Graph Neural Networks for Data Management

IN3020/4020 Database Systems

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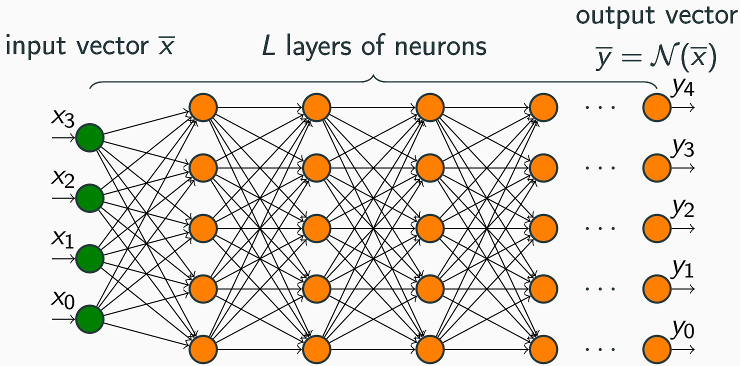
Fully Connected Feed-Forward Neural Networks (NNs)



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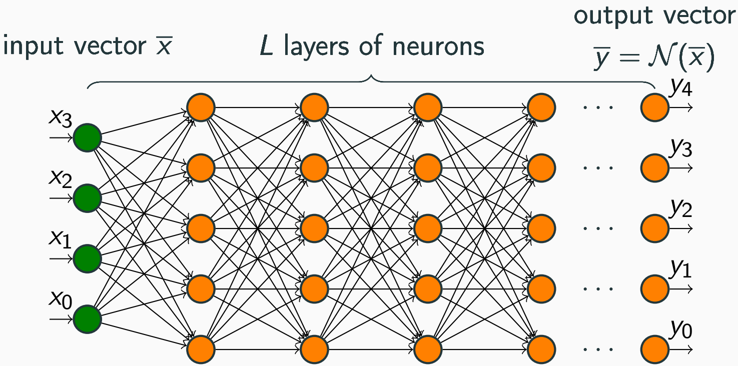

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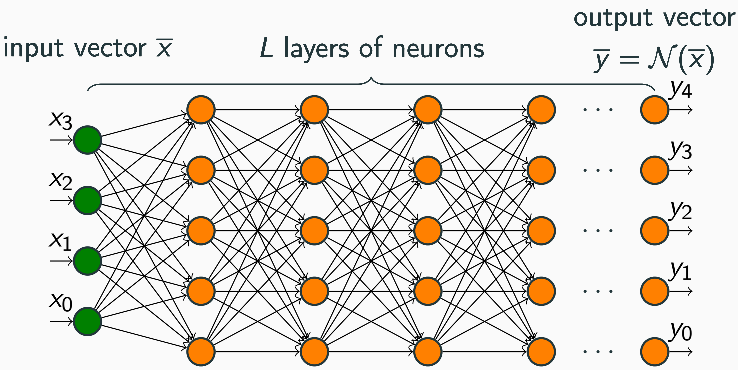

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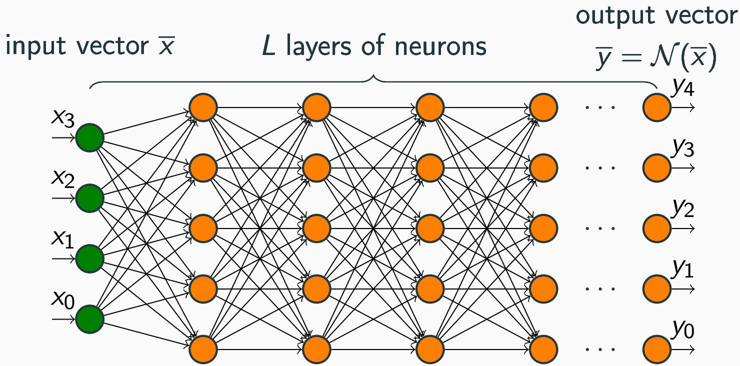

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- Goal: find the weights that "solve" your problem (classification, clustering, regression, etc.)

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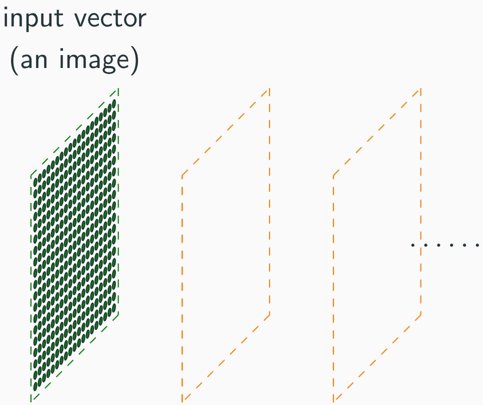
$\rightarrow$ example: input is a 250×250 pixels image, and we want to build a fully connected NN with 500 neurons per layer

$\rightarrow$ between the first two layers we have $250 \times 250 \times 500 = 31,250,000$ weights

Convolutional Neural Networks



A convolutional neural network

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

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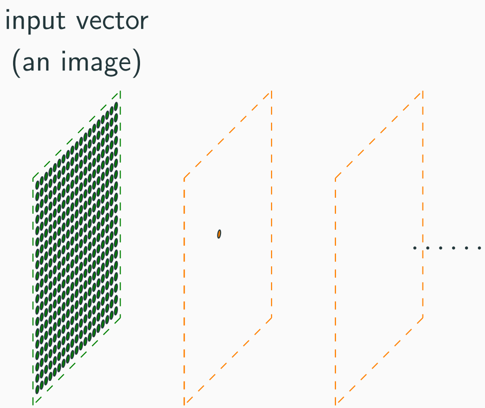

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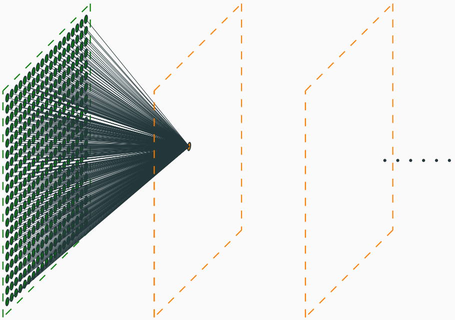
Convolutional Neural Networks

input vector
(an image)



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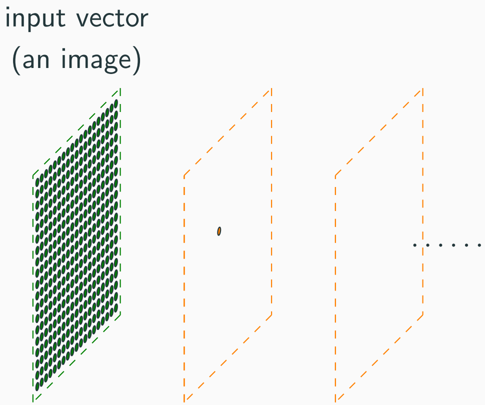

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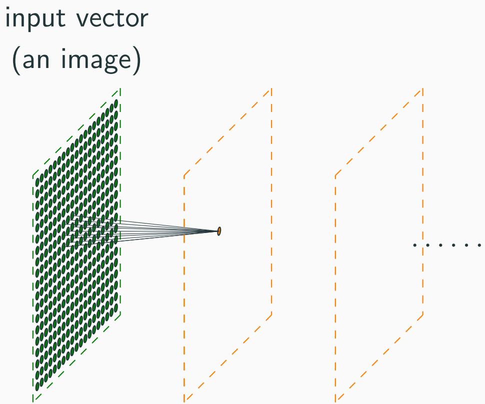

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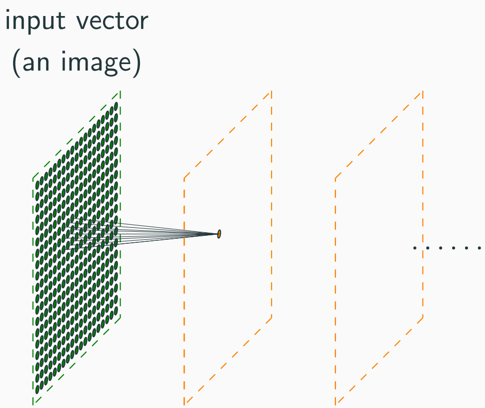

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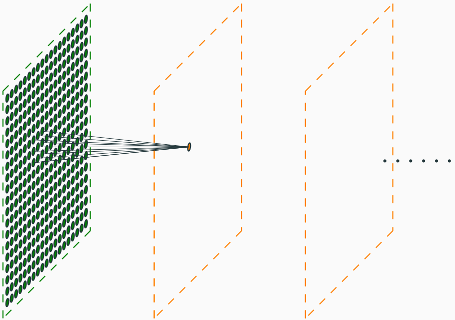

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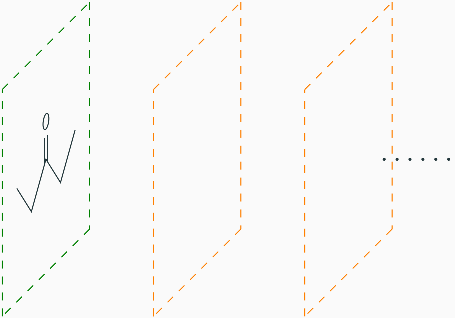
$\rightarrow$ fewer weights to learn (e.g, $500 * 9 = 4,500$ for the first layer)

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

Graph Neural Networks (GNNs)

input vector
(a molecule)

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



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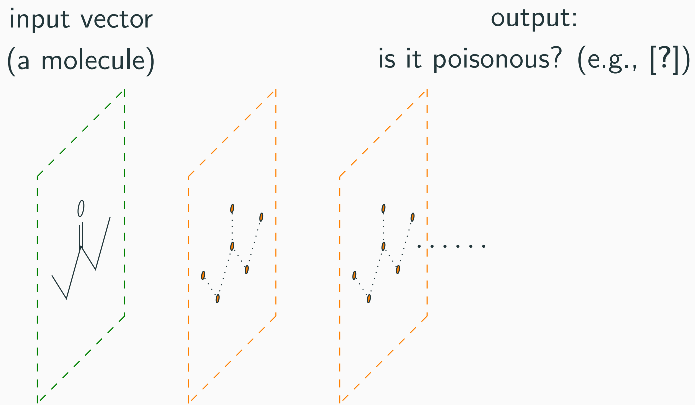

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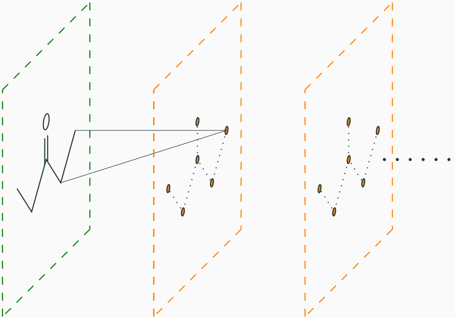

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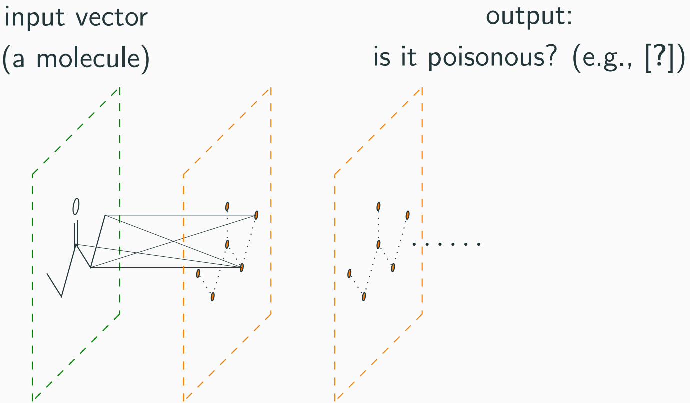

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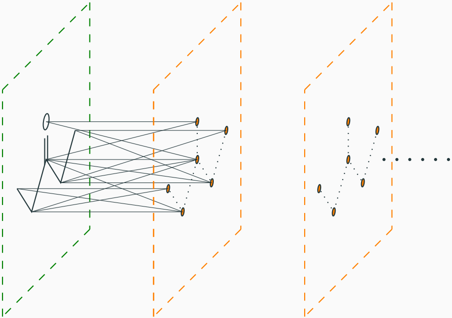

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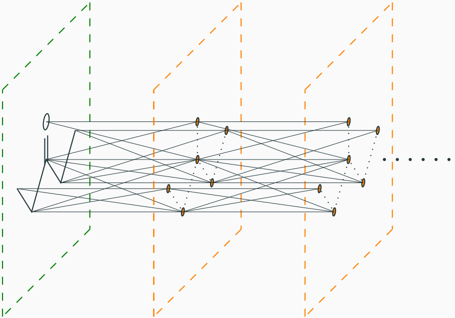

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- where $\mathbf{A}_i$ and $\mathbf{B}_i$ are trainable matrices and $\mathbf{c}_i$ are such vectors
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- Generalisation to ordered graphs with different types of edges is straightforward
- Knowledge graphs (RDF, Neo4j)?

Question:
Can we make use of GNNs in data management?

One problem: Supervised learning queries from examples

- Input:
  - set of positive examples (G, v) (graph-node pairs)
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- Question:
  - give me a simple query (SPARQL, Cypher) that mostly give these answers

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- Question:
  - give me a simple query (SPARQL, Cypher) that mostly give these answers
- Mostly, because input may be noisy
- Query (not a NN or other algorithm), because we want efficient evaluation on big graphs
- Simple, because we need something understandable (explainable!)

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- GNNs have potential to overcome these problems:
  - can process inputs of various size
  - work directly on graph structures
  - noise-tolerant
- Question: How to translate a (trained) GNN to a (SPARQL) query?
  - much less hopeless than for usual NNs
  - GNNs "keep" a lot of structure
  - some GNN architectures may be easier to translate than others

GNNs for data and knowledge management

- There are two paradigms for data and knowledge management
  - Symbolic (logic-based) methods (SQL, SPARQL, OWL)
  - Syb-Symbolic (statistic-based) methods (NNs)
- Both have strengths and weaknesses
- A major challenge is to deeply integrate these paradigms

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- I believe that GNNs can be a bridge between these paradigms
  - work on structured data of varying size
  - have a neural capabilities
- Can be potentially used to solve many problems as above:
  - incorporating logical knowledge into network-based models
  - knowledge graph completion
  - query answering over incomplete knowledge graphs
  - ontology learning
  - etc.