On Many-to-Many Mapping Between Concordance Correlation Coefficient and Mean Square Error

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Abstract

The concordance correlation coefficient (CCC) is one of the most widely used reproducibility indices, introduced by Lin in 1989. In addition to its extensive use in assay validation, CCC serves various different purposes in other multivariate population-related tasks. For example, it is often used as a metric to quantify an inter-rater agreement. It is also often used as a performance metric for prediction problems. In terms of the cost function, however, there has been hardly any attempt to design one to train the predictive deep learning models. In this paper, we present a family of lightweight cost functions that aim to also maximise CCC, when minimising the prediction errors. To this end, we first reformulate CCC in terms of the errors in the prediction; and then as a logical next step, in terms of the sequence of the fixed set of errors. To elucidate our motivation and the results we obtain through these error rearrangements, the data we use is the set of gold standard annotations from a well-known database called ‘Automatic Sentiment Analysis in the Wild’ (SEWA), popular thanks to its use in the latest Audio/Visual Emotion Challenges (AVEC’17 and AVEC’18). We also present some new and interesting mathematical paradoxes we have discovered through this CCC reformulation endeavour.
1 Introduction

The need to quantify inter-rater, inter-device or inter-method agreement arises often in the field of biometrics. The ‘inter-rater agreement’ and ‘inter-device agreement’ scenarios refer to the situations, where quantifying the extent of agreement between two or more examiners or devices is of primary interest. For example, before any new instrument can be introduced to the market, it is necessary to assess first whether the new assay reproduces the measurements consistent with the traditional gold-standard assay [21, 22, 43]. Inter-rater agreement is for example important, when severity of a specific disease is evaluated by different raters during a clinical trial, and the reliability of each of their subjective evaluation is to be determined by measuring agreement among the raters [13]. Inter-rater agreement evaluations are further popular in the fields such as psychology, psychobiology, anthropology, and cognitive science, where subjectivity coupled with a multitude of factors directly influences the assessment of the variable under observation [41]. Inter-method comparisons are made, when a bivariate population results from two disparate methods. For example, comparing the gold standard sequences (e.g., device measurements) against the prediction sequences from a trained machine learning model, or the annotation sequences from an independent observer.

A quest for a summary statistic, that effectively represents the extent of association between two variables, has led researchers to invent several different indices. As for the nominal and ordinal classification tasks, Cohen’s kappa coefficient ($\kappa$) [36, 12, 6], and intraclass correlation coefficient ($ICC$) [9, 17] are the more commonly used reproducibility indices. The Pearson correlation coefficient or simply the ‘correlation coefficient’ ($\rho$) [10, 11, 30], concordance correlation coefficient ($\rho_c$) [21] are arguably the most popular performance measures when it comes to the regression tasks and the ordinal classifications. In this paper, we focus on the problem involving only the bivariate population featuring the continuous regression values, or the ordinal classes.

While there exist multiple ways to interpret a correlation coefficient ($\rho$) [20, 38], $\rho$ essentially represents the extent to which a linear relationship between two variables exists. $\rho$ is the covariance of the two variables divided by the product of their standard deviations.
Thus, given a bivariate population \( X := (x_i)^N_1 \) and \( Y := (y_i)^N_1 \),

\[
\rho = \frac{\text{cov}(X, Y)}{\sigma_X \sigma_Y} = \frac{\sigma_{XY}}{\sigma_X \sigma_Y},
\]

\[
\sum_{i=1}^{n} (x_i - \mu_X)(y_i - \mu_Y)
\]

\[
\sqrt{\sum_{i=1}^{n} (x_i - \mu_X)^2} \sqrt{\sum_{i=1}^{n} (y_i - \mu_Y)^2}
\]

where, \( \mu_X = \frac{1}{N} \sum_{i=1}^{N} x_i \), \( \sigma_X = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (x_i - \mu_X)^2} \), \( \mu_Y = \frac{1}{N} \sum_{i=1}^{N} y_i \), \( \sigma_Y = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_i - \mu_Y)^2} \),

and \( \text{cov}(X, Y) = \sigma_{XY} = \frac{1}{N} \sum_{i=1}^{n} (x_i - \mu_X)(y_i - \mu_Y) \).

Covariance is a measure of the strength of the joint variability between two variables. When the greater values of one are often associated with the lesser values of another, the covariance is negative. When they grow together, the covariance is positive. The magnitude of the covariance is harder to interpret, as it depends largely on how deviated the magnitudes of the two variables are from their respective mean values. It is thus normalised by the standard deviations of both the variables to effectively yield \( \rho \). To compute the covariance in the numerator in Equation (2), \( X \) and \( Y \) are first centred around zero by subtracting the mean of each of the variables separately, before the sum of products of the centred variables is obtained. The scales of the variables, too, are then normalised by the denominator. \( \rho \) is, therefore, a centred and standardised sum of inner-product of the two variables. The magnitude of the denominator can only be greater than or equal to that of the numerator owing to the Cauchy-Schwarz inequality. Thus, \( \rho \in [-1, 1] \).

While \( \rho \) signifies a linear relationship, the \( \rho \) measure fails to quantitatively distinguish between a linear relationship and an identity relationship. The \( \rho \) measure also fails to quantitatively distinguish between the linear relationship with a constant offset, the one without any offset, and an identity relationship. In summary, it fails to capture any departure from the 45° (slope = 1) line, i.e., any shifts in the scale (slope) and the location (offset). Thus, while successful in capturing the precision of the linear relationship, the \( \rho \) measure completely misses out on the accuracy.

Lin in 1989 proposed CCC or Lin’s coefficient \( (\rho_c) \), which is a product of \( \rho \) with the term \( C_b \) that penalises such deviations in the scale and the location [21]. The \( C_b \) component captures the accuracy, while the \( \rho \) component represents the
precision. Formally,\[ C_b = \frac{2}{\left(v + \frac{1}{v} + u^2\right)}, \] (3)
where, \( v = \frac{\sigma_X}{\sigma_Y} \) = the scale shift, \( u = \frac{(\mu_X - \mu_Y)}{\sqrt{\sigma_X \sigma_Y}} \) = the location shift relative to the scale. (4)

Substituting Equation (4) and Equation (5) in Equation (3), we get
\[ C_b = \frac{2}{\left(\frac{\sigma_X}{\sigma_Y} + \frac{\sigma_Y}{\sigma_X} + \left(\frac{\mu_X - \mu_Y}{\sqrt{\sigma_X \sigma_Y}}\right)^2\right)}, \] (6)
\[ = \frac{2\sigma_X \sigma_Y}{\sigma_X^2 + \sigma_Y^2 + (\mu_X - \mu_Y)^2}. \] (7)

\( \rho_c \) is, thus, given by the following:
\[ \rho_c = \rho C_b, \]
\[ = \frac{2\rho}{\left(v + \frac{1}{v} + u^2\right)}, \]
\[ = \frac{2\rho}{\frac{\sigma_X}{\sigma_Y} + \frac{\sigma_Y}{\sigma_X} + \left(\frac{\mu_X - \mu_Y}{\sqrt{\sigma_X \sigma_Y}}\right)^2}, \]
\[ = \frac{2\rho \sigma_X \sigma_Y}{\sigma_X^2 + \sigma_Y^2 + (\mu_X - \mu_Y)^2}. \] (7)

The concordance correlation coefficient \( (\rho_c) \) has the following characteristics:
-1 \leq -|\rho| \leq \rho_c \leq |\rho| \leq 1.
\( \rho_c = 0 \) if and only if: \( \rho = 0. \)
\( \rho_c = \rho \) if and only if: \( \sigma_1 = \sigma_2 \) and \( \mu_1 = \mu_2. \)
\( \rho_c = \pm 1 \) if and only if:
\[ (\mu_X - \mu_Y)^2 + (\sigma_X - \sigma_Y)^2 + 2\sigma_X \sigma_Y (1 \mp \rho) = 0, \]
i.e., if and only if:
\[ \rho = \pm 1, \sigma_X = \sigma_Y, \text{ and } \mu_X = \mu_Y, \]
i.e., if and only if:
\[ x_i \text{ and } y_i \text{ are in perfect } (\rho_c = 1) \text{ agreement, or } \]
x_i and y_i are in perfect reverse \( (\rho_c = -1) \) agreement.

Since Lin’s pioneering work, numerous articles have been published advancing the field. The CCC-measure is based on the expected value of the squared
difference between X and Y. In terms of the distance function used, a more
generalised version has since been proposed \cite{16, 15}, also establishing its similarities to the kappa and weighted kappa coefficients. Some others have extended the applicability of CCC to more than two measurements by proposing new reliability coefficients, e.g., the overall concordance correlation coefficient \cite{3, 1, 2}. Alternative estimators for evaluating agreement and reproducibility based on the CCC have also been proposed \cite{31, 37}. Comparing the CCC against the previously existing four intraclass correlation coefficients presented in \cite{35, 24}, Nickerson presents a strong critique of the contributions of the CCC-measure in evaluating reproducibility \cite{26}. The usability and apparent paradoxes associated with the reliability coefficients have been thoroughly and vehemently debated upon \cite{8, 44, 18}. However, CCC remains arguably one of the most popular reproducibility indices, used in a wide range of fields, e.g., cancer detection and treatment \cite{27, 25}, comparison of the analysis method for MRI brain scans \cite{19}, or Magnetic resonance fingerprinting \cite{23}. The popularity of the measure has encouraged researchers to publish macros and software packages likewise \cite{4, 7}. When it comes to instance-based ordinal classification, regression, or a sequence prediction task, the machine learning community likewise has begun adapting CCC as the performance measure of choice \cite{39, 28, 29}. Take the case of the ‘Audio/Visual Emotion Challenge and Workshops’ (AVEC) for example. The shift is noticeable, with early challenges using RMSE as the winning criteria, to now CCC in those recently held \cite{32, 40, 33, 34}. Almost without exception, the winners of these challenges have lately used deep learning models, which are trained to model the input to output (the raw data or features to prediction) mapping through minimisation of a cost function. A cost function nominally captures the difference between a prediction from a model and the desired output; its job, consequently, is to encourage a model to drive the prediction of the model close to the desired value. While the shift in the community to use the CCC measure as a performance metric is definitely underway, no attempts have been made to design a cost function specifically tailored to boost CCC, barring a lone exception \cite{42}.

The cost function used in \cite{42} is directly the CCC, which is computationally expensive to use at every training step. This is because, the computation of CCC necessitates computation of standard deviations of the gold standard and the prediction, covariance between the gold standard and the prediction, and the difference between the mean values at every iteration. Also, because CCC is being used as a cost function, the partial derivative of CCC with respect to the outputs needs to be recalculated as well, to propagate the error down to the input layers using the backpropagation algorithm in neural networks – again, at every step in the training iteration. In this paper, we therefore identify and isolate workable lightweight functions which directly have an impact on the CCC metric. We achieve this by dividing the CCC into its constituent components through reformulation of the CCC in terms of the prediction errors. Recognising the terms that are affected by the error or the prediction ‘sequence’ alone, we propose a family of candidate cost functions.

We present next the overall organisation of the paper. In Section 3, we
formally define the problem we attempt to tackle. In Section 4 and Section 5 we rework the CCC formulation through two slightly different substitutions in terms of the prediction sequences. Interestingly, we arrive at mutually contradictory requirements in terms of the redistribution of error values. We present these interesting insights and paradoxes in Section 6. We then go on to establish conditions that help us conclusively determine which of the two reformulations yields us a better CCC in Section 7. We supplement our findings with illustrations in Section 8. Learning from these insights, we present a family of candidate cost functions in Section 9. In Section 10 we summarise our motivation, the resulting findings and our planned future work as we conclude.
2 Many to Many Mapping between MSE and CCC In General

\[
\therefore \sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY} = \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu_X)^2 + \frac{1}{N} \sum_{i=1}^{N} (y_i - \mu_Y)^2 - \frac{2}{N} \sum_{i=1}^{N} (x_i - \mu_X)(y_i - \mu_Y)
\]

\[
= \frac{1}{N} \sum_{i=1}^{N} [(x_i - \mu_X)^2 + (y_i - \mu_Y)^2 - 2(x_i - \mu_X)(y_i - \mu_Y)]
\] (8)

\[
= \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu_X - y_i + \mu_Y)^2
\] (9)

\[
= \frac{1}{N} \sum_{i=1}^{N} [(x_i - y_i) - (\mu_X - \mu_Y)]^2
\] (10)

\[
= \frac{1}{N} \sum_{i=1}^{N} [(x_i - y_i)^2 + (\mu_X - \mu_Y)^2 - 2(x_i - y_i)(\mu_X - \mu_Y)]
\]

\[
= MSE + \frac{1}{N} \sum_{i=1}^{N} [(\mu_X - \mu_Y)^2 - 2(x_i - y_i)(\mu_X - \mu_Y)]
\]

\[
= MSE + \frac{1}{N} \sum_{i=1}^{N} (\mu_X - \mu_Y)^2 - \frac{2}{N} \sum_{i=1}^{N} (x_i - y_i)(\mu_X - \mu_Y)
\]

\[
= MSE + \frac{1}{N} \cdot N \cdot (\mu_X - \mu_Y)^2
\]

\[
= MSE + \frac{1}{N} \cdot N \cdot (\mu_X - \mu_Y)^2
\]

\[
- \frac{2}{N} \cdot \left( \frac{x_1 + x_2 + \ldots + x_N}{N} - \frac{y_1 + y_2 + \ldots + y_N}{N} \right) \cdot \left( \frac{x_1 + x_2 + \ldots + x_N}{N} - \frac{y_1 + y_2 + \ldots + y_N}{N} \right)
\]

\[
= MSE + \frac{1}{N} \cdot N \cdot (\mu_X - \mu_Y)^2 - \frac{2}{N} \left( N\mu_X - N\mu_Y \right) \left( \mu_X - \mu_Y \right)
\]

\[
= MSE - (\mu_X - \mu_Y)^2
\]

\[
\therefore \sigma_X^2 + \sigma_Y^2 + (\mu_X - \mu_Y)^2 = MSE + 2\sigma_{XY}
\]
\[
\therefore \rho_c = \frac{2\sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 + (\mu_X - \mu_Y)^2} \\
= \frac{2\sigma_{XY}}{MSE + 2\sigma_{XY}} = \frac{1}{1 + \frac{MSE}{2\sigma_{XY}}} \\
= \left(1 + \frac{MSE}{2\sigma_{XY}}\right)^{-1}
\]

3 Many to Many Mapping for a Fixed Set of Prediction Errors

Inspired by the discovery that the predictions with identical mean square error can result in different values of CCC, we attempt to decouple the components of CCC that are dependent on merely the magnitudes of errors, from those directly impacted by the sequence of errors. We, thus, formulate our problem as follows.

Given (1) a gold standard time series, \(G := (g_i)_1^N\), and (2) a fixed set of error values, \(E := (e_i)_1^N\) (thus a fixed mean square error (MSE)), find the distribution(s) of error values that achieve(s) the highest possible CCC.

Let the prediction and the gold standard sequence be \(X := (x_i)_1^N\) and \(Y := (y_i)_1^N\), not necessarily in that order. As the formula for \(\rho_c\) is symmetric with respect to \(X\) and \(Y\), which variable represents what sequence does not matter, as far as \(\rho_c\) is concerned.

From Equation (2) and Equation (7), we note:

\[
\rho_c = \frac{2\sigma_{XY}}{(\mu_Y - \mu_X)^2 + \sigma_X^2 + \sigma_Y^2},
\]

where, \(\sigma_{XY} = \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu_X)(y_i - \mu_Y)\),

\[
\mu_X = \frac{1}{N} \sum_{i=1}^{N} x_i, \quad \sigma_X = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (x_i - \mu_X)^2},
\]

and \(\mu_Y = \frac{1}{N} \sum_{i=1}^{N} y_i, \quad \sigma_Y = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_i - \mu_Y)^2}\).

Now, let \(d_i := x_i - y_i\), and \(\mu_D := \frac{1}{N} \sum_{i=1}^{N} d_i\).

\[
\therefore \mu_D = \mu_X - \mu_Y, \quad \therefore \text{Equations (24) to (26)}
\]

\[
\therefore \text{MSE} := \frac{1}{N} \sum_{i=1}^{N} d_i^2, \quad \text{RMSE} := \sqrt{\frac{1}{N} \sum_{i=1}^{N} d_i^2} = \sqrt{\text{MSE}}, \quad \text{MAE} := \frac{1}{N} \sum_{i=1}^{N} |d_i|.
\]
\[ \rho_c = \frac{2}{N} \frac{\sum_{i=1}^{N} (x_i - \mu_X)(y_i - \mu_Y)}{(\mu_Y - \mu_X)^2 + \sigma_X^2 + \sigma_Y^2}. \]

\[ \therefore \quad \rho_c = \frac{2}{N} \frac{\sum_{i=1}^{N} (x_i - \mu_X)(y_i - \mu_Y)}{N(\mu_D)^2 + \sum_{i=1}^{N} (x_i - \mu_X)^2 + \sum_{i=1}^{N} (y_i - \mu_Y)^2}. \]

\[ \therefore \quad \text{Equations (22) and (23)} \quad (29) \]

\[ \therefore \quad \text{Equations (24) to (26)} \quad (30) \]

### 4 Formulation 1: Replacing \((x_i)\) with \((y_i + d_i)\)

\[ \rho_c = \frac{2}{N} \frac{\sum_{i=1}^{N} (y_i + d_i - \mu_Y - \mu_D)(y_i - \mu_Y)}{N(\mu_D)^2 + \sum_{i=1}^{N} (y_i + d_i - \mu_Y - \mu_D)^2 + \sum_{i=1}^{N} (y_i - \mu_Y)^2}. \]

\[ \text{Rewriting the individual terms in terms of } (y_i - \mu_Y) \]

\[ \rho_c = \frac{2}{N} \frac{\sum_{i=1}^{N} (y_i - \mu_Y)^2 - \sum_{i=1}^{N} \mu_D(y_i - \mu_Y) + \sum_{i=1}^{N} d_i(y_i - \mu_Y)}{N\mu_D^2 + 2 \sum_{i=1}^{N} (y_i - \mu_Y)^2 - 2 \sum_{i=1}^{N} \mu_D(y_i - \mu_Y) + 2 \sum_{i=1}^{N} d_i(y_i - \mu_Y) + \sum_{i=1}^{N} (d_i - \mu_D)^2}. \]

\[ \text{Now, } \sum_{i=1}^{N} \mu_D(y_i - \mu_Y) = \mu_D \sum_{i=1}^{N} (y_i - \mu_Y) = \mu_D(N\mu_Y - N\mu_Y) \therefore \text{Equation (25)} \quad (33) \]

which cancels out a term from both the numerator and the denominator.

\[ \rho_c = \frac{2}{N} \frac{\sum_{i=1}^{N} (y_i - \mu_Y)^2 - \sum_{i=1}^{N} \mu_D(y_i - \mu_Y) + \sum_{i=1}^{N} d_i(y_i - \mu_Y)}{N\mu_D^2 + 2 \sum_{i=1}^{N} (y_i - \mu_Y)^2 - 2 \sum_{i=1}^{N} \mu_D(y_i - \mu_Y) + 2 \sum_{i=1}^{N} d_i(y_i - \mu_Y) + \sum_{i=1}^{N} (d_i - \mu_D)^2} \]

\[ = \frac{2N\sigma_Y^2 + 2 \sum_{i=1}^{N} d_i(y_i - \mu_Y)}{N\mu_D^2 + 2N\sigma_Y^2 + 2 \sum_{i=1}^{N} d_i(y_i - \mu_Y) + \left( \sum_{i=1}^{N} \mu_D^2 - 2 \sum_{i=1}^{N} d_i \mu_D + \sum_{i=1}^{N} d_i^2 \right)}. \]

\[ \text{(35)} \]
The terms underlined in Equation (35) above, thus, sum to zero. That is,

\[\sum_{i=1}^{N} \mu_i^2 - 2 \sum_{i=1}^{N} d_i \mu_D = N \mu_D^2 + N \mu_D^2 - 2 N \mu_D^2 = 0.\]  

(36)

\[\therefore \rho_c = \frac{2 N \sigma_y^2 + 2 \sum_{i=1}^{N} d_i (y_i - \mu_Y)}{N \mu_D^2 + 2 N \sigma_Y^2 + 2 \sum_{i=1}^{N} d_i (y_i - \mu_Y) + \left( \sum_{i=1}^{N} \mu_D^2 - 2 \sum_{i=1}^{N} d_i \mu_D + \sum_{i=1}^{N} d_i^2 \right)}.
\]

(37)

\[= \frac{2 N \sigma_Y^2 + 2 \sum_{i=1}^{N} (y_i - \mu_Y) d_i}{2 N \sigma_Y^2 + 2 \sum_{i=1}^{N} (y_i - \mu_Y) d_i + N (MSE)} \therefore \sum_{i=1}^{N} d_i^2 = N (MSE).\]  

(38)

\[= 1 - \left( \frac{N (MSE)}{2 N \sigma_Y^2 + 2 \sum_{i=1}^{N} y_i d_i - 2 N \mu_Y \mu_D + N (MSE)} \right) \therefore \sum_{i=1}^{N} d_i = N \mu_D.
\]

(39)

For a given gold standard \(Y\) and a set of \(\{d_i\}\) values, maximisation of \(\rho_c\) requires that \(\sum_{i=1}^{N} (y_i) d_i\) is maximised.

5 Formulation 2: Replacing \((y_i)\) with \((x_i - d_i)\)

\[\rho_c = \frac{2 \sum_{i=1}^{N} (x_i - \mu_X)(x_i - d_i - \mu_X + \mu_D)}{N (\mu_D)^2 + \sum_{i=1}^{N} (x_i - d_i - \mu_X + \mu_D)^2 + \sum_{i=1}^{N} (x_i - \mu_X)^2}\therefore \text{Equation (30)}.\]  

(40)

Continuing as in Section 4 (cf. Appendix 1), we get

\[\rho_c = \frac{2 N \sigma_X^2 - 2 \sum_{i=1}^{N} (x_i - \mu_X)d_i}{2 N \sigma_X^2 - 2 \sum_{i=1}^{N} (x_i - \mu_X)d_i + N (MSE)}\]

(41)

\[= 1 - \left( \frac{N (MSE)}{2 N \sigma_X^2 - 2 \sum_{i=1}^{N} x_i d_i + 2 N \mu_X \mu_D + N (MSE)} \right) .\]  

(42)
For a given gold standard \( X \) and a set of \( \{d_i\} \) values, maximisation of \( \rho_c \) requires that \( \sum_{i=1}^{N} (x_i)d_i \) is minimised.

6 The Paradoxical Nature of the Conditions on the Error-set

The concluding remarks of Section 4 and Section 5 imply that we arrive at mutually contradictory requirements in terms of the rearrangement of values in the error set. Likely because, given a set of error values and a gold standard sequence, two different candidate sequences may be generated yielding a high CCC, for a given MSE.

However, when devising a cost function in terms of the predicted sequence itself, the requirements implied by both formulations converge to being the same fortunately. We discuss this rediscovery of consistency, arising interestingly out of contradictory insights next. To this end, we formally (and this time unambiguously) redefine the symbols for prediction sequence, gold standard sequence and the error sequence – instead of using \( X \) and \( Y \) interchangeably, albeit in different sections (Sections 4 and 5).

Let \( G := (g_i)_1^N \), \( E := (e_i)_1^N \), and \( P := (p_i)_1^N \) be the gold standard sequence, the error sequence and the prediction sequence respectively. Let \( \mu_G \), \( \mu_E \), and \( \mu_P \) be the arithmetic means of the sequences \( G \), \( E \), and \( P \) respectively.

6.1 Paradoxical requirements in terms of the \( \left(\sum_{i=1}^{N} g_ie_i\right) \) summation

As noted in Sections 4 and 5, the formulations 1 and 2 end up in exactly the contradictory requirements in terms of the product summation \( \left(\sum_{i=1}^{N} g_ie_i\right) \).

Specifically, to maximise \( \rho_c \):

- The formulation in the Section 4 requires maximisation of the \( \left(\sum_{i=1}^{N} g_ie_i\right) \) quantity.
- The formulation in the Section 5 requires minimisation of the \( \left(\sum_{i=1}^{N} g_ie_i\right) \) quantity.

6.2 Paradoxical requirements in terms of redistribution of the values in the error set

- The requirement posed by the formulation in the Section 4, i.e., the maximisation of \( \left(\sum_{i=1}^{N} g_ie_i\right) \), necessitates that the error values are in the same sorted order as of the gold standard values (cf. Appendix 2).
- That is, a larger \( e_i \) needs to get multiplied with the larger \( g_i \).
The requirement posed by the formulation in Section 5, i.e., the minimisation of \( \sum_{i=1}^{N} g_i e_i \), necessitates that the error values are in the opposite order as of the gold standard values (cf. Appendix 2).

That is, a smaller \( e_i \) needs to get multiplied with the larger \( g_i \).

In other words, taking into account not only the magnitudes, but also the signs, the error values need to be sorted in the same order as of the elements of the time series, when it comes to the first \( \rho_c \) formulation. In case of the second formulation, the errors need to be sorted in exactly the opposite order as of the elements of the time series.

Thus, there exist two prediction sequences that correspond to identical set of error values when compared against the gold standard sequence, but likely maximise \( \rho_c \).

6.3 Consistent requirements in terms of the \( \left( \sum_{i=1}^{N} g_i p_i \right) \) summation

While it has been established that there exist two distinct prediction sequences with identical mean square error and error value set, and despite the existence of the contradictory conditions on the underlying error redistribution, the conditions for the \( \rho_c \) maximisation in terms of the product summation \( \sum_{i=1}^{N} g_i p_i \) are consistent in both the formulations. In summary, the formulations 1 and 2 end up in identical requirements in terms of the product summation \( \left( \sum_{i=1}^{N} g_i p_i \right) \).

The consistency in the requirement can be proven as follows.

According to the first formulation,

- \( E = P - G \), i.e., \( (e_i)_1^N = (p_i)_1^N - (g_i)_1^N \), and the quantity \( \left( \sum_{i=1}^{N} g_i e_i \right) \) needs to be maximised.
- That is, the quantity \( \left( \sum_{i=1}^{N} g_i (p_i - g_i) \right) \) needs to be maximised,
- implying the quantity \( \left( \sum_{i=1}^{N} g_i (p_i) \right) \) needs to be maximised, since \( \left( \sum_{i=1}^{N} g_i^2 \right) \) is constant for any given gold standard.

According to the second formulation,

- \( E = G - P \), i.e., \( (e_i)_1^N = (g_i)_1^N - (p_i)_1^N \), and the quantity \( \left( \sum_{i=1}^{N} g_i e_i \right) \) needs to be minimised.
- That is, the quantity \( \left( \sum_{i=1}^{N} g_i (g_i - p_i) \right) \) needs to be minimised.
- implying the quantity \( \left( \sum_{i=1}^{N} g_i (p_i) \right) \) needs to be maximised, since \( \left( \sum_{i=1}^{N} g_i^2 \right) \) is constant for any given gold standard.
7 The Quest for Highest Achievable CCC

Having obtained the two prediction sequences corresponding to the same set of error values, let us now compare the two concordance correlation coefficients we obtain. Our attempt here is to determine conclusively which of the two prediction sequences will correspond to the higher of the two CCCs. If this is not possible, our aim here is to, at the very least, establish the conditions under which one can choose the prediction sequence conclusively.

The Chebyshev’s sum inequality [14] states that

$$\frac{1}{n} \sum_{k=1}^{n} a_k \cdot b_k \geq \left( \frac{1}{n} \sum_{k=1}^{n} a_k \right) \left( \frac{1}{n} \sum_{k=1}^{n} b_k \right),$$

(43)

and if

$$\frac{1}{n} \sum_{k=1}^{n} a_k \cdot b_k \leq \left( \frac{1}{n} \sum_{k=1}^{n} a_k \right) \left( \frac{1}{n} \sum_{k=1}^{n} b_k \right),$$

(44)

Let $iE := (i\bar{e})_1^N$, and $\bar{E} := (\bar{e})_1^N$ denote the two error sequences which relate to the optimal redistributions per the formulations in Section 4 and Section 5 respectively, such that indexing of $iE$ and $\bar{E}$ is consistent with the sorted rearrangement of $G$, i.e., $\bar{G} := (\bar{g})_1^N$.

If for $\bar{G}$, $\bar{g}_1 \geq \bar{g}_2 \cdots \geq \bar{g}_N$, then for $iE$, $i\bar{e}_1 \geq i\bar{e}_2 \cdots \geq i\bar{e}_N$, and for $\bar{E}$, $\bar{e}_1 \leq \bar{e}_2 \cdots \leq \bar{e}_N$, i.e., $\bar{E}, \bar{e}_1 \geq \bar{e}_2 \cdots \geq \bar{e}_N$, $\bar{e}_1 \leq \bar{e}_2 \cdots \leq \bar{e}_N$.

From Equations (39) and (42),

$$\rho_{c_1} = 1 - \left( \frac{N(MSE)}{2N\sigma^2_G + 2 \sum_{i=1}^{N} \bar{g}_i \bar{e}_i - 2N\mu G \mu E + N(MSE)} \right),$$

(50)

$$\rho_{c_2} = 1 - \left( \frac{N(MSE)}{2N\sigma^2_G - 2 \sum_{i=1}^{N} \bar{g}_i \bar{e}_i + 2N\mu G \mu E + N(MSE)} \right).$$

(51)

As per the Equations (46) and (47), the denominators for expressions for both $\rho_{c_1}$ and $\rho_{c_2}$ are strictly non-negative (referring to the Chebyshev’s sum inequality from the Equations (43) and (44)). Therefore, both the error redistributions result in the sequences that are guaranteed to be non-negatively correlated. $\rho_c$
approaches 0 only when the \( \text{MSE} \) is large.

Suppose \( \rho_{c_1} \geq \rho_{c_2} \)

This is true if and only if

\[
\frac{N(\text{MSE})}{2N\sigma_G^2 + 2\sum_{i=1}^N \bar{g}_i e_i - 2N\mu_G\mu_E + N(\text{MSE})} \leq \frac{N(\text{MSE})}{2N\sigma_G^2 - 2\sum_{i=1}^N \bar{g}_i e_i + 2N\mu_G\mu_E + N(\text{MSE})},
\]

which is true only if

\[
2N\sigma_G^2 + 2\sum_{i=1}^N \bar{g}_i e_i - 2N\mu_G\mu_E + N(\text{MSE}) \geq 2N\sigma_G^2 - 2\sum_{i=1}^N \bar{g}_i e_i + 2N\mu_G\mu_E,
\]

which is true only if

\[
\sum_{i=1}^N \bar{g}_i e_i + \sum_{i=1}^N \bar{g}_i e_i \geq 2N\mu_G\mu_E,
\]

which is true only if

\[
\frac{1}{N} \sum_{i=1}^N \bar{g}_i e_i + \frac{1}{N} \sum_{i=1}^N \bar{g}_i e_i \geq \left( \frac{1}{N} \sum_{k=1}^N \bar{g}_k \right) \left( \frac{1}{N} \sum_{k=1}^N \left( \bar{e}_i + \bar{e}_i \right) \right),
\]

which is true only if

\[
\frac{1}{N} \sum_{i=1}^N \bar{g}_i \left( \bar{e}_i + \bar{e}_N - i + 1 \right) \geq \left( \frac{1}{N} \sum_{k=1}^N \bar{g}_k \right) \left( \frac{1}{N} \sum_{k=1}^N \left( \bar{e}_i + \bar{e}_N - i + 1 \right) \right).
\]

We note that, the scatter plot of the series \((x, y) = \left( i, \left( \bar{e}_i + \bar{e}_N - i + 1 \right) \right)\) is symmetric with respect to \( x = \frac{N+1}{2} \). Because the sequence \((\bar{e}_i + \bar{e}_N - i + 1)\) features both the similarly ordered and the oppositely ordered error components, no guarantees can be made in terms of veracity of Equation (52) using either the Chebyshev’s sum inequality (Equations (43) and (44)) or the rearrangement inequality (Appendix 2). One can only compute the two sides of the Equation (52) to determine which redistribution of error values would result in the prediction sequence with the highest CCC.

### 8 Examples and Illustrations

Figure 1 illustrates what it means to ‘redistribute the errors’, and kinds of prediction sequences this translates to when using each of the two CCC reformulations. The data used to generate Figure 1 are the gold standard sequences of arousal levels from the SEWA database. The database has recently gained a lot of popularity, as it was used in the recent AVEC challenges [34, 33].

Prediction 1 in Figure 1 corresponds to maximisation of \( \rho_{c_1} \) (Equation (50)), while prediction 2 corresponds to \( \rho_{c_2} \) maximisation (Equation (51)). Because
Figure 1: Illustration of two candidate prediction sequences having an identical set of prediction errors (thus, the same mean square error), when compared against a common gold standard. Different ordering of these errors gives rise to different prediction sequences, resulting in different CCCs against the very same gold standard sequence. In the figure above, gold standard sequence used is the arousal level for one of the subjects from the SEWA German database (more specifically, from the challenge data of and ), shown in Green. The two prediction sequences are shown in red and blue in the first row of plots.

The error distribution we chose in this simulation happens to be strictly positive, the errors carry an identical sign and the minimum of the errors is close to zero. Corresponding to this minimum error, we note that the first prediction sequence attempts to closely follow the lower values in the gold standard, while the later closely follows the larger values present in the gold standard, thanks to the error rearrangement discussed in Section 6 and Appendix 3.

We also note that the shape of the two prediction sequences is quite similar to one another, but far from being identical. The overall shape is non-linearly stretched in the vertical direction, i.e., corresponding to the different error values. The two plots at the bottom provide a better insight into this vertical stretching in a comparative sense. Comparing the magenta and the green-coloured plot, it can be readily seen that the difference between the two prediction sequences is at its highest at the extremities of the gold standard. This is expected, as per the Equations (45) to (47).
9 Designing a cost function

Both the reformulations imply that, in order to achieve the highest possible $\rho_c$, it is necessary to minimise the $L_p$ norm of the error values (i.e., minimise $MSE = \frac{1}{N} \sum_{i=1}^{N} (g_i - p_i)^2$, while simultaneously maximising the DotProduct$(G, P) = DP = \sum_{i=1}^{N} g_i p_i$ (also called the Hadamard product).

In order to design the cost function $\phi(p_i, g_i)$, the only constraint we have, therefore, is that

$$\frac{\partial}{\partial p_i} MSE < 0 \quad \text{and} \quad \frac{\partial}{\partial p_i} DP > 0, \quad (53)$$

i.e.,

$$\frac{\partial}{\partial p_i} \sum_{i=1}^{N} (g_i - p_i)^2 < 0 \quad \text{and} \quad \frac{\partial}{\partial p_i} \sum_{i=1}^{N} g_i p_i > 0,$$

should imply that

$$\frac{\partial}{\partial p_i} f(g_i, p_i) < 0 \quad \forall p_i \in \mathbb{R} \quad (54)$$

A family of cost functions, such as the following, can now be easily designed.

$$f(g_i, p_i) = \sum_{i=1}^{N} (g_i - p_i)^2 - \alpha \sum_{i=1}^{N} g_i p_i, \quad \text{where} \quad \alpha > 0; \quad (55)$$

or more generally,

$$f(g_i, p_i) = \sum_{i=1}^{N} (g_i - p_i)^2 - \alpha \sum_{i=1}^{N} (g_i p_i)^\beta, \quad \text{where} \quad \alpha, \beta > 0; \quad (56)$$

even more generally,

$$f(g_i, p_i) = \sum_{i=1}^{N} (g_i - p_i)^2 - \sum_{j} \alpha_j \sum_{i=1}^{N} (g_i p_i)^\beta_j, \quad \text{where} \quad \alpha_j, \beta_j > 0. \quad (57)$$

Such a cost function, attempting to maximise $\sum_{i=1}^{N} g_i p_i$, i.e., the dot product between the predictions and the gold standard, makes intuitive sense as well. We essentially dictate the neural network to raise the prediction values as large as possible when dealing with large values in the gold standard sequence, and diminish the predictions to as small as possible corresponding to the smaller values in the gold standard sequence. The mean square error as a component of the cost function, too, attempts to achieve this. However, the inner workings are slightly different. The mean square component drives the prediction closer to the gold standard by the amount that is proportional to the error. The inner product component drives the prediction in the direction of gold standard by an amount proportional to the gold standard itself. Another way to look at the dot product term is that, we now effectively weigh the individual errors by the corresponding gold standard.

16
10 Concluding Remarks

Keeping the deep learning models in perspective – that are capable of mapping complex and non-linear input to output relationships, we propose a family of cost functions, whereby the model can also aim to maximise the concordance correlation coefficient, while simultaneously minimising the errors in the prediction.

Our proposed cost function consists of two components. The classical cost function, such as $MSE$ that reduces the difference between the prediction and the gold standard by an amount that is proportional to the difference itself in every training iteration. Our newly introduced component of the cost function drives every prediction closer to the corresponding gold standard by an amount that is proportional to the value of the gold standard itself. We derive these properties of the desired cost function by rigorously reformulating the CCC measure in terms of the error coefficients, i.e., the difference between the prediction and the gold standard population, in two different ways.

It is a well known fact that, while each of the $MAE$, $MSE$, and $RMSE$ cost functions aim to reduce the difference between the prediction and the desired output, they deal with the outliers in the data differently. $RMSE$ gives a relatively high weight to large errors when compared to $MAE$. For XGBoost alike frameworks, the twice differentiable functions are more favourable (unlike, e.g., as in the case of $MAE$) \cite{5}. In the same vein, we hope to accelerate the model convergence when maximising $\sum_{i=1}^{N} g_i p_i$ by introducing $-\alpha \sum_{i=1}^{N} (g_i p_i)^\beta$ to the cost function ($\beta \in \mathbb{R} : \beta > 0$).

With the mathematical foundations formally laid out in this paper, we now intend to rerun our emotion recognition experiments and relevant examples of application with newly invented cost functions. It would be interesting to investigate the effect of the hyperparameters present in the cost function. We intend to optimise a model’s predictive power and time-to-convergence by tuning the hyperparameters such as $\alpha_j$, $\beta_j$, presenting the run-time benchmarks as our future work.

11 Acknowledgements

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A 1: Formulation 2: Replacing \((y_i)\) with \((x_i - d_i)\)

\[
\rho_c = \frac{2 \sum_{i=1}^{N} (x_i - \mu_X)(x_i - d_i - \mu_Y + \mu_D)}{N(\mu_D)^2 + \sum_{i=1}^{N} (x_i - d_i - \mu_X + \mu_D)^2 + \sum_{i=1}^{N} (x_i - \mu_X)^2}. \tag{58}
\]

Rewriting the individual terms in terms of \((x_i - \mu_X)\)

\[
\rho_c = \frac{2 \left[ \sum_{i=1}^{N} (x_i - \mu_X)^2 + \sum_{i=1}^{N} \mu_D(x_i - \mu_X) - \sum_{i=1}^{N} d_i(x_i - \mu_X) \right]}{N \mu_D^2 + 2 \sum_{i=1}^{N} (x_i - \mu_X)^2 + 2 \sum_{i=1}^{N} \mu_D(x_i - \mu_X) - 2 \sum_{i=1}^{N} d_i(x_i - \mu_X) + \sum_{i=1}^{N} (d_i - \mu_D)^2}. \tag{59}
\]

Now, \[\sum_{i=1}^{N} \mu_D(x_i - \mu_X) = \mu_D \sum_{i=1}^{N} (x_i - \mu_X) = \mu_D (N \mu_X - N \mu_X) \therefore \text{Equation (25)} \tag{60}\]

which cancels out a term from both the numerator and the denominator.

\[
\rho_c = \frac{2 \left[ \sum_{i=1}^{N} (x_i - \mu_X)^2 - \sum_{i=1}^{N} d_i(x_i - \mu_X) \right]}{N \mu_D^2 + 2 \sum_{i=1}^{N} (x_i - \mu_X)^2 + 2 \sum_{i=1}^{N} \mu_D(x_i - \mu_X) - 2 \sum_{i=1}^{N} d_i(x_i - \mu_X) + \sum_{i=1}^{N} (d_i - \mu_D)^2} \tag{61}
\]

\[
= \frac{2N \sigma_X^2 - 2 \sum_{i=1}^{N} d_i(x_i - \mu_Y)}{N \mu_D^2 + 2N \sigma_X^2 - 2 \sum_{i=1}^{N} d_i(x_i - \mu_X) + \left( \sum_{i=1}^{N} \mu_D^2 - 2 \sum_{i=1}^{N} d_i \mu_D + \sum_i d_i^2 \right)}. \tag{62}
\]

The terms underlined in Equation (62) above, thus, sum to zero. That is,

\[N \mu_D^2 + \sum_{i=1}^{N} \mu_D^2 - 2 \sum_{i=1}^{N} d_i \mu_D = N \mu_D^2 + N \mu_D^2 - 2N \mu_D^2 = 0. \tag{63}\]

\[\therefore \rho_c = \frac{2N \sigma_X^2 - 2 \sum_{i=1}^{N} d_i(x_i - \mu_X)}{N \mu_D^2 + 2N \sigma_X^2 - 2 \sum_{i=1}^{N} d_i(x_i - \mu_X) + \left( \sum_{i=1}^{N} \mu_D^2 - 2 \sum_{i=1}^{N} d_i \mu_D + \sum_i d_i^2 \right)}. \tag{64}\]

\[= \frac{2N \sigma_X^2 - 2 \sum_{i=1}^{N} (x_i - \mu_X) d_i}{2N \sigma_X^2 - 2 \sum_{i=1}^{N} (x_i - \mu_X) d_i + N(MSE)} \therefore \sum_{i=1}^{N} d_i^2 = N(MSE). \tag{65}\]

\[= 1 - \left( \frac{N(MSE)}{2N \sigma_X^2 - 2 \sum_{i=1}^{N} x_i d_i + 2N \mu_X \mu_D + N(MSE)} \right) \therefore \sum_{i=1}^{N} d_i = N \mu_D. \tag{66}\]

For a given gold standard \(Y\) and a set of \(\{d_i\}\) values, maximisation of \(\rho_c\) requires that \[\sum_{i=1}^{N} (y_i) d_i\] is maximised.
**B 2: The Rearrangement Inequality**

The rearrangement inequality is a theorem concerning the rearrangements of two sets, to maximise and minimise the sum of element-wise products.

Denoting the two sets \((a) = \{a_1, a_2, \ldots a_n\}\) and \((b) = \{b_1, b_2, \ldots b_n\}\), let \((\bar{a})\) and \((\bar{b})\) be the sets where elements of \((a)\) and \((b)\) are arranged in the ascending order respectively such that

\[
\bar{a}_1 \leq \bar{a}_2 \leq \cdots \leq \bar{a}_n \quad (67)
\]

and

\[
\bar{b}_1 \leq \bar{b}_2 \leq \cdots \leq \bar{b}_n \quad (68)
\]

The rearrangement inequality states that

\[
\sum_{j=1}^{n} \bar{a}_j \bar{b}_{n+1-j} \leq \sum_{j=1}^{n} a_j b_j \leq \sum_{j=1}^{n} \bar{a}_j \bar{b}_j. \quad (69)
\]

More explicitly,

\[
\bar{a}_n \bar{b}_1 + \cdots + \bar{a}_1 \bar{b}_n \leq \bar{a}_{\sigma(1)} \bar{b}_1 + \cdots + \bar{a}_{\sigma(n)} \bar{b}_n \leq \bar{a}_1 \bar{b}_1 + \cdots + \bar{a}_n \bar{b}_n, \quad (70)
\]

for every permutation \(\{\bar{a}_{\sigma(1)}, \bar{a}_{\sigma(2)}, \ldots, \bar{a}_{\sigma(n)}\}\) of \(\{\bar{a}_1, \ldots, \bar{a}_n\}\).

For the unsorted ordered sets \((a)\) and \((b)\), the two sets are said to be ‘similarly ordered’ if \((a_\mu - a_\nu)(a_\mu - a_\nu) \geq 0\) for all \(\mu, \nu\), and ‘oppositely ordered’ if the inequality is always reversed. With this notion of ‘similar’ and ‘opposite’ ordering, the maximum summation corresponds to the similar ordering of \((a)\) and \((b)\). The minimum corresponds to the opposite ordering of \((a)\) and \((b)\).