Minimum levels of high energy particle bombardment on fusion reactor vessels:

Towards a computational multi-parameter scan for automated data reduction ("big data") applications

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February 2020

Contents

Abstract

Chapter 1

Introduction

The design process for a facility like a fusion power plant takes into account a manifold of aspects. Thereunder a cost analysis for the fusion device. To make an estimate of the cost analysis one has to consider the lifetime of machine parts. Most prominently the divertor and first wall suffer from shortened life spans due to erosion. Which is partly due to neutral particle induced sputtering.
To include considerations like these in the design of a power plant one uses so called systems codes like PROCESS [**?**]. These codes focus on optimizing design parameters of large scale systems like power plants, which consist of many smaller subsystems. Due to the amount of subsystems the need arises to simplify models in order to achieve reasonable run times for systems codes. The following work is concerned with deducing a fast surrogate in place of a simulation for the sputtering rate of a fusion device component.
The following chapter gives a brief overview of the motivating applications while also introducing the concept of reduced model approaches via machine learning algorithms. Furthermore it considers which methods are most applicable in the given situation.

1.1 Fusion Devices

Fusion technology has been an ongoing field of research for almost one century. The earliest records of fusion research go back to the 1920s when Francis William Aston discovered the potential energy gain of combining hydrogen atoms into helium atoms. Later in the 1920s Arthur Stanley Eddington proposed the proton-proton chain reaction as the primary working mechanism of the sun. add citation

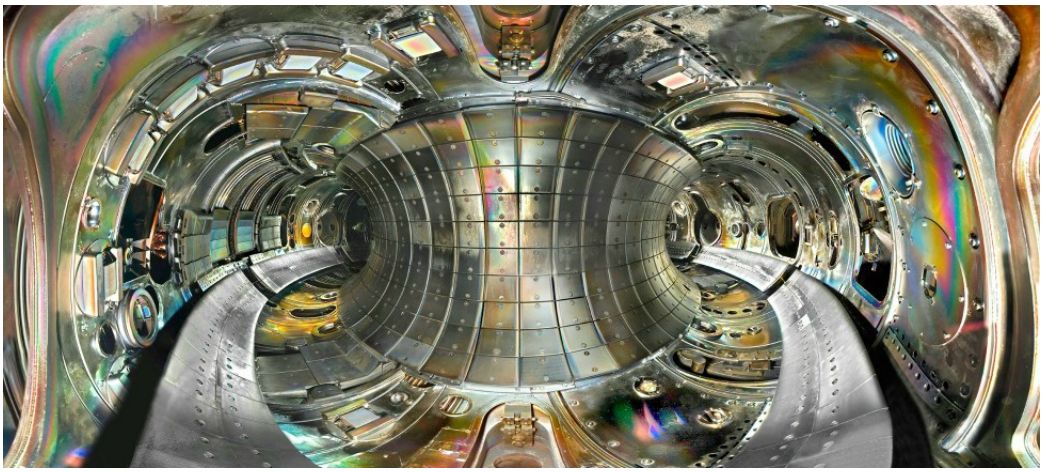

Figure 1.1: A picture of the TEXTOR Tokamak reactor. Depicting the inside with a wide angle camera shot.

The basic idea of fusion power generation is exploiting a difference in binding energy of different elements. A basic calculation as in 1.1 shows that by combining the hydrogen isotopes deuterium and tritium into helium a neutron with 14.1MeV is released which can be used to extract energy as heat, thus allowing fusion to be used as a means of generating electric power.

$$ {}^{2}_{1}\mathrm{D} + {}^{3}_{1}\mathrm{T} \Rightarrow {}^{4}_{2}\mathrm{He}(3.5\,\mathrm{MeV}) + \mathrm{n}(14.1\,\mathrm{MeV}) \tag{1.1} $$

maybe replace $^1_1$ with mathtools and MeV with units

add citation

Add footnote and/or citation

The containment principle for fusion plasma is based on the magnetic bottle/mirror phenomenon. This allows to encase charged particles inside a magnetic field. Neutral particles will not be confined by the magnetic field and quickly exit the fusion plasma towards the first wall of any fusion device. The impact of neutral particles will also lead to erosion of the wall. The erosion can be estimated by using monte carlo simulations via the EIRENE [**?**] code. To counter the erosion of integral machine parts a device called blanket is used as a replaceable first layer. The operating life of the blanket needs to be taken into consideration for maintenance cycles and operating cost of a fusion power plant.

1.2 PROCESS Systems Code

The systems code PROCESS [**?**] is concerned with the combination of physics, engineering and economical simulation and evaluation for a fusion power plant scenario[1]. It is based on TETRA (Tokamak Engineering Test Reac-

[1]So far most published work has been on ITER and DEMO Tokamak like scenarios.

tor Analysis) [?] and has been used for the Power Plant Conceptual Study [?].

PROCESS can be operated in two different modes, namely optimization mode and non-optimization mode. In non-optimization mode PROCESS will find a single set of parameters that form a viable fusion device within the given constraints, while the more commonly used optimization mode finds a set of parameters that minimize or maximize a chosen figure of merit. The list of figures of merit includes capital cost, cost of electricity or more physical/engineering related quantities such as neutron wall load.[2]
There are several hundred input parameters which can be chosen as iteration variable for a run in optimization mode. Studies of a given design for a fusion device might want to use the optimization mode to scan a range in multiple input parameters, easily resulting in a high number of runs and an accordingly high total run time. Hence underlying physical models have to be sufficiently simplified in an attempt to balance required runtime against a higher potential for error.

This work is concerned with finding a surrogate model replacing the monte carlo simulation of EIRENE for contexts like the PROCESS systems code. Whereas this work is concerned with a simple model, see chapter **??**, the methods used are examined for further use in full scale 3D models.

1.3 Reduced Model Approaches

Simulations based on complex models face the barrier of having long run times, which is often unsuited for studying general systematic behaviours. Reducing run time of numerical simulations can be achieved via model order reduction methods like dimensionality reductions.[3] Given that in many cases a complete analytical model can not be given there are approaches to model order reduction using machine learning algorithms that approximate the simulated system via surrogate functions. The resulting surrogates do not give further insight into working mechanisms of the system, but allow for much faster computation at reasonable approximation errors. Depending on the desired capabilities of the surrogate a machine learning methods should be chosen accordingly. The methods chosen in this work are Deep Neural

Fix citation

[2]Further information on the details of PROCESS code operation can be found in the publication of M. Kovari et. al [?].

[3]Ideally one would apply control theory to the given system with proper orthogonal decomposition and reduced basis methods. Though this method relies on an analytical model description.

Networks (NN) and Gaussian Processing (GP). Both methods feature high flexibility and NN also provide excellent scalability. Furthermore combining both methods allows to reduce downsides of a single method. For example GP achieves accurate prediction when interpolating but has much greater error margins when extrapolating. A more in depth discussion can be found in chapter [**?**].

Chapter 2

Model

2.1 EIRENE 1D

- What is Eirene
  - Monte Carlo Simulation of plasma particles
  - solving kinetic boltzmann equations to propagate particles
  - using plasma chemical reaction rates for interactions
  - Plasma Profiles
- Why 1DModel instead of full Eirene
  - Reduction of run time of each simulation step.
  - Removes geometric parameters from input parameter set.
- Additional assumptions
  - $T_I = T_e$ reasonable assumption to further reduce dimensionality of input.

2.1.1 Kinetic Boltzmann Equations

2.2 Plasma Profiles

For the inputs of Eirene plasma profiles are needed, that can be dynamically provided by other algorithms like SOLPS or EMC3. Central piece of this

Citation needed

Citation needed

work is to investigate if a substitute function can be found for the full range of possible plasma profiles by using big data methods. One can ascertain the physical limits of the parameters constituting the plasma profiles from table **??**. These limits are based on different phenomenons in plasma physics, which can be

Insert Plasma Profiles and table from RedMod Workshop

2.3 Choice of sampling set

Since the parameter space is high dimensional, the training points have not been selected randomly. According to randomly sampled points might form clusters, which could skew the training towards a subsection of the parameter space. To avoid this a low discrepancy sequence, namely the Sobol sequence, from which the training points are sampled has been chosen.

Add reference

2.3.1 Sobol Sequence

- short overview
- formula
- advantages

Add citation

The sobol sequence was first invented by the mathematician Ilya M. Sobol

2.3.1.1 Low-discrepency sequences

More details on advantages of low-discrepency sequences.

Chapter 3

Methods

This chapter is concerned with introducing the methods used to investigate the data reduction of the previously introduced model. The focus of this work will be on artificial neural networks (ANN in short) and Gaussian processes. The following list will provide a brief overview of other machine learning techniques that are frequently employed in machine learning approaches:

- Support Vector Machines (SVM):
  SVMs are used to classify data similar to ANNs. In contrast to ANNs SVMs are build up from theory and contain little Hyperparameters[1] making them easier to analyse and less prone to overfitting. Generally speaking a SVM tries to separate data by calculating a hyperplane using given training data. The separation has a margin[2] that is maximized. Classification of SVMs are based on which side of the separation the data point lies. For non-linear classification the kernel trick[3] can be used to create a high dimensional feature space. Better suited for classification tasks. Could be used in future endeavours to assess the viability of a certain configuration by classifying input toward a threshold value, e.g. Sputter rate for first wall lower than X
  There are variations of regression SVMs which are difficult to optimize for performance since SVMs rely on analytically calculating the separating hyperplane.

add citation

What is X?

- Random Forests :

Short description of Random Forests

add citation: https://www.oreilly.co on-machine-learning/978178934641 421e-4577-afc3-efdd4e02a468.xhtml

add citation: https://towardsdatasc

[1] Please refer to section 3.1.4 for further information.
[2] Area around separation plane that contains no data.
[3] add source for further information

- Random forest are ensembles of decision trees, hence the name forest. Each individual tree provides a classification prediction. The class with most votes is prediction of the random forest.
  A forest with many uncorrelated trees outperforms highly correlated forest. Random forests have good predictive performance, but slower prediction time which makes them unsuited for system codes.

- Adaptive Boosting:
  Not unlike random forests AdaBoost works with an ensemble of decision trees, though in contrast the decision trees used are single split trees called stumps. When training an AdaBoost algorithm the algorithm boosts weights of individual stumps based on their contribution to difficult to classify instances.

add citation: https://towardsdatascience.com/understanding-adaboost-2f94f22d5bfe

3.1 Neural Networks

The following section is concerned with discussing neural networks as a means of investigating functional dependencies.[4]

3.1.1 General Introduction To Neural Networks

An artificial neural network (ANN) in the following called neural network, abbreviated to NN, is "a computing system made up of a number of simple, highly interconnected processing elements, which process information by their dynamic state response to external inputs." [1] First concepts of learning algorithms based on neural plasticity have been introduced in the late 1940s by D. O. Hebb . In 1975 backpropagation became possible via an algorithm by Werbo, this led to an increase in machine learning popularity. During the 1980s other methods like support vector machines and linear classifiers became the preferred and/or dominating machine learning approach. With the rise in computational power in recent years neural networks have gained back a lot of popularity.

citation needed

citation needed

The concept idea of neural networks is to replicate the ability of the human brain to learn and to adapt to new information. The structure and naming convention reflect this origin.
A neural network is made up of small processing units called neurons. These are grouped together into so called layers. Every network needs at least two

[4] To aid with understanding the terminology used there is a glossary in the appendix section B.2.

layers, the input layer and the output layer. If a network has intermediary layers between input and output, they are called hidden layers. A network with at least two hidden layers is called a deep neural network (DNN). The amount of layers in a network is called the depth of the network. While the amount of neurons in a layer is called the layers width. In a typical NN information stored in neurons is transferred into the next layer by a weighted sum. The connected neuron of the following layer then applies a non-linear function, called activation function, to calculate it's final value. This process in repeated until the output layer is reached. The activation function as well as the amount and order of connections can vary in between layers. The system according to which a network is designed is called a network architecture. The most important architectures in the following work will be *dense deep feed forward* and *autoencoder*. To give insight into the basic working principle an example neural network is depicted and described in the following section 3.1.2.

reword "order"

Neural networks are usually used in two ways, optimization or classification. Well known examples are handwriting recognition as classification and least mean squares (LMS) optimization.

think of better example

3.1.2 Functionality

The working principle is to form a weighted sum $\sum_{k=1}^{N} w_{j,k} \cdot x_k$ over the values from neurons of the previous layer x_k weighted by the connecting weight $w_{j,k}$. The weighted sum is then evaluated by the activation function $\sigma()$ such that the new value $x_j = \sigma(\sum_{k=1}^{N} w_{j,k} \cdot x_k)$. Here k refers to the index of the neuron in the previous layer and j to the index of the neuron in the current layer.[5]

Since forming a weighted sum is a linear operation the activation function must be non-linear to enable the network to learn non-linear behaviour. The most common activation functions are the rectifier also called rectified linear unit (ReLU) and exponential linear unit (ELU) shown in figure **??**. Both are inspired by the asymmetrical behaviour of biological neural connections.

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reference needed

[5]The order of indices becomes more intuitive when talking about backpropagation and it's matrix notation in section 3.1.3.1

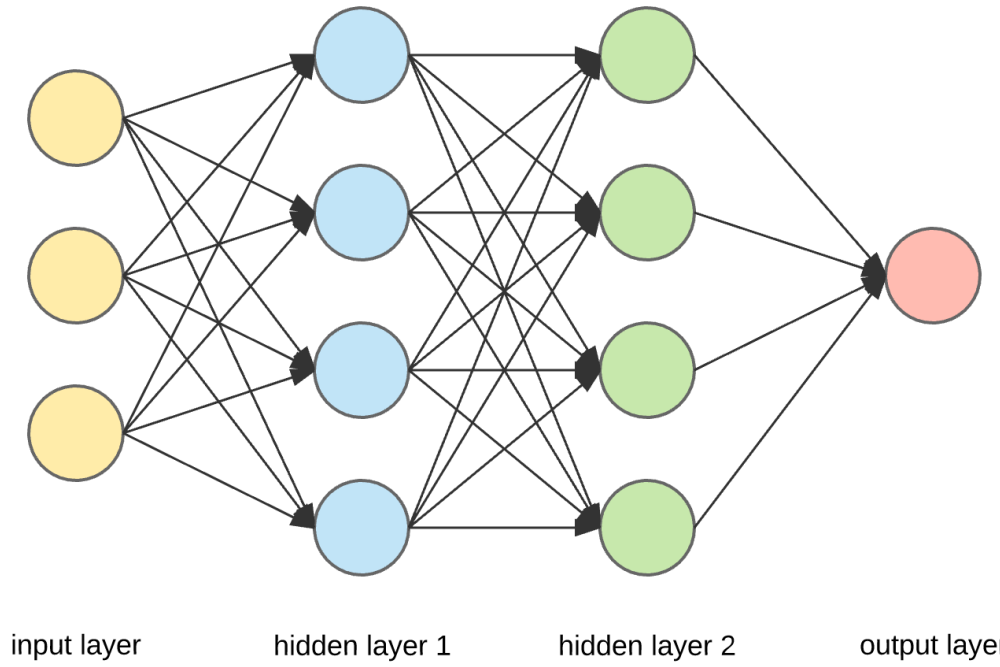

Figure 3.1: Schematic structure of the most basic fully connected deep neural network. Indicated are the input (yellow), output (red) and hidden layers (blue and green). Each neuron outputs to all neurons in the following layer, but there are no interconnection between neurons of the same layer. Note that while the network has the minimum depth (2 hidden layers) to qualify for a deep neural network, the width could be smaller.

3.1.3 Training

Before a neural network can be put to work it needs to be trained. To train a NN a set of training and test data has to be generated. This work uses the afore mentioned monte carlo simulations from the EIRENE code. The training data consists of input e.g. temperature and density of the plasma and output e.g. the sputtering rate of the first wall. The EIRENE input data is used as input of the network and the sputtering rate is compared to the output of the network via a cost function. Afterwards the weights of the network are adjusted by using backpropagation, which is a method that calculates partial weight derivatives of the output. A more detailed explanation can be found in section 3.1.3.1 .

add citation

3.1.3.1 Backpropagation

To talk about Backpropagation it is necessary to first set down a notation. In the following $w^l_{j,k}$ will denote the weight of the connection from neuron k in layer $l-1$ to neuron j in layer l. Furthermore we will reference the activation function as $\sigma(\,)$, the activation $a^l_j = \sigma\left(\sum_k w^l_{j,k} \cdot a^{l-1}_j + b^l_j\right)$ cost function as C. Later on the quantity $w^l_{j,k} \cdot a^{l-1}_j + b^l_j$ will be useful and called weighted input z^l_j. Many of the notation above can be understood as a vector across neurons of a layer, hence omitting the indices j and k.
This leads to the vector notation:

$$a^l = \sigma(w^l a^{l-1} + b_l) = \sigma(z^l) \tag{3.1}$$

The backpropagation algorithm aims to provide a computational fast way of calculating the partial derivatives 3.2 and 3.3.

add citation: http://neuralnetworks

$$\frac{\partial C}{\partial w^l_{j,k}} \tag{3.2}$$

$$\frac{\partial C}{\partial b^l_j} \tag{3.3}$$

Before looking at the partial derivatives of the cost function it is necessary to make two assumptions about the cost function C.

Assumptions of the cost function
The following two assumptions have to be made.

Maybe reformat?

1. The cost function can be written as an average of cost functions for individual training examples.

$$C = \frac{1}{n} \sum_x C_x \tag{3.4}$$

2. The cost function can be written as a function of the outputs a^L of the network:

$$C = C(a^L) \tag{3.5}$$

Where L is the number of layers in a network such that the activation a^L is the output of the network.

A good example for a cost function that fulfils these requirements is the quadratic cost function

$$C(a^L) = \frac{1}{2} \left\| y - a^L \right\|^2 = \frac{1}{2} \sum_j \left(y_j - a_j^L \right)^2 \tag{3.6}$$

Please note that y is a given parameter and not learned by the network therefore it is not a variable of the cost function. Furthermore the partial derivative $\frac{\partial C}{\partial a_j^L} = (a_j^L - y_j)$ is known and easily evaluated.

Change paragraph title

Back to Backpropagation A few more intermediate steps are necessary:

1. Define the error $\delta_j^l \equiv \frac{\partial C}{\partial z_j^l}$.

2. Start with the error of the output layer:

$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma' \left(z_j^L \right) \tag{3.7}$$

3. Express δ_L in a matrix equation[6]

$$\delta^L = \nabla_a C \odot \sigma' \left(z^L \right) \tag{3.8}$$

4. Express δ^l as a function of δ^{l+1}:

$$\delta^l = \left(\left(w^{l+1} \right)^T \delta^{l+1} \right) \odot \sigma' \left(z^l \right) \tag{3.9}$$

[6]Hadamard prodcut of two vectors x and y is given by $x \odot y = x_j \cdot y_j$

Now the partial derivative 3.2 can be expressed as:

$$\frac{\partial C}{\partial w^l_{j,k}} = a^{l-1}_k \delta^l_j \tag{3.10}$$

And the partial derivative 3.3 can be expressed as:

$$\frac{\partial C}{\partial b^l_j} = \delta^l_j \quad \Rightarrow \quad \frac{\partial C}{\partial b} = \delta \tag{3.11}$$

Equations 3.8 and 3.9 provide a fast functionality once the components are known. Luckily all $\sigma'(\ )$ and $\frac{\partial C}{\partial a^L_j}$ are known before start of training and all weight matrices w^{l+1} are calculated during forward pass of each training point. Lastly the error δ^l can be deduced from the following error δ^{l+1}. Hence, as the name suggests, the algorithm works from layer L backward to the first layer $l = 1$.
Therefore the main computational cost of backpropagation is to apply the matrix multiplication of $\left(w^{l+1}\right)^T$ to δ^{l+1}. This can be done in a computational efficient manner over multiple training samples called mini-batches.[7]

3.1.3.2 Choice of optimizer

With the partial derivative of the cost function in respect to any given weight and bias it is possible to adjust them. Additionally a learning rate η that depends on the type of optimizer used and architecture of the network has to be chosen. A basic optimizer is the first order Gradient Descend. It applies the following formula to update parameters θ:

$$\theta_{t+1} = \theta_t - \eta \nabla C(\theta_t) \tag{3.12}$$

Where theta can be any $w^l_{j,k}$ or b^l_j from the previous section 3.1.3.1.
There are multiple optimization techniques that improve upon gradient descend. A few concepts are briefly mentioned here, but for a more detailed explanation please refer to :

add citation

Mini Batches Applying a parameter update after each training example will cause fluctuations that can be helpful in finding minima, but also slow the convergence once close to them. On the other hand applying only one update per training set slows the learning rate immensely. It might not even be possible for training sets that are too large to fit in

[7] For a more detailed explanation and short proofs of equations 3.8 to 3.11 please refer to

memory at once. To compromise one uses a mini batch system where subsets of training data are accumulated for update steps. Typical mini batch sizes range from 50 to 256 training examples.

Momentum Using the gradient descend optimizer it is easy to see that moving along a slope one can imagine a ball rolling down a slope collecting momentum along the way. This is realized by adjusting the weight update with an additional term from the previous update.

$$\theta_{t+1} = \theta_t - V(t) \tag{3.13}$$
$$V(t) = \gamma V(t-1) + \eta \nabla C(\theta_t) \tag{3.14}$$

Where γ is a simple numerical factor to control the size of the momentum. A typical value for γ is around 0.9.[8]
While this method speeds up learning it can also lead to overshooting a minimum. To negate the negative effect a method called Nesterov Accelerated Gradient (NAG)[9] is used, in which a predictive term slows down momentum if the slope changes signs.

$$V_{NAG}(t) = \gamma V(t-1) + \eta \nabla C(\theta_t - \gamma V(t-1)) \tag{3.15}$$

Adaptive learning rates Some neurons activate more seldom than others and therefore it makes sense to put more emphasis on updates of infrequently activated neurons by adjusting learning rates of neurons individually. To do so manually is not feasible, but there are methods like the AdaDelta optimizer that utilise a running average $E[g_t^2]$ of past updates to decrease the learning rate of neurons.

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{E[g_t^2] + \epsilon}} g_t \tag{3.16}$$
$$E[g_t^2] = \gamma E[g_{t-1}^2] + (1-\gamma) g_t^2 \tag{3.17}$$

Here $g_t = \nabla C(\theta_t)$ is a shorthand for the gradient and g_t^2 the square not laplacian. ϵ is a small positiv number usually on the order of 10^{-8}.

The Adaptive Moment Estimation (Adam) optimizer combines adaptive learning rates, momentum and batch application in one optimizer. It is well suited

[8] This factor can be thought of as how many previous time steps influence the current update. See https://towardsdatascience.com/stochastic-gradient-descent-with-momentum-a84097641a5d for more information.

[9] More details on NAGs can be found at http://cs231n.github.io/neural-networks-3/.

add citation https://towardsdatascience.com/types-of-optimization-algorithms-used-in-neural-networks-and-ways-to-optimize-gradient-95ae5d39529f

Turn link in footnote into citation

for sparse problems and has been shown to yield fast convergence. It is therefore the optimizer of choice in the following work.

$$\hat{m}_t = \frac{m_t}{1-\alpha_t} \tag{3.18}$$

$$\hat{v}_t = \frac{v_t}{1-\beta_t} \tag{3.19}$$

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_t}+\epsilon}\hat{m}_t \tag{3.20}$$

Here $m_{t+1} = \alpha m_t + (1-\alpha)g_t$ denotes the mean of the gradient and $v_{t+1} = \beta v_t + (1-\beta)g_t^2$ the variance. α is typically as large as γ from AdaDelta, around 0.9. β is close to 1 with a default value of 0.999.

3.1.3.3 Regularization

From the description above it should be clear that the number of parameters in a neural network can easily exceed the one or even ten thousand, some state-of-the-art neural networks even exceed 40 million parameters. With that many parameters a model can fit to nearly any set of data reasonably well. John von Neumann famously said:"With four parameters I can fit an elephant, and with five I can make him wiggle his trunk."[10]
The aim of a network is to give accurate predictions on data it has never seen before. Therefore it is critical to ensure the learning gains generalize well to unknown data. Any method that aims to increase prediction accuracy on the test set at a disregard to the accuracy of the training predictions is called a regularization method. Inversely the increase in training accuracy with stagnating or even degrading of test prediction accuracy is called overtraining or overfitting.
In the following we will shortly introduce the most commonly used regularization methods.

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add citation: book Multi Media Modeling

Hold out In this work training and test sets have been mentioned before. This is the appropriate point to go into a little more depth at why the distinction is necessary. Furthermore a third set called validation set is introduced.
The naming of the three sets is already indicative of what their purpose is.

Make footnote contain citation

Training Set Set of examples used during the training process. The network iterates on these points to adjust weights and biases to minimize the cost function.

[10] See https://www.johndcook.com/blog/2011/06/21/how-to-fit-an-elephant/

Validation Set Set of examples used after training to evaluate the performance of the network. After which hyper parameters like architecture or learning rate are reassessed.

Test set Set of examples used after hyper parameters have been tuned. Used to judge final performance of the network.

At first glance validation and test set seem to fulfil a similar role in that they are used to validate the learning process of the network. Since overtraining is a major concern, it is also important to consider overfitting the hyper parameters. Considering the tuning of hyper parameters as an optimization task to improve test accuracy shows that the validation set really is more similar to the training set on a higher meta-level. Therefore it is necessary to split potential test data into a validation and test set. This allows to have a data set that the network does not see over the training and validation process.

L1 Regularization Adding an additional term to the cost function that is dependent on the weights forces the network to use small weights. For the L1 Regularization this term is $\frac{\lambda}{n}\sum_w |w|$ such that the new cost function becomes:

$$C = C_0 + \frac{\lambda}{n}\sum_w |w| \tag{3.21}$$

Here C_0 denotes the original cost function and λ is a hyper parameter called the regularization parameter. The effect of this regularization becomes apparent when considering its partial derivative $\frac{\partial C}{\partial w} = \frac{\lambda}{n}\text{sgn}(w)$ that is used to adjust the weights via backpropagation.
The new update rule becomes:

$$w_{t+1} = w_t - \frac{\eta\lambda}{n}\text{sgn}(w) - \eta\frac{\partial C_0}{\partial w_t} \tag{3.22}$$

Subtracting a constant amount drives the weights towards 0. This causes the network to focus on a few high importance neurons which can be an advantage but is not generally a wanted quality. The following L2 Regularization improves upon this idea.

L2 Regularization From the name and the previous L1 regularization it can be inferred that the L2 regularization adds the following term to the cost function:

$$C = C_0 + \frac{\lambda}{n}\sum_w \|w^2\| \tag{3.23}$$

Which leads to the following update rule:

$$w_{t+1} = w_t \left(1 - \frac{\eta\lambda}{n}\right) - \eta\frac{\partial C_0}{\partial w_t} \tag{3.24}$$

Where the L1 regularization shrank each weight by the same amount, the L2 regularization rescales the weights while penalising large weight terms harsher. This leads to many small weights contributing to the network performance. Reducing the size of weights is appealing because large weights can be used to learn single features like particularities of the training data.

Dropout Before discussing neural networks there was a brief mention of alternative machine learning methods. Many of which made use of an ensemble of weak classifiers to work together as a strong classifier. Dropout manages to achieve much the same in that it deactivates a portion of neurons randomly selected in each training phase. The remaining neurons form a subnetwork which is tasked with learning the same task as the full size network. Each configuration of neurons or subnetwork can be seen as a weak classifier that when dropout is deactivated for validation perform together as a strong classifier. Furthermore dropout regularizes the network by averaging over the results of the subnetworks. Therefore for a overfitting a feature it has to be learned by multiple subnetworks.

Data variation As explained overfitting happens when a model has more parameters than data points to fit. Hence procuring more training data would remedy this problem. Data variation provides a method to expand the pool of training examples without the need for new data.
It is more easily explained when thinking of images to classify. A common example is recognition of handwritten numbers. Here a training example is an image of a single digit, which can be streched, rotated or otherwise be transformed and still be recognizable as the same digit. Therefore applying a transformation to the training data allows to multiply the number of available training examples by the amount of transformations applied.
For the task at hand a data transformation can be applied and seen as measurement inaccuracy for the inputs and stochastic inaccuracy of the monte carlo data for the output.[11]
A neat side effect of data variation is that the model becomes more robust to exactly the transformations applied. Again this can be more easily understood in terms of image recognition. For example face recognition software

[11]This assumes that the functionality of the underlying model is smooth, which can be seen as given due to the network trying to learn such a smooth function anyways.

might be able to better recognize reflections if a flip transformation (mirror effect) has been applied to the training examples.

3.1.3.4 Choice of test data

To validate and test network performance in this work half as many points as for training were chosen via random input variables (between 0 and 1). Then the monte carlo simulation was run and recorded along the corresponding input.

3.1.4 Hyperparameters

3.1.4.1 Activation Functions

maybe change to subsubsubsection instead of paragraph

When designing a neural network it is important to consider which activation function to use. There are requirements of a suited activation as well as varying advantage of using one or another.
In the past a major problem of neural networks has been vanishing of gradients.[12]
To avoid vanishing gradients a better choice than the sigmoid can be found. The most common activation function for neural networks is the rectified linear unit (ReLU), shown in figure 3.2a.

$$f(x) = \begin{cases} 0 & x < 0 \\ x & x \geq 0 \end{cases} \tag{3.25}$$

The derivatives of this function is easily computed to 0 for $x < 0$ and 1 for $x \geq 0$. While an activation like the sigmoid function has two sided saturation[13]. The ReLU activation saturates only for negative values, which can be interpreted as neurons that work like switches specialising in detecting certain features . In some networks this is a wanted quality of the ReLU activation.

Write Transition

[12] As explained in section 3.1.3.1 in order to adjust the weights it is necessary to calculate the partial derivative of the cost function in respect to each weight. Backpropagation can be done without needing to apply the chain rule to calculate the partial derivatives, but using the chain rule obviously has to yield the same result, if our algorithm is working correctly.
Choosing a sigmoid $f(x) = \frac{1}{1+e^{-}x}$ as activation function leads to a derivative $f(x) = \frac{e^{-}x}{(e^{-}x+1)^2}$ with vanishing values at the fringes. For each layer between the current and the output applying the chain rule will result in a partial derivative factor with values between 0 and 1. Hence in a network with realistic depth e.g. 50, the partial derivative calculated for adjusting the weight will be almost always negligible for the beginning layers.

[13] Values at either end of the spectrum have small derivatives.

The downside of saturation, and it's vanishing gradient, whether one or two sided is that once a neuron has reached a saturating value it will change hardly or not at all from it, due to the small or even 0 gradient. This leads to a slow down or stagnation of the learning process.
To alleviate the 0 gradient of the ReLU activation one can introduce a leaky ReLU or Parametric ReLU (PReLU) function. That has a flatter linear part in the negative range:

$$f(x) = \begin{cases} \alpha x & x < 0 \\ x & x \geq 0 \end{cases} \tag{3.26}$$

If α is randomly initialized or static the function is called (Randomized) Leaky ReLU. If α is a parameter of the network and improved during training, the function is called PReLU. A typical value for a static parameter is $\alpha = 0.01$.[14]
An even better activation function is the Exponential Linear Unit (ELU), depicted in 3.2b, which offers a one sided saturation with a monotone and smooth gradient. The downside is that while it performs generally better in terms of accuracy, it is also slower in both training and predictions, since a lot of exponential functions have to be evaluated.

add citation see comment after PReLU

$$f(x) = \begin{cases} \alpha(e^x - 1) & x < 0 \\ x & x \geq 0 \end{cases} \tag{3.27}$$

add citation

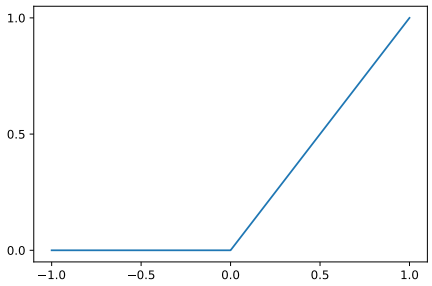
3.1.4.2 Architecture

The architecture of a network refers to its shape and type of connection. As previously done it is useful to first set down some fundamental terms:

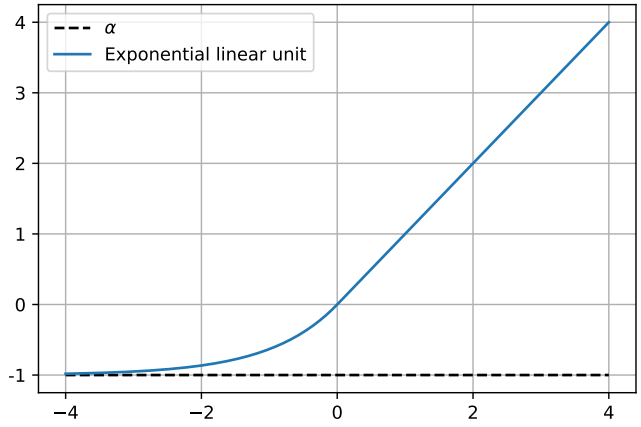
Depth The amount of layers in a network is referred to as the depth of the network. Commonly the input and output layers are omitted for this count, since they are essential for any network.

Width The width of a layer refers to the amount of neurons in that layer. Often networks are build of layers with the same width in each hidden layer. If that is the case one speaks of the width of the network.

[14] Also some works indicate that for a static parameter $\alpha = \frac{1}{5.5}$ is a better choice.



(a) Rectified Linear Unit



(b) Exponential Linear Unit

Figure 3.2: Example activation functions rectified linear unit (a) and exponential linear unit (b) used to introduce non-linearity into neural networks.

Dense layers A fully connected or dense neural network like depicted in figure 3.1 is characterized by connecting every neuron from the previous to all neurons of the following layer. In contrast to other networks this allows for a very high flexibility but also lacks the spatial context of data. This kind of network is especially well suited for data that is given in form of vectors or drawn from an arbitrary parameter space.

Feed Forward Networks Any network that propagates information only from input to output is called a feed forward network.

Recurrent networks Recurrent networks allow the use of outputs as inputs. They are typically used in speech and text recognition and processing. Recurrent networks excel in contextualizing information. For example recognizing words as part of a sentence structure.

Auto-Encoder Networks

Other types There is a wide range of different architectures, some of which can be seen in fig. 3.3. Most of which are not of further importance to this work, but at least convolutional, probabilistic and spiking networks should be mentioned. Since they excel in their respective fields.

insert reference

3.1.4.3 Cost function

The default cost function is the well known mean squared error formula 3.6, that has already been used as an example before. For the more general case of calculating the cost of multiple training examples the it has to be multiplied by $\frac{1}{n}$, where n is the number of examples.
Alternatively the cross-entropy function is used, if the output is on the scale of 0 to 1, which can be easily achieved by using a sigmoid or softmax activation function in the last layer.

$$C(x) = -\frac{1}{n}\sum_x [y \ln(a) + (1-y)\ln(1-a)] \tag{3.28}$$

Here n is the number of inputs x and corresponding labels y, a denotes the activation of the last neuron layer.
The main advantage of the cross entropy function is that its partial derivative to either weights or biases does not depend on the derivative of the activation function, but on the value of the activation function. Thus it prevents slowdown of the learning process.

https://www.asimovin

$$\frac{\partial C_{\text{quadratic}}}{\partial w} = a\sigma'(z) \tag{3.29}$$

$$frac\partial C_{\text{crossentropy}}\partial w = \frac{1}{n}\sum_x x_j(\sigma(z) - y) \tag{3.30}$$

Batch size and Epochs During training an update step can occur after each training example[15], after the whole training set has been processed[16] or a after a set amount, called batch size, of training examples has been fed to the network. Research[17] suggests that using a small batch size is optimal, but as with many other hyper parameters the exact size depends on the problem and other hyper parameters.
Smaller batch sizes lead to more noisy updates which has a regularizing effect on the network, though it increases computing time, since more updates are made.
An epoch marks the time when every training example has been shown to

[15] This is called stochastic gradient descend.
[16] This is called batch gradient descend.
[17] add citation see comment

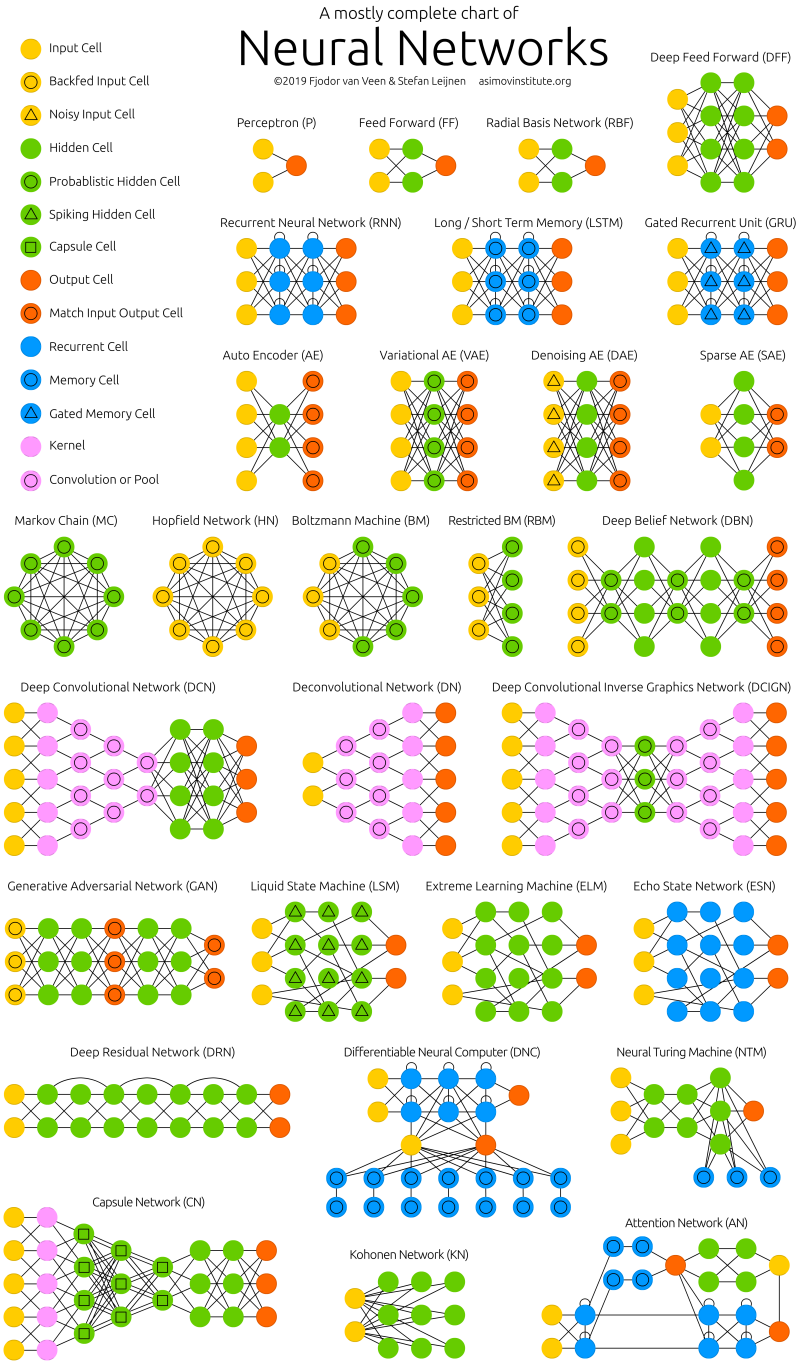


Figure 3.3: Zoo of Neural network architectures. Image taken from

the network once. At that time the next batches for training are created.[18] Epochs are a useful measure of training efficiency. Often training progress is depicted in graphs of epochs against prediction accuracy.

[18]For example with 100 data points and a batch size of 10, 10 random points are assigned to each batch. Meaning that batches over different epochs contain different training examples.

Chapter 4

Results

4.1 Physical Results

4.2 Neural Networks

4.2.1 Hyper Parameters

The following subsets of hyper parameters have been investigated: Beginning with investigating the effect of the data amount. Using same network size per

Number	Width	Depth (hidden)	Amount of Data	Activation	Droprate
1	100	10	2^17	Relu	0.25
2	X	X	2^16	X	X
3	X	X	2^15	X	X
4	X	X	2^14	X	X
5	80	X	2^17	X	X
6	X	X	2^16	X	X
7	X	X	2^15	X	X
8	X	X	2^14	X	X

4.2.1.1 Depth & Width

Depth and Width together determine the total number parameters and complexity of the network. The question is how complex does the network need to be to accurately learn the model. Ideally we'd like to trim the network as much as possible without loosing too much accuracy.

4.2.1.2 Activation

Elu, Relu, Sigmoid

4.2.1.3 Loss Function

SGD

4.2.2 Derivatives

4.3 Gaussian Processes

4.3.1 Subdivion of parameter space

4.3.2 Derivatives

4.4 Comparison

4.4.1 Accuracy

4.5 NNGP - Maybe

Appendix A

More Data probably

Appendix B

Background Neural Network

B.1 Overview of Hyper parameters

A hyper parameter refers to a parameter of the network that is not changed during training. Since these can have substantial influence on the performance of the network they will be explained in the following

Activation or Activation Function As previously discussed the activation function introduces non-linearity to the network. Some activation function will be better suited to model a certain problem than others. If information about the model or pattern to be predicted is known, an activation function close to this will have better performance. For example predicting outcome of a sine function will perform better with exponential activations or uneven polynomial activations than even polynomials.

Loss Function Choosing a loss function determines what criteria the network optimizes for which directly corresponds to which patterns it learns. For prediction one typically chooses a root mean square function. For classification cross entropy loss functions are most common.

Batch size The Dataset is divided into subsets called batches which are fed to the current network during training. After each batch the weights are adjusted. Splitting the dataset in this way is advantageous to the computational performance during training. Less memory is used during training and the number of epochs trained is reduced. The flip side of using a batch size smaller than the number of training data is that the gradient for optimization will be worse in comparison to the gradient calculated with the full data set.

Epochs An epoch describes a full training cycle of training, validating and adjusting weights for the entire training data set. If the batch size is smaller than the number of training points then multiple[1] adjustments are made.

Metrics Metrics are additional information gained from the network during training and evaluation. Metrics are not hyperparameters since they do not influence the resulting network but are an important source of information for further improving the network structure. For example a secondary loss function can be implemented as a metric to evaluate general optimization of the network in contrast to only the chosen loss quantity.

cite https://www.analyticsvidhya.com/blog/2018/04/fundamentals-deep-learning-regularization-techniques/

Regularization Regularization describes methods used to reduce the generalization error but not the training error. Commonly used regularization methods include L1, L2, Dropout and Early Stopping regularization. L1 and L2 regularization is applied by adding a penalty term to the loss function. This requires initial knowledge of input influences. For example an image with bad resolution might have a larger penalty term applied than an image with high resolution. Dropout regularization and early stopping are used to prevent overfitting. Since the amount of parameters in the network is often on the same order of magnitude as the amount of training data, neural networks are prone to overfitting. Early stopping interrupts the training process as soon as the validation loss stops improving by a user set minimum delta.

B.2 Introduction to Neural Networks

Glossary:

- Network: A series of layers. The first layer of a network is called the input layer, the last layer is called the output layer. Any layers in between are called hidden layers. The amount of hidden layers is called the **depth** of the network.

- Layer: A collection of neurons. The amount of neurons in a layer is called the **width** of a layer.

- Neuron: A single node in a layer. It contains a single number formed by a weighted sum of it's inputs evaluated by the activation function.

[1] Number of batches in one epoch = rounded up $\left(\frac{Amount of Training Data}{Batch Size}\right)$

- Activation function: A non-function applied to the weighted sum of a neuron. Used to introduce non linearity into the network in order to enable non linear model "fitting".
- Weight: Each connection between layers has it's own weight factor. These are adjusted during training to fit the data. Weights are often referred to as parameters.
- Regularization: Methods used to suppress overfitting.
- Metric: Additional information gathered during training/testing.
- Loss function: Function that dictates the optimization, e.g. Root Mean Squared.
- Training Data: Set of Data used during training phase. Weights are adjusted to these data.
- Validation Data: Set of Data used during training phase to evaluate training results intermediary.
- Test Data: Data set not seen during training to evaluate trained network performance.
- Input: Data fed to the network for training or evaluation.
- Output: Prediction of the network.
- Label: True output value for input data.
- Hyperparameter: A parameter not changed during training e.g. width and depth of the network.

B.3 Examples of neural networks in different contexts

Appendix C

Background Gaussian Processes

C.1 Baysian Statistics

Bibliography

[1] Maureen Caudill. Neural networks primer, part i. *AI Expert*, 2(12):46–52, December 1987.