Re-assessing the "Classify and Count" Quantification Method

Alejandro Moreo$^{(\boxtimes)}$ and Fabrizio Sebastiani

Istituto di Scienza e Tecnologie dell'Informazione,
Consiglio Nazionale delle Ricerche, 56124 Pisa, Italy
{alejandro.moreo,fabrizio.sebastiani}@isti.cnr.it

Abstract. *Learning to quantify* (a.k.a. *quantification*) is a task concerned with training unbiased estimators of class prevalence via supervised learning. This task originated with the observation that "Classify and Count" (CC), the trivial method of obtaining class prevalence estimates, is often a biased estimator, and thus delivers suboptimal quantification accuracy. Following this observation, several methods for learning to quantify have been proposed and have been shown to outperform CC. In this work we contend that previous works have failed to use properly optimised versions of CC. We thus reassess the real merits of CC and its variants, and argue that, while still inferior to some cutting-edge methods, they deliver near-state-of-the-art accuracy once (a) hyperparameter optimisation is performed, and (b) this optimisation is performed by using a truly quantification-oriented evaluation protocol. Experiments on three publicly available binary sentiment classification datasets support these conclusions.

Keywords: Learning to quantify · Quantification · Prevalence estimation · Classify and count

1 Introduction

Learning to quantify (a.k.a. *quantification*) consists of training a predictor that returns estimates of the relative frequency (a.k.a. *prevalence*, or *prior probability*) of the classes of interest in a set of unlabelled data items, where the predictor has been trained on a set of labelled data items [13]. When applied to text, quantification is important for several applications, e.g., gauging the collective satisfaction for a certain product from textual comments [8], establishing the popularity of a given political candidate from blog posts [17], predicting the amount of consensus for a given governmental policy from tweets [4], or predicting the amount of readers who will find a product review helpful [5].

The rationale of this task is that many real-life applications of classification suffer from *distribution shift* [22], the phenomenon according to which the distribution $p_y(U)$ of the labels in the set of unlabelled test documents U is different from the distribution $p_y(L)$ that the labels have in the set of labelled training documents L. It has been shown that, in the presence of distribution shift, the trivial strategy of using a standard classifier to classify all the unlabelled documents in U and counting the documents that have been assigned to each class

(the "Classify and Count" (CC) method), delivers poor class prevalence estimates. The reason is that most supervised learning methods are based on the IID assumption, which implies that the distribution of the labels is the same in L and U. "Classify and Count" is considered a *biased estimator* of class prevalence, since the goal of standard classifiers is to minimise (assuming for simplicity a binary setting) *classification* error measures such as (FP + FN), while the goal of a quantifier is to minimise *quantification* error measures such as |FP − FN|. (In this paper we tackle binary quantification, so FP and FN denote the numbers of false positives and false negatives, resp., from a binary contingency table.) Following this observation, several quantification methods have been proposed, and have been experimentally shown to outperform CC.

In this paper we contend that previous works, when testing advanced quantification methods, have used as baselines versions of CC that had not been properly optimised. This means that published results on the relative merits of CC and other supposedly more advanced methods are still unreliable. We thus reassess the real merits of CC by running extensive experiments (on three publicly available sentiment classification datasets) in which we compare properly optimised versions of CC and its three main variants (PCC, ACC, PACC) with a number of more advanced quantification methods. In these experiments we properly optimise all quantification methods, i.e., (a) we optimise their hyperparameters, and (b) we conduct this optimisation via a truly quantification-oriented evaluation protocol, which also involves minimising a quantification loss rather than a classification loss. Our results indicate that, while still inferior to some cutting-edge quantification methods, CC and its variants deliver near-state-of-the-art quantification accuracy once hyperparameter optimisation is performed properly. We make available all the code and the datasets that we have used for our experiments.[1]

2   "Classify and Count" and Its Variants

In this paper we use the following notation. We assume a binary setting, with the two classes $\mathcal{Y} = \{\oplus, \ominus\}$ standing for Positive and Negative. By $\mathbf{x}$ we denote a document drawn from a domain $\mathcal{X}$ of documents; by $L \subset \mathcal{X}$ we denote a set of labelled documents, that we typically use as a training set, while by U we denote a sample of unlabelled documents, that we typically use as the sample to quantify on. By $p_y(\sigma)$ we indicate the true prevalence of class y in sample σ, by $\hat{p}_y(\sigma)$ we indicate an estimate of this prevalence[2], and by $\hat{p}_y^M(\sigma)$ we indicate the estimate of this prevalence as obtained via quantification method M. Of course, for any method M it holds that $\hat{p}_\ominus^M(U) = (1 - \hat{p}_\oplus^M(U))$.

An obvious way to solve quantification is by aggregating the scores assigned by a classifier to the unlabelled documents. We first define two different aggregation methods, one that uses a "hard" classifier (i.e., a classifier $h_\oplus : \mathcal{X} \to \{0, 1\}$

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[2] Consistently with most mathematical literature, we use the caret symbol (ˆ) to indicate estimation.

that returns binary decisions, 0 for $\ominus$ and 1 for $\oplus$) and one that uses a "soft" classifier (i.e., a classifier $s_{\oplus} : \mathcal{X} \rightarrow [0, 1]$ that returns posterior probabilities $\Pr(\oplus|\mathbf{x})$, representing the probability that the classifier attributes to the fact that $\mathbf{x}$ belongs to the $\oplus$ class). Of course, $\Pr(\ominus|\mathbf{x}) = (1 - \Pr(\oplus|\mathbf{x}))$. The *classify and count* (CC) and the *probabilistic classify and count* (PCC) [3] methods then consist of computing

$$\hat{p}_{\oplus}^{\text{CC}}(U) = \frac{\sum_{\mathbf{x} \in U} h_{\oplus}(\mathbf{x})}{|U|} \qquad \hat{p}_{\oplus}^{\text{PCC}}(U) = \frac{\sum_{\mathbf{x} \in U} s_{\oplus}(\mathbf{x})}{|U|} \qquad (1)$$

Two popular, alternative quantification methods consist of applying an *adjustment* to the $\hat{p}_{\oplus}^{\text{CC}}(U)$ and $\hat{p}_{\oplus}^{\text{PCC}}(U)$ estimates. It is easy to show that, in the binary case, the true prevalence $p_{\oplus}(U)$ is such that

$$p_{\oplus}(U) = \frac{\hat{p}_{\oplus}^{\text{CC}}(U) - \text{FPR}_h}{\text{TPR}_h - \text{FPR}_h} \qquad p_{\oplus}(U) = \frac{\hat{p}_{\oplus}^{\text{PCC}}(U) - \text{FPR}_s}{\text{TPR}_s - \text{FPR}_s} \qquad (2)$$

where TPR_h and FPR_h (resp., TPR_s and FPR_s) here stand for the *true positive rate* and *false positive rate* that the classifier $h_{\oplus}$ (resp., $s_{\oplus}$) has on U. The values of TPR_h and FPR_h (resp., TPR_s and FPR_s) are unknown, but can be estimated via k-fold cross-validation on the training data. In the binary case this amounts to using the results that $h_{\oplus}(\mathbf{x})$ (resp., $s_{\oplus}(\mathbf{x})$) obtains in the k-fold cross-validation (i.e., when $\mathbf{x}$ ranges on the training documents) in equations

$$\begin{aligned} \hat{\text{TPR}}_h &= \frac{\sum_{\mathbf{x} \in \oplus} h_{\oplus}(\mathbf{x})}{|\oplus|} & \hat{\text{FPR}}_h &= \frac{\sum_{\mathbf{x} \in \ominus} h_{\oplus}(\mathbf{x})}{|\ominus|} \\ \hat{\text{TPR}}_s &= \frac{\sum_{\mathbf{x} \in \oplus} s_{\oplus}(\mathbf{x})}{|\oplus|} & \hat{\text{FPR}}_s &= \frac{\sum_{\mathbf{x} \in \ominus} s_{\oplus}(\mathbf{x})}{|\ominus|} \end{aligned} \qquad (3)$$

We obtain $\hat{p}_{\oplus}^{\text{ACC}}(U)$ and $\hat{p}_{\oplus}^{\text{PACC}}(U)$ estimates, which define the *adjusted classify and count* (ACC) [11] and *probabilistic adjusted classify and count* (PACC) [3] quantification methods, resp., by replacing TPR_h and FPR_h (resp., TPR_s and FPR_s) in Eq. 2 with their estimates from Eq. 3.

3 Quantification and Parameter Optimisation

3.1 Unsuitable Parameter Optimisation and Weak Baselines

The reason why we here reassess CC and its variants we have described above, is that we believe that, in previous papers where these methods have been used as baselines, their full potential has not been realised because of *missing or unsuitable optimisation* of the hyperparameters of the classifier on which the method is based.

Specifically, both CC and its variants rely on the output of a previously trained classifier, and this output usually depends on some hyperparameters. Not only the quality of this output heavily depends on whether these hyperparameters have been optimised or not (on some held-out data or via k-fold cross-validation), but *it also depends on what evaluation measure this optimisation has*

used as a criterion for model selection. In other words, given that hyperparameter optimisation chooses the value of the parameter that minimises error, it would make sense that, for a classifier to be used for quantification purposes, "error" is measured via a function that evaluates *quantification* error, and not classification error. Unfortunately, in most previous quantification papers, researchers either do not specify whether hyperparameter optimisation was performed at all [9,11,14,15,17,19,26,27], or leave the hyperparameters at their default values [1,3,10,16,21], or do not specify which evaluation measure they use in hyperparameter optimisation [8,12], or use, for this optimisation, a classification-based loss [2,25]. In retrospect, we too plead guilty, since some of the papers quoted here are our own.

All this means that CC and their variants, when used as baselines, have been turned into *weak* baselines, and this means that the merits of more modern methods relative to them have possibly been exaggerated, and are thus yet to be assessed reliably. In this paper we thus engage in a reproducibility study, and present results from text quantification experiments in which, contrary to the situations described in the paragraph above, we compare *carefully optimised* versions of CC and its variants with a number of (*carefully optimised* versions of) more modern quantification methods, in an attempt to assess the relative value of each in a robust way.

3.2 Quantification-Oriented Parameter Optimisation

In order to perform quantification-oriented parameter optimisation we need to be aware that there may exist two types of parameters that require estimation and/or optimisation, i.e., (a) the hyperparameters of the classifier on which the quantification method is based, and (b) the parameters of the quantification method itself.

The way we perform hyperparameter optimisation is the following. We assume that the dataset comes with a predefined split between a training set L and a test set U. (This assumption is indeed verified for the datasets we will use in Sect. 4.) We first partition L into a part L_{Tr} that will be used for training purposes and a part L_{Va} that will be used as a held-out validation set for optimising the hyperparameters of the quantifier. We then extract, from the validation set L_{Va}, several random validation samples, each characterised by a predefined prevalence of the $\oplus$ class; here, our goal is allowing the validation to be conducted on a variety of scenarios characterised by widely different values of class prevalence, and, as a consequence, by widely different amounts of distribution shift.[3] In order to do this, we extract each validation sample σ by randomly undersampling one or both classes in L_{Va}, in order to obtain a sample with

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[3] Note that this is similar to what we do, say, in classification, where the different hyperparameter values are tested on many validation documents; here we test these hyperparameter values on many validation *samples*, since the objects of study of text quantification are document samples inasmuch as the objects of study of text classification are individual documents.

prespecified class prevalence values. We draw samples with a desired prevalence value and a fixed amount q of documents; in order to achieve this, in some cases only one class needs to be undersampled while in some other cases this needs to happen for both classes. We use random sampling without replacement if the number of available examples of $\oplus$ (resp. $\ominus$) is greater or equal to the number of required ones, and with replacement otherwise. We extract samples with a prevalence of the $\oplus$ class in the set $\{\pi_1, ..., \pi_n\}$; for each of these n values we generate m random samples consisting of q validation documents each. Let Θ be the set of hyperparameters that we are going to optimise. Given the established grid of value combinations $\theta_1, ..., \theta_n$ that we are going to test for Θ, for each θ_i we do the following, depending on whether the quantification method has its own parameters (Case 1 below) or not (Case 2 below):

1. If the quantification method M we are going to optimise requires some parameters λ_i to be estimated, we first split L_{Tr} into a part $L_{\mathrm{Tr}}^{\mathrm{Tr}}$ and a part $L_{\mathrm{Tr}}^{\mathrm{Va}}$, training the classifier on $L_{\mathrm{Tr}}^{\mathrm{Tr}}$ using the chosen learner parameterised with θ_i, and estimate parameters λ_i on $L_{\mathrm{Tr}}^{\mathrm{Va}}$.[4] Among the variants of CC, this applies to methods ACC and PACC, which require the estimation of (the hard or soft version of) TPR and FPR. Other methods used in the experiments of Sect. 4 and that also require some parameter to be estimated are HDy and QuaNet (see Sect. 4.3.2).
2. If the quantification method M we are going to optimise does not have any parameter that requires estimation, then we train our classifier on L_{Tr}, using the chosen learner parameterised with θ_i, and use quantification method M on all the samples extracted from L_{Va}.

In both cases, we measure the quantification error via an evaluation measure for quantification that combines (e.g., averages) the results across all the validation samples. As our final value combination for hyperparameter set Θ we choose the θ_i for which quantification error is minimum.

Note that, in the above discussion, each time we split a labelled set into a training set and a validation set for parameter estimation/optimisation purposes, we could instead perform a k-fold cross-validation; the parameter estimation/optimisation would be more robust, but the computational cost of the entire process would be k times higher. While the latter method is also, from a methodological standpoint, an option, in this paper we stick to the former method, since the entire parameter optimisation process is, from a computational point of view, already very expensive.

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[4] Note that we do *not* retrain the classifier on the entire L_{Tr}. While this might seem beneficial, since L_{Tr} contains more training data than $L_{\mathrm{Tr}}^{\mathrm{Tr}}$, we need to consider that the estimates $\hat{\mathrm{TPR}}_h$ and $\hat{\mathrm{FPR}}_h$ have been computed on L_{Tr} and not on $L_{\mathrm{Tr}}^{\mathrm{Tr}}$.

Table 1. The three datasets used in our experiments; the columns indicate the class prevalence values of the $\oplus$ and $\ominus$ classes, and the numbers of documents contained in the training set L and the test set U.

	$\oplus$	$\ominus$	L	L_{Tr}	L_{Va}	U
IMDB	0.500	0.500	25,000	15,000	10,000	25,000
KINDLE	0.917	0.083	3,821	2,292	1,529	21,592
HP	0.982	0.018	9,533	5,720	3,813	18,401

4   Experiments

In order to conduct our experiments we use the same datasets and experimental protocol as used in [7]. Specifically, we run our experiments on three sentiment classification datasets, i.e., (i) IMDB, the popular *Large Movie Review Dataset* [20]; (ii) KINDLE, a set of reviews of Kindle e-book readers [7], and (iii) HP, a set of reviews of the books from the Harry Potter series [7].[5] For all datasets we adopt the same split between training set L and test set U as in [7]. The IMDB, KINDLE, and HP datasets are examples of balanced, imbalanced, and severely imbalanced datasets, since the prevalence values of the $\oplus$ class in the training set L are 0.500, 0.917, 0.982, resp. Some basic statistics from these datasets are reported in Table 1. We refer the reader to [7] for more details on the genesis of these datasets.

In our experiments, from each set of training data we randomly select 60% of the documents for training purposes, leaving the remaining 40% for the hyperparameter optimisation phase; these random splits are stratified, meaning that the two resulting parts display the same prevalence values as the set that originated them. In this phase (see Sect. 3.2) we use $n = 21$, $m = 10$, and $q = 500$, i.e., we generate $m = 10$ random samples of $q = 500$ documents each, for each of the $n = 21$ prevalence values of the $\oplus$ class in $\{0.00, 0.05, ..., 0.95, 1.00\}$.

In order to evaluate a quantifier over a wide spectrum of test prevalence values, we use essentially the same process that we have discussed in Sect. 3.2 for hyperparameter optimisation; that is, along with [7,11], we repeatedly and randomly undersample one or both classes in the test set U in order to obtain testing samples with specified class prevalence values. Here we generate $m = 100$ random testing samples of $q = 500$ documents each, for each of the $n = 21$ prevalence values of the $\oplus$ class in $\{0.00, 0.05, ..., 0.95, 1.00\}$.

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[5] The three datasets are available at https://doi.org/10.5281/zenodo.4117827 in pre-processed form. The raw versions of the HP and KINDLE datasets can be accessed from http://hlt.isti.cnr.it/quantification/, while the raw version of IMDB can be found at https://ai.stanford.edu/~amaas/data/sentiment/.

4.1 Evaluation Measures

As the measures of quantification error we use *Absolute Error* (AE) and *Relative Absolute Error* (RAE), defined as

$$\text{AE}(p, \hat{p}) = \frac{1}{|\mathcal{Y}|} \sum_{y \in \mathcal{Y}} |\hat{p}_y - p_y| \qquad \text{RAE}(p, \hat{p}) = \frac{1}{|\mathcal{Y}|} \sum_{y \in \mathcal{Y}} \frac{|\hat{p}_y - p_y|}{p_y} \qquad (4)$$

where $\mathcal{Y}$ is the set of classes of interest ($\mathcal{Y} = \{\oplus, \ominus\}$ in our case) and the sample σ is omitted for notational brevity. Note that RAE is undefined when at least one of the classes $y \in \mathcal{Y}$ is such that its prevalence in U is 0. To solve this problem, in computing RAE we smooth both all p_y's and $\hat{p}_y$'s via additive smoothing, i.e., we take $\underline{p}_y = \frac{\epsilon + p_y}{\sum_{y \in \mathcal{Y}} (\epsilon + p_y)}$, where $\underline{p}_y$ denotes the smoothed version of p_y and the denominator is just a normalising factor (same for the $\underline{\hat{p}}(y)$'s); following [11], we use the quantity $\epsilon = \frac{1}{2|U|}$ as the smoothing factor. We then use the smoothed versions of p_y and $\hat{p}_y$ in place of their original non-smoothed versions in Eq. 4; as a result, RAE is always defined.

The reason why we use AE and RAE is that from a theoretical standpoint they are, as it has recently been argued [28], the most satisfactory evaluation measures for quantification.

4.2 Data Processing

We preprocess our documents by using the stop word remover and default tokeniser available within the `scikit-learn` framework[6]. In all three datasets we remove all terms occurring less than 5 times in the training set and all punctuation marks, and lowercase the text. As the weighting criterion we use a version of the well-known tfidf method, i.e.,

$$\text{tfidf}(f, \mathbf{x}) = \log(\#(f, \mathbf{x}) + 1) \times \log \frac{|L|}{|\mathbf{x}' \in L : \#(f, \mathbf{x}') > 0|} \qquad (5)$$

where $\#(f, \mathbf{x})$ is the raw number of occurrences of feature f in document $\mathbf{x}$; weights are then normalised via cosine normalisation.

Among the learners we use for classification (see below), the only one that does not rely on a tfidf-based representation is CNN. This learner simply converts all documents into lists of unique numeric IDs, indexing the terms in the vocabulary. We pad the documents to the first 300 words.

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[6] http://scikit-learn.org/.

4.3   The Quantifiers

We here describe all the quantification systems we have used in this work.

4.3.1   CC and Its Variants

In our experiments we generate versions of CC, ACC, PCC, and PACC, using five different learners, i.e., support vector machines (SVM), logistic regression (LR), random forests (RF), multinomial naive Bayes (MNB), and convolutional neural networks (CNN). For the first four learners we rely on the implementations available from `scikit-learn`, while the CNN deep neural network is something we have implemented ourselves using the `pytorch` framework.[7] The setups that we use for these learners are the following:

– SVM: We use soft-margin SVMs with linear kernel and L2 regularisation, and we explicitly optimise the C parameter (in the range $C \in \{10^i\}$ with $i \in \{-4, -3, \ldots, 4, 5\}$) that determines the tradeoff between the margin and the training error (default: $C = 1$). We also optimise the $J_\oplus$ and $J_\ominus$ "rebalancing" parameters, which determine whether to impose that misclassifying a $\oplus$ document has a different cost than misclassifying a $\ominus$ document (in this case one sets $J_\oplus = \frac{p_\ominus(L)}{p_\oplus(L)}$ and $J_\ominus = 1$), or not (in this case one sets $J_\oplus = J_\ominus = 1$, which is the default configuration) [23].

– LR: As in SVM, we use L2 regularisation, and we explicitly optimise the rebalancing parameters and the regularisation coefficient C (default values are as in SVM).

– RF: we optimise the number of estimators in the range $\{10, 50, 100, 250, 500\}$, the max depth in $\{5, 15, 30, \max\}$,[8] and the splitting function in $\{$Gini, Entropy$\}$ (default: (100, max, Gini)).

– MNB: We use Laplace smoothing, and we optimise the additive factor α in the range $\{0.00, 0.05, \ldots, 0.95, 1.00\}$ (default: $\alpha = 1$).

– CNN: we use a single convolutional layer with γ output channels for three window lengths of 3, 5, and 7 words. Each convolution is followed by a ReLU activation function and a max-pooling operation. All convolved outputs are then concatenated and processed by an affine transformation and a sigmoid activation that converts the outputs into posterior probabilities. We use the Adam optimiser (with learning rate $1E^{-3}$ and all other parameters at their default values) to minimise the balanced binary cross-entropy loss, set the batch size to 100, and train the net for 500 epochs, but we apply an early stop after 20 consecutive training epochs showing no improvement in terms of F_1 for the minority class on the validation set. We explore the dimensionality of the embedding space in the range $\{100, 300\}$ (default: 100), the number of output channels γ in $\{256, 512\}$ (default: 512), whether to apply dropout to the last layer (with a drop probability of 0.5) or not (default: "yes"), and whether to apply weight decay (with a factor of $1E^{-4}$) or not (default: "no").

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[7] https://pytorch.org/.

[8] When the depth is set to "max" then nodes are expanded until all leaves belong to the same class.

Since we perform hyperparameter optimisation via grid search, the number of validations (i.e., combinations of hyperparameters) that we perform amounts to 20 for SVMs, 20 for LR, 40 for RF, 21 for MNB, and 16 for CNN.

In the following, by the notation M_l^m we will indicate quantification method M using learner l whose parameters have been optimised using measure m (where $M_l^\emptyset$ indicates that no optimisation at all has been carried out). We will test, on all three datasets, all combinations in which M ranges on {CC, ACC, PCC, PACC}, l ranges on {SVM, LR, RF, MNB, CNN}, and m ranges on {A, F_1, AE}, where A denotes vanilla accuracy, F_1 is the well-known harmonic mean of precision and recall, and AE is absolute error. We stick to the tradition of computing F_1 with respect to the minority class, which always turns out to be $\ominus$ in all three datasets (this means that, e.g., the true positives of the contingency table are the documents that the classifier assigns to $\ominus$ and that indeed belong to $\ominus$).

Note that PCC requires the classifier to return posterior probabilities. Since SVMs does not produce posterior probabilities, for PCC_{SVM} and $PACC_{SVM}$ we calibrate the confidence scores that SVMs return by using Platt's method [24].

4.3.2   Advanced Quantification Methods

As the advanced methods that we test against CC and its variants, we use a number of more sophisticated systems that have been top-performers in the recent quantification literature.

– We use the Saerens-Latinne-Decaestecker method [6,27] (SLD), which consists of training a probabilistic classifier and then exploiting the EM algorithm to iteratively shift the estimation of $p_y(U)$ from the one that maximises the likelihood on the training set to the one that maximises it on the test data. As the underlying learner for SLD we use LR, since (as MNB) it returns posterior probabilities (which SLD needs), since these probabilities tend to be (differently from those returned by MNB) well-calibrated, and since LR is well-known to perform much better than MNB.
– We use methods SVM(KLD), SVM(NKLD), SVM(Q), SVM(AE), SVM(RAE), from the "structured output learning" camp. Each of them is the result of instantiating the SVM_{perf} structured output learner [18] to optimise a different loss function. SVM(KLD) [10] minimises the Kullback-Leibler Divergence (KLD); SVM(NKLD) [9] minimises a version of KLD normalised via the logistic function; SVM(Q) [1] minimises the harmonic mean of a classification-oriented loss (recall) and a quantification-oriented loss (RAE). We also add versions that minimise AE and RAE, since these latter are now, as indicated in Sect. 4.1, the evaluation measures for quantification considered most satisfactory, and the two used in this paper for evaluating the quantification accuracy of our systems. We optimise the C parameter of SVM_{perf} in the range $C \in \{10^i\}$, with $i \in \{-4, -3, \ldots 4, 5\}$. In this case we do not optimise the $J_\oplus$ and $J_\ominus$ "rebalancing" parameters since this option is not available in SVM_{perf}.
– We use the HDy method of [15]. The method searches for the prevalence values that minimise the divergence (as measured via the Hellinger Distance)

between two cumulative distributions of posterior probabilities returned by the classifier, one for the unlabelled examples and the other for a validation set. The latter is a mixture of the distributions of posterior probabilities returned for the $\oplus$ and $\ominus$ validation examples, respectively, where the parameters of the mixture are the sought class prevalence values. We use LR as the classifier for the same reasons as discussed for SLD.

– We use the QuaNet system, a "meta-"quantification method based on deep learning [7]. QuaNet takes as input a list of document embeddings, together with and sorted by the classification scores returned by a classifier. A bidirectional LSTM processes this list and produces a quantification embedding that is then concatenated with a vector of predictions produced by an ensemble of simpler quantification methods (we here employ CC, ACC, PCC, PACC, and SLD). The resulting vector passes through a set of fully connected layers (followed by ReLU activations and dropout) that return the estimated class prevalence values. We use CNN as the learner since, among the learners we use in this paper, it is the only one that returns both posterior probabilities and document embeddings (we use the last layer of the CNN as the document embedding). We set the hidden size of the bidirectional LSTM to $128 + 128 = 256$ and use two stacked layers. We also set the hidden sizes of the fully connected layers to 1024 and 512, and the dropout probability to 0.5. We train the network for 500 epochs, but we apply early stopping with a patience of 10 consecutive validations without improvements in terms of mean square error (MSE). Each training epoch consists of 200 quantification predictions, each of which for a batch of 500 randomly drawn documents at a prevalence sampled from the uniform distribution. In our case, validation epochs correspond to 21 quantification predictions for batches of 500 documents randomly sampled to have prevalence values $0.00, 0.05, \ldots, 0.95, 1.00$. We use Adam as the optimiser, with default parameters, to minimise MSE. In order to train QuaNet, we split (using a 40%/40%/20% stratified split) the training set L_{Tr} in three sets $L_{\mathrm{Tr}}^{\mathrm{CTr}}$, for training the classifier; $L_{\mathrm{Tr}}^{\mathrm{QTr}}$, for training QuaNet; and $L_{\mathrm{Tr}}^{\mathrm{QVa}}$, for validating QuaNet. When optimising QuaNet we do not explore any additional hyperparameter apart from those for the CNN.

– We also report results for *Maximum Likelihood Probability Estimation* (MLPE), the trivial baseline for quantification which makes the IID assumption and thus simply assumes that $p_{\oplus}(U)$ is identical to the training prevalence $p_{\oplus}(L)$ irrespectively of the set U.

Note that ACC, PACC, HDy, and QuaNet need to estimate their own parameters on a validation set, which means that their performance depends on exactly which documents this set consists of. In order to mitigate the impact of this random choice, for these methods we run each experiment 10 times, each time with a different random choice. The results we report are the average scores across these 10 runs.

Table 2. Results showing how the quantification error of CC changes according to the measure used in hyperparameter optimization; a negative percentage indicates a reduction in error with respect to using the method with default parameters. The background cell color indicates improvement (green) or deterioration (red), while its tone intensity is proportional to the absolute magnitude.

	IMDB				KINDLE				HP			
	AE		RAE		AE		RAE		AE		RAE	
$CC^{\varnothing}_{SVM}$	0.065		6.029		0.305		15.928		0.471		24.058	
CC^{A}_{SVM}	0.059	(-9.6%)	5.408	(-10.3%)	0.245	(-19.8%)	13.220	(-17.0%)	0.401	(-14.9%)	20.645	(-14.2%)
$CC^{F_1}_{SVM}$	0.059	(-9.5%)	5.523	(-8.4%)	0.108	(-64.5%)	7.192	(-54.8%)	0.236	(-50.0%)	13.590	(-43.5%)
CC^{AE}_{SVM}	0.065	(+0.3%)	6.091	(+1.0%)	0.100	(-67.1%)	7.555	(-52.6%)	0.119	(-74.8%)	10.593	(-56.0%)
$CC^{\varnothing}_{LR}$	0.059		5.477		0.470		23.990		0.500		25.508	
CC^{A}_{LR}	0.062	(+6.0%)	5.839	(+6.6%)	0.202	(-57.0%)	11.215	(-53.3%)	0.451	(-9.8%)	23.035	(-9.7%)
$CC^{F_1}_{LR}$	0.062	(+5.3%)	5.725	(+4.5%)	0.163	(-65.3%)	9.278	(-61.3%)	0.229	(-54.3%)	13.505	(-47.1%)
CC^{AE}_{LR}	0.062	(+6.1%)	5.745	(+4.9%)	0.094	(-80.0%)	7.087	(-70.5%)	0.110	(-78.0%)	10.304	(-59.6%)
$CC^{\varnothing}_{RF}$	0.155		13.388		0.448		22.988		0.493		25.196	
CC^{A}_{RF}	0.080	(-48.1%)	7.446	(-44.4%)	0.463	(+3.5%)	23.744	(+3.3%)	0.500	(+1.3%)	25.482	(+1.1%)
$CC^{F_1}_{RF}$	0.079	(-49.1%)	7.396	(-44.8%)	0.451	(+0.7%)	23.142	(+0.7%)	0.499	(+1.2%)	25.469	(+1.1%)
CC^{AE}_{RF}	0.079	(-48.8%)	7.487	(-44.1%)	0.464	(+3.6%)	23.721	(+3.2%)	0.500	(+1.3%)	25.487	(+1.2%)
$CC^{\varnothing}_{MNB}$	0.096		8.147		0.500		25.513		0.500		25.510	
CC^{A}_{MNB}	0.098	(+1.6%)	8.529	(+4.7%)	0.443	(-11.4%)	22.641	(-11.3%)	0.499	(-0.2%)	25.459	(-0.2%)
$CC^{F_1}_{MNB}$	0.097	(+0.8%)	8.311	(+2.0%)	0.444	(-11.3%)	22.731	(-10.9%)	0.499	(-0.2%)	25.470	(-0.2%)
CC^{AE}_{MNB}	0.097	(+0.9%)	8.431	(+3.5%)	0.443	(-11.4%)	22.701	(-11.0%)	0.499	(-0.2%)	25.464	(-0.2%)
$CC^{\varnothing}_{CNN}$	0.072		6.683		0.087		8.138		0.255		17.042	
CC^{A}_{CNN}	0.073	(+2.0%)	6.620	(-1.0%)	0.107	(+23.8%)	8.680	(+6.7%)	0.159	(-37.5%)	14.255	(-16.4%)
$CC^{F_1}_{CNN}$	0.078	(+8.7%)	7.142	(+6.9%)	0.085	(-2.2%)	7.951	(-2.3%)	0.149	(-41.5%)	14.030	(-17.7%)
CC^{AE}_{CNN}	0.074	(+3.2%)	6.613	(-1.0%)	0.109	(+26.2%)	8.591	(+5.6%)	0.343	(+34.3%)	19.008	(+11.5%)

4.4   Results

Tables 2, 3, 4, and 5 report the results obtained for CC, ACC, PCC, and PACC. At a first glance, the results do not seem to give any clearcut indication on how the CC variants should be optimised. However, a closer look reveals a number of patterns. One of these is that SVM and LR (the two best-performing classifiers overall) tend to benefit from optimised hyperparameters, and tend to do so to a greater extent when the loss used in the optimisation is quantification-oriented. Somehow surprisingly, not all methods improve after model selection in every case. However, there tends to be such an improvement especially for ACC and PACC. A likely reason for this is the possible existence of a complex tradeoff between obtaining a more accurate classifier and obtaining more reliable estimates for the TPR and FPR quantities.

Regarding the different datasets, it seems that there is no clear improvement from performing model selection when the training set is balanced (see IMDB), neither by using a classification-oriented measure nor by using a quantification-oriented one. A possible reason is that any classifier (with or without hyperparameter optimisation) becomes a reasonable quantifier if it learns to pay equal importance to positive and negative examples, i.e., if the errors it produces are unbiased towards either ⊕ or ⊖. In this respect, RF and MNB prove strongly biased towards the majority class, and only when corrected via an adjustment (ACC or PACC) they deliver results comparable to those obtained for other learners.

Table 3. Same as Table 2, but with ACC instead of CC.

	IMDB		KINDLE		HP	
	AE	RAE	AE	RAE	AE	RAE
$ACC^{\varnothing}_{SVM}$	0.023	1.084	0.068	2.958	0.341	17.350
ACC^{A}_{SVM}	0.019 (-17.6%)	0.889 (-18.0%)	0.070 (+4.1%)	3.093 (+4.6%)	0.181 (-47.0%)	9.245 (-46.7%)
$ACC^{F_1}_{SVM}$	0.022 (-5.2%)	1.153 (+6.3%)	0.052 (-22.9%)	2.309 (-21.9%)	0.110 (-67.8%)	7.019 (-59.5%)
ACC^{AE}_{SVM}	0.020 (-11.4%)	0.933 (-13.9%)	0.069 (+1.6%)	3.193 (+7.9%)	0.108 (-68.4%)	7.225 (-58.4%)
$ACC^{\varnothing}_{LR}$	0.017	0.569	0.279	9.997	0.500	25.508
ACC^{A}_{LR}	0.020 (+21.2%)	0.933 (+63.9%)	0.060 (-78.6%)	2.628 (-73.7%)	0.185 (-62.9%)	9.629 (-62.3%)
$ACC^{F_1}_{LR}$	0.019 (+15.9%)	0.896 (+57.4%)	0.057 (-79.5%)	2.507 (-74.9%)	0.098 (-80.5%)	6.534 (-74.4%)
ACC^{AE}_{LR}	0.018 (+10.8%)	0.850 (+49.3%)	0.065 (-76.9%)	2.891 (-71.1%)	0.092 (-81.7%)	5.849 (-77.1%)
$ACC^{\varnothing}_{RF}$	0.034	1.254	0.136	4.199	0.439	23.528
ACC^{A}_{RF}	0.021 (-38.7%)	0.643 (-48.8%)	0.180 (+31.7%)	6.603 (+57.3%)	0.482 (+9.7%)	24.654 (+4.8%)
$ACC^{F_1}_{RF}$	0.019 (-42.7%)	0.526 (-58.1%)	0.155 (+13.4%)	4.282 (+2.0%)	0.460 (+4.7%)	24.205 (+2.9%)
ACC^{AE}_{RF}	0.019 (-43.0%)	0.554 (-55.8%)	0.197 (+44.2%)	6.057 (+44.3%)	0.499 (+13.5%)	25.436 (+8.1%)
$ACC^{\varnothing}_{MNB}$	0.049	2.316	0.473	23.280	0.500	25.508
ACC^{A}_{MNB}	0.051 (+4.4%)	2.479 (+7.0%)	0.189 (-59.9%)	9.065 (-61.1%)	0.435 (-13.1%)	22.170 (-13.1%)
$ACC^{F_1}_{MNB}$	0.049 (+0.5%)	2.404 (+3.8%)	0.197 (-58.3%)	9.285 (-60.1%)	0.428 (-14.5%)	22.025 (-13.7%)
ACC^{AE}_{MNB}	0.051 (+3.9%)	2.591 (+11.9%)	0.213 (-54.9%)	10.376 (-55.4%)	0.451 (-9.7%)	23.146 (-9.3%)
$ACC^{\varnothing}_{CNN}$	0.021	1.082	0.074	1.596	0.173	10.642
ACC^{A}_{CNN}	0.019 (-8.2%)	0.811 (-25.0%)	0.064 (-12.7%)	1.515 (-5.1%)	0.223 (+28.6%)	9.939 (-6.6%)
$ACC^{F_1}_{CNN}$	0.023 (+10.1%)	1.067 (-1.4%)	0.061 (-17.4%)	1.424 (-10.8%)	0.182 (+5.3%)	10.344 (-2.8%)
ACC^{AE}_{CNN}	0.023 (+9.1%)	1.072 (-0.9%)	0.068 (-7.8%)	1.399 (-12.4%)	0.174 (+0.7%)	10.810 (+1.6%)

Table 4. Same as Table 2, but with PCC instead of CC.

	IMDB		KINDLE		HP	
	AE	RAE	AE	RAE	AE	RAE
$PCC^{\varnothing}_{SVM}$	0.101	9.460	0.255	14.514	0.375	20.158
PCC^{A}_{SVM}	0.100 (-0.4%)	9.517 (+0.6%)	0.283 (+10.9%)	16.174 (+11.4%)	0.385 (+2.6%)	20.653 (+2.5%)
$PCC^{F_1}_{SVM}$	0.101 (+0.0%)	9.425 (-0.4%)	0.251 (-1.8%)	14.239 (-1.9%)	0.385 (+2.7%)	20.594 (+2.2%)
PCC^{AE}_{SVM}	0.100 (-0.4%)	9.484 (+0.2%)	0.254 (-0.6%)	14.461 (-0.4%)	0.386 (+2.8%)	20.607 (+2.2%)
$PCC^{\varnothing}_{LR}$	0.122	11.564	0.356	20.405	0.464	24.608
PCC^{A}_{LR}	0.091 (-25.5%)	8.563 (-26.0%)	0.279 (-21.5%)	15.031 (-26.3%)	0.352 (-24.2%)	18.605 (-24.4%)
$PCC^{F_1}_{LR}$	0.092 (-25.0%)	8.606 (-25.6%)	0.172 (-51.6%)	11.222 (-45.0%)	0.212 (-54.2%)	16.117 (-34.5%)
PCC^{AE}_{LR}	0.079 (-35.3%)	7.348 (-36.5%)	0.154 (-56.6%)	13.066 (-36.0%)	0.211 (-54.6%)	19.597 (-20.4%)
$PCC^{\varnothing}_{RF}$	0.199	18.865	0.376	21.592	0.461	24.267
PCC^{A}_{RF}	0.198 (-0.7%)	18.753 (-0.6%)	0.368 (-2.0%)	21.209 (-1.8%)	0.482 (+4.7%)	25.349 (+4.5%)
$PCC^{F_1}_{RF}$	0.195 (-2.1%)	18.459 (-2.2%)	0.372 (-0.9%)	21.319 (-1.3%)	0.466 (+1.1%)	24.563 (+1.2%)
PCC^{AE}_{RF}	0.196 (-1.4%)	18.565 (-1.6%)	0.366 (-2.5%)	21.088 (-2.3%)	0.462 (+0.3%)	24.379 (+0.5%)
$PCC^{\varnothing}_{MNB}$	0.171	15.928	0.478	24.702	0.498	25.453
PCC^{A}_{MNB}	0.168 (-1.7%)	15.663 (-1.7%)	0.381 (-20.3%)	20.396 (-17.4%)	0.497 (-0.2%)	25.397 (-0.2%)
$PCC^{F_1}_{MNB}$	0.167 (-2.2%)	15.617 (-2.0%)	0.380 (-20.4%)	20.369 (-17.5%)	0.473 (-5.0%)	24.487 (-3.8%)
PCC^{AE}_{MNB}	0.160 (-6.4%)	14.907 (-6.4%)	0.380 (-20.4%)	20.396 (-17.4%)	0.473 (-5.0%)	24.479 (-3.8%)
$PCC^{\varnothing}_{CNN}$	0.110	9.994	0.111	10.448	0.257	18.368
PCC^{A}_{CNN}	0.105 (-4.8%)	9.893 (-1.0%)	0.154 (+39.2%)	10.775 (+3.1%)	0.389 (+51.6%)	21.093 (+14.8%)
$PCC^{F_1}_{CNN}$	0.099 (-10.3%)	9.377 (-6.2%)	0.111 (+0.3%)	9.474 (-9.3%)	0.251 (-2.2%)	17.005 (-7.4%)
PCC^{AE}_{CNN}	0.145 (+31.3%)	11.146 (+11.5%)	0.148 (+33.8%)	14.017 (+34.2%)	0.156 (-39.3%)	14.644 (-20.3%)

CNN works well on average almost in all cases, and seems to be the least sensitive learner to model selection.

Table 5. Same as Table 2, but with PACC instead of CC.

	IMDB		KINDLE		HP	
	AE	RAE	AE	RAE	AE	RAE
$PACC^{\emptyset}_{SVM}$	0.021	1.166	0.059	2.464	0.137	8.368
$PACC^{A}_{SVM}$	0.021 (-3.2%)	1.215 (+4.3%)	0.065 (+10.0%)	2.893 (+17.4%)	0.106 (-22.8%)	6.425 (-23.2%)
$PACC^{F_1}_{SVM}$	0.021 (-3.4%)	1.202 (+3.1%)	0.066 (+11.4%)	2.979 (+20.9%)	0.148 (+8.2%)	8.723 (+4.2%)
$PACC^{AE}_{SVM}$	0.022 (+5.1%)	1.363 (+17.0%)	0.059 (-1.4%)	2.333 (-5.3%)	0.114 (-16.6%)	7.497 (-10.4%)
$PACC^{\emptyset}_{LR}$	0.017	0.846	0.064	2.456	0.119	9.639
$PACC^{A}_{LR}$	0.021 (+22.0%)	1.087 (+28.4%)	0.053 (-16.7%)	2.177 (-11.4%)	0.147 (+23.1%)	8.316 (-13.7%)
$PACC^{F_1}_{LR}$	0.021 (+24.5%)	1.176 (+39.0%)	0.065 (+2.2%)	2.060 (-16.1%)	0.091 (-23.2%)	7.748 (-19.6%)
$PACC^{AE}_{LR}$	0.021 (+26.5%)	1.237 (+46.3%)	0.068 (+5.5%)	2.253 (-8.3%)	0.104 (-12.3%)	8.812 (-8.6%)
$PACC^{\emptyset}_{RF}$	0.030	1.221	0.074	2.923	0.168	10.322
$PACC^{A}_{RF}$	0.022 (-28.4%)	0.877 (-28.2%)	0.082 (+10.4%)	3.367 (+15.2%)	0.180 (+7.1%)	11.095 (+7.5%)
$PACC^{F_1}_{RF}$	0.021 (-29.8%)	0.952 (-22.0%)	0.079 (+6.9%)	3.331 (+13.9%)	0.160 (-5.1%)	10.350 (+0.3%)
$PACC^{AE}_{RF}$	0.020 (-33.2%)	0.914 (-25.1%)	0.081 (+8.9%)	3.286 (+12.4%)	0.140 (-17.1%)	10.067 (-2.5%)
$PACC^{\emptyset}_{MNB}$	0.055	3.253	0.180	7.352	0.195	10.930
$PACC^{A}_{MNB}$	0.058 (+4.8%)	3.412 (+4.9%)	0.130 (-27.7%)	6.058 (-17.6%)	0.335 (+71.6%)	17.883 (+63.6%)
$PACC^{F_1}_{MNB}$	0.060 (+8.1%)	3.487 (+7.2%)	0.122 (-32.2%)	5.570 (-24.2%)	0.363 (+86.0%)	18.138 (+65.9%)
$PACC^{AE}_{MNB}$	0.063 (+14.9%)	3.815 (+17.3%)	0.144 (-19.6%)	6.626 (-9.9%)	0.248 (+27.2%)	13.999 (+28.1%)
$PACC^{\emptyset}_{CNN}$	0.022	1.205	0.064	1.414	0.181	9.808
$PACC^{A}_{CNN}$	0.019 (-11.1%)	0.970 (-19.5%)	0.079 (+23.0%)	1.664 (+17.7%)	0.161 (-11.3%)	9.293 (-5.3%)
$PACC^{F_1}_{CNN}$	0.019 (-14.4%)	0.928 (-23.0%)	0.073 (+13.0%)	1.464 (+3.5%)	0.169 (-6.5%)	9.034 (-7.9%)
$PACC^{AE}_{CNN}$	0.018 (-17.3%)	0.830 (-31.2%)	0.069 (+6.9%)	1.367 (-3.3%)	0.165 (-9.1%)	8.829 (-10.0%)

In order to better understand whether or not, on average and across different situations, CC and its variants benefit from performing model selection using a quantification-oriented loss, we have submitted our results to a statistical significance test. Table 6 shows the outcome of a two-sided t-test on *related* sets of scores, across datasets and learners, from which we can compare pairs of model selection methods. The test reveals that optimising AE works better than

Table 6. Two-sided t-test results on *related* samples of error scores across datasets and learners. For a pair of optimization measures X vs. Y, symbol $\gg$ (resp. $>$) indicates that method X performs better (i.e., yields lower error) than Y, and that the difference in performance, as averaged across pairs of experiments on all datasets and learners, is statistically significant at a confidence score of $\alpha = 0.001$ (resp. $\alpha = 0.05$). Symbols $\ll$ and $<$ have a similar meaning but indicate that X performs worse (i.e., yields higher error) than Y. Symbol $\sim$ instead indicates that the differences in performance between X and Y are not statistically significantly different, i.e., that p-value ≥ 0.05.

			CC		ACC		PCC		PACC	
			AE	RAE	AE	RAE	AE	RAE	AE	RAE
AE	vs	F_1	$\gg$	$\sim$	$\ll$	$\ll$	$\gg$	$\ll$	$\gg$	$\gg$
AE	vs	A	$\gg$	$\gg$	$\gg$	$>$	$\gg$	$\gg$	$\gg$	$\gg$
AE	vs	$\emptyset$	$\gg$	$\gg$	$\gg$	$\gg$	$\gg$	$\gg$	$\gg$	$\sim$
F_1	vs	A	$\gg$	$\gg$	$\gg$	$\gg$	$\gg$	$\gg$	$\sim$	$\sim$
F_1	vs	$\emptyset$	$\gg$	$\gg$	$\gg$	$\gg$	$\gg$	$\gg$	$\ll$	$\ll$
A	vs	$\emptyset$	$\gg$	$\gg$	$\gg$	$\gg$	$\gg$	$\gg$	$\ll$	$\ll$

Table 7. Results showing how CC and its variants, once optimised using a quantification-oriented measure, compare with more modern quantification methods. **Boldface** indicates the best method. For columns AE and RAE, the best/worst results are highlighted in bright green/red; the colour for the other scores is a linearly interpolation between these two extremes. For columns r_{AE} and r_{RAE}, green/red is used to denote methods which have obtained higher/lower rank positions once the CC variants have been optimised for AE, with respect to the case in which they have not been optimised at all. All scores are different, in a statistically significant sense, from the best one according to a paired sample, two-tailed t-test at a confidence level of 0.001.

		IMDB		KINDLE		HP		IMDB		KINDLE		HP	
		AE	RAE	AE	RAE	AE	RAE	r_{AE}	r_{RAE}	r_{AE}	r_{RAE}	r_{AE}	r_{RAE}
	CC^{AE}_{SVM}	0.065	6.091	0.100	7.555	0.119	10.593	20 (20)	20 (20)	13 (21)	15 (21)	8 (22)	11 (20)
	ACC^{AE}_{SVM}	0.020	0.933	0.069	3.193	0.108	7.225	7 (8)	7 (6)	8 (6)	9 (9)	5 (16)	4 (15)
	PCC^{AE}_{SVM}	0.100	9.484	0.254	14.461	0.386	20.607	25 (23)	25 (23)	24 (19)	24 (20)	21 (17)	22 (18)
	$PACC^{AE}_{SVM}$	0.022	1.363	0.059	2.333	0.114	7.497	9 (6)	11 (7)	3 (3)	7 (7)	7 (5)	5 (3)
	CC^{AE}_{LR}	0.062	5.745	0.094	7.087	0.110	10.304	14 (14)	15 (14)	12 (26)	14 (26)	6 (29)	10 (28)
	ACC^{AE}_{LR}	0.018	0.850	0.065	2.891	0.092	5.849	4 (2)	5 (3)	4 (20)	8 (17)	3 (28)	3 (27)
	PCC^{AE}_{LR}	0.079	7.348	0.154	13.066	0.211	19.597	22 (25)	22 (25)	19 (22)	22 (22)	16 (21)	20 (22)
	$PACC^{AE}_{LR}$	0.021	1.237	0.068	2.253	0.104	8.812	8 (3)	10 (4)	5 (4)	6 (6)	4 (3)	6 (5)
	CC^{AE}_{RF}	0.079	7.487	0.464	23.721	0.500	25.487	23 (26)	23 (26)	29 (25)	28 (24)	29 (24)	29 (23)
	ACC^{AE}_{RF}	0.019	0.554	0.197	6.057	0.499	25.436	5 (11)	3 (11)	21 (14)	11 (10)	27 (19)	26 (19)
	PCC^{AE}_{RF}	0.196	18.565	0.366	21.088	0.462	24.379	28 (28)	28 (28)	25 (23)	26 (23)	24 (20)	24 (21)
	$PACC^{AE}_{RF}$	0.020	0.914	0.081	3.286	0.140	10.067	6 (10)	6 (10)	10 (9)	10 (8)	10 (6)	9 (7)
	CC^{AE}_{MNB}	0.097	8.431	0.443	22.701	0.499	25.464	24 (22)	24 (22)	28 (29)	27 (29)	28 (26)	28 (29)
	ACC^{AE}_{MNB}	0.051	2.591	0.213	10.376	0.451	23.146	12 (12)	12 (12)	23 (27)	20 (25)	23 (27)	23 (26)
	PCC^{AE}_{MNB}	0.160	14.907	0.380	20.396	0.473	24.479	27 (27)	27 (27)	26 (28)	25 (27)	25 (25)	25 (25)
	$PACC^{AE}_{MNB}$	0.063	3.815	0.144	6.626	0.248	13.999	16 (13)	13 (13)	16 (17)	12 (12)	19 (10)	17 (9)
	CC^{AE}_{CNN}	0.074	6.613	0.109	8.591	0.343	19.008	21 (21)	21 (21)	14 (11)	17 (14)	20 (14)	19 (14)
	ACC^{AE}_{CNN}	0.023	1.072	0.068	1.399	0.174	10.810	10 (5)	8 (5)	6 (8)	3 (3)	13 (7)	12 (8)
	PCC^{AE}_{CNN}	0.145	11.146	0.148	14.017	0.156	14.644	26 (24)	26 (24)	17 (12)	23 (18)	11 (15)	18 (16)
	$PACC^{AE}_{CNN}$	0.018	0.830	0.069	1.367	0.165	8.829	2 (7)	4 (9)	7 (5)	2 (2)	12 (8)	7 (6)
	SLD^{AE}_{LR}	**0.014**	**0.216**	**0.048**	1.606	**0.042**	**0.195**	1 (1)	1 (1)	1 (1)	4 (4)	1 (1)	1 (1)
	$SVM(KLD)^{AE}$	0.064	5.936	0.122	7.866	0.185	12.185	18 (18)	18 (18)	15 (13)	16 (13)	14 (9)	14 (11)
	$SVM(NKLD)^{AE}$	0.065	5.927	0.085	6.693	0.121	9.566	19 (19)	16 (16)	11 (10)	13 (11)	9 (4)	8 (4)
	$SVM(Q)^{AE}$	0.064	5.928	0.208	11.384	0.386	19.956	17 (17)	17 (17)	22 (18)	21 (19)	22 (18)	21 (17)
	$SVM(AE)^{AE}$	0.060	5.572	0.159	9.705	0.219	13.090	13 (15)	14 (15)	20 (16)	19 (16)	17 (12)	15 (12)
	$SVM(RAE)^{RAE}$	0.063	5.957	0.152	9.242	0.239	13.575	15 (16)	19 (19)	18 (15)	18 (15)	18 (13)	16 (13)
	HDy^{AE}_{LR}	0.018	0.420	0.055	**1.027**	0.058	2.970	3 (4)	2 (2)	2 (2)	1 (1)	2 (2)	2 (2)
	$QuaNet^{AE}_{CNN}$	0.027	1.175	0.070	2.119	0.210	11.433	11 (9)	9 (8)	9 (7)	5 (5)	15 (11)	13 (10)
	$MLPE^{\emptyset}_{\emptyset}$	0.262	24.874	0.429	25.266	0.484	25.447	29 (29)	29 (29)	27 (24)	29 (28)	26 (23)	27 (24)

optimising A or than using default settings (Ø). The test does not clearly say whether optimising AE or F_1 is better, but it suggests that PACC (the strongest CC variant) works better when optimised for AE than when optimised for F_1.

Finally, Table 7 compares the CC variants against more recent state-of-the-art quantification systems. Columns AE and RAE indicate the error of each method for each dataset. Columns r_{AE} and r_{RAE} show the rank positions for each pair (dataset, error) and, in parentheses, the rank position each method would have obtained in case the CC variants had not been optimised.

Interestingly, although some advanced quantification methods (specifically: SLD and HDy) stand as the top performers, many among the (supposedly more sophisticated) quantification methods fail to improve over CC's performance. At a glance, most quantification methods tend to obtain lower ranks when compared

with properly optimised CC variants. Remarkable examples of rank variation include CC and ACC with SVM and LR: when evaluated on KINDLE and HP, they climb several positions (up to 25), often entering the group of the 10 top-performing methods. In the most extreme case, ACC_{LR}^{AE} moves from position 28 (out of 29) to position 3 once properly optimised for quantification.

5   Conclusions

One of the takeaway messages from the present work is that, when using CC and/or its variants as baselines in their research on learning to quantify, researchers should properly optimise these baselines (i.e., use a truly quantification-oriented protocol, which includes the use of a quantification-oriented loss, in hyperparameter optimisation), lest these baselines become strawmen. The extensive empirical evaluation we have carried out shows that, in general, the performance of CC and its variants improves when the underlying learner has been optimised with a quantification-oriented loss (AE). The results of our experiments are less clear about whether optimising AE or F_1 (which, despite being a *classification*-oriented loss, is one that rewards classifiers that balance FPs and FNs) is better, although they indicate that optimising AE is preferable for PACC, the strongest among the variants of CC.

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