A survey and taxonomy of loss functions in machine learning

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Most state-of-the-art machine learning techniques revolve around the optimisation of loss functions. Defining appropriate loss functions is therefore critical to successfully solving problems in this field. We present a survey of the most commonly used loss functions for a wide range of different applications, divided into classification, regression, ranking, sample generation and energy based modelling. Overall, we introduce 33 different loss functions and we organise them into an intuitive taxonomy. Each loss function is given a theoretical backing and we describe where it is best used. This survey aims to provide a reference of the most essential loss functions for both beginner and advanced machine learning practitioners.

1 INTRODUCTION

In the last few decades there has been an explosion in interest in machine learning [52, 76]. This field focuses on the definition and application of algorithms that can be trained on data to model underlying patterns [11, 73, 77, 88]. Machine learning approaches can be applied to many different research fields, including biomedical science [59, 84, 95, 126], natural language understanding [22, 83], [97] anomaly detection [17], image classification [71], database knowledge discovery [32], robot learning [3], online advertising [86], time series forecasting [13], brain computer interfacing [78] and many more [98]. To train these algorithms, it is necessary to define an objective function, which gives a scalar measure of the algorithm's performance [77, 116]. They can then be trained by optimising the value of the objective function.

Within the machine learning literature, such objective functions are usually defined in the form of loss functions, which are optimal when they are minimised. The exact form of the loss function depends on the nature of the problem to be solved, the data available and the type of machine learning algorithm being optimised. Finding appropriate loss functions is therefore one of the most important research endeavours in machine learning.

As the field of machine learning has developed, lots of different loss functions have been proposed. It is therefore very useful to summarise and understand them. However, there are few works that attempt to do this for the whole field [119]. The existing reviews of loss functions in the literature either lack a good taxonomy to structure and contextualise the different losses, or are specifically focused on a particular subset of machine learning applications [49, 117]. There is also no single source that puts the most commonly used loss functions in the same formal setting, listing the advantages and drawbacks of each one.

For this reason, we have worked to build a proper taxonomy of loss functions, where we show the advantages and disadvantages for each technique. We hope this will be useful for new users who want to familiarise themselves with the most common loss functions used in the machine learning literature and find one that is suitable for a problem that they are trying to solve. We also hope this summary will be useful as a comprehensive reference for advanced users, allowing them to quickly find the best loss function without having to broadly search the literature. Additionally, this can be helpful for researchers to find possible avenues for further research, or to understand where to place any new techniques that they have proposed. They could, for example, use this

survey to understand if their new proposals fit somewhere inside the taxonomy we present, or if they are in a completely new category, maybe combining disparate ideas in novel ways.

Overall, we have included 33 of the most widely used loss functions. In each section of this work, we break down the losses based on the broad classification of tasks that they can be used for. Each loss function will be defined mathematically, and its most common applications listed highlighting advantages and drawbacks.

The main contribution of this work can be found in the proposed taxonomy depicted in Fig. 1. Each loss function is first divided according the specific task on which they are exploited: regression, classification, ranking, sample generation and energy-based modelling. Furthermore, we divide them by the type of learning paradigm on which they can be applied to, from supervised to unsupervised. Finally, we classify them according to the underling strategy on which they are based, such as if they rely on a probabilistic formalization, or are based on errors or a margin between the prediction and the actual values.

This work is organized as follows: In Section 2, we provide a formal definition of a loss function and introduce our taxonomy. In Section 3, we describe the most common regularization methods used to reduce model complexity. In Section 4, we describe the regression task and the key loss functions used to train regression models. In Section 5, we introduce the classification problem and the associated loss functions. In Section 6, we present generative models and their losses. Ranking problems and their loss functions are introduced in Section 7, and energy based models and their losses are described in Section 8. Finally, we draw conclusions in Section 9.

2 DEFINITION OF OUR LOSS FUNCTION TAXONOMY

In a general machine learning problem, the aim is to learn a function f that transforms an input, defined by the input space Φ into a desirable output, defined by the output space $\mathcal{Y}$:

$$f \colon \Phi \to \mathcal{Y}$$

Where f is a function that can be approximated by a model, f_Θ, parameterised by the parameters Θ.

Given a set of inputs $\{\mathbf{x}_0, ..., \mathbf{x}_N\} \in \Phi$, they are used to train the model with reference to target variables in the output space, $\{\mathbf{y}_0, ..., \mathbf{y}_N\} \in \mathcal{Y}$. Notice that, in some cases (such as autoencoders) $\mathcal{Y} = \Phi$.

A loss function, L, is defined as a mapping of $f(\mathbf{x}_i)$ with it's corresponding $\mathbf{y}_i$ to a real number $l \in \mathbb{R}$, which captures the similarity between $f(\mathbf{x}_i)$ and $\mathbf{y}_i$. Aggregating over all the points of the dataset we find the overall loss, $\mathcal{L}$:

$$\mathcal{L}(f|\{\mathbf{x}_0, ..., \mathbf{x}_N\}, \{\mathbf{y}_0, ..., \mathbf{y}_N\}) = \frac{1}{N} \sum_{i=1}^{N} L(f(\mathbf{x}_i), \mathbf{y}_i) \tag{1}$$

The optimisation function to be solved is defined as:

$$\min_{f} \mathcal{L}(f|\{\mathbf{x}_0, ..., \mathbf{x}_N\}, \{\mathbf{y}_0, ..., \mathbf{y}_N\}) \tag{2}$$

Notice that, it is often convenient to explicitly introduce a regularisation term (R) which maps f to a real number $r \in \mathbb{R}$. This term is usually used for penalising the complexity of the model in the optimisation [77]:

$$\min_{f} \frac{1}{N} \sum_{i=1}^{N} L(f(\mathbf{x}_i), \mathbf{y}_i) + R(f) \tag{3}$$

In practice, the family of functions chosen for the optimisation can be parameterised by a parameter vector Θ, which allows the minimisation to be defined as an exploration in the parameter space:

$$\min_{\Theta} \frac{1}{N} \sum_{i=1}^{N} L(f_{\Theta}(\mathbf{x}_i), \mathbf{y}_i) + R(\Theta) \tag{4}$$

2.1 Optimisation techniques for loss functions

2.1.1 Loss functions and optimisation methods. In this section, we list out the most common mathematical properties that a loss may or may not satisfy and then we briefly discuss the main optimisation methods employed to minimise them. For the sake of simplicity, visualisation and understanding we define such properties in a two dimensional space, but they can be easily generalised to a d-dimensional one.

- **Continuity** (*CONT*): A real function, that is a function from real numbers to real numbers, can be represented by a graph in the Cartesian plane; such a function is continuous if the graph is a single unbroken curve belonging to the real domain. A more mathematically rigorous definition can be given by defining continuity in terms of limits. A function f with variable x is continuous at the real number c, if $\lim_{x \to c} f(x) = f(c)$.
- **Differentiability** (*DIFF*): A differentiable function f on a real variable is a function derivable in each point of its domain. A differentiable function is smooth (the function is locally well approximated as a linear function at each interior point) and does not contain any break, angle, or cusp. A continuous function is not necessarily differentiable, but a differentiable function is necessarily continuous.
- **Lipschitz Continuity** (*L-CONT*): A Lipschitz continuous function is limited in how fast it can change. More formally, there exists a real number such that, for every pair of points on the graph of this function, the absolute value of the slope of the line connecting them is not greater than this real number; this value is called the Lipschitz constant of the function.
  To understand the robustness of a model, such as a neural network, some research papers [39, 115] have tried to train the underlying model by defining an input-output map with a small Lipschitz constant. The intuition is that if a model is robust, it should not be too affected by perturbations in the input, $f(x + \delta x) \approx f(x)$, and this would be ensured by having f be ℓ-Lipschitz where ℓ is small [85].
- **Convexity** (*CONV*): a real-valued function f is *convex* if each segment between any two points on the graph of the function lies above the graph between the two points. Convexity is a key feature, since the local minima of convex function is also the global minima. Whenever the second derivative of a function exists, then the convexity is easy to check, since the Hessian of the function must be positive semi-definite.
- **Strict Convexity** (*S-CONV*): a real-valued function is *strictly convex* if the segment between any two points on the graph of the function lies above the graph between the two points, except for the intersection points between the straight line and the curve. Strictly convex functions have a positive definitive Hessian. Positive-definite matrices are invertible and the optimisation problem can be so solved in a closed form.

Algorithm 2.1 Gradient Descent
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Input: initial parameters $\Theta^{(0)}$, number of iterations T, learning rate α
Output: final learning $\Theta^{(T)}$
1.   **for** $t = 0$ **to** $T - 1$
2.   estimate $\nabla \mathcal{L}(\Theta^{(t)})$
3.   compute $\Delta \Theta^{(t)} = -\nabla \mathcal{L}(\Theta^{(t)})$
4. $\Theta^{(t+1)} := \Theta^{(t)} + \alpha \Delta \Theta^{(t)}$
5.   **return** $\Theta^{(T)}$
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2.1.2 Relevant optimisation methods. An optimisation method is a technique that, given a formalised optimisation problem with an objective function, returns the solution to obtain the optimal value of that optimisation problem. Most of the optimisation methods presented in this work rely on algorithms that may not guarantee the optimality of the solution, but imply a degree of approximation.

- **Closed form solutions** are systems of equations that can be solved analytically by finding the values of Θ that lead to a zero value for the derivative of the loss function. An optimization problem is closed-form solvable if its objective function is differentiable with respect to Θ and the differentiation can be solved for Θ. In general differentiability and strict convexity are required to have a closed form solution. Closed-form solutions should always be used instead of iterative algorithms if they're available and computationally feasible.
- **Gradient Descent** is a first-order[1] iterative optimization algorithm for finding a local minimum of a differentiable function. The procedure takes repeated steps in the opposite direction of the gradient of the function at the current point, with a step-size defined by a parameter α, often called the learning rate.
  The loss function employed must be differentiable, so that the gradient can be computed. In order to overcome this limitation and employ also non-differentiable loss function, approximation of gradient and other techniques can be used [56, 99]. The procedure for gradient descent is formalized in Algorithm 1.
- **Stochastic Gradient Descent** (SGD [77]) is a stochastic approximation of gradient descent optimization. It replaces the actual gradient, calculated from the entire dataset, by an estimate, which is calculated from a randomly selected subset of the data. The stochastic gradient is an unbiased estimate of the real gradient.
  In high-dimensional optimization problems, such as in artificial neural networks, this reduces the time cost. The stochasticity of this method reduces the probability of the optimisation to get stuck in a local minimum. SGD shares the same constraints (i.e. differentiability, convexity for optimal solution) of traditional Gradient Descent.
- **Derivative Free Optimisation** In some cases the derivative of the objective function may not exist, or may not be easy to calculate. This is where derivative-free optimisation comes into the picture. Classical simulated annealing arithmetic, genetic algorithms and particle swarm optimisation are a few such examples. Conventional derivative free optimisation methods are usually difficult to scale to large-size problems. To learn more about derivative free optimisation you can refer to [24, 91].
- **Zeroth Order optimisation** Zeroth-Order (ZOO) optimisation is a subset of gradient-free optimisation that emerges in various signal processing as well as machine learning applications [70]. ZOO optimisation methods are the gradient-free counterparts of first-order

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[1]In numerical analysis, methods that have at most linear local error are called first order methods. They are frequently based on finite differences, a local linear approximation.

optimisation techniques. ZOO approximates the full gradients or stochastic gradients through function value-based gradient estimates. Some recent important applications include generation of prediction-evasive, black-box adversarial attacks on deep neural networks [19], generation of model-agnostic explanation from machine learning systems [26], and design of gradient or curvature regularised robust ML systems in a computationally-efficient manner [70]. Zeroth optimisation can be a convenient option, compared to the conventional derivative free optimisation approach, as it's easy to implement inside commonly used gradient based algorithm (e.g SGD), it approximates derivatives efficiently and has comparable convergence rates to first-order algorithms.
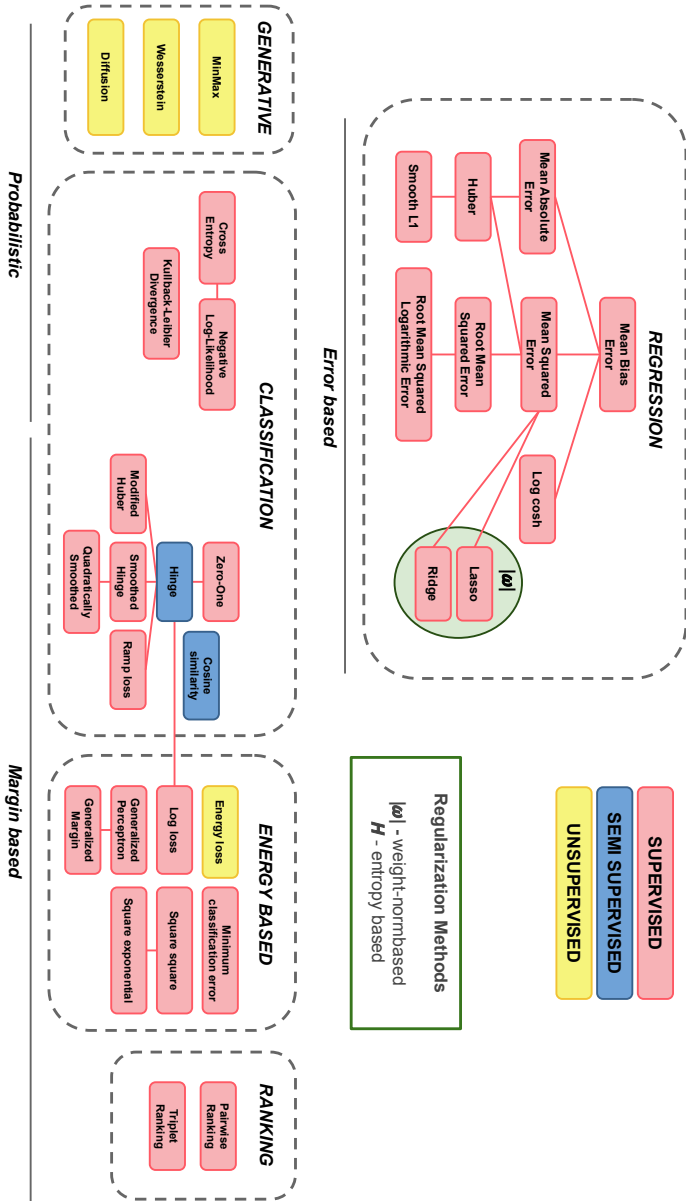
Fig. 1. The proposed taxonomy. Five major tasks are identified on which loss function are applied to, namely regression, classification, ranking, generating samples (generative) and energy based. With different colors we specify the type of learning paradigm, from supervised to unsupervised of each loss function. Finally the underlying strategy to optimize them, namely margin based, probabilistic and error based is illustrated under each group of losses.

2.2 Our taxonomy

Our taxonomy is summarized in Fig 1 . To define it, we started by categorizing the losses depending on which machine learning problem they are best suited to solve. We have identified the following categories:

- Regression (Sec. 4)
- Classification (Sec. 5)
- Generative modelling (Sec. 6)
- Ranking (Sec. 7)
- Energy based modelling (Sec. 8)

We also made a distinction based on the mathematical concepts used to define the loss obtaining the following sub-categories:

- Error based
- Probabilistic
- Margin based

Exploiting this approach we find a compact and intuitive taxonomy, with little redundancy or overlap between the different sections. We have employed well known terminology to define the taxonomy, which will make it easier for any user to intuitively understand it.

3 REGULARISATION METHODS

Regularisation methods can be applied to almost all loss functions. They are employed to reduce model complexity, simplifying the trained model and reducing it's propensity to overfit the training data [5, 30, 61]. Model complexity, is usually measured by the number of parameters and their magnitude [5, 77, 79]. There are many techniques which fall under the umbrella of regularisation method and a significant number of them are based on the augmentation of the loss function [30, 77]. An intuitive justification for regularization is that it imposes Occam's razor on the complexity of the final model. More theoretically, many loss-based regularization techniques are equivalent to imposing certain prior distributions on the model parameters.

3.1 Regularisation by Loss Augmentation

One can design the loss function to penalise the magnitude of model parameters, thus learning the best trade-off between bias and variance of the model and reducing the generalization error without affecting the training error too much. This prevents overfitting, while avoiding underfitting, and can be done by augmenting the loss function with a term that explicitly controls the magnitude of the parameters, or implicitly reduces the number of them. The general way of augmenting a loss function in order to regularise the result is formalized in the following equation:

$$\widehat{L}(f(\mathbf{x}_i), \mathbf{y}_i) = L(f(\mathbf{x}_i), \mathbf{y}_i) + \lambda \rho(\mathbf{\Theta}) \tag{5}$$

where $\rho(\mathbf{\Theta})$ is called regularization function and λ defines the amount of regularisation (the trade-off between fit and generalisation).

This general definition makes it clear that we can employ regularization on any of the losses proposed in this paper.

We are now going to describe the most common regularisation methods based on loss augmentation.

3.1.1 L2-norm regularisation. In L_2 regularization the loss is augmented to include the weighted L_2 norm of the weights [12, 77], so the regularisation function is $\rho(\mathbf{\Theta}) = \|\mathbf{\Theta}\|_2^2$:

$$\widehat{L}(f(\mathbf{x}_i), \mathbf{y}_i) = L(f(\mathbf{x}_i), \mathbf{y}_i) + \lambda \|\mathbf{\Theta}\|_2^2 \tag{6}$$

when this is employed to regression problems it is also known as Ridge regression [46, 77].

3.1.2 L_1-norm regularisation. In L_1 regularization the loss is augmented to to include the weighted L_1 norm of the weights [12, 77], so the regularisation function is $\rho(\Theta) = \|\Theta\|$

$$\widehat{L}(f(\mathbf{x}_i), \mathbf{y}_i) = L(f(\mathbf{x}_i), \mathbf{y}_i) + \lambda \|\Theta\|_1 \tag{7}$$

when this is employed to regression problems it is also known as Lasso regression [77, 109].

3.2 Comparison between L_2 and L_1 norm regularisations

L_1 and L_2 regularisations are both based on the same concept of penalising the magnitude of the weights composing the models. Despite that, the two methods have important differences in their employability and their effects on the result.

One of the most crucial differences is that L_1, when optimised, is able to shrink weights to 0, while L_2 results in non-zeros (smoothed) values [7, 12, 73, 77, 81]. This allows L_1 to reduce the dimension of a model's parameter space and perform an implicit feature selection. Indeed, it has been shown by [81] that by employing L_1 regularization on logistic regression, the sample complexity (i.e., the number of training examples required to learn "well") grows logarithmically in the number of irrelevant features. On the contrary, the authors show that any rotationally invariant algorithm (including logistic regression) with L_2 regularization has a worst case sample complexity that grows at least linearly in the number of irrelevant features. Moreover, L_2 is more sensitive to the outliers than L_1-norm since it squares the error.

L_2 is continuous, while L_1 is a piece-wise function. The main advantage of L_2 is that it is differentiable, while L_1 is non-differentiable at 0, which has some strong implications. Precisely, the L_2 norm can be easily trained with gradient descent, while L_1 sometimes cannot be efficiently applied. The first problem is the inefficiency of applying the L_1 penalty to the weights of all the features, especially when the dimension of the feature space tends to be very large [110], producing a significant slow down of the weights updating process. Finally the naive application of L_1 penalty in SGD does not always lead to compact models, because the approximate gradient used at each update could be very noisy, so the weights of the features can be easily moved away from zero by those fluctuations and L_1 looses its main advantages with respect to L_2 [110].

4 REGRESSION LOSSES

The aim of a regression model is to predict the outcome of a continuous variable y (the dependent variable) based on the value of one or multiple predictor variables $\mathbf{x}$ (the independent variables). More precisely, let f_Θ be a generic model parameterized by Θ, which maps the independent variables $\mathbf{x} \in \{\mathbf{x}_0, ..., \mathbf{x}_N\}, \mathbf{x}_i \in \mathbb{R}^D$ into the dependent variable $y \in \mathbb{R}$. The final goal is to estimate the parameters of the model Θ that most closely fits the data by minimizing a loss function L.
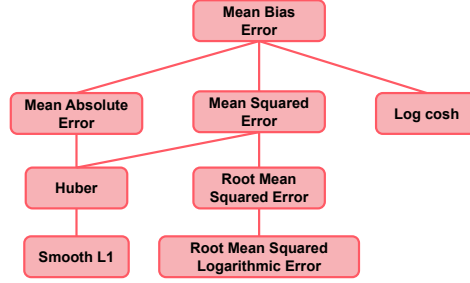
Fig. 2. Schematic overview of the regression losses showing the connection

All the losses considered for the regression task are based on functions of the residuals, i.e. the difference between the observed value y and the predicted value $f(\mathbf{x})$. In the following, let $f(\mathbf{x}_i)$ be the outcome of the prediction over $\mathbf{x}_i$, and y be the ground truth of the ith variable of interest.

As highlighted by Fig. 2 the Mean Bias Error (MBE) loss can be considered a base pillar for regression losses, characterized by many variations. Among them the most relevant are: Mean Absolute Error (MAE), Mean Squared Error (MSE), and Root Mean Squared Error (RMSE) losses. In this section we are also going to introduce the Huber loss and the smooth L1, which are a blend between the MAE and the MSE. Finally, the Log-cosh and the Root Mean Squared Logarithmic Error losses are presented.

4.0.1 Mean Bias Error Loss (CONT, DIFF). The most straightforward loss function is the Mean Bias Error loss, illustrated in Equation 8. It captures the average bias in the prediction, but is rarely adopted as loss function to train regression models, because positive errors may cancel out the negative ones, leading to a potential erroneous estimation of the parameters. Nevertheless, it is the starting point of the loss functions defined in the next subsections and it is commonly used to evaluate the performances of the models [60, 111, 112].

$$\mathcal{L}_{MBE} = \frac{1}{N} \sum_{i=1}^{N} y_i - f(\mathbf{x}_i) \tag{8}$$

Directly connected to MBE there are respectively the Mean Absolute Error, the Mean Squared Error and the Log-cosh losses, which basically differs from MBE in how they exploit the bias.

4.0.2 Mean Absolute Error Loss (L-CONT,CONV). The Mean Absolute Error loss or L1 loss is one of the most basic loss functions for regression, it measures the average of the absolute bias in the prediction. The absolute value overcomes the problem of the MBE ensuring that positive errors do not cancel the negative ones. Therefore each error contributes to MAE in proportion to the absolute value of the error. Notice that, the contribution of the errors follows a linear behavior, meaning that many small errors are important as a big one. This implies that the gradient magnitude is not dependent on the error size, thus may leading into convergence problems when the error is small. A model trained to minimize the MAE is more effective when the target data conditioned on the input is symmetric. It is important to highlight that the derivative of the absolute value at zero is not defined.

As for MBE, MAE is also used to evaluate the performances of the models [68, 121].

$$\mathcal{L}_{MAE} = \frac{1}{N} \sum_{i=1}^{N} |y_i - f(\mathbf{x}_i)| \tag{9}$$

4.0.3 Mean Squared Error Loss (CONT, DIFF, CONV). The Mean Squared Error loss, or L2 loss, is the average of squared distances between the observed value y and the predicted value $\hat{y}$. As for *MAE*, it is a well-known and straightforward loss function for regression. The squared term makes all the biases positive and magnifies the contribution made by outliers, making it more suitable for problems where noise in the observations follows a normal distribution. The main drawback is the sensitivity to the outliers.

$$\mathcal{L}_{MSE} = \frac{1}{N} \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i))^2 \tag{10}$$

4.0.4 Root Mean Squared Error Loss(CONT,DIFF,CONV). Directly connected to MSE, we have the Root Mean Squared Error loss, which is similar to MSE except for the square root term. The main advantage is to make sure that the loss has the same units and scale of the variable of interest. Since the only difference between the MSE and the RMSE consists in the application of the root term, the minimization process converge to the same optimal value. However, depending on the optimisation technique used, the RMSE may take different gradient steps. As the previously presented loss functions, it is also used as a metric to compare the performances of the model [68, 112], and it shares the same limitations.

$$\mathcal{L}_{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i))^2} \tag{11}$$

4.0.5 Huber loss (L-CONT,DIFF,S-CONV). The Huber loss [48] is a variant of the MAE that becomes MSE when the residuals are small. It is parameterized by δ, which defines the transition point from MAE to MSE. When $|\mathbf{y}_i - f(\mathbf{x}_i)| \le \delta$ the Huber loss follows the MSE, otherwise it follows the MAE. This allows it to combine the advantages of both the MAE and the MSE, when the difference between the prediction and the output of the model is huge errors are linear, make the Huber loss less sensitive to the outliers. Conversely, when the error is small, it follows the MSE making the convergence much faster and differentiable at 0. The choice of δ is fundamental and it can be constantly adjusted during the training procedure based on what is considered an outlier. The main limitation of the Huber loss resides in the additional extra hyperparameter δ.

$$L_{Huberloss} = \begin{cases} \frac{1}{2} (y_i - f(\mathbf{x}_i))^2 & for \ |y_i - f(\mathbf{x}_i)| \le \delta, \\ \delta \left(|y_i - f(\mathbf{x}_i)| - \frac{1}{2}\delta\right) & otherwise \end{cases} \tag{12}$$

Notice that, when $\delta = 1$, we obtain the smooth L1 loss.

4.0.6 Log-cosh loss(CONT, DIFF). The log-cosh loss is the logarithm of the hyperbolic cosine of the residuals between the observed value y and the predicted value $\hat{y}$. It has all the advantages of the Huber loss, without the requirement of setting a hyperparameter, at the cost of being more computationally expensive. Furthermore, another benefit of the log-cosh loss is related to the fact that is differentiable twice everywhere, making it suitable for methods that requires solving the second derivative. As $log(cosh(\mathbf{x}))$ is approximately equal to $\frac{\mathbf{x}^2}{2}$ for small values of $\mathbf{x}$ it behave similarly to the MSE. For larger value of $\mathbf{x}$ instead, is nearly equivalent to $|\mathbf{x}| - log(2)$ making it similar to MAE.

$$\mathcal{L}_{logcosh} = \frac{1}{N} \sum_{i=1}^{N} log(cosh(f(\mathbf{x}_i) - y_i)) \tag{13}$$

Another drawback of $\mathcal{L}_{logcosh}$ is related to the fact that, compared to the Huber loss, it is less customizable.

4.0.7 *Root Mean Squared Logarithmic Error Loss*(CONT,DIFF,CONV). The Root Mean Squared Logarithmic Error (RMSLE) loss (formalized in Eq. 14) is the RMSE of the log-transformed observed value y and log-transformed predicted value $\hat{y}$. The only difference with respect to RMSE is that the logarithm is applied to both the predicted and the observed values. The plus one term inside the logarithm allows values of $f(\mathbf{x}_i)$ to be zero.

Due to the properties of the logarithm, the error between the predicted and the actual values is relative, making the RMSLE more robust to outliers. Precisely, the magnitude of the RMLSE does not scale accordingly to the magnitude of the error. Indeed, data points with big residuals are less penalized when the predicted and the actual values have high values too. This make the RMSLE suitable for problems where targets have an exponential relationship, or it is preferable to penalize more under estimates than over estimates. However, this loss is not appropriate for problems that allows negative values.

$$\mathcal{L}_{RMSLE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left(\log(y_i + 1) - \log(f(\mathbf{x}_i) + 1) \right)^2} \tag{14}$$

5 CLASSIFICATION LOSSES

5.1 Problem Formulation and Notation

Classification is a subset of problems belonging to supervised learning. The goal is to assign an input $\mathbf{x}$ to one of K discrete classes. This goal can be pursued by training a model f_Θ and its parameters Θ by minimizing a loss function L. Let the target space of f discrete and consider a model returning the output label, f can be defined as:

$$f : \Phi \rightarrow \Lambda^K$$
$$\Lambda = \{0, 1\}$$

The above definition is working also for multi-label classification, since more than one label could be associated to a sample, e.g. $f(\mathbf{x}) = [0, 1, 0, 1, 0, 0]$. In order to define single label classification we need to add the constraint that the output sum up to 1, $\sum_k \lambda_k = 1$.

We can also consider models with continuous outputs, in case they return a probability $p_k(\mathbf{x}) \in [0, 1]$ to a sample $\mathbf{x}$ for each possible assignable label $k \in 1, ..., K$:

$$f : \Phi \rightarrow P^K$$
$$P = [0, 1]$$

As before, to switch between multi-label and single-label classification, we need to constraint the probabilities output to sum up to one, $\sum_k p_k = 1$, if we want to force a single label assignment.

A more narrow notation for classification can be introduced in order to describe binary classification problems. This notation is useful in this work because margin based losses are designed to solve binary classification problems and cannot be generalised to multi-class or multi label classification. For the subset of binary classification problems the target space of f is discrete and it is defined as follows:

$$f : \Phi \rightarrow B$$
$$B = \{-1, 1\}$$

We define two different macro categories of classification losses accordingly to the underlying strategy employed to optimize them, namely the margin based and the probabilistic ones as illustrated in Fig. 3. In the next section, we introduce the margin based loss function starting by the most basic and intuitive one, the Zero-One loss. Subsequently, we present the Hinge loss

and its variants (the Smoothed and Quadratically Smoothed Hinge losses). Then, the Modified Huber loss, the Ramp loss, and the Cosine Similarity loss are described. Moreover, we introduce the probabilistic loss by introducing the Cross Entropy loss and Negative Log-Likelihood loss, which, from a mathematical point of view, coincides. Finally, the Kullback-Leibler Divergence loss is presented.
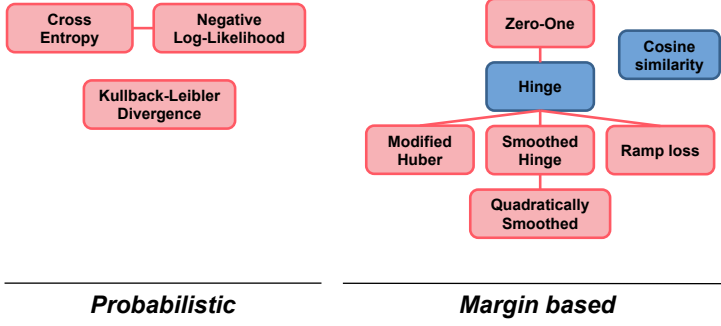

Fig. 3. Overview of the classification losses divided in two major groups: margin based losses and probabilistic ones.

5.2 Margin Based Loss Functions

In this section, we introduce the most known margin based loss functions.

5.2.1 Zero-One loss. The basic and more intuitive margin based classification loss is the Zero-One loss. It assigns 1 to a misclassified observation and 0 to a correctly classified one.

$$L_{\text{ZeroOne}}(f(\mathbf{x}), y) = \begin{cases} 1 & \text{if } f(\mathbf{x}) \cdot y < 0 \\ 0 & \text{otherwise} \end{cases} \tag{15}$$

ZeroOne loss is not directly usable since it lacks convexity and differentiability. However, it is possible to derive employable surrogate losses that are classification calibrated, which means that they are a relaxation of $L_{ZeroOne}$, or an upper bound, or an approximation of such loss. A significant achievement of the recent literature on binary classification has been the identification of necessary and sufficient conditions under which such relaxations yield Fisher consistency [6, 50, 72, 74, 105, 124]. All the following losses satisfy such conditions.

5.2.2 Hinge loss and Perceptron loss (L-CONT,CONV). The most famous surrogated loss is the Hinge loss [35], which linearly penalizes every prediction where the resulting agreement is <= 1.

$$L_{\text{Hinge}}(f(\mathbf{x}), y) = \max(0, 1 - (f(\mathbf{x}) \cdot y)) \tag{16}$$

The Hinge loss is not strictly convex, but it is Lipschitz continuous and convex, so many of the usual convex optimizers used in machine learning can work with it. The Hinge loss is commonly employed to optimise the Support Vector Machine (SVM [14, 75]).

To train the Perceptron [93] a variation of this loss, the Perceptron loss, is employed. This loss slightly differs from the Hinge loss, because it does not penalise samples inside the margin, surrounding the separating hyperplane, but just the ones that are mislabeled by this hyperplane with the same linear penalisation.

$$L_{\text{Perceptron}}(f(\mathbf{x}), y) = \max(0, -(f(\mathbf{x}) \cdot y)) \tag{17}$$

There are two main drawbacks using the hinge loss. Firstly, its adoption use to make the model sensible to outliers in the training data. Secondly, due to the discontinuity of the derivative at $(f(\mathbf{x}) \cdot y) = 1$, i.e. the fact that is not continuously differentiable, Hinge loss results difficult to optimise.

5.2.3 *Smoothed Hinge loss* *(L-CONT,CONV).* A smoothed version of the Hinge loss was defined in [90] with the goal of obtaining a function easier to optimise as shown by the following equation:

$$L_{\text{SmoothedHinge}}(f(\mathbf{x}), y) = \begin{cases} \frac{1}{2} - (f(\mathbf{x}) \cdot t) & (f(\mathbf{x}) \cdot y) <= 0 \\ \frac{1}{2}(1 - (f(\mathbf{x}) \cdot t))^2 & 0 < (f(\mathbf{x}) \cdot y) < 1 \\ 0 & (f(\mathbf{x}) \cdot y) >= 1 \end{cases} \tag{18}$$

This smoothed version of the Hinge loss is differentiable. Clearly, this is not the only possible smooth version of the Hinge loss. However, it is a canonical one that has the important property of being zero for $z >= 1$ and it has constant (negative) slope for $z <= 0$. Moreover, for $0 < z < 1$, the loss smoothly transitions from zero slope to a constant negative one. This loss inherit sensibility to outliers from the original Hinge loss.

5.2.4 *Quadratically Smoothed Hinge loss* *(L-CONT,CONV,DIFF).* With the same goal of the Smoothed Hinge loss a quadratically smoothed version has been defined in [125], to make it easier to be optimised:

$$L_{\text{QSmoothedHinge}}(f(\mathbf{x}), y) = \begin{cases} \frac{1}{2\gamma} \max(0, -(f(\mathbf{x}) \cdot y))^2 & (f(\mathbf{x}) \cdot y) >= 1 - \gamma \\ 1 - \frac{\gamma}{2} - (f(\mathbf{x}) \cdot y) & \text{otherwise} \end{cases} \tag{19}$$

The hyperparameter γ determines the degree of smoothing, for $\gamma \to 0$ the loss becomes the original hinge. In contrast with the Smoothed Hinge loss, this version is not differentiable in the whole domain.

5.2.5 *Modified Huber loss* *(L-CONT, DIFF, S-CONV).* The Modified Huber loss is a slight variation of the Huber loss for regression and a special case of the Quadratic Smoothed Hinge loss with $\gamma = 2$ (For more details refer to section 4.0.5):

$$L_{\text{ModHuber}}(f(\mathbf{x}), y) = \begin{cases} \frac{1}{4} \max(0, -(f(\mathbf{x}) \cdot y))^2 & (f(\mathbf{x}) \cdot y) >= -1 \\ -(f(\mathbf{x}) \cdot y) & \text{otherwise} \end{cases} \tag{20}$$

5.2.6 *Ramp loss* *(CONT,CONV).* The Ramp loss, or Truncated Hinge, is a piece-wise linear, continuous and convex loss that has been presented in [122]. Under multi-class setting, this loss is more robust to outliers. When employed in SVM, it produces more accurate classifiers using a smaller, and more stable, set of support vectors than the multi-class SVM that employes L_{Hinge} [66], also preserving fisher consistency.

$$L_{\text{Ramp}}(f(\mathbf{x}), y) = \begin{cases} L_{\text{Hinge}}(f(\mathbf{x}), y)) & (f(\mathbf{x}) \cdot y) <= 1 \\ 1 & \text{otherwise} \end{cases} \tag{21}$$

5.2.7 *Cosine Similarity loss* *(L-CONT,DIFF).* Cosine similarity is generally used as a metric to measure distance when the magnitude of vectors is not important [12]. A typical example is related to text data representation by means of word counts [12, 77]. When the label and output can be

interpreted as vectors it is possible to derive a distance metric between them, which can be adapted into a loss function as follows:

$$L_{cos-sim}(f(\mathbf{x}), \mathbf{y}) = 1 - \frac{\mathbf{y} \cdot \mathbf{f}(\mathbf{x})}{\|\mathbf{y}\| \, \|\mathbf{f}(\mathbf{x})\|} \tag{22}$$

It is important to underline that, when using Cosine Similarity loss, the range of possible values is restricted to the interval [-1, 1], which may not be suitable for all types of data or applications, particularly when interpretability is a key requirement.

5.3 Probabilistic loss Functions

Let q be the probability distribution underlying the dataset and f_Θ the function generating the output, probabilistic loss functions provide some distance function between q and f_Θ. By minimizing that distance, the model output distribution converges to the ground truth one. Usually, models trained with probabilistic loss functions can provide a measure of how likely a sample is labeled with one class instead of another [12, 43, 77] providing richer information w.r.t. margin based .

5.3.1 *Cross Entropy loss and Negative Log-Likelihood loss (CONT,DIFF,CONV)*. Maximum likelihood estimation (MLE) is a method to estimate the parameters of a probability distribution by maximizing the likelihood [12, 77, 80]. From the point of view of Bayesian inference, MLE can be considered a special case of maximum a-posteriori estimation (MAP) that assumes a uniform prior distribution of the parameters. Formally, it means that, given a dataset of samples $\mathcal{D}$, we are maximizing the following quantity:

$$P(\mathcal{D}|\Theta) = \prod_{n=1}^{N} f_\Theta(\mathbf{x}_i)^{y_i} \cdot (1 - f_\Theta(\mathbf{x}_i))^{1-y_i} \tag{23}$$

The aim is to find the maximum likelihood estimate by minimizing a loss function. To maximize Eq. 23, we can turn it into a minimisation problem by employing the negative log likelihood. To achieve this goal we need to define the following quantity:

$$log(P(\mathcal{D}|\Theta)) = \sum_{i=1}^{N} (y_i \log(f_\Theta(\mathbf{x}_i)) + (1 - y_i) \log(1 - f_\Theta(\mathbf{x}_i)))) \tag{24}$$

and we can obtain the loss function by taking the negative of the log:

$$\mathcal{L}_{NLL} = - \sum_{i=1}^{N} (y_i \log(f_\Theta(\mathbf{x}_i)) + (1 - y_i) \log(1 - f_\Theta(\mathbf{x}_i))) \tag{25}$$

Often, the above loss is also called the cross-entropy loss, because it can be derived by minimising the cross entropy between f_Θ and q.

$$H(q, f_\Theta) = - \int q(\mathbf{x}) \log(f_\Theta(\mathbf{x})) d\mathbf{x} \tag{26}$$

For the discrete case (which is the one we are interested in) the definition of the cross entropy is:

$$H(q, f_\Theta) = - \sum_{i=1}^{N} q(\mathbf{x}_i) \log(f_\Theta(\mathbf{x}_i)) \tag{27}$$

Maximizing the likelihood with respect to the parameters Θ is the same as minimizing the cross-entropy as shown by the following equations:

$$\sum_{i=1}^{N} (y_i \log(f_\Theta(\mathbf{x}_i)) + (1 - y_i) \log(1 - f_\Theta(\mathbf{x}_i))) = \frac{1}{N} \prod_{n=1}^{N} f_\Theta(\mathbf{x}_i)^{N y_i} \tag{28}$$

$$= \sum_{i=1}^{N} q(\mathbf{x}_i) \log(f_\Theta(\mathbf{x}_i) \tag{29}$$

$$= - H(q, f_\Theta) \tag{30}$$

The classical approach to extend this loss to the multi-class scenario is to add as a final activation of the model a softmax function, defined accordingly to the number of (K) classes considered. Given a score for each class $f_k(\mathbf{x}) = s$, it's output can be squashed to sum up to 1 by mean of a softmax function f_S obtaining:

$$\widehat{f_k}(\mathbf{x}_i) = f_S(f_k(\mathbf{x})) \tag{31}$$

where, the softmax is defined as follows:

$$f_S(s_i) = \frac{e^{s_i}}{\sum_{j=1}^{K} e^{s_j}} \tag{32}$$

The final loss (usually named as categorical cross entropy) is:

$$L_{CCE} = -\frac{1}{K} \sum_{j=1}^{K} \log(\widehat{f_k}(\mathbf{x})) \tag{33}$$

5.3.2 Kullback-Leibler divergence (CONT, CONV, DIFF). The Kullback-Leibler (KL) divergence is an information-based measure of disparity among probability distributions. Precisely, it is a non-symmetrical measurement of how one probability distribution differs from another one [12, 53, 77]. Technically speaking, KL divergence is not a distance metric because it doesn't obey to the triangle inequality ($KL(q||f_\Theta)$ is not equal to $KL(f_\Theta||q)$). It is important to notice that, in the classification use case, minimizing the KL divergence is the same as minimising the cross entropy. Precisely, the KL between two continuous distributions is defined as:

$$\text{KL}(q||f_\Theta) = \int q(\mathbf{x}) \log(\frac{q(\mathbf{x})}{f_\Theta(\mathbf{x})}) d\mathbf{x} = - \int q(\mathbf{x}) \log(f_\Theta(\mathbf{x})) d\mathbf{x} + \int q(\mathbf{x}) \log(q(\mathbf{x})) d\mathbf{x} \tag{34}$$

If we want to minimise KL on the parameter Θ, since the second integral is non-dependant on Θ, we obtain:

$$\min_\Theta \text{KL}(q||f_\Theta) = \min_\Theta - \int q(\mathbf{x}) \log(f_\Theta(\mathbf{x})) d\mathbf{x} = \min_\Theta H(q, f_\Theta) \tag{35}$$

In general, it is preferable using cross entropy, instead of KL divergence, because it is typically easier to compute and optimize. The cross entropy only involves a single sum over the data, whereas the KL divergence involves a double sum. This can make it more computationally efficient, especially when working with large datasets.

6 GENERATIVE LOSSES

In recent years, generative models have become particularly useful for both understanding the complexity of data distributions and being able to regenerate them [36, 37]. In this section, as shown in the Fig. 4, we describe the losses relevant to Generative Adversarial Networks (GANs) and Diffusion Models. However, generative models are not limited to these cases, but extend to include

more models. For example, Variational Auto-Encoders (VAEs) [2, 55, 87] in which the KL-divergence, described in section 5.3.2, is the loss function employed. The objective of the VAE loss is to reduce the discrepancy between the original distribution and its predicted distribution. Other models such as the pixel recurrent neural networks [113] and real-valued Non-Volume Preserving (realNVP) models [27] are not considered in this survey.

Fig. 4. Overview of the generative losses.

6.1 Generative Adversarial Networks

Generative Adversarial Networks (GANs) are used to create new data instances that are sampled from the training data. GANs have two main components:

- The **generator**, referred as $G(\{\mathbf{z}_0, \cdots, \mathbf{z}_N\})$, which generates data starting from random noise and tries to replicate real data distributions
- The **discriminator**, referred as $D(\{\mathbf{x}_0, \cdots, \mathbf{x}_N\})$, which learns to distinguish the generator's fake data from real one. It applies penalties in the generator loss for producing distinguishable fake data compared with real data.

The GAN architecture is relatively straightforward, although one aspect remains challenging: GAN loss functions. Precisely, the discriminator is trained to provide the loss function for the generator. If generator training goes well, the discriminator gets worse at telling the difference between real and fake samples. It starts to classify fake data as real, and its accuracy decreases.

Both the generator and the discriminator components are typically neural networks, where the generator output is connected directly to the discriminator input. The discriminator's classification provides a signal that the generator uses to update its weights through back-propagation.

As GANs try to replicate a probability distribution, they should use loss functions that reflect the distance between the distribution of the data generated by the GAN and the distribution of the real data.

Two common GAN loss functions are typically used: **minimax loss** [38] and **Wasserstein loss** [4]. The generator and discriminator losses derive from a single distance measure between the two aforementioned probability distributions. The generator can only affect one term in the distance measure: the term that reflects the distribution of the fake data. During generator training, we drop the other term, which reflects the real data distribution. The generator and discriminator losses look different, even though they derive from a single formula.

In the following, both minimax and Wasserstein losses are written in a general form. The properties of the loss function (*CONT*, *DIFF*, etc.) are identified based on the function chosen for the generator or discriminator.

6.1.1 Minimax loss. The generative model G learns the data distributions and is trained simultaneously with the discriminative model D. The latter estimates the probability that a given sample is identical to the training data rather than G. G is trained to maximize the likelihood of tricking D [38]. In other words, the generator tries to minimize the following function while the discriminator tries

to maximize it:

$$\mathcal{L}_{minimax}(D, G) = E_{\{\mathbf{x}_0,\cdots,\mathbf{x}_N\}}[\log(D(\{\mathbf{x}_0,\cdots,\mathbf{x}_N\}))] + E_{\{\mathbf{z}_0,\cdots,\mathbf{z}_N\}}[\log(1 - D(G(\{\mathbf{z}_0,\cdots,\mathbf{z}_N\})))],$$
(36)

where:

- $D(\{\mathbf{x}_0,\cdots,\mathbf{x}_N\})$ is the discriminator's estimate of the probability that real data instance $\{\mathbf{x}_0,\cdots,\mathbf{x}_N\}$ is real,
- $E_{\{\mathbf{x}_0,\cdots,\mathbf{x}_N\}}$ is the expected value over all real data instances,
- $G(\{\mathbf{z}_0,\cdots,\mathbf{z}_N\})$ is the generator's output when given noise $\{\mathbf{z}_0,\cdots,\mathbf{z}_N\}$,
- $D(G(z))$ is the discriminator's estimate of the probability that a fake instance is real,
- $E_{\{\mathbf{z}_0,\cdots,\mathbf{z}_N\}}$ is the expected value over all random inputs to the generator (in effect, the expected value over all generated fake instances $G(\{\mathbf{z}_0,\cdots,\mathbf{z}_N\})$).

The loss function above directly represents the cross-entropy between real and generated data distributions. The generator can't directly affect the $\log(D(\{\mathbf{x}_0,\cdots,\mathbf{x}_N\}))$ term in the function, and it only minimizes the term $\log(1 - D(G(\{\mathbf{z}_0,\cdots,\mathbf{z}_N\})))$. A disadvantage of this formulation of the loss function is that the above minimax loss function can cause the GAN to get stuck in the early stages of the training when the discriminator received trivial tasks. Therefore, a suggested modification to the loss [38] is to allow the generator to maximize $\log(D(G(\{\mathbf{z}_0,\cdots,\mathbf{z}_N\})))$.

6.1.2 Wasserstein loss. The Wasserstein distance gives an alternative method of training the generator to better approximate the distribution of the training dataset. In this setup, the training of the generator itself is responsible for minimizing the distance between the distribution of the training and generated datasets. The possible solutions are to use distribution distance measures, like Kullback-Leibler (KL) divergence, Jensen-Shannon (JS) divergence, and the Earth-Mover (EM) distance (also called Wasserstein distance). The main advantage of using Wasserstein distance is due to its differentiability and having a continuous linear gradient [4].

A GAN that uses a Wasserstein loss, known as a WGAN, does not discriminate between real and generated distributions in the same way as other GANs. Instead, the WGAN discriminator is called a "critic," and it scores each instance with a real-valued score rather than predicting the probability that it is fake. This score is calculated so that the distance between scores for real and fake data is maximised.

The advantage of the WGAN is that the training procedure is more stable and less sensitive to model architecture and selection of hyperparameters.

The two loss functions can be written as:

$$\mathcal{L}_{critic} = D(\{\mathbf{x}_0,\cdots,\mathbf{x}_N\}) - D(G(\{\mathbf{z}_0,\cdots,\mathbf{z}_N\})), \ \mathcal{L}_{Generator} = D(G(\{\mathbf{z}_0,\cdots,\mathbf{z}_N\}))$$
(37)

The discriminator tries to maximize $\mathcal{L}_{critic}$. In other words, it tries to maximize the difference between its output on real instances and its output on fake instances. The generator tries to maximize $\mathcal{L}_{Generator}$. In other words, It tries to maximize the discriminator's output for its fake instances.

The benefit of Wasserstein loss is that it provides a useful gradient almost everywhere, allowing for the continued training of the models. It also means that a lower Wasserstein loss correlates with better generator image quality, meaning that it explicitly seeks a minimization of generator loss. Finally, it is less vulnerable to getting stuck in a local minimum than minimax-based GANs [4]. However, accurately estimating the Wasserstein distance using batches requires unaffordable batch size, which significantly increases the amount of data needed [104].

6.2 Diffusion models

Diffusion Models are generative models that rely on probabilistic likelihood estimation to generate data samples. They were originally inspired by the physical phenomena called diffusion. Diffusion Modelling is a learning procedure in which a model can learn the systematic decay of information due to adding a slight noise factor iteratively [100, 101]. The learning procedure enables the possibility of recovering the decayed information from the noise again. They model a series of noise distributions in a Markov Chain and they decode the original data by systematically removing the noises hierarchically [20, 44].

The diffusion process consists of two steps, the forward process and the reconstruction (reverse) process. Gaussian noise is gradually added during the forward diffusion process until the data sample loses its distinguishable features. The reverse process removes the noise and restores the original data by utilizing a neural network model to learn the conditional probability densities.

6.2.1 Forward diffusion process. Given a data point $\mathbf{x_0}$ sampled from a real data distribution $q(\mathbf{x})$. The forward process aims to add a small noise iteratively T times. For every data point $\mathbf{x_0}$ the process produces a sequence of noisy samples $\mathbf{x_1}, \cdots, \mathbf{x_T}$. The noise distributions is usually chosen to be Gaussian. Because the forecast of probability density at time t is only dependent on the immediate predecessor at time $t-1$, the conditional probability density can be calculated as:

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I}) \quad q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}) \tag{38}$$

With a $\beta_t \in (0, 1)$ is a hyperparameter that can be taken as constant or variable and $t \in [1, T]$. As $T \to \infty, \mathbf{x_T}$ becomes a pure Gaussian distribution. We can only sample the new states of the system using the gradient of the density function in Markov Chain updates, according to stochastic gradient Langevin dynamics [120]. The following formula can then be employed to calculate the sampling of a new data point at time t with a step size δ dependent on the prior point at time $t-1$:

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \frac{\delta}{2}\nabla_\mathbf{x} \log q(\mathbf{x}_{t-1}) + \sqrt{\delta}\epsilon_t, \quad \text{where } \epsilon_t \sim \mathcal{N}(0, \mathbf{I}) \tag{39}$$

when $T \to \infty, \epsilon \to 0$ equals to the true probability density $p(\mathbf{x})$. The forward step does not require training a neural network; it only requires an iterative process for adding random Gaussian noises to the original data distribution.

6.2.2 Reverse diffusion process. Given the system's current state, the reverse process requires the calculation of probability density at a previous time step. Calculating the $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ at the time $t = T$ is equal to producing data from an isotropic Gaussian noise. However, contrary to the forward process, the estimation of the past state from the present state requires the knowledge of every previous gradient, which is not feasible without the aid of a learning model that can forecast such estimates. This problem is resolved by training a neural network model that, using the learnt weights Θ and the current state at time t, estimates the value of $p_\Theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ as formalized by the following equation:

$$p_\Theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^{T} p_\Theta(\mathbf{x}_{t-1}|\mathbf{x}_t) \quad p_\Theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\Theta(\mathbf{x}_t, t), \Sigma_\Theta(\mathbf{x}_t, t)) \tag{40}$$

where $\boldsymbol{\mu}_\Theta(\mathbf{x}_t, t)$ is the mean function proposed in [44]. The sample at time $t-1$ can then be computed as:

$$\mathbf{x}_{t-1} = \mathcal{N}\left(\mathbf{x}_{t-1}; \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\Theta(\mathbf{x}_t, t)\right), \Sigma_\Theta(\mathbf{x}_t, t)\right) \tag{41}$$

6.2.3 Diffusion model loss function (CONT, DIFF). The main task of the network model is to minimize the following loss:

$$L_{diffusion} = \mathbb{E}_t \left[\log p(\mathbf{x}_T) - \sum_{t \geq 1} \log \frac{p_\Theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})} \right] \tag{42}$$

In [44, 100], it is shown that a simplified version of $L_{diffusion}$ is able to achieve better results:

$$L_{diffusion}^{\text{simple}} = \mathbb{E}_{t \sim [1,T], \mathbf{x}_0, \epsilon_t} \left[\| \epsilon_t - \epsilon_\Theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\epsilon_t, t) \|^2 \right] \tag{43}$$

It is important to notice that diffusion Models perform significantly better in some applications despite being computationally more expensive than alternative deep network structures [25, 45, 89, 92, 94, 102].

7 RANKING LOSSES

Machine learning can be employed to solve ranking problems, which have important industrial applications, especially in information retrieval systems. These problems can be typically solved by employing supervised, semi-supervised, or reinforcement learning [15, 47].

The goal of ranking losses, in contrast to other loss functions like the cross-entropy loss or MSE loss, is to anticipate the relative distances between inputs rather than learning to predict a label, a value, or a set of values given an input. This is also sometimes called *metric learning*. Nevertheless, the cross-entropy loss can be used in the top-one probability ranking. In this scenario, given the scores of all the objects, the top-one probability of an object in this model indicates the likelihood that it will be ranked first [16].

Ranking loss functions for training data can be highly customizable because they require only a method to measure the similarity between two data points, i.e., similarity score. For example, consider a face verification dataset, pairs of photographs which belong to the same person will have a high similarity score, whereas those that don't will have a low score [118].[2]

In general, ranking loss functions require a feature extraction for two (or three) data instances, which returns an embedded representation for each of them. A metric function can then be defined to measure the similarity between those representations, such as the euclidean distance. Finally, the feature extractors are trained to produce similar representations for both inputs in case the inputs are similar or distant representations in case of dissimilarity.

Similar to Section 6, both pairwise and triplet ranking losses are presented in a general form, as shown in the Fig. 5. The properties of the loss function (*CONT, DIFF*, etc.) are identified based on the metric function chosen.

Fig. 5. Overview of the ranking losses.

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[2]Different tasks, applications, and neural network configurations use ranking losses (like Siamese Nets or Triplet Nets). Because of this, there are various losses can be used, including Contrastive loss, Margin loss, Hinge loss, and Triplet loss.

7.1 Pairwise Ranking loss

In the context of Pairwise Ranking loss, positive and negative pairs of training data points are used [15, 21, 42, 69]. Positive pairs are composed of an anchor sample $\mathbf{x}_a$ and a positive sample $\mathbf{x}_p$, which is similar to $\mathbf{x}_a$ in the metric. Negative pairs are composed of an anchor sample $\mathbf{x}_a$ and a negative sample $\mathbf{x}_n$, which is dissimilar to $\mathbf{x}_a$ in that metric. The objective is to learn representations with a small distance d between them for positive pairs and a greater distance than some margin value m for negative pairs. Pairwise Ranking loss forces representations to have a 0 distance for positive pairs and a distance greater than a margin for negative pairs.

Given $\mathbf{r}_a$, $\mathbf{r}_p$, and $\mathbf{r}_n$ the embedded representations (the output of a feature extractor) of the input samples $\mathbf{x}_a$, $\mathbf{x}_p$, $\mathbf{x}_n$ respectively and d as a distance function the loss function can be written as:

$$L_{pairwise} = \begin{cases} d(\mathbf{r}_a, \mathbf{r}_b) & \text{if positive pair} \\ \max(0, m - d(\mathbf{r}_a, \mathbf{r}_n)) & \text{if negative pair} \end{cases} \tag{44}$$

For positive pairs, the loss will vanish if the distance between the embedding representations of the two elements in the pair is 0; instead, the loss will increase as the distance between the two representations increases. For negative pairs, the loss will vanish if the distance between the embedding representations of the two elements is greater than the margin m. However, if the distance is less than m, the loss will be positive, and the model parameters will be updated to provide representations for the two items that are farther apart. When the distance between $\mathbf{r}_a$ and $\mathbf{r}_n$ is 0, the loss value will be at most m. The purpose of the margin is to create representations for negative pairs that are far enough, thus implicitly stopping the training on these pairs and allowing the model to focus on more challenging ones. If $\mathbf{r}_0$ and $\mathbf{r}_1$ are the pair elements representations, y is a binary flag equal to 0 for a negative pair and to 1 for a positive pair, and the distance d is the euclidean distance:

$$L_{pairwise}(\mathbf{r}_0, \mathbf{r}_1, y) = y||\mathbf{r}_0 - \mathbf{r}_1|| + (1 - y)\max(0, m - ||\mathbf{r}_0 - \mathbf{r}_1||) \tag{45}$$

Unlike typical classification learning, this loss requires more training data and time because it requires access to all the data of all potential pairs during training. Additionally, because training involves pairwise learning, it will output the binary distance from each class, which is more computationally expensive if there is incorrect classification [58].

7.2 Triplet Ranking loss

Employing triplets of training data instances instead of pairs can produce better performance [18, 47, 118]. The resultant loss is called Triplet Ranking loss. A triplet consists of an anchor sample $\mathbf{x}_a$, a positive sample $\mathbf{x}_p$, and a negative sample $\mathbf{x}_n$. The objective is that the distance between the anchor sample and the negative sample representations $d(\mathbf{r}_a, \mathbf{r}_n)$ is greater (and bigger than a margin m) than the distance between the anchor and positive representations $d(\mathbf{r}_a, \mathbf{r}_p)$. The same notation applies:

$$L_{triplet}(\mathbf{r}_a, \mathbf{r}_p, \mathbf{r}_n) = \max(0, m + d(\mathbf{r}_a, \mathbf{r}_p) - d(\mathbf{r}_a, \mathbf{r}_n)) \tag{46}$$

This loss is characterized by three different scenarios based on the values of $\mathbf{r}_a$, $\mathbf{r}_p$, $\mathbf{r}_n$, and m:

- Easy Triplets: $d(\mathbf{r}_a, \mathbf{r}_n) > d(\mathbf{r}_a, \mathbf{r}_p) + m$. In the embedding space, the distance between the negative sample and the anchor sample is already large enough. The model parameters are not changed, and the loss is 0.

- Hard Triplets: $d(\mathbf{r}_a, \mathbf{r}_n) < d(\mathbf{r}_a, \mathbf{r}_p)$. Compared to the positive sample, the negative sample is closer to the anchor. The loss is positive (and $> m$). The model's parameters are subject to change.
- Semi-Hard Triplets: $d(\mathbf{r}_a, \mathbf{r}_p) < d(\mathbf{r}_a, \mathbf{r}_n) < d(\mathbf{r}_a, \mathbf{r}_p) + m$. The loss is still positive (and $< m$) nevertheless, the negative sample is further away from the anchor than the positive sample. The model's parameters are subject to change, and the loss is not 0.

This loss is sensitive to small changes in the input samples, so it cannot be generalized. This means that once the model has been trained on a specific dataset, it cannot be applied to other datasets [58].

8 ENERGY-BASED LOSSES

An Energy-Based Model (EBM) is a probabilistic model that uses a scalar energy function to describe the dependencies of the model variables [28, 31, 33, 34, 40, 41, 64]. An EBM can be formalised as $F : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$, where $F(\mathbf{x}, \mathbf{y})$ stands for the relationship between the $(\mathbf{x}, \mathbf{y})$ pairings.

Given an energy function and the input $\mathbf{x}$, the best fitting value of $\mathbf{y}$ is computed with the following inference procedure:

$$\tilde{\mathbf{y}} = argmin_{\mathbf{y}}\{F(\mathbf{x}, \{\mathbf{y}_0, \cdots, \mathbf{y}_N\})\} \qquad (47)$$

Energy-based models provide fully generative models that can be used as an alternative to probabilistic estimation for prediction, classification, or decision-making tasks [29, 40, 41, 64, 82].

The energy function $E(\mathbf{x}, \mathbf{y}) \equiv F(\mathbf{x}, \mathbf{y})$ can be explicitly defined for all the values of $\mathbf{y} \in \mathcal{Y} = \{\mathbf{y}_0, \cdots, \mathbf{y}_N\}$ if and only if the size of the set $\mathcal{Y}$ is small enough. In contrast, when the space of $\mathcal{Y}$ is sufficiently large, a specific strategy, known as the inference procedure, must be employed to find the $\mathbf{y}$ that minimizes $E(\mathbf{x}, \{\mathbf{y}_0, \cdots, \mathbf{y}_N\})$.

In many real situations, the inference procedure can produce an approximate result, which may or may not be the global minimum of $E(\mathbf{x}, \{\mathbf{y}_0, \cdots, \mathbf{y}_N\})$ for a given $\mathbf{x}$. Moreover, it is possible that $E(\mathbf{x}, \{\mathbf{y}_0, \cdots, \mathbf{y}_N\})$ has several equivalent minima. The best inference procedure to use often depends on the internal structure of the model. For example, if $\mathcal{Y}$ is continuous and $E(\mathbf{x}, \{\mathbf{y}_0, \cdots, \mathbf{y}_N\})$ is smooth and differentiable everywhere concerning $\mathbf{y}$, a gradient-based optimization algorithm can be employed [8].

In general, any probability density function $p(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^D$ can be rewritten as an EBM:

$$p_\theta(\mathbf{x}) = \frac{\exp(-E_\theta(\mathbf{x}))}{\int_{\mathbf{x}'} \exp(-E_\theta(\mathbf{x}'))d\mathbf{x}'}, \qquad (48)$$

where the energy function (E_θ) can be any function parameterised by $\theta \in \Theta$ (such as a neural network). In these models, a prediction (e.g. finding $p(\mathbf{x}_0 | \mathbf{x}_1, \mathbf{x}_2, ...)$) is done by fixing the values of the conditional variables, and estimating the remaining variables, (e.g. $\mathbf{x}_0$), by minimizing the energy function [106, 108, 123].

An EBM is trained by finding an energy function that associates low energies to values of $\mathbf{x}$ drawn from the underlying data distribution, $p_\theta(\mathbf{x}) \sim p_D(\mathbf{x})$, and high energies for values of $\mathbf{x}$ not close to the underlying distribution.

8.1 Training

Given the aforementioned conceptual framework, the training can be thought as finding the model parameters that define the good match between the output ($\mathbf{y} \in \mathcal{Y}$) and the input ($\mathbf{x} \in \mathcal{X}$) for every step. This is done by estimating the best energy function from the set of energy functions ($\mathcal{E}$) by scanning all the model parameters Θ [62, 103], where $\mathcal{E} = \{F(\Theta, X, Y) : \Theta \in \mathcal{W} = \Theta\}$. A loss function should behave similarly to the energy function described in Equation 47, i.e., lower

energy for a correct answer must be modeled by low losses, instead, higher energy, to all incorrect answers, by a higher loss.

Considering a set of training samples $S = \{(\mathbf{x}_i, \mathbf{y}_i) : i = 1, \cdots, N\}$, during the training procedure, the loss function should have the effect of pushing-down $E(\Theta, \mathbf{y}_i, \mathbf{x}_i)$ and pulling-up $E(\Theta, \tilde{\mathbf{y}}_i, \mathbf{x}_i)$, i.e., finding the parameters Θ that minimize the loss:

$$\Theta^* = min_{\Theta \in \mathcal{W}} L_{ebm}(\Theta, S) \tag{49}$$

The general form of the loss function $\mathcal{L}_{ebm}$ is defined as:

$$\mathcal{L}_{ebm}(\Theta, S) = \frac{1}{N} \sum_{i=1}^{N} L_{ebm}(\mathbf{y}_i, E(\Theta, \mathcal{Y}, \mathbf{x}_i)) + \text{regularizer term} \tag{50}$$

Where:

- $L_{ebm}(\mathbf{y}_i, E(\Theta, \mathcal{Y}, \mathbf{x}_i))$ is the per-sample loss
- $\mathbf{y}_i$ is the desired output
- $E(\Theta, \mathcal{Y}, \mathbf{x}_i))$ is energy surface for a given $\mathbf{x}_i$ as $\mathbf{y} \in \mathcal{Y}$ varies

This is an average of a per-sample loss functional, denoted $L_{ebm}(\mathbf{y}_i, E(\Theta, \mathcal{Y}, \mathbf{x}_i))$, over the training set. This function depends on the desired output $\mathbf{y}_i$ and on the energies derived by holding the input sample $\mathbf{x}_i$ constant and changing the output scanning over the sample $\mathcal{Y}$. With this definition, the loss remains unchanged when the training samples are mixed up and when the training set is repeated numerous times [64]. As the size of the training set grows, the model is less likely to overfit [114].

8.2 Loss Functions for EBMs

Following Fig. 6, in this section, we introduce the energy loss first since it is the most straightforward. Then we present common losses in machine learning that can be adapted to the energy based models, such as the Negative Log-Likelihood loss, the Hinge loss, and the Log loss. Subsequently, we introduce more sophisticated losses like the Generalized Perceptron loss and the Generalized Margin loss. Finally, the Minimum classification error loss, the Square-square loss, and its variation Square-exponential loss are presented.
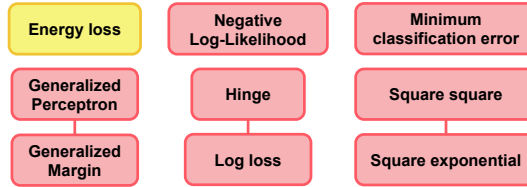

Fig. 6. Schematic overview of the energy based losses with their connection.

8.2.1 Energy loss. The so-called energy loss is the most straightforward loss due to its simplicity. It can be simply defined by using the energy function as the per-sample loss:

$$L_{energy}(\mathbf{y}_i, E(\Theta, \mathcal{Y}, \mathbf{x}_i)) = E(\Theta, \mathbf{x}_i, \mathbf{y}_i) \tag{51}$$

This loss is often used in regression tasks. Accordingly to its definition, it pulls the energy function down for values that are close to the correct data distribution. However, the energy

function is not pulled up for incorrect values. The assumption is that, by lowering the energy function in the correct location, the energy for incorrect values is left higher as a result. Due to this assumption, the training is sensitive to the model design and may result in energy collapse, leading to a largely flat energy function.

8.2.2 Generalized Perceptron loss (L-CONT, CONV).
The Generalized Perceptron loss is defined as:

$$L_{perceptron}(\mathbf{y}_i, E(\mathbf{\Theta}, \mathcal{Y}, \mathbf{x}_i)) = E(\mathbf{\Theta}, \mathbf{y}_i, \mathbf{x}_i) - [\min_{\mathbf{y} \in \mathcal{Y}}]\{E(\mathbf{\Theta}, \{\mathbf{y}_0, \cdots, \mathbf{y}_N\}, \mathbf{x}_i)\} \tag{52}$$

This loss is positive definite as the second term is the lower bound of the first one, i.e., $E(\mathbf{\Theta}, \mathbf{y}_i, \mathbf{x}_i) - [min_{\mathbf{y} \in \mathcal{y}}]\{E(\mathbf{\Theta}, \{\mathbf{y}_0, \cdots, \mathbf{y}_N\}, \mathbf{x}_i)\} \geq 0$. By minimizing this loss, the first term is pushed down and the energy of the model prediction is raised. Although it is widely used [23, 63], this loss is suboptimal as it does not detect the gap between the correct output and the incorrect ones, and it doesn't restrict the function from assigning the same value to each wrong output $\mathbf{y}_i$ and it may produce flat energy distributions [64].

8.2.3 Negative Log-Likelihood loss (CONT,DIFF,CONV).
In analogy with the description in Section 5.3.1, the Negative Log-Likelihood loss (NLL) in the energy-based context is defined as:

$$\mathcal{L}_{NLL}(\mathbf{\Theta}, \mathcal{S}) = \frac{1}{N} \sum_{i=1}^{N} \left(E(\mathbf{\Theta}, \mathbf{y}_i, \mathbf{x}_i) + \frac{1}{\beta} \log \int_{\mathbf{y} \in \mathcal{y}} e^{\beta E(\mathbf{\Theta}, \mathbf{y}, \mathbf{x}_i)} \right) \tag{53}$$

where $\mathcal{S}$ is the training set.

This loss reduces to the perceptron loss when $\beta \rightarrow \infty$ and to the log loss in case $\mathcal{Y}$ has only two labels (i.e., binary classification). Since the integral above is intractable, considerable efforts have been devoted to finding approximation methods, including Monte-Carlo sampling methods [96], and variational methods [51]. While these methods have been devised as approximate ways of minimizing the NLL loss, they can be viewed in the energy-based framework as different strategies for choosing the $\mathbf{y}$'s whose energies will be pulled up [64, 65]. The NLL is also known as the cross-entropy [67] loss and is widely used in many applications, including energy-based models [9, 10]. This loss function formulation is subject to the same limitations listed in section 5.3.1.

8.2.4 Generalized Margin loss.
The generalized margin loss is a more reliable version of the generalized perceptron loss. The general form of the generalized margin loss in the context of energy-based training is defined as:

$$L_{margin}(\mathbf{\Theta}, \mathbf{x}_i, \mathbf{y}_i) = Q_m(E(\mathbf{\Theta}, \mathbf{x}_i, \mathbf{y}_i), E(\mathbf{\Theta}, \mathbf{x}_i, \bar{\mathbf{y}}_i)) \tag{54}$$

Where $\bar{\mathbf{y}}_i$ is the so-called *"most-offending incorrect output"* which is the output that has the lowest energy among all possible outputs that are incorrect [64], m is a positive margin parameter, and Q_m is a convex function which ensures that the loss receives low values for $E(\mathbf{\Theta}, \mathbf{x}_i, \mathbf{y}_i)$ and high values for $E(\mathbf{\Theta}, \mathbf{x}_i, \bar{\mathbf{y}}_i)$. In other words, the loss function can ensure that the energy of the most offending incorrect output is greater by some arbitrary margin than the energy of the correct output.

This loss function is written in the general form and a wide variety of losses that use specific margin function Q_m to produce a gap between the correct output and the wrong output are formalised in the following part of the section.

Hinge loss (L-CONT,CONV). Already explained in section 5.2.2, the hinge loss can be rewritten as:

$$L_{hinge}(\mathbf{\Theta}, \mathbf{x}_i, \mathbf{y}_i) = max(0, m + E(\mathbf{\Theta}, \mathbf{x}_i, \mathbf{y}_i) - E(\mathbf{\Theta}, \mathbf{x}_i, \bar{\mathbf{y}}_i)) \tag{55}$$

This loss enforces that the difference between the correct answer and the most offending incorrect answer be at least m [1, 107]. Individual energies are not required to take a specific value because

the hinge loss depends on energy differences. This loss function shares limitations with the original Hinge loss defined in eq. 16.

Log loss (DIFF,CONT,CONV). This loss is similar to the hinge loss, but it sets a softer margin between the correct output and the most offending outputs. The log loss is defined as:

$$L_{log}(\Theta, \mathbf{x}_i, \mathbf{y}_i) = \log(1 + e^{E(\Theta, \mathbf{x}_i, \mathbf{y}_i) - E(\Theta, \mathbf{x}_i, \bar{\mathbf{y}}_i)}) \tag{56}$$

This loss is also called soft hinge and it may produce overfitting on high dimensional datasets [57].

Minimum classification error loss (CONT, DIFF, CONV). A straightforward function that roughly counts the total number of classification errors while being smooth and differentiable is known as the Minimum Classification Error (MCE) loss [54]. The MCE is written as a sigmoid function:

$$L_{mce}(\Theta, \mathbf{x}_i, \mathbf{y}_i) = \sigma(E(\Theta, \mathbf{x}_i, \mathbf{y}_i) - E(\Theta, \mathbf{x}_i, \bar{\mathbf{y}}_i)) \tag{57}$$

Where σ is defined as $\sigma(x) = (1 + e^{-x})^{-1}$. While this function lacks an explicit margin, it nevertheless produces an energy difference between the most offending incorrect output and the correct output.

Square-square loss (CONT,CONV). Square-square loss deals differently with the energy of the correct output $E(\Theta, \mathbf{x}_i, \mathbf{y}_i)$ and the energy of the most offensive output $E(\Theta, \mathbf{x}_i, \bar{\mathbf{y}}_i)$ as:

$$L_{sq-sq}(\Theta, \mathbf{x}_i, \mathbf{y}_i) = E(\Theta, \mathbf{x}_i, \mathbf{y}_i)^2 + (\max(0, m - E(\Theta, \mathbf{x}_i, \bar{\mathbf{y}}_i)))^2 \tag{58}$$

The combination aims to minimize the energy of the correct output while enforcing a margin of at least m on the most offending incorrect outputs. This loss is a modified version of the margin loss. This loss can be only used when there is a lower bound on the energy function [42, 65].

Square-exponential loss (CONT, DIFF, CONV). This loss is similar to the square-square loss function, and it only differs in the second term:

$$L_{sq-exp}(\Theta, \mathbf{x}_i, \mathbf{y}_i) = E(\Theta, \mathbf{x}_i, \mathbf{y}_i)^2 + \gamma e^{-E(\Theta, \mathbf{x}_i, \bar{\mathbf{y}}_i)} \tag{59}$$

While γ is a positive constant, the combination aims to minimize the energy of the correct output while pushing the energy of the most offending incorrect output to an infinite margin [21, 65, 82]. This loss is considered a regularized version of the aforementioned square-square loss. This loss, as for the Square-square loss, can be only used when there is a lower bound on the energy function [42, 65].

9 CONCLUSION

The definition of an appropriate loss function is a critical part of solving many machine learning problems. In this survey we have described 33 of the most commonly used loss functions from across the machine learning literature. These functions are appropriate for solving a wide range of problems, including classification, regression, sample generation and ranking. Overall, we made an effort to provide a useful resource for newcomers to the machine learning literature and advanced practitioners alike.

Each of the loss functions we describe have also been put into context and compared in a novel taxonomy, introduced in Sec. 2. This gives practitioners a quick view of the different techniques and how they fit together, allowing them to decide and choose the most appropriate approach for their technique quickly and efficiently. We also hope this framing helps researchers to contextualise newly developed loss functions.

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