KTH Computer Science
and Communication

A Framework for Anomaly Detection with Applications to Sequences

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Abstract

Anomaly detection is an important issue in data mining and analysis, with applications in almost every area of science, technology and business that involves data collection. The development of generally applicable anomaly detection methods can therefore have a large impact on data analysis across many domains. However, due to the highly subjective nature of anomaly detection, there are no generally applicable methods, and for each new application a large number of possible methods must be evaluated. In spite of this, little work has been done to automate the process of anomaly detection research for new applications.

In this report, a novel approach to anomaly detection research is presented, in which the task of finding appropriate anomaly detection methods for some specific application is formulated as an optimisation problem over a set of possible problem formulations. In order to facilitate the application of this optimisation problem to applications, a high-level framework for classifying and reasoning about anomaly detection problems is also introduced.

An application of this optimisation problem to anomaly detection in sequences is also presented; algorithms for solving general anomaly detection problems in sequences are given, along with tractable formulations of the optimisation problem for the main anomaly detection tasks in sequences.

Finally, a software implementation of the optimisation problem and framework is presented, along with a preliminary investigation into how it can be used to facilitate anomaly detection research.

Contents

Chapter 1

Introduction

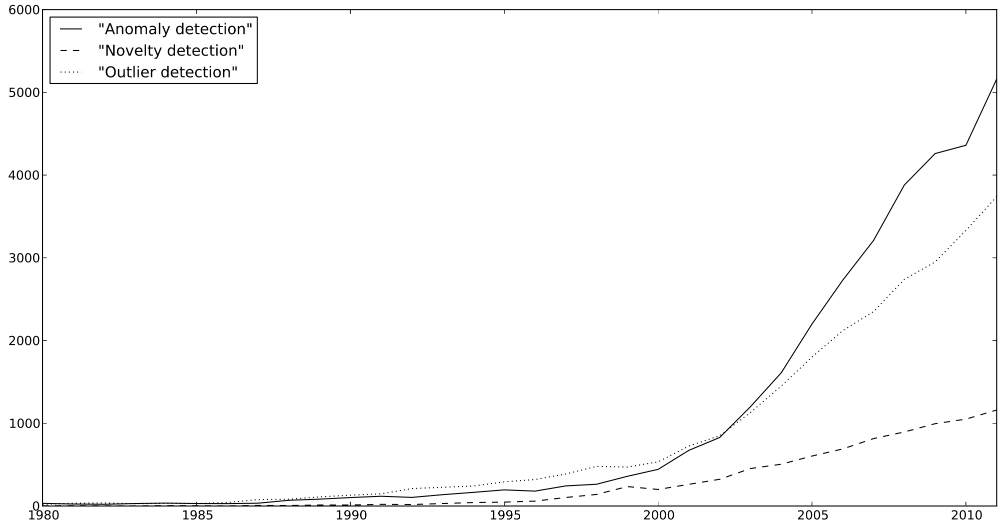


Figure 1.1. Approximate number of papers (by year) published between 1980 and 2011 containing the terms “anomaly detection”, “outlier detection” and “novelty detection”. All three terms exhibit strong upward trends in recent years. Source: Google Scholar.

This report is the result of a master’s thesis project at the KTH Royal Institute of Technology, performed partly in conjunction with an internship at Splunk Inc., based in San Francisco, California, USA.

Roughly defined as the automated detection within datasets of elements that are somehow abnormal, anomaly detection encompasses a broad set of techniques and problems. In recent years, anomaly detection has become increasingly important in a variety of domains in business, science and technology. In part due to the emergence of new application domains, and in part due to the evolving nature of many traditional domains, new applications of and approaches to anomaly detection and related subjects are being developed at an increasing rate, as indicated in

Figure 1.1.

Anomaly detection tasks are encountered in almost every domain of science, business and technology, and providing efficient methods for solving these tasks ahs potentially enormous benefits. Typically, however, finding appropriate anomaly detection methods for a given application is a laborious process, which requires expertise both both in the specific application and in anomaly detection methods. This affects the uptake of anomaly detection methods negatively. A key challenge in anomaly detection research is providing automated tools that can be used to streamline and simplify the research process.

With the above in mind, it was decided that the aim of this thesis project would be to investigate efficient automated methods for anomaly detection research. The main contributions of this thesis are:

1. A optimisation problem formulation of the task of finding appropriate anomaly detection methods.

2. A framework for reasoning about anomaly detection problems and guiding the optimisation.

3. A software implementation of the optimisation problem and framework.

In Chapter 2, some background information useful to the rest of the report is presented. Specifically, the subject of anomaly detection is discussed in more depth, along with a few basic concepts. Some of the major problems faced in anomaly detection research are also discussed. Finally, the optimisation problem approach is introduced.

As a means of overcoming these hurdles, in Chapter 3, a framework for reasoning about anomaly detection problems is introduced. As part of the framework, a few novel concepts and generalisations of existing concepts are introduced.

Next, in Chapter 4, an application of the framework to anomaly detection in sequences is presented. How existing methods fit in with the framework is also dicussed.

In Chapter 5 a software implementation, called ADRT of the optimisation problem and framework is presented.

Chapter 6 consists of a preliminary investigation into how ADRT can be used to perform the optimisation and gain insights into how well different types of problems perform for a given application.

The report is concluded in Chapter 7 with a summary of the project and a few possible directions for future work.

Chapter 2

Background

In this chapter the subject of anomaly detection is briefly introduced, along with a discussion of some of the major challenges in anomaly detection research. Finally, the task of finding appropriate anomaly detection methods for a given application is formulated as an optimisation problem.

2.1 Anomaly detection

In essence, anomaly detection is the task of automatically detecting items (*anomalies*) in datasets that in some sense do not fit in with the rest of those datasets (i.e. items that are *anomalous* with regard to the rest of the data). The nature of both the datasets and anomalies are dependent on the specific application in which anomaly detection is applied, and vary drastically between application domains. As an illustration of this, consider the two datasets shown in Figures 2.2 and 2.2. While these are similar in the sense that they both involve sequences, they differ in the type of data points (real-valued vs. categorical), the structure of the dataset (a long sequence vs. several sequences), as well as the nature of the anomalies (a subsequence vs. one sequence out of many).

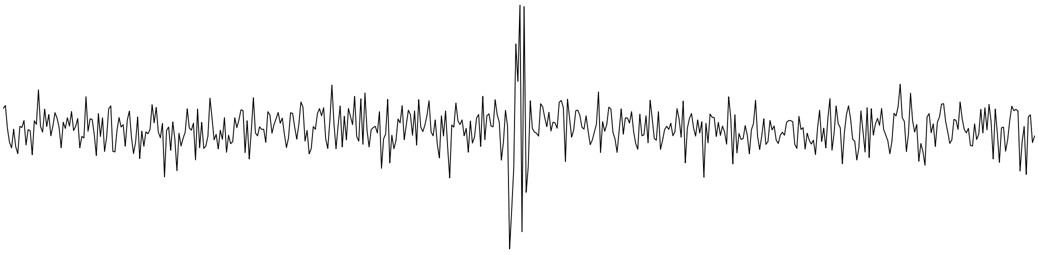


Figure 2.1. Real-valued sequence with an anomaly at the center.

Like many other concepts in machine learning and data science, the term 'anomaly detection' does not refer to any single well-defined problem. Rather, it is an umbrella term encompassing a collection of loosely related techniques and problems. Anomaly detection problems are encountered in nearly every domain in business and science in which data is collected for analysis. Naturally, this leads to a great diversity in the applications and implications of anomaly detection techniques. Due to this wide scope, anomaly detection is continuously being applied to new domains despite having been researched for decades.

$\mathbf{S_1}$	login	passwd	mail	ssh	...	mail	web	logout
$\mathbf{S_2}$	login	passwd	mail	web	...	web	web	logout
$\mathbf{S_3}$	login	passwd	mail	ssh	...	web	web	logout
$\mathbf{S_4}$	login	passwd	web	mail	...	web	mail	logout
$\mathbf{S_5}$	login	passwd	login	passwd	login	passwd	...	logout

Figure 2.2. Several sequences of user commands. The bottom sequence is anomalous compared to the others.

In other words, anomaly detection as a subject encompasses a diverse set of problems, methods, and applications. Different anomaly detection problems and methods often share few similarities, and no unifying theory exists. Indeed, the eventual discovery of such a theory seems highly unlikely, considering the subjectivity inherent to most anomaly detection problems. Even the term ‘anomaly detection’ itself has evaded any widely accepted definition [6] in spite of multiple attempts.

Despite this diversity, anomaly detection problems from different domains often share some structure, and studying anomaly detection as a subject can be useful as a means of understanding and exploiting such common structure. Anomaly detection methods are vital analysis tools in a wide variety of domains, and the set of scientific and commercial domains which could benefit from improved anomaly detection methods is huge. Indeed, due to increasing data volumes, exhaustive manual analysis is (or will soon be) prohibitively expensive in many domains, rendering effective automated anomaly detection critical to future development.

As a consequence of the diversity of the subject, a thorough survey of existing methods would not fit within the scope of this report. The interested reader is instead referred to any of several published surveys [6] [11] [3] [7] and books [8] [9] [10].

A few classifications, which are useful in reasoning about anomaly detection problems, are now presented.

2.1.1 Training data

As is customary in most areas of machine learning, anomaly detection problems are classified as either *supervised*, *semi-supervised* or *unsupervised* [1] based on the availability of training data.

[1] Note that we here adopt the convention used in [3], and take supervised learning to mean that both classes of training data are available, and semi-supervised to mean that only one class of training data is available. Conventionally, supervised learning is usually taken to mean any

In *supervised* anomaly detection, training data containing both normal and anomalous items is available. In essence, this constitutes a traditional supervised classification problem. As such, it can be handled by any two-class classifier, such as regular support vector machines. Unfortunately, supervised approaches are usually not suitable for anomaly detection, for a few reasons. First, anomalous training data is almost always relatively scarce, potentially leading to skewed classes (described in [12] and [13]). Second, supervised anomaly detection methods are by definition unable to detect types on anomalies that are not represented in the training data, and so can not be used to find *novel* anomalies. This is problematic as it is often not possible to obtain training data containing all possible anomalies.

Semi-supervised anomaly detection, on the other hand, assumes the availability of only one class of training data. While anomaly detection with only anomalous training data has been discussed (for instance in [14]), the vast majority of semi-supervised methods assume that normal training data is available. Considering the difficulties involved in obtaining anomalous training data mentioned above, this should not be surprising. Semi-supervised methods are used more frequently than supervised methods in part due to the relative ease of producing normal training data to anomalous training data.

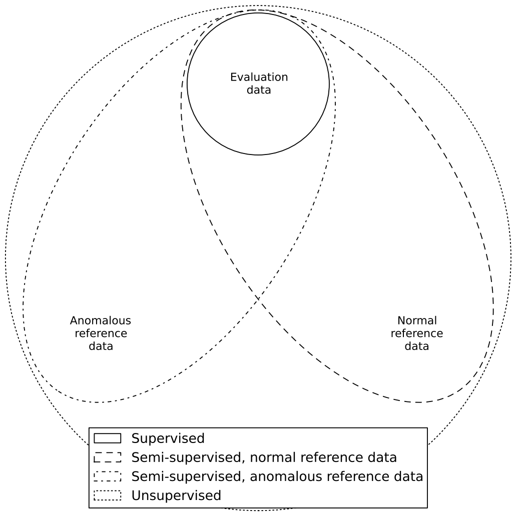


Figure 2.3. Euler diagram of the available training data for the four types of supervision.

Finally, *unsupervised* anomaly detection requires no training dataset. Since training data is not always available, unsupervised methods are typically considered to be of wider applicability than both supervised and semi-supervised methods [3]. However, unsupervised methods are unsuitable for certain tasks. Since training data can not be manually specified, it is more difficult to sift out uncommon but uninteresting items in unsupervised anomaly detection than in semi-supervised anomaly detection. Furthermore, unsupervised methods will not detect anomalies that are common but unexpected (although such items are arguably not anomalies by definition).

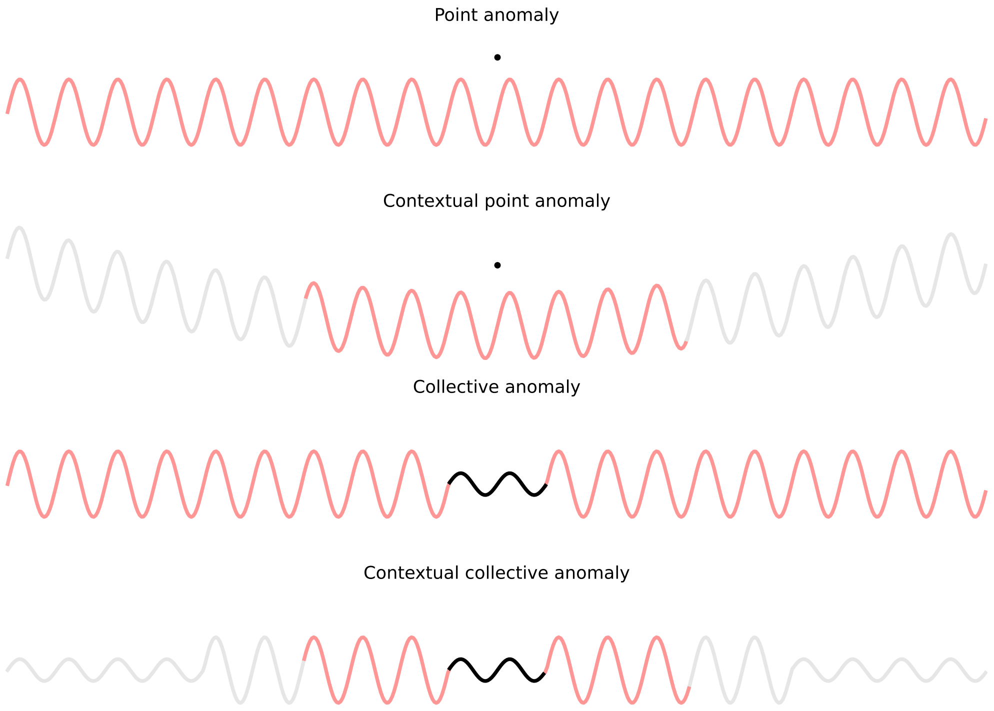


Figure 2.4. Different types of anomalies in a real-valued continuous sequence. In the middle of each series is an aberration—colored black—corresponding to a specific type of anomaly. Appropriate contexts for these anomalies are colored red, while items not part of the contexts are colored grey. The top panel contains a point anomaly—a point anomalous with regard to all other points in the series. The second panel contains a contextual anomaly—a point anomalous with regard to its context (in this case, the few points preceding and succeeding it), but not necessarily to the entire series. The third panel contains a collective anomaly—a subsequence anomalous with regard to the rest of the time series. The fourth contains a contextual collective anomaly—a subsequence anomalous with regard to its context.

2.1.2 Anomaly types

It is also useful to classify problems based on what types of anomalies they can be used to detect. To this end, we now describe four *anomaly types* [2], which can be used to classify the types of anomalies handled by problems. In order of increasing generality, these are *point anomalies*, *contextual point anomalies*, *collective anoma-*

learning from training data, while semi-supervised learning is taken to mean that both labeled and unlabeled data is available.

[2] While the concept of an anomaly type as defined here is novel, it is based on the concepts of contextual and collective anomalies discussed in [3].

lies, and *contextual collective anomalies.* An illustration of these anomaly types in the context of real-valued sequences is shown in Figure 2.4.

Point anomalies is the simplest of the anomaly types. These correspond to single points in the dataset that are considered anomalous with regard to the entire training set. Point anomalies are often referred to as *outliers* and arise in many domains [16]. Compared to the other anomaly types, detecting point anomalies is relatively straightforward. Statistical anomaly measures have been shown to be well suited for handling point anomalies, and are often used. Essentially, point anomalies are the only anomaly type it makes sense to look for when the individual elements of the input dataset are unrelated.

When the individual elements of the input dataset *are* related (for instance, through an ordering or a metric), however, not all interesting anomalies will be point anomalies. The concept of *contextual point anomalies* generalises point anomalies to take context into account, and is thus better suited for such cases. We here take the context to be the set of items with which an item is compared; when the input dataset admits a concept of proximity, the context of an item is usually those items which are closest to that item. Contextual anomalies are defined as individual items that are anomalous with regards to their context; i.e. while they might seem normal when compared with all elements in the training data, they are anomalous when compared to the other items in their context. Formally, contextual point anomalies can be defined as follows: Given a dataset D and a context function $C(d)$ which associates a context with each $d \in D$, a contextual point anomaly d is a point anomaly in $C(d)$. Thus, contextual point anomalies are a generalisation of point anomalies, in the sense that a point anomaly is a contextual point anomaly with regard to the trivial context $C(d) = D \setminus d$.

Of course, detecting individual anomalous points $d \in D$ might not always suffice, and the concept of *collective anomalies* might be required to capture relevant anomalies. Collective anomalies correspond to subsets of the input data that, when taken as a whole, are anomalous with regards to the entire training set. The task of detecting such anomalies can be formulated with the help of filter functions, which are map an input dataset D to a set of candidate anomalies $F(D)$ (where $\forall f_i \in F(D) : f_i \subset D$). Formally, given a set D and a filter F, the collective anomalies of D are the point anomalies of $F(D)$. Of course, point anomalies are a special case of collective anomalies, corresponding to the case where $F(D) = \{D\}$.

Finally, the concept of *contextual collective anomalies*, which generalises contextual point anomalies and collective anomalies, can be introduced. Contextual collective anomalies correspond to subsets of the input dataset that are anomalous with regard to their context. Formally, given a dataset D, a filter F, and a context function C, the contextual collective anomalies of D are the elements of $X \in F(D)$ that are point anomalies in $C(X)$. As expected, all of the three previous anomaly types can be considered special cases of contextual collective anomalies.

An illustration of the above concepts in real-valued sequences is shown in Figure 2.4. Assuming that unsupervised anomaly detection is used, Detecting point anomalies amounts to disregarding the information provided by the ordering and detecting only ‘rare’ items. While the task can capture the aberration in the first sequence in Figure 2.4, none of the aberrations in the other sequences would be considered point anomalies.

While the value at the anomalous point at the center of the second sequence occurs elsewhere in that sequence, it is anomalous with regards to its context, and as such, should be considered a contextual point anomaly and can be captured by problem formulations that use contextual point anomalies.

Since the third time series is continuous, the aberration present at its center can not be a (contextual) point anomaly. It is, however, a collective anomaly, and can be accurately captured by problem formulations that use collective anomalies.

Finally, neither of the first three types of anomalies can capture the aberration in the fourth sequence, as it is both continuous and occurs elsewhere in the sequence. However, with an appropriate choice of context, it can be deemed a contextual collective anomaly, and can be captured by problem formulations that use contextual collective anomalies.

It should be noted that while contextual point anomalies, collective anomalies, and contextual collective anomalies are all generalisations of point anomalies, it is sometimes possible to reduce each of these anomaly types to of point anomalies, as well. As outlined above, each of these anomaly types can be defined using point anomalies. Furthermore, data normalisation be utilized to solve some contextual anomaly detection problems using point anomaly detection (see [17], for instance).

2.2 On Anomaly Detection Research

Most anomaly detection research involves either applying existing methods to new applications (i.e. on new types of data) or investigating new methods in the context of previously studied applications. In order to handle the increasing need for effective anomaly detection in many areas of business and science it is vital that these activities can be performed in a highly automated manner. However, little work has been done on developing automated methods and tools for anomaly detection research.

There are a few difficulties which complicate research into anomaly detection for new applications. For one, comparing different anomaly detection methods found in the literature is difficult, since even though it might not appear so at first glance, papers on anomaly detection often target subtly different problems. This renders direct comparisons problematic and makes it hard to assess which methods might be appropriate to use in new applications. A systematic way of comparing anomaly detection methods would be helpful in mitigating this problem.

Furthermore, reproducing existing results as well as applying existing methods to new datasets is often difficult. Due in part to the subjective nature of the subject, and in part to a historical lack of freely available datasets, new methods are often not adequately compared to previous methods. Furthermore, the performance of many anomaly detection methods is often highly dependent on parameter choices, and only the results for the best parameter values (which might be difficult to find) are often presented [30]. Finally, there is often a lack of freely available software implementations of methods.

An important distinction to make is that between problems and methods. Informally, the process of finding an appropriate anomaly detection method for some application can be described as a two-step process. As a first step, an appropriate problem is formulated, which accurately captures intuitive notions of what constitutes an anomaly in the specific application. Once such a problem formulation has been found, an efficient method of solving or finding approximate solutions to the problem is constructed.

Due to the subjective nature of anomaly detection, radically different problem formulations might be appropriate for applications that are superficially very similar. Furthermore, there is often no obvious connection between the intuitive notion of what constitutes an anomaly in some application and the problem formulations which most accurately capture that notion, so prospective problem formulations must themselves be empirically evaluated.

This means that unless specific information is available on what problems are appropriate for a given application, finding the correct problem formulations should take priority over formulating methods. Finding efficient methods should be done only after it has been shown that the problem the methods are solving is relevant to the application. In the literature, methods, rather than problems, are often emphasised, and it can often be unclear exactly what problem a given method is meant to solve. In this report, the focus is instead placed almost entirely on problems.

This work attempts to simplify the research process by providing tools which help address the hurdles described above. As a means of mitigating the first problem, a general framework for systematically comparing anomaly detection problem formulations is presented, the purpose of which is to facilitate high-level reasoning about anomaly detection problems, and which thereby can help simplify the application of existing methods to new domains.

Furthermore, the process of finding appropriate anomaly detection methods for a given application is studied as an optimisation problem. A software implementation of this optimisation problem for anomaly detection in real-valued sequences is presented, which can help mitigate the reproducibility issues outlined above, as well as streamline the research process by enabling researchers to automatically evaluate a large amount of problem formulations.

2.3 Problem formulation

As a first step towards the goal of automated tools for anomaly detection research, the task we are trying to automate—-that of finding appropriate anomaly detection methods for some given application—must be formalised. In this section, the first step of the anomaly detection research process—finding an appropriate problem—is formulated as an optimization problem.

To motivate our optimisation problem formulation, one can consider a stylized variant of the typical anomaly detection research process, in which a researcher equipped with a working hypothesis (in the form of a problem formulation, which associates a set of anomaly scores with each possible input from the application) is given a dataset sampled from the target application, for which she constructs a set of anomaly scores in line with her hypothesis (i.e. a solution to her problem formulation). She then shows her results to a domain expert, who rates them based on how well aligned he deems them to be with his notion of what is anomalous and not in the specific application. This process is iterated, with the researcher successively improving her problem formulation until the domain expert tends to agree with sufficiently well with it.

A significant share of the work involved in finding appropriate methods could be avoided if this process could be automated, and one way to automate it is to formulate it as an optimisation problem that can be algorithmically solved. To do this, the concepts presented above must be formalised.

To begin with, the sets of valid problem inputs (datasets) and outputs (solutions) must be defined. Here, we simply assume that some set $\mathcal{D}$ has been defined containing all possible datasets for the application, along with some set $\mathcal{S}$ consisting of all valid corresponding solutions.

Next, a formal description of all allowed problem formulations must be constructed. Here, we simply assume that this description consists of a set of formulae in some logic sufficiently expressive to capture all relevant problem formulation. Let us call this set $\mathcal{P}$.

The role of the domain expert can be modeled by means of an error function $\epsilon(D, S) : \mathcal{D} \times \mathcal{S} \to \mathbb{R}^+$, which associates a score to any solution S based on how accurately it captures the anomalies in the data D.

The researcher, on the other hand, really has two roles; finding a new P based on the feedback from the domain expert, and computing a solution S given some dataset D and problem P. The former role corresponds to the heuristic driving the optimisation—searching the problem set $\mathcal{P}$ for an appropriate problem—and does not need be formalised yet. The latter role can be formalised as an oracle $O(P, D) : \mathcal{P} \times \mathcal{D} \to \mathcal{S}$, which takes a problem $P \in \mathcal{P}$ and an input dataset $D \in \mathcal{D}$, and computes the associated solution $S \in \mathcal{S}$.

The success of P in capturing the anomalies in D can then be stated as $\epsilon(D, O(P, D))$. Finally, since the goal is to minimise the *expected* error for datasets sampled from the given application, a random variable X over $\mathcal{D}$ ought to be introduced, modelling the probability of encountering any given $D \in \mathcal{D}$. A suitable objective function would then be $\mathbb{E}_X[\epsilon(D, O(P, D))]$.

The optimisation problem can then be stated as:

$$P_{opt} = \operatorname*{argmin}_{P \in \mathcal{P}} \mathbb{E}_X[\epsilon(D, O(P, D))].$$

Here, P_{opt} corresponds to the best possible problem formulation, and $O(P_{opt}, D)$

to the solution of this problem for D.

Of course, this optimisation problem (and specifically the oracle O) is not tractable unless heavy restrictions are placed on the problem set $\mathcal{P}$. A major challenge is thus to find a reduced problem set $\mathcal{P}^*$ which has a tractable oracle O^* and which contains a majority of interesting problem formulations.

Another problem is that it is generally not possible to compute either ϵ or X. Indeed, an algorithmic formulation of ϵ presupposes knowledge of the optimal problem formulation and would consequently render the optimisation process redundant. Likewise, the generation of a stream of data in accordance with X would require an exact model of the underlying process, which could just as well be used directly to detect anomalies. Even if an external stream of datasets would be available, an actual domain expert would be required to represent ϵ.

To get around these issues, the random vairable X can be replaced with a set of labeled training data, i.e. a set $\mathcal{T} \subset \mathcal{D}$ in which each $T_i \in \mathcal{T}$ has an associated $s(T_i) \in \mathcal{S}$. Correspondingly, $\epsilon(D, S)$ can then be replaced with some $\epsilon^*(T_i, S) = \delta(s(T_i), S)$, where $\delta : \mathcal{S} \times \mathcal{S} \to \mathbb{R}^+$ is some distance measure. This approach leads to the following estimate of P_{opt}:

$$P^*_{opt} = \operatorname*{argmin}_{P \in \mathcal{P}^*} \sum_{T_i \in \mathcal{T}} \delta(s(T_i), O^*(P, T_i)).$$

A major focus of this report is the construction of restricted problem sets P^* and corresponding tractable oracles O^*. In Chapter 3, a framework for reasoning about anomaly detection problems is outlined, which can be used to construct appropriate problem sets for specific applications. This framework is then applied to sequences in Chapter 4, in order to construct a problem sets that generalise a majority of previously studied problem formulations for sequences while admitting a simple oracle.

Chapter 3

A Framework for Anomaly Detection

In this chapter, a framework for reasoning about anomaly detection problem formulations is presented. This framework can be utilised in order to limit the scope of the optimisation problem outlined in the previous chapter by enabling the systematic construction of tractable problem sets.

The core idea of the framework is that anomaly detection problems can be almost exhaustively classified based on a few independent factors, and that by studying the factor choices handled in the anomaly detection literature, insights may be obtained into what problem formulations are appropriate for specific applications as well as how to formulate algorithms which solve these problem formulations.

As mentioned in Section 2.3, a problem formulation is a specification that associates with each element in the set $\mathcal{D}$ of possible datasets a unique element of the set $\mathcal{S}$ of possible solutions. In other words, problem formulations can be seen as functions $P : \mathcal{D} \to \mathcal{S}$, and the problem set $\mathcal{P}$ can be seen as the set of all such functions. Correspondingly, the task of selecting an appropriate restricted problem set $\mathcal{P}^*$ is equivalent to the task of finding an appropriate restricted subset of such functions.

One interesting aspect of anomaly detection is that almost all problem formulations found in the literature share common structure, in that they involve selecting a set of subsets of the input data, comparing each element of this set to some set of reference elements to produce a set of anomaly scores, and aggregating these anomaly scores into a result.

If this common structure could be captured by decomposing P into a collection of functions between sets, then the task of finding an appropriate $\mathcal{P}^*$ could be simplified to the task of placing appropriate restrictions on these individual functions. Correspondingly, formulating an oracle which can solve arbitrary $P \in \mathcal{P}^*$ could be simplified to the task of computing each individual function. If an efficient such oracle could be found, then software could be constructed which could, given a problem set in the form of a set of restrictions on the functions, automatically solve the optimisation problem for arbitrary applications.

3.1 The problem decomposition

We now present such a decomposition of P, which covers almost all previously studied problem formulations by capturing the common structure mentioned above. This decomposition is now presented in detail, assuming that $\mathcal{D}$ and $\mathcal{S}$ are fixed by the application. In parallel, illustrations are presented of a decomposition of an actual anomaly detection problem.

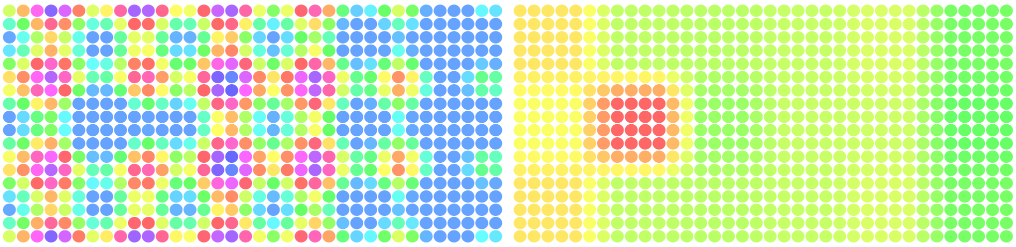


Figure 3.1. The example input data $D \in \mathcal{D}$ and the corresponding solution $P(D) = S \in \mathcal{S}$.

Roughly, our example problem associates an anomaly score with each element in a grid of colour values. These anomaly scores are also colours; red and green signify high and low anomaly scores, respectively. Specifically, the problem involves finding contextual collective anomalies—i.e. contiguous subsets of the data which are anomalous with regards to their surroundings—in such grids. To illustrate this problem, we will use the dataset shown in figure 3.1. This dataset contains an interesting anomaly to the left; a blue region that is larger than and has a different shape than nearby blue regions. The problem P we will decompose can be used to identify this anomaly, and the corresponding solution is shown to the right in the figure.

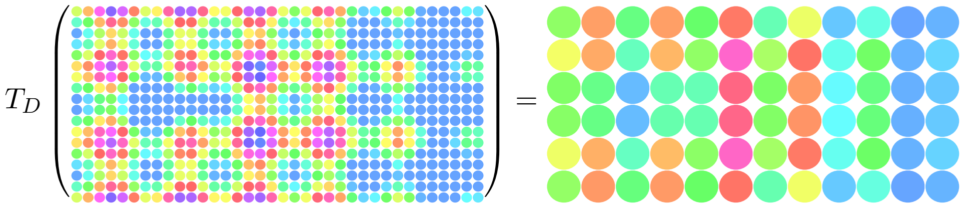
We make the assumption that the input data is an ordered set, i.e. a list [1], of homogeneous items, which we denote by $\mathcal{D} = [D]$ for some arbitrary set D. Likewise, we take the solution format to be a list anomaly scores: $\mathcal{S} = [\mathbb{R}^+]$. This means that we consider the set of problems to be equivalent to the set of all functions $P : [D] \to [\mathbb{R}^+]$.

The proposed decomposition splits each such P into a composition of the following functions:

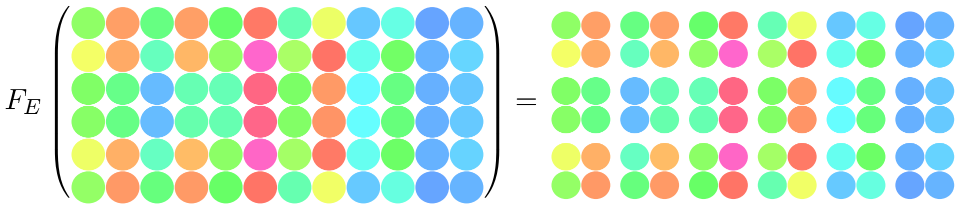
1. A transformation $T_D : [D] \to [D']$,which transforms a list of input data with elements in some set D to a list of elements in some other set D'. Typically,

[1] We will denote the ordered set consisting of a, followed by b and c by $[a, b, c]$, and we will denote the set of all ordered set with items in some set X by $[X]$. We will also assume that items in lists implicitly carry indices, and that any function $f : [X] \to [X]$ that maps a list to one of its sub-lists will preserve these indices, i.e. if $f([a, b, c]) = [b]$, then it is apparent that $f([a, b, c])$ is the second element of $[a, b, c]$, even if $b = a$ or $b = c$.

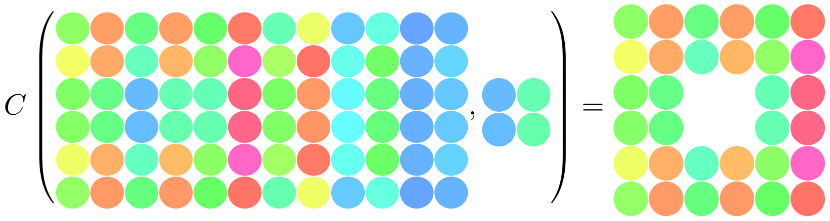
this is done in order to speed up or simplify the analysis. In our example [2], this transformation reduces the dimensionality of the dataset, by averaging the values of adjacent elements:



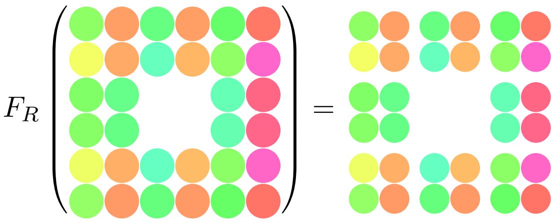
2. An evaluation filter $F_E : [D'] \to [[D']]$,which maps the transformed data to an *evaluation set*—a list of subsets of the transformed data, corresponding to potential anomalies. In our example, F_E simply partitions its input into collections of four elements:



3. A context function[3] $C : ([D'], [D']) \to [D']$,which takes a dataset and a corresponding candidate anomaly (i.e. a sublist of the dataset), and produces an associated *context*. In our example, the context function $C(X, Y)$ produces a set of elements in X adjacent to Y:



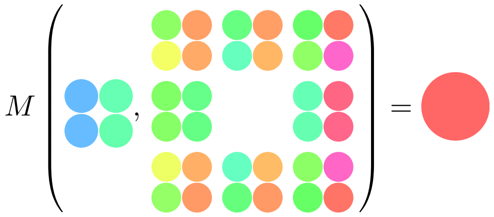
4. A reference filter $F_R : [D'] \mapsto [[D']]$,which works analogously to the evaluation filter, but operates on contexts instead of input data. In our case, F_R is identical to F_E; it partitions the context into subsets of four items:



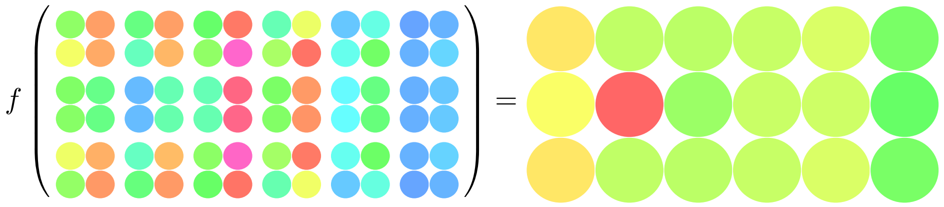
[2] Note that we here implicitly assume that a well-defined ordering of the elements in the example is provided, such that the data can be treated as a list.

[3] We will take (X, Y) to mean the set of tuples with the first element in X and the second element in Y. In other words, (X, Y) is just the Cartesian product $X \times Y$.

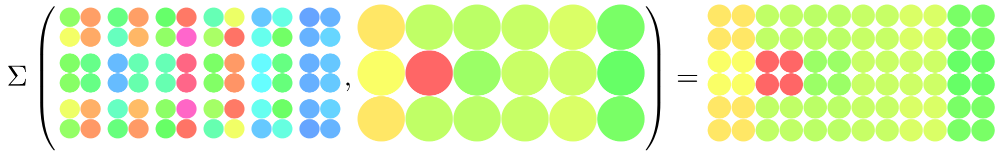
5. An anomaly measure $M : ([D'], [[D']]) \to \mathbb{R}^+$, which takes an item $x \in [D']$ and a list $[x_1, x_2, \ldots, x_n] \in [[D']]$ of reference items, and computes an anomaly score based on how anomalous x is with regards to $[x_1, x_2, \ldots, x_n]$. In our example, M works by computing an average distance between x and the x_i, which is here shown as a colour (red for high average distance, green for low agverage distance):



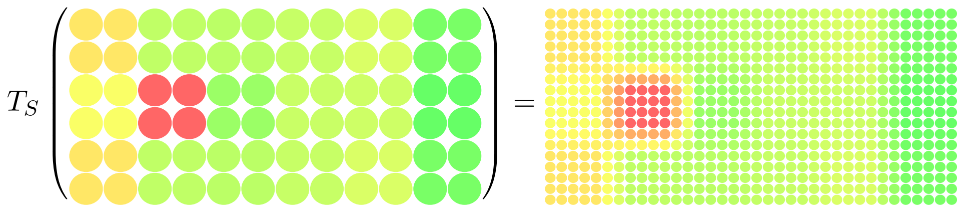
Computing $f(E) = [m(e_1), m(e_2), \ldots, m(e_n)]$, where $E = [e_1, e_2, \ldots, e_n]$ is the evaluation set, X is the input dataset and $m(e) = M(e, F_R(C(X, e)))$ gives:



6. An aggregation function $\Sigma : ([[D']], [\mathbb{R}^+]) \to [\mathbb{R}^+]$, which aggregates the anomaly scores for the elements of the evaluation set to form a 'preliminary' solution, i.e. a list of anomaly scores for the transformed data $[D']$. In our example, the aggregation function associates with each element the anomaly score of the candidate anomaly to which that element belongs:



7. A transformation $T_S : [\mathbb{R}^+] \to [\mathbb{R}^+]$, which transforms the preliminary solution (a list of anomaly scores for the transformed input data) into an actual solution (a list of anomaly scores for the input data). In our example, T_S uses bilinear interpolation to produce anomaly scores for all elements of the input data:



The process of computing a solution to a problem P with associated T_D, F_E, C, F_R, M, Σ, and T_S for an input dataset $d \in [D]$ can be seen as a series of transformations on d.

Now, the sets $\mathcal{D}$ and $\mathcal{S}$, as well as the functions T_D, F_E, C, F_R, M, Σ, and T_S are discussed in detail.

3.2 The input data format $\mathcal{D}$

As mentioned above, we represent the set of possible input datasets by means of a set $\mathcal{D} \subset [D]$, i.e. a set of lists over some application-specific set D. A problem formulation associates with each element of $\mathcal{D}$ a solution in the set of solutions $\mathcal{S}$.

Methods are commonly classified based on characteristics of D. For instance, a distinction is typically made between categorical, discrete, and real-valued data based on the cardinality of D. The input data is said to be *categorical* (or *symbolic*) if D is finite, *discrete* if D is countable and *real-valued* if $D \subseteq \mathbb{R}^n$ for some n (other uncountable sets are typically not encountered). It is also frequently the case that D consists of some combination of categorical, discrete and real-valued data, in which case the input data is referred to as *mixed*.

Another classification, also based on characteristics of D, is that between uni- and multivariate data. If $D = X^n$ for some set X, the input data is called *multivariate*; otherwise it is called *univariate*. An illustration of uni- and multivariate time series is shown in figure 3.2.

Characteristics such as the dimensionality of the data typically prove important in applications. For instance, categorical data is typically both computationally and conceptually easier to handle than either discrete or real-valued data. Likewise, univariate data is typically much easier to handle than multivariate data.

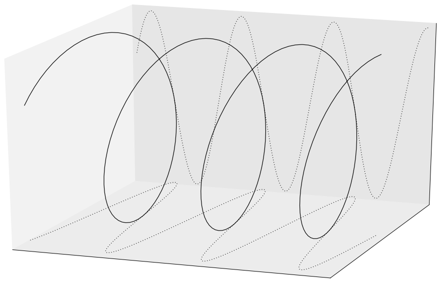


Figure 3.2. Two sine curves regarded as two separate univariate time series (dotted lines) and as one multivariate time series (solid lines).

3.3 The set of solutions $\mathcal{S}$

In this section, typical choices of collection of possible solutions $\mathcal{S}$ are discussed. To simplify the exposition, $\mathcal{S}$ is taken to be $[\mathbb{R}^+]$ in the framework. The discussion in this section assumes a list of input data $d = [d_1, d_2, \ldots, d_n]$.

Typically, the solution consists of a list $[s_1, s_2, \ldots, s_n]$ of *anomaly scores*, indicating how anomalous each element of d is. Another common approach is to let the solution consist of a sublist of d, containing those elements which are anomalous.

Two approaches can be distinguished here. Either, the solution has a fixed size (this is typically referred to as finding *discords* [26]), or the solution contain the indices of all elements which are considered sufficiently anomalous. In either case, the solution can be seen as a list $[s_1, s_2, \ldots, s_n]$ where s_i is 1 if d_i is considered anomalous, and 0 otherwise. With this in mind, it is easily seen that a list of anomalous items is really just a special case of anomaly scores.

Finally, it might be desirable to let the solution consist of a list of anomalous sublists of the input data. While potentially interesting, this seems to be uncommon, and for the sake of brevity is not incorporated into the framework. To accomodate for this, the solution format could be taken to be $\mathcal{S} = [\mathbb{R}^+]$ for either $S = \mathbb{R}^+$ or $S = [D]$.

3.4 The transformations T_D and T_S

It is common for the input data to be preprocessed to make it more amenable to analysis. To account for this, two transformations $T_D : [D] \to [D']$ and $T_S : [\mathbb{R}^+] \to [\mathbb{R}^+]$ are included in the framework. These transformations are complementary, in the sense that T_D maps the input data to some set $[D']$, while T_S takes a a list of anomaly scores for the transformed data and maps it to a list of anomaly scores for the data fed into T_D.

Typically, T_D involves either dimensionality or numerosity reduction. *Dimensionality reduction* involves reducing the dimensionality in the individual elements of the input dataset; i.e. a transformation $T_D : [D] \to [D']$ is a dimensionality reduction transformation if D' is of lower dimensionality than D.

Such transformations invariably involve some degree of information loss. Ideally, the information which they retain should be that which is most relevant to the analysis. Many methods have been designed with this goal in mind. A distinction is typically made between feature selection and feature extraction methods. *Feature selection* methods select a subset of the features present in the original data, while *feature extraction* methods create new features from the original data. An example of feature extraction is shown in figure 3.3.

Numerosity reduction, on the other hand, serves to reduce the cardinality of the data, either by converting real-valued data to discrete or categorical data, by converting discrete data to categorical data, or by compressing categorical data. An example of numerosity reduction in time series is shown in figure 4.1.

3.5 The evaluation filter F_E

An important aspect of any problem is which subsets of the transformed data are considered candidate anomalies; i.e. which sublists of the transformed data $[d'_1, d'_2, \ldots, d'_n] \in [D']$ constitute the *evaluation set* $E \in [[D']]$. Letting the evaluation set consist of all sublists is not computationally feasible, and considering only single element lists is likely to be overly limiting for many applications. To allow for

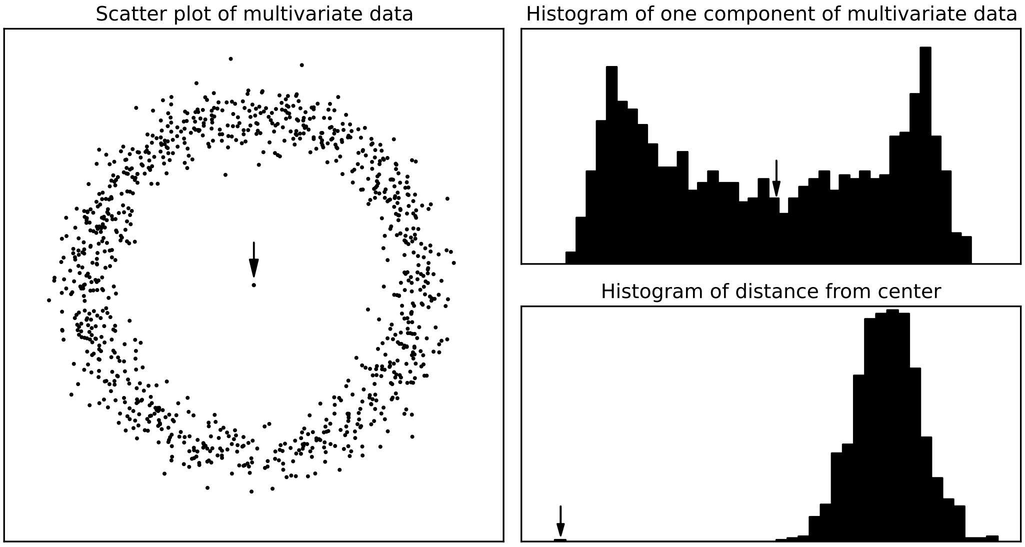


Figure 3.3. An example of dimensionality reduction in a point anomaly detection problem in $\mathbb{R}^2$. The left figure shows a set of 500 data points (x_i, y_i) containing one anomaly. The top right figure shows a histogram of the x_i, while the bottom right figure shows a histogram of the distance from the center point. In each figure, the location of the anomalous point is marked by an arrow. While the anomaly is easy to detect in the left and bottom right figures, it can not be seen in the top right figure. This is due to the linear inseparability of the data, and illustrates how dimensionality reduction can lead to information losses if not performed properly.

greater flexibility in the choice of evaluation set, the framework includes a function, the *evaluation filter* $F_E : [D'] \to [[D']]$, which includes the choice of evaluation set as part of the problem formulation.

What F_E is appropriate depends on whether or not there is any structure that relates the elements of the input data. If no such structure is present, allowing candidate anomalies with more than one element is not meaningful, and F_E should be given by $F_E([d'_1, d'_2, \ldots, d'_n]) = [[d'_1], [d'_2], \ldots, [d'_n]]$. On the other hand, if any such structure (such as an ordering of or distance between the elements) exists (and is pertinent to the analysis), then F_E ought to take that structure into account.

As an example, consider the case where the input elements $X = [d'_1, d'_2, \ldots, d'_k]$ constitute a sequence. Here, a concept of locality is naturally induced by the sequence ordering, and it is reasonable that $F_E(X)$ consist of contiguous sublists of X:

$$F_E(X) = [[d'_{a_1}, d'_{a_1+1}, \ldots, d'_{b_1}], [d'_{a_2}, d'_{a_2+1}, \ldots, d'_{b_2}], \ldots, [d'_{a_n}, d'_{a_n+1}, \ldots, d'_{b_n}]]$$

for some arbitrary n, $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$, where $\forall i : b_i > a_i$.

An evaluation filter which extracts contiguous sublists of a fixed length is illustrated in Figure 3.4.

3.6 The context function C

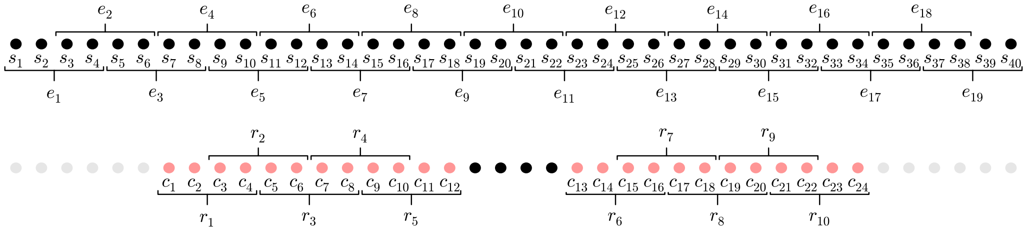

e_2 e_4 e_6 e_8 e_{10} e_{12} e_{14} e_{16} e_{18}
s_1 s_2 s_3 s_4 s_5 s_6 s_7 s_8 s_9 s_{10} s_{11} s_{12} s_{13} s_{14} s_{15} s_{16} s_{17} s_{18} s_{19} s_{20} s_{21} s_{22} s_{23} s_{24} s_{25} s_{26} s_{27} s_{28} s_{29} s_{30} s_{31} s_{32} s_{33} s_{34} s_{35} s_{36} s_{37} s_{38} s_{39} s_{40}
e_1 e_3 e_5 e_7 e_9 e_{11} e_{13} e_{15} e_{17} e_{19}
r_2 r_4 r_7 r_9
c_1 c_2 c_3 c_4 c_5 c_6 c_7 c_8 c_9 c_{10} c_{11} c_{12} c_{13} c_{14} c_{15} c_{16} c_{17} c_{18} c_{19} c_{20} c_{21} c_{22} c_{23} c_{24}
r_1 r_3 r_5 r_6 r_8 r_{10}

Figure 3.4. Schematic illustration of filters and contexts acting on a sequence $\mathbf{s} = [s_1, s_2, \ldots, s_{40}]$. The top panel shows the evaluation set $E = F_E(\mathbf{s}) = [e_1, e_2, \ldots, e_{19}]$ extracted by an evaluation filter which selects contiguous subsequences of fixed length. The bottom panel shows the context (in red) of e_{10} given by $C(\mathbf{s}, e_{10}) = [c_1, c_2, \ldots, c_{24}]$, as well as the corresponding reference set $F_R(e_{10}) = [t_1, t_2, \ldots, t_{10}]$ extracted by a reference filter identical to the evaluation filter.

Once the candidate anomalies have been identified, a *context* must be associated with each candidate anomaly. The context for a candidate anomaly represents the set of elements with which that candidate anomaly is to be compared. To this end, the decomposition associates with each problem a *context function* $C : ([D'], [D']) \to [D']$, which takes the transformed input data and a list of candidate anomalies, and associates with each candidate anomaly a context (in $[D']$).

As with the evaluation filter, what constitutes an appropriate context function is entirely dependent on what structure is present in the input data. If no such structure is present, the only reasonable choices of C are to let $C(X, Y)$ be those elements of X not in Y, or to let $C(X, Y) = T$ for some fixed dataset $T \in [D']$ (this corresponds to semi-supervised anomaly detection). If, on the other hand, there is such structure present, a context function which takes it into account might be preferable. As a concrete example of such an application with such structure, consider a long sequence: often how an item compares to those items ‘closest’ to it (in the ordering) is more relevant to the analysis than how it compares to the rest of the sequence.

Context functions generalise several of the concepts discussed in the previous chapter; semi-supervised anomaly detection with normal training data and unsupervised anomaly detection correspond to $C(X, Y) = T$ and $C(X, Y) \subset X$ respectively, while contextual and point anomalies are just special cases of $C(X, Y) \subset X$. Context functions also generalise anomaly detection problems to various tasks that have traditionally been considered separate from anomaly detection. For instance,

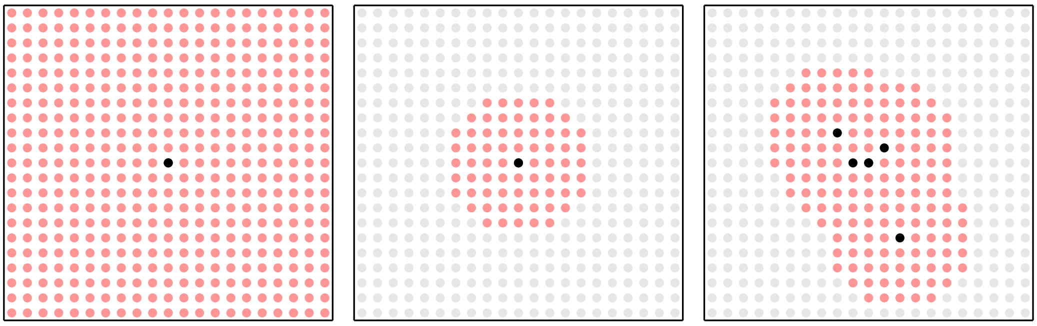


Figure 3.5. Schematic view of a dataset illustrating a few contexts. In each panel, the black dots represent selected items, the red dots represent items in the context of the selected items, and the grey dots indicate items not in the context of the selected items. The left panel shows the trivial context—all items are part of the context. The middle panel shows a local context of a single item. The right panel shows a local context of a subset of the dataset.

novelty detection [3], which refers to the detection of novel—or previously unseen—items or subsequences in a sequence [4], is really just the use of a one-sided context

$$C([s_1, s_2, \ldots, s_n], [s_i, s_{i+1}, \ldots s_j]) = [s_{i-w}, s_{i-w+1}, \ldots, s_{i-1}],$$

for some w, in an anomaly detection problem.

A few possible context functions are shown in Figures 3.4 and 3.5.

3.7 The reference filter F_R

Once a set of candidate anomalies has been produced and a context has been associated with each candidate anomaly, all that remains is to assign anomaly scores to each candidate anomaly (and then combine the results of this computation into a solution). However, a candidate anomaly and its context are likely to be of different sizes, which can be inconvenient, since most anomaly measures only work on elements of the same size. To get around this, the context can be split into chunks of the same size as the candidate anomaly.

To accommodate for this step, the framework includes a *reference filter* $F_R : [D'] \to [[D']]$, which (analogously to the evaluation filter) maps a context to a *reference set* of items with which the candidate anomaly can be effectively compared. A possible reference filter for sequences is illustrated in Figure 3.4. If the anomaly measure can operate on elements of different sizes, then $F_R(X) = [X]$ might be a good choice.

[4] It should be noted that the term 'novelty detection' is occasionally used in the literature to refer to what is referred to as semi-supervised anomaly detection in this report.

3.8 The anomaly measure M

The anomaly measure $M : ([D'], [[D']]) \rightarrow \mathbb{R}^+$ takes a candidate anomaly and a reference set and produces an anomaly score. The anomaly measure essentially defines (often in unpredictable ways) what types of features will be considered anomalous, so it is vital that it is chosen appropriately.

A large number of different anomaly measures are used in the literature, and listing them all is not possible within the scope of this report. Methods are often categorised based on what type of anomaly measure they employ; for instance, a method might be classified as statistical, classifier-based, distance-based, or information-theoretic based on the anomaly measure. A good presentation of these categories is given in [3].

3.9 The aggregration function Σ

The aggregation function $\Sigma : ([[D']], [\mathbb{R}^+]) \rightarrow [\mathbb{R}^+]$ takes a list of candidate anomalies and a list of corresponding anomaly scores, and produces a list of anomaly scores for the transformed data. If a problem does not involve any transformation, i.e. if $D' = D$ and T_D is the identity transformation, then T_S must also be the identity transformation, and Σ will produce the actual solution.

How this is done depends on which types of anomalies are sought. If only point anomalies are sought (i.e. if all candidate anomalies are single-element lists), then no aggregation needs to be performed and one can let[5] $\Sigma(X, Y) = Y$. The situation is similar when the evaluation set consists of non-overlapping multiple-element lists.

If on the other hand the evaluation set contains overlapping elements, then the anomaly scores must somehow be weighted together for all overlapping elements. Reasonably, such an aggregation function ought to be on the form (for $e = [e_1, e_2, \ldots, e_n]$ and $a = [a_1, a_2, \ldots, a_n]$):

$$\Sigma(e, a) = [\sigma(\{a_i : d'_1 \in e_i\}), \sigma(\{a_i : d'_2 \in e_i\}), \ldots, \sigma(\{a_i : d'_n \in e_i\})],$$

where $\sigma : [\mathbb{R}^+] \rightarrow \mathbb{R}^+$.

3.10 Constructing an oracle

Assuming that each of the functions in some problem formulation $P = (T_D, F_E, C, F_R, M, \Sigma, T_S)$ can be computed, the construction of an oracle O that computes the solution to P is an easy task. Specifically, the following algorithm solves P:

```
Require: Some $X \in [D]$.
  $X' \leftarrow T_D(X)$
  $A \leftarrow []$                          ▷ initialize anomaly scores to empty list
  for $E \in F_E(X')$ do                     ▷ iterate over the evaluation set
```

[5] Assuming that the inputs have the same order as the expected anomaly score order.

```
        $R_E \leftarrow F_R(C(X', E))$                ▷ compute a reference set
        $append(A, M(E, R_E))$                ▷ compute and store anomaly scores
    end for
    return $F_S(\Sigma(F_E(X'), A))$                ▷ aggregate scores to form anomaly vector
```

The filters F_E and F_R, the context function C and the aggregation function Σ can all be expected to be simple to compute, since they really just involve selecting subsets of or aggregating their input data; given a description of any of these functions, producing an algorithm that computes it is trivial.

On the other hand, the transformations T_D and T_S, as well as the anomaly measure M can in principle be arbitrarily difficult to compute. Consequently, special attention must be paid to ensure that these functions are dealt with properly.

3.11 Constructing a problem set

Using the framework presented in this chapter, the construction of an appropriate problem set for some specific application can be approached in a systematic manner.

First, the format of the input and solution elements D and S must be formally defined. The set of all possible problems then corresponds to the set of functions $P : [D] \to [\mathbb{R}^+]$. Assuming that all interesting problems can be decomposed as a combination of the components T_D, F_E, C, F_R, M, Σ, and T_S, an appropriate restricted problem set can be constructed by individually restricting the components.

As has been previously pointed out, what restrictions should reasonably be placed on the filters and context function F_E, F_R and C depends entirely on the presence of structure in the input data $D \in \mathcal{D}$ which relates the $d_i \in D$. If the d_i are completely unrelated, then it is reasonable to bypass these components by restricting them to only consider point anomalies. If, on the other hand, there is a relation between the $d_i \in D$, then it is reasonable to restrict these components to take this structure into account.

The aggregation function Σ is similarly limited. When candidate anomalies do not overlap, Σ is naturally constrained to a single value. Otherwise, Σ is uniquely determined by the weighting function σ described in Section 3.9. Typically, constraining the allowed σ to a few different values should suffice.

Restricting T_D and T_S is more difficult, since it is typically not known what types of transformations are appropriate for a given application. With this in mind, it might be appropriate to simply restrict T_D and T_S to some set of transformations which have been used in the specific application or similar applications. That way, the problem set can be said to generalise previously studied methods while remaining tractable.

Finally, the anomaly measure M must be appropriately restricted. Since M can not be appropriately restricted based on information about the application, it is reasonably to take a similar approach as with the transformations and restrict M to some set of anomaly measures which have been previously studied in conjunction with the specific application.

While restricting the components individually simplifies problem set construction, it might lead to a problem set that is overly permissive, in the sense that some combinations of components might not be useful. In this case, it is reasonable to place additional restrictions on the problem set based on combinations of components.

3.12 Error measures

Before the optimisation problem

$$P^*_{opt} = \operatorname*{argmin}_{P \in \mathcal{P}^*} \sum_{T_i \in \mathcal{T}} \delta(s(T_i), O^*(P, T_i)).$$

can be solved, the training set $\mathcal{T}$ and the error function δ must be defined. As was mentioned in the previous chapter, we assume that the set $\mathcal{T}$ of training data consists of a finite set of pairs $T_i = (D_i, S_i)$ in $([D], [\mathbb{R}^+])$. This means that the training set is entirely application-specific, and discussing it in a general context is not likely to be useful.

The choice of error measure, which is formally a distance function for $\mathcal{S} = [\mathbb{R}^+]$, i.e. $\delta : ([\mathbb{R}^+], [\mathbb{R}^+]) \to \mathbb{R}^+$, however, has more to do with the solution format than with the application itself. A few simple error measures which are likely to work well across most applications are now discussed.

If the solution format is a list of anomalous items, then S can be seen as the binary set $\{0, 1\}$ and the solution $[s_1, s_2, \ldots, s_n]$ as a binary list, where s_i indicates whether or not the corresponding input element d_i is considered anomalous. Reasonably the Hamming distance, corresponding to

$$\delta([a_1, a_2, \ldots, a_n], [b_1, b_2, \ldots, b_n]) = \sum_i \delta'(a, b),$$

where $\delta'(a, b) = 1$ if $a \neq b$ and 0 otherwise, ought to be used for such cases.

If the solution format is a list of anomaly scores the situation becomes more complex. Assuming that $S = \mathbb{R}$, one might imagine that any ordinary real-valued distance measure, such as the Euclidean distance could be used. However, an error measure must be invariant under scalings and transformations of its input data in order to be useful, and this is not the case for the Euclidean distance. To get around this, the input data can be normalised to some interval (i.e. $[a_1, a_2, \ldots, a_n] \mapsto [\frac{a_1 - a_{min}}{a_{max} - a_{min}}, \frac{a_2 - a_{min}}{a_{max} - a_{min}}, \ldots, \frac{a_n - a_{min}}{a_{max} - a_{min}}]$, where a_{min} and a_{max} are the minimum and maximum elements of a, respectively) before the error measure is applied. We will denote this normalised Euclidean error measure by ϵ_N

However, since providing meaningful real-valued training data can be difficult, it might be more reasonable to restrict the training data to be a set of anomalous items, and convert the solution to a binary list before applying the error measure. Reasonably, this conversion ought to be done by mapping all values above some threshold τ to 1, and the rest of the values to 0.

This approach gives gives rise to a number of possible error measures, corresponding to different methods of selecting τ. The following measures are used later in this report:

ϵ_E, which corresponds to setting τ such that the number of non-zero elements in both lists are equal.

ϵ_F, which corresponds to using the largest τ for which all non-zero elements of the training data vector are non-zero in the solution vector.

ϵ_B, which corresponds to using the τ that gives the smallest error value.

3.13 Optimisation

Once the sets D and S of input and solution items, the training data $\mathcal{T}$, and the error measure δ have been defined, and appropriate restrictions have been placed on T_D, F_E, C, F_R, M, Σ, and T_S, all that remains is to perform the actual optimisation.

Of course, effectively performing the optimisation is a difficult task, and evaluating the entire problem set is not feasible. Thus, efficient heuristics for searching the problem set are required. To help develop such heuristics, it can be useful to consider each of the components T_D, F_E, C, F_R, M, Σ, and T_S separately, and to divide the set of allowed component choices into a set of parametrised functions. Let us denote the set of such functions for component X by $\{X^i\}_i$ and the corresponding sets of parameters by $\{\theta_{X^i}\}$. A hierarchal view of the problem set $\mathcal{P}$ can then be taken, in which it consists of a set of tuples $(T_D^a, F_E^b, C^c, F_R^d, M^e, \Sigma^f, T_S^g)$ indexed by (a, b, c, d, e, f, g), in which each element has a corresponding parameter space $(\theta T_D^a, \theta F_E^b, \theta C^c, \theta F_R^d, \theta M^e, \theta \Sigma^f, \theta T_S^g)$. A hierarchal optimisation can then be performed, in which a preliminary search identifies appropriate (a, b, c, d, e, f, g), the parameter spaces of which are then more thoroughly searched.

Essentially, each choice of (a, b, c, d, e, f, g) corresponds to a traditional machine learning problem, and can be optimised using traditional techniques. The meta-problem of finding suitable (a, b, c, d, e, f, g) must be equipped with some method of assessing the potential of candidate problems. Reasonably, such a method ought to employ some method of probabilistically sampling the parameter spaces of candidate problems. The meta-problem can then be regarded as an optimisation problem with uncertainty.

It further seems likely that the optimisation could itself be learnt, so that a preliminary analysis of the data could be used to guide the process.

Chapter 4

An application to sequences

Recall that the optimisation problem is stated as

$$P^*_{opt} = \operatorname*{argmin}_{P \in \mathcal{P}^*} \sum_{T_i \in \mathcal{T}} \epsilon^*(s(T_i), O^*(P, T_i)),$$

where the objects that need to defined are the input and solution formats $[D]$ and $[S]$, the problem set $\mathcal{P}^*$, the test data $\mathcal{T}$, the error function ϵ^*, and the oracle O. The framework presented in the previous chapter makes the assumption that all relevant problems P can be decomposed into a set of functions $P = (T_D, F_E, C, F_R, M, \Sigma, T_S)$.

In this chapter, the objects mentioned above are defined for the two most common tasks in anomaly detection in sequences. Furthermore, suitable choices of and restrictions on T_D, F_E, C, F_R, M, Σ and T_S for anomaly detection are discussed in depth.

From here on, a *sequence* will be taken to mean any list ($[X]$ for some set X) for which the list order reflects the natural ordering of the elements. A *time series* is defined to be any sequence in $[(\mathbb{R}^+, X)]$, where the elements are ordered such that their first component (the timestamp) is increasing.

In Section 4.1, the two anomaly detection tasks we will study are presented. Corresponding oracles are presented.

The remaining sections consist of a discussion of how the components T_D, F_E, C, F_R, M, Σ, and T_S relate to anomaly detection in sequences, and which component choices are appropriate.

4.1 Tasks

Two main tasks can be distinguished in anomaly detection in sequences: *finding anomalous sequences in a set of sequences*, and *finding anomalous subsequences in a long sequence* [3]. The former task can be seen as the detection of point anomalies in an unstructured set of sequences, while the latter corresponds to finding contextual anomalies in a totally ordered set.

4.1.1 Finding anomalous sequences

The task of finding anomalous sequences in a set of sequences involves taking a list of similar sequences and producing a list of corresponding anomaly scores. The input elements are not related, i.e. the input data is unstructured. Thus, the task can be seen as one of detection of point anomalies in a collection of sequences. This task has been the subject of intense research. Thorough reviews are found in [4] and [5].

For an example of this task, see figure 2.2. Here, dataset consists of a set of sequences of user commands extracted from a system log, and task corresponds to detecting individual anomalous sequences in this dataset. While sequences $\mathbf{S_1}$ through $\mathbf{S_4}$ are originate from ordinary user sessions, sequence $\mathbf{S_5}$ could indicate an attack. Accurately detecting such anomalous sequences is an important problem in computer security.

The input data has the format $[D]$, where D is itself a set of sequences, i.e. $D = [X]$ for some set X. In the example above X is a set of commands, but it could just as well be $\mathbb{R}$ or any other set. The solution format is $[S]$, where either $S = \mathbb{R}^+$ or $S = \{0, 1\}$ depending on the application requirements.

Since the input data is unstructured, any transformation T_D must produce lists with the same length as it is given. Correspondingly, we can let $S' = S$. This renders T_S redundant, so it can be ignored.

Since the task deals with unstructured data, the components F_E, F_R, and Σ can be ignored. An oracle can then be formulated as:

```
Require: Some $X \in [D]$.
  $X' \leftarrow T_D(X)$
  $A \leftarrow []$                          ▷ initialize anomaly scores to empty list
  for $E \in X'$ do                          ▷ iterate over elements
      $append(A, M(E, C(X', E)))$            ▷ compute and store anomaly scores
  end for
  return $A$                                 ▷ aggregate scores to form anomaly vector
```

As per the discussion in the previous chapter, C can only be one of two functions, corresponding to unsupervised and semi-supervised anomaly detection, respectively.

4.1.2 Finding anomalous subsequences

The task of finding anomalous subsequences of long sequences corresponds to finding anomalous contiguous sublists of the input data $[D]$. In contrast to the task of finding anomalous sequences, the input data is structured, and the sequence ordering naturally gives rise to concepts of proximity and context. This task is relatively poorly understood, but is highly relevant in many application domains. As a consequence, automated methods can be expected to be very useful for this task. Essentially any monitoring or diagnosis application could benefit from a better understanding of the task.

For examples of sequences to which this task might be applied, see Figures 2.1

and 2.4. These are all real-valued sequences which contain anomalous items or subsequences.

As with the previous task, either $S = \mathbb{R}^+$ or $S = \{0, 1\}$ depending on the application. However, it here makes sense to allow T_D to compress the data (i.e. return a shorter list than it is given). Correspondingly, a corresponding T_S is required in order to transform the preliminary solution (in $[S']$) to a list of anomaly scores with the same length as the input data.

Since all components must be used for this task, the oracle is identical to the one presented in Section 3.10.

4.2 The input data format $\mathcal{D}$

Categorical, discrete, and real-valued sequences have all been extensively studied. Categorical sequences arise naturally in applications such as bioinfomatics and intrusion detection. Discrete sequences are typically encountered when monitoring the frequency of events over time. Finally, real-valued sequences are encountered in any application that involves measuring physical phenomena (such as audio, video and other sensor-based applications).

Which the origins and nature of the data obviously differs heavily between these different categories of sequences, the choice of components (with the exception of the transformations and anomaly measures) can be made independently of the type of data. For this reason, we can disregard the data format in most of the following discussion.

4.3 The transformations T_D and T_S

Transformations are commonly used to facilitate the analysis of sequences, and a large number of different such transformations are found in the literature.

Feature extraction is commonly performed to reduce the dimensionality of sequences, and especially of real-valued ones. Essentially, the task of feature extraction in real-valued sequences corresponds to, given a sequence $s = [s_1, s_2, \ldots, s_n]$, finding a collection of basis functions $[\phi_1, \phi_2, \ldots, \phi_m]$ where $m < n$ that s can be projected onto, such that s can be recovered with little error. Many different methods for obtaining such bases have been proposed, including the discrete Fourier transform [19], discrete wavelet transforms [21] [32], various piecewise linear and piecewise constant functions [28] [31], and singular value decomposition [28]. An overview of different representations is provided in [40].

Arguably the simplest of these bases are piecewise constant functions $[\phi_1, \phi_2, \ldots, \phi_n]$:

$$\phi_i(t) = \begin{cases} 1 & \text{if } \tau_i < t < \tau_{i+1} \\ 0 & \text{otherwise.} \end{cases}$$

where $(\tau_1, \tau_2, \ldots \tau_n)$ is a partition of $[t_1, t_n]$.

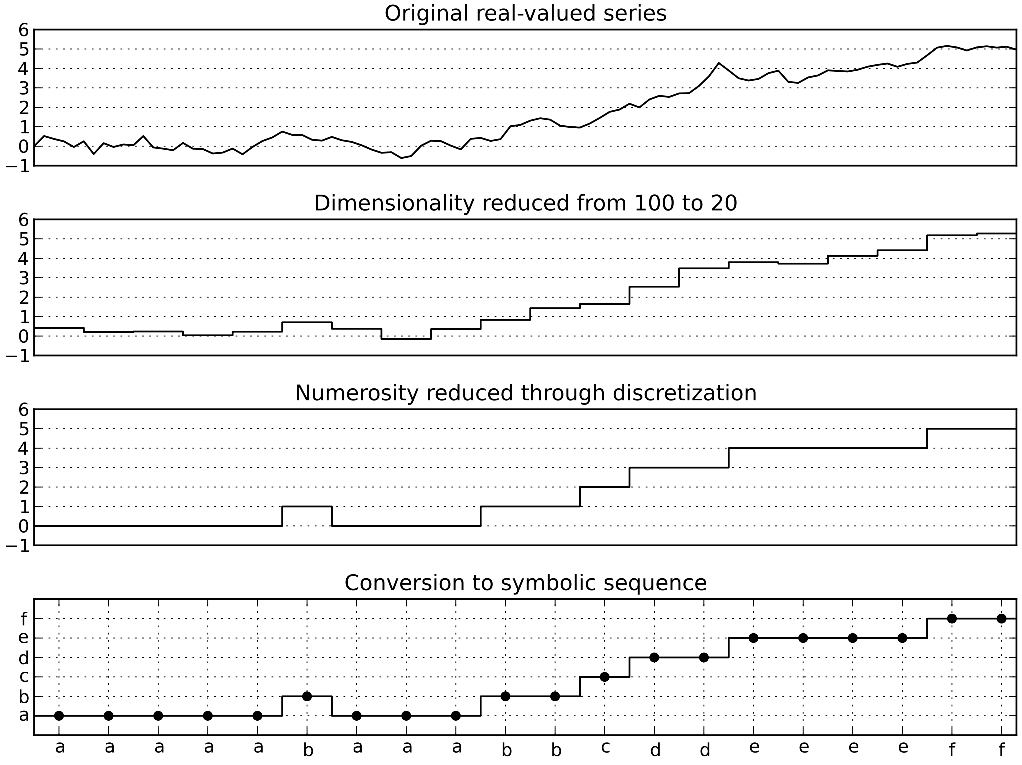


Figure 4.1. Illustration of numerosity and dimensionality reduction in a conversion of a real-valued sequence to a symbolic sequence. The top frame shows a real-valued sequence sampled from a random walk. The second frame shows the resulting series after a (piecewise constant) dimensionality reduction has been performed. In the third frame, the series from the second frame has been numerosity-reduced through rounding. The bottom frame shows how a conversion to a symbolic sequence might work; the elements from the third series is mapped to the set $\{a, b, c, d, e, f\}$.

Different piecewise constant representations have been proposed, corresponding to different partitions. The simplest of these, corresponding to a partition with constant $\tau_{i+1} - \tau_i$ is proposed in [29] and [20] and is usually referred to as *piecewise aggregate approximation (PAA)*. As shown in [30], [28] and [20], PAA rivals the more sophisticated representations listed above.

Numerosity reduction is also commonly utilised in analysis of real-valued sequences. One scheme that combines numerosity and dimensionality reduction in order to give real-valued sequences into a categorical representation is *symbolic aggregate approximation* (SAX) [39]. This representation has been used to apply categorical anomaly measures to real-valued data with good results. A simplified variant of SAX is demonstraded in figure 4.1.

In general, real-valued sequences are much easier to deal with than time series. For this reason, irregular time series are commonly transformed to form regular time series, which can be treated as sequences. Formally, such transformations map a sequence in $[(\mathbb{R}^+, X)]$ to a sequence in $[X]$.

The simplest such transformation involves simply dropping the timestamp component of each item. This is useful when the order of items is important, but how far apart they are in time is not. This is often the case when dealing with categorical sequences. An example of such an application is shown in figure 2.2.

Another common class of transformations involves estimating the (weighted) frequency of events. This is useful in many scenarios, especially in applications involving machine-generated data. Several methods can be used to generate sequences appropriate for this task from time series, such as histograms, sliding averages, etc.

Transformations that transform the data into some alternative domain can also be useful. For example, transformations based on the *discrete Fourier transform* (DFT) and *discrete wavelet transform* (DWT) [32] have shown promise. The DFT is parameter-free, while the DWT can be said to be parametrised due to the variety of possible wavelet transforms.

4.4 The filters F_E and F_R

As was previously mentioned, filters are really only interesting for the task of finding anomalous subsequences. Here, the role of the filter is to map a sequence in $[D']$ to a list candidate anomalies (subsequences of the input sequence).

By far the most frequently used filters are *sliding window* filters. These map a sequence $X = [x_1, x_2, \ldots, x_n]$ to

$$F_E(X) = [[x_1, x_2, \ldots, x_w], [x_{s+1}, x_{s+2}, \ldots, x_{s+w}], \ldots, [x_{n-w}, x_{n-w+1}, \ldots, x_n]],$$

where w and s are arbitrary integers (typically $s \leq w$)[1].

4.5 The context function C

The ordering present in sequences naturally give rise to a few interesting contexts, which are now demonstrated for a sequence $s = [s_1, s_2, \ldots, s_n]$ and a candidate anomaly $s'[s_i, s_{i+1}, \ldots, s_j]$, where $1 \leq i \leq j \leq n$. It is here assumed that all candidate anomalies are contiguous. As mentioned in the previous chapter, contexts can be used to generalise the concept of training data. Semi-supervised anomaly detection corresponds to the *semi-supervised context* $C(s, s') = T$, where T is some fixed set of training data.

Likewise, traditional unsupervised anomaly detection for subsequences can be formulated using the *trivial context* $C(s, s') = [[s_1, s_2, \ldots, s_{i-1}], [s_{j+1}, s_{j+2}, \ldots, s_n]]$.

[1] We here assume that $s|n - w$. Otherwise, the last element above might look a bit different.

This corresponds to finding either point anomalies or collective anomalies in a sequence.

Another interesting context is the *novelty context* $C(s, s') = [[s_1, s_2, \ldots, s_{i-1}]]$. This context captures the task of novelty detection in sequences, which is especially interesting in monitoring applications.

Finally, a family of *local contexts*

$$C(s, s') = [[s_{\max(1,i-a)}, s_{\max(2,i-a+1)}, \ldots, s_{i-1}], [s_{j+1}, s_{j+2}, \ldots s_{min(n,j+b)}]]$$

may be defined for $a, b \in \mathbb{N}$, in order to handle anomalies such as the one in the last sequence of figure 2.4.

4.6 The anomaly measure M

As was mentioned previously, an anomaly measure is a function $M : ([D'], [[D']]) \to \mathbb{R}^+$ that takes a candidate anomaly $c \in [D']$ and a reference set $R \in [[D']]$, and produces an anomaly score based on how anomalous C is with regards to R. A large number of such measures have been used in the literature, and a thorough discussion of these is not possible within the scope of this report. Instead, we will limit our consideration to distance-based anomaly measures, since these are flexible and have been shown to perform well in general for sequences [5].

Distance-based anomaly measures operate by, given some distance measure $\delta : [D'] \times [D'] \to \mathbb{R}^+$, somehow aggregating the set $\{\delta(c, r) | r \in R\}$ into an anomaly score in $\mathbb{R}^+$. A class of especially interesting distance-based anomaly measure is k-nearest-neighbour-based anomaly measures. These assign as anomaly score the mean of the k largest values of $\{\delta(c, r) | r \in R\}$.

Possible interesting choices of δ for real-valued data include the *Euclidean distance* or the more general *Minkowski distance*; measures focused on time series, such as *dynamic time warping* [50], *autocorrelation measures* [49], or the *Linear Predictive Coding cepstrum* [47].

There are also several or measures developed for series of categorical data, such as the *compression-based dissimilarity measure* [27]. Often, coupling a distance measure with a data transformation step (in order to, for instance, to apply a distance measure defined on categorial data to a real-valued seqeuence) can yield good results.

4.7 The aggregation function Σ

Examples of anomaly detection problems which involve aggregation are hard to find in the literature. For this reason, suggesting appropriate choices of Σ is difficult. A few choices which are likely to produce good results are Σ on the form suggested in Section 3.9, with σ that produce either the *maximum*, *minimum*, *median*, or *mean* of its input values. The resulting Σ will henceforth be referred to as Σ_{max}, Σ_{min}, Σ_{median} and Σ_{mean}, respectively.

Chapter 5

Implementation

As part of this thesis project, a software implementation of the framework was constructed. Called, *Anomaly Detection Research Tool*, or ADRT, it can be found at `http://github.com/aeriksson/ad-eval`. While it currently serves mainly as a proof of concept, it has been designed with extensibility in mind, and should be easily extendible to handle real-world applications.

The implementation is split into two parts. The first is an implementation of the oracle discussed in Section 3.10; i.e. a program that takes an input element $x \in [D]$ and a set of components (T_D, F_E, C, F_R, M, Σ, T_S), and which produces a solution to the problem defined by these inputs. The second part is a set of utilities which can be used to solve the optimisation problem. The idea behind this separation is for the oracle to be deployable as a separate components once the optimisation problem has been solved for a given type of data.

In order to limit the scope of the project, ADRT currently only contains the components required for the task of finding anomalous subsequences in real-valued sequences. However, extending it to handle any given anomaly detection task should be as simple as implementing a set of components suited for the given task.

In this chapter, the oracle and utility implementations are discussed.

5.1 The oracle

The oracle part of ADRT is a straightforward implementation of the oracle described in Section 3.10:

```
Require: Some $X \in [D]$.
  $X' \leftarrow T_D(X)$
  $A \leftarrow []$                          ▷ initialize anomaly scores to empty list
  for $E \in F_E(X')$ do                     ▷ iterate over the evaluation set
      $R_E \leftarrow F_R(C(X', E))$         ▷ compute a reference set
      $append(A, M(E, R_E))$                 ▷ compute and store anomaly scores
  end for
  return $F_S(\Sigma(F_E(X'), A))$           ▷ aggregate scores to form anomaly vector
```

Currently, the following components have been implemented:

The transformations T_D and T_S: Only the identity transformations $T_D(D) = D$ and $T_S(A) = A$.

The filters F_E and F_R: Sliding windows, as described in Section 4.4.

The context function C: The trivial context, the novelty context, and local contexts as described in Section 4.5.

The anomaly measure M: A kNN-based anomaly measure, along with the distance measures listed in Section 3.8 and a few optional transformations (SAX, DWT and DFT), as well as the support vector machine-based measure described in [5].

The aggregation function Σ: Σ_{min}, Σ_{max}, Σ_{mean}, and Σ_{median} as described in Section 4.7.

Since the initial focus of ADRT is on real-valued sequences, it is currently assumed that $D = D' = \mathbb{R}$. However, all the components listed above with the exception of the anomaly measures, are defined independently of D, so other types of data could be handled by implementing more anomaly measures.

Note that while the focus is currently on the task of finding anomalous subsequences, the task of finding anomalous sequences can be handled using the same oracle by fixing F_E, F_R, and Σ to identity transformations, and so could be handled by *ADRT* essentially without any modifications.

5.2 Utilities

Given an implementation of the oracle and a suitable set of components, all that's needed to solve the optimisation problem is an implementation of some error measure and optimisation method.

These are provided as part of the utilities package in ADRT. Specifically, the error measures ϵ_N, ϵ_E, and ϵ_F mentioned in Section 3.12 are provided, as well as a few rudimentary optimisation tools (for constraining the problem set and naively optimising over the resulting reduced set). Better optimisation heuristics such as simulated annealing could greatly improve running times, as well as enable more relaxed problem set constraints. However, since the implementation and evaluation of such methods would not fit within the scope of this project, these have yet to be added to ADRT.

For purposes of assessing the accuracy of the results and suitability of the error measure and optimisation method, tools for generating and visualising performance metrics are also provided.

Finally, a set of utilities for generating and manipulating time series are provided. These are meant to facilitate testing and perturbation analysis.

One of the main benefits of the framework presented in this report is that since it provides a unified language for dealing with diverse anomaly detection problems, it could be used as a basis for the sharing and replication of results in anomaly detection research. Thereby, it could help solve some of the issues in modern anomaly detection research outlined in Section 2.2.

In order to capitalise on this, the utilities package was written with scripting in mind. Essentially, this means that the typical anomaly detection research process (evaluating new methods and sharing the results) could become as a simple matter of implementing a few additional components, writing a few scripts to produce the results, and sharing these (along with the data used) publicly. Verifying or building upon others' results would then be as simple as downloading and running their scripts.

To highlight how this could work, the results in the next chapter (including the graphs) have all been produced using scripts, which have been made available in the ADRT repository.

Chapter 6

Results

In this chapter, a few basic results obtained by analysing time series using ADRT are presented. Since appropriate data could not be obtained for this project, and in order to limit the scope of this report, a comprehensive analysis could not be performed. Instead, a preliminary, qualitative evaluation was performed, with the twofold goal of gaining some insight into the how component choices affect accuracy and performance, as well as demonstrating how ADRT can be used to simplify and standardize the process of evaluating anomaly detection methods.

Specifically, the analysis presented in this chapter concerns the task of finding anomalous subsequences in long real-valued sequences. This task was chosen since it is a very interesting task that has not been extensively researched, and which is complex enough to require the full oracle as presented in Section 3.10.

All graphs and data in this chapter were obtained through scripts written using ADRT. Since one of the main goals of the evaluation was to demonstrate how ADRT can be used to perform standardized evaluations, all scripts used to obtain the figures and results in this chapter are available in the ADRT source code repository. Modifying these scripts to use other datasets or to evaluate other components (such as the SVM anomaly measure implemented in ADRT) is trivial.

6.1 Method

As the main goal of the analysis was to demonstrate the utility of the framework in reasoning about and evaluating anomaly detection approaches, the focus of this chapter is on using the framework and ADRT to assess how problem accuracy and performance varies over the problem set.

Since an analysis of the entire problem set would be prohibitively expensive, this is instead achieved by means of parametrising a constrained problem set, fixing a point (in other words, a problem) in this set, and measuring accuracy and performance in a neighbourhood (as defined by the parametrisation) of this point.

Since both the specific task studied and approach taken are novel, the error measures ϵ_E, ϵ_F, and ϵ_N implemented in ADRT must themselves be empirically evaluated to verify that they accurately capture intuitive error notions. Were this not the case, using them could invalidate the entire analysis. For this reason, an analysis of their performance is presented prior to the problem set analysis.

Due to difficulties in obtaining appropriate real-world test data, and due to the fact that evaluating anomaly detection methods on artificial data is dubious at best, the decision was made to limit the analysis to a qualitative one. Instead, necessary tools are provided (in the form of ADRT scripts) to make it trivial to perform a thorough analysis once the appropriate data is available.

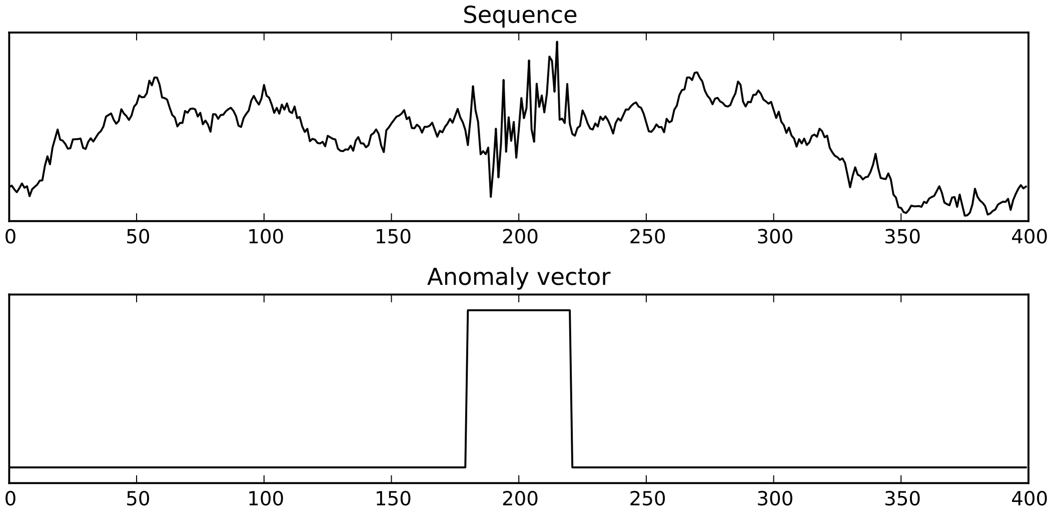


Figure 6.1. The sequence s^* and corresponding reference anomaly vector a^*.

To emphasise this qualitative nature, the analysis in this chapter has been performed on a single artificial sequence, using scripts which can be run on bigger datasets without modification. The chosen sequence, which will be referred to as s^*, is shown in Figure 6.1, along with the reference anomaly vector used.

6.2 Problem set

Evaluating the set of all problems solvable by ADRT would make for a rather lengthy and dull analysis. To avoid this situation, a few constraints were placed on the problem set. Specifically, M was restricted to kNN-based anomaly measures (as defined in Section 4.6, and C was restricted to local contexts (as defined in Section 4.5) with $a = b = m$.

Next, a parametrisation of this problem set was defined by parametrising each of the allowed components separately. The filters F_E and F_R, being sliding window filters, are naturally parametrised by the step length s and window length w. The context function C, has only a single parameter m given the above restrictions. The kNN anomaly measures can be considered to be parametrised by the value of k and the distance measure δ. Specific δ can in turn be parametrised individually. Since only four distinct values of Σ are available, it does not need to be parametrised.

Finally, a single point in the restricted problem set was selected, and performance and accuracy characteristics were assessed in the neighbourhood of this point. The specific point, which will henceforth be referred to as s^*, is given by $s = 1$, $w = 10$, $m = 400$, $k = 1$, δ is the standard Euclidean distance, and $\Sigma = \Sigma_{mean}$. This point was chosen by using ADRT to optimise for ϵ_B over the given problem set.

To simplify the following discussion, we now introduce some notation. We will denote our fixed point by P^*, and let $P^*_{\alpha_1,\alpha_2,\ldots,\alpha_n}$ be the set of problems where $\alpha_1, \alpha_2, \ldots, \alpha_n$ are allowed to take on any value, and all other parameters are given by P^* (e.g., P^*_k corresponds to the set of problems where all parameters other than k agree with the P^*). We will further denote the set of corresponding solutions for s^* by $A_{\alpha_1,\alpha_2,\ldots,\alpha_n}$.

6.3 Error measures

In Section 3.12, three error measures for anomaly vectors were proposed: ϵ_N, ϵ_E, and ϵ_F. In this section, an investigation into how well these error measures capture intuitive notions of error is presented.

This investigation was performed by computing and graphing the errors $\epsilon(O^*(P^*_{k,w}, s^*), a^*)$ for $\epsilon = \epsilon_N, \epsilon_E$ and ϵ_F and $k, w \in \{0, 2, \ldots, 50\}$. Heat maps of the resulting values are shown in Figure 6.2. A few of the $A_{k,w}$ which were given the lowest values by each of the error measures are shown in Figure 6.3.

As shown in the heat maps, the three error measures give similar results, attaining minima and maxima in the same regions. Since ϵ_E and ϵ_F operate on binary strings and thus have discrete domains, they often assign identical errors to nearby points. This is the cause of the relatively jagged appearance in the plots of these errors compared to the smoother appearance of the ϵ_N plot.

Figure 6.3 shows the anomaly vectors with the nth lowest errors for the three distance measures. All three measures give similar anomaly vectors for $n = 1$ and $n = 10$, with ϵ_N and ϵ_F giving the same anomaly vector in both cases. For $n = 50$ and $n = 100$, however, ϵ_F seems to prioritize smooth anomaly vectors, while the other two anomaly measures prioritize anomaly vectors with few false positives.

One interesting aspect evidenced in the heat map plot is that while ϵ_E and ϵ_F are both very large for $A_{k,w}$ with small w, this tendency is not shared by ϵ_N. As seen in Section 6.4.4, anomalies significantly larger than w will not be detected by kNN methods, which means that assigning a large value to these anomaly vectors is reasonable. Since the ϵ_N (unlike the other two error measures) gives equal weight to every component, it will assign relatively low values to anomaly vectors that only partially capture anomalies as long as most of their elements are close to zero. Indeed, this is the case for the $A_{k,w}$ with small w since these anomaly vectors are

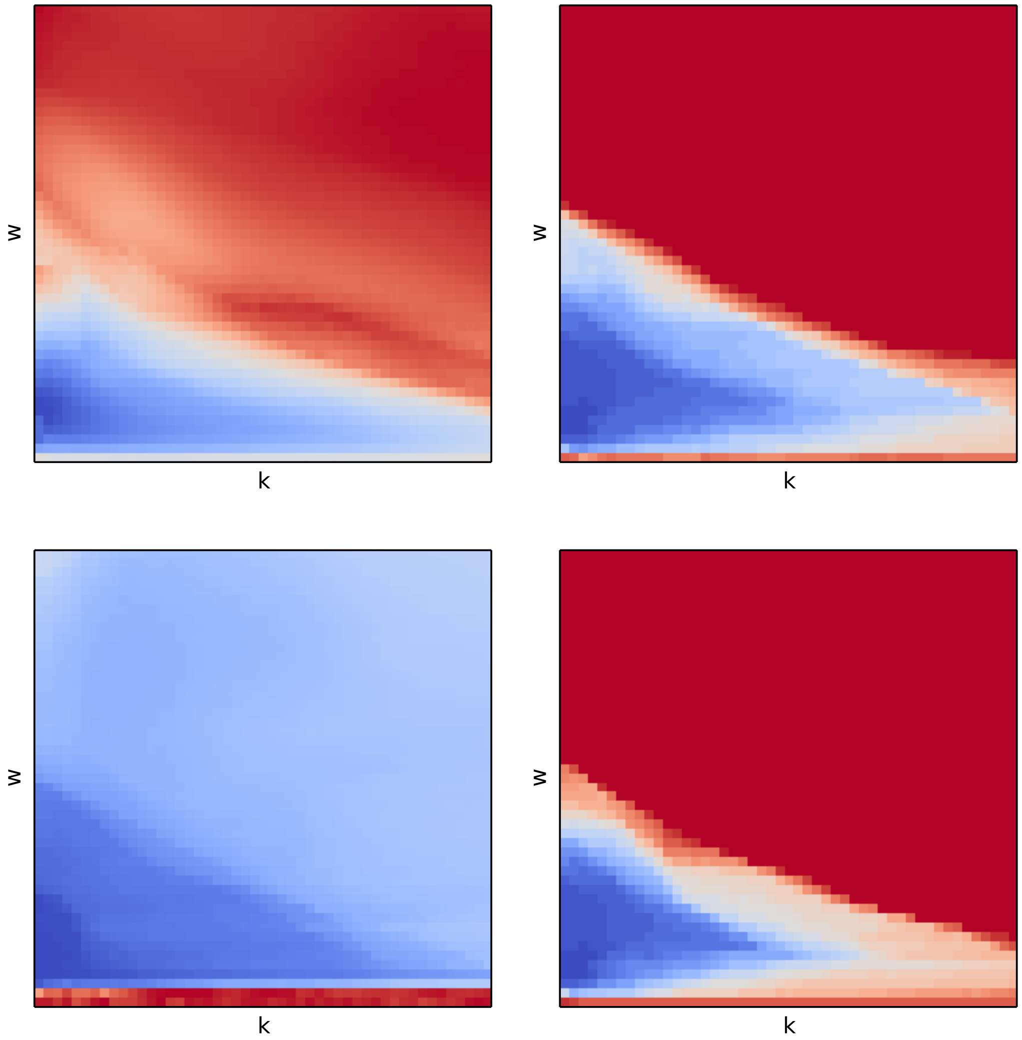


Figure 6.2. Heat maps showing the normalized values of $\epsilon(A(P^*_{k,w}, s^*), a^*)$ for the three errors and $k, w = 1, 2, \ldots, 50$. Blue and red correspond to low and high error values, respectively.

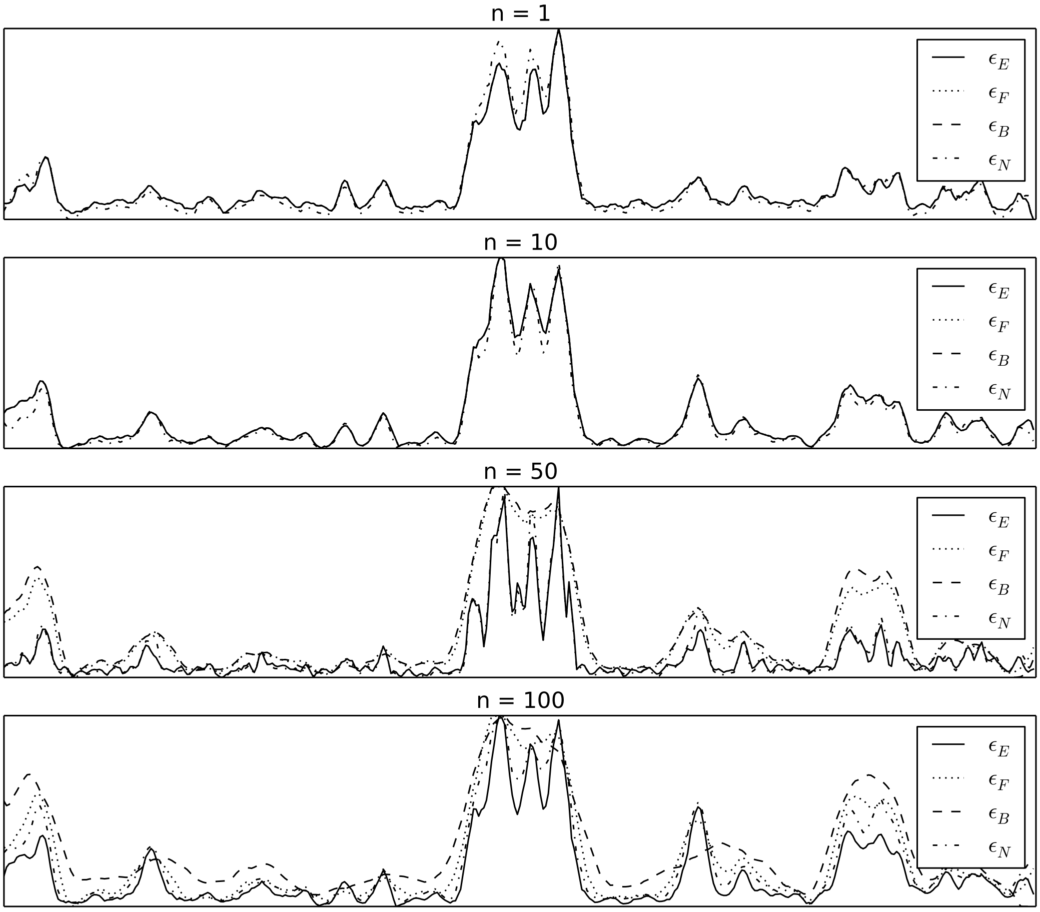


Figure 6.3. The nth best $A_{k,w}$ according to the three error measures for $n = 1, 10, 50$ and 100.

close to constant everywhere except for a few spikes.

As an illustration of the potential problems this could cause, see Figure 6.4, which shows one reference anomaly vector and two candidate anomaly vectors for a long sequence. Here, the first anomaly vector, while noisy, accurately captures the anomaly while the second not only misses the anomaly, but also introduces two false positives. While ϵ_F and ϵ_E are significantly smaller for the first candidate than for the second, the reverse is true for ϵ_N. This problem is amplified as the sequence length grows. These results indicate that ϵ_N should be used with caution, and that since other two error measures are preferable since they were defined specifically to avoid problems such as this.

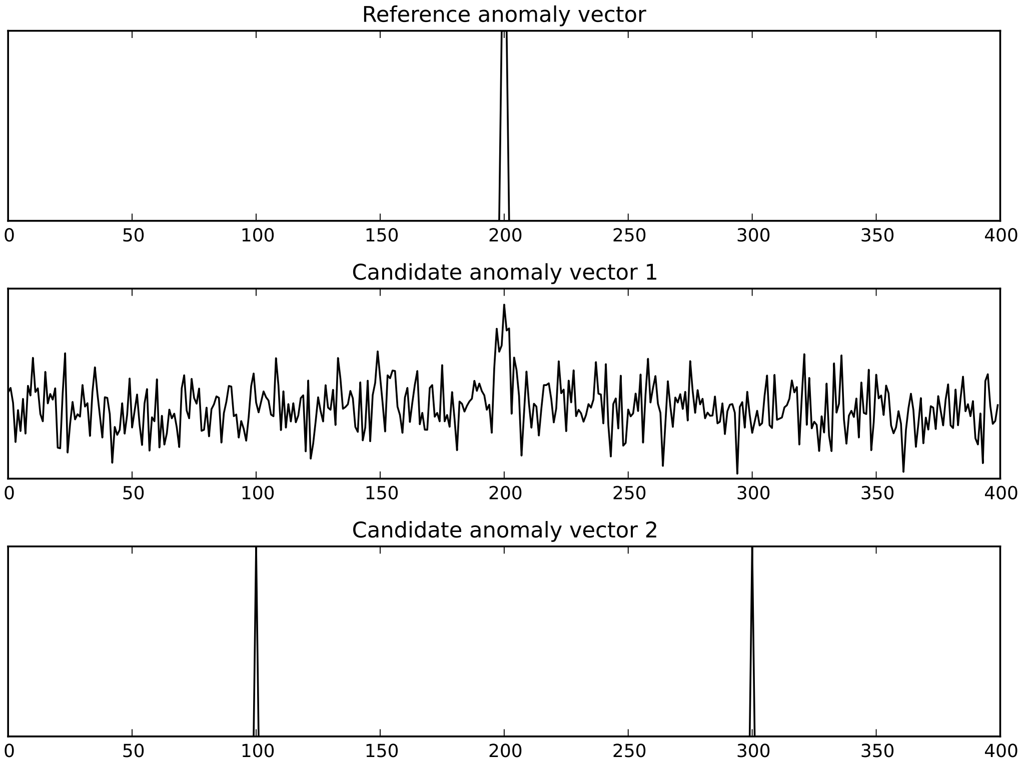


Figure 6.4. A reference anomaly vector for a long sequence and two corresponding candidate anomaly vectors. The first candidate vector, while noisy, correctly marks the anomaly. The second candidate does not mark the anomaly and marks two false anomalies. ϵ_N, ϵ_E and ϵ_F for the two sequences are 8.3 and 2.2; 0.010 and 0.99; and 0.0050 and 0.99, respectively.

6.4 Parameter values

The accuracy and performance of problems around P^* is now studied for the sequence s^*, by means of varying each of k, δ, t, w, s, m, and Σ individually and looking at the resulting anomaly vectors and oracle execution times.

As mentioned previously, since only a small subset of the problem space is studied, and only a single sequence is used, no conclusions about the global characteristics of the problem space, or about how well the results might extend to other sequences can be drawn. Instead, the analysis in this Section should be considered a first step towards establishing a broader understanding of how problem accuracy can vary over the problem sets for distance-based problems, and as an introduction to ADRT, including some useful ways to explore performance and accuracy characteristics.

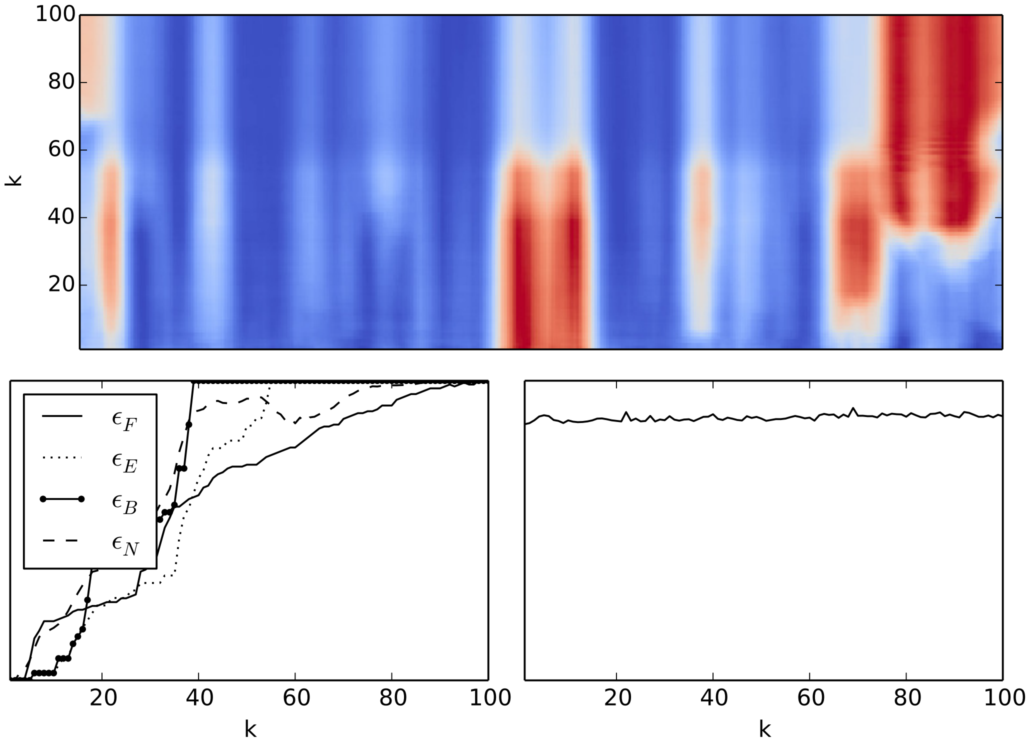


Figure 6.5. Results for P_k^*, where $k = 1, 2, \ldots, 100$. The top panel shows the anomaly vectors A_k (red and blue indicate high and low anomaly scores, respectively). The anomaly vectors have been individually normalised to lie in the unit interval. In the upper right panel, the errors ϵ_N, ϵ_E and ϵ_F are plotted as a function of k. The errors curves have been individually normalised. Finally, oracle computation times for a single execution are plotted as a function fo k in the lower right panel.

6.4.1 The k value

It is important to study how the anomaly vectors vary with k; first, because the choice of k is likely to have a large impact on the appearance of the anomaly vector, regardless of the dataset; and second, because the kNN anomaly measure only operates on a single k value at a time, it is in a sense the simplest distance-based anomaly measure, and thus an ideal tool for better understanding how the choice of k impacts the analysis. This understanding is crucial in effectively designing other types of distance-based anomaly measures.

In order to understand how the k value affects the resulting anomaly vectors, the problems P_k^* for $k = 1, 2, \ldots, 100$ were solved for s^*. The results are shown in Figure 6.5.

The smoothness with which the A_k vary with k indicate that using several nearby k in distance-based anomaly measures is not likely to significantly improve accuracy. Furthermore, at least in this case, $k = 1$ minimizes all three error measures, and there is no indication that considering additional k might help. While higher k do lead to other regions being marked as anomalous, these regions do not correspond to relevant features. Were this to hold in general, considering k higher than 1, or using linear combinations of several k is not likely to lead to any significant increase in accuracy. It is highly doubtful, however, that this holds fin general.

Since the implemented kNN method operates by brute force, the entire reference set must be evaluated regardless of k, so the constant evaluation time exhibited in the bottom right of the figure is expected. For any distance measure that is also a metric—such as the Euclidean distance—more efficient methods exist.

6.4.2 The distance function

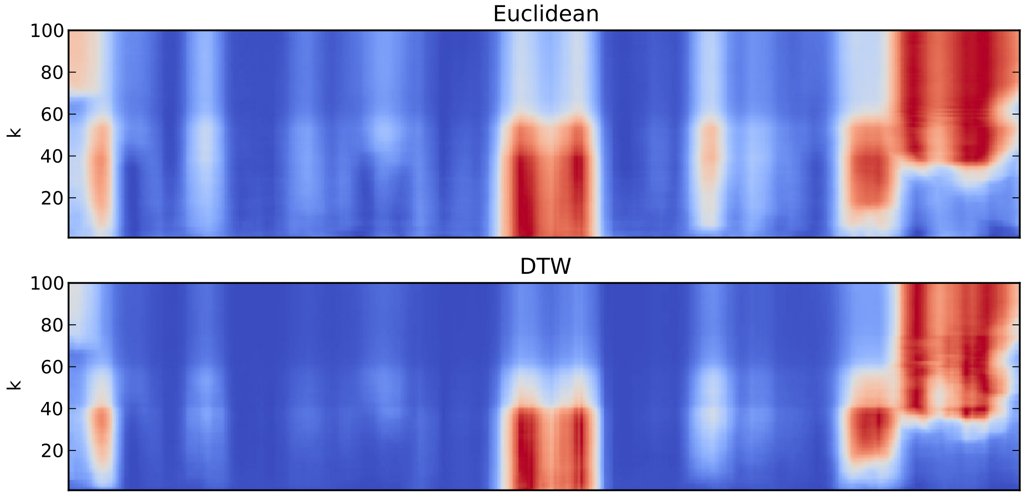


Figure 6.6. Heat maps showing $A_{k,\delta}$ for the Euclidean and DTW distances.

For obvious reasons, the choice of the distance function δ can have a great impact on the anomaly vectors when using distance-based methods. The distance measures implemented in ADRT are the Euclidean distance, the dynamic time warp (DTW) distance, and the compression-based dissimilarity measure (CDM). To investigate the relative performance of these, the anomaly vectors $A_{k,\delta}$ were examined. Note that since A_δ consists of only one value per distance measure, calculating only A_δ would have yielded insufficient data.

Since the CDM distance measure performed seemed to perform poorly both in terms of accuracy and performance around P^*, it is not included in this analysis. Most likely, this was caused by the elements of reference set

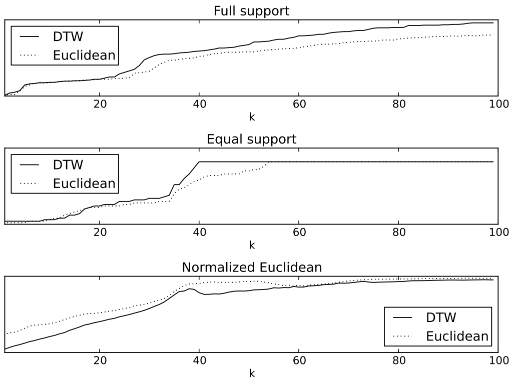


Figure 6.7. Errors for $A_{k,\delta}$.

being relatively small; letting F_E be the identity transformation should give better results.

Instead, the focus was placed on comparing the Euclidean and DTW distances. Heat maps of the resulting anomaly vectors are shown in Figure 6.6 and a plot of the corresponding errors is shown in Figure 6.7. As is seen in the heat maps, there is generally little difference between the outcomes of the two distance measures; the DTW distance gives slightly 'cleaner' (i.e., with non-anomalous regions closer to 0) anomaly vectors for very low values of k, while the Euclidean distance assigns a slightly lower score to the false anomalies encountered at high values of k. While there are some differences in the obtained errors—the DTW distance gives a better normalized Euclidean error, while the Euclidean distance generally gives better values of the other two errors—the evaluation is not sufficient to draw any conclusions about the relative merits of the two measures.

However, the fact that the DTW distance does not perform worse than the Euclidean distance in this evaluation is interesting. Since the DTW was designed to recognize long, shifted but relatively similar continuous sequences, it might be expected to perform poorly on other types of data, such as the short, noisy sequence used in this evaluation. The fact that this is not the case is a positive indication.

6.4.3 Transformations

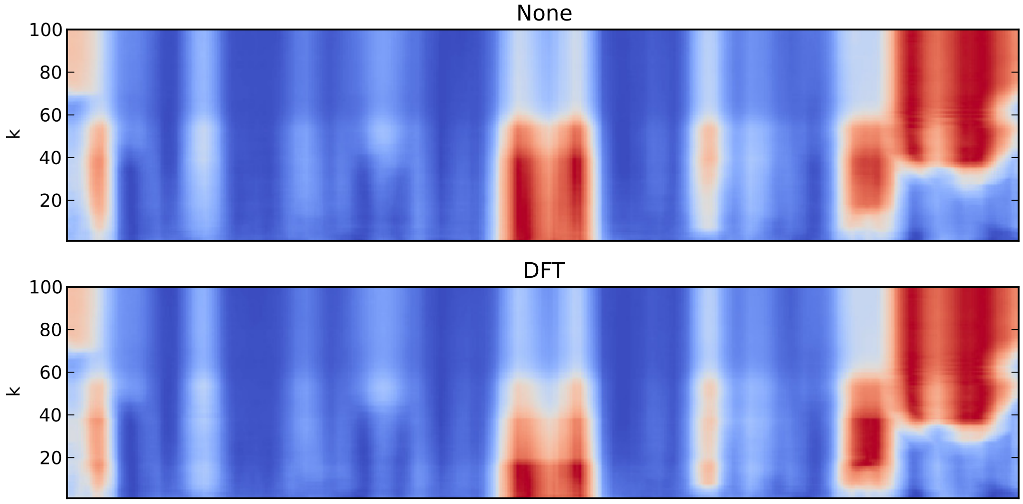


Figure 6.8. Anomaly vectors $A_{k,t}$ for $k = 1, 2, \ldots, 100$ with and without the discrete Fourier transform.

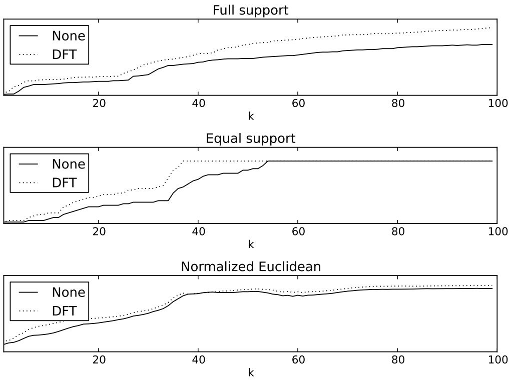


Figure 6.9. Errors of the $A_{k,t}$.

As discussed in Chapter 4, applying transformations to extracted subsequences prior to evaluation, such as to perform dimensionality reduction, might assist in discovering certain types of anomalies. While a large number of compressions and other transformations deserving investigation have been proposed, due to time constraints, only the discrete Fourier transform (DFT) was properly implemented in ADRT.

The performance of the DFT was investigated by evaluating s^* for $k = 1, 2, \ldots, n$ with and without the DFT. A heat map of the results is shown in Figure 6.8, and a plot of the corresponding errors is shown in Figure 6.9.

While the DFT gave fairly accurate anomaly vectors for low values of k, it performed poorly overall, returning less accurate anomaly vectors and higher error values over all k. This is reasonable: the DFT is not expected to perform well on random data. A proper evaluation of the performance characteristics of kNN methods using the DFT would require a more diverse dataset.

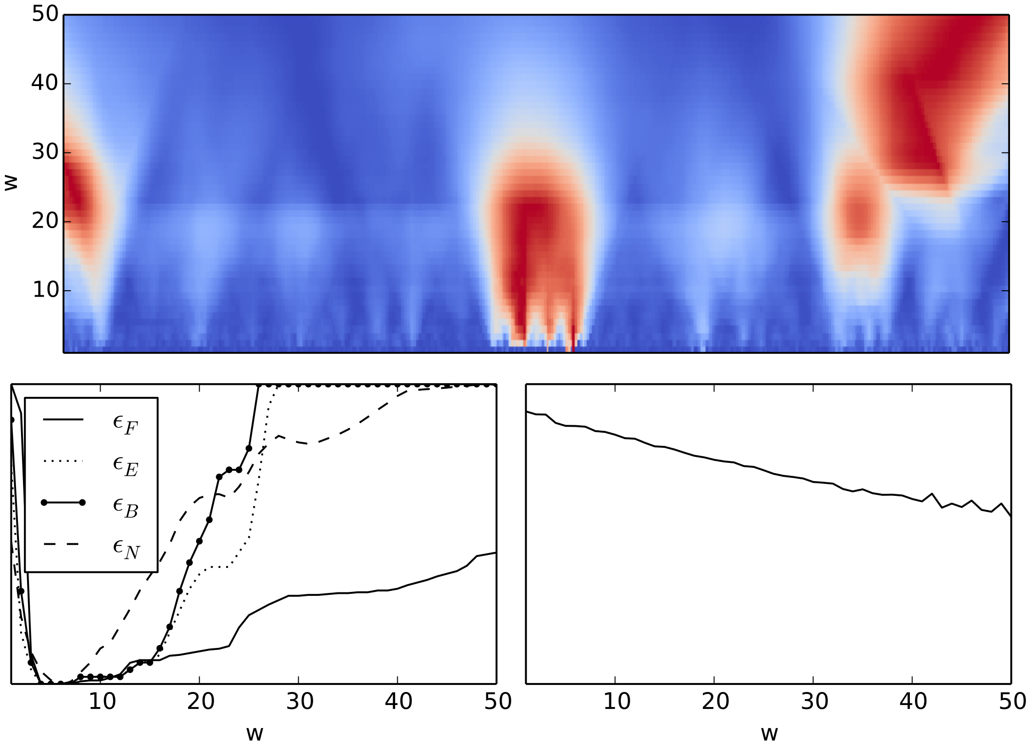


Figure 6.10. Results for P_w^*, where $w = 1, 2, \ldots, 50$.

6.4.4 The sliding window width

Since the sliding window width w determines the size of the elements used by the anomaly measure, it can be expected to have a significant impact on the size of detected features. To determine if this was the case, the anomaly vectors A_w for $w = 1, 2, \ldots, 50$ were computed and examined. The results are shown in Figure 6.10.

As seen in the figures, very low values of this parameter are associated with a very high error. This is expected, since as w tends to 1, the target anomaly type is reduced to point anomalies. Furthermore, all errors increase sharply as w nears 20, indicating that large values of w can lead to inaccurate results.

Interestingly, as seen in the figure, beyond $w \approx 3$, increasing w essentially amounts to smoothing the resulting anomaly vectors. Since the anomaly in s^* has a relatively small width of 40, and since its surroundings have low anomaly values for low values of w, this could help explain why the anomaly is not detected after $w \approx 40$.

It is further interesting to note that while the errors are at a minimum when $w \approx 5$, the anomaly vectors in this area contain three separate spikes in the vicinity of the anomaly, rather than a single smooth bump. Arguably, the anomaly vectors

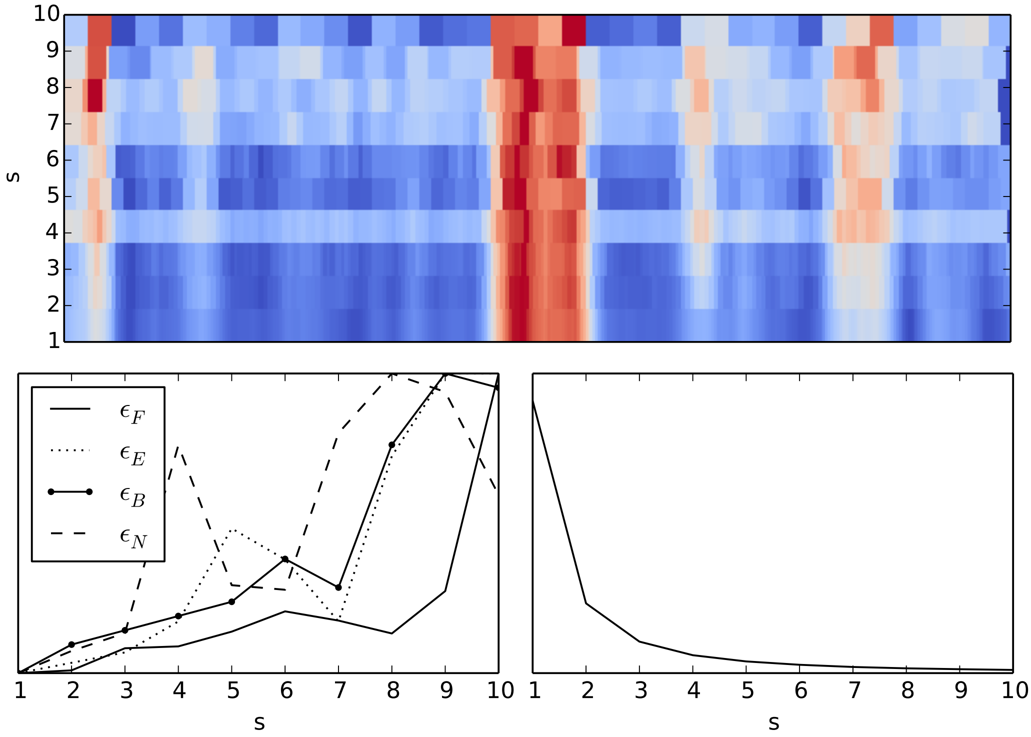


Figure 6.11. Results for P^*_s, where $s = 1, 2, \ldots, 10$. As expected, the oracle execution times scale as $O(1/s^2)$

at $w \approx 10$ are preferable, since they more clearly mark the anomaly. This suggests that the error measures may need refinement.

Finally, while the evaluation time ought to be roughly independent of w (or proportional to the evaluation time of the distance metric with vectors of length w), there is a clear decrease in the computation time as w grows. This is unsurprising, considering that the relatively small width of the evaluation sequence means fewer elements are evaluated as w grows.

6.4.5 The sliding window step

The sliding window step length, s, is interesting mainly for the large effect it has on the execution time. For a brute-force kNN anomaly measure with the trivial context and sliding window filters, the number of comparisons performed on a sequence of length L is $O((L/s)^2)$. It is therefore desirable to choose a value of s that is as large as possible. However, it is likely that all three errors increase with s for all sequences, and large s values might lead to poor results.

To gain some insight into how kNN methods perform with higher s, the anomaly vectors A_s were computed for $s = 1$ to 10 (the value of w is 10 in the default

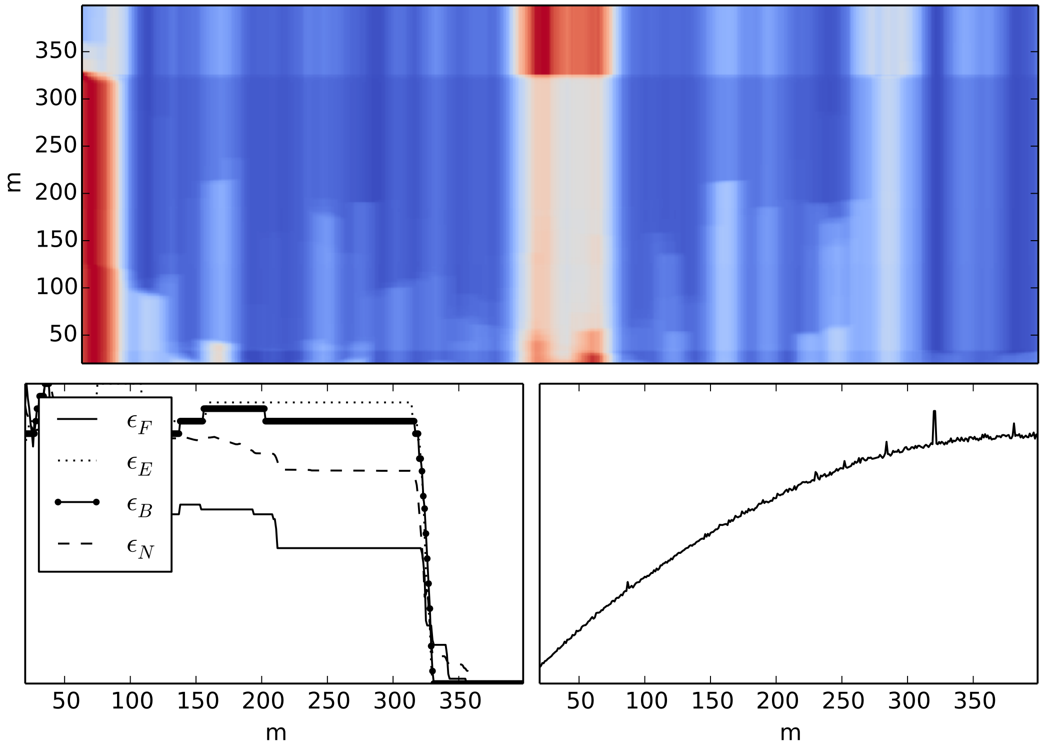


Figure 6.12. Results for P_m^*, where $m = 20, 21, \ldots, 400$. Note the false anomaly present at the left end of the anomaly vectors until $m \approx 330$.

configuration). The results are shown in Figure 6.11.

As seen, the anomaly vectors are fairly accurate for all s. No major false anomalies are exhibited for $s < 8$, and the actual anomaly is still clearly detected over all s. This is reflected in the error plot: all errors are low until $s \geq 8$. Additionally, the evaluation time plot follows the expected $O(1/s^2)$ trend.

In light of these results, perhaps a multi-resolution scheme should be considered, in which a preliminary, ‘coarse’ evaluation (corresponding to high s), and a ‘fine’ evaluation (corresponding to low s) is performed only on those subsequences which are given the highest anomaly scores in the coarse evaluation. Depending on how the subsequences for the fine evaluation are selected, and on the context type, such an algorithm could achieve either lower computational complexity or an evaluation time reduction by a constant factor. If, as indicated in this evaluation, false positives but no false negatives are introduced as s increases, fine evaluation would only rule out false anomalies, and there would be no loss of analytical power.

6.4.6 The context width

Which values of the context width m are appropriate depends heavily on the application domain and on the types of anomalies present in the data. Ideally, the importance of the context width should be evaluated by considering several sequences with a natural context concept, such as the bottom series in Figure 2.4. Constructing representative artificial datasets of such sequences is likely to be difficult, so real-world series should be used for such an evaluation.

While such datasets are not available, a simple evaluation on the available data can still prove illuminating. The sequence s^* is highly homogeneous and admits no non-standard contexts. Thus, all errors should be expected to decrease monotonically with increasing m. To confirm this, the anomaly vectors A_m were computed for $m = 20$ to 400. The results of this evaluation are shown in Figure 6.12.

As these figures demonstrate, the anomaly vectors identify a false anomaly at the left end until $m \approx 330$, at which point the false anomaly disappears and the errors decline sharply. That this false anomaly appears for small context widths is understandable since, as seen in Figure 6.1, the sequence includes values at its left end that are not seen again until the right end. As expected, the error is minimized when the trivial context (corresponding to $m > 390$) is incorporated.

Finally, it should be noted that while the size of the reference set, and consequently the evaluation time, grows linearly with the size of the context, the average context size only grows linearly with m when m is much smaller than the sequence length. When m is close to the sequence length, the context size for a large portion of the subsequences extracted by the evaluation filter will be limited by the sequence edges. This leads to the curve in the bottom right of the figure.

6.4.7 The aggregation function

To get an idea of how the choice of aggregation function Σ affects the analysis, the anomaly vectors $A_{k,\Sigma}$ were computed and analyzed for the minimum, maximum, median and mean aggregation functions, with $k = 1, 2, \ldots, 100$. Heat map plots of the results are shown in Figure 6.13, and plots of the corresponding error measures are shown in Figure 6.14. Single anomaly vectors for $k = 1$ are shown in Figure 6.15.

As seen in Figures 6.14 and 6.15, Σ_{min} and Σ_{max} produce blocky, piecewise constant anomaly vectors, while Σ_{mean} (and, to a lesser extent, Σ_{median}) produces smooth anomaly vectors.

As is seen in the plots, Σ_{mean} and Σ_{median} performed almost identically for all error measures.

As could be expected, Σ_{min} consistently leads to the highest values of ϵ_F. It is likely to give a low score to a point if a single element containing that point has a low anomaly score, which effectively means that parts of anomalies will tend to be undervalued—something ϵ_F is sensitive to. In contrast, Σ_{max} consistently led to the lowest values for ϵ_F. This is also as expected, since Σ_{max} will assign high values to any point contained in an anomalous subsequence.

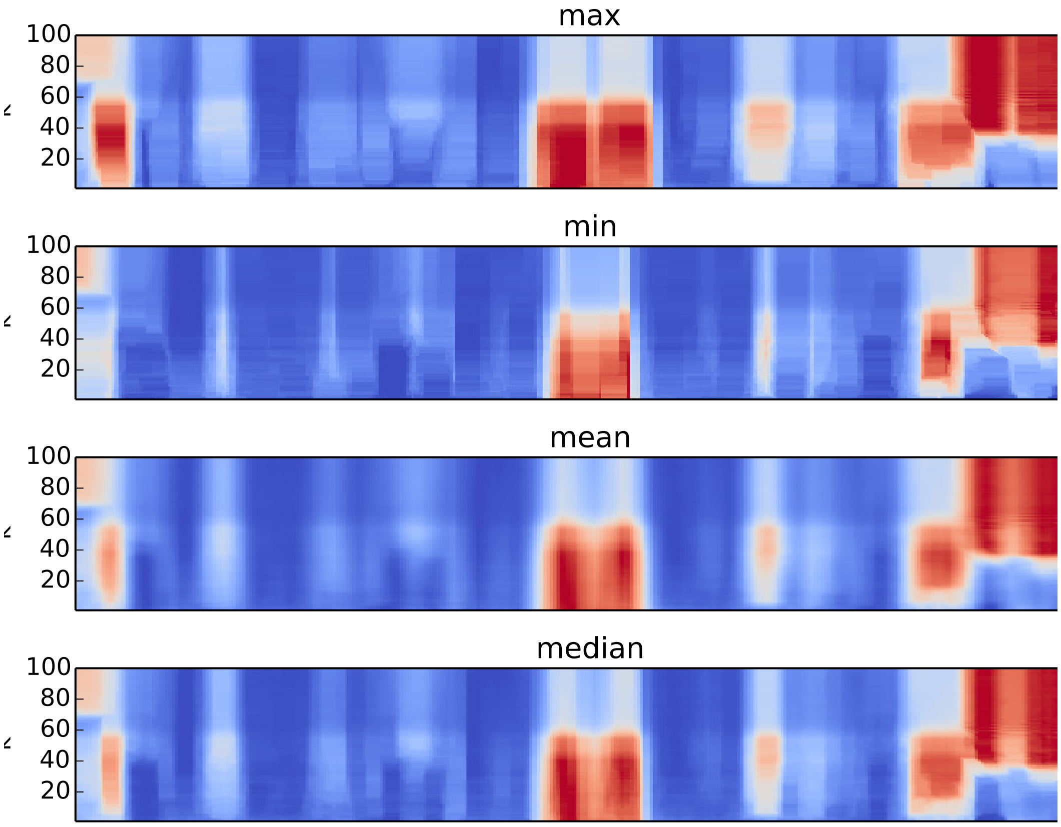


Figure 6.13. Heat maps showing $A_{k,\Sigma}$ for the four aggregation functions.

Similar, but less clear, results were obtained for ϵ_E. Σ_{min} consistently performed the worst with low k, while Σ_{max} performed the best, on average, with k up to 40.

Finally, ϵ_N was consistently lower for Σ_{min} than for Σ_{max}. This is likely a consequence of the fact that Σ_{min} tends to assign scores close to zero to all elements except for a few, while Σ_{max} tends to assign scores close to zero to only a few elements. As discussed in Section 6.3, ϵ_N has a bias in favor of anomaly vectors where most elements are close to zero.

In conclusion, all evaluated choices of Σ performed roughly equally well on s^* (arguably, the minimum Σ performed slightly worse than the others). If this holds in general, then it appears that the choice of Σ is mainly one of aesthetics.

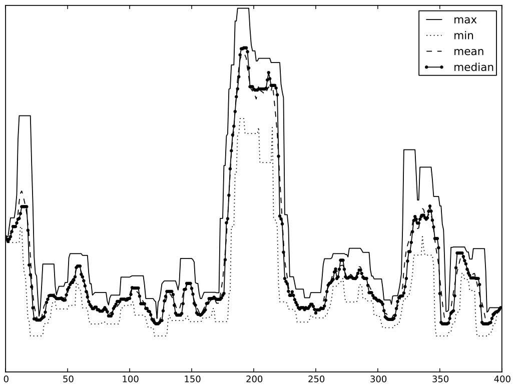


Figure 6.15. Plot of the $A_{k,\Sigma}$ for $k = 1$.

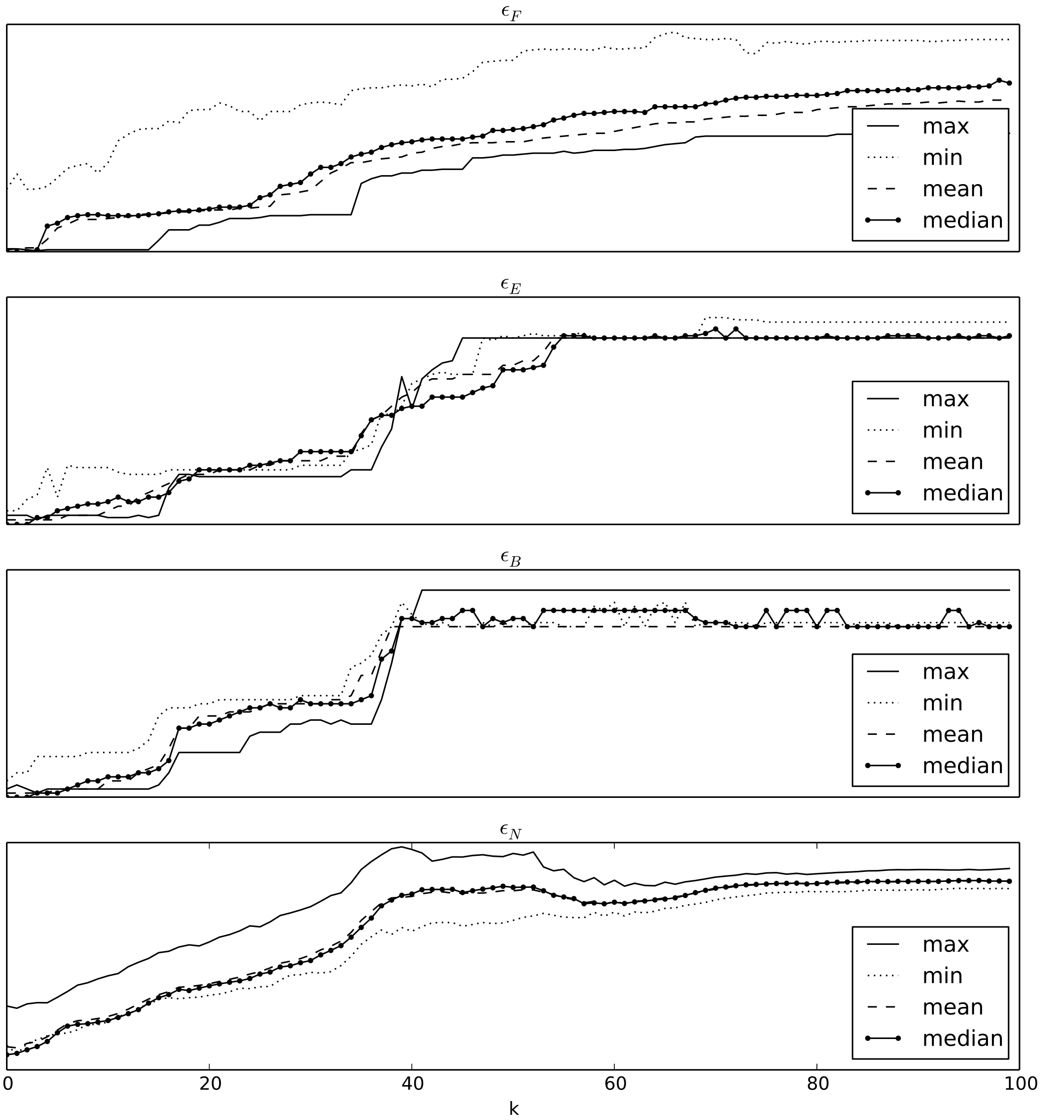


Figure 6.14. Errors of the anomaly vectors $A_{k,\Sigma}$.

Chapter 7

Conclusions

The report is concluded with a short summary and a discussion of a few possible directions for future work.

7.1 Summary

Overall, the project was successful. The new theory introduced in the form of the optimisation problem formulation and the framework represent a step towards powerful, user-friendly tools for automated anomaly detection research. Additionally, ADRT has shown that the framework can be implemented and used to effectively find anomaly detection methods for real applications. Furthermore, the evaluation utilities and evaluation scripts in ADRT have shown that producing open, reproducible anomaly detection research need not be difficult. Finally, as summarized in the next section, the project illuminated several new frontiers for future work.

However, there were some shortcomings. Initially, the project focus was on the implementation and evaluation of a few specific methods for specific datasets. This focus gradually shifted towards a more theoretical one throughout the course of the project, which meant that a large body of work was produced that was ultimately discarded.

Moreover, a proper evaluation of ADRT could not be performed due to lack of data and time. As a result, exactly how practical and useful the framework really is for actual research is still an open question. However, this has been partially mitigated by the provision of reusable evaluation scripts and utilities, which can be used to properly answer this question when the right data becomes available.

7.2 Future work

Several interesting directions for future work have been opened up through this project, a few of which are now discussed.

7.2.1 Optimisation

Developing efficient optimisation methods is key to the successful implementation of the optimisation problem and framework. Currently, only naive optimisation methods have been implemented in ADRT; faster and better methods must be implemented for it to be practical for real-world applications.

There are several interesting paths to take towards this goal. As indicated in the previous chapter, at least for distance-based anomaly measures, errors seem to vary rather smoothly over problem sets, with few non-global error minima or other irregularities. Thus, it can be expected that improved optimisation heuristics, such as simulated annealing, could have a large impact.

Another possibility would be perform the optimisation over a larger set of problems, for instance by allowing combinations of elements of the problem set. This would be a fairly trivial extension, and would allow for the optimisation to produce ensemble-style combinations of methods.

Finally, it seems likely that the optimisation itself could be learned to some degree. For instance, if correlations between the accuracy of problems and the underlying characteristics of the data being analyzed could be found, then these could likely be exploited to provide very efficient optimisation methods. Another, related possibility would be to allow for user-assisted optimisation.

The optimisation process could also be made more efficient through performance improvements. Performance has been deliberately deemphasized in favor of simplicity in the development of ADRT, and it can be expected that dramatic performance improvements could be reaped fairly easily by, for instance, enabling parallelism or rewriting ADRT in a programming language better suited for numeric computations. A performance optimisation that can be expected to have drastic results is the multi-resolution heuristic suggested in Section 6.4.5.

7.2.2 New applications

There is much work to be done still on applying the framework to sequences. To begin with, task involving finding anomalous sequences, as well as tasks involving discrete and categorical data have yet to be studied and implemented in ADRT. There are also several interesting transformations and anomaly measures which are encountered in the literature, but which have yet to be implemented in ADRT. Finally, how ADRT performs on sets of more diverse real-valued sequences needs to be researched.

Of course, applying the framework and ADRT to entirely different application domains, such as fraud detection or bioinformatics would also be interesting. Essentially, this should be as simple as defining the data and problem sets, as well as (optionally) implementing a few more component choices.

7.2.3 Deployment

A major goal in the design of ADRT was for it to be as modular and flexible as possible, so that creating a user interface for it or hooking it up for use with data analysis software such as Splunk would be easy. This was achieved in two ways: first, by designing it as a collection of command line tools, and second, by making it scriptable. Extending ADRT to work with existing data analysis software or a custom user interface could help further elucidate just how sound and practical the framework is for everyday analysis use, as well as how user-friendly it can be made.

One of the main benefits of the optimisation problem formulation and framework is that they provide a venue for automating the work-intensive aspects anomaly detection research, and replacing them with an automated optimisation process. As was mentioned in Chapter 2, anomaly detection research typically necessitates the involvement of both a domain expert and an export on anomaly detection, and is a laborious process involving plenty trial and error. In contrast, ADRT lets users focus almost entirely on more significant aspects of the process: finding methods suitable for a given domain becomes a matter of writing a script which defines the data, places a few restrictions on the problem set, and runs an optimisation. The declarative nature of this work could be taken one step further by defining a domain-specific language for describing the data and the problem set. Reimplementing ADRT in a language with an expressive type system, such as Haskell, would be a good first step in this direction.

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