

Spline Optimization of Soft Connectives in Machine Learning Models

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Abstract

In this study, the problem of limited accuracy of machine learning models using soft logical connectives is investigated. Such connectives have shown their effectiveness in models with fuzzy initial data. On the one hand, the fundamental disadvantage of soft connectives is their non-associativity. On the other hand, the disadvantages of the currently used soft connectives include the loss of monotonicity and the inability to control several factors simultaneously. We minimized the difference between the connective and the associative connective, the latter in our study was the minimum function. In the resulting solution, the rate of deviation reduction is the highest among known connectives. We have achieved not only a small deviation from associativity, but also the presence of a large domain of exact associativity. This area is up to a third of the volume of all triples of arguments. A comparative analysis of the currently used soft connectives with the constructed model was carried out. It was shown that the spline approximation is able to reduce the influence of all negative factors and is more flexible in setting. Moreover, the constructed spline model allows numerous modifications depending on the factor that requires the most attention for different tasks

Keywords: fuzzy sets; spline; soft connective; soft signum.

1 Introduction

In 1970, Bellman and Zadeh [1] suggested using fuzzy set theory to solve multicriteria choice problems. Criteria reduction is considered as an operation with fuzzy sets using analogues of set-theoretic operations on them. The decision maker chooses an operation on fuzzy sets after evaluating his potential actions. In that work, Bellman and Zadeh use the minimum and maximum functions as the AND and OR connectives corresponding to the intersection and union of goals. These connectives later became known as rigid. However, experiments have shown that this preset does not always reflect the behavior of the decision maker [2]. This circumstance gave impetus to the search for alternative connectives. The use of the latter has fully justified itself, for example, when describing complex linguistic categories [3]. It was shown that logical connectives with a compensation effect are more effective from the point of view of control. Such connectives are the average values between the maximum and minimum and are called soft connectives.

Summing up the study of averaging operations, Zimmerman lists the most studied generalized averages in terms of applications [4]: arithmetic and geometric means [5], symmetric sum and difference [6], “fuzzy and” and “fuzzy or” [7], compensatory AND and OR, convex combinations of maximum and minimum, of products and sums [8], OWA-operators [9].

Bobyry [10] justified the use of soft connectives in machine learning models and presented the results of computer experiments. The use of a rigid minimum in traditional fuzzy inference algorithms does not allow obtaining

satisfactory indicators of model accuracy. As it was shown in [11], dead zones of the ML model are formed. In that work a method of teaching MISO-fuzzy (Multiple Input Single Output) systems was reviewed and the results of numerical modeling were shown. As test functions, authors used a table of observations consisting of randomly obtained points in the range of values corresponding to the distribution of the output membership function (fig. 1, a). From the presented plot (fig. 1, b) it can be seen that for model using rigid arithmetic operations, there are dead zones in which the response of the resulting variable does not occur. Thus, for the range $x_1 \in [0, 20]$ and $[90, 100]$, and the variable $x_2 \in [280, 300]$, the response of the resulting value is not observed. Moreover, the RMSE coefficient for the rigid MISO system was $RMSE_{rigid} = 1.4945$, and for the soft MISO system $RMSE_{soft} = 0.01232$.

The main reason is that the minimum has a specific nature of the value dependence on the argument. Let us consider function $\min(x, y_0)$ with a fixed second argument. When the diagonal point $x = y_0$ is crossed, the uniform increase in values is abruptly replaced by a loss of dependence.

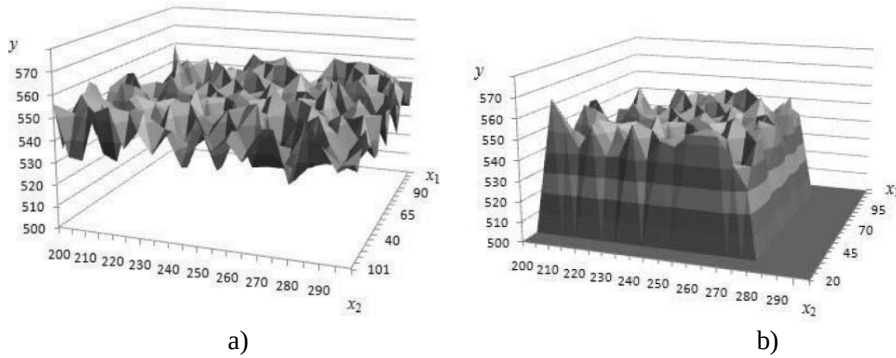


Figure 1. a) Graphical representation of points in the observation table, b) Training a neuro-fuzzy network using rigid arithmetic operations. (Source: [11])

There are two standard tricks to solve this problem. The first one is to decrease the angle between the tangents at the diagonal point (for the minimum function, this angle is 45°). The second one is the smoothing of the function. However, there are two other circumstances that negatively affect the quality of the model using soft connectives: possible violation of monotonicity in arguments and non-associativity. The latter is inevitable, since all smooth averages are non-associative [12]. So, the main problem of soft computing is that there are no monotonic, smooth, and associative soft connectives. The classical approach to solving this problem is to use a one-parameter family of soft connectives approximating the minimum. The optimal parameter for the accuracy of the ML model is selected experimentally.

The general disadvantage of the used approximations is the impossibility of achieving an independent influence on the behavior of soft connective near the diagonal point and on the measure of non-associativity. We suggest using a spline to smooth the minimum with the smallest possible deviation from associativity.

2 Materials and methods

A good overview of the axiomatic foundations of fuzzy set theory can be found in [13]. Let us give some basic definitions.

Definition 1 [14]. If Ω is a collection of objects denoted generically by x , then a fuzzy set $\tilde{A}$ is a set of ordered pairs:

$$\tilde{A} = \{(x, \mu_{\tilde{A}}(x)) | x \in \Omega, \mu_{\tilde{A}}(x) \in [0, 1]\},$$

where $\mu_{\tilde{A}}(x)$ is called the membership function.

The values of the membership function are interpreted as a subjective degree of confidence that the element x belongs to the fuzzy set $\tilde{A}$. The set of all fuzzy subsets of the universal space Ω is identified with the function space $[0, 1]^\Omega$.

Definition 2. A connective H is a continuous monotone commutative function

$$H: [0,1] \times [0,1] \rightarrow [0,1].$$

Using a connective H one can define *H -operation of two fuzzy sets by defining their membership function.

Definition 3. The membership function of the *H -operation of two fuzzy sets $\tilde{A}$ and $\tilde{B}$ is defined as:

$$\mu_{\tilde{A} {}^*H \tilde{B}}(x) = H(\mu_{\tilde{A}}(x), \mu_{\tilde{B}}(x)).$$

If we add the requirement of additivity [15]

$$H(x + \delta, y + \delta) = H(x, y) + f(\delta),$$

for all δ for which the left and right parts of the relation make sense, then we obtain a class of functions of the form

$$H(x, y) = \min(x, y) + f(|x - y|),$$

where $f: [0,1] \rightarrow [0,1]$, $0 \leq f(\alpha) \leq \alpha$, $f(0) = 0$, $f(x) = H(x, 0)$. All these functions are generalized averages [16]:

$$\min(x, y) \leq H(x, y) \leq \max(x, y).$$

It seems natural that if the degrees of our confidence in some two statements have increased by the same amount, then our confidence in the logical connectives AND and OR of these statements will also increase. This leads to averages, which have an unintuitive non-associativity. All the illogicality of this statement lies in the independence of the increment $f(\delta)$ from the values x and y of the membership function. This class of soft connectives is much narrower than generalized averages. However, they have performed well in ML models [11].

Any additive connective can be obtained by generalizing the function $\text{sgn}(x)$. The minimum can be written in the form

$$\min(x, y) = \frac{x + y - (x - y)\text{sgn}(x - y)}{2}.$$

Definition 4. A soft signum is a family of functions $\varphi_\delta(z)$ converging pointwise to the function $\text{sgn}(z)$ as $\delta \rightarrow 0$ on the interval $[-1, 1]$.

Definition 5. A soft minimum is a function of the form

$$\min_\delta(x, y) = \frac{x + y - (x - y)\varphi_\delta(x - y)}{2}.$$

When choosing the optimal parameter δ , two trends collide. On the one hand, softening eliminates a sharp change in the growth rate of values, but on the other hand, a soft minimum is increasingly different from an associative operation. The latter becomes a negative factor for the learning process. Almost all triplets (x_1, x_2, x_3) in the cube $[0, 1]^3$ are not associative:

$$\tilde{\Delta}(x_1, x_2, x_3) = \min_\delta(\min_\delta(x_1, x_2), x_3) - \min_\delta(x_1, \min_\delta(x_2, x_3)) \neq 0. \quad (1)$$

The smaller the angle between the left and the right tangents at the diagonal point of soft minimum with fixed second argument, the greater the difference. The optimal parameter δ is the compromise between two tendencies. We can use different measures of non-associativity, for example

$$\iiint_{[0,1]^3} |\tilde{\Delta}(x_1, x_2, x_3)| dx_1 dx_2 dx_3 \sim \min, \quad (2)$$

where the integral is calculated over the $[0,1]^3$. However, we implement a simpler approach by comparing the plots of signums in the integral 1-metric:

$$\Delta(\varphi_\delta) = \int_{-1}^1 |\operatorname{sgn}(z) - \varphi_\delta(z)| dz. \quad (3)$$

Let us list several connectives of this type used in various applications.

1) The convex combinations of the minimum and the arithmetic mean [4]. A family of soft minima, $\delta \in [0,1]$, is used in linear programming, mixed-integer linear programming, and natural language processing models where they are most computationally efficient. Here

$$\varphi_\delta(z) = (1 - \delta) \cdot \operatorname{sgn}(z).$$

For practical applications, it is recommended to select a parameter in the range $0,1 \leq \delta \leq 0,4$, starting with 0,25. For the specified parameter value, the angle between the left and the right tangents at the diagonal point of soft minimum with fixed second argument is within $(27^\circ; 41^\circ)$. Finally,

$$\Delta(\varphi_\delta) = 2\delta.$$

2) Soft minimum of the first type [17]

$$\operatorname{sgn}_\delta^I(z) = 2 \frac{\sqrt{z^2 + \delta^2} - \delta}{z}.$$

Using this soft sign smooths the function $\min_\delta$ for any value of the parameter, $\operatorname{sgn}_\delta^I(0) = \frac{1}{2\delta}$. However, the closer to the signum, the greater the curvature k of the plot of $\min_\delta(x, y_0)$ at the diagonal point $x = y_0$:

$$k = \frac{|(\min_\delta(x, y_0))'_x|}{\sqrt{1 + (\min_\delta(x, y_0))'_x}} \Big|_{x=y_0} = \frac{2}{\sqrt{5}} |\operatorname{sgn}_\delta^I(0)| = \frac{1}{\delta\sqrt{5}}.$$

Almost all triplets are non-associative. The closer to the associative signum, the greater the curvature. The compromise between these two tendencies is $\delta \approx 0,05$. The measure of deviation (3) from the signum is equal to

$$\Delta(\operatorname{sgn}_\delta^I) = 2 \left(\delta + 1 - \sqrt{1 + \delta^2} + \delta \ln \left(\frac{\sqrt{1 + \delta^2} + \delta}{2\delta} \right) \right).$$

3) Soft minimum of the second type [18]

$$\operatorname{sgn}_\delta^{II}(z) = \frac{z}{\sqrt{z^2 + \delta^2}}$$

For this soft signum holds $(\operatorname{sgn}_\delta^{II})'(0) = \frac{1}{\delta}$, $\Delta(\operatorname{sgn}_\delta^{II}) = 2(\delta + 1 - \sqrt{1 + \delta^2})$.

Here the analysis of the previous point can be applied. However, the authors did not notice the fact that the use of this soft signum leads to a function that is not monotonic in its arguments, it has an extremum at $|x - y| \approx \delta/3$. A smooth soft minimum is monotonic in its arguments if holds:

$$sgn_{\delta}(z) + z \cdot sgn'_{\delta}(z) \leq 1.$$

Anyway, good accuracy of the models was achieved with $\delta \approx 0,1$.

4) The additive average operator [19]

$$softMIN(x, y) = \frac{xe^{-kx} + ye^{-ky}}{e^{-kx} + e^{-ky}}.$$

For this operator, the practical accuracy of the models is achieved for $\delta \approx 0,01$. Here

$$sgn_{\delta}(z) = \frac{1 - e^{-\frac{1}{\delta}z}}{1 + e^{-\frac{1}{\delta}z}}, \quad sgn'_{\delta}(0) = \frac{1}{2\delta}.$$

Again, the soft minimum is not monotonic here. It has an extremum at $|x - y| \approx 2/k$. The deviation (3) is equal to

$$\Delta(sgn_{\delta}) = 4\delta \ln \left(\frac{2}{1 + e^{-\frac{1}{\delta}}} \right).$$

For the smooth soft minima listed above, a common feature is observed. The accuracy of all methods is limited by objective reasons. In an attempt to get closer to the signum, reducing the non-associativity, one has to increase the curvature of the plot of $\min_{\delta}(x, y_0)$ at the diagonal point $x = y_0$. The reason is the particular choice of approximation in the form of smooth functions of a fixed type. In these classes of functions, there is no possibility to improve one factor by fixing another. For this to be possible, the value of the derivative at zero should not affect the behavior of the generalized signum outside some neighborhood of zero. We suggest using the spline method. The soft signum must be an odd C^1 -function on the interval $[-1, 1]$ and is defined by two splines on the interval $[0, 1]$. The first spline is responsible for the curvature, the second one generates a connective that differs little from the associative one. As a parameter, we choose the value of the derivative of the soft signum at zero. In addition, it is necessary to guarantee the commutativity, monotonicity, and pointwise convergence to signum of the generated connectives.

Definition 6. A function φ_k is k -admitted, $k > 0$, if the properties hold

1. $\varphi_k \in C^1[-1, 1]$.
2. There exists $z_0 \in [0, 1]$ such that $\varphi_k(z) = kz$ for $z \in [-z_0, z_0]$.
3. For all $z \in [-1, 1]$ holds $\varphi_k(z) + z \cdot \varphi'_k(z) \leq 1$.

Problem. To find k -admitted function φ_k for which the measure of non-associativity $\Delta(\varphi_k)$ is minimal. As k increases, the function φ_k must converge pointwise to the signum. In this formulation, the problem has an exact solution

3 Results

Theorem. For every $k > 0$ there exist z_0 and the k -admitted function minimizing Δ .

Proof. Consider the differential equation for the function $\varphi(z) \in C^1[z_0, 1], \varphi(z_0) = C_0 < 1$:

$$\varphi(z) + z\varphi'(z) = 1.$$

The only solution of this equation has the form

$$\varphi(z) = 1 - \frac{(1 - C_0)z_0}{z}.$$

For all functions $\psi(z)$ satisfying the inequality

$$\psi(z) + z\psi'(z) \leq 1, \quad (4)$$

with $\psi(z_0) \leq C_0$, holds $\psi(z) \leq \varphi(z)$ on $[z_0, 1]$. Therefore $\Delta(\varphi) \leq \Delta(\psi)$. We have found a minimizing function for a given z_0 and $\varphi'(z_0) = \frac{1-C_0}{z_0}$. Consider condition (4) for the first spline $\varphi(z) = kz$:

$$\begin{aligned} \varphi(z) + z\varphi'(z) &= kz + zk = 2kz \leq 1, \\ z &\leq \frac{1}{2k}. \end{aligned}$$

Therefore $z_0 \leq \frac{1}{2k}$. On the other hand, C^1 -smoothness of spline means

$$k = \varphi'(z_0) = \frac{1-C_0}{z_0} \text{ and } kz_0 = C_0.$$

It follows that $C_0 = \frac{1}{2}$, $z_0 = \frac{1}{2k}$. We have found the optimal solution for $z_0 = \frac{1}{2k}$ (Fig. 2, a):

$$\text{sgn}_k^0(z) = \begin{cases} kz, z \in [0, \frac{1}{2k}], \\ 1 - \frac{1}{4kz}, z \in [\frac{1}{2k}, 1]; \end{cases} \quad \text{sgn}_k^0(-z) = -\text{sgn}_k^0(z). \quad (5)$$

Finally, if we consider $z_0 < \frac{1}{2k}$, then for every admitted spline satisfying (4) we can choose another one with less Δ . To do this, it suffices to smoothly conjugate the line with any hyperbola intersecting it (Fig. 2, b). Thus, for values $z_0 < \frac{1}{2k}$, there is no smooth solution to the problem. The problem has only a non-smooth solution, which is union of a line segment and an arc of a hyperbola. The theorem has been proven. ■

So, let's now calculate the deviation (3):

$$\frac{1}{2}\Delta(\text{sgn}_k^0) = \int_0^{z_0} (1 - kz) dz + \int_{z_0}^1 \frac{z_0}{2z} dz = z_0 - \frac{kz_0^2}{2} - \frac{z_0}{2} \ln z_0 = \frac{3 + 2 \ln(2k)}{8k}.$$

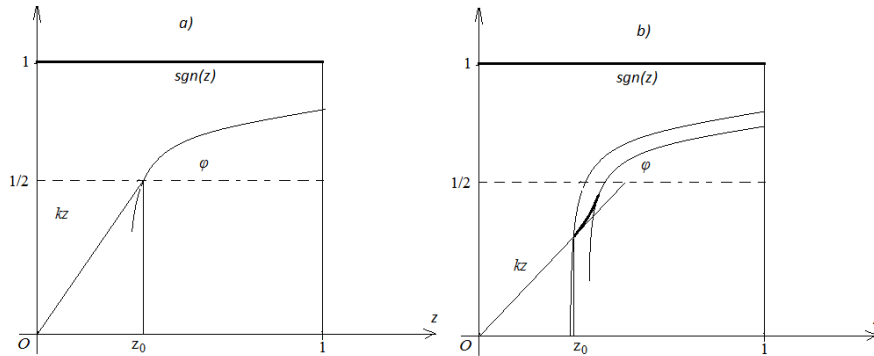


Figure 2. a) Optimal solution, b) non-existence of an optimal solution for $z_0 < \frac{1}{2k}$.
(Source: compiled by the authors)

An explicit expression for the resulting soft minimum is:

$$\min_k(x, y) = \begin{cases} \frac{x + y - k(x - y)^2}{2}, & \text{if } |x - y| < \frac{1}{k}; \\ \min(x, y) + \frac{1}{8k}, & \text{if } |x - y| \geq \frac{1}{k}. \end{cases}$$

For every $(x_0, y_0) \in [0, 1]^2$ soft minimum converges to minimum, i.e. we got an approximation

$$\lim_{k \rightarrow \infty} \min_k(x_0, y_0) = \min(x_0, y_0).$$

We note an important circumstance regarding the behavior of the soft minimum outside the diagonals. It differs from the minimum only by a constant. For all triplets $(x_1, x_2, x_3), x_2 < x_1, x_2 < x_3, |x_i - x_j| > \frac{1}{8k}$, associativity holds:

$$\min_k(\min_k(x_1, x_2), x_3) = \min_k(x_1, \min_k(x_2, x_3)).$$

Indeed, according to the conditions $\min_k(x_1, x_2) = x_2 + \frac{1}{8k}$, $\min_k(x_2 + \frac{1}{8k}, x_3) = x_2 + \frac{2}{8k}$, and $\min_k(x_2, x_3) = x_2 + \frac{1}{8k}$, $\min_k(x_1, x_2 + \frac{1}{8k}) = x_2 + \frac{2}{8k}$. The specified range of values is approximately one third of the cube $[0, 1]^3$ (Fig. 3). Here the domain ABCDF is the solution of two inequalities $x_2 < x_1, x_2 < x_3$.

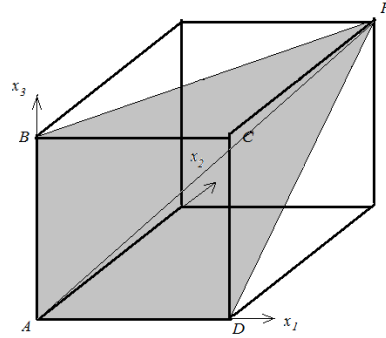


Figure 3. The associativity domain of the optimal soft minimum is ABCDF without diagonal neighborhood $|x_i - x_j| < \frac{1}{k}$ (Source: compiled by the authors).

For other triplets of the cube out of diagonals, the difference (1) is equal to $|\tilde{\Delta}(x_1, x_2, x_3)| = \frac{1}{8k}$. For instance, if $x_1 < x_2 < x_3, |x_i - x_j| > \frac{1}{8k}$, then $\min_k(x_1, x_2) = x_1 + \frac{1}{8k}$, $\min_k(x_1 + \frac{1}{8k}, x_3) = x_1 + \frac{2}{8k}$, and $\min_k(x_2, x_3) = x_2 + \frac{1}{8k}$, $\min_k(x_1, x_2 + \frac{1}{8k}) = x_1 + \frac{1}{8k}$. Other cases are calculated similarly. So, the integral measure of non-associativity (2) is

$$\iiint_{[0,1]^3} |\tilde{\Delta}(x_1, x_2, x_3)| dx_1 dx_2 dx_3 = \frac{1}{12k} + o\left(\frac{1}{k}\right).$$

This is the best result for a given curvature.

4 Discussion

The results obtained in the previous section can be compared with the soft signums listed earlier. Since one of the quality factors of the models is the curvature, which is determined by the derivative of the soft signum at zero, we will compare by the equality of this indicator.

Table 1. Comparative characteristics of soft signums with the same curvature.

Soft signum	$\varphi'_k(0) = k$			Associativity	Monotonicity of soft minimum
	$\Delta(\varphi_k)$	optimal k_0	$\Delta(\varphi_{k_0})$		
$\varphi_\delta(z)$	δ^*	$0,1 \leq \delta \leq 0,4$	$0,1 \leq \delta \leq 0,4$	non-associative for almost all triplets	yes
$sgn_\delta^I(z)$	$\frac{1}{k} + o\left(\frac{1}{k}\right)$	≈ 100	0.063	non-associative for almost all triplets	yes
$sgn_\delta^{II}(z)$	$\frac{2}{k} + o\left(\frac{1}{k}\right)$	≈ 100	0.0198	non-associative for almost all triplets	no
$sgn_\delta(z)$	$\frac{1.48}{k} + o\left(\frac{1}{k}\right)$	≈ 50	0.0276	non-associative for almost all triplets	no
$sgn_k^0(z)$	$\frac{0.74}{k} + o\left(\frac{1}{k}\right)$	$\approx 100^{**}$	0.0338	About one third of triplets associative	yes

* This parameter is not determined by the curvature, since the signum is discontinuous.

** Taken for comparison only. (Source: compiled by the authors).

Analyzing the results of the comparison, we can conclude that when solving the problem of optimizing the parameters of a soft signum, three factors have to be balanced: non-associativity, preservation of monotonicity, and curvature (angle) at the critical point. The soft signum $\varphi_\delta(z)$ retains monotonicity, but is not associative to a very large extent and is not differentiable at the critical point. The soft signum of the first type $sgn_\delta^I(z)$ is smooth at zero and remains monotonic, but the deviation cannot be improved. Soft signs of the second type and Berenji are smooth and have a relatively small deviation only due to the loss of monotonicity. The solution we found is devoid of all shortcomings. The spline-signum $sgn_k^0(z)$ defined by (5) is smooth, retains monotonicity, has a large associativity region for any curvature, and has the highest deviation decay rate as the curvature increases (column 2).

The described model can be improved in several ways. Due to the fact that the weight of the curvature factor at the critical point is not known, one can try to design the experiment with zero curvature. To do this, it suffices to specify on the segment $[-z_0, z_0]$ not a linear dependence, but a monomial of odd degree, for example, kz^3 . In this case, for any k the curvature will remain zero as the rate of decrease of deviation will drop. What will be the optimal value of the parameter in this case, needs to be set experimentally.

We can forego the smoothness of a continuous soft signum outside zero, which will improve the deviation, but form the original problem of a sharp jump in the dependence on the argument in the neighborhood of the diagonal.

Alternatively, you can keep the break at the critical point by allowing the soft spline-signum to break at zero, greatly reducing the deflection.

In all proposed variants of modifications, spline-signums have more advantageous positions in comparison with regular functional classes of high smoothness.

5 Conclusion

In the presented study, a new approach was proposed for constructing connective approximations for soft computations in machine learning. Instead of using smooth functions, we suggested using spline approximations. Thanks to this, the problem of separating the negative factors that worsen the accuracy of ML-models was solved. Such factors include curvature, non-monotonicity and non-associativity of soft connectives. We have built a spline-connective that has a vast area of exact associativity, which was not previously noticed by specialists.

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