Deep learning theory and application for astrophysics

From machine learning basics to deep learning

Hypotheses and models

Objective

Build a smart thermostat that regulates heating/cooling, predicting what the temperature will be on a given day.

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Build a smart thermostat that regulates heating/cooling, predicting what the temperature will be on a given day.

Challenge

Predicting the temperature is complex:

- Physical laws
- Influencing variables (e.g., external temperature)

Alternative approach

- Historical temperature measurements
- Formulation of a **hypothesis**
- Estimate a mathematical function

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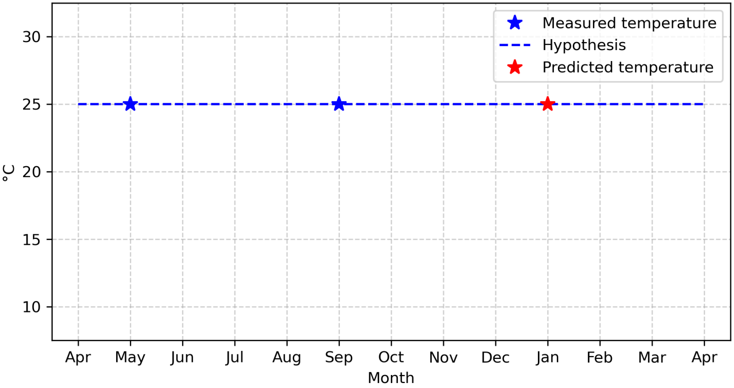
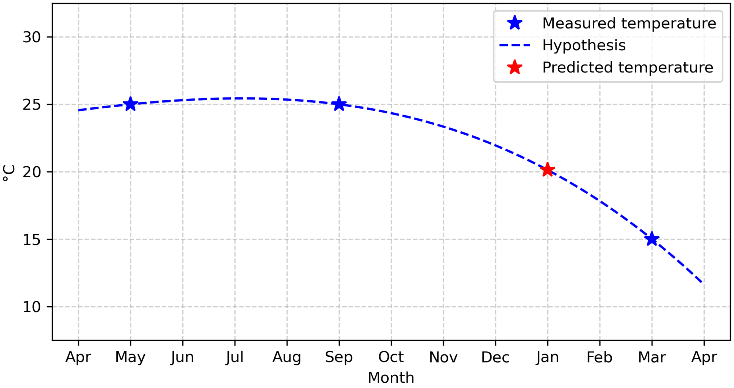
Machine Learning

Science that recognizes **patterns** from limited examples.

Importance of examples



Importance of examples



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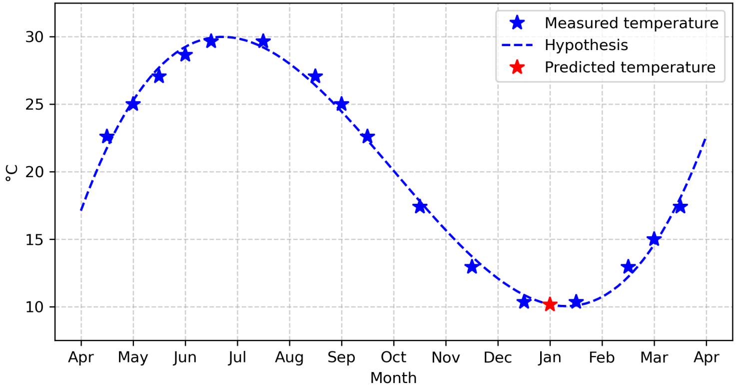

Supervised machine learning

- **Dataset** $\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$
- **Feature** x_i: data for prediction
- **Target** y_i: what we want to predict

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Objective

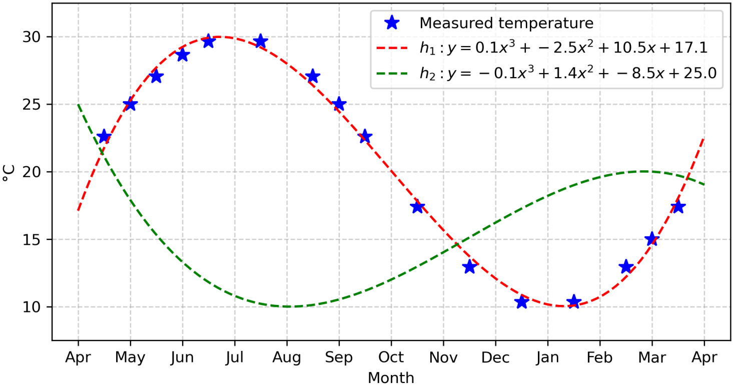
Find the hypothesis h:

$$h(x) \approx f(x), \forall x$$

Models and hypotheses

- Subset of hypotheses: **model**
- Family of hypotheses varies with **parameters**

Models and hypotheses



Model training

Model training

Loss function

Measures the error of the model

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Measures the error of the model

- **Training objective**:
  - Find parameters $\boldsymbol{\theta}^*$ that minimize the loss function $\mathcal{L}$
- Formally:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \mathcal{L}\left(\mathcal{D}, \boldsymbol{\theta}\right)$$

Solving a machine learning problem

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1. **Model selection**
    - Suitable model for the problem
    - Risks of incorrect choice

Solving a machine learning problem

1. **Model selection**
   - Suitable model for the problem
   - Risks of incorrect choice
2. **Parameter optimization**
   - Find parameters for the best hypothesis
   - Exploration of the parameter space $\mathbb{R}^d$

Generalization

Loss optimization

- It is not enough for the model to perform well on training data
- We want it to perform well on data **never seen** during training

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Generalization capability

Correct predictions on **test** data

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Generalization capability

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Dataset split

- **Training set** $\mathcal{D}_{\text{train}}$: training and optimization
- **Test set** $\mathcal{D}_{\text{test}}$: performance evaluation

Training and test loss

- **Training loss** $\mathcal{L}(\mathcal{D}_{\text{train}}, \boldsymbol{\theta})$
- **Test loss** $\mathcal{L}(\mathcal{D}_{\text{test}}, \boldsymbol{\theta})$

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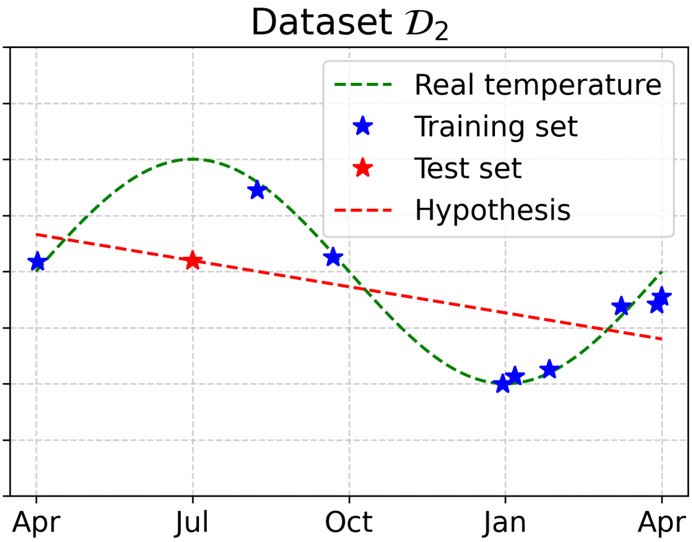
Discrepancy

A model that performs well in training does not necessarily perform well in testing

Underfitting



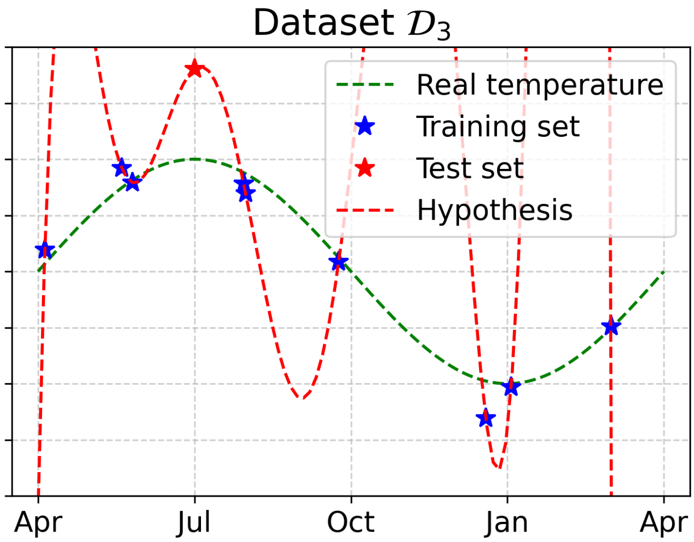
Underfitting

Definition

Inability to approximate the training data

- High errors on both training and test sets
- Limitation due to the simplicity of the model

Overfitting



Overfitting

Definition

The model learns the training data too well

- $\mathcal{L}(\mathcal{D}_{\text{train}}, \boldsymbol{\theta}) \approx 0$
- $\mathcal{L}(\mathcal{D}_{\text{test}}, \boldsymbol{\theta}) \gg 0$

Model choice

Possible approach

- Train different models on $\mathcal{D}_{\text{train}}$
- Evaluate performance on $\mathcal{D}_{\text{test}}$
- Choose the model with the best performance on $\mathcal{D}_{\text{test}}$

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Problem

- Test set used for model selection
- "Contaminated" its role in generalization

Validation set

Validation set

Estimate of generalization performance during training, without using the test set

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New division of the dataset

- **Training set**: training the parameters
- **Validation set**: model selection
- **Test set**: final evaluation

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Correct approach

- Divide $\mathcal{D}$ into $\mathcal{D}_{\text{train}}$, $\mathcal{D}_{\text{val}}$, $\mathcal{D}_{\text{test}}$
- Train models on $\mathcal{D}_{\text{train}}$
- Evaluate on $\mathcal{D}_{\text{val}}$
- Select the model with the best performance on $\mathcal{D}_{\text{val}}$
- Evaluate the chosen model on $\mathcal{D}_{\text{test}}$

Introduction to artificial neural networks

History

- Peaks of popularity: 1950s-60s and 80s
- Decline: design and training complexity
- Revival: 2000s thanks to technological and algorithmic advances

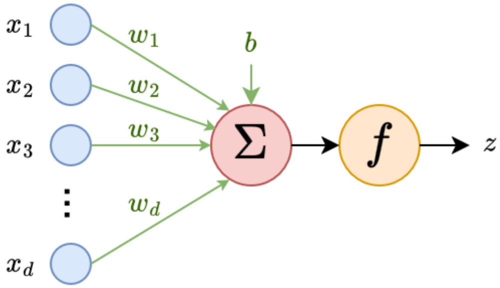
Artificial neuron

Definition

- Observation: $\mathbf{x} = [x_1, \ldots, x_d]^\intercal$
- Parameters:
  - **weights** $\mathbf{w} = [w_1, \ldots, w_d]^\intercal \in \mathbb{R}^d$
  - **bias** $b \in \mathbb{R}$
- f: **activation function**

Neuron output

$$z = f\left(\mathbf{x}^\intercal \mathbf{w} + b\right)$$



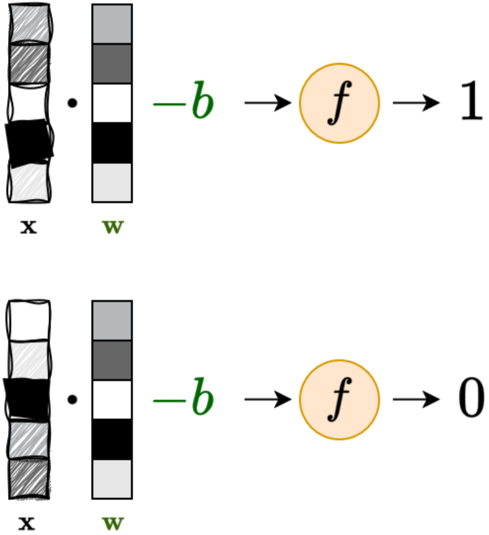
Interpretations of the artificial neuron

Neuron output

$$z = f\left(\mathbf{x}^\intercal \mathbf{w} + b\right)$$

Prototypical interpretation

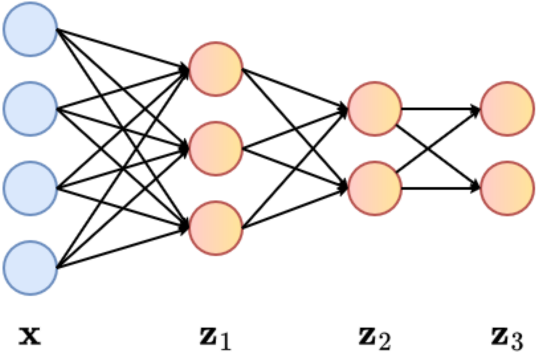
- $\mathbf{w}$: feature prototype
- $\mathbf{x}^\intercal \mathbf{w}$: measure of similarity
- Similarity threshold: $-b$



Multi-layer perceptron (MLP)

- Model equipped with **multiple layers** to approximate non-linear functions
- **Concatenation of layers**: output of one layer becomes input to the next

(Example)



Training a neural network

Objective

Minimize loss function $\mathcal{L}$

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Gradient descent

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}$$

- $\boldsymbol{\theta}$: vector of network parameters
- $\nabla_{\boldsymbol{\theta}} \mathcal{L} = \left[\frac{\partial \mathcal{L}}{\partial \theta_1}, \frac{\partial \mathcal{L}}{\partial \theta_2}, \ldots, \frac{\partial \mathcal{L}}{\partial \theta_p} \right]^\mathsf{T}$: gradient of the loss with respect to the parameters

Backpropagation

Definition

- Algorithm for computing gradients of a neural network
- Efficient and suitable for computer implementation
- Requires that layers are **differentiable**

Role of the learning rate

- Key hyperparameter in the gradient descent algorithm
- Determines the size of update steps

Choosing the learning rate η

- η too small: slow progress, difficulty escaping local minima
- η too large: risk of oscillations or divergence

Deep neural networks

Complex data

- Hierarchical and compositional nature
  - Images: pixels $\rightarrow$ edges $\rightarrow$ shapes $\rightarrow$ objects $\rightarrow$ scenes
  - Text: letters $\rightarrow$ words $\rightarrow$ sentences $\rightarrow$ complex meaning

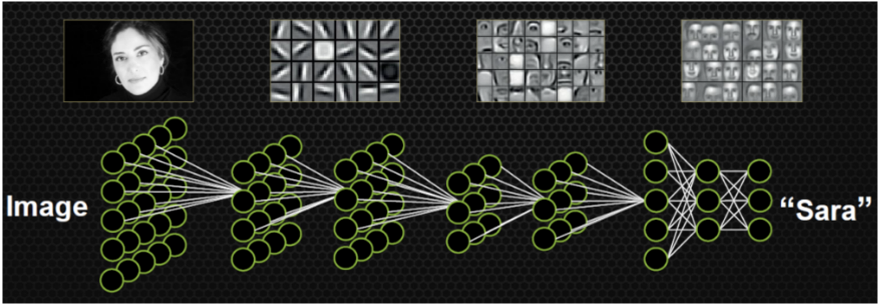
Deep neural networks

- Hierarchical representations
- Initial layers: low-level patterns
- Final layers: abstract and complex representations

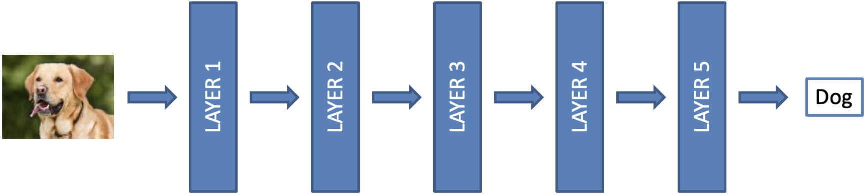
Convolutional neural networks

Suitable for 2D/3D data analysis

Network layers apply image processing filtering **convolutions**)



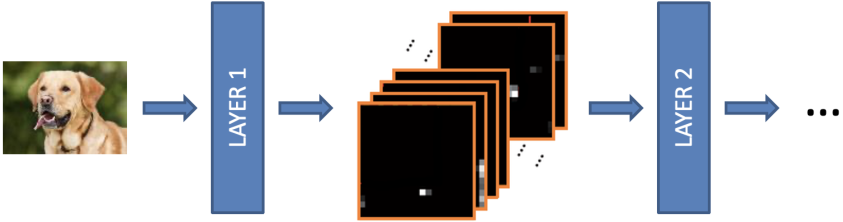
Convolutional neural networks



Convolutional neural networks

Representation

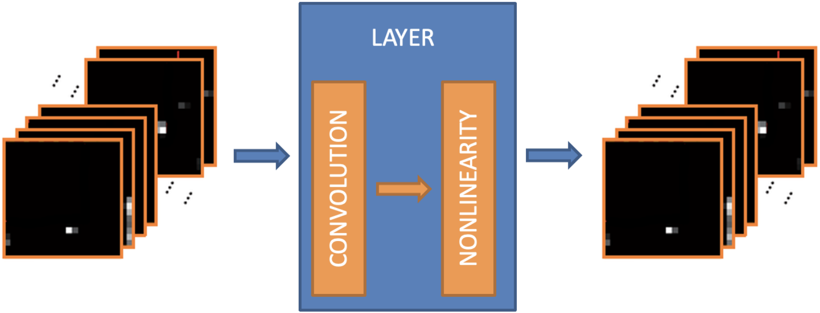
Each layer extracts a set of **feature maps**



Convolutional neural networks

Minimal layer configuration

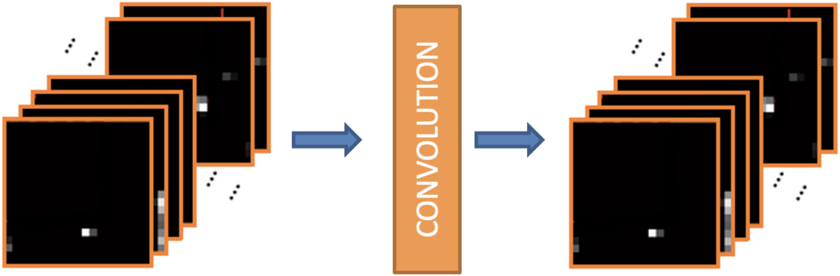
- Convolution operator
- Nonlinear activation



Convolutional neural networks

Convolution

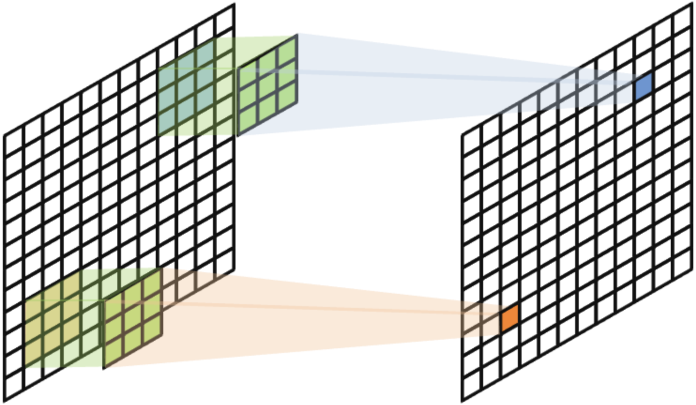
- Each feature map emphasizes specific visual characteristics
- Computed by aggregating information from previous layers



Convolutional neural networks

Convolution

- Each "neuron" is computed by filtering a window from the previous feature maps using a **kernel** matrix



Convolutional neural networks

Main parameters

- **Kernel size**
  - Larger size $\rightarrow$ more context, but more parameters
  - Must be tuned to input data
- **Stride**
  - Stride 1: process every pixel
  - Stride N: process one pixel every N
  - Suitable at high resolution

Convolutional neural networks

Feature map resolution

- Deep layers encode more and more aggregate information
- No need to keep original resolution

Convolutional neural networks

Feature map resolution

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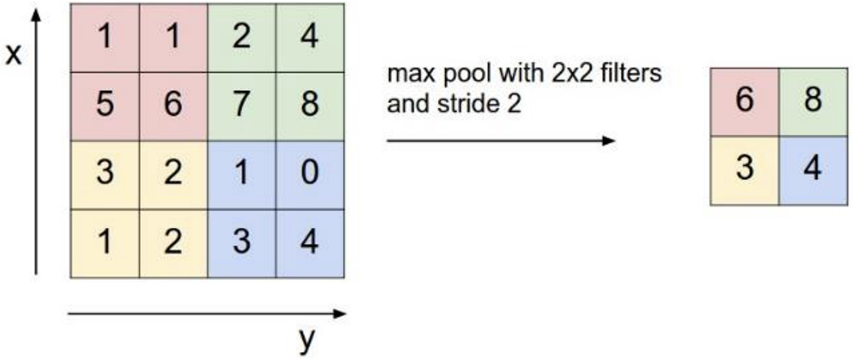
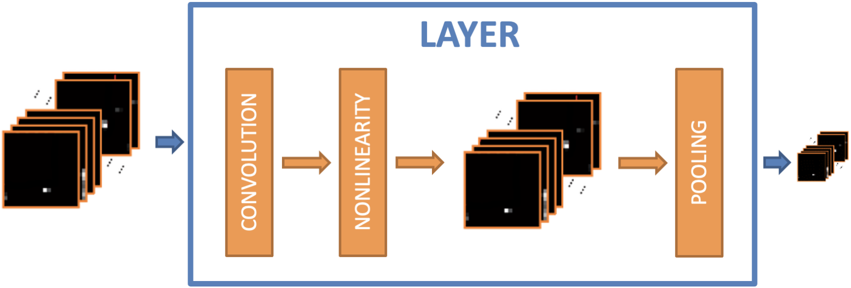
- **Max pooling**



Convolutional neural networks

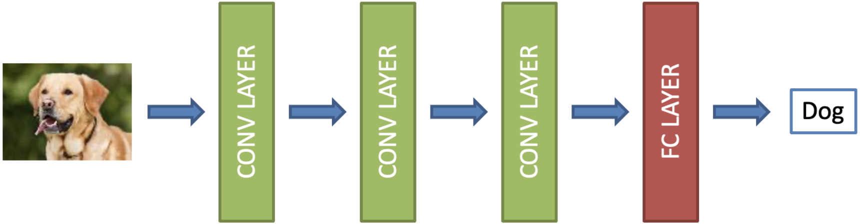
Basic layer implementation



Convolutional neural networks

CNN architecture

- Initial **feature extraction** stage
- Final **fully-connected** stage (traditional MLP)
- Task-specific output



Improve CNN training

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Dropout

- At training time, randomly disable neurons in fully-connected layers
- Reduces model complexity, help preventing overfitting
- At test time, use full model

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Batch normalization

- Feed **batches** of samples at a time
- At each layer, standardize feature maps based on batch statistics
- Reduces variations of intermediate data distributions

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Data augmentation

- Create "variations" of input samples
- Increase dataset variability, help preventing overfitting
- Examples: random crop, flip, color jitter

Convolutional neural networks

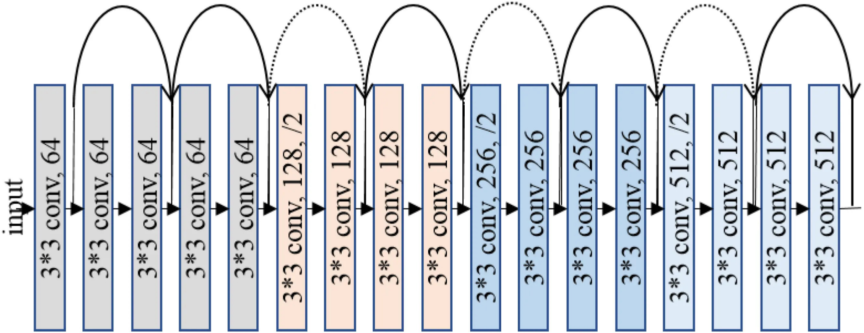
Pretrained models

- Adapt public trained models, rather than train from scratch

Convolutional neural networks

Pretrained models

- Adapt public trained models, rather than train from scratch
- Example: **ResNet** models



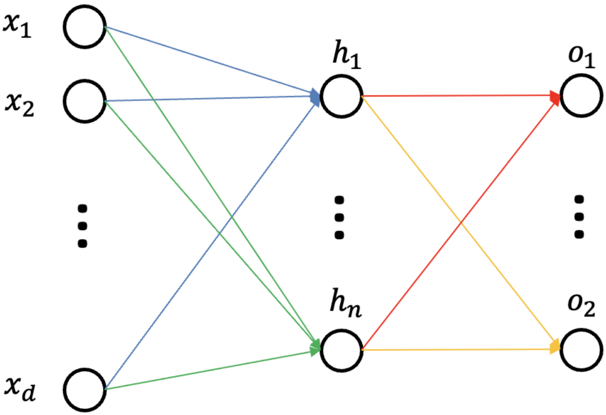
Recurrent neural networks

How to process sequential data?

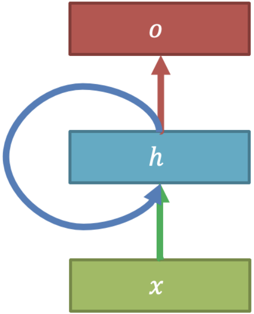
- Video
- Text
- Audio
- Time series

Recurrent neural networks

Feed-forward neural network



Recurrent neural networks



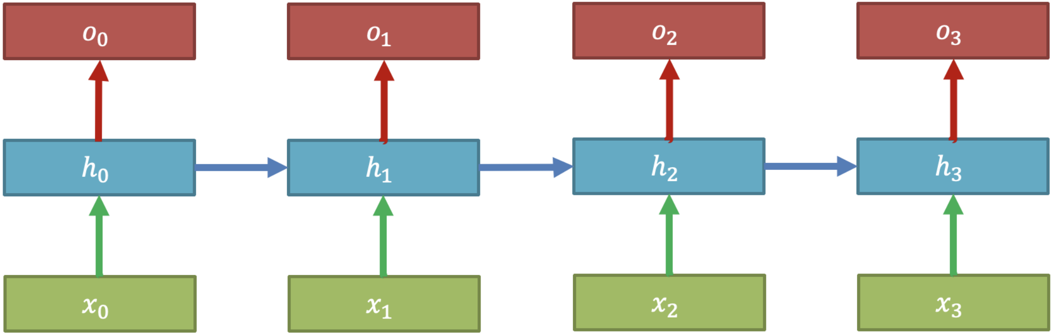
Output layer (e.g. classification)

Recurrent layer (nonlinear)

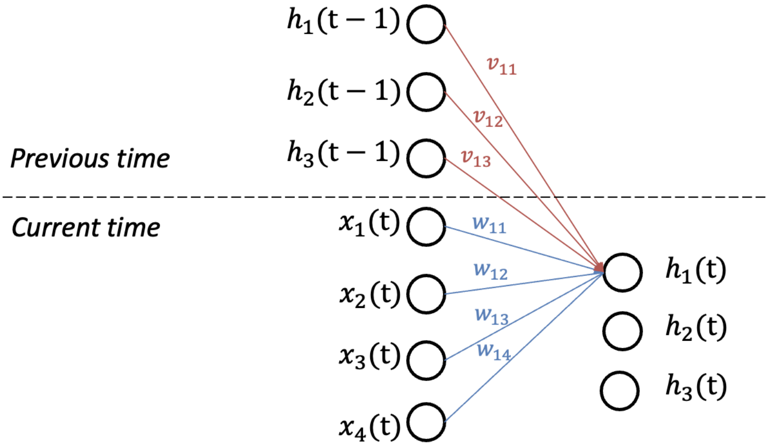
Input layer

Recurrent neural networks

"Unrolled" visualization



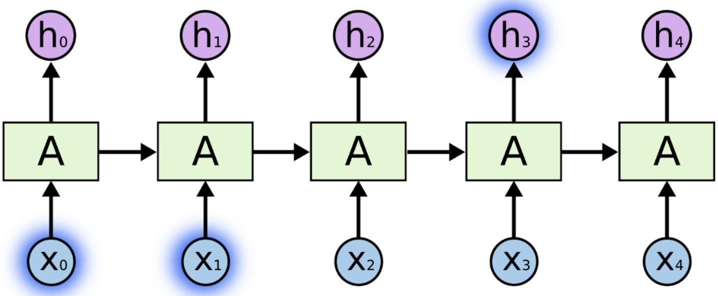
Recurrent neural networks



Recurrent neural networks

Long-term dependencies

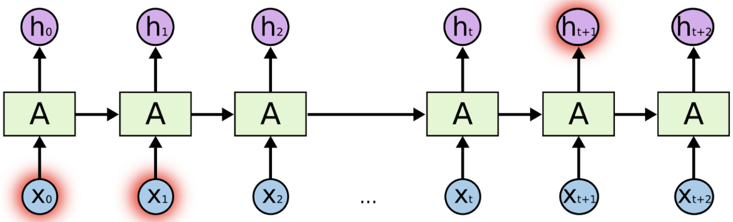
- RNNs store a representation of **context**
- Based on past information, make predictions on the future



Recurrent neural networks

Long-term dependencies

- **Recent** history affects state more than old history
- Old samples have little impact on future predictions



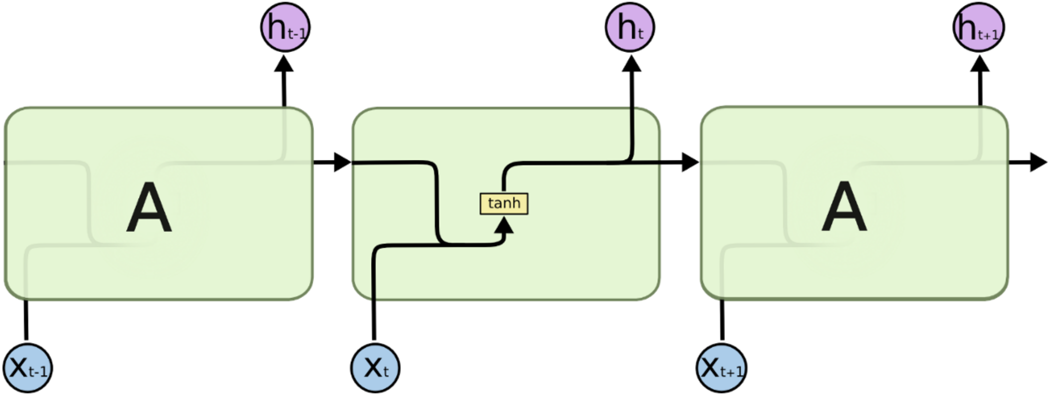
LSTM

Long short-term memory

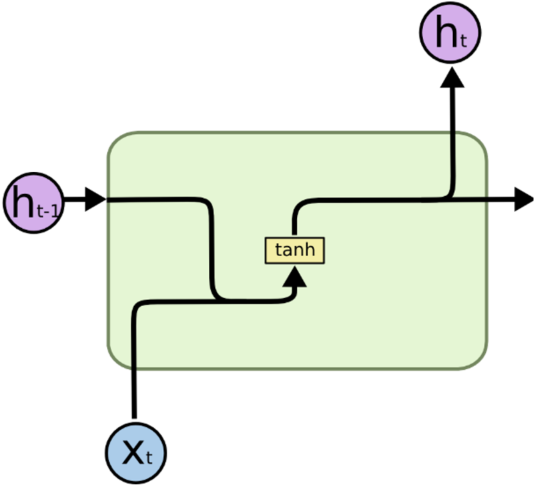
- Introduce a **memory** mechanism in the cell
- **Long**: memory enables to retain context information of a long time
- **Short-term**: stored information are dynamically selected based on the current input
- **Gates** control information flow
- Technical insight: improve backpropagation by preventing decreases in loss gradients

LSTM

Standard RNN layer

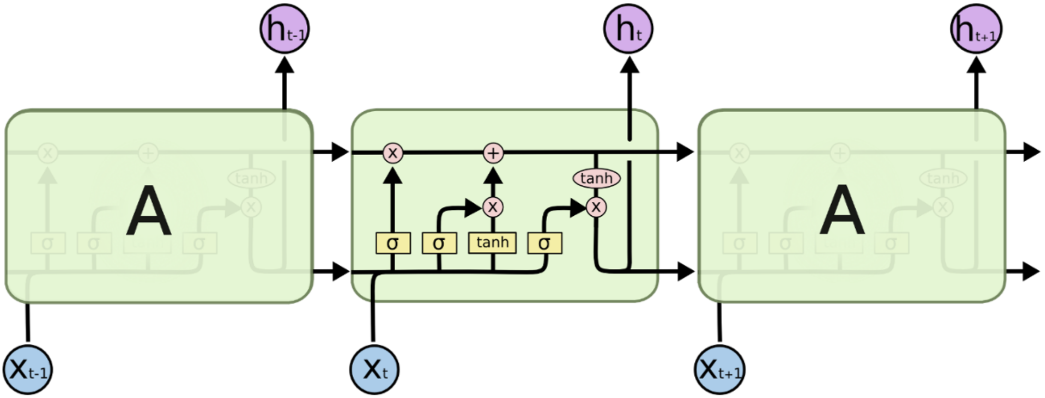


LSTM

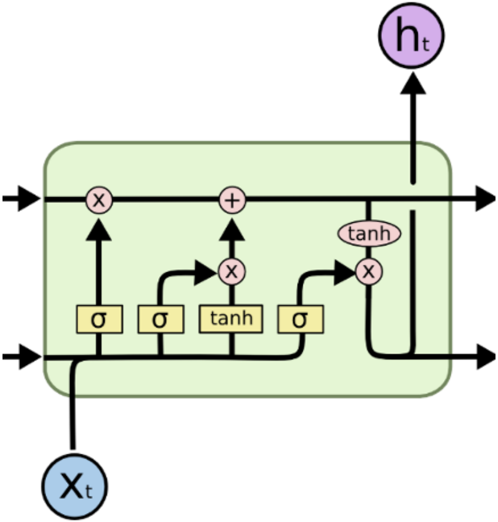


LSTM

LSTM layer



LSTM



LSTM

Long short-term memory

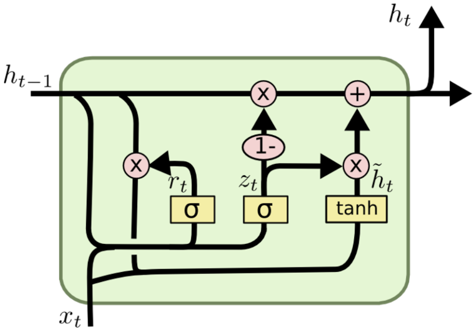
The cell internally controls:

- when information should be stored in memory
- when information should be removed
- when information should be provided as output

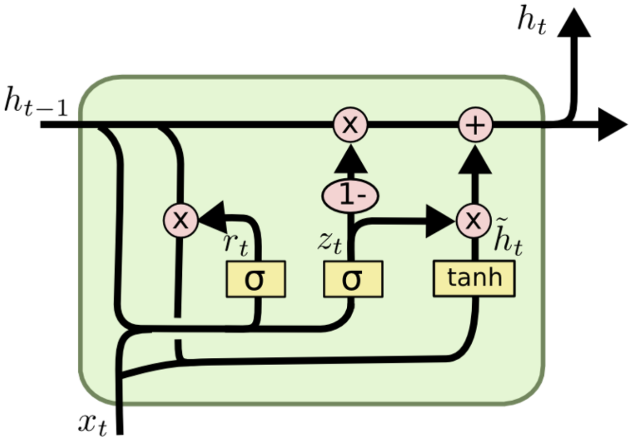
GRU

Gated recurrent unit

- Single cell state/output
- Single input/forget gate $\rightarrow$ **update** gate



GRU



Conclusions

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Recap

- Fundamental ML concepts
- Common deep architectures

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- Common deep architectures

New frontiers in astrophysics

- **Scalability:** tackle massive datasets (e.g., LSST, SKA).
- **Knowledge discovery:** identify subtle patterns missed by traditional methods.
- **Surrogate modeling:** accelerate computationally expensive simulations.

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Recap

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Challenges

- **Interpretability:** uncover the "black box"
- **Data scarcity/bias:** handling rare phenomena and observational biases.
- **Computational resources:** training large models can be demanding.