A First Step Towards Distribution Invariant Regression Metrics

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ABSTRACT
Regression evaluation has been performed for decades. Some metrics have been identified to be robust against shifting and scaling of the data but considering the different distributions of data is much more difficult to address (imbalance problem) even though it largely impacts the comparability between evaluations on different datasets. In classification, it has been stated repeatedly that performance metrics like the F-Measure and Accuracy are highly dependent on the class distribution and that comparisons between different datasets with different distributions are impossible. We show that the same problem exists in regression. The distribution of odometry parameters in robotic applications can for example largely vary between different recording sessions. Here, we need regression algorithms that either perform equally well for all function values, or that focus on certain boundary regions like high speed. This has to be reflected in the evaluation metric. We propose the modification of established regression metrics by weighting with the inverse distribution of function values \( Y \) or the samples \( X \) using an automatically tuned Gaussian kernel density estimator. We show on synthetic and robotic data in reproducible experiments with the inverse distribution of function values using an automatically tuned Gaussian kernel density estimator.\(^\text{†}\)

1 INTRODUCTION
Knowledge discovery for robot is becoming increasingly complex and learning algorithms like regression have to be used to model their dynamics or environment. Consider for example a case of an autonomous vehicle where we record data and want to estimate certain parameters of its odometry model like velocity and acceleration. Due to external factors, we might have more, small accelerations in one experiment and more, high accelerations in another experiment (see also Fig. 1 for examples with non-uniform distributions). We are interested in regression algorithms that are either equally good for all accelerations or prioritize higher accelerations. However, an evaluation on the dataset with small accelerations could produce excellent mean-squared error (MSE), even though the algorithm might be completely off for higher accelerations. The reason could be that high accelerations did not occur that often in the dataset and that the dynamics in those regions are more complicated. When the vehicle moves slowly, parameter relationships might behave linearly whereas for higher accelerations, nonlinear relationships have to be considered. So the evaluation metric might prefer a linear algorithm in contrast to a nonlinear one because it matches the overrepresented small accelerations slightly better. But the nonlinear approach might work perfectly for high accelerations where the linear approach fails. Apart from this, there is the issue that evaluation results on a different dataset will not be comparable because the underlying distributions of samples \( X \) and function values \( Y \) are completely different (also called imbalance problem). We claim that good performance metrics should be independent from dataset properties to enable a good comparison of the regression algorithm. We suggest to compensate for those distribution differences by using a correction by inverse weights from kernel-density estimates.

This approach is closely related to importance sampling in statistics [19]. Given data with a density \( g(x) \), the expected value of a function \( f(x) \) is estimated by sampling \( x_1, \ldots, x_N \) with \( q \) and then calculating: \( E[f|q] = \frac{1}{N} \sum f(x_i) \). The simplified basic idea of importance sampling is to sample with a density \( g(x) \) instead and correct for it by the weighted average

\[
E[f|q] = \frac{\sum f(x_i) w_i}{\sum w_i} \quad \text{with weights } w_i = \frac{g(x_i)}{g(x_i)} .
\]

Importance sampling is usually applied in Monte Carlo methods to calculate an expected value more efficiently or reduce the variance. The main difference to our application is that we don’t look only
at expected values, but rather at different error functions. Furthermore, the evaluation dataset has already been chosen by the data recording. Hence, it is not possible to modify it to calculate the error function more efficiently or reduce the variance—usually all data is used for evaluation. However, from the perspective of importance sampling, metrics like MSE are calculated in the wrong way, assuming data from X has been sampled with density q which is different from the desired density p. The density q could represent the “true density”, the density of a different dataset that we want to compare with, or a density that describes the relevance for the application. Practically, we don’t want to sample from a different density function but use the estimated density of the data being given to correct for the bias in the regression metrics.

Definition: Distribution Invariant Metric Let D1 and D2 be two differently distributed datasets that cover the whole range of interest for the application. A1 and A2 be the true function values, P1 and P2 be the predictions coming from the same regression function (trained on some other data beforehand), and f be a regression metric. We say f is distribution invariant, if and only if \( f(D_1, A_1, P_1) = f(D_2, A_2, P_2) \) for any choice of \( D_1 \) and \( D_2 \).

We are assuming that the true underlying functional relationship stays the same, namely the probability of \( P_i \) given \( D_i \). This makes this topic slightly different to classical covariate shifts and transfer learning [23].

An overview over the imbalance problem in classification, as well as regression, is provided by Branco et al. [2]. They focus on the application perspective, where some prediction values have more relevance/costs than others. A major part of the literature introduces asymmetric loss functions to differentiate between positive and negative errors like a ROC curve for regression [9] and the LIN-LIN loss [4, 6]. For balancing the data, the SMOTE approach for regression has been introduced [33]. For transferring a regression function between different contexts, a reframing concept was presented [10] where the trained model was adapted to new loss functions. This approach does not handle different distributions in the data. A highly related topic is the area of cost sensitive learning. A straightforward approach is to introduce weights in the classical metrics to emphasize certain errors. Still, it remains open how to define those weights and how to handle different \( Y \)-distributions. The same holds for the approaches by Ribeiro et al. [24, 32]. They point out that for some applications, rare values in \( Y \) might be very important and there should be very low error in their prediction.

Furthermore, false predictions that assign those rare values to samples where the true value is not rare, should be avoided. To solve this problem, the user has to define a special handmade relevance function and a threshold for calculating metrics that were inspired by precision and recall.

In contrast, we propose a parameter free solution that also generalizes over evaluations on different datasets and makes them better comparable. So far, the imbalance problem has not been tackled from the distribution perspective by reusing existing metrics. Especially, the lack of comparability between evaluations with different distributions has not yet been addressed at all. Note, different \( Y \)-distributions are a result of the mapping function as well as the underlying distribution of samples (\( X \)). Hence, we compare both approaches. The \( X \)-perspective is motivated by importance sampling and the \( Y \)-perspective by classical approaches for metrics. Apart from evaluation metrics, our approach can be also applied to loss functions as they occur in most regression algorithms.

In Section 2, we review the related work. Our method is introduced in Section 3. For the evaluation in Section 4, we first explore the required kernel-density estimation (KDE, Section 4.1) and then we look at specifically designed synthetic data examples (Section 4.2), as well as a real world application on robotic data (Section 4.3). Finally, we provide a conclusion and discuss future steps in Section 5.

2 RELATED WORK

Looking into the literature, it turns out that classification problems are much more prominent in the machine learning literature than regression problems. For classification tasks, the problem of data imbalance/bias [2, 13, 23, 31, 34] and its effect on the metrics has been discussed exhaustively (see Straube et al. [30] for a review). Kubat et al. [16] point out that accuracy is not a good evaluation metric for data with imbalanced class ratio because good results can be obtained with a constant prediction of the overrepresented class (areas without oil spills in their case). Straube et al. emphasized that the resulting famous F-Measure is not a good way out because it is highly sensitive to the class ratio. This was confirmed from a different perspective by Lipton et al. [18]. Possible solution approaches in classification are metrics that are based on rates like geometric mean, balanced accuracy, or area under roc curve [1, 16, 30]. These methods treat the two different classes equally. An approach from the data perspective is to oversample the underrepresented class or reduce the overrepresented class, which has a similar effect.
So far, there is few literature that tackles the much more challenging counterpart in the regression area. For regression, we do not have two classes, but we have a distribution of the dependent variable, \( Y \), as well as the independent variables, \( X \). The task of the regression model is to construct a function \( f \) that approximates \( f(x_i) = y_i \). Depending on the application, the distribution of \( X \) and \( Y \) cannot be assumed to be fixed or uniform. Note, that a uniform distribution would be the generalization of the balanced class ratio in a classification problem.

### 2.1 Regression Metrics

Relevant regression metrics have been summarized by Witten et al. [36]. The most widely used metric is probably the means-squared error (MSE). This is the error minimized in linear regression, which assumes that the residuals are Gaussian distributed. It is also commonly used for neural networks. Given the predictions \( p_i \) and the actual measured values \( a_i \) from a training set \( x_i \) with \( n \) samples it is defined as

\[
MSE(a, p) = \frac{1}{n} \sum_{i=1}^{n} (p_i - a_i)^2,
\]

\[
RMSE(a, p) = \sqrt{MSE(a, p)}.
\]

Instead of squares it is also possible to use absolute values for the mean absolute error (MAE) [35]:

\[
MAE(a, p) = \frac{1}{n} \sum_{i=1}^{n} |p_i - a_i|.
\]

It is common for classification, to calculate metrics that correspond to random guessing or estimating just one class. The respective counterpart in regression is to look at the average actual values and consider \( p_i = \bar{a} \) as the worst case. Whereas for linear regression, the relative metrics (RSE, RRSE, RAE) should not exceed 1 due to this worst case, this can happen for nonlinear regression problems.

Apart from those straightforward sums, there are also metrics that come from statistics. The (Pearson) correlation coefficient \( \text{PCC} \) [21], takes the correlation of actual and predicted values (relative to the mean values) and normalizes the results by the respective autocorrelations:

\[
PCC(a, p) = \frac{\sum_{i=1}^{n} (p_i - \bar{p})(a_i - \bar{a})}{\sqrt{\sum_{i=1}^{n} (p_i - \bar{p})^2 \cdot \sum_{i=1}^{n} (a_i - \bar{a})^2}}.
\]

If the values are anti-correlated, values of \(-1\) are possible, whereas the maximum value is again \( +1 \).

Another metric from statistics is the \( R^2 \) score or “coefficient of determination” (COD) [3], which is usually defined as \( COD = 1 - RSE \). COD is a statistic for linear regression but widely used for any regression evaluation, whereas the generalization to nonlinear regression [5] is rarely used. If the prediction is worse than the average, COD can obtain large negative numbers lower than \(-1\) in the nonlinear case. Otherwise, it provides scores between \(-1\) for the worst result and a maximum of \(+1\) for the best result. If the prediction is always constant disregarding the input features, COD would then give a score of 0. The explained variance score (EVS) is similar but corrects the nominator of COD by the mean, as it is common for the variance [12]:

\[
EVS(a, p) = 1 - \frac{\sum_{i=1}^{n} ((p_i - a_i) - (\bar{p} - \bar{a}))^2}{\sum_{i=1}^{n} (a_i - \bar{a})^2}.
\]

In this paper, we will not discuss the choice of an appropriate metric but provide an approach to improve all of them using KDE.

### 2.2 Kernel Density Estimation (KDE)

Even though histograms are still quite famous, they are usually not a good approach to represent distributions because histograms can look completely different depending on the underlying discretization (number of bins) [22]. Instead, the more general KDE should be applied to estimate the probability density function [20, 25]. It can be considered as a smooth version of the histogram. The general notation for a KDE is:

\[
g(a) = \frac{1}{n} \sum_{i=1}^{n} K \left( \frac{a - a_i}{h} \right)
\]

where the \( h \) is usually assumed to be independent identically distributed. The kernel function \( K \) is non-negative, with zero mean and an integral of one. Established examples are Gaussian, Tophat, Epanechnikov, exponential, linear, and cosine kernel functions [22]. The parameter \( h \) defines the bandwidth and it is crucial to choose it carefully.

There are several approaches implemented in Python libraries to automatically estimate this bandwidth. Scipy [11] implements two simple heuristics called Scott’s rule [26] \( n^{-1/(d+4)} \) and Silverman’s rule [28] \( n^{-1/(d+2)/4} \) where \( d \) is the dimension of \( Y \). Note that for a good fit, it is required to adapt the bandwidth to the data and optimize it. Hence, cross-validation based optimization is usually a better choice than heuristics. The statsmodels [27] library provides cross-validation, using the maximum likelihood and the integrated mean square error [17].

### 3 METHODS

For classification, a standard approach for imbalanced classification is to determine the correct classifications for each class separately and normalize them by the overall number of instances in this class to obtain ratios like true positive/negative rate and then average them in some sense (geometric/arithmetical mean).

A direct transfer to regression would be to discretize the \( Y \) distribution into bins and calculating the respective histogram. Then, the regression results are divided by the number of occurrences in the respective bin. This means that each bin gets the same relevance in the evaluation. If the large majority of the data is in one bin where the regression algorithm performs perfect but it is “far” off for the other bins, this can be reflected by this measure whereas the common other measures would basically ignore the other bins, if there is just enough data in the correctly estimated bin.

Motivated by the state of the art in KDE (Section 2.2) and our evaluation in Section 4.1, we suggest to use this generalization (i.e., smooth version) of the histogram with a Gaussian kernel and automatic bandwidth tuning with efficient cross-validation using
the maximum likelihood and the integrated mean square. We chose
the Gaussian kernel because of its smoothing properties and general
validity. The KDE model is trained on the actual values \( a_i \) in
the respective testing set. Eventually, the results are weighted by
the inverse of the probability density function applied again to the
respective \( a_i \). The predictions \( (p_i) \) should not be used because they
should not influence this part of the normalization.

Note that this maps the distribution of \( a_i \) basically to a uniform
distribution. If a uniform distribution is considered appropriate,
the weights can be corrected by multiplying it with the target
distribution \( q \) afterwards as it is also done in importance sampling.
This way, too high weights on noisy values at the boundary region
can be avoided. The target distribution could be for example derived
from the training set. Another example in location estimation, when
you want to limit the evaluation to images from Paris. Then you
put zero weight to images from the USA to compare with results
on a different dataset that is solely based on images from Paris.

Let \( g \) be the density function, constructed from the \( a_i \). Our
approach is now to reformulate all sums occurring in the definitions
of metrics in Section 2.1 to arithmetic means \((1/n \sum i=1 \sum (a_i, p_i) )\) and then
replace those by weighted means \(( \sum i=1 \sum g(a_i)^{-1} \cdot (a_i, p_i) / \sum g(a_i)^{-1} )\)
with the inverse distribution function values. With \( (a_i, p_i) \) we de-
note any kind of occurring loss functions. In some examples, there
is a loss function in the nominator as well as the denominatore,
such that multiplying the respective fraction with \( \frac{1}{n \prod i=1} \) provides the
given structure. Hence, our new weighted COD would for example read:

\[
\text{COD}_g(a, p) = 1 - \frac{\sum_{i=1}^{n} \sum g(a_i)^{-1} \cdot (p_i - a_i)^2}{\sum_{i=1}^{n} g(a_i)^{-1} \cdot (a_i - \bar{a})^2},
\]

(5)

All other respective formulas can be found in the Appendix.
Similarly, a correction by the sample distribution \( (X) \) instead of
using the function values \( a_i \) can be performed. Therefore, the KDE
\( g \) is trained on the samples \( x_1 \) that correspond to the true function
values \( a_i \) and \( g(x_1)^{-1} \) is used instead of \( g(a_i)^{-1} \).

Last but not least, this weighting can be combined with other
weightings. Approaches that address costs, priorities, or confidence
could be incorporated on top by weight multiplication. Furthermore,
the distributions from other datasets could be used to make results
comparable to the literature.

4 EVALUATION
First, we evaluate different KDE parameters to select an approach
for the weight correction. Then we carefully analyze the properties
of our new type of metrics on synthetic data and eventually on real
world data for modeling the dynamics of an unmanned underwater
vehicle (UUV).

All code is provided as Jupyter notebooks in Python and data is
uploaded on Github [14]. The provided implementation of our new
approach uses existing libraries like statsmodels and NumPy and
can be directly integrated into existing evaluation frameworks like
scikit-learn [22] and pySPACE [15].

4.1 Analysis of Automatically Tuned Kernel Density Estimation
A general important advice, independent of the evaluation strategy,
is to look at the Y-distribution of the data as a histogram as well as
using a KDE. This can also provide important insights into the data
and raise awareness of the differences between the Y-distribution
and a uniform distribution.

Since we prefer a smooth and non-vanishing density function,
we chose a Gaussian kernel, which showed sufficiently good approx-
imation capabilities on predefined distributions even with small
sample size [14]. If the aforementioned visualization strongly sug-
gests a different kernel, we suggest to provide our weighted metrics
normalized with the Gaussian kernel as well as with the differently
chosen one, to remain comparable.

In a preliminary analysis, we analyzed the approximation ca-
pacities and processing time of KDEs on different distributions:
Gaussians, sum of Gaussians, Laplace, Chi square, and sum of uni-
form and Gaussian distribution (see also Supplement [14]) with
the simple heuristics (Scott’s and Silverman’s rule) and the cross-
validation approaches. In some cases, the simple heuristics
performed much worse than the cross-validation approaches.
Hence they are not a good choice, even though they were much more faster
with around 0.02 seconds, whereas the other approaches needed
around 1 second for 1000 samples with linear increase, for simple
distributions with only one peak. We also tested the efficiency
parameter in statsmodels, which performs the cross-validation on
separate sub-samples of the data to determine the bandwidth \( h \).
For simple distributions, it provided no speed up but turned out to be a
good regularizer for the cross-validation methods which sometimes
showed random drops in performance, when the efficiency option
was not used. For more complex distributions, like the sum of 3
normal distributions, the efficiency parameter is crucial (10 instead
of 75 seconds for 10000 samples). If the time for the KDE fitting
is crucial and too long due to a large number of more than 10000
samples, Scott’s rule could be used instead.

For the following evaluation, we focus on cross-validation with
the mean square error as metric instead of maximum likelihood,
because it slightly performed better in some cases. For training the
KDE, having only 100 samples was sometimes too few and resulted
in a performance below 0.9 COD. Whereas for 200 samples, we
always got a COD better than 0.9 with our chosen method with a
slight increase when using more samples (up to 0.99). Depending
on the data at hand, this approach has to be adapted, when the KDE
is too far off.

In Fig. 1, we show the fitting of the chosen KDE approach to
target variable’s (acceleration, damping) distribution (displayed as
histogram) for three different robotic datasets from UUVs.

If the number of samples is large enough (at least > 1000) and
only a one-dimensional distribution has to be modeled, it is also
possible to use the histogram as a density estimator instead. Similar
to the kernel width, there are heuristics that can determine the
optimal number of bins. A brief comparison showed that from all 6
heuristics in numpym only the approach by Freedman et al. [8] was
sufficient for noisy non-Gaussian distributions and was very close
to the estimated KDE and sometimes even better.
Figure 2: Comparison between classical metrics without weighting (denoted by nw) and our weight correction (denoted by yw and xw) for three different synthetic functions (f1, f2, f3) using the Y-distribution (a) or the X-distribution (b). The x-axis displays the mean of the moving normal distribution (see Section 4.2). A distribution invariant metric would be constant for all means.
4.2 Evaluation on Synthetic Data

For this analysis, we changed the distribution of $Y$ by changing the distribution in $X$ and applying three functions of increasing complexity ($2 \cdot x \cdot |x|, 10 \cdot \cos^2(x)$) with random noise, uniformly sampled from $[0, 0.1]$. The scaling factors $(2, 10)$ are used to map the MSE and MAE to similar ranges at the end. For training we used 300 samples from a uniform distribution from the interval $[-4, 4]$ and 700 samples from a normal distribution with mean $-3$ and standard deviation 0.1. For comparing different distributions and the effect on established metrics as well as our new modification, we consecutively shifted the mean by 1 up to a value of 3 to obtain 7 different testing sets.

As regression algorithm, we used support vector regression [29] from scikit-learn [22] with $\epsilon = 0.1$, kernel='rbf', $\gamma = 10$, and $C = 0.1$. For Function 2 ($x \cdot |x|)$, we chose $C = 0.5$, instead, to get errors in a similar range to simplify joint visualization with the other two functions.

The results are depicted in Fig. 2(a). They show the change of 6 metrics depending on the shifted mean. It can be seen that all classical metrics (without weighting correction) change with the shifting mean in the testing sample distribution but with different patterns for the functions as well as the metrics. This proves the need for distribution invariant regression metrics. Interestingly, our new correction of the metrics by the $Y$-distribution worked very well for Function 1 and 3 but not that well for Function 2 for MSE and MAE, for a mean value of 0 for the $X$-distribution. A possible reason for that might be that even for a uniform distribution of $X$, we would get an accumulation of weights around 0 in $Y$. This indicates that the distribution of $X$ might be more relevant.

Hence, we also tested a correction in the weighting by the probabilities of the underlying samples in $X$. The results are depicted in Fig. 2(b). Now, the modified metrics are almost insensitive to the changing distribution. Slight deviations might be due to inaccuracies in the KDE calculation, because the chosen Gaussian kernel is not that well suited to fit uniform distributions. But note that in normal experiments, uniform sampling rarely occurs.

All in all, for one-dimensional function approximation, weighting based on the $X$-distribution is the best approach to obtain distribution invariant performance values. But when more dimensions are considered for a regression problem, modeling the $X$-distribution might be too computationally expensive or too inaccurate. In such a case, our correction by the $Y$-distribution is still feasible and improves the state of the art in regression evaluation.

4.3 Evaluation on Robotic Data

In this section, we introduce a real world example where we learn the damping term or resistive force of a UUV in one degree of freedom (DOF). Following the definition of [7], the damping term is modeled as a function of the robot’s velocity. For simplicity, we only tackle the yaw DOF of the damping term, which therefore reduces the equation to the following: $d(\nu) = \tau - I_2 \ddot{\nu}$, where $(\nu, \dot{\nu})$ are the robot’s velocity and acceleration respectively, $\tau$ is the control effort due to actuation, and $I_2$ the the robot’s moment of inertia in the yaw DOF. The regression task can be summarized as fitting a function $f$ that maps $f(x_i) = y_i$, where $[x = \nu, y = d(\nu)]$.

5 CONCLUSION AND FUTURE WORK

In this paper, we showed that non-uniform distributions of target variables in regression tasks have an effect on the established regression metrics that cannot be ignored (up to 100% difference). To handle this imbalance, we propose several steps that should be followed to overcome this problem. First, the distribution of actual regression values should be visualized. Second, a KDE, e.g., with a Gaussian kernel if it provides sufficient accuracy, should be fitted to the input samples. Therefore, the efficient cross-validation scheme based on the integrated mean square error ("cv_1s") from the statsmodels library could be used. Third, the distribution fit is used as a (hyperparameter free) methodology to adapt existing evaluation metrics to imbalanced data by using the inverse density values as weights in the the definitions of established metrics. The results on synthetic and robotic data from UUVs show that our modified metrics compensate for the imbalance almost perfect. If a corrections by the $X$-distribution is not possible, the $Y$-distribution can be used instead and still provides much better results than the state of the art.

In future, we would like to look into other applications such as location estimation and origami difficulty estimation. We want to analyze more functions with more dimensions as input, or output, and with sparse distributions. Last but not least, we want to incorporate our new evaluation concept into the loss function of support vector regression or deep neural networks.

APPENDIX

This section lists the detailed formulas for the new distribution invariant regression metrics.
Figure 3: Comparison between classical metrics without weighting (denoted by nw) and our weight correction using the X-distribution (xw) as well as the Y-distribution (yw) on dataset 1 (d1) and the reformulated dataset 3 (d3) for modeling the damping. The x-axis displays the index of the overrepresented chunk (see Section 4.3). A distribution invariant metric would be constant for all indices.

\[
\begin{align*}
MSE_x(a, p) &= \frac{\sum_{i=1}^{n} g(a_i)^{-1} \cdot (p_i - a_i)^2}{\sum_{i=1}^{n} g(a_i)^{-1}} \\
RMSE_x(a, p) &= \sqrt{MSE_x(a, p)} \\
MAE_x(a, p) &= \frac{\sum_{i=1}^{n} g(a_i)^{-1} \cdot |p_i - a_i|}{\sum_{i=1}^{n} g(a_i)^{-1}} \\
RSE_x(a, p) &= \frac{\sum_{i=1}^{n} g(a_i)^{-1} \cdot (p_i - a_i)^2}{\sum_{i=1}^{n} g(a_i)^{-1} \cdot (a_i - \bar{a})^2} \\
RRSE_x(a, p) &= \sqrt{RSE_x(a, p)} \\
RAE_x(a, p) &= \frac{\sum_{i=1}^{n} g(a_i)^{-1} \cdot |p_i - a_i|}{\sum_{i=1}^{n} g(a_i)^{-1} \cdot |a_i - \bar{a}|} \\
PCC_x(a, p) &= \frac{\sum_{i=1}^{n} (p_i - \bar{p})(a_i - \bar{a}) g(a_i)}{\sqrt{\sum_{i=1}^{n} (p_i - \bar{p})^2 g(a_i) \cdot \sum_{i=1}^{n} (a_i - \bar{a})^2 g(a_i)}} \\
EVSE_x(a, p) &= 1 - \frac{\sum_{i=1}^{n} ((p_i - a_i) - \bar{p} - \bar{a})^2}{\sum_{i=1}^{n} g(a_i)^{-1} \cdot (a_i - \bar{a})^2}
\end{align*}
\]

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