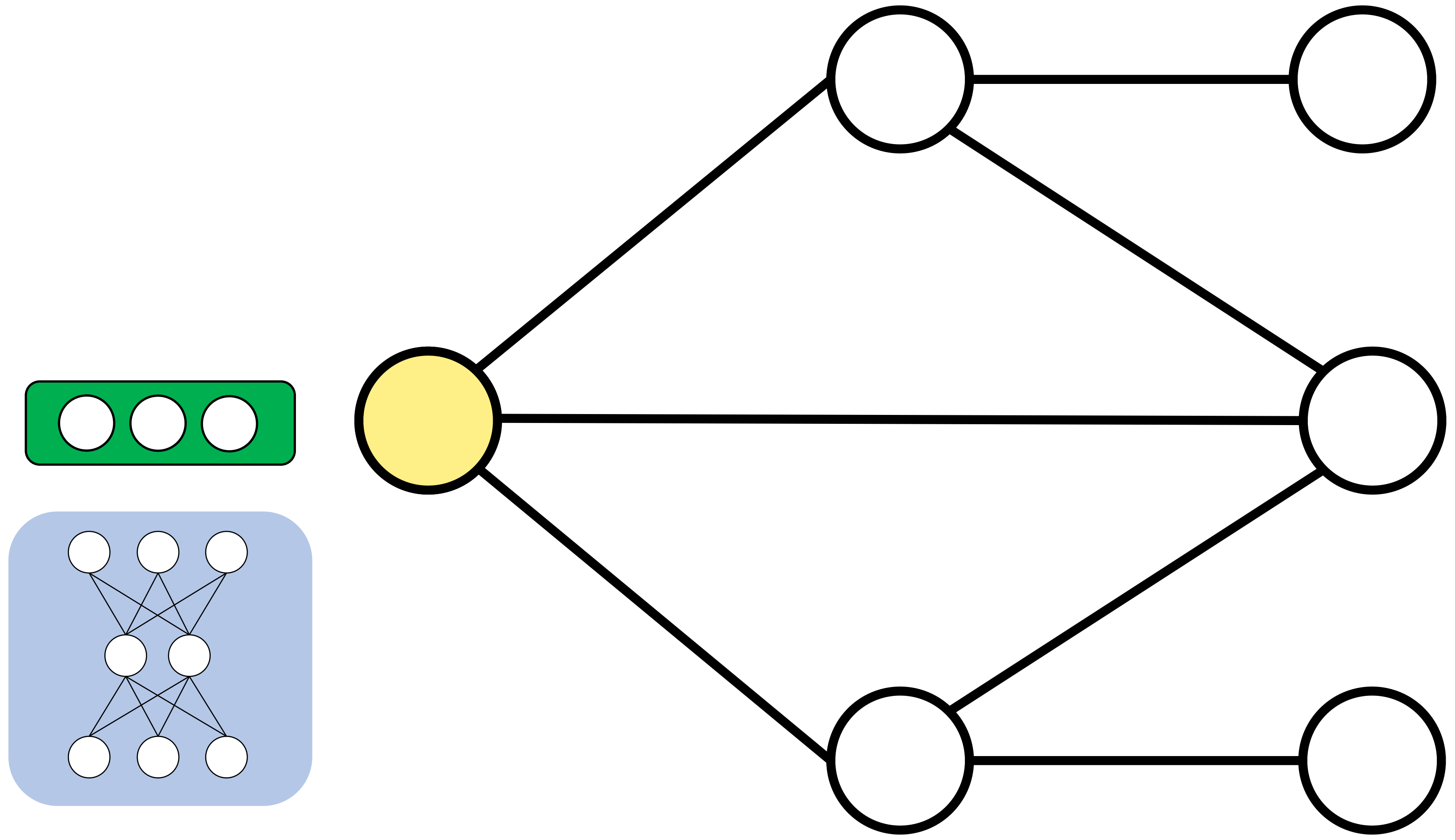




Message Passing in GNNs

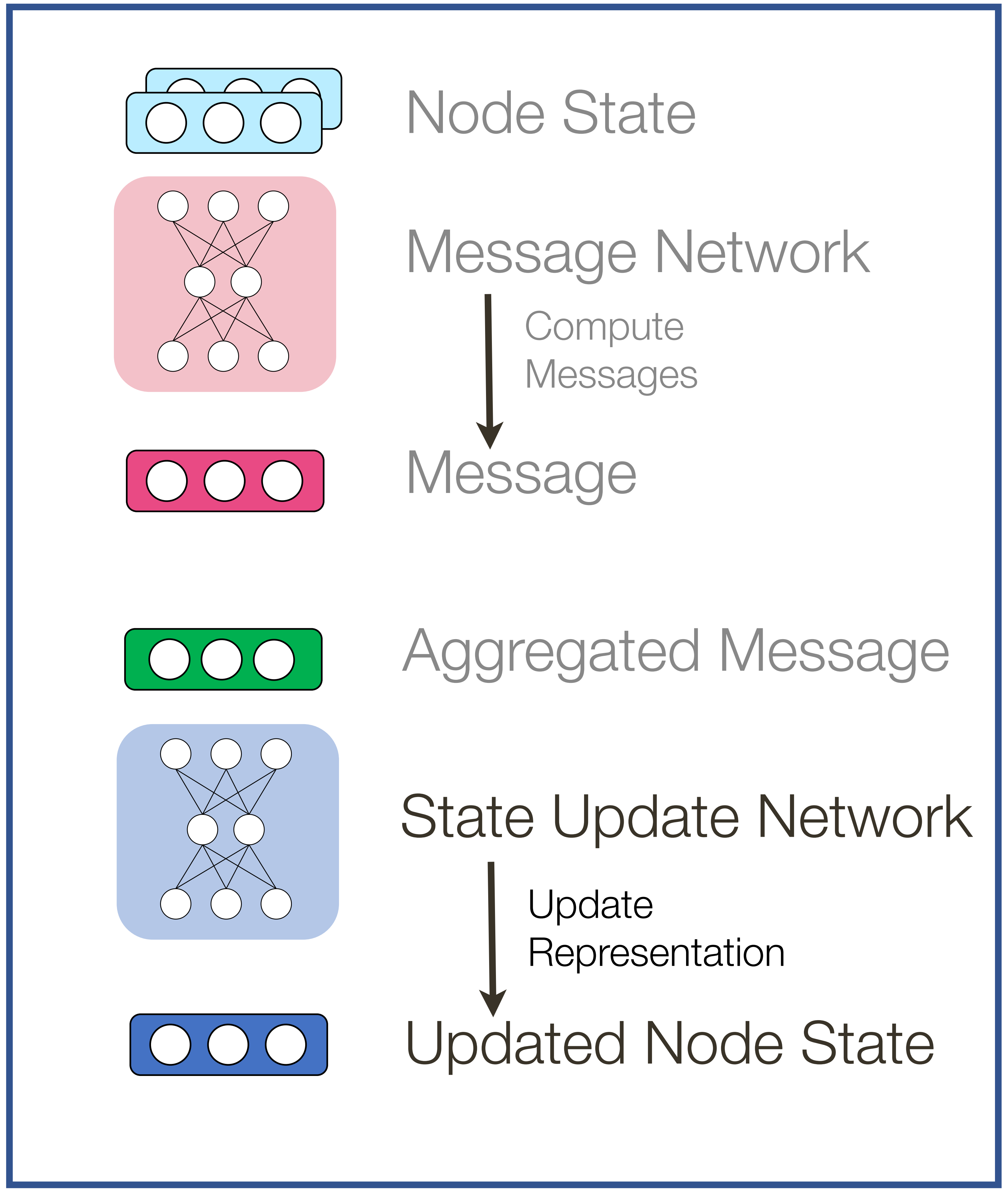
(t+1)-th message passing step/layer

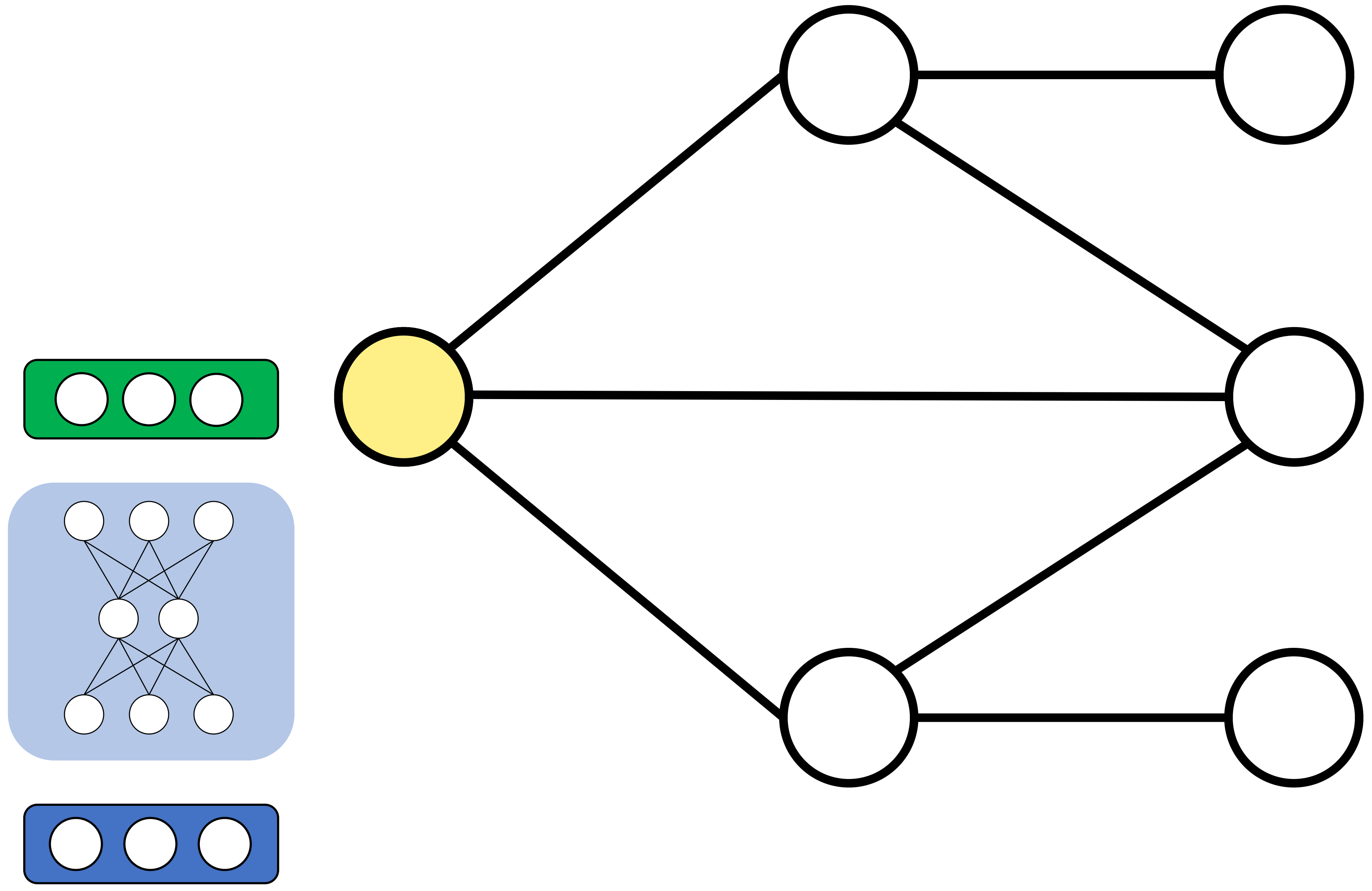
$$\mathbf{h}_i^t \quad \mathbf{h}_j^t$$

$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

$$\bar{\mathbf{m}}_i^t = f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

$$\mathbf{h}_i^{t+1} = f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$





Slide from Renjie Liao

Message Passing in GNNs

(t+1)-th message passing step/layer

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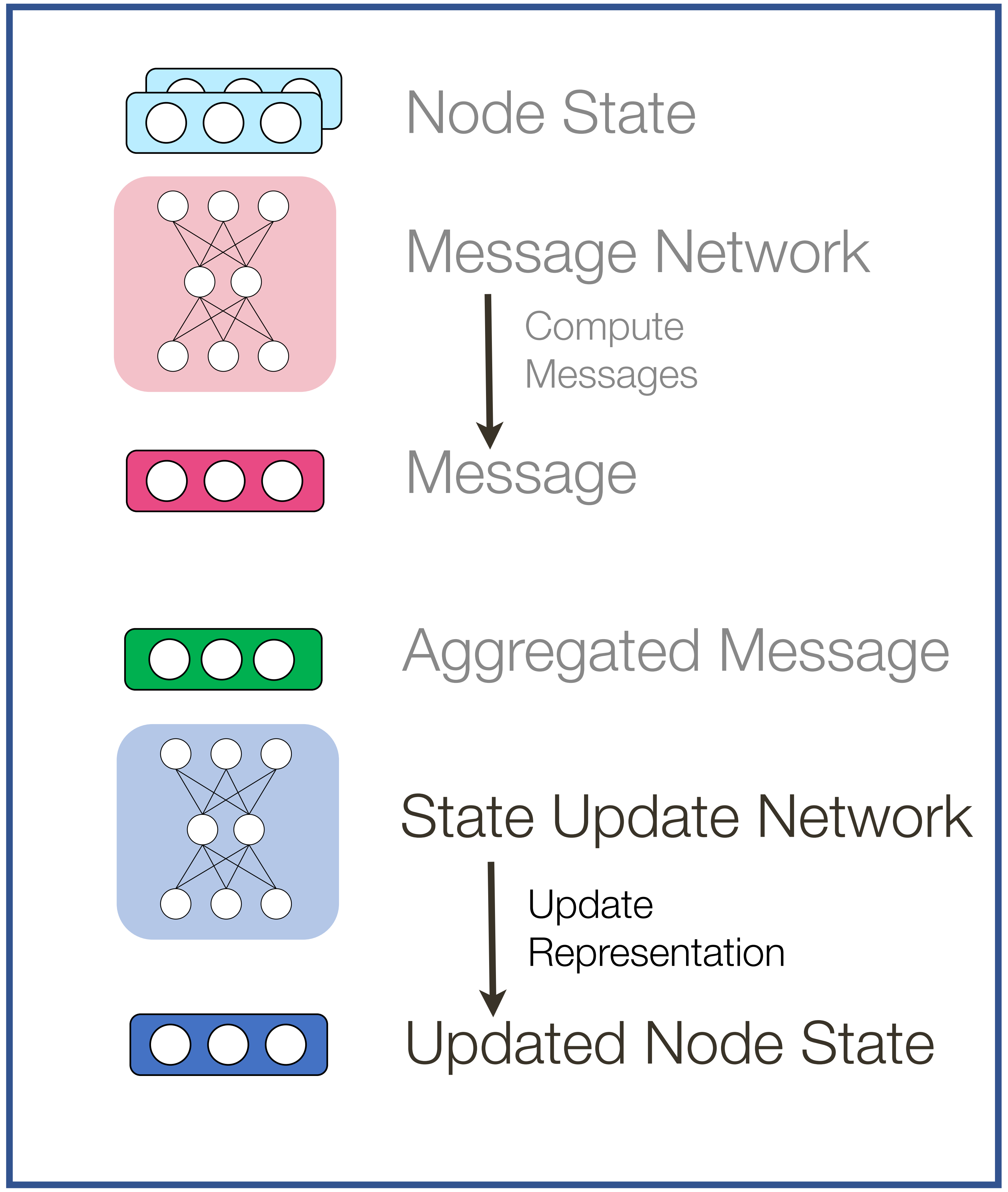
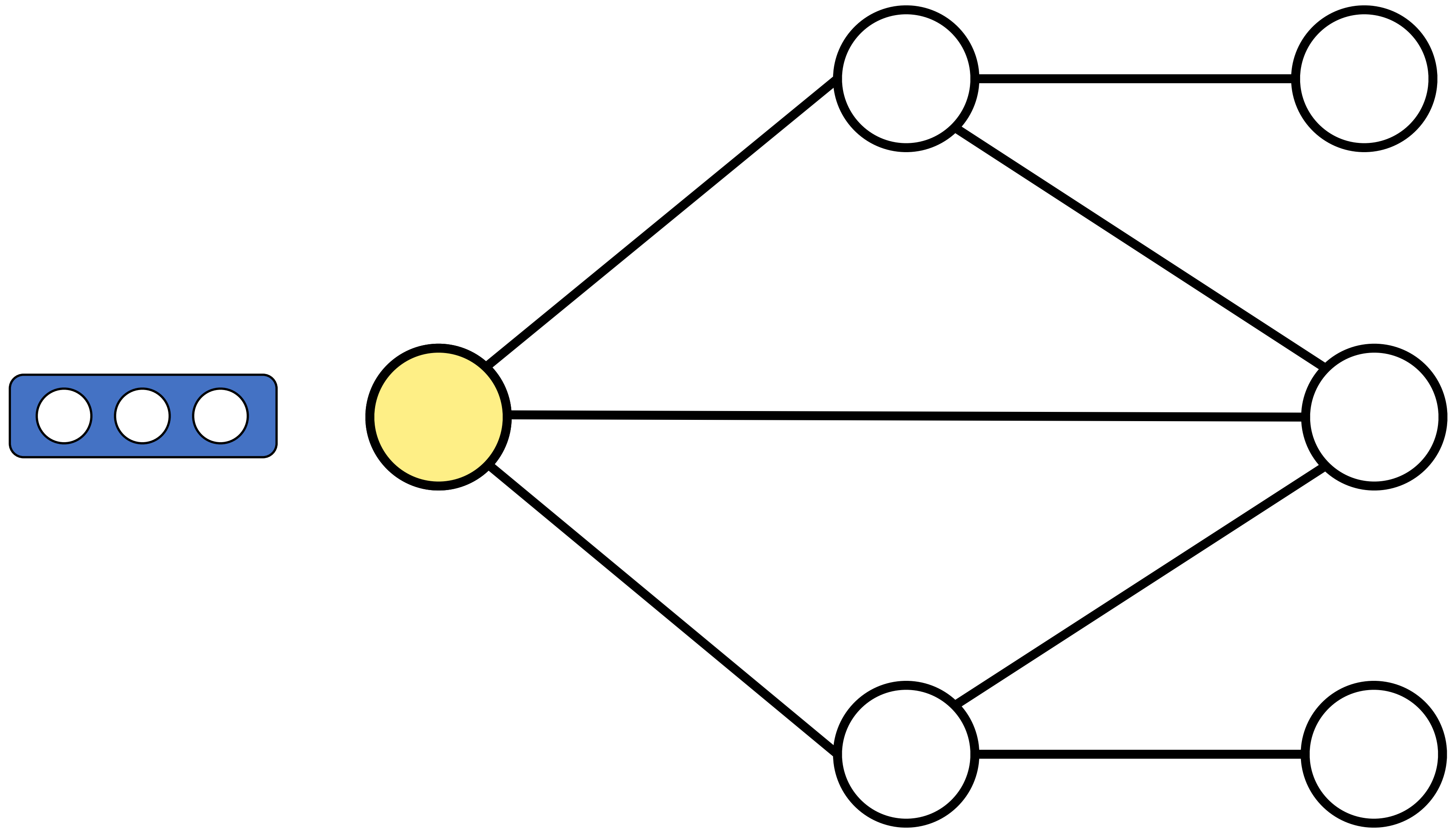




Slide from Renjie Liao

Message Passing in GNNs

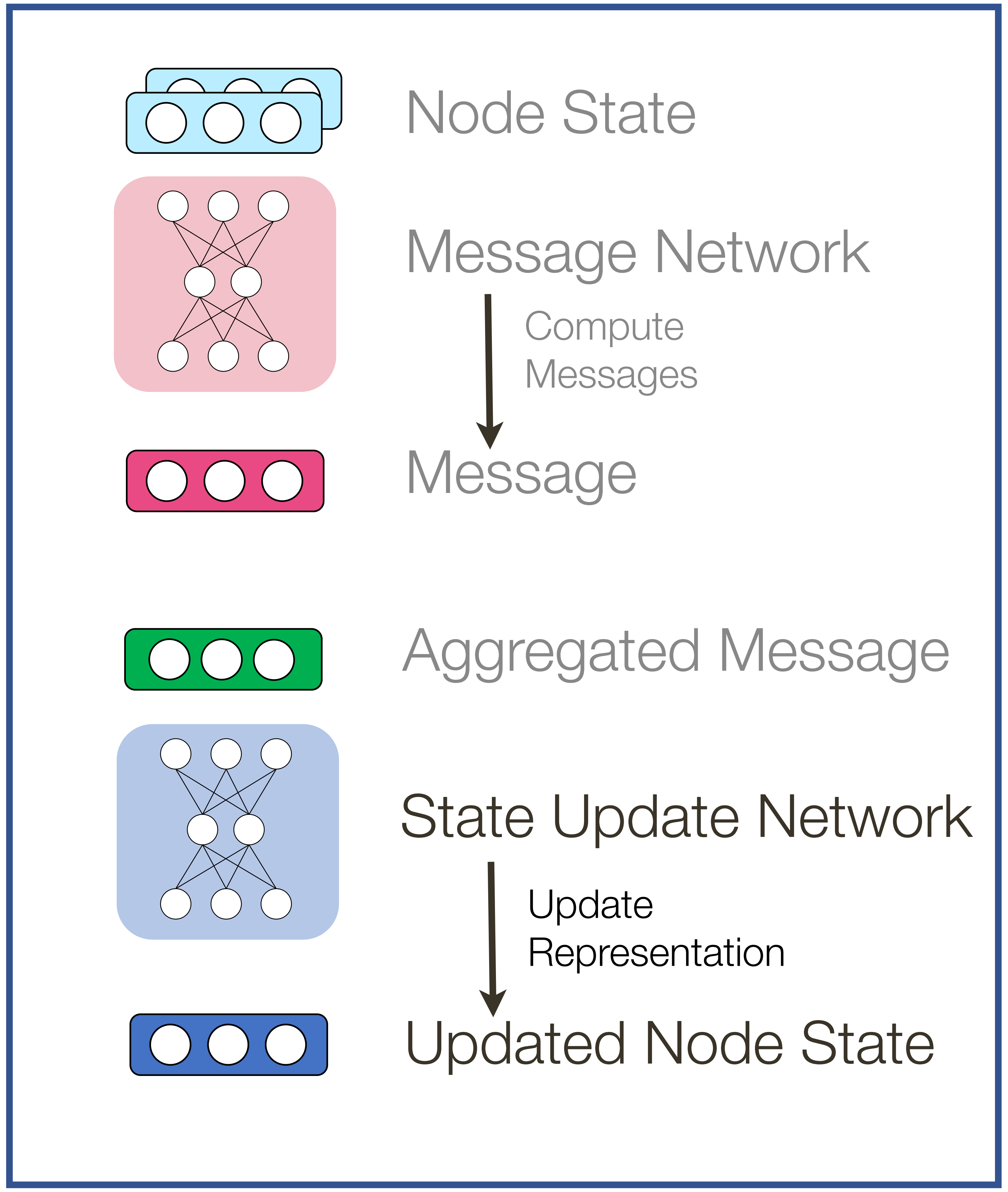
(t+1)-th message passing step/layer

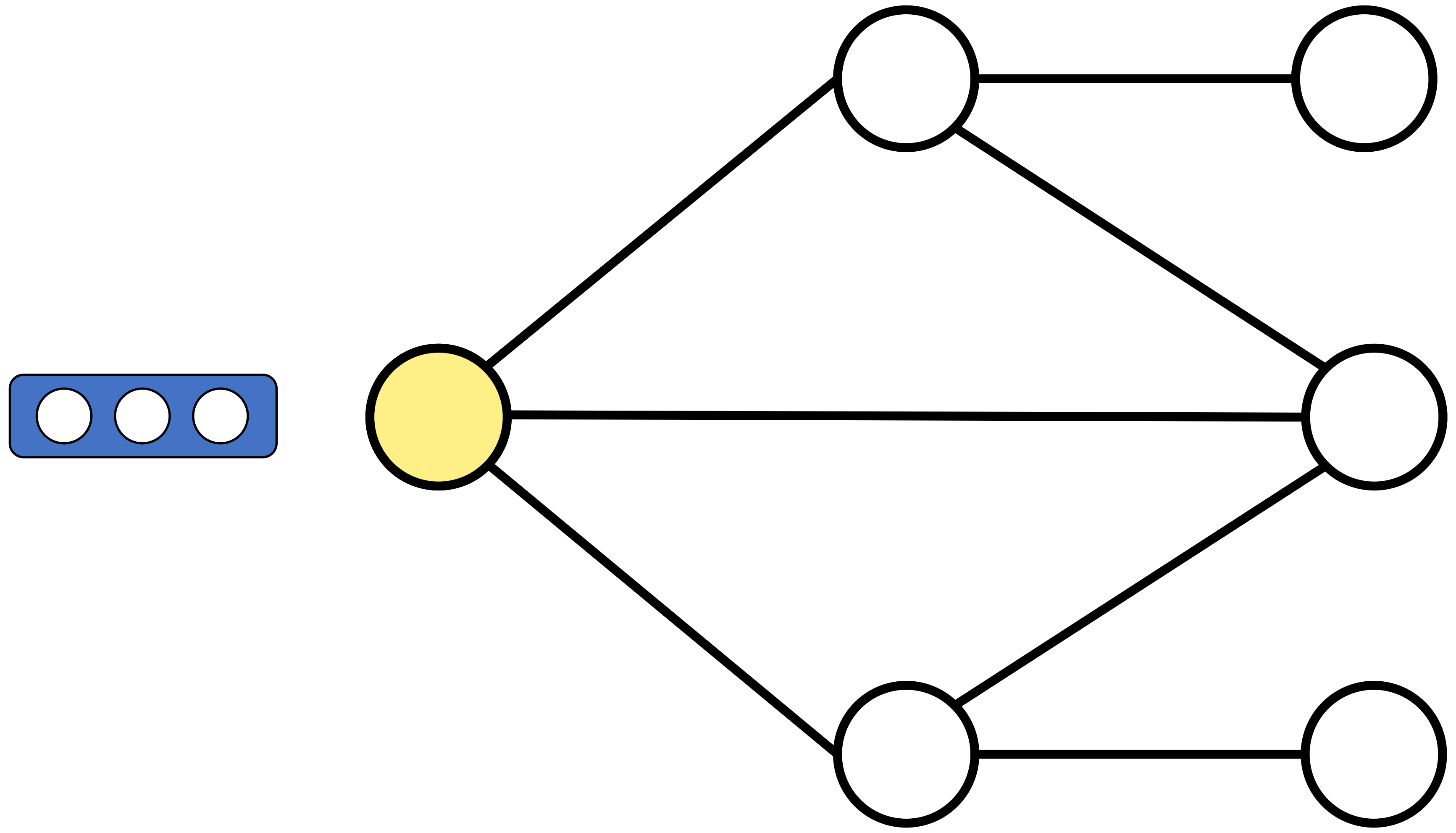
$$\mathbf{h}_i^t \quad \mathbf{h}_j^t$$

$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

$$\bar{\mathbf{m}}_i^t = f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

$$\mathbf{h}_i^{t+1} = f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$





Note: We can do all updates in parallel! (but can also be serial)

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GNN **Instantiations**

1. Compute Messages

$$\mathbf{m}_{ji}^{t} = f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

2. Aggregate Messages

$$\bar{\mathbf{m}}_i^t = f_{\mathrm{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

3. Update Node Representations

$$\mathbf{h}_i^{t+1} = f_{\mathrm{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$

GNN **Instantiations**

1. **Compute Messages**

$$\mathbf{m}_{ji}^{t} = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathrm{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [4]

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GNN **Instantiations**

1. **Compute Messages**

$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [4]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [5]

GNN **Instantiations**

1. **Compute Messages**

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$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t, \boxed{\mathbf{e}_{ji}}) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}])$$ [4]

Edge Feature

GNN **Instantiations**

1. Compute Messages

$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [4]

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Edge Feature

2. **Aggregate Messages**

$$\bar{\mathbf{m}}_i^t = f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [4,5,7]

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GNN **Instantiations**

1. Compute Messages

$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

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$$\bar{\mathbf{m}}_i^t = f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [4,5,7]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [6]

GNN **Instantiations**

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$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [4]

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$$\bar{\mathbf{m}}_i^t = f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

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$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \max_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [6]

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$$\bar{\mathbf{m}}_i^t = f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

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$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t \quad [6]$$

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \max_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t \quad [6]$$

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \text{LSTM}\left([\mathbf{m}_{ji}^t | j \in \mathcal{N}_i]\right) \quad [6]$$

GNN **Instantiations**

1. Compute Messages

$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [4]

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$$\bar{\mathbf{m}}_i^t = f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

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3. **Update Node Representations**

$$\mathbf{h}_i^{t+1} = f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$

$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{GRU}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$ [4,7]

Slide from Renjie Liao

GNN **Instantiations**

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$$\bar{\mathbf{m}}_i^t = f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

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$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{GRU}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$ [4,7]

$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{MLP}_1(\mathbf{h}_i^t) + \text{MLP}_2(\bar{\mathbf{m}}_i^t)$$ [5]

GNN **Instantiations**

1. Compute Messages

$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t]) \quad [4]$$

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Edge Feature

2. Aggregate Messages

$$\bar{\mathbf{m}}_i^t = f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \textstyle\sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t \quad [4,5,7]$$

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$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{MLP}_1(\mathbf{h}_i^t) + \text{MLP}_2(\bar{\mathbf{m}}_i^t) \quad [5]$$

$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{MLP}([\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t]) \quad [6]$$

Slide from Renjie Liao

GNN **Readout**

1. Node Readout

$$\mathbf{y}_i = f_{\text{readout}}(\mathbf{h}_i^T)$$

2. Edge Readout

$$\mathbf{y}_{ij} = f_{\text{readout}}(\mathbf{h}_i^T, \mathbf{h}_j^T)$$

3. Graph Readout

$$\mathbf{y} = f_{\text{readout}}(\{\mathbf{h}_i^T\})$$

Slide from Renjie Liao

GNN **Readout**

1. **Node Readout**

$$\mathbf{y}_i = f_{\text{readout}}(\mathbf{h}_i^T) \qquad f_{\text{readout}}(\mathbf{h}_i^T) = \text{MLP}(\mathbf{h}_i^T)$$

GNN **Readout**

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$$f_{\text{readout}}(\mathbf{h}_i^T) = \text{MLP}(\mathbf{h}_i^T)$$

2. **Edge Readout**

$$\mathbf{y}_{ij} = f_{\text{readout}}(\mathbf{h}_i^T, \mathbf{h}_j^T)$$

$$f_{\text{readout}}(\mathbf{h}_i^T, \mathbf{h}_j^T) = \text{MLP}([\mathbf{h}_i^T, \mathbf{h}_j^T])$$

$$f_{\text{readout}}(\mathbf{h}_i^T, \mathbf{h}_j^T, \boxed{e_{ij}}) = \text{MLP}([\mathbf{h}_i^T, \mathbf{h}_j^T, e_{ij}])$$

Edge Feature

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$$f_{\text{readout}}(\mathbf{h}_i^T, \mathbf{h}_j^T, \boxed{e_{ij}}) = \text{MLP}([\mathbf{h}_i^T, \mathbf{h}_j^T, e_{ij}])$$

Edge Feature

3. **Graph Readout**

$$\mathbf{y} = f_{\text{readout}}(\{\mathbf{h}_i^T\})$$

$$f_{\text{readout}}(\{\mathbf{h}_i^T\}) = \sum_i \sigma(\text{MLP}_1(\mathbf{h}_i^T))\text{MLP}_2(\mathbf{h}_i^T)$$

$$f_{\text{readout}}(\{\mathbf{h}_i^T\}, \boxed{\mathbf{g}}) = \sum_i \sigma(\text{MLP}_1(\mathbf{h}_i^T, \mathbf{g}))\text{MLP}_2(\mathbf{h}_i^T, \mathbf{g})$$

Graph Feature

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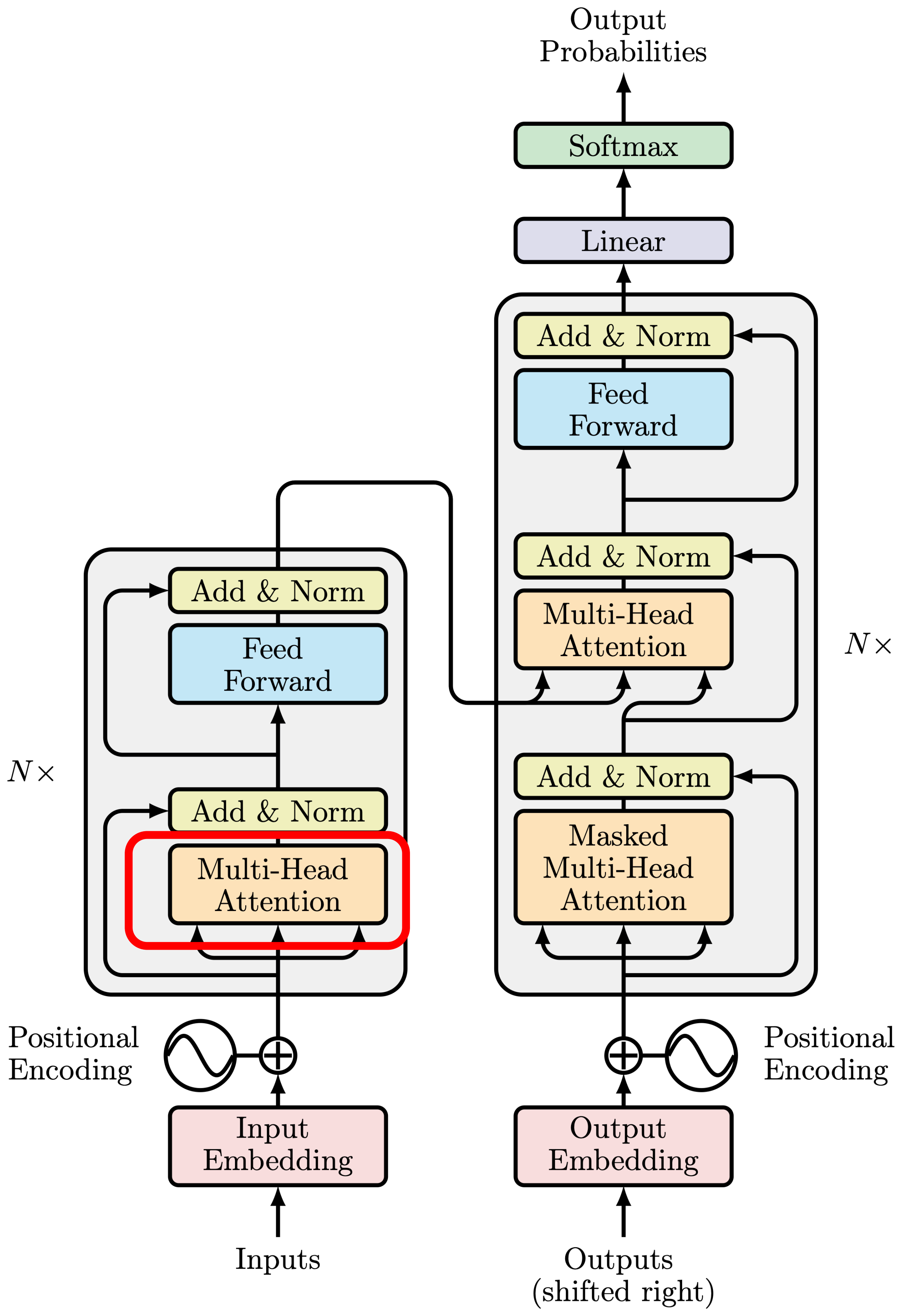
GNN **Relationship** to **Transformers**



— Attention can be viewed as the weighted adjacency matrix of a fully connected graph!

— Transformers (esp. encoder) can be viewed as GNNs applied to fully connected graphs!

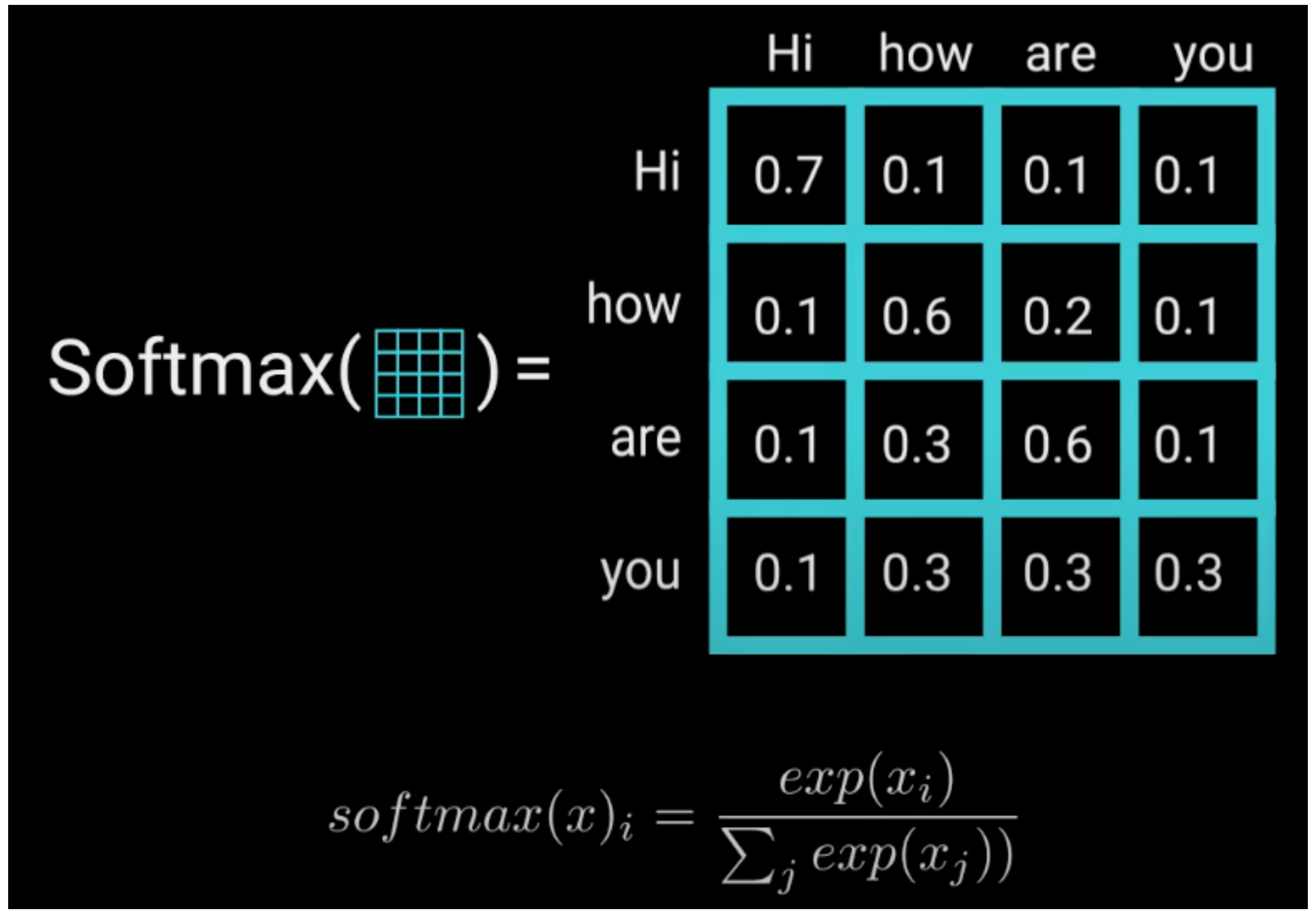


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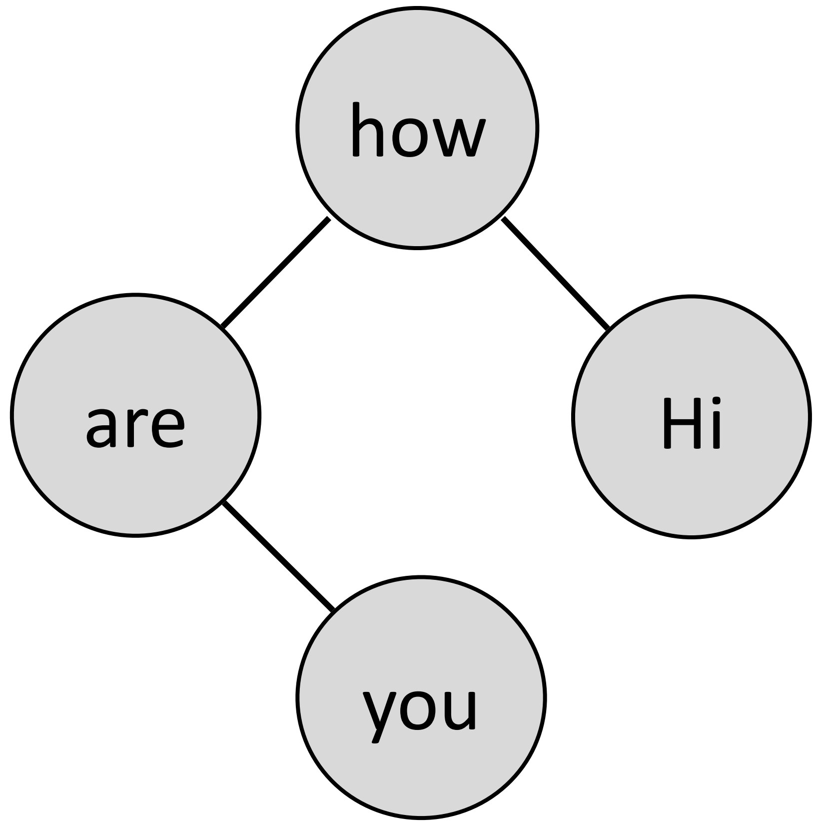
Image Credit: [9] & https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

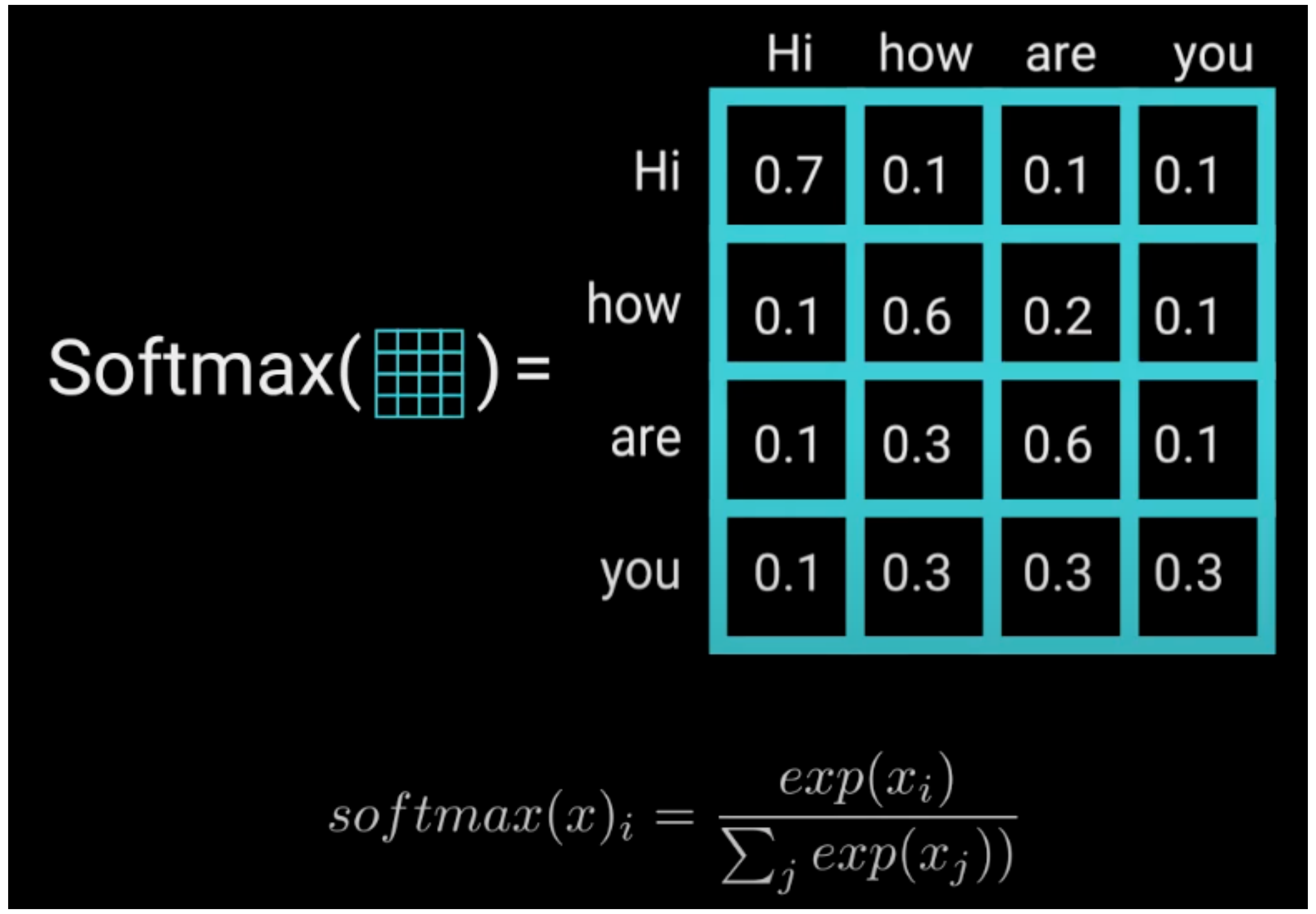
GNN **Relationship** to **Transformers**

— Apply the adjacency matrix as a mask to the attention and renormalize it, is like Graph Attention Networks (GAT) [10]

— Encoder connectivities/distances as bias of the attention [11]



	Hi	how	are	you
Hi	0	1	0	1
how	1	0	0	0
are	0	0	0	1
you	1	0	1	0



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