Principles of Deep Learning

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Part 1

- Minimal requirements, programming basics, and good practices
- Global Information Tracker (GIT): how to and setup

Part 2

- A (very brief) historical perspective.
- A hands-on analysis of the mathematical principles underlying deep learning.
- How to build a complete data analysis pipeline.
- From equations to code.

Python setup

- Python installation
- PIP
- Virtual environments
- Project blueprint

Good practices

- Single-responsibility principle

```
def function_11(a_in, opt_in):
  return a_in if opt_in is None else 0

...

def function1(a_in, b_in, opt_in = None):
  c_t = function_11(a_in, opt_in)
  return c_t + function_12(a_in, b_in)
```

- Unit test

```
def test_function_11():
  function_11(_, None) == 0
```

- Error management

```
class ACustomException(Exception):
  def __init__(self, my_arg):
    self.message = "A meaningful comment)
    super().__init__(self.message)
```

Good practices

- Write clear documentation

```
ss InvalidTravelType(Exception):
 """Exception raised for errors in travel type setting.

 Attributes:
     travel_type (int) -- input travel_type
 """
 def __init__(self, travel_type):
     self.message = "Travel type {} is invalid. Choose a value in
     super().__init__(self.message)
```

- Seopcify types and ouputs

```
def __init__(self, travel_type: int) -> None:
    self.message = "Travel type {} is invalid.
    "Choose a value in {}".format(travel_type, TRAVEL_TYPES)
    super().__init__(self.message)
```

- Provide examples and sample calls

```
if __name__ == "__main__":
  ...
```

GIT setup

- Install GIT
- Create an account on GitHub
- Clone a repository

```
git clone
```

- Create a repository
- Push a commit

The overarching purpose of deep learning

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Example problems

- Classification: What category does a given input belong to?
- Regression: What is the expected value of an unknown variable given a set of predictors?
- Control theory: What are the optimal control parameters given sensor data?
- ...

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The key difficulty is the choice of the parametric function f.

Early attempts

- The first neurally-inspired artificial decision-maker was Rosenblatt's *perceptron* (1958).
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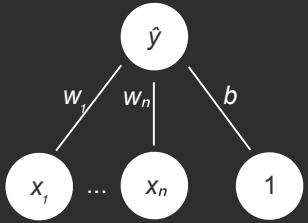

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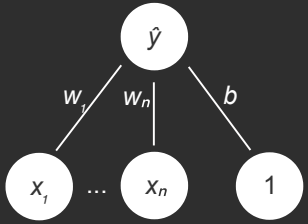

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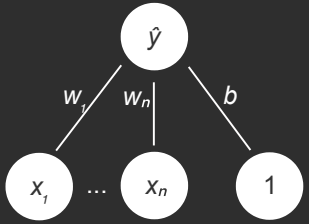
- In matrix notation, $\hat{y} = \sigma(Wx + b)$.
- Limitations of the perceptron were discovered quickly.
- For instance, this network cannot learn to implement the XOR function for binary inputs. That is to say, for inputs taking values either 0 or 1, return 1 if exactly one of the inputs is 1, return 0 otherwise. **Exercise.** Why?



Solution to XOR problem

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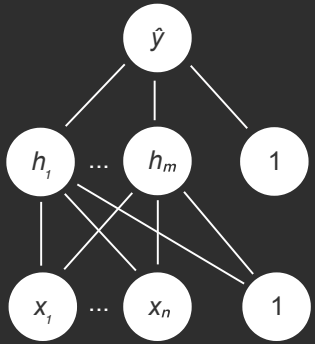
$1 = \sigma(w_1 + b) > \sigma(b) = 0$ and $1 = \sigma(w_2 + b) > \sigma(w_1 + w_2 + b) = 0$, hence $w_1 > 0$ and $w_1 < 0$, which is a contradiction.

The multilayer perceptron

The proposed solution was to "stack" perceptrons:



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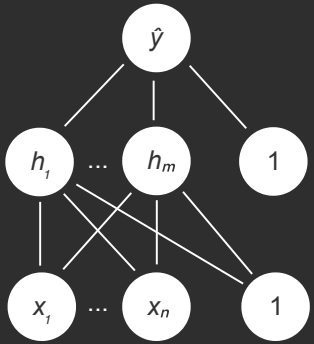

In formulas:

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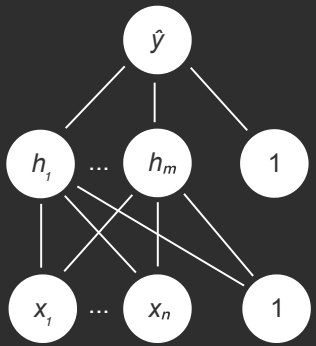

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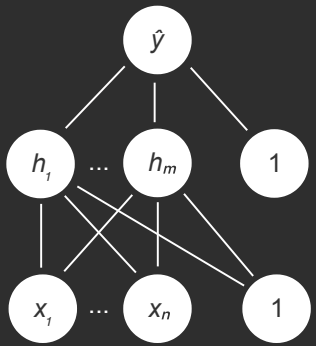

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The matrices W_1, W_2 and the vectors b_1, b_2 are our parameters. How can we optimize $\mathcal{L}(\hat{y})$ as a function of the parameters?

A concrete example

Let x, y be vectors. Let us define

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A general recipe: backpropagation

Backpropagation is the generalization of the above technique.

- During the forward pass, we compute *and store* all intermediate values from x to $\hat{y}$.
- For each one of these values, we compute the derivatives of the loss with respect to it, in *reversed order*.
- In the practical session, we will implement it.

Automatic differentiation

- In the above example, given a *primitive* $v = g(u)$ (matrix multiplication, addition, or pointwise nonlinearity), we wish to compute $\frac{\partial \mathcal{L}}{\partial u}$ as a function of $\frac{\partial \mathcal{L}}{\partial v}$.

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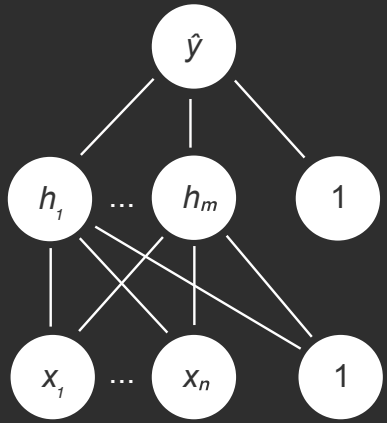

The road so far

- We have constructed a parametric function $\hat{y} = f(x, p)$: the *multilayer perceptron*.
- The parameters p contain all the weight matrices W and bias vectors b.
- Given a loss $\mathcal{L}(y, \hat{y})$ we can compute its derivatives with respect to p via backpropagation.

Stochastic (i.e., batched) gradient descent

- Let us now consider a dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{N}$.
- We wish to minimize $\mathcal{L}(y_i, \hat{y}_i)$, across all $(x_i, y_i) \in \mathcal{D}$, where $\hat{y}_i = f(x_i, p)$.
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Unfortunately, computing $\frac{\partial \mathcal{L}}{\partial p}$ requires averaging over the whole dataset, which can be very expensive.

A more practical approach (batched optimization) is to the following.

- Compute $\frac{\partial \mathcal{L}}{\partial p}$ for a given subset (batch) of data.
- Apply a step of gradient descent.
- Select a novel batch of data and repeat the procedure.

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Remark

In the above procedure, gradient descent on a batch of data is not the only option.

Many other batched optimizers can be used.

The overall procedure

- Start with a dataset of samples $\{x_i\}_{i=1}^N$ and correct outcomes $\{y_i\}_{i=1}^N$.

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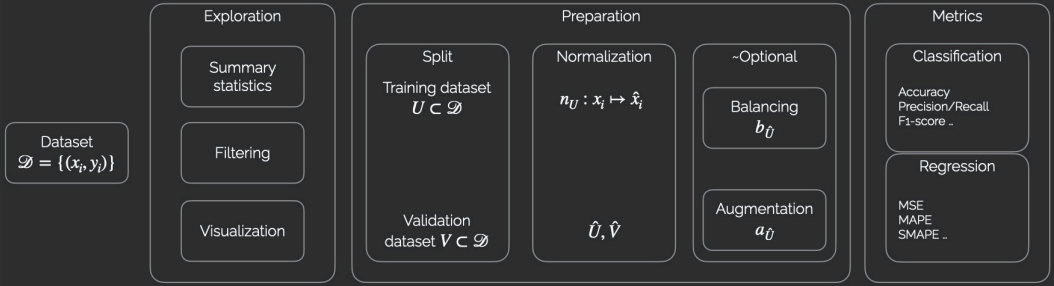
- Test the trained multilayer perceptron on novel samples.

From data to prediction



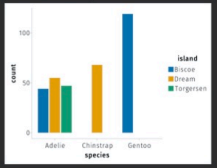
From data to prediction

Exploration

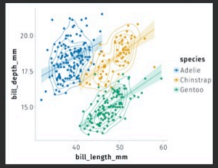
Summary statistics

Visualization

Frequency, distribution,...



Density, linear trend,...



Dimensionality reduction

PCA
t-SNE
UMAP
...

From data to prediction

Split

Training dataset $U \subset \mathscr{D}$

Validation dataset $V \subset \mathscr{D}$

Aim: gain insight on the performance of the model on actual data points

Hard-split

- Permute the dataset (if possible).
- Choose a ratio (e.g., 66% training and 33% test)

Folding

From data to prediction

Normalization

$n_U : x_i \mapsto \hat{x}_i$

$\hat{U}, \hat{V}$

Aim: scale the data uniformly.

Scaling

Let $I = [a, b] \subset \mathbb{R}$, $M = \max U$, and $m = \min U$

$$n_U = \frac{\square - m}{M - m}(b - a) + b$$

Standardization

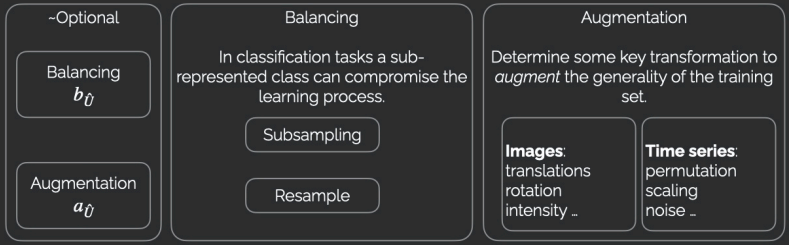
Let $\mu_U = \text{mean}(U)$ and $\sigma_U = \text{std}(U)$

$$n_U = \frac{\square - \mu_U}{\sigma_U}$$

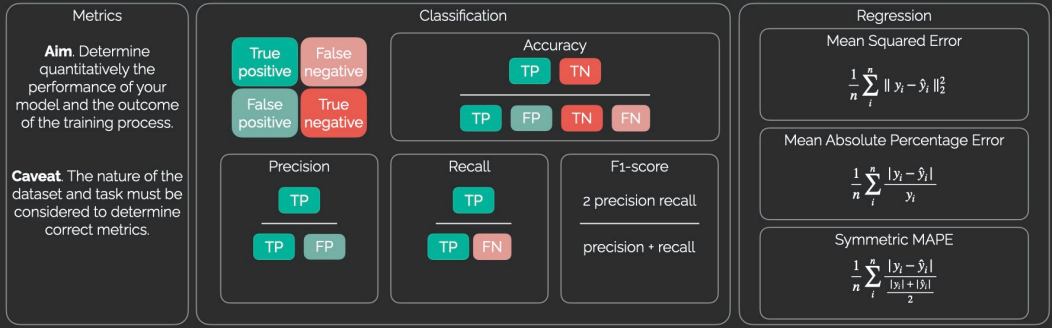
Caveat:

1. n_U should be either agnostic or dependent only on the training data
2. n_U should preferably be invertible

From data to prediction



From data to prediction



From data to prediction

Model
$M(\vartheta) = ?$

Equivariance

Main topic of lecture 2.

Loss

The loss function must be continuous and differentiable.
Beyond these assumptions it has to be tuned to one's problem.

Try to imagine possible loss functions to:
Classify images
Forecast time series
Generate images

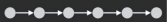
Architecture

There is no ultimate answer in establishing the optimal architecture for a given (dataset, task, model) triplet.

Heuristics and differentiable algorithms can learn architectures. Their optimality is still unclear.

Optimizer

Exercise. Let



be a minimization process through Gradient Descent. How the same process could be represented for SGD and SGD with momentum?

Monitoring

During training, we usually store the following quantities for the training and validation dataset:

- Running loss
- Running metrics

This allows us to spot overfitting and in case add early-stopping to our pipeline

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