ABSTRACT
We empirically investigate the (negative) expected accuracy as an alternative loss function to cross entropy (negative log likelihood) for classification tasks. Coupled with softmax activation, it has small derivatives over most of its domain, and is therefore hard to optimize. A modified, leaky version is evaluated on a variety of classification tasks, including digit recognition, image classification, sequence tagging and tree tagging, using a variety of neural architectures such as logistic regression, multilayer perceptron, CNN, LSTM and Tree-LSTM. We show that it yields comparable or better accuracy compared to cross entropy. Furthermore, the proposed objective is shown to be more robust to label noise.

1 INTRODUCTION
Classification is perhaps the most prominent supervised learning task in machine learning [1]. In classification, we are interested in assigning a given instance to a set of predetermined categories, based on prior observations in our training data. Typically, in classification, we use the maximum likelihood approach to estimate model parameters [21, 31]. In this approach, we aim to find the most likely model parameters that could explain the observations in our training set. This leads to the popular negative log likelihood objective function. However, there is an established mismatch in preeminent approaches: Even though we optimize for the negative log likelihood, we still compare models on their test accuracy, or error rate [15, 16, 22, 33]. This leads us to ask: why not optimize for accuracy directly? A simple answer would be that it is not differentiable, since it is not even continuous at the decision boundary. Another reason might be the desirable properties of the likelihood approach: if the true class label is probabilistic given by a joint distribution of instances and labels, the likelihood objective would converge to the actual distribution, given enough data [2, 13]. Still, in most settings we might actually only care about accuracy and think of log likelihood as a surrogate function to it [34]. A mistake might have the same cost regardless of how close it is to the decision boundary.

This is certainly not a new question. Prior work has investigated the notion of a surrogate loss function that upper bounds the 0-1 loss, with the assumption that, optimizing the surrogate risk results in a better true risk [3, 24]. Alternatively, margin based loss functions such as the hinge loss in support vector machines provide alternatives to the probabilistic log likelihood approaches [19, 32, 35]. Other work investigates the Fischer-consistent loss functions (proper scoring rules), such as squared error loss or boosting loss [6].

In this work we investigate a very simplistic loss function: negative expected accuracy (or error rate). We show that even though we define the expectation over the model distribution rather than the data distribution, this still gives us a loss function that is close to the actual accuracy (or 0-1 loss). We subsequently see that this particular loss function introduces difficulty in its optimization, and therefore further explore a leaky version of it. In a variety of experiments that cover a wide range of architectures and settings, we compare it to the traditional log likelihood loss and examine its strengths.

In Section 2, we provide the rigorous formulation of the expected accuracy and the leaky expected accuracy. In Section 3.1, we perform preliminary experiments that compare different loss functions. Based on these preliminary results, in Section 3.2 we lay out the further experimental setting and in Section 3.3 we present the main experimental results. Finally, we present our conclusions in Section 4.

2 METHODOLOGY
Consider a classification setting where a prediction function \( f \) assigns a categorical distribution \( \mathcal{Y} \), to an input instance \( x \in X \), and the final class assignment is done randomly by sampling a class label from \( \mathcal{Y} \):

\[
\mathcal{Y} = f(x) \quad \mathcal{Y} \in [0, 1]^k, |\mathcal{Y}| = 1
\]

\[
y \sim \mathcal{Y} \quad y \in \{1, \ldots, k\}
\]

This is slightly different than the traditional setting where the most likely class is picked \((y = \arg\max_i \mathcal{Y}_i)\). However since exact accuracy would be discontinuous, the stochastic setting allows us to define a continuous and differentiable proxy.

Given a dataset of instances - true label pairs \( \{(x^{(i)}, r^{(i)})\}_i \), the expected accuracy of the prediction function \( f \) would be:

\[
\mathbb{E}[\text{Acc}] = \frac{1}{N} \sum_i \mathbb{E}[1(y^{(i)} = r^{(i)})]
\]

\[
= \frac{1}{N} \sum_i \mathbb{P}(y^{(i)} = r^{(i)})
\]

\[
= \frac{1}{N} \sum_i \mathcal{Y}_r^{(i)}
\]

This is simply the sum of all probabilities assigned to the correct class labels (up to a constant factor of \( 1/N \)).

We can negate this quantity to turn into a loss function \((-\frac{1}{N} \sum_i \mathcal{Y}_r^{(i)})\).

We can additionally translate it to get the expected error rate \((1 - \frac{1}{N} \sum_i \mathcal{Y}_r^{(i)})\), which would yield the same objective up to a constant additive factor.

2.1 Comparison to negative log likelihood
Negative expected accuracy as defined above looks similar to negative log likelihood except that we sum the probabilities themselves rather than their logs. Both loss functions optimize for high probability values assigned to the correct class, but weighted differently.
We can consider the composition of loss functions and the softmax where both would be similar for the expected accuracy. We posit view. We visualize the compositions as such in Figure 1 (b).

There is an argument that a better training objective surrogate (or even the exact one) could be worse for test accuracy. We discuss this in the final section.

**Surrogate for the 0-1 loss.** If we look at the task of classification from an optimization point of view, we can describe the approach as follows:

1. Our main goal is to optimize for the test set accuracy.
2. Since we cannot optimize over unseen data, we settle for optimizing for the training set accuracy and hope to have good test set accuracy as a side effect.
3. Since we cannot optimize for accuracy using a gradient-based method (due to its nondifferentiability), we settle for optimizing a differentiable surrogate function that approximates it well enough.\(^1\)

In this regard, we can compare both losses with respect to the 0-1 loss (error rate for a single instance) as a function of the probability value assigned to the true class label. We visualize the functions in Figure 1 (a). Negative log likelihood diverges from 0-1 loss as we approach 0. It values an increase in probability values (of the true class), say, from 0.1 to 0.2 more than an increase from 0.45 to 0.55, whereas both would be similar for the expected accuracy. We posit that instead of prioritizing correction of those instances that we perform very poorly on, by weighing probability errors equally, we might just be able to push more instances to the other side of the decision boundary. Note that in the cases that we can perform well on the training set for the negative log likelihood, both functions behave similarly.

**As functions of pre-activations.** Commonly the softmax activation (or sigmoid in the binary classification case) is used to convert unbounded scores (pre-activations) to probability values. We can consider the composition of loss functions and the softmax as a function of these pre-activations \(a\), which gives us another view. We visualize the compositions as such in Figure 1 (b).

Logarithm and the exponential within sigmoid cancel each other asymptotically for \(-\log(\text{sigmoid}(a))\) for negative values of \(a\). This approximately linear behavior allows it to have (absolutely) large derivatives \((\approx -1)\) which is desirable for its optimization. On the other hand, expected error rate, coupled with the sigmoid has an asymptotically zero derivative around the negative region, which potentially make it hard to optimize. For the instances that we are the most incorrect on, progress could be very little. Still, the main motivating idea behind it is to provide more incentive (larger absolute derivatives) over the instances that are closer to the decision boundary, to grab the lower hanging fruit first.

As we will see in the later sections, difficulty of optimizing the negative expected accuracy will indeed present itself as a practical issue. To combat this, we explore a leaky version of it, by combining it with the traditional log likelihood function:

\[
L = -\frac{1}{N} \sum_{i} \left( \frac{y_{r(i)}}{r_{r(i)}} \log \frac{y_{r(i)}}{r_{r(i)}} + a \log y_{r(i)}^{(i)} \right)
\]

for some small value of \(a\). We use \(a = 0.1\) in this work. As seen in Figure 1, this gives us a similar curve while having a nonzero asymptotic derivative in the negative region.

**Bayes optimal predictors.** In general, in classification we assume the true label of an instance is a random variable rather than a deterministic value, since \((x, r)\) is assumed to be from a joint distribution. Negative log likelihood objective has the desirable property that the predicted conditional distribution \((\mathcal{Y}|X)\) converges to the true distribution \((R|X)\) as we have more observations. This does not hold for the expected accuracy. In fact the Bayes optimal predictor for it is to assign a one-hot probability distribution which marks the most likely class. Maximum likelihood approach strives for matching the predicted and true distributions of labels, where expected accuracy wants to simply improve the counts for matching class predictions. Since from an accuracy perspective the best label that we can predict is the one that has the most instances in the population, such a Bayes optimal predictor is intuitive for its objective.

**Noisy labels.** Since negative likelihood diverges the most from 0-1 loss in the most negative region, we hypothesize that the impact of the proposed alternative will be the most apparent in the noisy label setting where each instance has a probability of its label being flipped. This setting simulates practical issues such as annotation errors.

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\(^1\)There is an argument that a better training objective surrogate (or even the exact accuracy) could be worse for test accuracy. We discuss this in the final section.
3 EXPERIMENTS

3.1 Preliminary Experiments

For preliminary experimentation, we use the logistic regression method over the MNIST digit recognition dataset, which has 60k train and 10k test instances of digits which are of 28×28 dimensional. The task is to classify each digit into one of the ten classes. We train the model over 200 epochs using the Adam update rule [14] with a learning rate of 1e-4.

Results are given in Figure 2 as training and test curves. We see that in terms of both training and test performance, expected accuracy performs better. However, as we suspected, we observe a temporary plateauing of performance in the early stages of training for the expected accuracy.

To account for randomness, and investigate consistency of the behavioral patterns, we perform 10-fold cross-validation by splitting the entire training set into training-development partitions of ratio 9:1. Development set is used for early stopping for a patience value of 15 epochs.

Results for the replicated experiments are given in Figure 3. We observe that initial plateauing is consistent across different runs. Furthermore, even though we see good performance compared to negative log likelihood for many runs, there is a particular run that the expected accuracy cannot overcome the initial plateau, resulting in a suboptimal performance by a wide margin.

Magnitudes of gradients. A possible culprit that would explain the early plateauing is simply the low magnitudes of gradients for the loss function of interest. We plot the average norms of the gradients of both losses (composed with the softmax) with respect to the softmax pre-activations in Figure 4 for one of the runs.

As we confirm a two order of magnitude difference in the norms, we rerun the experiments with a learning rate of 1e-2 for the negative expected accuracy loss, since merely having a larger learning rate might resolve getting stuck early on. However we observe a behavior that is very similar to Figure 3 (henceforth, the plot is omitted), which confirms that the issue is more fundamental.

This justifies the use of the leaky expected accuracy as defined in Equation 6 as a simple workaround.

3.2 Main Experimental Setting

Architectures. For further experiments we explore several classification related tasks using various architectures:

- **Multilayer perceptron (MLP).** We use a three hidden layer feedforward neural network with ReLU activations [22]. Number of hidden units are set to 300, 200 and 100 for each layer respectively. We use dropout regularization for both the input as well as the hidden layers in which we randomly drop each unit with probability p [28].

- **Convolutional neural network (CNN).** As a CNN we use the ResNet18 deep residual network architecture [10]. To combat overfitting, we provide small random translations or horizontal flips of each training image to the network.

- **Bidirectional LSTM.** For sequence tagging tasks, we use a bidirectional long short-term memory architecture [11, 25]. We use 100 hidden units / memory cells in each direction.

- **Tree LSTM.** For tree tagging (e.g. sentiment classification over parse trees of sentences) we use a tree LSTM architecture [29] which generalizes the traditional LSTM such that it can operate over tree structures. Again, we fix the number of hidden units to 100.

For architectures that operate over textual data, we represent each word using a dense word embedding. To this end, we use the pretrained 300-dimensional Glove word embeddings [23].

Data. For logistic regression, we use six relatively small datasets from the UCI repository [7]: magic [4], musk2 [8], pima [26], polyadenylation, ringnorm [5], satellite47. Number of instances, dimensionality and number of class labels for each dataset are shown in Table 1.

For the MLP architecture, we use the MNIST dataset which we used for our preliminary experiments.

For the CNN architecture (ResNet) we use the CIFAR10 dataset which poses an image classification task, where each 32×32×3 image is to be classified into one of the ten categories [16].

![Figure 2: Logistic regression on MNIST.](image)

![Figure 3: Logistic regression on MNIST over ten folds.](image)
For sequence tagging tasks (in which we use the LSTM architecture), we focus on part-of-speech tagging (POS) and named entity recognition (NER) [12]. We use Penn Treebank (PTB) dataset [20] for POS and CoNLL 2003 dataset [30] for NER.

For tree tagging, we use the Stanford Sentiment Treebank (SSTB) [27]. SSTB includes a supervised sentiment label for every node in the binary parse tree of each sentence. Therefore, not only the sentences but every possible phrase within a sentence is labeled with a sentiment score.

See Table 2 for a breakdown of the datasets.

For a subset of the data, we also experiment in the noisy label setting where we randomly assign random labels (with a probability of 0.05) to each instance in the training and development sets. Noisy versions of the dataset are denoted with an asterisk in the results.

Learning. For each task, we use the Adam update rule [14] and Xavier random initialization of parameters [9]. Since batching is nontrivial, for Tree LSTM (over SSTB), we use the purely online setting of stochastic gradient descent (SGD), whereas for every other task we use minibatched training. For all tasks we perform early stopping, i.e. we pick the best iteration out of all epochs based on the development set performance. Additionally, we tune the learning rate (and dropout rate when appropriate) over the same development set. For logistic regression, we use a minimum number of 100 epochs after which we start applying an 15 epoch patience rule (a lack of improvement for 15 epoch over the development set ends the run). This is because logistic regression is the least costly method and the datasets are small. For MLP and LSTMs, we apply a 30 epoch patience with no minimum or maximum number of epochs. For CNNs and Tree LSTMs, we apply 200 epochs without a patience value. These hyperparameters are intentionally left different to cover a wider range of settings.

Replication. For purposes of replication and to account for extraneous randomness such as data splits, initialization, or the order of instances in SGD, we perform cross-validation (CV). After the original test set is left apart, we randomly split the remaining data into training and development partitions. For MNIST and CIFAR, we use 10-fold CV (there is no development partition readily available). For PTB and SSTB we first combine the original training and development partitions into a bigger set and then apply 5-fold CV, by respecting the original training and development set sizes of each dataset. For UCI datasets, we apply 5×2-CV, which simply reappplies 2-fold CV five times. The only exception to cross-validation is the CoNLL03 data: Since training / development / test partitions are temporally ordered, shuffling and resplitting is not possible. For this data we replicate 5 different random initializations over the same partition.

Finally, we report average accuracy / error rates (with standard deviations) over the test set and compare them using the paired t-test.

3.3 Main Experiments

Logistic regression experiments using the UCI datasets are shown in Table 3. We report mean error rate with the standard deviation across replications. Best results, as well as the ones that perform no worse than the best results in a statistically significant fashion are shown underlined (α = 0.05). Comparing leaky expected error (LEErr) and negative log likelihood (NegLog), we see three wins for LEErr (magic, musk2, ringnorm) and three ties (pima, polyadenylation, satellite47). We see that LEErr consistently performs best (or no worse that best). Unmodified expected error rate (EErr) has four instances in which it is no worse than the best, however for
two datasets, it is significantly worse than the other two (pima, polyadenylation). For later experiments we omit EErr.

Table 4 lists the results for the MLF architecture using MNIST. We observe that LEErr outperforms NegLog by a slight but (statistically) significant margin. When we rerun the experiment using the noisy label case (denoted as MNIST*), we observe a similar result with an increase in the margin. This is in line with our hypothesis about the differences of the two function possibly being more noticeable in the noisy labeling setting since more instances will lie in the negative region.

ResNet18 results over CIFAR10 are presented in Table 5. For this setting, we observe no discernible difference with the two approaches. On average, LEErr performs about single standard deviation better than NegLog, however the difference is not statistically significant.

Results for sequence tagging using bidirectional LSTMs are given in Table 6. For part-of-speech tagging over PTB, we see a statistically significant improvement using LErr (96.95 vs 96.82). For named entity recognition over CoNLL03 however we see a very close tie. When we inject noise to the labels, there is no degradation for LErr (the test accuracy stays at 97.37) whereas NegLog drops from 97.36 to 97.12. In that setting, the difference between NegLog and LEErr is significant.

Finally, results for sentiment classification over binary parse trees are demonstrated in Table 7. Since the data contains sentiment labels all phrases (all tree nodes) as well as sentences (only root nodes), we can evaluate the accuracy for both. For both measurements we see a tie: LEErr performs slightly worse than NegLog, however the difference is not significant.

4 CONCLUSION AND FUTURE WORK
We experimentally investigate the expected accuracy / error rate (and in particular, its leaky version) as an alternative classification objective over a number of architectures and tasks. For some settings, we observe improvements over log likelihood, such as logistic regression, multilayer perceptron and sequence tagging with RNNs. For others, it performs comparably, e.g. for CNNs and Tree LSTMs. We find the results promising since LEErr overall performs better or no worse than NegLog.

One of the main motivations behind expected accuracy is to provide a more faithful approximation to accuracy. However there is a chance that optimizing for training accuracy (or expected accuracy) to be worse for generalization accuracy. For instance, this is an argument for the margin based loss approaches, since having a large margin around the decision boundary tends to improve generalization (even though accuracy itself does not have any margin) [19]. In this work, we compare loss functions over the test set to ensure that their generalization performance is evaluated.

Log likelihood is perhaps the most commonly used probabilistic objective for classification, and is well studied. Many of the recent innovations in deep learning that led to being able to train better models, such as improved regularization [28], better activation functions [22], or improved update rules [14] are studied using the cross entropy classification objective, therefore expected to synergize well with it. Similarly, recent results on loss surfaces or convergence dynamics of neural networks use softmax with log likelihood losses [17, 18]. We believe that future work that uses the (leaky) expected accuracy objective could discover more compatible hyperparameters with improved performance.

REFERENCES
[1] Ethem Alpaydin. 2009. Introduction to machine learning. MIT press.
[2] Rajiv D Banker. 1993. Maximum likelihood, consistency and data envelopment analysis: a statistical foundation. Management science 39, 19 (1993), 1261–1273.
[3] Peter L Bartlett, Michael I Jordan, and Jon D McAuliffe. 2006. Convexity, classification, and risk bounds. J. Amer. Statist. Assoc. 101, 473 (2006), 138–156.
[4] RK Bock, A Chilingarian, M Gaug, F Hakl, T Hengstebeck, M Júrša, J Klaschka, E Kostel, P Savicky, S Towers, et al. 2004. Methods for multidimensional event classification: a case study using images from a Cherenkov gamma-ray telescope. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 516, 2-3 (2004), 511–528.
[5] Leo Breiman. 1996. Bias, variance, and arcing classifiers. (1996).
[6] Andreas Buja, Werner Stuetzle, and Yi Shen. 2005. Loss functions for binary classification: Structure and applications. Working draft, November 3 (2005).
[7] Dua Dheeru and Efi Karra Taniskidou. 2017. UCI Machine Learning Repository. http://archive.ics.uci.edu/ml
[8] Thomas G Dietterich, Ajay N Jain, Richard H Lathrop, and Tomas Lozano-Perez. 1994. A comparison of dynamic repositing and tangent distance for drug activity prediction. In Advances in Neural Information Processing Systems. 216–223.
[9] Xavier Glorot and Yoshua Bengio. 2010. Understanding the difficulty of training deep feedforward neural networks. In Proceedings of the thirteenth international conference on artificial intelligence and statistics. 249–256.
[10] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. 2016. Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition. 770–778.
[11] Sepp Hochreiter and Jürgen Schmidhuber. 1997. Long short-term memory. Neural computation 9, 8 (1997), 1735–1780.
[12] Zhiheng Huang, Wei Xu, and Kai Yu. 2015. Bidirectional LSTM-CRF models for sequence tagging. arXiv preprint arXiv:1508.01991 (2015).
[13] Jack Kiefer and Jacob Wolfowitz. 1956. Consistency of the maximum likelihood estimator in the presence of infinitely many incidental parameters. The Annals of Mathematical Statistics (1956), 887–906.
[14] Diederik K Kingma and Jimmy Ba. 2014. Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980 (2014).
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[15] Sotiris B Kotsiantis. 2007. Supervised machine learning: A review of classification techniques. (2007).
[16] Alex Krizhevsky and Geoffrey Hinton. 2009. Learning multiple layers of features from tiny images. Technical Report. Citeseer.
[17] Hao Li, Zheng Xia, Gavin Taylor, Christoph Studer, and Tom Goldstein. 2018. Visualizing the Loss Landscape of Neural Nets. In Advances in Neural Information Processing Systems 31, S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett (Eds.). Curran Associates, Inc., 6891–6901.
[18] Yuanzhi Li, Zheng Xu, Gavin Taylor, Christoph Studer, and Tom Goldstein. 2018. Visualizing the Loss Landscape of Neural Nets. In Advances in Neural Information Processing Systems 31, S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett (Eds.). Curran Associates, Inc., 6391–6401.
[19] Yi Lin. 2004. A note on margin-based loss functions in classification. Statistics & probability letters 68, 1 (2004), 73–82.
[20] Mitchell P Marcus, Mary Ann Marcinkiewicz, and Beatrice Santorini. 1993. Building a large annotated corpus of English: The Penn Treebank. Computational linguistics 19, 2 (1993), 313–330.
[21] Russell B Millar. 2011. Maximum likelihood estimation and inference: with examples in R, SAS and ADMB. Vol. 111. John Wiley & Sons.
[22] Vinod Nair and Geoffrey E Hinton. 2010. Rectified linear units improve restricted boltzmann machines. In Proceedings of the 27th international conference on machine learning (ICML-10). 807–814.
[23] Jeffrey Pennington, Richard Socher, and Christopher Manning. 2014. Glove: Global vectors for word representation. In Proceedings of the 2014 conference on empirical methods in natural language processing (EMNLP). 1532–1543.
[24] Bernardo Ávila Pires and Csaba Szepesvári. 2016. Multiclass classification calibration functions. ArXiv preprint arXiv:1609.06385 (2016).
[25] Mike Schuster and Kuldip K Paliwal. 1997. Bidirectional recurrent neural networks. IEEE Transactions on Signal Processing 45, 11 (1997), 2673–2681.
[26] Jack W Smith, JE Everhart, WC Dickson, WC Knowler, and RS Johannes. 1988. Using the ADAP learning algorithm to forecast the onset of diabetes mellitus. In Proceedings of the Annual Symposium on Computer Application in Medical Care. American Medical Informatics Association, 261.
[27] Richard Socher, Alex Perelygin, Jean Wu, Jason Chuang, Christopher D Manning, Andrew Ng, and Christopher Potts. 2013. Recursive deep models for semantic compositionality over a sentiment treebank. In Proceedings of the 2013 conference on empirical methods in natural language processing. 1631–1642.
[28] Nitish Srivastava, Geoffrey Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. 2014. Dropout: A Simple Way to Prevent Neural Networks from Overfitting. Journal of Machine Learning Research 15 (2014), 1929–1958. http://jmlr.org/papers/v15/srivastava14a.html
[29] Kai Sheng Tai, Richard Socher, and Christopher D Manning. 2015. Improved semantic representations from tree-structured long short-term memory networks. arXiv preprint arXiv:1503.00075 (2015).
[30] Erik F Tjong Kim Sang and Fien De Meulder. 2003. Introduction to the CoNLL-2003 shared task: Language-independent named entity recognition. In Proceedings of the seventh conference on Natural language learning at HLT-NAACL 2003-Volume 4. Association for Computational Linguistics, 142–147.
[31] Vladimir Vapnik. 2013. The nature of statistical learning theory. Springer science & business media.
[32] Grace Wahba et al. 1999. Support vector machines, reproducing kernel Hilbert spaces and the randomized GACV. Advances in Kernel Methods-Support Vector Learning 6 (1999), 69–87.
[33] Sholom M Weiss and Ioannis Kapouleas. 1990. An empirical comparison of pattern recognition, neural nets and machine learning classification methods. Readings in machine learning (1990), 177–183.
[34] Ian H Witten, Eibe Frank, Mark A Hall, and Christopher J Pal. 2016. Data Mining: Practical machine learning tools and techniques. Morgan Kaufmann.
[35] Yichao Wu and Yufeng Liu. 2007. Robust truncated hinge loss support vector machines. J. Amer. Statist. Assoc. 102, 479 (2007), 974–983.