A novel approach to error function minimization for feedforward neural networks

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Abstract

Feedforward neural networks with error backpropagation (FFBP) are widely applied to pattern recognition. One general problem encountered with this type of neural networks is the uncertainty, whether the minimization procedure has converged to a global minimum of the cost function. To overcome this problem a novel approach to minimize the error function is presented. It allows to monitor the approach to the global minimum and as an outcome several ambiguities related to the choice of free parameters of the minimization procedure are removed.

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1 Introduction

In high energy physics the separation of signal to background usually turns out to be a multi-
dimensional classification problem with many variables involved in order to achieve a reasonable
rejection factor. This is the domain, where neural networks with their intrinsic ability to deal
with many dimensions, are worth to be applied. The output values of neural networks (NN)
can be interpreted as estimators of \( a \text{ posteriori} \) Bayesian probabilities which provide the link
to classification problems of higher order [?].

A neural network can be regarded as a non-linear combination of several transformation ma-
trices, with entries (denoted as weights) adjusted in the training phase by a least squares
minimization of an error function. There are several technical problems associated with the
training of the neural network. Real world applications rarely allow a perfect separation of
patterns, i.e. given a problem with patterns of two classes \( C_1 \) and \( C_2 \), a certain fraction of
patterns belonging to class \( C_1 \) will look like patterns from class \( C_2 \) and vice versa. This ef-
fect may be denoted as the confusing teacher problem. In high energy physics one deals with
overlapping distributions which will cause an \( a \text{ priori} \) contamination, i.e. indistinguishable
patterns assigned to different classes. The non-linearity of the problem and the number of free
parameters involved, enhance the possibility of the minimization procedure to converge to a
local minimum of the error function. This leads to a deterioration of the separation ability and
therefore a poorer estimate of the Bayesian probabilities, which are lower limits to the prob-
ability of error in any problem of classification. The type of network used in this analysis is
known as feedforward neural network with error backpropagation (FFBP) [?]. The name orig-
inates from the specific architecture of the transformation matrices and the method applied to
optimize their entries. A pattern is represented by an input vector whose entries are processed
by the network in several layers of units. Each unit feeds only the units of the following layer
(feedforward). During the minimization procedure the calculated difference between the actual
network output and the desired output is used to adjust the weights (error backpropagation) [?].

A general description rule to avoid problems with local minima in the minimization procedure
for feedforward neural networks with a quadratic cost function will be presented in this article.
The basic features of the new model are demonstrated by a one-dimensional problem.

2 Mathematical foundation of feedforward neural net-
works

Each pattern to be classified is represented by a vector \( X \) of dimension \( K \) (called the input
vector). For the purpose of estimating the Bayesian \( a \text{ posteriori} \) probabilities the input vector
\( X \) is projected into the output space by means of the neural network formula

\[
Y = f(X) ,
\]

(1)
in which $Y$ is of dimension $I$, equal to the total number of possible classes $C_l$, with $l \epsilon [1, I]$. Standard FFBP use for $f$

$$f(X) = g \left( A_{ij} g \left( \frac{B_{jk} X_k - \alpha_j}{t} \right) - \text{eta}_i \right)$$

$$g(...) = \frac{1}{2} \left( 1 + \tanh(...) \right)$$

with $i \epsilon [1, I], j \epsilon [1, J], k \epsilon [1, K]$ and where the Einstein convention for same indices was used. For two overlapping Gaussian distributions the function $g$ represents the exact solution for the Bayesian probabilities which is the motivation for the choice of this particular sigmoid function [?]. The weights $A_{ij}, B_{jk}, \alpha_j$ and $\beta_i$ are the free parameters of the fit function $f$, and $J$ denotes the number of hidden nodes. In analogy to spin Ising models $t$ is called temperature and is usually set to one. For any classification problem the aim is to achieve for an input vector $X$ belonging to class $C_l$ the output value $Y = O(C_l)$, where $O(C_l)$ is a unit vector whose components are all zero except for the entry with index $l$. For any $A_{ij}, B_{jk}, \alpha_j$ and $\beta_i$, initialized at random in an interval $[-\epsilon, +\epsilon]$, one defines the error function

$$E = \frac{1}{2 N} \sum_{n=1}^{N} \sum_{i=1}^{I} ( Y_i(X(C_l,n)) - O_i(C_l) )^2$$

where the first sum runs over all $N$ patterns available and the second sum runs over all possible classes $I$. This error function is minimized iteratively by a gradient descent method

$$A_{ij}^{(\mu+1)} = A_{ij}^{(\mu)} - \eta \Delta A_{ij}^{(\mu)}$$

$$\Delta A_{ij}^{(\mu)} = \frac{\partial E^{(\mu)}}{\partial A_{ij}} + \kappa \Delta A_{ij}^{(\mu-1)}$$

where $\eta$ is the step size ($\eta \epsilon (0, \infty)$) and $0 \leq \kappa < 1$ is the weight of the momentum term. The same procedure applies to the matrices $B, \alpha$ and $\beta$. The upper index $(\mu)$ denotes the iteration step. The momentum term serves to damp possible oscillations and to speed up the convergence in regions where $E$ is almost flat [?].

Typically FFBP consist of many free parameters which need to be adjusted by the minimization procedure. Due to the non-linearity of the neural net function $f(X)$ it is very likely that local minima of the error function $E$ will prevent the convergence to the global minimum which results in a deterioration of the classification ability. One common method to avoid this problem is to change the definition of $E$; i.e. instead of averaging over all patterns $N$, the sum for $n$ in equation (3) extends only over $\tilde{N}$ patterns with $1 \leq \tilde{N} < N$ (called incremental updating). This introduces some randomness into the minimization procedure which might help to overcome local minima but introduces at the same time a new free parameter $\tilde{N}$ which can only be optimized by trials. For $\tilde{N} = N$ the method is called batch mode updating.

For standard FFBP the temperature $t$ does not affect the performance of the minimization procedure. As for the entries of the matrices, no constraints are imposed, any change of $t$ can be compensated by an overall rescaling of the weights.

The least squares fit procedure requires several input parameters whose values are to be assumed and tested, i.e.
• the temperature ($t$),
• the initial range of the weights ($\epsilon$),
• the weight of the momentum term ($\kappa$),
• the step size ($\eta$), and
• the number of patterns over which the sum for $E$ extends ($\tilde{N}$).

The performance of the FFBP is strongly influenced by the choice of these parameters. For instance the possibility of getting trapped in a local minimum is enhanced for a wrong choice of $\epsilon$. Often the surface of $E$ is probed by initializing the matrices of $f(X)$ at different points in the parameter space and by choosing different sets of values for the above listed parameters. Each of the networks will achieve a different performance on an independent test sample, which has not been part of the sample used to minimize the cost function. This usually happens if the minimization procedure converges to a local minimum. It can be shown, that an average over the output values of the different networks improves significantly the overall performance on the test sample. This method is referred to as the ensemble method [?]. However, it does not ensure an optimal solution and the results depend on the number of trials. Another approach is denoted as weight decay and reduces the number of weights by adding a penalty term to the cost function. This term depends on the size of the weights and thus gives each weight a tendency to decay to zero. Thereby it is less likely that the error function exhibits local minima because it depends on less weights [?].

The problem of restricting the parameter space to a region which ensures convergence to the global minimum remains thus to a large extend unsolved.

3 Modified FFBP model

Let’s assume the entries of the input vector $X$ to be of the order of unity. The matrices $A_{ij}$ and $B_{jk}$ can be normalized for each row, i.e.

$$
A_{ij} \rightarrow A_{ij} , \quad B_{jk} \rightarrow B_{jk} ,
$$

$$
\sum_{j=1}^{J} A_{ij}^2 = 1 , \quad \forall \ i ; \quad \sum_{k=1}^{K} B_{jk}^2 = 1 , \quad \forall \ j . \quad (6)
$$

Thereby $B_{jk}$ and $\alpha_j$ denote the normal and the Euclidean distance to zero of the $j$’s hyperplane in the space of the input variables as depicted in figure 1. The hyperplanes are defined by the equations $B_{jk} X_k - \alpha_j = 0$. The same is true for the hyperplanes in the space of the hidden variables, with the replacement $B_{jk} \rightarrow A_{ij} , \quad \alpha_j \rightarrow \beta_i$ and $X_k \rightarrow g_j$. These constraints remove the dependence of the minimization procedure on $\epsilon$. The weights $\alpha_j$ and $\beta_i$ are initially set to zero such that only the orientation of the hyperplanes vary. Due to this modification the role of $t$ becomes a major one and rules the overall structure of the error function. For $t \rightarrow \infty$
the values of $Y_i$ are all equal to 0.5 for any finite $X$. The value of $E$ will thus converge to a constant, i.e.
\[
\lim_{t \to \infty} E = \frac{1}{2N} \sum_{n=1}^{N} \sum_{i=1}^{I} \left( \frac{1}{2} - O_i(C_l, n) \right)^2 = \frac{I}{8}.
\]
(7)

In the limit of $t \approx 0$ the sigmoid function $g$ becomes the step function $\Theta$. This results in probabilities $Y$ equal to 1 or 0, thus in non overlapping distributions in the input space, i.e. the input distributions are completely separated. In terms of the parameter $t$, the error function $E$ acquires a well defined structure. The contribution to $E$ of patterns belonging to class $C_l$ is determined by the following expression:

\[
E(C_l) = \int dX \ P(C_l) \ P(X|C_l) \frac{1}{2} \sum_{i=1}^{I} \frac{1}{t} \left( \frac{Y_i(X(C_l)) - O_i(C_l)}{\Lambda(C_l)} \right)^2.
\]
(8)

If an input vector $X$ belongs to class $C_l$ the function $P(X|C_l)$ denotes the probability distribution of $X$ and $P(C_l)$ the probability of class $C_l$. Both functions depend upon the problem under investigation, thus $\Lambda(C_l)$ is the only part of equation (8) which changes as a function of the parameter $t$. To analyse the high $t$-behavior of $E(C_l)$ one can expand $\Lambda(C_l)$ in $\frac{1}{t}$.

Denoting $h_j := B_{jk} X_k - \alpha_j$,
\[
\lim_{t \to 0} \Lambda(C_l) = \left( g \left[ \frac{A_{ij} g(h_j)}{t} - \frac{\beta_i}{t} \right] - O_i(C_l) \right)^2
\]
\[
= \left( \frac{1}{2} \left( 1 + \frac{A_{ij}}{2t} + \frac{A_{ij} h_j}{2t^2} - \frac{\beta_i}{t} + O\left( \frac{1}{t^3} \right) \right) - O_i(C_l) \right)^2
\]
\[
= O^2_i(C_l) - O_i(C_l) \left( 1 + \frac{A_{ij}}{2t} + \frac{A_{ij} h_j}{2t^2} - \frac{\beta_i}{t} \right) +
\]
\[
\frac{1}{4} \left( 1 + \frac{A_{ij}}{t} + \frac{A_{ij}^2}{4t^2} + \frac{A_{ij} h_j}{t^2} - \frac{2 \beta_i}{t} - \frac{A_{ij} \beta_i}{t^2} + \frac{\beta_i^2}{t^2} \right) + O\left( \frac{1}{t^3} \right)
\]
(9)

For small $\frac{1}{t}$, when terms of the order $O\left( \frac{1}{t^3} \right)$ or higher can be neglected, the error function becomes a quadratic sum of the weights with only one minimum. In the next section this will be illustrated with an example.

Thus, while for high temperatures the error function has a smooth behavior, at low temperatures all its structures are present. This transition is continuous and it is reasonable to assume that the global minimum of the error function becomes at high temperatures the only minimum of $E$. The idea is then to start the minimization at high values of $t$ and converge to the region of the minimum of $E$ in this regime. The resulting weights are expected to be already close to those corresponding to the global minimum. If so, further decrease of the temperature should lead to the global minimum without the risk of being trapped in a local minimum. Therefore the summation in equation (8) must extend over the whole pattern sample to determine the
position of the global minimum as precisely as possible, i.e. the free parameter $\tilde{N}$ is set to $N$.

In the minimization procedure the temperature is changed in the same way as the weights but the step size for the temperature is reduced by one order of magnitude. This ensures a faster convergence behavior for the weights, therefore

\begin{align}
  t^{(\mu+1)} &= t^{(\mu)} - \frac{\eta}{10} \Delta t^{(\mu)} \\
  \Delta t^{(\mu)} &= \frac{\partial E^{(\mu)}}{\partial t} + \kappa \Delta t^{(\mu-1)}
\end{align}

In the low $t$ region $E$ becomes very steep which might lead during the minimization to oscillations in $t$. Any step in the wrong direction and the error function could yield huge derivatives for $t$. Thus given that the functional dependence of $E$ on $t$ is of the form $E \sim \tanh^2 \frac{1}{t}$, the step size $\eta$ must be $t$-dependent, i.e.

\begin{equation}
  \eta(t) = 1 + \gamma - \tanh^2 \frac{1}{t},
\end{equation}

where the new parameter $\gamma$ is the pedestal value for $\eta(t)$. A value of $\gamma$ of 0.1 ensures that only about 10% of the calculated derivatives will contribute to the change of the weights for $t \leq 0.5$.

### 3.1 Determination of $t^{(0)}$

Usually one aims to separate two distinct distributions. In that case the neural net formula (2) can be simplified. We set $I = 1$, change the sigmoid function to $g(...) = \tanh(...)$ and assign two output values to the now scalar variable $O(C_l)$:

\[ O(C_l) = \begin{cases} +1, & \text{if } X \text{ belongs to class } C_1 \\ -1, & \text{if } X \text{ belongs to class } C_2 \end{cases} \]

Therefore $Y$ is a scalar and becomes an estimator for the probability function

\[ Y \approx P(C_1|X) - P(C_2|X) \]

with $P(C_i|X)$ being the a posteriori Bayesian probability that $X$ belongs to the class $C_i$. For the case of two overlapping Gaussian distributions $g(...)$ represents the exact solution for the Bayesian probabilities. If we consider a one-dimensional problem ($K = 1$) and allow for simplicity just one cut ($J = 1$) formula (2) can be reduced to:

\[ Y(X(C_l)) = \tanh \left[ \frac{X(C_l) - d}{t} \right] \]

with $d$ as the only remaining weight, corresponding to $\alpha_j$ in equation (2). Let us assume a flat conditional probability distribution for the different classes, i.e.

\[ P(X|C_l)_{ij} = \begin{cases} \frac{1}{X_j-X_i}, & \text{if } X_i \leq X \leq X_j \\ 0, & \text{elsewhere} \end{cases} \]

The contribution of $P(X|C_l)_{ij}$ to the error function $E$ can be evaluated analytically:
\[ E_{ij}(C_l) = \frac{1}{2} \frac{P(C_l)}{X_j - X_i} \left[ O^2(C_l)(X_j - d) - 2tO(C_l) \ln \cosh \frac{X_j - d}{t} + (X_j - d - t \tanh \frac{X_j - d}{t}) \right] - \]
\[
\frac{1}{2} \frac{P(C_l)}{X_j - X_i} \left[ O^2(C_l)(X_i - d) - 2tO(C_l) \ln \cosh \frac{X_i - d}{t} + (X_i - d - t \tanh \frac{X_i - d}{t}) \right] .
\] (16)

For high values of \( t \) the non-linear functions in equation (16) are expanded in powers of \( \frac{X-d}{t} \).

Neglecting terms of the order of \( O(\frac{X-d}{t})^5 \) and higher will leave a \( d^4 \) dependence in \( E_{ij}(C_l) \) which might lead to a local minimum. It’s partial derivative relative to \( d \) turns out to be only quadratic:

\[
\partial_d E_{ij}(C_l) = P(C_l) \left( d^2 \left( -\frac{O(C_l)}{t^3} \right) + d(\ldots) + (\ldots) \right) \quad (17)
\]

\[
\partial_d E = \partial_d E_{ij}(C_1) + \partial_d E_{kl}(C_2) \quad (18)
\]

This already proves that \( E \) has only one maximum and one minimum. The quadratic dependence of the partial derivative \( \partial_d E \) on the weight \( d \) vanishes for \( P(C_l) = 0.5 \) due to the definition of \( O(C_l) \). With this additional requirement the error function \( E \) depends only quadratically on the weight \( d \). Thereby the optimal a priori probability for the minimization procedure is determined to be 0.5. As \( Y \) will be an estimator for an a posteriori probability it is possible afterwards to reweigh the result to any a priori probability under investigation. The \( t \)-dependence of \( E_{ij}(C_l) \) is determined by a sum of 2 terms

\[
E_{ij}(C_l) \sim t \ln \cosh \frac{1}{t} + t \tanh \frac{1}{t} ,
\] (19)

which are depicted in figure [2]. The two terms exhibit a different behavior for \( t \to 0 \) and \( t \to \infty \). The first term \((I)\) dominates in the low \( t \) region and therefore determines the structure of the error function \( E \) in this temperature range. For high values of \( t \) the second term \((II)\) dominates over the first one. Both terms have almost equal weight for \( 1/t = 1.5 \). Since the proposed method of minimizing the error function requires that initially \( t(0) \) be chosen such that \( E \) exhibits only one minimum, it implies \( 1/t(0) < 1.5 \). At \( t = 5 \) the second term \((II)\) has a 10-times bigger weight than the first term \((I)\) which should satisfy the requirements necessary for the approximation done in equation (19). With the assumption that the values of the input vector \( X \) are of order one, the general prescription for the initial value of the temperature \( t \) is thus

\[
t(0) \geq 5 . \quad (20)
\]

This will be illustrated by a numerical example. Suppose one aims to separate the two one-dimensional overlapping distributions with flat conditional probabilities as defined in equation (15) and assumes that:

\[
P(X|C_1) = 0.7 P(X|C_1)_{12} + 0.3 P(X|C_1)_{34}
\]
\[
P(X|C_2) = 1.0 P(X|C_2)_{56}
\]
\[
X_1 = -4.0 \quad X_2 = 0.5 \quad X_3 = 3.0 \\
X_4 = 3.1 \quad X_5 = -0.5 \quad X_6 = 4.0
\]

With \( P(C_1) = P(C_2) = 0.5 \) one gets a surface of the error function \( E \) as depicted in figure 3.

If the minimization procedure were to start at any value of \( d \) and \( t^{(0)} \geq 5 \) it would converge to the global minimum of \( E \) without the possibility of getting trapped in a local minimum. In the case of non-overlapping distributions the temperature \( t \) will converge to zero to model probabilities equal to one. If the distributions overlap to 100\% the temperature will converge to infinity. Thereby the final value of \( t = t^{(\infty)} \) becomes a measure of the overlap of the two distinct distributions, i.e.

\[
\text{Overlap} \approx \frac{t^{(\infty)}}{1 + t^{(\infty)}}.
\]  \hspace{1cm} (21)

Thus to summarize, the proposed modified neural network differs from networks using standard backpropagation as follows:

| Parameter | Name                              | New model                                      | Standard FFBP                                  |
|-----------|-----------------------------------|------------------------------------------------|-----------------------------------------------|
| \( t^{(0)} \) | The initial value of the temperature | \( t^0 \geq 5 \). The temperature is **not** constant and changes for each iteration step. | Not well defined. Usually \( t \) is not changed throughout the minimization procedure and thus set to \( t = 1 \). |
| \( \epsilon \) | The absolute range of the initial weights | Cancelled, as the weights \( A \) and \( B \) are row-wise normalized to one, and \( \alpha \) and \( \beta \) are initially set to zero. | Not well defined. Usually \( \epsilon \leq 0.01 \). |
| \( \kappa \) | The weight of the momentum term | Not well defined. | Not well defined |
| \( \eta \) | The step size | \( \eta(t) = 1.0 + \gamma - \tanh^2 \frac{\gamma}{t} \) | Not well defined. Usually \( \eta \leq 0.001 \). |
| \( \gamma \) | The pedestal for \( \eta \) | Not well defined. Usually set to 0.1 | Does not exist in this model |
| \( \tilde{N} \) | The # of patterns to sum over in \( E \) | \( \tilde{N} = N \) | Not well defined. Usually set to \( \tilde{N} \approx 10 \) |
| \( P(C_l) \) | The a priori probability of class \( C_l \) | For the case of two classes determined to \( P(C_l) = 0.5 \), otherwise not well defined. | Not well defined |

### 4 Conclusions

A novel method to minimize the quadratic cost function of a neural network with error backpropagation has been presented. The essential modification is the row-wise normalization of the matrices \( A \) and \( B \) which represent part of the weights of the neural network. Thus, the entries of each row of \( A \) and \( B \) acquire the meaning of normals which define the orientation of hyperplanes. Due to the normalization, the error function \( E \) obtains a well defined structure as a function of the free parameter \( t \), denoted as the temperature. It has been proven that for high values of \( t \), when terms of the order \( \mathcal{O}(\frac{1}{t}) \) or higher can be neglected, the cost function \( E \)
always exhibits a quadratic dependence on the weights and thus only one minimum. For low temperatures all structures of $E$ are apparent and local minima might exist. This transition is continuous and it is natural to assume, that the single minimum of the cost function at high values of $t$ leads to the global minimum of $E$ at low temperatures. However, there is no rigorous proof as yet, that this should be the case.

The minimization procedure starts at high temperatures and converges first to the single minimum of the error function in this range of $t$. Further decrease of $t$ should lead to the global minimum without the risk to converge to a local minimum. Similar to the weights, the temperature becomes a parameter whose value is determined by the minimization procedure. Assuming the entries of the input vector $X$ to be of the order of one, the initial value of $t$ should be $t^{(0)} \geq 5$ as derived from an one-dimensional example. Multi-dimensional problems are nested superpositions of the one-dimensional example, therefore this range for $t^{(0)}$ should still ensure the quadratic dependence of the cost function on the weights. Several free parameters of the standard minimization procedure for FFBP, whose values are to be assumed and tested, are constrained. Thus, without any fine tuning, the new model is applicable to any classification problem.

The new method described in this paper has been successfully applied to the problem of electron identification \[?] in the ZEUS ldetector \[?] at HERA. At HERA electrons of 30 GeV collide with protons of 820 GeV. High energetic particles and jets of particles, mainly hadronic particles, emerge from the interaction point and deposit energy in the spatially segmented uranium-scintillator calorimeter (CAL) of the ZEUS detector. A certain fraction of the interactions between electrons and protons are characterized by the presence in the final state of the electron scattered under a large angle, which is thus in the geometrical acceptance of the CAL. The aim is to select this type of events which are believed to originate from the scattering of the electron on a point like constituent of the proton. The showering properties of electrons and hadrons in an absorber material are different and it is possible to identify the particle type by the pattern of the energy deposits in the CAL. The longitudinal and transversal segmentation of the CAL provides 54 values reflecting the spatial shape of the shower. The shape depends also on the angle of incidence of the showering particle. After including this angle the input patterns are 55-dimensional. Using the new method, a neural network has been trained on patterns originating from electrons and hadrons. In comparison with a classical approach, the neural network separates the distinct distributions better, giving a typical increase of about 10% in efficiency and purity. A principle component analysis has shown that this improvement is achieved through the use of all the 55 variables.

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5 Appendix

This new minimization procedure has been implemented in a FORTRAN program called dEXTRA. The program is controlled by a configuration file named dextra.cnf where all parameters, paths and options are set. It must be located in the directory from which dEXTRA is started. The value of the error function $E$ for $t = 0$ for both the training and an independent test pattern sample can be calculated during the minimization procedure. This method is denoted as cross-validation and serves to check for over-fitting, i.e. when the network starts to pick up fluctuations from the training sample [?]. After the training procedure the final set of matrices and parameters can be written to a file which afterwards can be read in again for application to new pattern samples.

The program is available on request from the author. For further questions please contact sinkus@zow.desy.de.
Figure 1: Graphical representation of the first transformation of the neural net formula (2). The matrix operation $B_{jk} X_k - \alpha_j$ calculates the Euclidean distances of the input vector $X$ to the $J$ hyperplanes in the space of the input variables (Hesse’s normal form). An example for the first hyperplane ($j = 1$) in 3 dimensions ($K = 3$) is depicted. Each row of the matrix $B_{jk}$ denotes a normal of a hyperplane in the space of the input variables. The value $\alpha_j$ determines the distance of the $j$’s hyperplanes to zero.
Figure 2: The t-dependence of the individual terms contributing to the error function $E_{ij}(C_i)$ for a one-dimensional distribution with a flat conditional probability.

Figure 3: Structure of the error function $E$ for the one-dimensional example (described in the text) as a function of the weight $d$ and the temperature $t$. The global minimum of this specific error function is placed at $d \approx 0.5$ and $t \approx 4.5$. Local minima of $E$ lie below $t \approx 1.3$. 