Recurrent Graph Neural Networks

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TIM[2]
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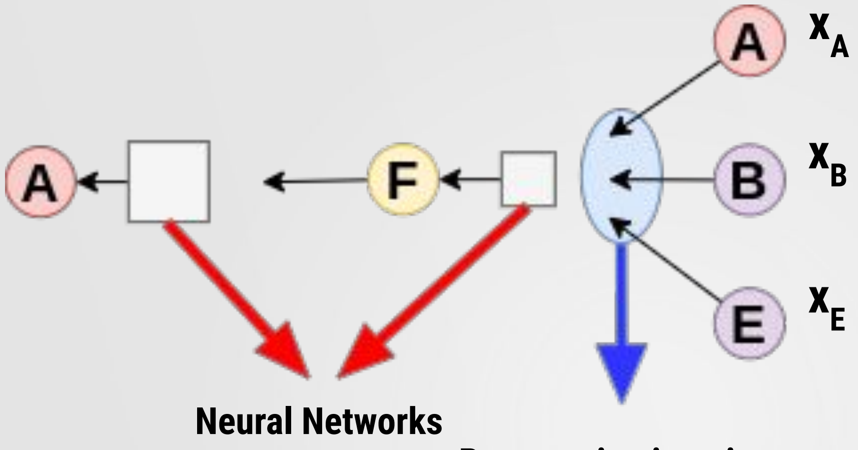
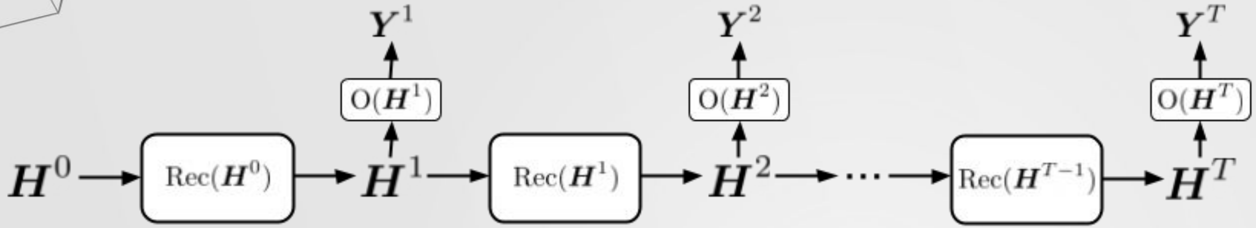
01 GNNs so far

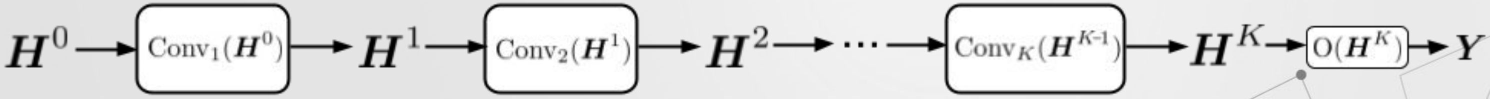


<u>Permutation invariant</u>
Aggregation

Sum
Average
Max

02 Recurrent VS Convolutional





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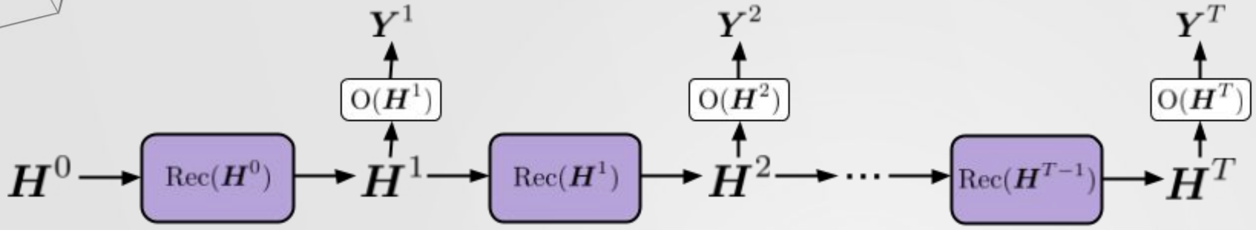

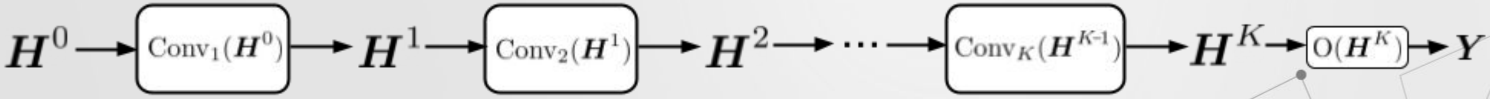

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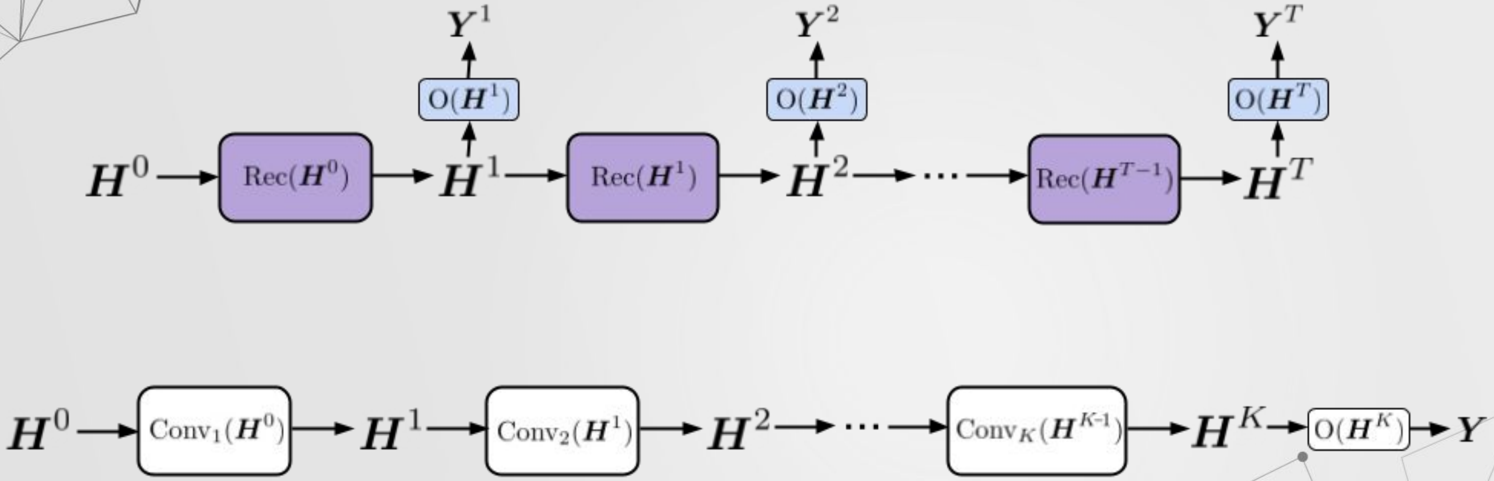

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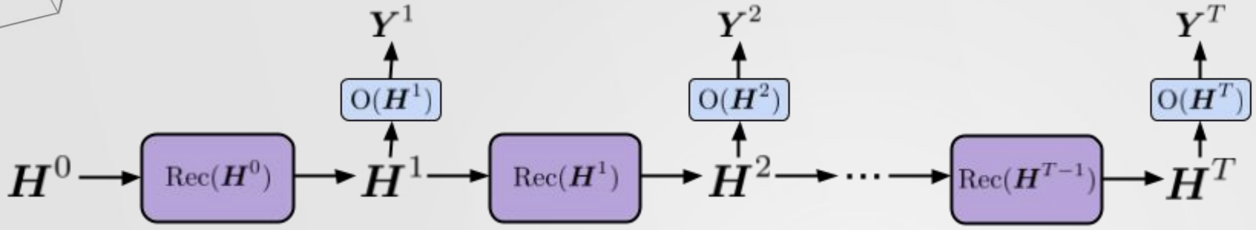

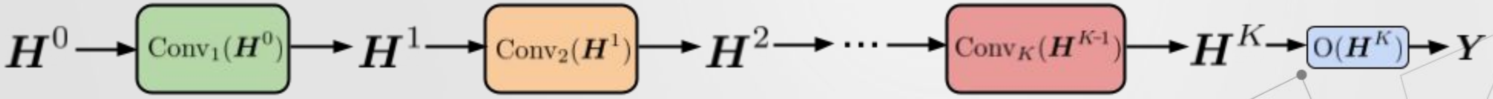

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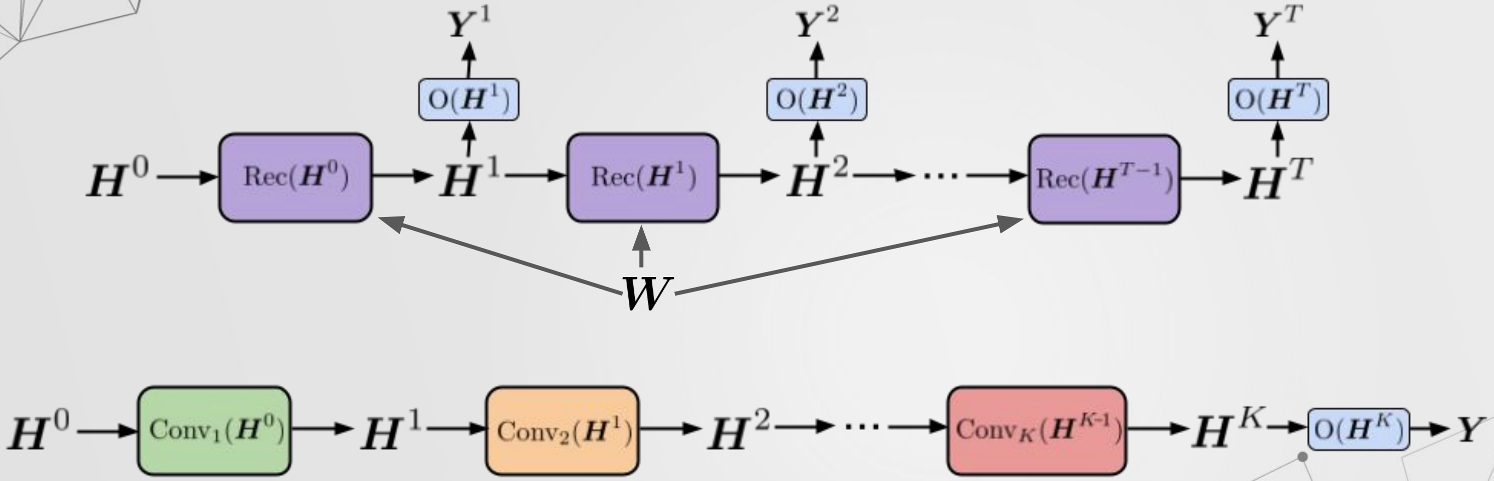

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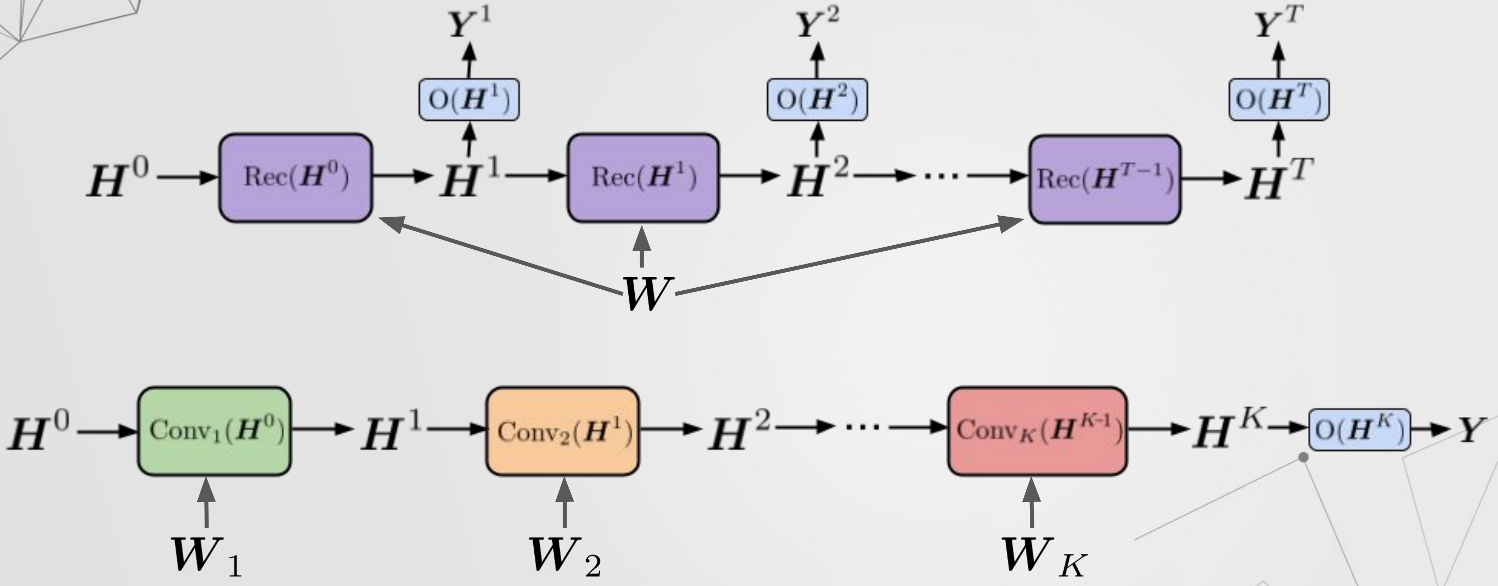

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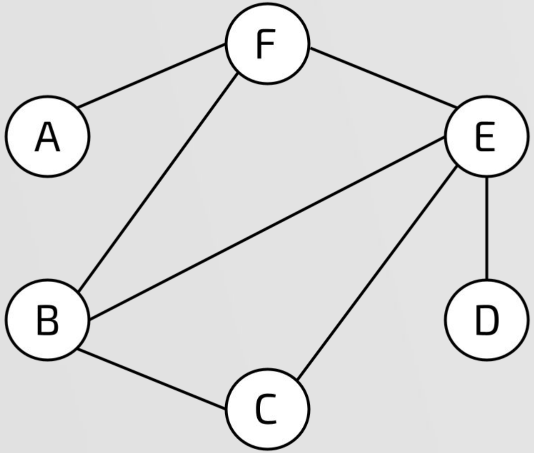
03 Graph Neural Network Model[1]

- Pioneer work on Graph Neural Network
- Diffusion mechanism (convolution)
- General framework for graph processing

[1] Scarselli, et al., *The graph neural network model*, IEEE Transactions on Neural Networks, 2009

03 Graph Neural Network Model



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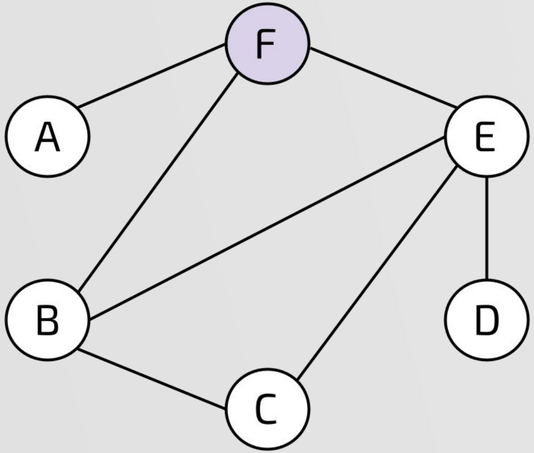
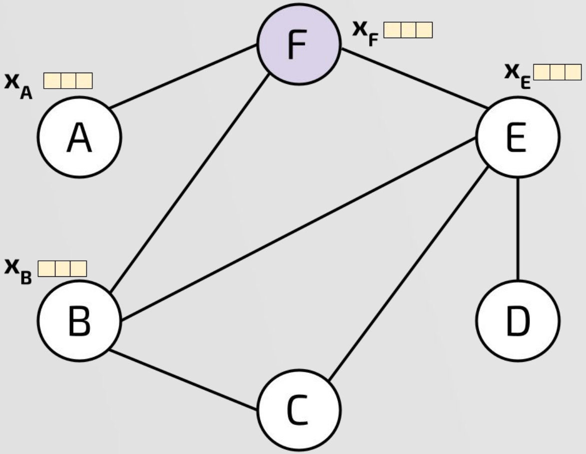


03 Graph Neural Network Model

$$\boldsymbol{x}_v = \mathbb{R}^d$$



03 Graph Neural Network Model

$$\boldsymbol{x}_v = \mathbb{R}^d$$
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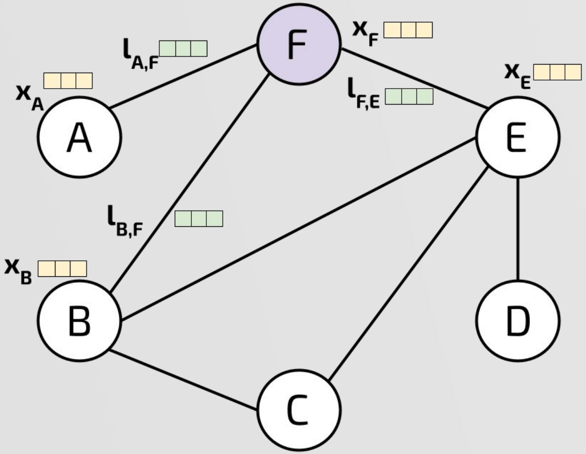

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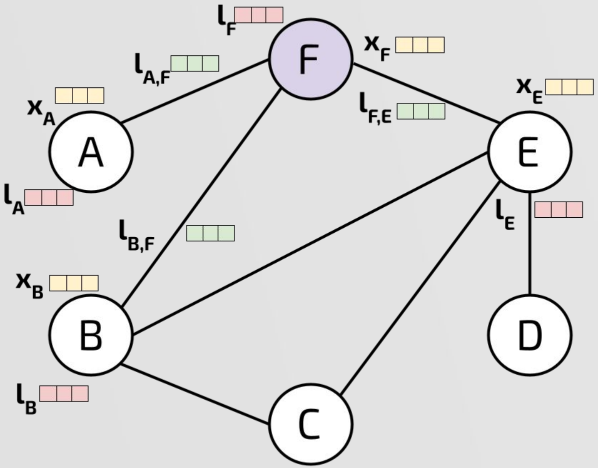

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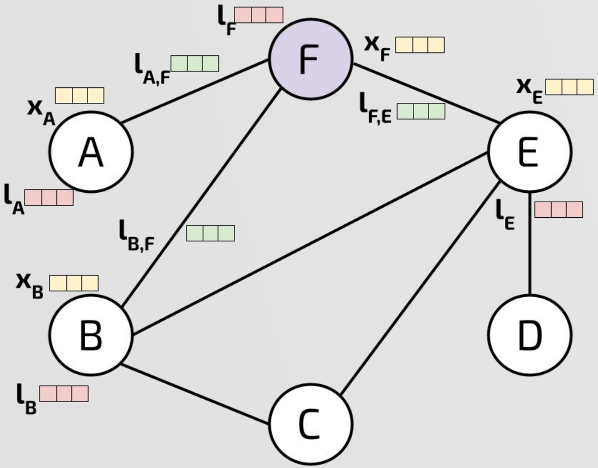
$co(v)$ = edges connected to v

$ne(v)$ = neighbours of v



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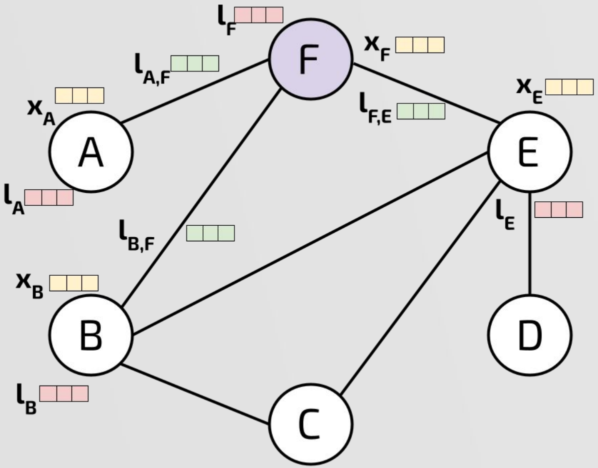

$$\boldsymbol{x}_v^{t+1} = f_{\boldsymbol{w}}(\boldsymbol{l}_v, \boldsymbol{l}_{co(v)}, \boldsymbol{x}^t_{ne(v)}, \boldsymbol{l}_{ne(v)})$$

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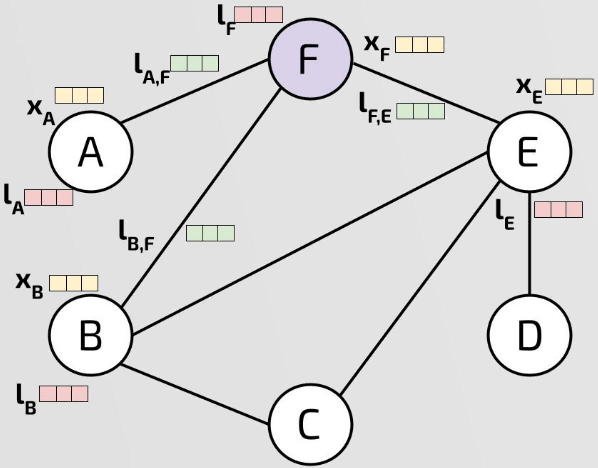

$$\boldsymbol{x}_v^{t+1} = f_{\boldsymbol{w}}(\boldsymbol{l}_v, \boldsymbol{l}_{co(v)}, \boldsymbol{x}_{ne(v)}^t, \boldsymbol{l}_{ne(v)})$$

$$\boldsymbol{o}_v^t = g_{\boldsymbol{w}}(\boldsymbol{x}_v^t, \boldsymbol{l}_v)$$

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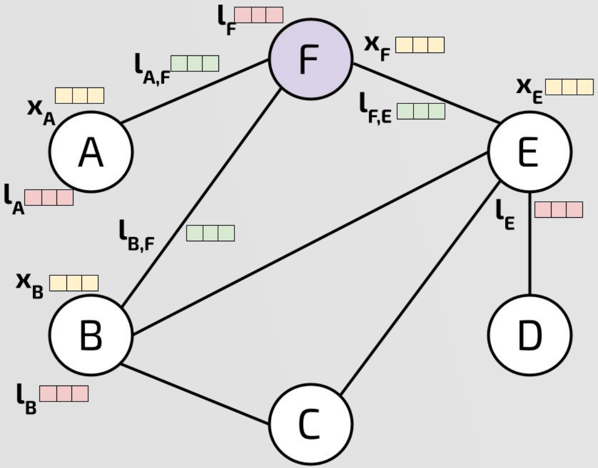

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learnable parameters

$$\boldsymbol{o}_v^t = g_{\boxed{\boldsymbol{w}}}(\boldsymbol{x}_v^t, \boldsymbol{l}_v)$$

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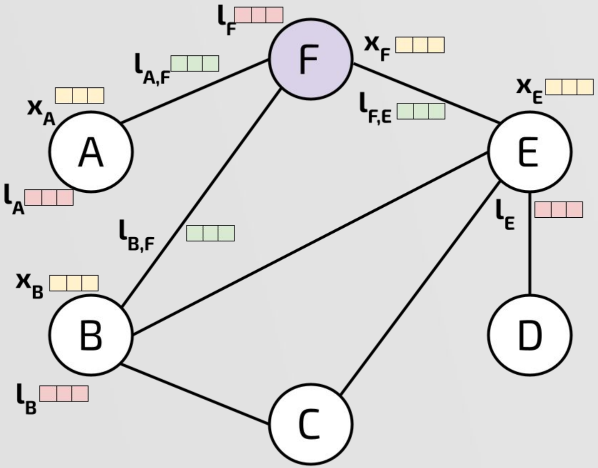

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learnable parameters

$$\boldsymbol{o}_v^t = g_{\boxed{\boldsymbol{w}}}(\boldsymbol{x}_v^t, \boldsymbol{l}_v)$$

$f_{\boldsymbol{w}}$ = transition function

$g_{\boldsymbol{w}}$ = output function

03 Graph Neural Network Model

Repeated forward of the transition function create an **encoding network** $\varphi_{\boldsymbol{w}}$

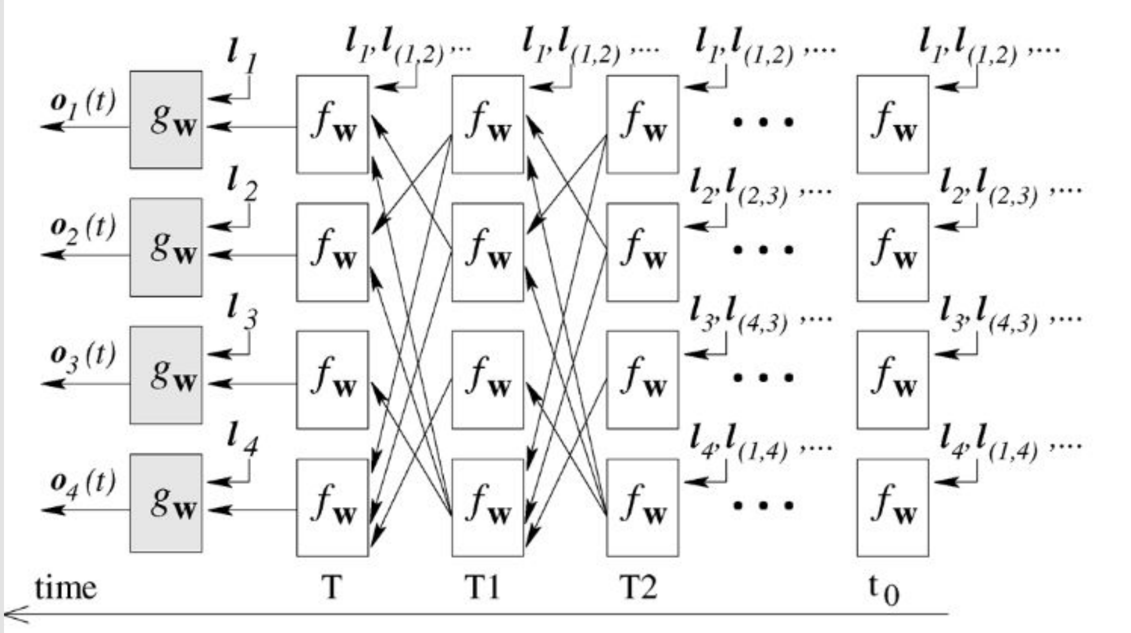

Image taken from the original publication

03 Graph Neural Network Model

Goal: converge to a unique solution for $\mathbf{x}_v$ and $\mathbf{o}_v$

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If the transition function $f_{\boldsymbol{w}}$ is a **contraction mapping**, there exists a fixed point solution

$$\|\boldsymbol{x}_v^{t+1} - \boldsymbol{x}_v^{t}\| < \epsilon$$

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If the transition function $f_{\boldsymbol{w}}$ is a **contraction mapping**, there exists a fixed point solution

$$\|\boldsymbol{x}_v^{t+1} - \boldsymbol{x}_v^t\| < \epsilon$$

If $f_{\boldsymbol{w}}$ is a NN, to ensure the contraction mapping a penalty based on the norm of the Jacobian is added to the loss function

MAIN

initialize $\boldsymbol{w}$;

$\boldsymbol{x}$=**Forward**($\boldsymbol{w}$);

repeat

$\frac{\partial e_{\boldsymbol{w}}}{\partial \boldsymbol{w}}$=BACKWARD($\boldsymbol{x}, \boldsymbol{w}$);

$\boldsymbol{w}$=$\boldsymbol{w} - \lambda \cdot \frac{\partial e_{\boldsymbol{w}}}{\partial \boldsymbol{w}}$;

$\boldsymbol{x}$=FORWARD($\boldsymbol{w}$);

until (a stopping criterion);

return $\boldsymbol{w}$;

end

03 Graph Neural Network Model

```
MAIN
    initialize w;
    x=Forward(w);
    repeat
        ∂e_w/∂w = BACKWARD(x, w);
        w = w − λ · ∂e_w/∂w;
        x = FORWARD(w);
    until (a stopping criterion);
    return w;
end
```

```
FORWARD(w)
    initialize x(0), t = 0;
    repeat
        x(t + 1) = F_w(x(t), l);
        t = t + 1;
    until ||x(t) − x(t − 1)|| ≤ ε_f
    return x(t);
end
```

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    initialize $\boldsymbol{w}$;
    $\boldsymbol{x}$=**Forward**($\boldsymbol{w}$);
    repeat
        $\frac{\partial e_{\boldsymbol{w}}}{\partial \boldsymbol{w}}$=BACKWARD($\boldsymbol{x}, \boldsymbol{w}$);
        $\boldsymbol{w}=\boldsymbol{w} - \lambda \cdot \frac{\partial e_{\boldsymbol{w}}}{\partial \boldsymbol{w}}$;
        $\boldsymbol{x}$=FORWARD($\boldsymbol{w}$);
    until (a stopping criterion);
    return $\boldsymbol{w}$;
end

FORWARD($\boldsymbol{w}$)
    initialize $\boldsymbol{x}(0)$, $t = 0$;
    repeat
        $\boldsymbol{x}(t+1) = F_{\boldsymbol{w}}(\boldsymbol{x}(t), \boldsymbol{l})$;
        t=$t+1$;
    until $\|\boldsymbol{x}(t) - \boldsymbol{x}(t-1)\| \leq \varepsilon_f$
    return $\boldsymbol{x}(t)$;
end

BACKWARD($\boldsymbol{x}$,$\boldsymbol{w}$)
    $\boldsymbol{o} = G_{\boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{l}_{\boldsymbol{N}})$;
    $\boldsymbol{A} = \frac{\partial F_{\boldsymbol{w}}}{\partial \boldsymbol{x}}(\boldsymbol{x}, \boldsymbol{l})$;
    $\boldsymbol{b} = \frac{\partial e_{\boldsymbol{w}}}{\partial \boldsymbol{o}} \cdot \frac{\partial G_{\boldsymbol{w}}}{\partial \boldsymbol{x}}(\boldsymbol{x}, \boldsymbol{l}_{\boldsymbol{N}})$;
    initialize $\boldsymbol{z}(0)$, t=0;
    repeat
        $\boldsymbol{z}(t) = \boldsymbol{z}(t+1) \cdot \boldsymbol{A} + \boldsymbol{b}$;
        t=$t-1$;
    until $\|\boldsymbol{z}(t-1) - \boldsymbol{z}(t)\| \leq \varepsilon_b$;
    $\boldsymbol{c} = \frac{\partial e_{\boldsymbol{w}}}{\partial \boldsymbol{o}} \cdot \frac{\partial G_{\boldsymbol{w}}}{\partial \boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{l}_{\boldsymbol{N}})$;
    $\boldsymbol{d} = \boldsymbol{z}(t) \cdot \frac{\partial F_{\boldsymbol{w}}}{\partial \boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{l})$;
    $\frac{\partial e_{\boldsymbol{w}}}{\partial \boldsymbol{w}} = \boldsymbol{c} + \boldsymbol{d}$;
    return $\frac{\partial e_{\boldsymbol{w}}}{\partial \boldsymbol{w}}$;
end

03 Graph Neural Network Model

```
MAIN
    initialize w;
    x=Forward(w);
    repeat
        ∂e_w/∂w = BACKWARD(x, w);
        w = w − λ · ∂e_w/∂w;
        x = FORWARD(w);
    until (a stopping criterion);
    return w;
end
```

```
FORWARD(w)
    initialize x(0), t = 0;
    repeat
        x(t + 1) = F_w(x(t), l);
        t = t + 1;
    until ||x(t) − x(t − 1)|| ≤ ε_f
    return x(t);
end
```

```
BACKWARD(x,w)
    o = G_w(x, l_N);
    A = ∂F_w/∂x (x, l);
    b = ∂e_w/∂o · ∂G_w/∂x (x, l_N);
    initialize z(0), t=0;
    repeat
        z(t) = z(t + 1) · A + b;
        t = t − 1;
    until ||z(t − 1) − z(t)|| ≤ ε_b;
    c = ∂e_w/∂o · ∂G_w/∂w (x, l_N);
    d = z(t) · ∂F_w/∂w (x, l);
    ∂e_w/∂w = c + d;
    return ∂e_w/∂w;
end
```

Almeida - Pineda algorithm

04 Gated Graph Neural Network[2]

- Adaptation of the GNNM
- Uses GRU (Gated Recurrent Units) as transition function
- Iterate over T timesteps (instead of until convergence)
- Uses BTT (BackProp Through Time) to compute gradient

[1] Li et al, *Gated graph sequence neural networks*, ICLR, 2015.

04 Gated Graph Neural Network

Node annotations: node embeddings with additional information

Propagation Model:

$$\mathbf{h}_v^{(1)} = [\boldsymbol{x}_v^\top, \mathbf{0}]^\top \tag{1}$$

$$\mathbf{a}_v^{(t)} = \mathbf{A}_{v:}^\top \left[\mathbf{h}_1^{(t-1)\top} \dots \mathbf{h}_{|\mathcal{V}|}^{(t-1)\top}\right]^\top + \mathbf{b} \tag{2}$$

$$\mathbf{z}_v^t = \sigma\left(\mathbf{W}^z \mathbf{a}_v^{(t)} + \mathbf{U}^z \mathbf{h}_v^{(t-1)}\right) \tag{3}$$

$$\mathbf{r}_v^t = \sigma\left(\mathbf{W}^r \mathbf{a}_v^{(t)} + \mathbf{U}^r \mathbf{h}_v^{(t-1)}\right) \tag{4}$$

$$\widetilde{\mathbf{h}_v^{(t)}} = \tanh\left(\mathbf{W}\mathbf{a}_v^{(t)} + \mathbf{U}\left(\mathbf{r}_v^t \odot \mathbf{h}_v^{(t-1)}\right)\right) \tag{5}$$

$$\mathbf{h}_v^{(t)} = (1 - \mathbf{z}_v^t) \odot \mathbf{h}_v^{(t-1)} + \mathbf{z}_v^t \odot \widetilde{\mathbf{h}_v^{(t)}}. \tag{6}$$

04 Gated Graph Neural Network

Node annotations: node embeddings with additional information

Propagation Model:

Node state

Node annotation

$$\boxed{\mathbf{h}_v^{(1)}} = [\boxed{\boldsymbol{x}_v^\top}, \mathbf{0}]^\top \tag{1}$$

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Propagation Model:

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$$\mathbf{z}_v^t = \sigma\left(\mathbf{W}^z \mathbf{a}_v^{(t)} + \mathbf{U}^z \mathbf{h}_v^{(t-1)}\right) \quad (3)$$

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$$\widetilde{\mathbf{h}_v^{(t)}} = \tanh\left(\mathbf{W}\mathbf{a}_v^{(t)} + \mathbf{U}\left(\mathbf{r}_v^t \odot \mathbf{h}_v^{(t-1)}\right)\right) \quad (5)$$

$$\mathbf{h}_v^{(t)} = (1 - \mathbf{z}_v^t) \odot \mathbf{h}_v^{(t-1)} + \mathbf{z}_v^t \odot \widetilde{\mathbf{h}_v^{(t)}}. \quad (6)$$

$$\mathrm{o}_\mathrm{v} = \mathrm{g}(\mathbf{h}_\mathrm{v}{}^{(\mathrm{T})}, \mathrm{x}_\mathrm{v})$$

05 Gated Graph Sequence Neural Network

What if we want to produce sequences of output values?

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GGSNN : multiple GGNNs operate in sequence to produce $\boldsymbol{o}_v^{(1)}, \ldots, \boldsymbol{o}_v^{(k)}$

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$\mathcal{F}_x^{(k)}$ Computes $\mathbf{X}^{(k+1)}$ from $\mathbf{X}^{(k)}$

$\mathcal{F}_o^{(k)}$ Computes $\mathbf{o}^{(k)}$ from $\mathbf{X}^{(k)}$

05 Gated Graph Sequence Neural Network

What if we want to produce sequences of output values?

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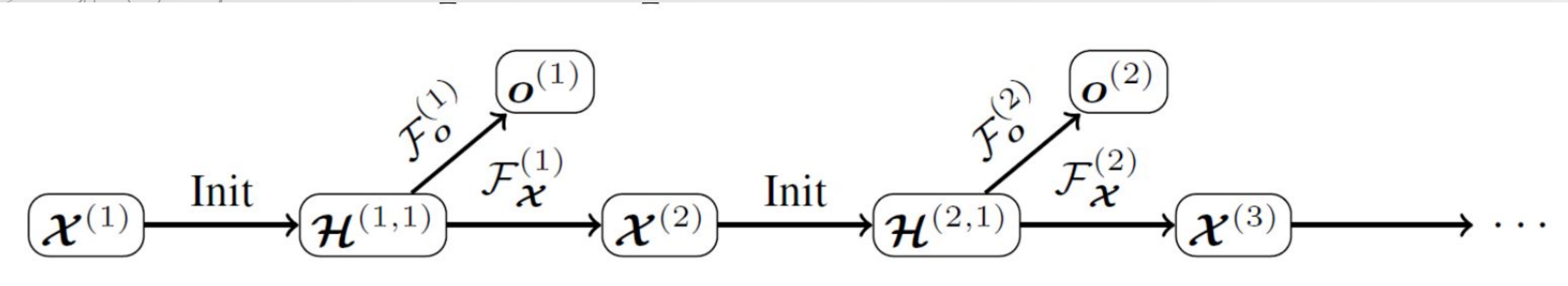
$\mathcal{F}_o^{(k)}$ Computes $\mathbf{o}^{(k)}$ from $\mathbf{X}^{(k)}$

$\mathcal{F}^{(k)}$ implements both the **transition** and **output** function!

05 Gated Graph Sequence Neural Network



$$\boldsymbol{X}^{(k)} = [\boldsymbol{x}_1^{(k)}, \dots, \boldsymbol{x}_v^{(k)}]$$

$$\boldsymbol{H}^{(k,t)} = [\boldsymbol{h}_1^{(k,t)}, \dots, \boldsymbol{h}_v^{(k,t)}]$$

k = length of the sequence

t = timesteps

06 PyG tutorial

Let's go to the Jupyter notebook….