Distance Metric Learning for Conditional Anomaly Detection

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Abstract

Anomaly detection methods can be very useful in identifying unusual or interesting patterns in data. A recently proposed conditional anomaly detection framework extends anomaly detection to the problem of identifying anomalous patterns on a subset of attributes in the data. The anomaly always depends (is conditioned) on the value of remaining attributes. The work presented in this paper focuses on instance–based methods for detecting conditional anomalies. The methods depend heavily on the distance metric that lets us identify examples in the dataset that are most critical for detecting the anomaly. To optimize the performance of the anomaly detection methods we explore and study metric learning methods. We evaluate the quality of our methods on the Pneumonia PORT dataset by detecting unusual admission decisions for patients with the community–acquired pneumonia. The results of our metric learning methods show an improved detection performance over standard distance metrics, which is very promising for building automated anomaly detection systems for variety of intelligent monitoring applications.

Introduction

Anomaly detection methods can be very useful in identifying interesting or concerning events. Typical anomaly detection attempts to identify unusual data instances that deviate from the majority of examples in the dataset. Such instances indicate anomalous (out of ordinary) circumstances, for example, a network attack (Eskin 2000) or a disease outbreak (Wong *et al.* 2003). In this work, we study conditional anomaly detection framework that extends standard anomaly detection by identifying partial patterns in data instances that are anomalous with respect to the remaining data features. Such a framework has been successfully applied to identify unusual patient–management decisions made for patients suffering from different conditions (Hauskrecht *et al.* 2007).

Data attributes (features) in the conditional anomaly detection are divided into two disjoint groups: context (or condition) attributes C and target attributes A. The conditional anomaly methods then attempt to identify anomalies in target attributes A with respect to context C. The conditional aspect allows us to identify patterns that are typical in one context but anomalous in the other. To illustrate the potential of the method assume two patients with different conditions are given the same drug. In one of these conditions the administration of the drug is normal, but for the other one it is unusual. The conditional anomaly detection methods with target variables corresponding to the treatment should be able to identify the anomaly in the treatment.

The conditional anomaly detection method evaluates and identifies anomalies one data example at the time. To make an anomaly call for a data instance **x**, (Hauskrecht *et al.* 2007) proposed a probabilistic predictive model M that aims to capture stochastic dependencies among the target and context attributes. The predictive model defines a conditional probability distribution $p(A/C)$ of target attributes given the values of context variables. Given the

predictive model, the anomaly call for a data instance **x** is made if the probability of the target attributes observed in **x** is small.

A predictive probabilistic model used for detection purposes can be built in different ways. In this paper, we focus on instance–based approaches. The instance–based methods do not try to learn a universal predictive model for all possible instances at the same time, instead the model is optimized for every data instance **x** individually. The instance–specific model $M_\mathbf{x}$ may provide a better option if the predictive model is less complex and the dataset is small.

Instance–specific models often rely on a distance metric that aims to pick examples most relevant for the prediction of **x**. However, the question of what is the best distance metric to reflect the relevancy of the example to the prediction is the most challenging part of the task. Standard metrics such as Euclidean or Mahalanobis metrics are not the best for the anomaly detection task since they may be biased by feature duplicates or features that are irrelevant for predicting target attributes. Thus, instead of choosing one of the standard distance metrics we investigate and test metric–learning methods that let us adapt predictive models to specifics of the currently evaluated example **x**.

We explore two metric–learning methods that were originally used for building non–parametric classification models. The first method is NCA (Goldberger *et al.* 2004). The method adjusts the parameters of the generalized distance metric so that the accuracy of the associated nearest neighbor classifier is optimized. The second method, RCA (Bar-Hillel *et al.* 2005), optimizes mutual information between the distribution in the original and the transformed space with restriction that distances between same class cases do not exceed a fixed threshold.

To evaluate the quality of metric learning methods in anomaly detection we apply them to the problem of identification of unusual patient–management decisions, more specifically, to the problem of detection of unusual hospitalization patterns for patients with the community acquired pneumonia. We show that on this problem metric learning approaches outperform standard distance metrics.

Methodology

Conditional anomaly detection

In anomaly detection, we are interested in detecting an unusual data pattern the occurrence of which deviates from patterns seen for other examples. In the conditional anomaly, a partial data pattern is evaluated in context of other data variables and their values. Briefly, the data attributes (features) are divided into two disjoint groups: context (or condition) attributes *C* and the target attributes *A*. The objective of conditional anomaly detection methods is to identify anomalies in target attributes *A* with respect to context attributes *C*.

Let $E = \{\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^n\}$ be a set of examples in the dataset and let **x** be an example we want to analyze and determine if it is conditionally anomalous with respect to examples in *E*. The context of the example **x** is defined by the projection of **x** to context attributes *C*, which we denote by *C*(**x**). Similarly, *A*(**x**) denotes the projection of **x** to target attributes.

Our goal is to identify the anomaly in **x** with respect to examples in the dataset *E*. The examples and their relation to **x** can be captured indirectly by an auxiliary probabilistic predictive model *M*. This approach was proposed recently by (Hauskrecht *et al.* 2007). The predictive model *M* defines a conditional probability distribution of target variables given the value of context variables: *p*(*A*/*C*) and it is induced (learned) from examples in *E*. Given *M* we say the case **x** is *anomalous* in target attributes *A*, if the probability *p*(*A*(**x**)/*C*(**x**)) for the model is small and falls below some threshold. In summary, stochastic relations in between the context and target

attributes observed in examples *E* are incorporated into a probabilistic model *M*, which is in turn applied to example **x**. The anomaly is detected by evaluating the probability of target variable values for the **x** given the values of its context variables *C*(**x**) in model *M*.

To build a working anomaly detection algorithm, we need to provide methods for building a probabilistic model *M* from the dataset and methods for detecting the anomaly using the model.

Building a probabilistic model

Our conditional anomaly framework builds upon the existence of an underlying probabilistic model *M* that describes stochastic relations among context and target data attributes. We consider two types of models to achieve this task: (1) parametric and (2) non–parametric models.

Parametric predictive models—In the parametric approach we assume a predictive model *p*(*A*/*C*) is defined using a small set of parameters Θ that reflect accurately the stochastic relation among the context and target attributes expressed in data *E*. Examples of parametric models are: a Bayesian belief network (Pearl 1988), a Naive Bayes model (Domingos & Pazzani 1997), Linear discriminant analysis (Hastie, Tibshirani, & Friedman 2001)or a logistic regression model (Hastie, Tibshirani, & Friedman 2001). In this work we focus on the Naive Bayes model that is used frequently in classification tasks. We adopt the Bayesian framework to learn the parameters of the model from data *E* and to support probabilistic inferences. In such a case the parameters *M* of the model are treated as random variables and are described in terms of a density function $p(\theta_M)$. The probability of an event is obtained by averaging over all possible parameter settings of the model *M*.

To incorporate the effect of examples *E*, $p(\theta_M)$ corresponds to the posterior $p(\theta_M /E)$. The posterior is obtained via Bayes theorem:

$$p(\theta_M|E)=p(E|\theta_M)p(\theta_M)/p(E),$$

where $p(\theta_M)$ defines the prior for parameters θ_M. To simplify the calculations we assume (Heckerman 1995) (1) parameter independence and (2) conjugate priors. In such a case, the posterior follows the same distribution as the prior and updating reduces to updates of sufficient statistics. Similarly, many probabilistic calculations can be performed in the closed form.

Instance–specific models—In general, a predictive probabilistic model used for anomaly detection purposes can be of different complexity. However, if the dataset used to learn the model is relatively small, a more complex model may become hard to learn reliably. In such a case a simpler parametric model of *P*(*A*/*C*) with a smaller number of parameters may be preferred. Unfortunately, a simpler model may sacrifice some flexibility and its predictions may become biased towards the population of examples that occurs with a higher prior probability. To make accurate predictions for any instance we use *instance–specific* predictive methods and models (Visweswaran & Cooper 2005; Aha, Kibler, & Albert 1991).

Briefly, instance–based methods do not try to learn a universal predictive model for all possible instances, instead the model is optimized for every data instance **x** individually. To reflect this, we denote the predictive model for **x** as $M_\mathbf{x}$. The benefit of instance–based parametric models is that they can be fit more accurately to any data instance; the limitation is that the models must be trained only on the data that are relevant for **x**. Choosing the examples that are most relevant for training the instance–specific model is the bottleneck of the method. We discuss methods to achieve this later on.

Non–parametric predictive models—Non–parametric predictive models do not assume any compact parametrization of $P(A/C)$. Instead, the model is defined directly on the dataset of examples E. A classic example of a non–parametric model is the k Nearest Neighbor (k–NN) classifier in which the predicted class of the instance is the majority vote of the classes of its k nearest neighbors.

Non–parametric models are instance specific by definition. For example, the k–NN classifier for instance x executes by finding k examples closest to $\mathbf{x}$ first and making the prediction afterwards. The problem of finding the k closest neighbors is the bottleneck of the method. Non–parametric models depend on the choice of examples closest to $\mathbf{x}$, and the quality of these choices influences the quality of the model.

The anomaly detection approach applied in this work builds upon the model $M_{\mathbf{x}}$ which defines the probability distribution $P(A/C(\mathbf{x}))$ for $\mathbf{x}$. But how to define a non-parametric predictive model $M_{\mathbf{x}}$? The key here is to define the probability with which a neighbor example predicts the values of target attributes A for $\mathbf{x}$. Intuitively, closer neighbors should contribute more and hence their prediction should come with a higher probability. To reflect this intuition (Goldberger *et al.* 2004) define the probability that a data example $\mathbf{x}'$ predicts $\mathbf{x}$ using the softmax model (Mc-cullagh & Nelder 1989). In this model, the probability with which $\mathbf{x}'$

contributes to the prediction of $\mathbf{x}$ is proportional to: $\exp(-\left\|\mathbf{x} - \mathbf{x}'\right\|_m^2)$ where m is a distance metric reflecting the similarity of the samples. The softmax model normalizes this quantities so that their sum is 1.

The above definition of a non–parametric probabilistic predictive model expects a distance metric defining the similarity among examples. We return to the problem of distance metrics in the next section.

Anomaly detection

Multiple approaches can be used to make anomaly calls based on the probabilistic metric. Typically, they rely on a variety of thresholds. These include: absolute, relative or the k standard deviation thresholds. In our work, we build upon the absolute threshold test. In the absolute threshold test, the example $\mathbf{x}$ is anomalous if $p(A(\mathbf{x})/C(\mathbf{x}), M_{\mathbf{x}})$ falls below some fixed probability threshold p_ε. Intuitively, if the probability of the target attributes $A(\mathbf{x})$ for x is low with respect to the model $M_{\mathbf{x}}$ and its other attributes $C(\mathbf{x})$, then the value of the target attribute is anomalous. Note that the absolute threshold test relies only on the model $M_{\mathbf{x}}$ and there is no direct comparison of predictive statistics for $\mathbf{x}$ and examples in E. However, if instance–based methods are used the most important examples in E are used to construct the model $M_{\mathbf{x}}$ and hence their effect is reflected in the statistic.

Defining the similarity metric

Parametric instance–based models are sensitive of examples used to train them. Similarly, the instance–based non–parametric models are sensitive to examples incorporated into the model. The key question is what examples from E should be used for training or defining the instance–specific predictive model $M_{\mathbf{x}}$.

Exact match

Clearly, the best examples are the ones that exactly match the attributes $C(\mathbf{x})$, of the target case $\mathbf{x}$. However, it is very likely that in real–world databases none or only few past cases match the target case exactly so there is no or very weak population support to draw any statistically sound anomaly conclusion.

Similarity–based match

One way to address the problem of insufficient population available through the exact match is to define a distance metric on the space of attributes $C(\mathbf{x})$ that let us select examples closest to the target example $\mathbf{x}$. The distance metric defines the proximity of any two cases in the dataset, and the k closest matches to the target case define the best population of size k. Different distance metrics are possible. An example is the generalized distance metric r^2 defined:

$$r^2(\mathbf{x}^i, \mathbf{x}^j) = (\mathbf{x}^i - \mathbf{x}^j)^T \Gamma^{-1} (\mathbf{x}^i - \mathbf{x}^j), \tag{1}$$

where Γ^{-1} is a matrix that weights attributes of patient cases proportionally to their importance. Different weights lead to a different distance metric. For example, if Γ is the identity matrix I, the equation defines the Euclidean distance of x^i relative to x^j. The Mahalanobis distance (Mahalanobis 1936) is obtained from 1 by choosing Γ to be the population covariance matrix Σ which lets us incorporate the dependencies among the attributes.

The Euclidean and Mahalanobis metrics are standard off–shelf distance metrics often applied in many learning tasks. However they come with many deficiencies. The Euclidean metric ignores feature correlates which leads to 'double–counting' when defining the distance in between the points. The Mahalanobis distance resolves this problem by reweighting the attributes according to their covariances. Nevertherless, the major deficiency of both Mahalanobis and Euclidean metrics is that they may not properly determine the relevance of an attribute for predicting the target attributes.

The relevance of context attributes for anomaly detection is determined by their influence on target attributes A. Intuitively, a context attribute is relevant for the predictive model if is able to predict changes in values of target attributes A. To incorporate the relevance aspect of the problem into the metric we adapt (learn) the parameters of the generalized distance metric with the help of examples in the dataset E.

Metric–learning—The problem of distance metric learning in context of classification tasks has been studied by (Goldberger *et al.* 2004) and (Bar-Hillel *et al.* 2005). We adapt these metric learning methods to support probabilistic anomaly detection. In the following we briefly summarize the two methods.

(Goldberger *et al.* 2004) explores the learning of the metric in context of the nearest neighbor classification. They learn a generalized metric:

$$\begin{aligned}
d^2(x_1, x_2) &= (x_1 - x_2)^T Q(x_1 - x_2) \\
&= (x_1 - x_2)^T A^T A(x_1 - x_2) \\
&= (Ax_1 - Ax_2)^T (Ax_1 - Ax_2)
\end{aligned}$$

by directly learning its corresponding linear transformation A. They introduce a new optimization criterion (NCA), that is, as argued by the authors, more suitable for the nearest–neighbor classification purposes. The criterion is based on a new, probabilistic version of the cost function for the leave–one–out classification error in the k–NN framework. Each point i can now select any other point j with some probability p_{ij} defined as softmax function over distances in the transformed space:

$$p_{ij} = \frac{\exp(-\|Ax_i - Ax_j\|^2)}{\sum_{k \neq i} \exp((-\|Ax_k - Ax_j\|^2)}$$

A linear transformation *A* is then sought to maximize the expected number of correctly classified cases (with *k*–NN):

$$\arg \max_A g(A) = \arg \max_A \sum_i \sum_{j \in C_i} p_{ij}$$

where C_i is the set of cases that belong to the same class as *i*. Intuitively, the criterion aims to learn a generalized distance metric by shrinking the distance between similar points to zero, and expanding the distance between dissimilar points to infinity.

The algorithm and the metric it generates was shown to outperform other metrics for a number of learning problems. The method climbs the gradient of *g*(*A*), which is (x_{ij} being $x_i - x_j$):

$$\frac{\partial g}{\partial A} = 2A \sum_i \left(p_i \sum_k p_{ik} x_{ik} x_{ik}^T - \sum_{j \in C_i} p_{ij} x_{ij} x_{ij}^T \right)$$

(Bar-Hillel *et al.* 2005) and (Shental *et al.* 2002) define a different optimization criterion based on the mutual information. The advantage of their method (relevant component analysis – RCA) is the existence of the closed form (efficient) solution. Briefly, under the mutual information criterion, the class information is incorporated and optimized by computing the averages of class covariance matrices. The resulting matrix is obtained by

$$\sum_{\text{RCA}} = \sum_{i=1}^{k} \widehat{\sum}_i \quad A = \sum^{-\frac{1}{2}}$$

(2)

where $\hat{\Sigma}_i$ sample covariance matrix of class *i* and *A* is the resulting transformation for the data. The disadvantage of the method is that it assumes Gaussian distribution for the classes.

Experimental evaluation

We study our metric–learning methods and compare them to alternative methods on the problem of identification of anomalous patient–management decisions for patients with community acquired pneumonia. The data used in the experiment come from the Pneumonia PORT dataset (Kapoor 1996; Fine *et al.* 1997). The Pneumonia PORT dataset is based on the study conducted from October 1991 to March 1994 on 2287 patients with community–acquired pneumonia from three geographical locations at five medical institutions. The original PORT data were analyzed by (Fine *et al.* 1997), who derived a prediction rule with 30–day hospital mortality rate as the outcome. The authors developed a logistic regression model, which helped to identify 20 attributes that contribute the most to the mortality rate of pneumonia. To explore the anomaly detection methods, we have experimented with a simpler version of the PORT dataset that records, for every patient, only the attributes identified by Fine's study (Fine *et al.* 1997). The attributes are summarized in Figure 1. All attributes are binary with true/false (positive/negative) values.

Our objective was to detect unusual admission decisions (treat the patient at home versus in the hospital) which are captured by the variable 'Hospitalization'.

Study design

To study the performance of our anomaly detection methods, we used 100 patient cases (out of a total of 2287 of cases). The cases picked for the study consisted of 21 cases that were found anomalous according to a simple Naive Bayes detector (with detection threshold 0.05) that was trained on all cases in the database. The remaining 79 cases were selected randomly from the rest of the database. Each of the 100 cases was then evaluated independently by a panel of three physicians. The physicians were asked whether they agree with the hospitalization decision or not. Using panel's answers, the admission decision was labeled as anomalous when (1) at least two physicians disagreed with the actual admission decision that was taken for a given patient case or (2) all three indicated they were unsure (gray area) about the appropriateness of the management decision. Out of 100 cases, the panel judged 23 as anomalous hospitalization decisions; 77 patient cases were labeled as not being anomalous. The assessment of 100 cases by the panel represented the correct assessment of unusual hospitalization decisions.

Experiments

All the experiments followed the leave–one–out scheme. That is, for each example in the dataset of 100 patient cases evaluated by the panel, we first learn the metric. Next, we identified the cases in E most similar to it with respect to that metric. The cases chosen were either the closest 40 cases, or all the other cases (2286) in the dataset. We then learned the NB model and calculated the posterior probability of the decision. Alternatively, we calculated the probability of the decision using the softmax model and the learned metric.

The target example was declared anomalous if its posterior probability value fell below the detection threshold. The anomaly calls made by our algorithms were compared to the assessment of the panel and resulting statistics (sensitivity, specificity) were calculated. To gain insight on the overall performance of each method we varied its detection threshold and calculated corresponding receiver operating characteristic (ROC). For the hospital deployment no all thresholds are acceptable. Consequently, for the evaluation we selected only that part of the ROC curve, that corresponds to specificity equal or greater than 95% (see Figure 2). The 95% specificity limit means that at most 1 in 20 normal cases analyzed may yield a false alarm.

Results and Discussion

Table 1 shows the ROC statistics for the feasible detection range. For the softmax model, the NCA metric outperformed all other methods, whether it was using all cases (patients) or just the closest 40. We ascribe it to the fact, that NCA uses class information to weigh the features. The only other method that used class information was RCA. However, RCA uses class information only to consider (and average) covariance matrices for each class separately. Therefore, it still treats all features within the class the same way as the Mahalanobis metric, assuming the same relevance of all features. Comparing the global (all other patients) and local (closest 40 patients), local did always better: Close patients let us fit better the predictive model to the target patient, while taking all samples into the consideration biases the population. The local methods were also better for the Naive Bayes model. They were also more robust with respect to the metric. The intuition behind this result is that when using NB model, all cases are treated the same way, the metric was only used to select them. On the other hand, in softmax model, the distance from the case in hand does matter and the method treats closer patients with a higher weight. Accordingly, it is more sensitive to the metric changes.

Figure 2 shows the ROC curve for the best method in Table 1. The area of interest is bounded by the values [0, 0.13], [0.03, 0.30], and [0.05, 0.33]. The point [0.05 0.33] corresponds to the performance of 6.66 correct alarms in 10 alarms for 100 evaluated patients. However, we note that the prior for the evaluation dataset was biased towards anomalies. A rough correction using only anomalies that were randomly selected from the full database yields approximately 1 correct in 4 alarms, which is still very encouraging performance.

Conclusions

Summing up, our conditional anomaly detection is a very promising methodology for detecting unusual events such as network attacks or medical errors. We have demonstrated its potential by exploring and analyzing patient–management decisions for a dataset of patients suffering from pneumonia. The advantage of the anomaly detection approach over knowledge–based error detection approaches is that the method is evidence–based, and hence requires no or minimum input from the domain expert.

Despite initial encouraging results, our current approach can be further refined and extended. For example, instance–based (local) models tested in this paper always used a fixed number of 40 closest patients (or more, if the distances were the same). However, the patient's *neighborhood* and its size depend on the patient and data available in the database. We plan to address the problem by developing methods that are able to automatically identify and select only patients that are close enough for the case in hand.

Acknowledgments

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Target attributes

X_1 Hospitalization

Prediction attributes

Demographic factors

X_2 Age > 50

X_3 Gender (male = true, female = false)

Coexisting illnesses

X_4 Congestive heart failure

X_5 Cerebrovascular disease

X_6 Neoplastic disease

X_7 Renal disease

X_8 Liver disease

Physical-examination findings

X_9 Pulse ≥ 125 / min

X_{10} Respiratory rate ≥ 30 / min

X_{11} Systolic blood pressure < 90 mm Hg

X_{12} Temperature $< 35\,°C$ or $\geq 40\,°C$

Laboratory and radiographic findings

X_{13} Blood urea nitrogen ≥ 30 mg / dl

X_{14} Glucose ≥ 250 mg / dl

X_{15} Hematocrit $< 30\%$

X_{16} Sodium < 130 mmol / l

X_{17} Partial pressure of arterial oxygen < 60 mm Hg

X_{18} Arterial pH < 7.35

X_{19} Pleural effusion

Figure 1.
Attributes from the Pneumonia PORT dataset used in the anomaly detection study.
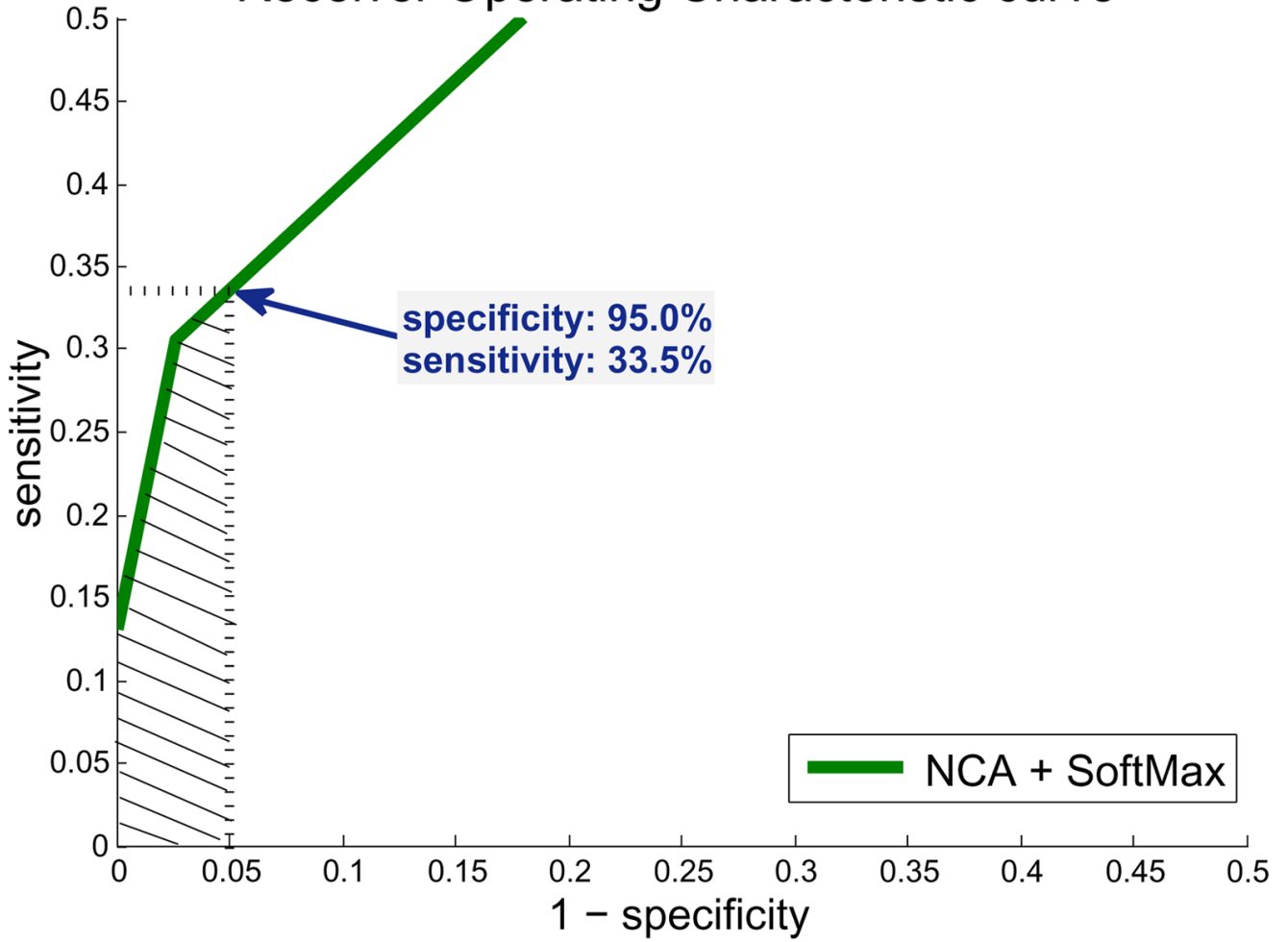
Figure 2.
An example of the ROC curve for the method that performed the best on the pneumonia dataset. The statistic of interest is the leftmost region of the ROC curve and its area.

Table 1

Area under the ROC curve in the feasible range of 95%–100% specificity. Please note that the baseline value for the random choice is 2.5%.

model	selection		
non–parametric	**global**	**#cases**	**area**
NCA	softmax	2286	18.0 %
Mahal	softmax	2286	12.2 %
RCA	softmax	2286	11.6 %
Euclidean	softmax	2286	8.0 %
non–parametric	**local**	**#cases**	**area**
NCA	softmax	40	20.2 %
Mahalanobis	softmax	40	15.0 %
RCA	softmax	40	12.8 %
Euclidean	softmax	40	8.0 %
parametric	**global**	**#cases**	**area**
any	NB	2286	11.6 %
parametric	**local**	**#cases**	**area**
NCA	NB	40	16.8 %
Mahalanobis	NB	40	17.6 %
RCA	NB	40	17.6 %
Euclidean	NB	40	16.4 %