

Expressive Power of Graph Neural Networks

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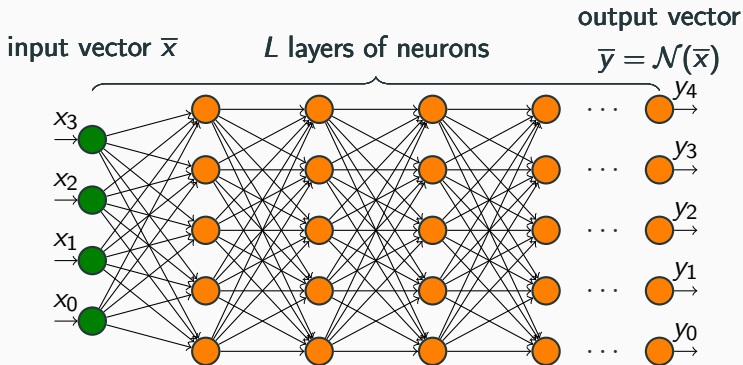
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²Oxford University, UK

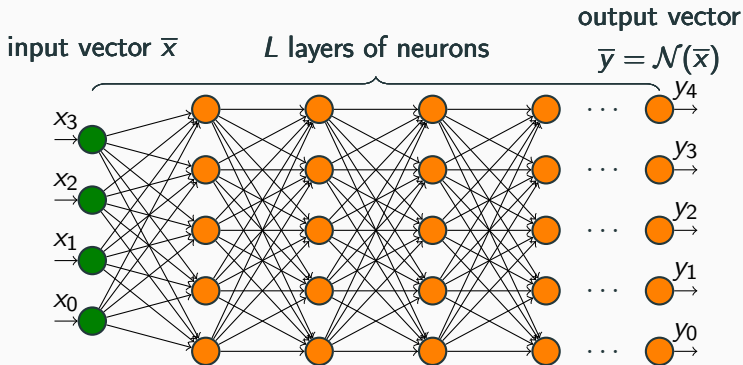
Motivation: why *graph* neural networks?

Neural Networks (NNs)



A fully connected neural network \mathcal{N} .

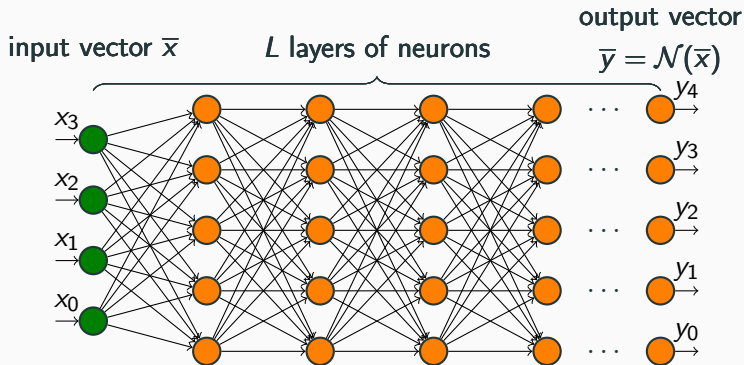
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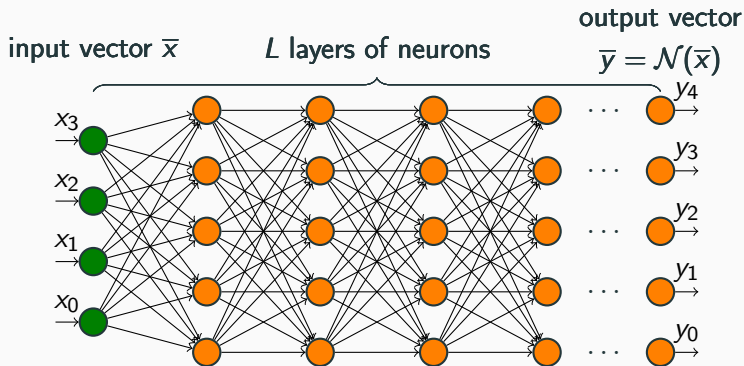
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- **Goal:** find the weights that “solve” your problem (classification, clustering, regression, etc.)

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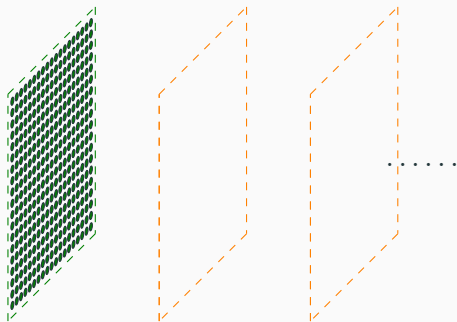
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 - example: input is a 250×250 pixels image, and we want to build a fully connected NN with 500 neurons per layer
 - between each consecutive layers we have $250 \times 250 \times 500 = 31,250,000$ weights

Convolutional Neural Networks

input vector
(an image)

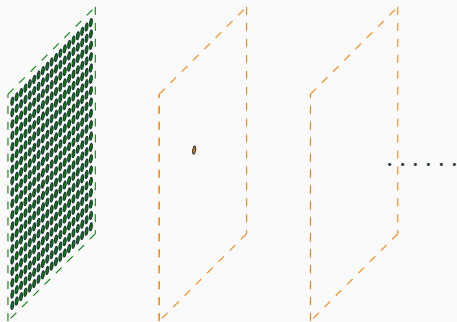


A convolutional neural network.

- Idea: use the **structure** of the data (here, a grid)

Convolutional Neural Networks

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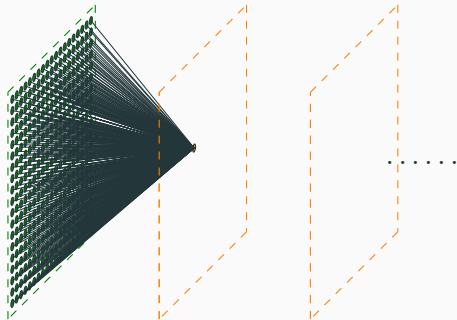


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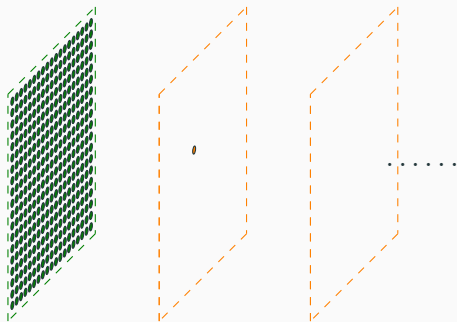


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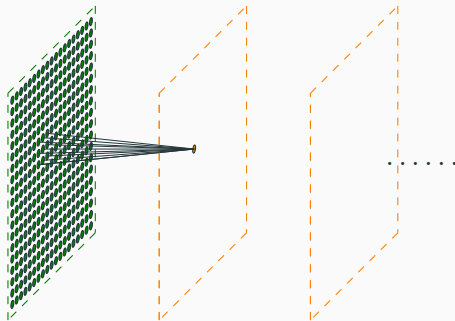


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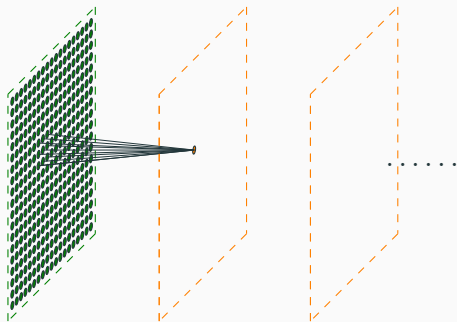


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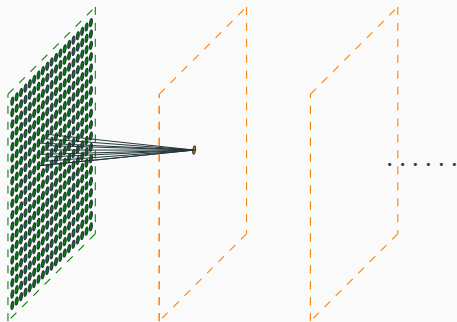


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→ fewer weights to learn (e.g, $500 * 9 = 4,500$ for the first layer)

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 - fewer weights to learn (e.g, $500 * 9 = 4,500$ for the first layer)
 - other advantage: recognize patterns that are **local**

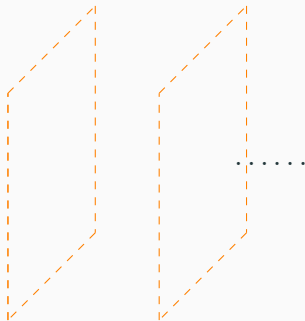
Graph Neural Networks (GNNs)

input vector
(a molecule)



output:

is it poisonous? (e.g., [1])



A graph neural network.

- **Idea:** use the **structure** of the data (here, a grid)
- GNNs generalize this idea to allow *any* graph as input (in particular, not constrained with fixed-size inputs anymore)

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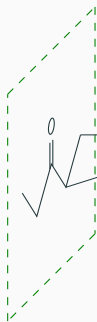


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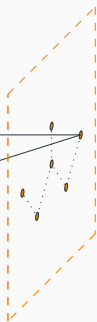
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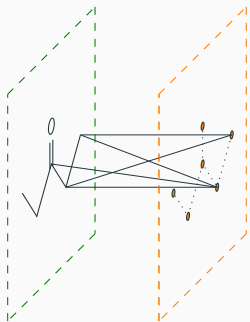


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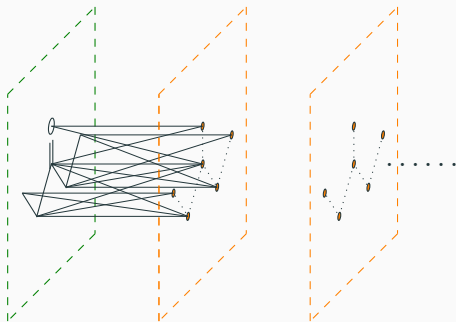
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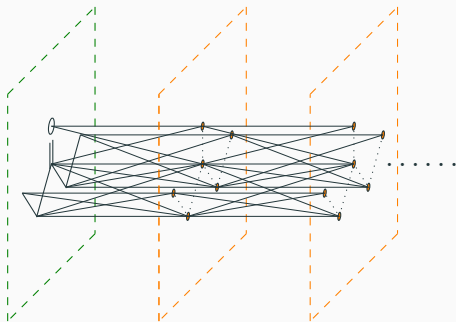
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Goal of the project: what can we do with graph neural networks?
(from a *theoretical* perspective)

Thanks for your attention!



David K Duvenaud, Dougal Maclaurin, Jorge Iparraguirre, Rafael Bombarell, Timothy Hirzel, Alán Aspuru-Guzik, and Ryan P Adams.

Convolutional networks on graphs for learning molecular fingerprints.

In *Advances in neural information processing systems*, pages 2224–2232, 2015.