Fundaments of Machine learning for and with engineering applications

Enrico Riccardi[1]

Department of Mathematics and Physics, University of Stavanger (UiS).[1]

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University of Stavanger

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Loss function

One of the main core concepts behind machine learning is the **loss function**.

In mathematical optimization and decision theory, a loss function or cost function (sometimes also called an error function) is a function that maps an event or values of one or more variables onto a real number intuitively representing some "cost" associated with the event. [Wiki]

Loss function in Machine Learning

It quantifies the difference between the predicted outputs of a machine learning algorithm and the actual target values.

Loss function aims

It provides a set of core quantifications/possibilities:

1. Performance measurement: it provides the metric of the prediction performances
2. Direction for improvement: it allows the identification of convergent solutions
3. Balancing bias and variance: it allows to account for artefact in the sampling phase
4. Influencing model behaviour: it allows to bridge data driven methods with mathematics/physics

Most common loss function in machine learning

Most popular entries:

1. Mean Square Error (regression): Fast computations, good convergence.
2. Mean Absolute Error (regression): No focus on the outliers, poor convergence.
3. Entropy Loss (classification): measures the difference between the model probability distribution outcomes and the predicted values

Losses

Mean absolute error, L1 loss

$$MAE = \frac{1}{n}\sum_{i=1}^{n}(|y_i - \bar{y}|)$$

Mean square error, L2 loss

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2$$

Log Loss for binary classification

$$Log\_Loss = -[y\ log(f(x)) + (1-y)log(1-f(x))]$$

MSE in Vanilla Python

```python
def mean_squared_error(observed, predicted):
    """ Compute the mean squared error.

    Parameters:
    ---------
    observed : list,
        The observed values.
    predicted : list,
        The predicted values.

    Output:
    ------
    sys[0] : float,
       Mean squared error.

    """
    if len(observed) != len(predicted):
        raise ValueError(
            "The lengths of input lists are" +
            f"not equal {len(observed)} {len(predicted)}.")

    # Initialize the sum of squared errors
    sum_squared_error = 0
```

MSE in Vanilla Python

```
    sum_squared_error = 0

    # Loop through all observations
    for obs, pred in zip(observed, predicted):
        # Calculate the square difference, and add it to the sum
        sum_squared_error += (obs - pred) ** 2

    # Calculate the mean squared error
    mse = sum_squared_error / len(observed)

    return mse
```

MSE in Numpy Python

```
import numpy as np

def mean_squared_error(observed, predicted):
    observed_np = np.array(observed)
    predicted_np = np.array(predicted)
    mse = np.mean((observed_np - predicted_np) ** 2)
    return mse
```

MSE in Python

```
from mse_vanilla import mean_squared_error as vanilla_mse
from mse_numpy import mean_squared_error as numpy_mse
import sklearn.metrics as sk

observed = [2, 4, 6, 8]
predicted = [2.5, 3.5, 5.5, 7.5]


mse_vanilla = vanilla_mse(observed, predicted)
print("Mean Squared Error, vanilla :", mse_vanilla)

mse_numpy = numpy_mse(observed, predicted)
print("Mean Squared Error, numpy :  ", mse_numpy)

sk_mse = sk.mean_squared_error(observed, predicted)
print("Mean Squared Error, sklearn :", sk_mse)

assert(mse_vanilla == mse_numpy == sk_mse)
```

MSE in benchmark

```
from mse_vanilla import mean_squared_error as vanilla_mse
from mse_numpy import mean_squared_error as numpy_mse
import sklearn.metrics as sk
import timeit as it

observed = [2, 4, 6, 8]
predicted = [2.5, 3.5, 5.5, 7.5]

mse_vanilla = vanilla_mse(observed, predicted)
time_v = it.timeit('vanilla_mse(observed, predicted)',
                   globals=globals(), number=10) / 100
mse_numpy = numpy_mse(observed, predicted)
time_np = it.timeit('numpy_mse(observed, predicted)',
                    globals=globals(), number=10) / 100
sk_mse = sk.mean_squared_error(observed, predicted)
time_sk = it.timeit('sk.mean_squared_error(observed, predicted)',
                    globals=globals(), number=10) / 100

for mse, mse_type, time in zip([mse_vanilla, mse_numpy, sk_mse],
                               ['vanilla', 'numpy', 'sklearn'],
                               [time_v, time_np, time_sk]):
    print(f"Mean Squared Error, {mse_type}:", mse,
          f"Average execution time: {time} seconds")

assert(mse_vanilla == mse_numpy == sk_mse)
```

Coding MSE

```
from mse_vanilla import mean_squared_error as vanilla_mse
from mse_numpy import mean_squared_error as numpy_mse
from sklearn.metrics import mean_squared_error as sk_mse
import timeit as it

observed = [2, 4, 6, 8]
predicted = [2.5, 3.5, 5.5, 7.5]

karg = {'observed': observed, 'predicted': predicted}

factory = {'mse_vanilla' : vanilla_mse,
           'mse_numpy' : numpy_mse,
           # 'mse_sk' : sk_mse
           }

for talker, worker in factory.items():
    exec_time = it.timeit('{worker(**karg)}',
                          globals=globals(), number=100) / 100
    mse = worker(**karg)
    print(f"Mean Squared Error, {talker} :", mse,
          f"Average execution time: {exec_time} seconds")
```

Regularization

Conventionally, MSE is used as loss function:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2$$

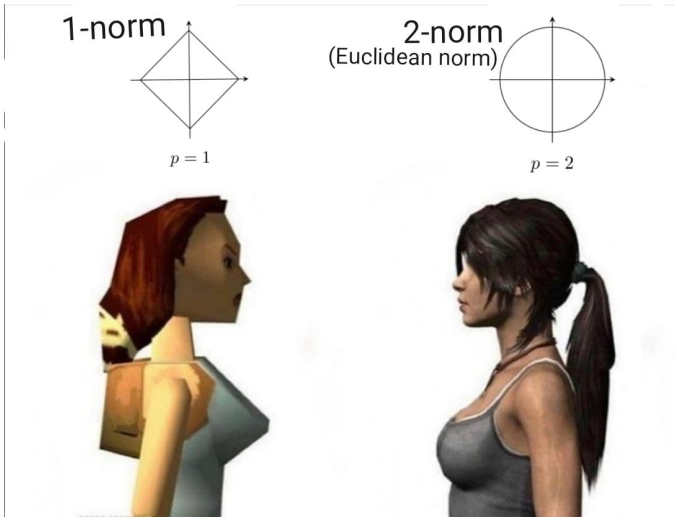
We might want to force our model not not fit so well the data, i.e. we *penalise* the model.

$$L1\_loss\_regularized = MSE + \lambda\sum_{i=1}^{m}|b_i|$$

$$L2\_loss\_regularized = MSE + \lambda\sum_{i=1}^{m}b_i^2$$

$$Elastic\ Net = MSE + \lambda_1\sum_{i=1}^{m}|b_i| + \lambda_2\sum_{i=1}^{m}b_i^2$$

Norms



Outcomes

Regularization

λ is the regularisation strength. The larger value it has, the more the target function is "wrong". For $\lambda = 0$, no regularisation is imposed.

Forcing a model to be "wrong" might sound rather counter-intuitive. Furthermore, we have introduced one more parameter that has not much meaning?!

Bias - variance trade off

$$Error = bias^2 + variance + statistical\ error$$

Bias

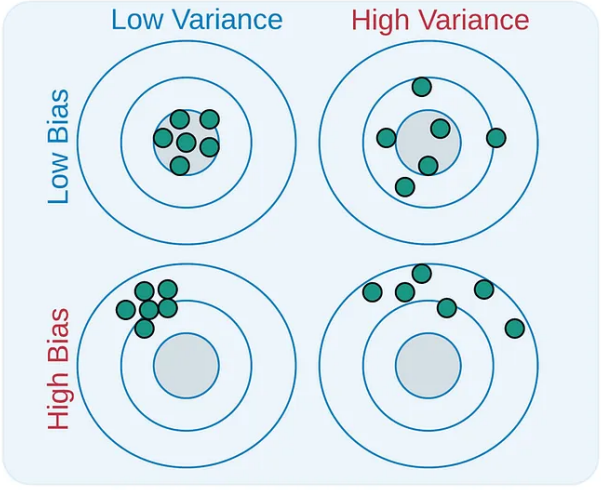
Bias is the difference of the average value of predictions (q) from the true relationship function (f):

$$bias[q(x)] = \mathbb{E}[q(x)] - f(x)$$

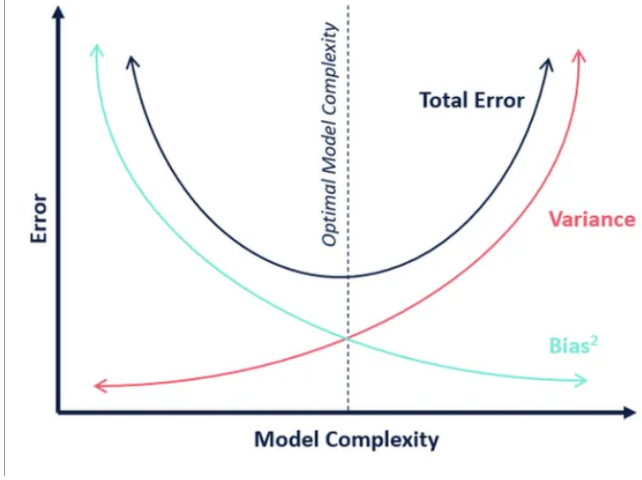
Variance is the expectation of the squared deviation of q(x) from its expected value $\mathbb{E}[q(x)]$.

$$var[q(x)] = \mathbb{E}[(q(x) - \mathbb{E}[q(x))^2]$$

Bias-Variance



Bias-Variance



Neural Network -NN-

One of the most famous models in Machine Learning is **Neural Network**.

The name comes from how the brain functions: a set of connected neurons that are either off or active.

In its essence,

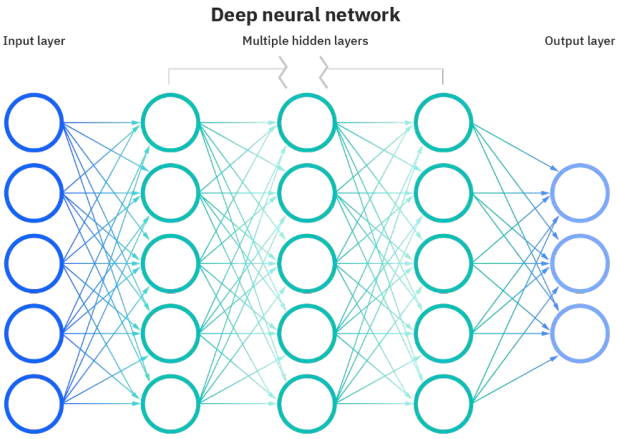
NN is a large set of (linear) regressions executed both in parallel and in series.

Conventional NN are composed by:

1. Input layer
2. Hidden layers
3. Output layers

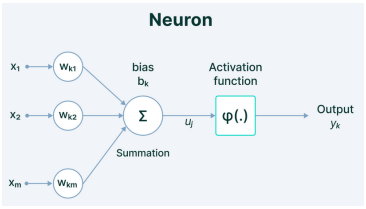
which, together, can approximately approximate any function in any dimension.

deep Neural Network



How do they work?

Each node is called neuron



Use many of these, many times, and you have builded a NN!

- It is really just a $Y = f(X)$, where w_i and b_i are the unknowns to solve for.
- As in linear regression, this becomes mainly a number of numerical recipes.
- As the problem's dimensionality is significant, several strategies have been developed.

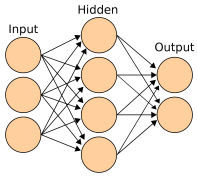
How do they work?

1. We thus need also an activation function.
2. The NN structure
3. Also, we might need to specify the number of epochs.

Using NN is essentially running a simulation campaign: a set of numerical experiments

Please say yes

Have you already heard of experimental design?



Activation function

Each node applies an activation function on the weighted sum of the previous nodes.

Such functions are called activation functions. There are MANY!

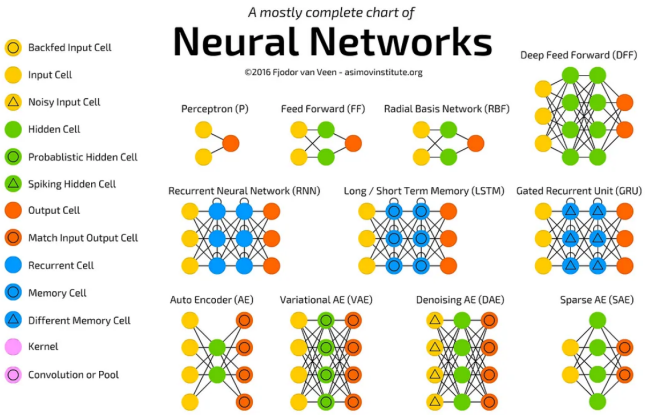
The most popular has been the logistic

	$\sigma(x) \doteq \frac{1}{1+e^{-x}}$	$g(x)(1-g(x))$

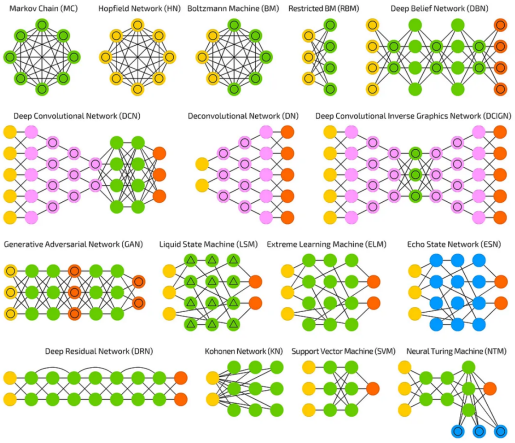
Now the most common is ReLU (Rectified linear unit)

	$(x)^+ \doteq \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases}$ $= \max(0, x) = x\mathbf{1}_{x>0}$	$\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \end{cases}$

NN Architecture



NN Architecture



NN Architecture

Neural net suffers from overfitting problems.

Even more parameters

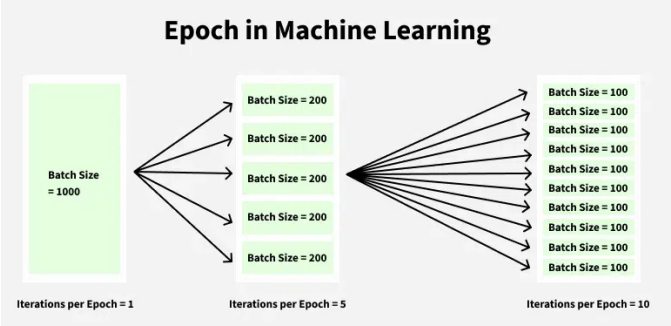
The number of nodes, the architecture, the number of hidden layer etc are NN hyperparameters

Unfortunately, at the current status of knowledge, the best architecture can be found only by trial and error.

The best fitting NN usually has a poor validation (generalizability).

NN is a very expensive approach and it should be used only if really needed.

Epoch



Epoch

Pro

1. Better performance
2. Progress tracking
3. Memory efficiency
4. Improved stopping criteria
5. More effective training

Cons

1. Overfitting risk
2. Computational cost
3. One more hyperparameter

NN types

There are many types of NN:

- ANN (artificial NN), just another name for NN
- DNN (deep) deep neural network
- RNN (recurrent NN) for audio
- CNN (convolutional NN) for images
- Autoencoder (for PCA) to compress to a latent space and decompress data
- Deep autoencoder (for interpretability)
- Physics informed NN (to merge NN to differential equations)
- ... and more ...

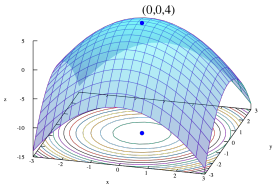
tensorflow, pytorch and keras are the most popular and popular libraries for NN.

Optimization

Optimization is a field on its own.

Definition

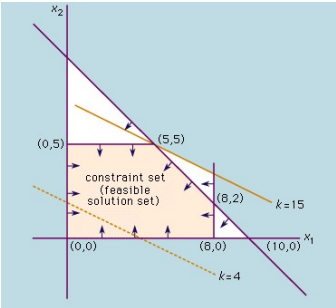
- Finding the "optimus" (latin), the best.
- Collection of mathematical principles and methods used for solving quantitative problems.



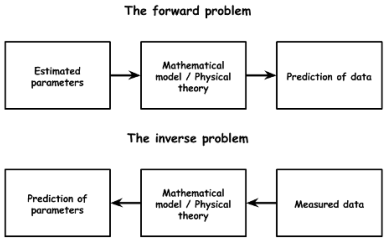
Constrains

Not only we want to find the best solution, we also need to respect the constraints.

Finding the minimum and maxima of functions subjected to constraints.



Forward and backward methods



Requirements:

1. Existence
2. Uniqueness
3. Stability
4. Efficiency

Gradient descend

Let's reconsider a linear model:

$$\hat{y}_i = \sum_{j=0}^{m} x_{ij} b_j$$

Let's get back the residuals

$$R = e^T e$$

What we do is to calculate the derivative of the residuals in respect to the coefficients b_j.

and the ideal solution is when

$$\frac{\partial R}{\partial b_j} = 0 \quad \forall j \in [0, n]$$

Gradient descent

ok, but what if we do not know

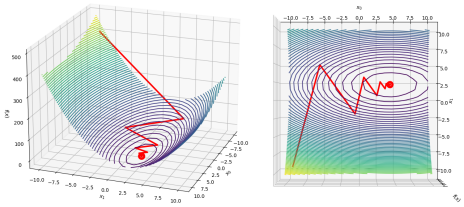
$$\frac{\partial R}{\partial b_j} = 0$$

We hopefully be able to numerically calculate $\frac{\partial R}{\partial b_j}$

When f is convex:

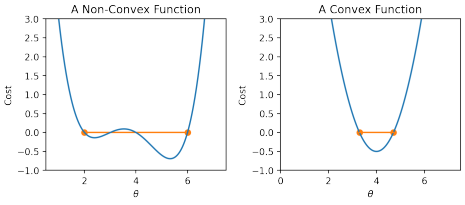
The learning rate η is used to move towards the global minimum:

$a_{n+1} = a_n + \eta \nabla f(a_n)$



Gradient descent

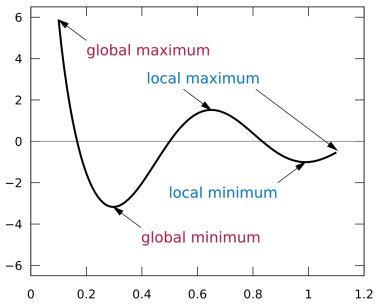
When f is convex:



$a_{n+1} = a_n + \eta \nabla f(a_n)$

Gradient descent

Multiple minima are commonly present in large dataset



Learning rate

The learning rate is a tuning parameter in an optimization algorithm that determines the step size at each iteration while moving toward a minimum of a loss function.

This is not that easy... Learning rate can be:

- Constant
- Variable (a given function)
- Block-set up (sparse data)
- Adaptive (as a function of the loss function)