Expressive Power of Graph Neural Networks

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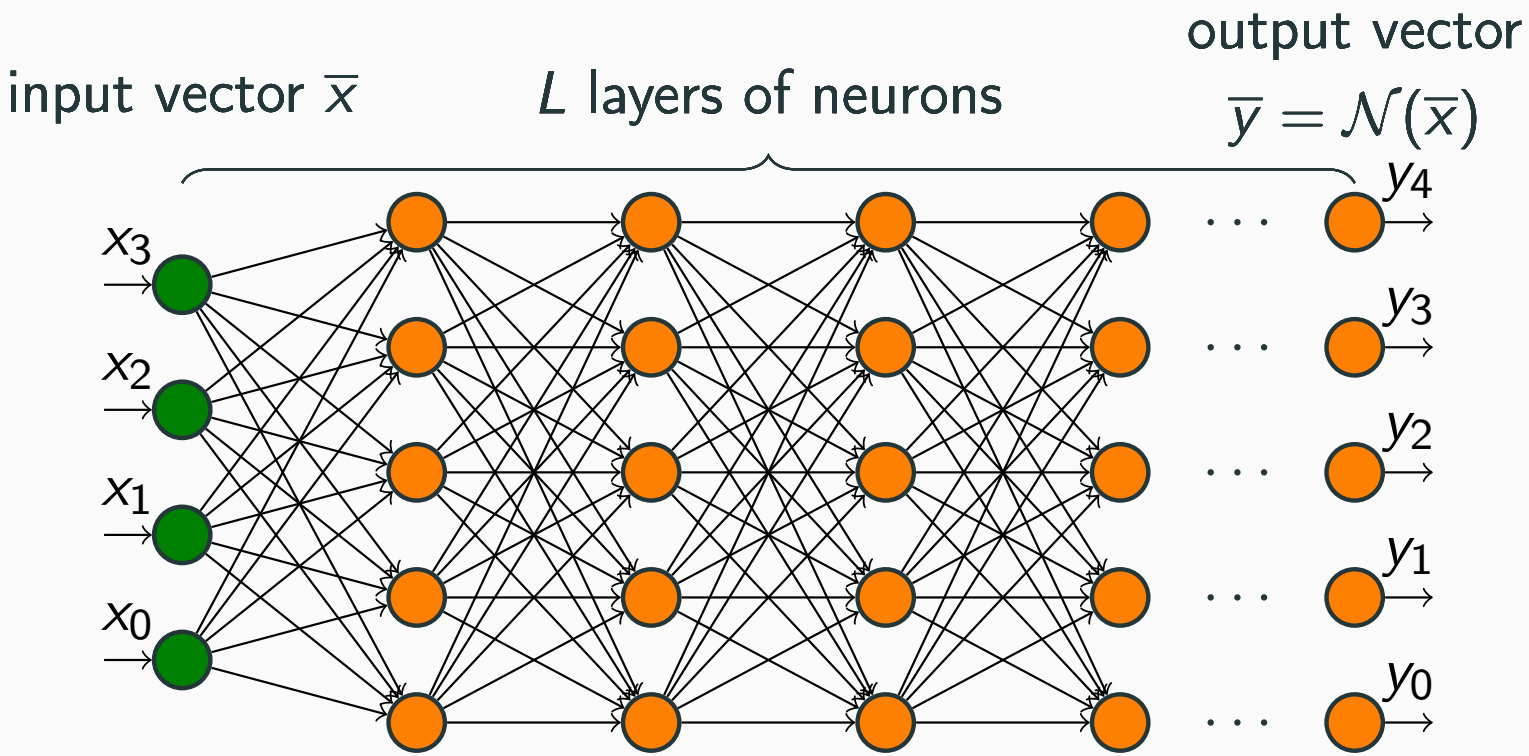
Motivation: why *graph* neural networks?

Neural Networks (NNs)



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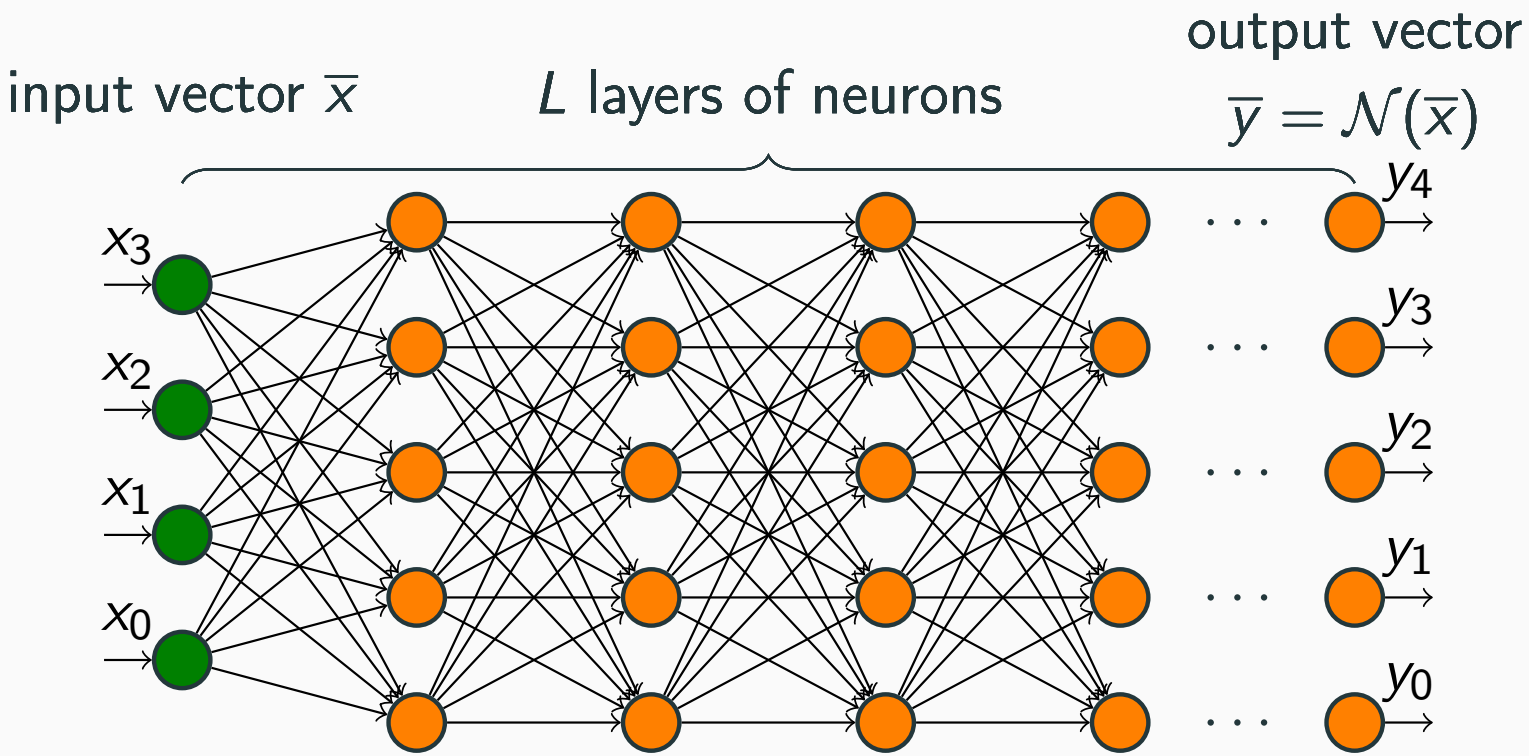

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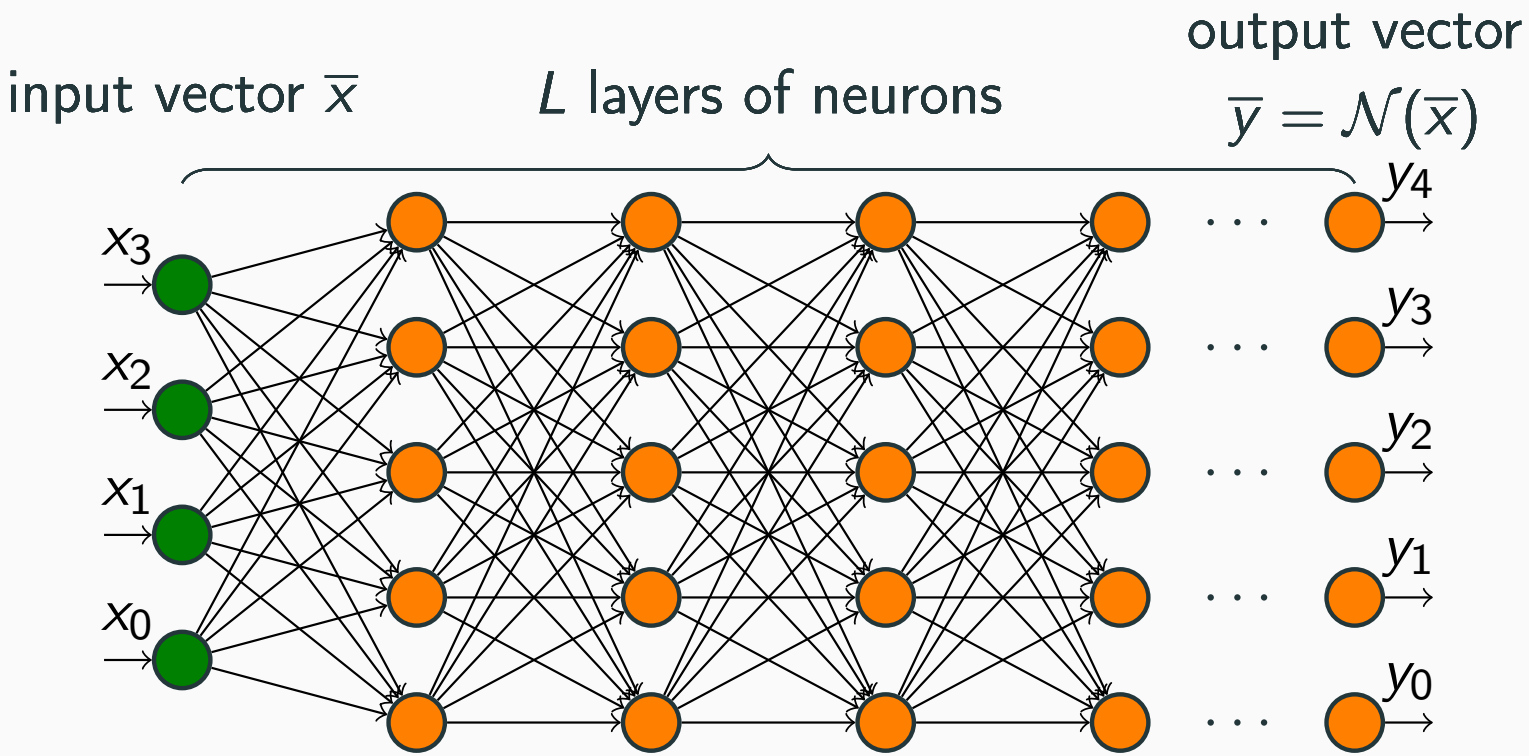

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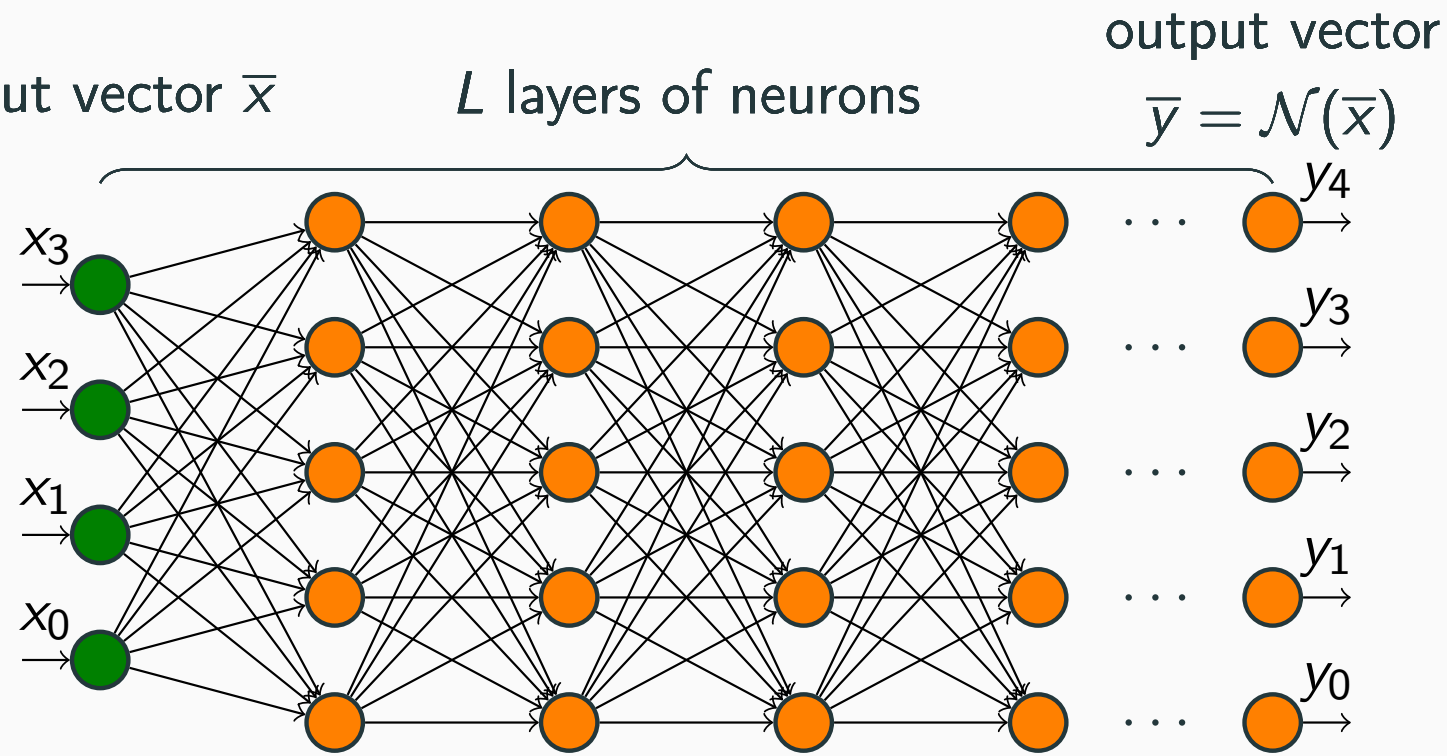

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- Goal: find the weights that "solve" your problem (classification, clustering, regression, etc.)

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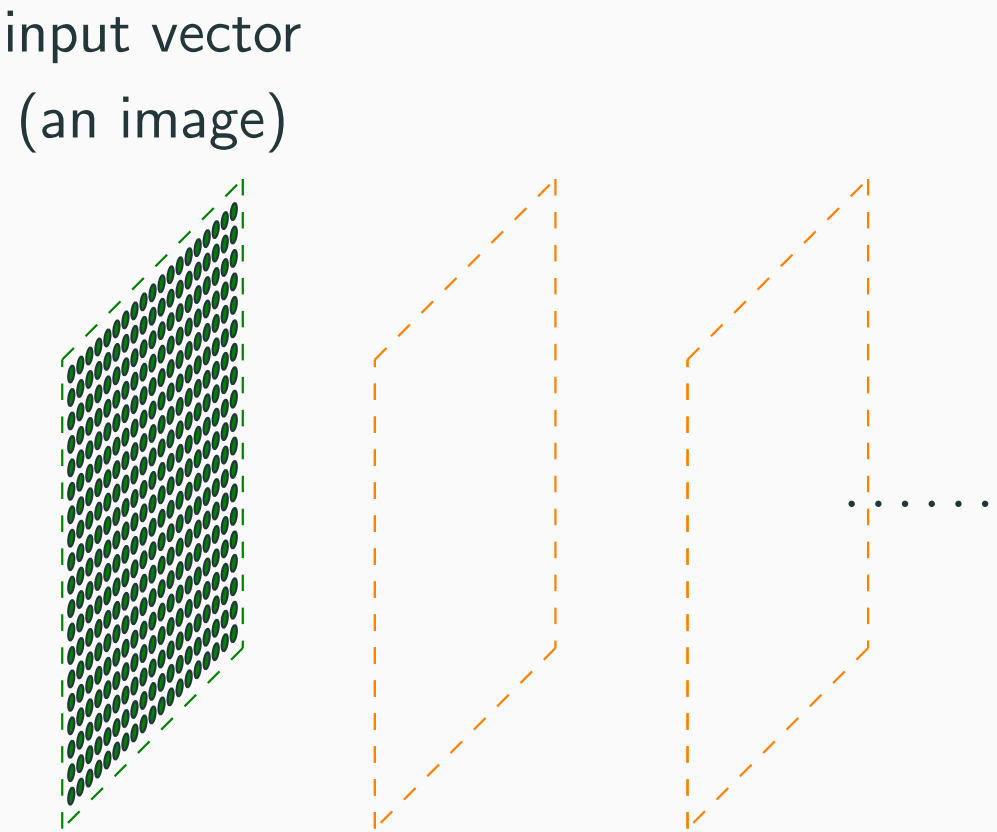
$\rightarrow$ example: input is a 250×250 pixels image, and we want to build a fully connected NN with 500 neurons per layer

$\rightarrow$ between each consecutive layers we have $250 \times 250 \times 500 = 31,250,000$ weights

Convolutional Neural Networks



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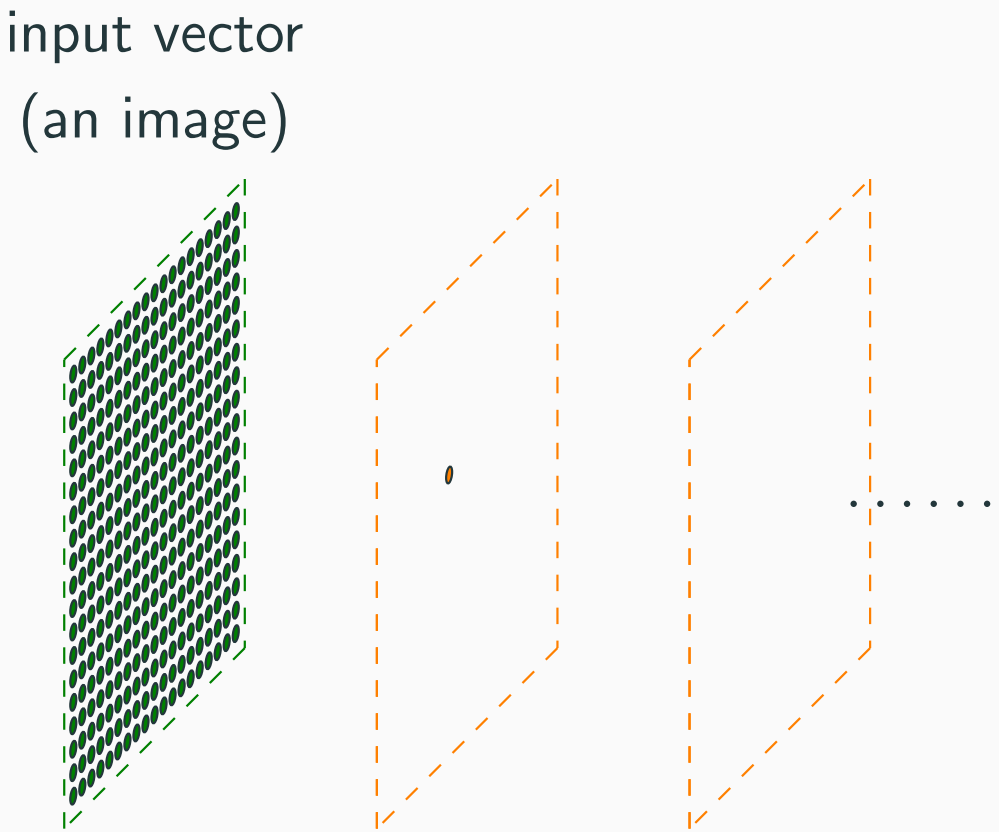

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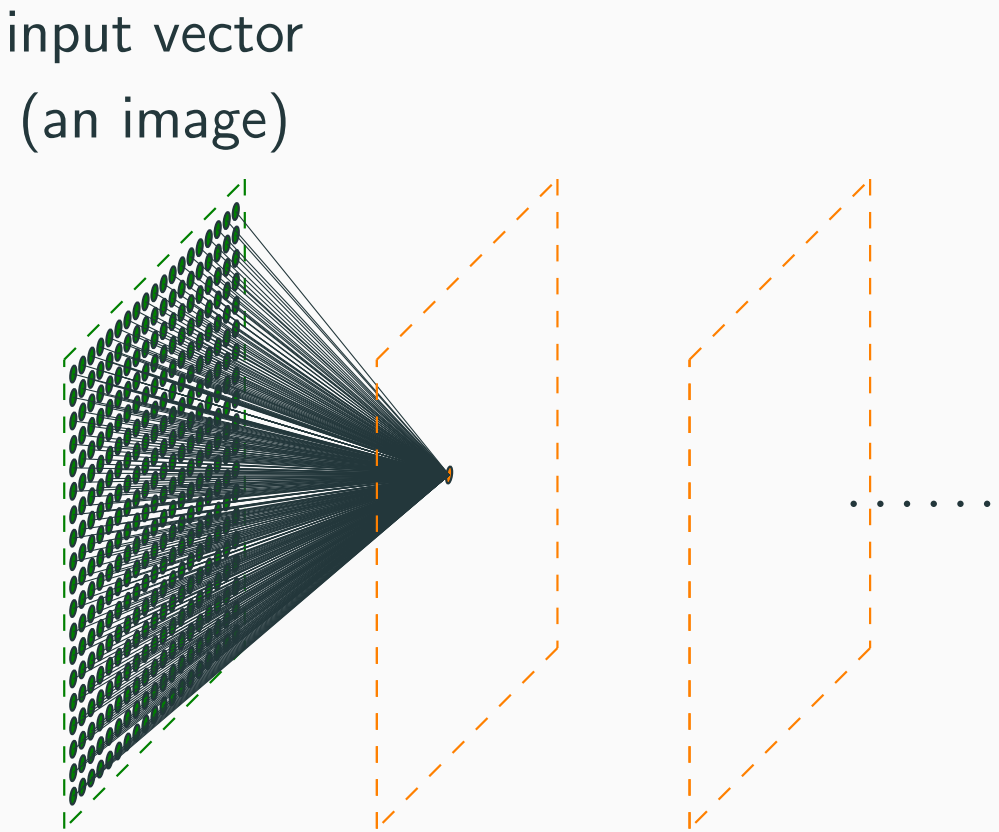

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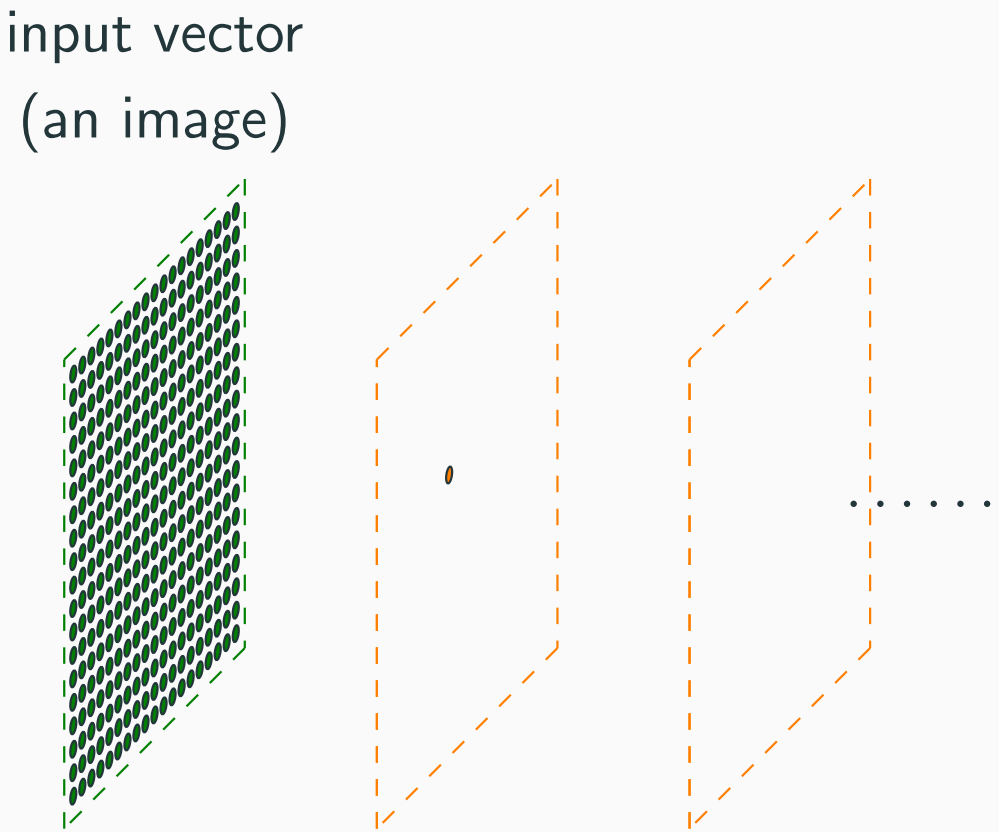

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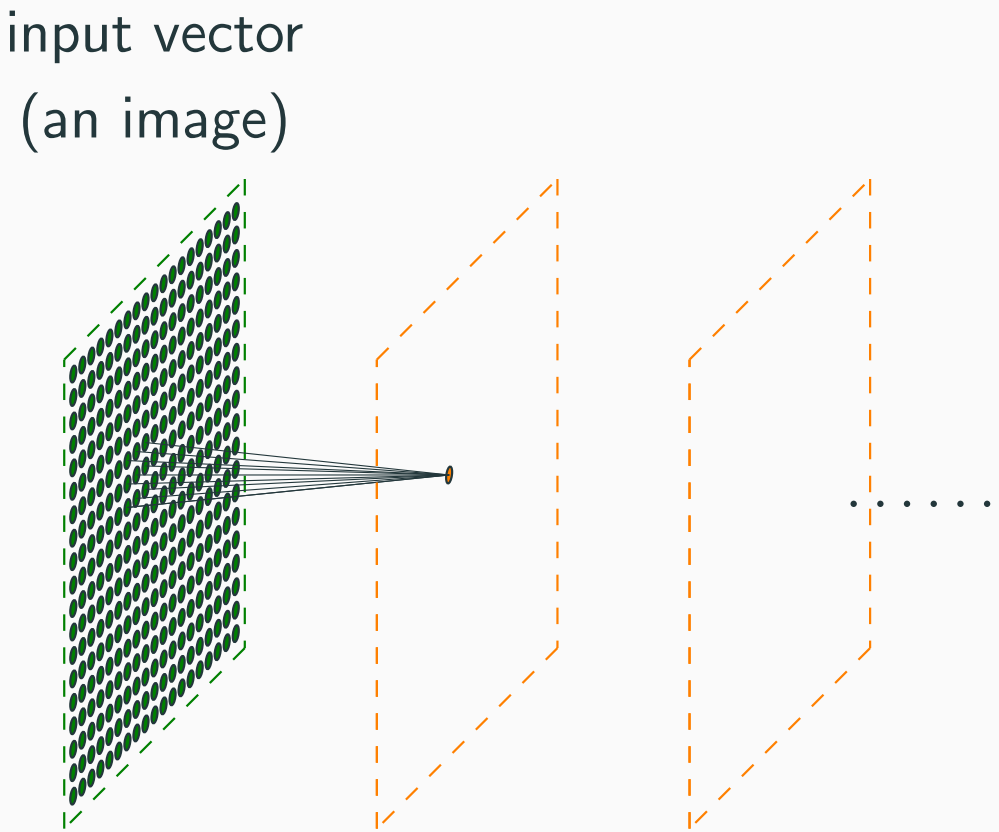

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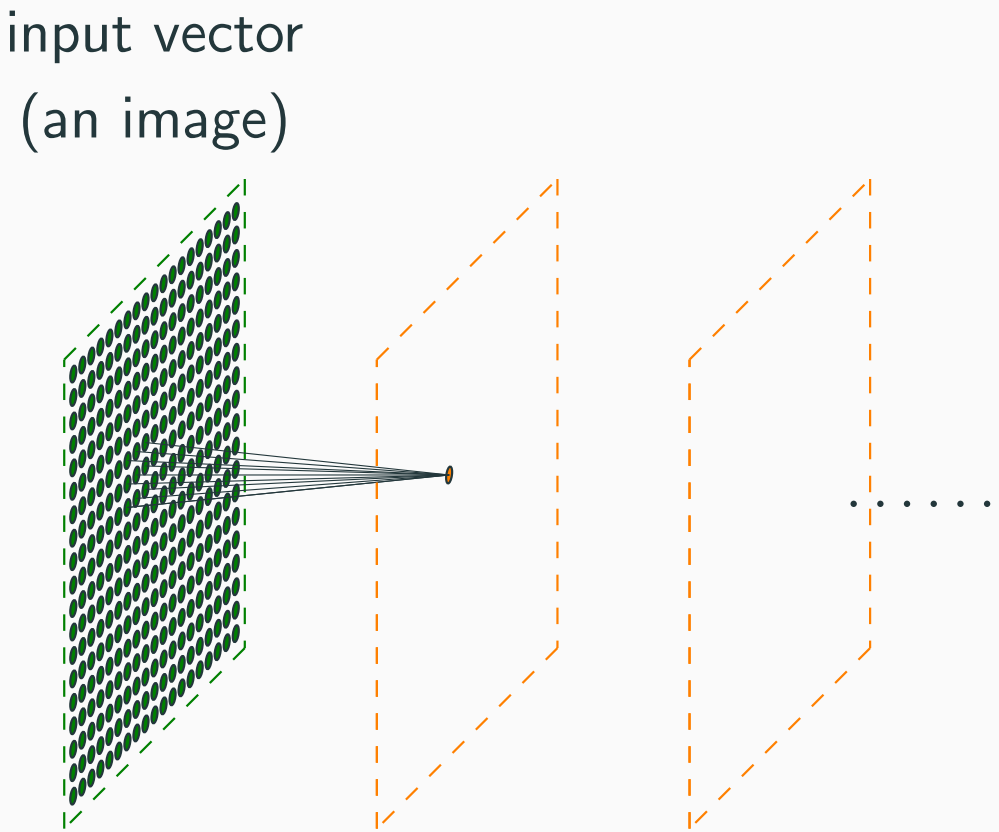

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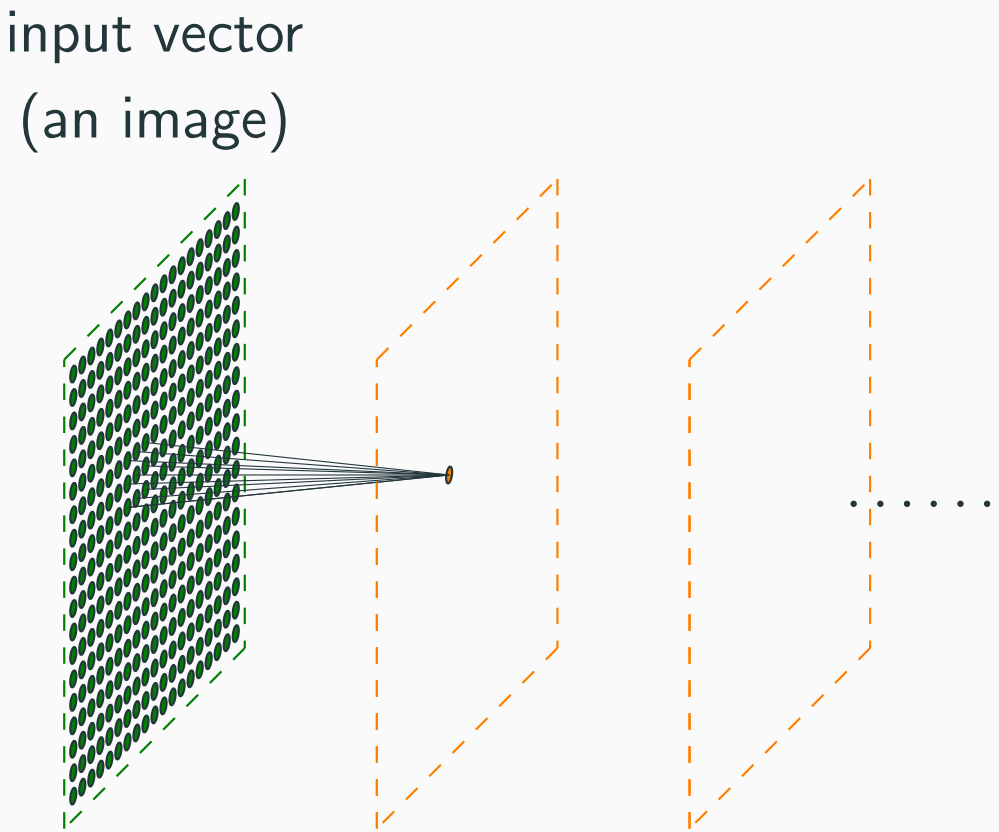

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$\rightarrow$ other advantages: recognize patterns that are local

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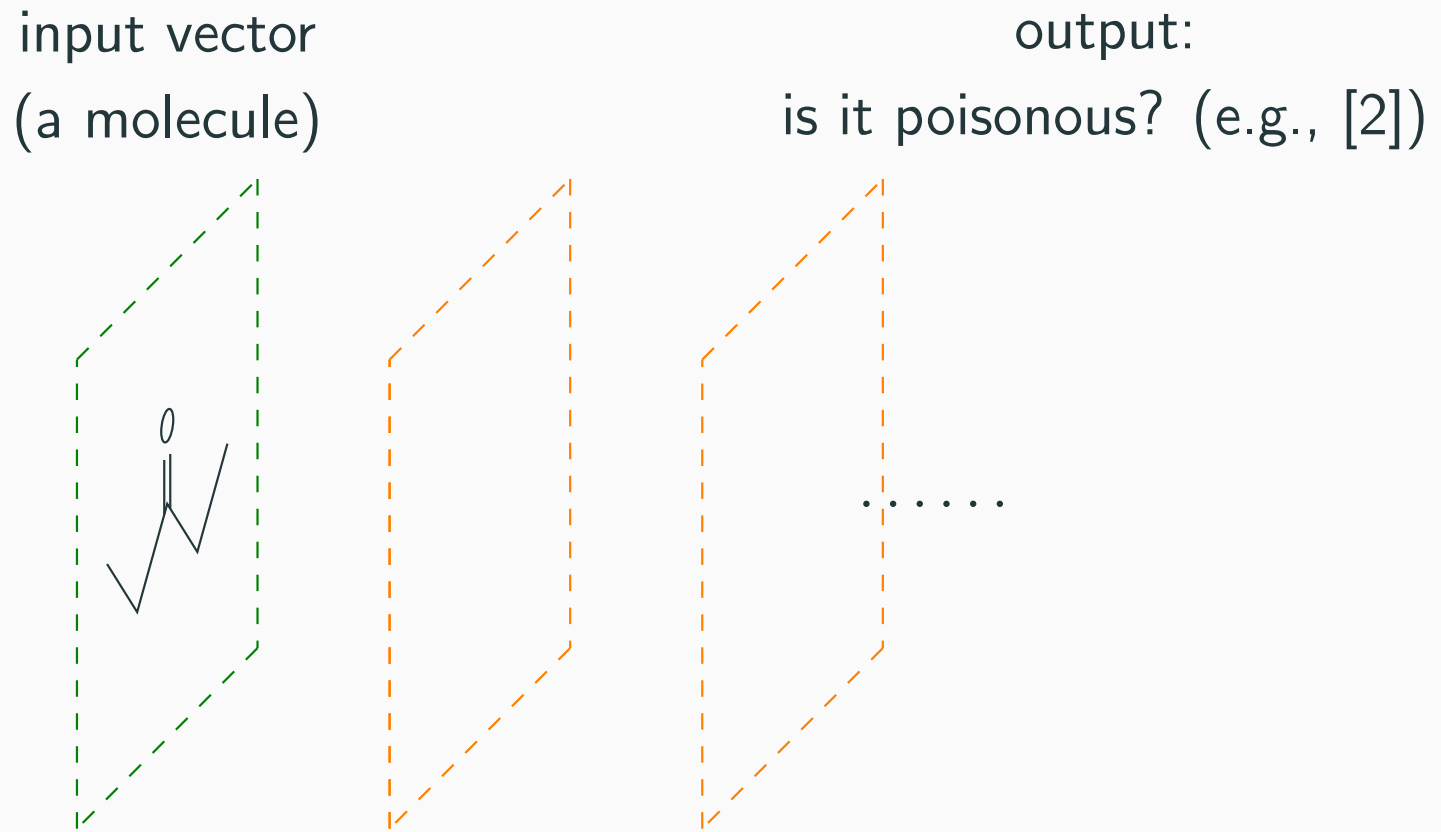

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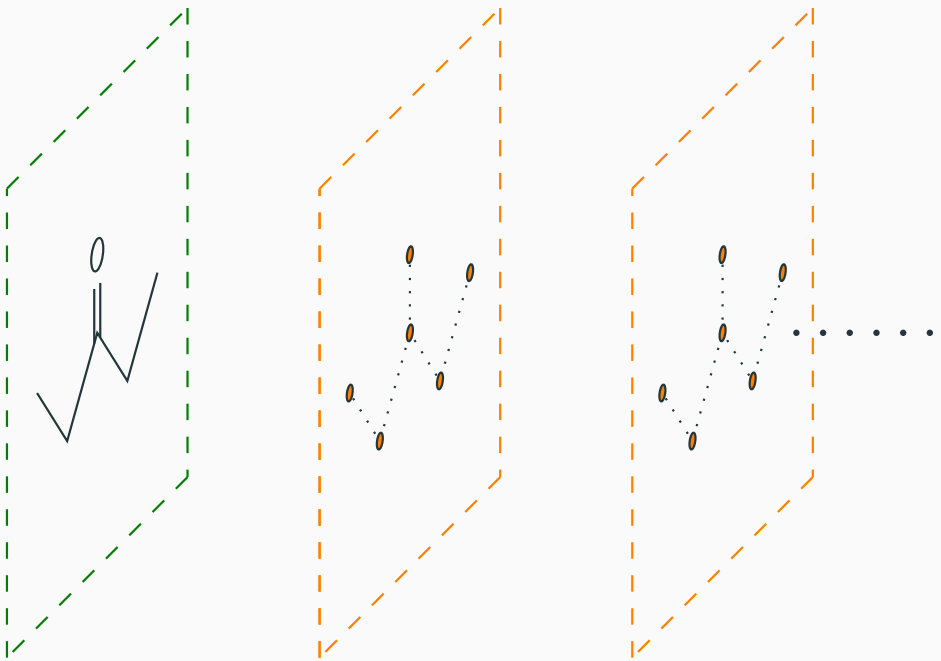

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output:
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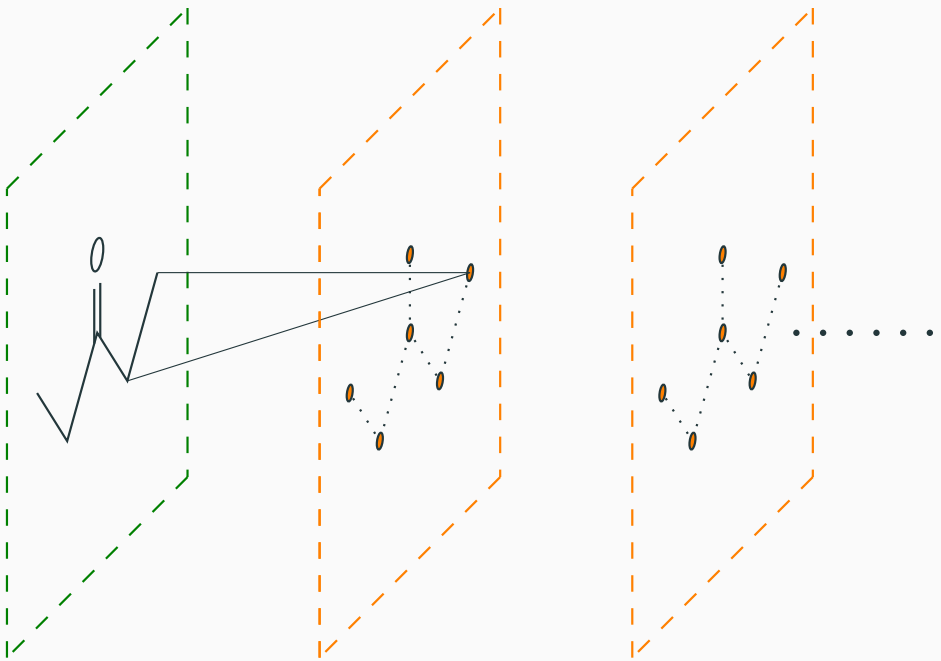

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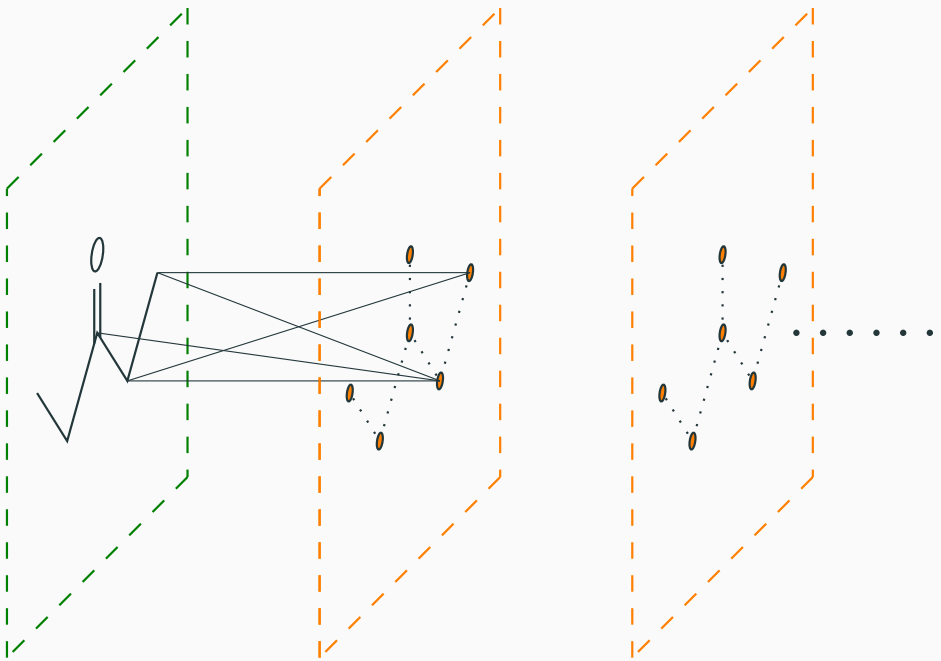

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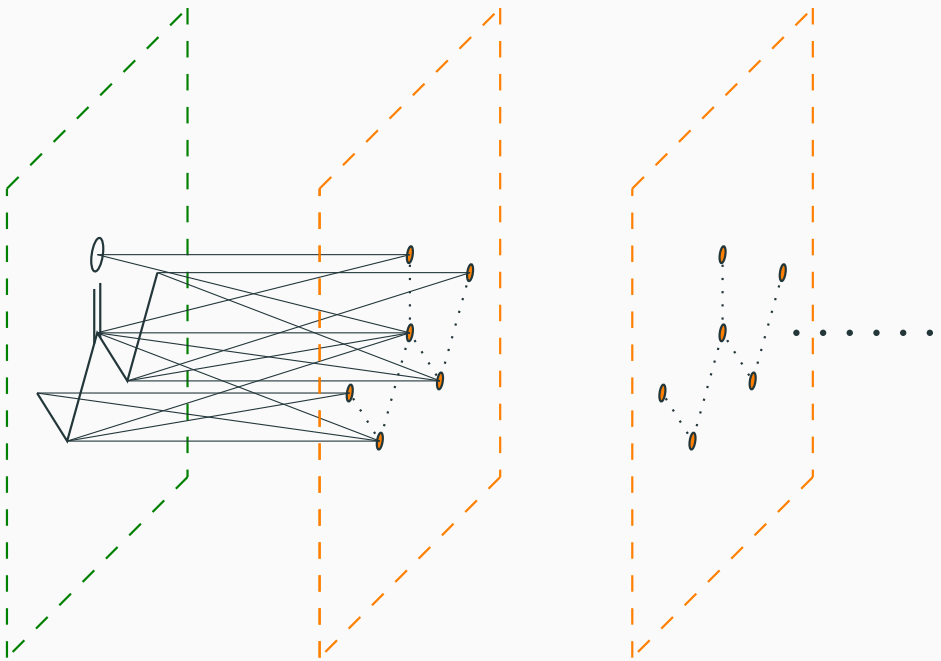

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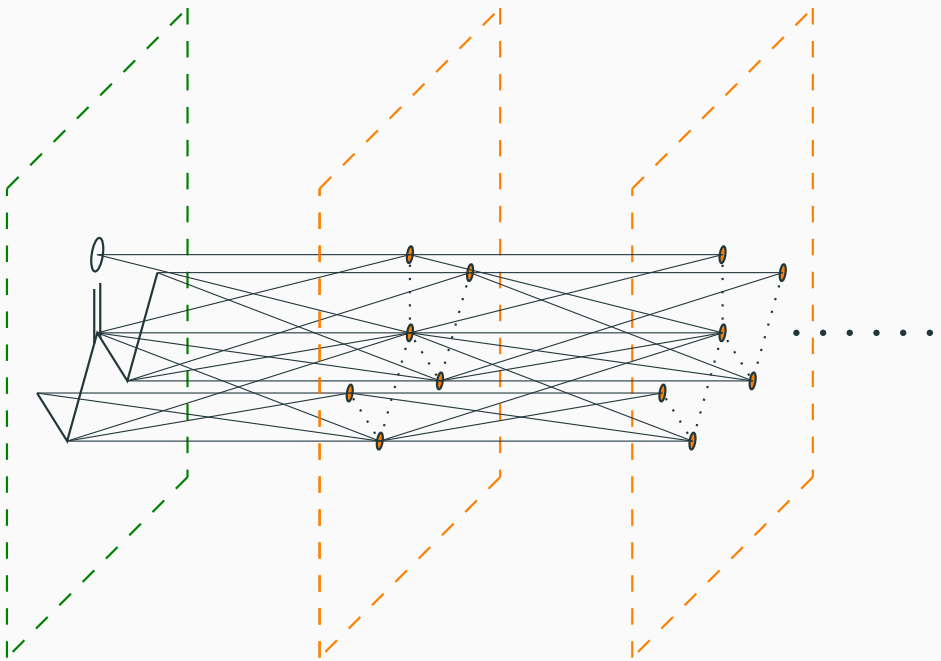

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Question: what can we do with graph neural networks? (from a *theoretical* perspective)

GNNs: formalisation

- $\mathcal{N}_G(u) \stackrel{\text{def}}{=}$ closed neighborhood of node u in **labeled** graph $G = (V, E, \lambda)$, where $\lambda : V \to \mathbb{R}^d$

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Where AGGREGATE and READOUT are what define $\mathcal{A}$

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- [3, 4]: moreover, there is a way to construct a GNN $\mathcal{A}_{\text{WL}}$ such that $\mathcal{A}$ is as discriminative as WL

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- There is a link between the WL test and FO with 2 variables and counting (FOC_2)

$\rightarrow$ example: $(\exists^{\geq 10} x).(\exists^{\geq 5} y).E(x,y) \vee (\exists^{\geq 2} x).E(y,x) \wedge C(x)$

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- [1]: we have $\mathrm{WL}^i(G_1) = \mathrm{WL}^i(G_2)$ if and only if G_1 and G_2 agree on all FOC_2 sentences of quantifier depth $\leq i$

However, we think that the links between GNNs and logics are not very well understood

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Thanks for your attention!

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