# Extremal learning: extremizing the output of a neural network in regression problems

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ABSTRACT: Neural networks allow us to model complex relationships between variables. We show how to efficiently find extrema of a trained neural network in regression problems. Finding the extremizing input of an approximated model is formulated as the training of an additional neural network with a loss function that minimizes when the extremizing input is achieved. We further show how to incorporate additional constraints on the input vector such as limiting the extrapolation of the extremizing input vector from the original training data set. An instructional example of this approach using TensorFlow is included.

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# 1 Introduction

Neural networks (NNs) [1] allow us to model complex relationships between certain input  $(x_n)$  and output data sets  $(y_n)$  when the underlying functional dependence is unknown. Advances in hardware, the advent of big data, and computational methods e.g. [2–8] have made it possible to apply (deep) NNs to a plethora of regression problems [9]. While it is extremely useful to obtain a prediction function  $y = f(\theta; x)$  with parameters  $\theta$  in the first place, one is often interested in properties such as minima or maxima of this function f.

For example, take radiotherapy cancer treatment. In a first step, one would like to find out how the output y, the tumor size, depends on the input x, the kinds and dosages of certain radiotherapies. Once the NN is trained via fitting the parameter values  $\theta$  and can predict the outcome of a certain treatment to the desired accuracy, one would like to know: what is the ideal treatment for the patient's cancer? In this case, we want to find the input vector  $x_{\min}$  that minimizes the tumor size. Were f a simple analytic function, one would simply proceed by finding extrema via solving for zeros of the derivative function w.r.t. x. However, due to the NN's complicated nonlinear functional structure, generally high dimensionality and potential recursive input dependencies [10] this easily becomes a highly complicated system of equations that is extremely difficult to solve. The strength of NNs also becomes a weakness in a sense: while NNs can reveal the elusive black box functions presented by certain processes, it can only do so in a complicated web of weights and biases that make an analytical analysis of the NN challenging.

In this paper, we present an alternative solution to this problem via a process that we term *extremal learning*: Finding the extremizing input  $\hat{x}$  is formulated as the training of

<sup>&</sup>lt;sup>1</sup>For a simple example, consider a single layered neural network with activation  $a(z) = \tanh(z)$ . Then the derivative of  $a(x) = \tanh(W \cdot x + b)$  with weights W and biases b allows us to find the optimal vector  $x_{\text{ext}}$  for the network.

an NN itself. The parameters  $\theta$  of the NN are frozen while the input vector x is promoted to a trainable variable itself. A loss function  $\mathcal{L}$  is defined such that its minimization, e.g. via gradient descent [3, 11], is equivalent to achieving an extremal value for f. Hence, custom machine learning frameworks such as TensorFlow [12] can be used to calculate extrema of NNs via this method of extremal learning. For an implementation of extremal learning in TensorFlow, we provide example code at: https://github.com/ZakariaPZ/Extremal-Learning.

The loss function  $\mathcal{L}$  may also include further constraints on the problem at hand. A common constraint in regression problems is that  $\hat{x}$  should not stray too far from the input data set  $(x_n)$ . Respecting this constraint avoids extrapolating into a no-data regime where the predictions of the NN are becoming unreliable. This can be achieved by limiting the extrapolation of the input vector to within some set number of standard deviations. For instance, consider fitting a car's fuel expenditure as a function of its speed v using data from low speeds. The data reflects a situation in which the rolling resistance force  $F_r$  that does not depend on speed is dominating the fuel expenditure. For higher speeds, the force dominating the fuel expenditure is the drag force  $F_d \propto v^2$ . Clearly, extrapolating to higher speeds with a model trained on low speed data will yield far too low a fuel expenditure. In a similar spirit, we risk making misleading predictions if we look for extremizing inputs far from the data set the model was trained on. Our initial data may not confidently reflect the behaviour of our system at points lying far from our observations. We will demonstrate how to include these or other constraints into extremal learning via the definition of custom loss functions as also discussed in [13, 14].

#### Relationship to GANs

Extremal learning has some similarities with Generative Adversarial Networks (GANs) [15–17]. In a typical example of extremal learning, we have a trained model for image classification and now want to find an image that maximizes the output for a given class. A GAN operates with a similar goal, yet executes it differently. Given a random noise input z, the generator in a GAN is trained to minimize the loss

$$\mathcal{L} = \log\left\{1 - D\left[G(z)\right]\right\}\,,\tag{1.1}$$

where G(z) is the output of a generator network and D is a discriminator network. The goal of the discriminator is to identify which inputs are real and which inputs are counterfeits of the generator, while the generator attempts to fool the discriminator into classifying its output as a true input. By minimizing the above loss, the generator should learn a generative model capable of transforming a random noise sample into an output G(z) which closely resembles the nature of a true instance y. Then, if we passed G(z) into a discriminator network, it should classify the input similarly to that of the true instance y. Succinctly, a GAN works to minimize the dissimilarity between an artificially produced data distribution and a true distribution. For extremal learning, instead of a generator-discriminator pair, we consider a lone discriminator whose loss function we try to minimize. An important distinction here is that extremal learning directly changes the input vector x,

rather than using other optimization methods such as Markov Chains to create a generative model.

#### Relationship to adversarial training

We can also draw parallels to adversarial training [15, 18, 19]. In image classification, adversarial attacks involve injecting an adversarial vector  $x_{\text{adv}}$  into the input vector x, where  $x_{\text{adv}}$  acts as a perturbation, imperceptible to the human eye yet causing misclassification in a machine learning model. Adversarial training aims to achieve the generation of such noise vectors  $x_{\text{adv}}$ , known as adversarial examples. This involves training an input vector x. One technique to generate adversarial examples is the fast method [20].

This method aims to maximize a linearized loss function  $\mathcal{L}$  that is approximated to first order as

$$\mathcal{L}(\tilde{x};\theta) \approx \mathcal{L}(x;\theta) + (\tilde{x} - x)^T \nabla_x \mathcal{L}(x;\theta), \qquad (1.2)$$

where  $\tilde{x}$  is the perturbed vector, i.e. the adversarial example in training. The above loss is maximized subject to the following max-norm constraint on  $\tilde{x}$  [21]:

$$||\tilde{x} - x||_{\infty} \le \epsilon \,, \tag{1.3}$$

i.e. each pixel can only be changed by a value  $\epsilon$ . The adversarial example is then generated by training the input as

$$\tilde{x} = x + \epsilon \operatorname{sign}[\nabla_x \mathcal{L}(x; \theta)].$$
 (1.4)

The extremal learning technique introduced in this paper also seeks to train inputs, but instead hopes to minimize a nonlinearized loss function via backpropagation. The input perturbations are not limited by a max-norm constraint, but the learning rate of the backpropagation.

#### A road map

This paper is structured as follows: in Section 2, we describe the general formalism of extremal learning for regression problems. In Section 3, we present a toy example of this approach by finding a maximizing input vector using an implementation of extremal learning in TensorFlow. We conclude in Section 4.

#### 2 Finding extrema

We first recap supervised learning in regression problems: given a set of labeled observations  $(x_n)$  and  $(y_n)$  with an NN function  $f(\theta;x)$  with parameters  $\theta$ , for supervised learning, the goal is to find the best-fit parameters

$$\hat{\theta} = \arg\min_{\theta} \left\{ \sum_{n} \mathcal{L}_{t} \left[ f(\theta; x_{n}), y_{n} \right] \right\}. \tag{2.1}$$

Here,  $\mathcal{L}_t(y', y)$  is the training loss function that measures the distance between the predicted output  $y' = f(\hat{\theta}; x)$  is from the true output y. Common choices in regression problems include mean squared error (MSE), mean squared logarithmic error or mean absolute error [9].

Once a model has been trained, i.e. once we have a set of parameters  $\hat{\theta}$ , predictions can be made. Given an input vector x, evaluating the function  $f(\hat{\theta}; x)$  is called inference - the rules dictating how  $f(\hat{\theta}; x)$  behaves are now approximately encoded within the NN's parameters.

### 2.1 Extremal learning

In this paper, we want to find an extremizing input  $\hat{x}$  because we are interested in maximizing or minimizing the output of f that can represent a quantity that we would like to optimize as for instance a return of investment, effectiveness of a treatment, amount spent etc. We formulate this extremization as yet another optimization problem: given a trained model  $f(\hat{\theta}; x)$ , we want to find the input(s)  $\hat{x}$  that maximize the output of the model, i.e.

$$\hat{x} = \begin{cases} \arg\max_{x} f(\hat{\theta}; x) & \text{for maximization,} \\ \arg\min_{x} f(\hat{\theta}; x) & \text{for minimization.} \end{cases}$$
 (2.2)

We call this task extremal training, because we are looking for an input vector that is extremizing the output. We can implement this optimization as fitting f via the following steps:

- Freeze the parameters  $\theta$  of the model to the value  $\hat{\theta}$  from the first training iteration, i.e. make them not trainable anymore.
- Promote the input vector x to a trainable variable. From the fitting procedure point of view, there is no input data anymore as  $\theta = \hat{\theta}$  is fixed and x is now effectively a parameter. We now have a different NN, albeit with the same architecture as the original NN.
- Define a loss function  $\hat{\mathcal{L}}$  such that its minimization is equivalent to the optimization problem at hand, i.e. finding the extremizing input  $\hat{x}$ . Reasonable, MSE inspired, loss functions are

$$\hat{\mathcal{L}} = \begin{cases} \left[ f(\hat{\theta}; x)^2 + \kappa \right]^{-1} & \text{for maximization,} \\ f(\hat{\theta}; x)^2 & \text{for minimization,} \end{cases}$$
 (2.3)

with constant  $\kappa > 0$  to avoid the zero divergence.

• Minimize the loss  $\hat{\mathcal{L}}$  via common fitting procedures, such as gradient descent and backpropagation [3, 11]. The gradient descent rule is applied to update the input vector x using the partial derivatives of the loss with respect to the input x [22].

$$x \to x - \alpha \nabla_x \hat{\mathcal{L}}$$
, (2.4)

where  $\alpha$  is the learning rate. One has to provide an initial vector  $x_{\text{init}}$  to start the gradient descent. This may be chosen at random or from the training data and may be chosen with caution in case of non-convexity [8].

#### 2.2 Constraints via additional loss functions

We may also introduce a variety of k additional loss functions  $\mathcal{L}_i$  to penalize undesirable inputs x or outputs y

$$\mathcal{L} = \hat{\mathcal{L}} + \sum_{i=1}^{k} \mathcal{L}_i. \tag{2.5}$$

In practice, one may introduce as many  $\mathcal{L}_i$  as desired to constrain the search for  $\hat{x}$  to a space that is desirable for the problem at hand for both the inputs and outputs.

A common constraint is that the global or local extrema of f may not be the most feasible solution to the optimization problem. Optimizing an input demands that we appreciate that there exists some boundary beyond which the input may become unrealistic. This is the extrapolation problem: we do not want to extrapolate too far from the original data set  $(x_n)$  as the predictions  $f(\hat{\theta}; x)$  may become arbitrarily unrealistic. Using extremal learning in conjunction with custom loss functions  $\mathcal{L}_i$  facilitates convergence towards an optimum within an error and constraint window that is often more useful in real-life applications than global or local extrema of the function f.

One way to define a loss function that penalizes extrapolation is as follows: if x deviates more than c-times the standard deviation  $\sigma$  of the data set  $(x_n)$  from the mean of the data set, those input vectors are penalized:

$$\mathcal{L}_{1} = \kappa_{1} \sum_{i=0}^{m} \begin{cases} (x_{i} - \mu_{i} + c\sigma_{i})^{2} & x_{i} < \mu_{i} - c\sigma_{i}, \\ 0 & \mu_{i} - c\sigma_{i} \leq x_{i} \leq \mu_{i} + c\sigma_{i}, \\ (x_{i} - \mu_{i} - c\sigma_{i})^{2} & x_{i} > \mu_{i} + c\sigma_{i}, \end{cases}$$
(2.6)

where  $x_i$  are the individual components of the m-dimensional input vector x and  $\kappa_1$  is a normalization constant. To avoid problems during gradient descent, one may choose continuous functions for the additional loss functions  $\mathcal{L}_i$  and ensure their relative weighting through normalization constants  $\kappa_i$  is inline with how strict the different constraints should be enforced relative to each other [13, 14].

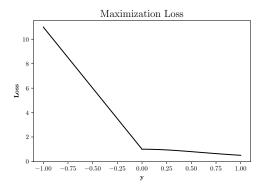
One may also combine additional constraints with the extremal loss function  $\hat{\mathcal{L}}$ . For instance, let us consider a situation in which negative outputs are ill defined as is the case for example if y represents a temperature that we want to maximize. In this case, we can define the loss function as

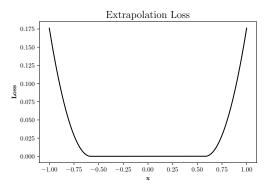
$$\mathcal{L}_{2} = \begin{cases} -\kappa_{2}y + \hat{\kappa} & y < 0, \\ (y^{2} + \hat{\kappa}^{-1})^{-1} & y \ge 0, \end{cases}$$
 (2.7)

where the first term ensures that the output is indeed positive. To give this physical constraint priority over maximization we would choose  $\kappa_2 \gg \hat{\kappa}$ . For a visualization of the maximization and extrapolation loss, see Figure 1.

If (some of) the components of the input vector are required to be positive this can be enforced via a loss function similar to (2.7):

$$\mathcal{L}_3 = \kappa_3 \sum_{i=0}^m \begin{cases} -x_i & x_i < 0, \\ 0 & x_i \ge 0, \end{cases}$$
 (2.8)





**Figure 1.** (a) Plot of maximization loss defined in (2.7) with  $\kappa_2 = 10$  and  $\hat{\kappa} = 1$ . (b) Plot of extrapolation loss defined in (2.6) with  $\kappa_1 = 1$ .

# 3 Example and case study

We now consider a simple toy example to demonstrate extremal learning. We first generate fake data that is used to fit a feed forward NN. After fitting, we apply the extremal learning approach described above to find a maximizing input. We provide the source code to this example using TensorFlow at: https://github.com/ZakariaPZ/Extremal-Learning.

Consider a simple problem in which  $x \in \mathbb{R}^4$  represents a specific intake of food classes to be optimized with respect to some arbitrary measure of "goodness of health" y. The classes are as follows:

•  $x_0$ : carbohydrate intake

•  $x_1$ : protein intake

•  $x_2$ : cake intake

•  $x_3$ : candy intake

All inputs are chosen to be in the range  $x_i \in [-1, 1]$ . We want to know how health depends on the different intakes and, in the next step, determine which intake composition is the most optimal for health.

### 3.1 Data generation

To generate a data set, we come up with a function that measures "goodness of health" as a function of the four different inputs in arbitrary units:

$$g_{\text{true}}(x) = 1 - |x_0| - x_1^2 - x_2 - e^{x_3} + \epsilon.$$
 (3.1)

In moderation,  $x_0$  and  $x_1$ , representing protein and carbs respectively, are good to intake, but as with anything, excess is deleterious to our health.  $x_2$  and  $x_3$  contribute negatively - the more intake of these foods, the worse your health becomes. The  $\epsilon$  term contributes Gaussian noise with mean  $\mu = 0$  and standard deviation  $\sigma = 0.05$ . Note that the function has no biological foundation - it is purely for data generation in this toy example.

The data set  $(x_n)$  and  $(y_n)$  with  $y_n = g_{\text{true}}(x_n)$  is created by sampling (3.1) over n = 1000 inputs sampled from a uniform distribution where  $-1 \le x_{n,i} \le 1$ . We plot the data set as health vs the various inputs in each dimension in Figure 2.

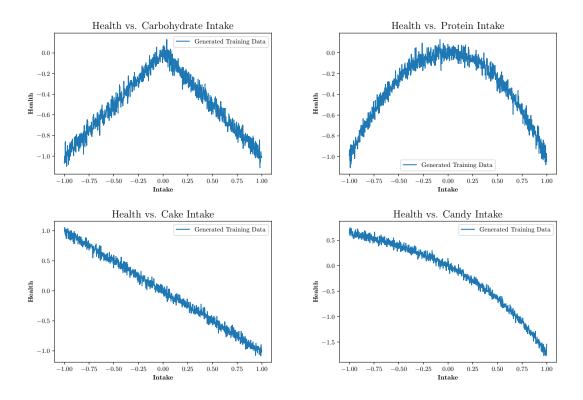


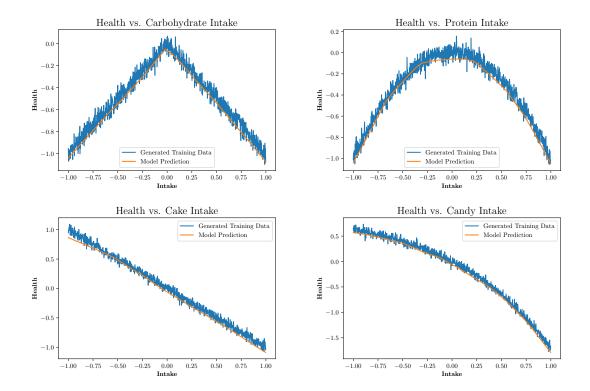
Figure 2. Each input  $x_i$  is plotted against the output health y. We want to maximize the output with respect to some constraints. Accordingly, we see that both  $x_0$  and  $x_1$  maximize y at  $x_0 = x_1 = 0$ , while  $x_2$  and  $x_3$  formally maximize  $g_{\text{true}}$  at  $x_2 = x_3 = -\infty$  (though of course, our extrapolation constraint impose limits on the domain within which we will search for a solution).

# 3.2 Finding a maximizing input

Ideally, we would like the network to learn the underlying functional dependence (3.1). To this extend, we define a feed forward NN  $f(\theta; x)$  that is trained via gradient descent on the data  $(x_n)$ ,  $(y_n)$ . Subsequently, we have a set of parameters  $\hat{\theta}$  containing the weights and biases of the NN which are conducive to a good approximation of  $g_{\text{true}}$ . We show the fitted NN in Figure 3.

Following 2.1, we can now apply extremal learning. First we freeze the parameters  $\theta$  to  $\hat{\theta}$ , i.e. they are not trainable parameters anymore. Secondly, we promote the input x to trainable parameters. We now have a second NN that has identical architecture to the original NN with the only difference being what is considered a parameter and what is considered an input. The extremal learning NN has no input, just trainable parameters x that were the input of the previous NN.

When training the extremal learning NN, one has to provide a starting value  $x_{\text{init}}$ . We randomly initialize the gradient descent with an input vector  $x_{\text{init}}$  from a normal distribution



**Figure 3.** The trained NN is superimposed onto the training data for each intake  $x_i$ . The NN describes the underlying functional dependence  $g_{\text{true}}$  of the data to sufficient accuracy.

such that  $x_{\text{init},i} \in [-1,1]$ .

Next, we set constraints using additional loss functions defined in Section 2.2 tailored to this specific problem. We use the extrapolation loss function (2.6) and penalize in the search for the optimal input if it is more than two standard deviations away from the mean. For the maximizing loss we use (2.7) with  $\kappa_2 = 10$  and  $\hat{\kappa} = 1$ . Hence, the total loss is

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 \,, \tag{3.2}$$

with

$$\mathcal{L}_{1} = \frac{1}{2} \sum_{i=0}^{3} \begin{cases} (x_{i} - \mu_{i} + 2\sigma_{i})^{2} & x_{i} < \mu_{i} - 2\sigma_{i}, \\ 0 & \mu_{i} - 2\sigma_{i} \leq x_{i} \leq \mu_{i} + 2\sigma_{i}, \\ (x_{i} - \mu_{i} - 2\sigma_{i})^{2} & x_{i} > \mu_{i} + 2\sigma_{i}, \end{cases}$$
(3.3)

and

$$\mathcal{L}_2 = \begin{cases} -10 \, y + 1 & y < 0 \,, \\ \left( y^2 + 1 \right)^{-1} & y \ge 0 \,, \end{cases} \tag{3.4}$$

The mean and standard deviation of the data set generated in Section 3.1 numerically evaluate to  $^{2}\,$ 

In the limit  $n \to \infty$ , we expect  $\mu = [0,0,0,0]$  as the data is sampled from a uniform distribution with mean zero. However, we see some noise remnants due to finite n = 1000. The standard deviation of a uniform distribution sampled over the interval  $a \le x \le b$  is approximately  $\sigma = \frac{(b-a)}{\sqrt{12}}[1,1,1,1]$ , which evaluates to  $\sigma \simeq [0.577, 0.577, 0.577, 0.577, 0.577]$  in this case.

$$\mu \simeq [0.007, -0.028, 0.005, 0.006],$$

$$\sigma \simeq [0.555, 0.577, 0.577, 0.567].$$
(3.5)

From here, we perform gradient descent to train the extremal learning NN via subsequently applying (2.4) until we converge on a maximizing input  $\hat{x}$ . We expect that the extremal NN's output should approach a maximum which is not the analytical maximum since we are using a numerical technique with additional constraints arising from the loss functions. However, considering the form of  $g_{\text{true}}$ , there is no true maximum as decreasing  $x_1$  and  $x_2$  towards  $-\infty$  will continuously increase the value of  $g_{\text{true}}(x)$ . We should instead see that the new output of the input-optimized model converges towards a value limited by the extrapolation loss. Indeed, we numerically find the maximizing input to be

$$\hat{x} \simeq [-0.167, -0.0861, -1.193, -1.153],$$
 (3.6)

which is reasonably close to the true optimal value under the limits of the extrapolation loss we have chosen:

$$\hat{x}_{\text{true}} = [0, 0, -2\sigma_2, -2\sigma_3] \simeq [0, 0, -1.154, -1.134].$$
 (3.7)

Similarly, the optimal output value calculated via extremal learning  $\hat{y} \simeq 1.702$  is reasonably close to the true optimal value of the underlying function in this optimization problem  $\hat{y}_{\text{true}} = 1 + 2\sigma_2 - e^{-2\sigma_3} \simeq 1.832$ 

#### 4 Conclusions

In this paper, we have introduced extremal learning which allows to calculate extremizing inputs of a trained NN in regression problems. This is a pressing issue in many applications of modern machine learning, where one is not just interested in inference, i.e. making predictions from a trained NN, but also finding the input vector that extremizes a certain output. Examples are finding the optimal cancer treatment after an NN has been trained that represents how the patient's tumor size responds to different cancer treatments, or the toy example discussed in Section 3: what is the healthiest diet for an individual based on an NN that evaluates health as a function of the intake of various food classes. There are many other real-world examples where solving extremization questions of this kind are very valuable. Analytically solving for extrema is generally not a feasible option as one is dealing with a coupled system of nonlinear equations of high dimensionality, with potentially recursive structure [10], due to the generally complicated underlying functional dependence defining NNs.

Extremal learning relies on the same NN infrastructure created to train the NN network in the first place to perform the optimization task of extremization. This way we can take advantage of how machine learning overcomes the curse of dimensionality which also plagues the task of extremization. The basic components of extremal learning are freezing the parameters such as weights and biases of the original NN and promoting the input vector

x to a trainable variable. Via choosing an appropriate loss function, common machine learning optimization techniques such as gradient descent and backpropagation [3, 11] can then be used to compute the extremizing input. Common machine learning frameworks such as TensorFlow have sufficient flexibility to perform this task with minimal configuration effort, see https://github.com/ZakariaPZ/Extremal-Learning. While there are certain parallels with GANs [15–17] and adversarial training [15, 18, 19], extremal learning presents an efficient way to find extrema of NNs in regression problems.

We also demonstrate how to incorporate further constraints on the input and/or output vector via additional loss functions, see Section 2.2. A common feature of many extremization tasks is to constrain the input vector not to measure too far a distance from the data set the NN was originally trained on. The distance from the original data set can be penalized via such an additional loss function and, in practice, prevent the NN to look for an extremizing input where the predictions may become unrealistic. We further demonstrate that it is straightforward to further constrain the input or output to one's liking via additional loss functions.

In the future, we would like to study the numerical performance of extremal learning in a variety of regression examples. An interesting question remains what extremal learning can add in the context of convolutional neural networks, in particular if it can be combined with GANs and/or adversarial training to solve input optimization problems.

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