

April 28, 2016

Dr J.K. Hillier
Associate Editor, ESurf

Dear Dr Hillier,

We enclose an updated version of our manuscript, ‘An introduction to learning algorithms and potential applications in geomorphometry and earth surface dynamics’. We are grateful to the reviewers and commenters for their constructive criticisms on the original draft. Our responses to their substantive points are set out below. A copy of the manuscript marked up to highlight the changes we have made is appended to this letter.

RC1 (Ian Evans)

This is a general survey, essentially a tutorial, of a broad field of methods. It provides a lot of common-sense advice. It is readable (more than anticipated!), and well written except for some overuse of ‘we’. I am in favour of the use of personal pronouns for emphasis, even in scientific writing, but four ‘we’s in four lines (p.2, lines 17-20) seems excessive. Also ‘we aim to give readers...’ (p.1 line 22) comes across as condescending: I would say ‘This review is intended to provide...’

We have replaced the phrase on p. 1, line 22 and reduced the use of ‘we’ overall.

Figs. 2, 3, 6 and 7 use hypothetical data sets (bivariate scatters of points). This is less persuasive than the use of real examples. If made-up data have to be used, however, could they at least be more realistic? Bivariate scatters of real data tend to fade away toward the edges, and clusters are hardly ever as separated as in Figs. 6 and 7. It should not be difficult to replace these Figs. – or even to find comparable scatters that are real observations.

We agree with the reviewer that the use of ‘real’ data sets could be regarded as more persuasive or impressive. However, this has to be offset against the complications that inevitably accompany such examples. Realistic datasets tend to be high-dimensional, making it difficult to illustrate concepts clearly using only one or two two-dimensional figures. In addition, a significant amount of explanation may be required to make examples meaningful to the full spectrum of potential readers. This diverts readers’ attention from the main focus of the paper, and may introduce unnecessary sources of confusion. On balance, we are not convinced that the benefits of using more real examples outweighs the potential costs. In particular, we feel that simple, synthetic examples are generally necessary to illustrate how a particular method works; real examples would have to be in addition to, rather than instead of, these figures.

However, we agree that some of the original figures exhibited unnecessarily unrealistic features, and we have attempted to improve this in the current version.

Many papers use K-Means as a ‘black box’: Fig.2 commendably provides a good illustration of how this algorithm works. The same cannot be said, however, about Fig.7 (SOM): I do not see how (b) leads on to (c), and neither the text nor the caption enlightens me.

We have altered this figure and its caption, and we hope the result is clearer.

One reason for resorting to more complex methods is because of the non-linearity of relationships (some are triangular) and the non-sphericity of clusters in property space. This can be hinted at, even in 2-D graphs: e.g. the separating line in a redrawn Fig. 6 could be curved.

In designing the figures for this paper, we have attempted to strike a balance between simplicity and realism. While the relationships used for illustrative purposes could be made more complex, it is not clear to us that this would necessarily enhance readers' understanding.

In the specific case of Fig. 6, the 'support vector machine' method is based around construction of linear boundaries separating clusters. Thus, the separating line cannot be drawn as a curve. We have modified the figure and caption in an effort to make it clearer.

The case for black boxes or learning algorithms needs to be based on the inadequacy of simpler approaches. On p.8 (line 4), porosity is considered a function of water depth and distance. That would seem to be a case for straightforward regression with two quantitative controls, on transformed scales if necessary.

The cited example (Martin et. al., 2015) makes use of a range of different datasets when generating porosity estimates, and not just the two observables we list for illustrative purposes. We have rephrased this passage in an attempt to make this clearer.

The paper provides a good read and a useful overview and juxtaposition of decision trees, K-Means, PCA, Neural networks, SVM and SOM. It covers the range of statistics from Pearson to Bayes. Although I am not about to use learning algorithms, I found a few useful references. But the case made would be much more persuasive if the paper were thoroughly revised to use real examples throughout (that in Fig. 4 is appreciated); to focus on situations where use of these methods can be shown to improve results considerably over 'traditional' methods; and even to show where they have led to new insights into environmental relationships.

I am relieved that the authors 'do not advocate... wholesale replacement' of 'traditional' approaches. My approach is to keep to the simplest methods that work, and to turn 'black boxes' into transparent boxes wherever possible. If a classification produces highly overlapping classes on most dimensions, I am not interested.

As already discussed, we are sympathetic to the call for greater use of 'real-world' examples. However—somewhat by definition—it is difficult to find problems which are straightforward to explain and illustrate, yet which cannot be convincingly tackled via 'traditional' methods. The rationale underpinning this paper is that learning algorithms are currently relatively unknown in geomorphology: thus, there are relatively few examples in the literature to draw on, and most of these are concentrated within one or two sub-fields. One option would be to make use of examples from fields other than geomorphology; however, this may introduce additional sources of confusion. We have tried to balance these competing factors by using generic examples to illustrate how the techniques work whilst increasing the number and range of references given at the end of the various subsections to provide real-world examples.

DETAILS:

(page/line) 2/13 in which software context should readers 'begin by writing their own...'?

2/16 what are 'optimised libraries'?

We have modified this passage.

2/34 'as black boxes'

Corrected.

3/12 the example is of ‘diverse’ observations, not just multiple.

Changed to ‘multiple, diverse’.

3/17 the title of section 2 led me to expect specific applications. These actually come in later sections: as 2 is very general, perhaps that should be in the heading.

We have re-titled this section.

4/8 to 11 this is a bit too general. Surely a classification can be evaluated only when the aspects of the data on which it is based can be understood?

Unfortunately, we are not sure we understand the reviewer’s point in the context of the cited passage. A learning algorithm classification scheme inherently uses the input data in an unprescribed way, but the performance can still be evaluated by comparison to manual classification. However, we have made some alterations to our text in an effort to make it clearer.

5/9 why do coordinates ‘generally have little physical meaning’?

We have attempted to clarify this point.

6/14 & 15 a desktop computer is contrasted with ‘a modern machine’. This is very vague. Desktops can be modern?

We have altered this to refer to a ‘modern high-performance machine’.

Fig.1 I prefer ‘standardised’ to ‘normalised’ here: the latter may imply a normal distribution.

Our use of the word ‘normalised’ is in accordance with its (mathematical) definition.

7/3 ‘the data are perfect’

Corrected.

9/29 I think it is the components / new variables / dimensions that are uncorrelated – not ‘each parameter’.

Unfortunately, we do not understand the distinction that the reviewer is attempting to draw here. We have changed the text to refer to ‘parameter or component’, in the hope that this resolves any confusion.

Fig.3 shows an even distribution of data points within a sharply-bounded rectangle. I never saw an earth science data set like that: could we have a more realistic scatter?

We have updated the figure appropriately.

Fig.4 is interesting: I see differences between the three rows. In the top row, $N=100$ captures the original thoroughly; in the second, $N=200$ is required: and in the bottom row only $N=500$ captures the lineations in the original. Thus I disagree with ‘using only 100-200 dimensions’, at the end of the caption.

Obviously, this ultimately depends on how accurately one wishes to represent the original data, and which features are regarded as ‘significant’. This may well vary according to application. We have updated the caption to reflect this.

Fig.6 Actually one dimension (y) DOES separate blue from red: they overlap only in x. This is because an unrealistically wide separation has been portrayed: again, the hypothetical example could at least approach realism.

We have updated the figure and caption.

19/6 & 7 I am unsure about ‘various’, but as it implies more than one, it should read ‘statistical distributions of the ... classifications’.

We have re-written this sentence.

19/16 There is no point mentioning CPU hours unless some idea of the machine involved is given.

We now state the clock speed.

19/26 ‘as well as skill’

Corrected.

RC2 (Niels Anders)

This paper sums up the most widely used learning algorithms to extract information from geospatial data sources. The geospatial analysis and geomorphometry related research is becoming more and more data-driven and I encourage papers advocating making use of modern computational techniques in geomorphology. This paper is particularly interesting to those unfamiliar to learning algorithms. Below I have addressed some comments that could improve the paper.

General

The paper explains well the most widely used methods in current literature with effective illustrations. Each topic is supported with one or few references to applications in the geosciences, mostly landslide susceptibility. However, to justify the part in the title concerning ‘...and potential applications in geomorphometry and earth science dynamics’ I think the paper should cover a more in depth section on the potential applications of learning applications in the geosciences. Or perhaps remove ‘potential’ from the title and at least provide more references in the 3.1-3.7 subsections to current research that are applying these algorithms.

We have increased the number of examples of current research, ensuring that at least three examples are given for each technique in subsections 3.1–3.7. We have also tried to ensure that a range of examples are given where possible. However, these techniques have been much more widely used in the subfield of landslide susceptibility, so studies on this topic do form a large part of the existing literature on applications of machine learning to geomorphology. One potential, if coincidental, benefit of this is that it demonstrates that a range of machine learning techniques can be successfully applied to very similar problems — there is not a single correct approach for a given problem.

Throughout the paper, we have tried to emphasise the general types of geomorphological problem or task that these techniques may be useful for, to highlight the wide range of potential applications — Section 2, in particular, focuses on this. The examples given in both Section 2 and Section 3 are also presented more to illustrate the range of what is possible than to attempt to explain in any detail what the previous authors have done or the conclusions they reached. We thus feel that ‘potential applications’ is a reasonable title.

Also in the subsections there are occasional statements such as ‘it is claimed that’ (P4L8)

or ‘literature describes a rule of thumb’ (P6L9), which are not followed by references. I think it is required to provide references to support such statements in general.

In both of these cases, we are expressing some disagreement with statements or misconceptions that—in our experience—occur quite frequently within the literature, usually introduced as ‘received wisdom’ without any attempt at justification. In such circumstances, we feel it is unfair to identify one or two randomly-selected papers as apparent targets for our criticism.

I suggest presenting an overview of strengths and weaknesses in different scenarios (data sets), or what learning algorithm could be appropriate for particular data sets or different scenarios, possibly as a table. For example when should scientists choose random forests over neural networks. There is probably not a single best method for each scenario, but I guess some algorithms are ruled out because of certain data types or data properties (maybe due to statistical limitations). This would also broaden the audience reading this paper.

We have added a table that summarises the various methods discussed in the paper. This does not go as far (perhaps) as the reviewer hoped: it is not possible to enumerate all the considerations that apply when deciding which method(s) should be adopted in a given situation. Nevertheless, we hope the addition will assist readers.

Although the English is much better than my own, there are a few singular/plural errors throughout the paper. I suggest to have the paper thoroughly checked.

We have eliminated a few typos and editing errors.

Specific P3L11: I would not say LiDAR ‘image’. In remote sensing an image is often associated with spectral measurements captured by a sensor creating this image. The authors probably mean a derived grid of interpolated elevation values from a LiDAR point dataset, hence LiDAR DEM or DTM is more appropriate than ‘image’. Also the abbreviation style LiDAR (with capital A) is more commonly used than LiDaR.

We have corrected this, and ensured all abbreviations are set as ‘LiDAR’.

P4L33: It is unclear to me what exactly this ‘data vector’ means with respect to a grid and why a 100m x 100m grid with with 10 m cells (thus 10x10=100 cells) would have (11x11=) 121 dimensions.

There are two possible interpretations of ‘a 100 m × 100 m grid... sampled at 10 m intervals’. One—as assumed by the reviewer—involves dividing the region into 100 equal cells, and sampling at the centre of each cell, leading to 100 measurements. The second involves sampling at the corners of each cell, resulting in 121 measurements. (This is often described as a ‘fence-post problem’: a ten-panel garden fence requires eleven fence-posts.)

We have edited this passage in an effort to reduce the potential for confusion, and make the link to ‘data vectors’ more explicit.

P5L6-10: I wonder if dimension reduction by means of visualization is appropriate to mention in this section, as dimension reduction in the context of learning algorithms is primarily used to reduce complexity of calculations and/or computing. To me the way how results are visualized and whether dimensions or detail are lost is a different discussion.

We feel that the use of learning algorithms to assist in dataset visualisation is an topic worth mentioning here. Certainly, it is an approach that is used more in some fields than in others, but we believe it is important to alert readers to this possibility. We wonder if the reviewer slightly misunderstood our

intentions here, and we have rephrased it to make things clearer.

P5L11-15: While vegetation of course has indirectly also geomorphological implications I'd like to, rather shamelessly, self-advertise our recent paper that is a more pure example of cluster analysis in (palaeo-glacial) geomorphology, see Smith et al (2016) in ESPL: <http://onlinelibrary.wiley.com/doi/10.1002/esp.3828/abstract>

We have adopted this suggestion.

P6L10: is 'performance' here meant in terms of computation time, or in terms of accuracy, or both.

We intended this to refer mainly to 'accuracy'. We have edited the text to make this clearer.

P9L18: now LiDAR is abbreviated as LIDAR. I suggest selecting one style of abbreviation, preferably Lidar, LiDAR or LIDAR.

We have now converged on 'LiDAR'.

Section 3.3. I think PCA should be explained in more detail. It is for example not mentioned what the axes actually mean and that what information is derived from the point distribution along the axes. For example that the axes do likely resemble an average of multiple dimensions is not mentioned. For example in the example of a PCA of plant species distribution with respect abiotic factors such as soil type, ph, and water availability a single PCA axis could resemble both ph and water availability and could make interpretation of PCA more complex. When describing PCA I think such information is essential to mention.

We have updated our discussion in the light of these comments, and added an example where the components relate to multiple observables in this way.

SC1 (Evan Goldstein)

In section 4.1 the authors discuss training data. They state, on P. 17 L. 1-2: "To avoid problems, it is important to choose training data with care, and to develop strategies for evaluating and monitoring the performance of the trained system." My own experience with machine learning suggests that this is crucial: if the training data is bad (e.g., not enough, too much, too noisy, doesn't cover the solution space adequately, etc.), the learner cannot do its job effectively (hence the expression 'garbage in, garbage out'). My recommendation is the authors present specific guidance on how to select appropriate training data and point the reader toward such guidance in the literature (i.e., selection routines). Note that this goes beyond offering advice on how to represent data to the learner (discussed on p. 17, line 2-8).

We have tried to incorporate this point into our discussion in Section 4.1. However, we do not feel there is much 'specific guidance' that can usefully be given in the present paper: anything beyond the most general remarks must surely depend upon the data and application being considered.

SC2 (J.J. Becker)

Page 9 line 5: As the 3rd author of Martin 2015, and the main author and "debugger" of the code used there, I wanted to throw in my two cents worth about how important it is to normalize both the "features" (aka predictors) and the "response" (aka measurements). This doesn't need to be complex, simply "Student-ize" by removing the mean of every column of the training data, (store that number), and dividing the detrended data by its standard deviation, (also store that). When making a prediction after training, it is important to apply the mean and std dev of the TRAINING data to the data used in the

PREDICTION. Often “software packages” do this automatically (aka Random Forests in MATLAB), but other times this is not the case and it will dramatically hurt the prediction. For example, the recent advances in “deep learning” for Machine Vision were only achieved after the researchers understood they needed to subtract the “average image” obtained from all the training images -BEFORE- training and prediction...

We have now included this point in Section 4.1.

Yours sincerely,

Andrew Valentine

An introduction to learning algorithms and potential applications in geomorphometry and earth surface dynamics

Andrew Valentine¹ and Lara Kalnins²

¹Department of Earth Sciences, Universiteit Utrecht, Postbus 80.021, 3508TA Utrecht, The Netherlands.

²Department of Earth Sciences, Science Labs, Durham University, Durham, DH1 3LE, UK.

Correspondence to: Andrew Valentine (a.p.valentine@uu.nl)

Abstract. ‘Learning algorithms’ are a class of computational tool designed to infer information from a dataset, and then apply that information predictively. They are particularly well-suited to complex pattern recognition, or to situations where a mathematical relationship needs to be modelled, but where the underlying processes are not well-understood, are too expensive to compute, or where signals are over-printed by other effects. If a representative set of examples of the relationship can be constructed, a learning algorithm can assimilate its behaviour, and may then serve as an efficient, approximate computational implementation thereof. A wide range of applications in geomorphometry and earth surface dynamics may be envisaged, ranging from classification of landforms through to prediction of erosion characteristics given input forces. Here, we provide a practical overview of the various approaches that lie within this general framework, review existing uses in geomorphology and related applications, and discuss some of the factors that determine whether a learning algorithm approach is suited to any given problem.

1 Introduction

The human brain has a remarkable capability for identifying patterns in complex, noisy datasets, and then applying this knowledge to solve problems or negotiate new situations. The research field of ‘learning algorithms’ (or ‘machine learning’) centres around attempts to replicate this ability via computational means, and is a cornerstone of efforts to create ‘artificial intelligence’. The fruits of this work may be seen in many different spheres—learning algorithms feature in everything from smartphones to financial trading. As we shall discuss in this paper, they can also prove useful in scientific research, providing a route to tackling problems that are not readily solved by conventional approaches. We will focus particularly on applications falling within geomorphometry and earth surface dynamics, although the fundamental concepts are applicable throughout the geosciences, and beyond.

This paper does not attempt to be comprehensive. It is impossible to list every problem that could potentially be tackled using a learning algorithm, or to describe every technique

that might somehow be said to involve ‘learning’. Instead, we aim to ~~give readers a general understanding~~ provide a broad overview of the possibilities and limitations associated with these approaches. We also hope to highlight some of the issues that ought to be considered when deciding whether to approach a particular research question by exploring the use of learning algorithms.

The artificial intelligence literature is vast, and can be confusing. The field sits at the interface of computer science, engineering, and statistics: each brings its own perspective, and sometimes uses different language to describe essentially the same concept. A good starting point is the book by Mackay (2003), although this assumes a certain level of mathematical fluency; Bishop (2006) is drier and has a somewhat narrower focus, but is otherwise aimed at a similar readership. Unfortunately, the nature of the field is such that there are few good-quality reviews targeted to the less mathematically-inclined, although one example can be found in Olden et al. (2008). There is also a wealth of tutorials and other course material available online, varying in scope and quality. Finally, we draw readers’ attention to a recent review by Jor-

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dan and Mitchell (2015), offering a broad ~~overview~~ survey of machine learning and its potential applications.

Learning algorithms are computational tools, and a number of software libraries are available which provide users with a relatively straightforward route to solving practical problems. Notable examples include `pybrain` and `scikit-learn` for Python (Schaul et al., 2010; Pedregosa et al., 2011), and the commercially-available ‘Statistics and Machine Learning’ and ‘Neural Networks’ toolboxes for Matlab. Most major techniques are also available as packages within the statistical programming language, R. Nevertheless, we encourage readers with appropriate interest and skills to ~~begin by~~ spend some time writing their own implementations for basic algorithms: our experience suggests that this is a powerful aid to understanding how methods behave, and provides an appreciation for potential obstacles or pitfalls. ~~Armed with this knowledge, the user is then better-placed to benefit from~~ In principle, this can be achieved using any mainstream programming language, although it is likely to be easiest in a high-level language with built-in linear algebra support (e.g. Matlab, Python with NumPy). Efficient ‘production’ applications are likely to benefit from use of the feature-intensive tools contained within optimised libraries and highly-optimised tools available within the specialist software libraries mentioned above.

This paper begins with a brief overview of the general framework within which learning algorithms operate. We then introduce three fundamental classes of problem that are often encountered in geomorphological research, and which ~~we see as seem~~ particularly suited to machine learning solutions. Motivated by this, we survey some of the major techniques within the field, highlighting some existing applications in geomorphology and related fields. Finally, ~~we discuss~~ some of the practical considerations that affect implementation of these techniques ~~, and are discussed, and we highlight some~~ issues that should be noted when considering exploring learning algorithms further.

1.1 Learning algorithms: A general overview

Fundamentally, a learning algorithm is a set of rules that are designed to find and exploit patterns in a dataset. This is a familiar process when patterns are known (or assumed) to take a certain form—consider fitting a straight line to a set of data points, for example—but the power of most learning algorithm approaches lies in their ability to handle complex, arbitrary structures in data. Traditionally, a distinction is drawn between ‘supervised’ learning algorithms, which are aimed at training the system to recognise known patterns, features, or classes of object; and ‘unsupervised’ learning, aimed finding patterns in the data that have not previously been identified or that are not well defined. Supervised learning typically involves optimising some pre-defined measure of the algorithm’s performance—perhaps minimising the difference be-

tween observed values of a quantity and those predicted by the algorithm—while in unsupervised learning, the goal is usually for the system to reach a mathematically-stable state.

At a basic level, most learning algorithms can be regarded as ~~a ‘black-box’~~ ‘black boxes’: they take data in, and then output some quantity based upon that data. The detail of the relationship between inputs and outputs is governed by a number of adjustable parameters, and the ‘learning’ process involves tuning these to yield the desired performance. Thus, a learning algorithm typically operates in two modes: a learning or ‘training’ phase, where internal parameters are iteratively updated based on some ‘training data’, and an ‘operational’ mode in which these parameters are held constant, and the algorithm outputs results based on whatever it has learned. Depending on the application, and the type of learning algorithm, training may operate as ‘batch learning’—where the entire dataset is assimilated in a single operation—or as ‘on-line learning’, where the algorithm is shown individual data examples sequentially and updates its model parameters each time. This may be particularly useful in situations where data collection is ongoing, and it is therefore desirable to be able to refine the operation of the system based on this new information.

In the context of learning algorithms, a ‘dataset’ is generally said to consist of numerous ‘data vectors’. For our purposes, each data vector within the dataset will usually correspond to the same set of physical observations made at different places in space or time. Thus, a dataset might consist of numerous stream profiles, or different regions extracted from a ~~LiDaR image~~ LiDAR-derived digital elevation model (DEM). It is possible to combine multiple, diverse physical observations into a single data vector: for example, it might be desirable to measure both the cross-section and variations in flow rate across streams, and regard both as part of the same data vector. It is important to ensure that all data vectors constituting a given dataset are obtained and processed in a similar manner, so that any difference between examples can be attributed solely to physical factors. In practice, pre-processing and ‘standardising’ data to enhance features that are likely to prove ‘useful’ for the desired task can also significantly impact performance: we return to this in Section 4.1.

2 ~~Geomorphological problems and applications~~ Some general classes of geomorphological problem

Broadly speaking, we see three classes of problem where learning algorithms can be particularly useful in geomorphology: classification and cataloguing; cluster analysis and dimension reduction; and regression and interpolation. All represent tasks that can be difficult to implement effectively via conventional means, and which are fundamentally data-driven. However, there can be considerable overlap between

all three, and many applications will not fit neatly into one category.

2.1 Classification and cataloguing

Classification problems are commonplace in observational science, and provide the canonical application for supervised learning algorithms. In the simplest case, we have a large collection of observations of the same type—perhaps cross-sections across valleys—and we wish to assign each to one of a small number of categories (for example, as being of glacial or riverine form). In general, this kind of task is straightforward to an experienced human eye. However, it may be difficult to codify the precise factors that the human takes into account, preventing their implementation as computer code: simple rules break down in the face of the complexities inherent to real data from the natural world. With a learning algorithm approach, the user typically classifies a representative set of examples by hand, so that each data vector is associated with a ‘flag’ denoting the desired classification. The learning algorithm then assimilates information about the connection between observations and classification, seeking to replicate the user’s choices as closely as possible. Once this training procedure has been completed, the system can be used operationally to classify new examples, in principle without the need for further human involvement.

Beyond an obvious role as a labour-saving device, automated systems may enable users to explore how particular factors affect classification. It is straightforward to alter aspects of data processing, or the labelling of training examples, and then re-run the classification across a large dataset. Another advantage lies in the repeatable nature of the classification: observations for a new area, or obtained at a later date, can be processed in exactly the same manner as the original dataset, even if personnel differ. It is also possible to use multiple datasets simultaneously when performing the classification—for example, identification of certain topographic features may be aided by utilising high-resolution local imagery, plus lower-resolution data showing the surrounding region, or land use classification may benefit from using topography together with satellite imagery.

It is sometimes claimed that it is possible to somehow ‘interrogate’ the learning algorithm, to discover its internal state and understand which aspects of the data are used to make a particular classification. This information could offer new insights into the physical processes underpinning a given problem. For the simplest classifiers, this may be possible, but in general we believe it ought to be approached with some scepticism. Classification systems are complex, and subtle interactions between their constituent parts can prove important. Thus, simplistic analysis may prove misleading. A more robust approach, where feasible, would involve classifying synthetic (artificial) data, and exploring how parameters controlling the generation of this affect results. It may also be

instructive to explore how performance varies when different subsets of observables are used.

Conventionally, classification problems assume that all examples presented to the system can be assigned to one category or another. A closely-related problem, which we choose to call ‘cataloguing’, involves searching a large dataset for examples of a particular feature—for example, locating moraines or faults in regional-scale topographic data. This introduces additional challenges: each occurrence of the feature should be detected only once, and areas of the dataset that do not contain the desired feature may nevertheless vary considerably in their characteristics. As a result, cataloguing problems may require an approach that differs from other classification schemes.

Examples of classification problems in geomorphology where machine learning techniques have been applied include classifying elements of urban environments (Miliaresis and Kokkas, 2007), river channel morphologies (Beechie and Imaki, 2014), and landslide susceptibility levels (e.g. Brenning, 2005). An example of a cataloguing problem is given in Valentine et al. (2013), aimed at identifying seamounts in a range of tectonic settings.

2.2 Cluster analysis and dimension reduction

Classification problems arise when the user has prior knowledge of the features they wish to identify within a given dataset. However, in many cases we may not fully understand how a given process manifests itself in observable phenomena. Cluster analysis and dimension reduction techniques provide tools for ‘discovering’ structure within datasets, by identifying features that frequently occur, and by finding ways to partition a dataset into two or more parts, each with a particular character. An accessible overview of the conceptual basis for cluster analysis, as well as a survey of available approaches, can be found in Jain (2010).

In many applications, data vectors are overparameterised: the representations used for observable phenomena have more degrees of freedom than the underlying physical system. For example, local topography might be represented as ~~100m × 100m a grid of terrain heights, sampled at 10m intervals. Each data vector would therefore contain~~ If samples are taken every ten metres, then eleven samples span a distance of 100m, and a 100m × 100m area is represented by 121 elements (and, mathematically, can be regarded as a distinct measurements. A single 121-dimensional object), while data vector is obtained by ‘unwrapping’ the grid according to some well-defined scheme—perhaps by traversing lines of latitude. Nevertheless, the underlying process of interest might be largely governed by a handful of parameters. This implies that there is a high level of redundancy within ~~each the~~ data vector, and ~~they can it could~~ therefore be transformed to a lower-dimensional state without significant loss of information. This may be beneficial, either in its own right or as an

adjunct to other operations: low dimensional systems tend to be easier to handle computationally, and similarities or differences between examples may be clearer after transformation. Dimension reduction algorithms aim to find the optimal low-dimension representation of a given dataset.

One particularly important application of dimension reduction lies in visualisation. Where individual data vectors are high-dimensional, it may be difficult to ~~see how devise effective means of plotting them in (typically) two dimensions. This makes it difficult to appreciate the structure of a dataset, and how different examples relate to each other. It is therefore common to attempt to map all examples into one another. In order to tackle this problem, learning algorithms may be used to identify a two-dimensional space, enabling each to be plotted as a point on a graph. The representation of the dataset that somehow preserves the higher-dimensional relationships between examples. This process involves identifying correlations and similarities between individual data vectors, and generally does not explicitly incorporate knowledge of the underlying physical processes. Thus, the coordinates of each point will generally have little physical meaning~~ example within the low-dimensional space may not have any particular physical significance, but examples that share common characteristics will yield closely-spaced points. Thus, it may be possible to identify visual patterns, and hence discover relationships within the high-dimensional data.

Geomorphological applications of cluster analysis include identifying flow directions from glacial landscapes (Smith et al., 2016), identifying different types of vegetation (Belluco et al., 2006) ~~and, or~~ extracting common structural orientations from a laser scan of a landslide scarp (Dunning et al., 2009). An example of dimension reduction comes again from landslide susceptibility studies, this time aimed at identifying the most influential observables within a suite of possibilities (Baeza and Corominas, 2001).

2.3 Regression and interpolation

The third class of problem involves learning relationships between physical parameters, in order to make predictions or to infer properties. Very often, it is known that one set of observable phenomena are closely-related to a different set—but the details of that relationship may be unknown, or it may be too complex to model directly. However, if it is possible to obtain sufficient observations where both sets of phenomena have been measured, a learning algorithm can be used to represent the link, and predict one given the other—for example, an algorithm might take measurements of soil properties and local topography, and output information about expected surface run-off rates. Alternatively, the same training data could be used to construct a system that infers the soil parameters given topography and run-off measurements. This may be useful when there are fewer measurements available for one of the physical parameters, perhaps because it is harder or

more expensive to measure: once trained on examples where this parameter has been measured, the algorithm can be used to estimate its value in other locations based on the more widely available parameters.

Questions of this sort may be framed deterministically—so that the system provides a single prediction—or statistically, where the solution is presented as a probability distribution describing the range of possible outcomes. The choice of approach will depend upon the nature of the underlying problem, and upon the desired use of the results. In general, probabilistic approaches are desirable, since they provide a more realistic characterisation of the system under consideration—deterministic approaches can be misleading when more than one solution is compatible with available data, or where uncertainties are large. However, in some cases it may be difficult to interpret and use information presented as a probability distribution. For completeness, we observe that most learning algorithms have their roots in statistical theory, and even when used ‘deterministically’, the result is formally defined within a statistical framework.

In geomorphology, a common application of machine learning for regression and interpolation is to link widely available remote sensing measurements with underlying parameters of interest that cannot be measured directly: for example, sediment and chlorophyll content of water from colour measurements (Krasnopolsky and Schiller, 2003) or marine sediment properties from bathymetry and proximity to the coast (Li et al., 2011; Martin et al., 2015).

3 Some popular techniques

The aforementioned problems can be tackled in almost any number of ways: there is rarely a single ‘correct’ approach to applying learning algorithms to any given question. As will become clear, once a general technique has been selected, there remains a considerable array of choices to be made regarding its precise implementation. Usually, there is no clear reason to make one decision instead of another—often, literature describes some ‘rule of thumb’, but its underlying rationale may not always be obvious. A certain amount of trial-and-error is generally required to ~~optimise performance~~ obtain optimal results with a learning algorithm. This should perhaps be borne in mind when comparisons are drawn between different approaches: although many studies can be found in the literature that conclude that one method outperforms another for a given problem, it is unlikely that this has been demonstrated to hold for all possible implementations of the two methods. It is also worth noting that the relationship between performance and computational demands may differ between algorithms: a method that gave inadequate performance on a desktop computer a decade ago may nevertheless excel given the vastly-increased resources of a modern, high-performance machine.

Method	Generally used for:				Learning mode		Deterministic
	Classification	Clustering	Dimension reduction	Regression	Supervised	Unsupervised	
Decision trees	✓				✓		
K-Means		✓				✓	
PCA			✓			✓	✓
Neural networks	✓		✓	✓	✓	✓	
SVMs	✓		✓			✓	
SOMs		✓	✓			✓	
Bayesian inference	✓	✓		✓	✓	✓	(✓)

Table 1. Summary of methods discussed in this paper. For each of the ‘popular techniques’ discussed in Section 3, we indicate the classes of problem for which they are generally used (as described in Section 2); whether the method generally operates as ‘supervised’ learning (based on optimising a pre-determined performance measure), or unsupervised (attempting to reach a stable state); and whether the method is typically ‘deterministic’, so that it is guaranteed to yield identical results each time it is applied to a given dataset. Note that Bayesian inference is itself deterministic, but it is most often encountered in contexts where it is applied to randomly-chosen observations. The indications given here are not intended to be exhaustive: it may be possible to adapt each technique to suit the full range of applications.

In what follows, we outline a selection of common methods, with an emphasis on conveying general principles rather than providing precise formal definitions. There is no particular rationale underpinning the methods we choose to include here, beyond a desire to cover a spectrum of important approaches. Other authors would undoubtedly make a different selection (for example, see Wu et al. (2008), although this has a narrower scope than the present work). In an effort to promote readability, we order our discussion roughly according to complexity, although this is not an objective assessment. [A brief summary of the methods discussed can be found in Table 1.](#)

3.1 Decision trees and Random Forests

A decision tree is a system that takes a data vector, and processes it via a sequence of `if-then-else` constructs (‘branch points’) until an output state can be determined (see Fig. 1). This is clearly well-suited to addressing simple classification problems, and to predicting the states of certain physical systems: essentially, the system resembles a flowchart. In this context, ‘learning’ involves choosing how the dataset should be partitioned at each branch.

Typically, each data vector contains a number of ‘elements’—distinct observations, perhaps made at different points in space or time, or of different quantities relevant to the phenomenon of interest. Each vector is also associated with a particular ‘desired outcome’—the classification or state that the tree should output when given that example. Basic decision tree generation algorithms aim to identify a test that can be applied to any one element, which separates desired outcomes as cleanly as possible (e.g. [Fig. 1a,b](#)). This is typically quantified using a measure such as ‘information entropy’, which assesses the degree to which a system behaves predictably. Once the training data has been partitioned into two sets, the algorithm can be applied recursively on

each, until a complete tree has been constructed. Commonly-encountered tree generation schemes include ID3 (Quinlan, 1986) and its successor C4.5 (Quinlan, 1993).

Tree generation assumes that the data ~~is~~ are perfect, and will therefore continue adding branch points until all training data can be classified as desired. When real-world datasets—which invariably contain errors and ‘noise’—are used, this tends to result in overly complex trees, with many branches. This phenomenon is known as ‘overfitting’, and tends to result in a tree with poor generalisation performance: when used to process previously unseen examples, the system does not give the desired outcome as often as one might hope. It is therefore usual to adopt some sort of ‘pruning’ strategy, by which certain branches are merged or removed. Essentially, this entails prioritising simple trees over perfect performance for training data; a variety of techniques exist, and the choice will probably be application-specific.

Another approach to this issue, and to the fact that in many problems the number of data elements vastly exceeds the number of possible outcomes, lies in the use of ‘random forests’ (Breiman, 2001). By selecting data vectors from the training set at random (with replacement), and discarding some randomly-chosen elements from these, we can construct a number of new datasets. It is then straightforward to build a decision tree for each of these. Typically, this results in trees that perform well for some—but not all—examples. However, if we use each tree to predict an outcome for a given data vector, and then somehow compute the average of these predictions, performance is usually significantly better than can be achieved with any one tree. This strategy, where a number of similar, randomised systems are constructed and then used simultaneously, is sometimes referred to as an ‘ensemble’ method. Again, when treated in more detail, a variety of approaches are possible, and the intended application may help dictate which should be used.

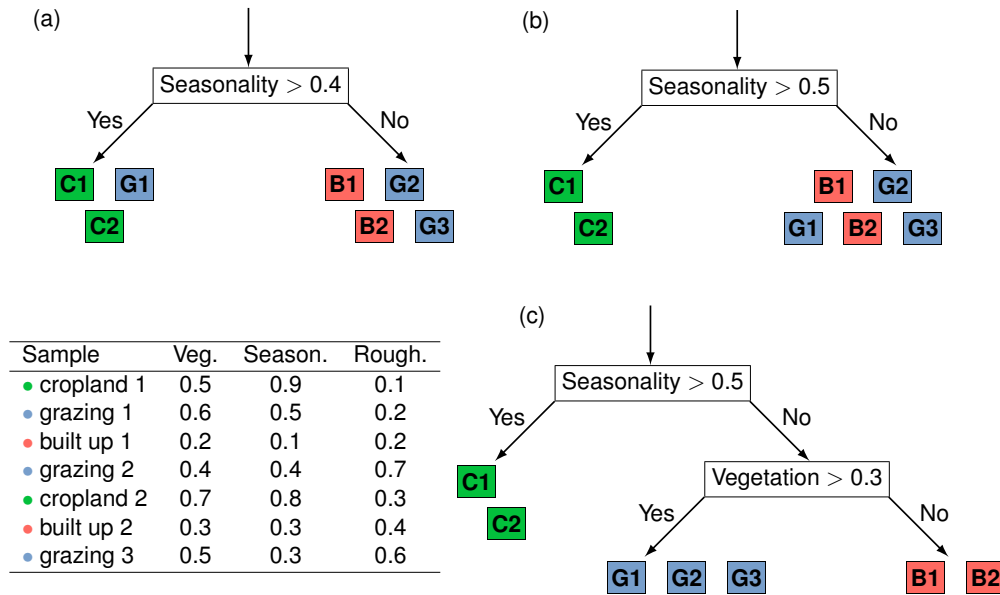


Figure 1. Evolution of a decision tree for land use data based on normalised parameters for vegetation index, seasonal colour variability, and topographic roughness. (a) The algorithm tests a variety of conditions for the first branch point, looking for a condition such as (b) that cleanly separates different classes. (c) A second branch point is added to differentiate between built up and grazing land.

A recent example of an application of random forests to Earth surface data can be found in Martin et al. (2015). Here, the goal is to predict the porosity of sediments lying on the ocean floor from [data—a range of different data, including measures](#) such as water depth [and-or](#) distance from sediment-producing features. Such observations are much easier to obtain than direct measurement of the seafloor, which obviously requires ocean-bottom sampling. Using training data from locations where such samples have been collected, a random forest is constructed that enables porosity predictions to be made throughout the oceans. This concept could readily be adapted to a variety of other situations where local physical properties must be estimated from remotely-sensed data. Further discussion of the use of random forests for interpolation between samples can be found in, for example, Li et al. (2011), [who test a variety of techniques including random forests and support vector machines in order to produce a regional map of mud content in sediments based on discrete sampling.](#) Another example comes from Bhattacharya et al. (2007), [who construct models of sediment transport using a variant of decision trees where each ‘leaf’ is a linear regression function, rather than a single classification; the decision tree is essentially used to choose which mathematical model to apply in each particular combination of circumstances.](#)

3.2 The K-Means Algorithm

By far the most well-known technique for cluster analysis, K-means is usually said to have its origins in work eventually

published as Lloyd (1982), but disseminated earlier (thus, for example, Hartigan and Wong (1979) sets out a specific implementation). The algorithm is designed to divide a set of N data vectors, each consisting of M elements, into K clusters. These clusters are defined so that the distance of each point in the cluster from its centre is as small as possible.

The algorithm is readily understood, and is illustrated in Fig. 2. We begin by generating K points, which represent our initial guesses for the location of the centre of each cluster—these may be chosen completely at random, or based on various heuristics which attempt to identify a ‘sensible’ initial configuration. We then assign each element of our training data to the cluster with the nearest centre (Fig. 2b). Once this has been done, we recompute the position of the central point, by averaging the locations of all points in the cluster (Fig. 2c). This process of assignment and averaging is repeated (Fig. 2d) until a stable configuration is obtained (Fig. 2e). The resulting clusters may then be inspected to ascertain their similarities and differences, and new data can be classified by computing its distance from each cluster centre.

In order to implement this, it is necessary to define what the word ‘distance’ means in the context of comparing any two data vectors. There are a number of possible definitions, but it is most common to use the ‘Euclidean’ distance: the sum of the squared difference between each element of the two vectors. Thus, if \mathbf{x} is a vector with M elements (x_1, x_2, \dots, x_M) and \mathbf{y} a second vector (y_1, y_2, \dots, y_M) , then the Euclidean distance between them is defined

$$d = \sum_{i=1}^M (x_i - y_i)^2. \quad (1)$$

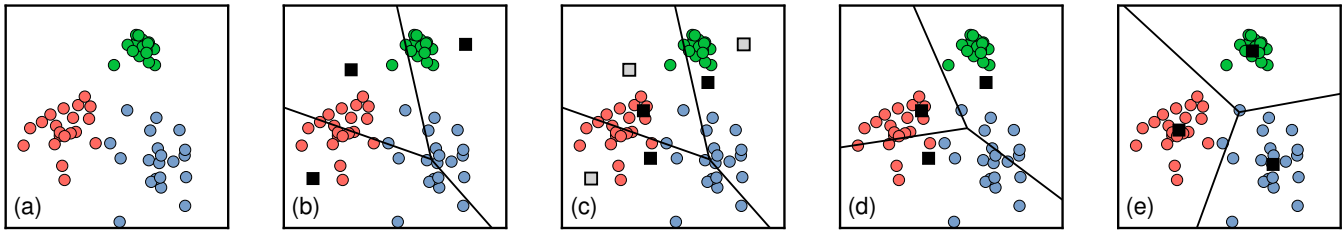


Figure 2. The K-Means algorithm. (a) A dataset contains points clustered around three distinct locations (colour-coded for ease of reference). (b) We first guess locations for these centres at random (black squares) and assign each datum to the nearest cluster (shown divided by black lines). (c) We then re-compute the location of each cluster centre by averaging all points within the cluster (old centres, grey squares; new centres, **black squares**), and (d) update the cluster assignment of each point to reflect this. It may be necessary to repeat steps (c) and (d) for several iterations until a stable partitioning of the dataset is found (e).

This definition is a natural extension of our everyday understanding of the concept of ‘distance’. However, where data vectors are comprised of more than one class of observation—perhaps combining topographic heights with soil properties—problems can arise if the measurements differ considerably in typical scale. The Euclidean distance between two two-element data vectors $(1, 10^{-9})$ and $(1, 10^{-5})$ is very small, despite the second elements differing by four orders of magnitude, because both are negligible in comparison to the first element. It may be necessary to rescale the various measurements that make up a data vector, to ensure that they have a similar magnitude and dynamic range. Alternatively, and equivalently, the definition of ‘distance’ can be adapted to assign different weights to various data types.

In its basic form, the K-means algorithm requires the user to specify the number of clusters to be sought as *a priori* information. In many cases, this may not be known, and a range of different solutions have been proposed—see, for example, Jain (2010). Fundamentally, these entail balancing increased complexity (i.e., an increased number of clusters) against any resulting reduction in the average distance between samples and the cluster centre. In general, this reduction becomes insignificant once we pass a certain number of clusters, and this is taken to provide an appropriate description of the data.

Clustering algorithms such as K-means have seen use in geomorphology as an aid to analysis or interpretation of a variety of datasets. It is common to first apply some transformation or pre-processing to raw data, to improve sensitivity to particular classes of feature. For example, Miliareis and Kokkas (2007) take **LIDAR-LiDAR** DEMs, apply various filters designed to enhance the visibility of the built environment within the image, and then use K-means to distinguish different areas of urban environment (such as differentiating between vegetation, buildings, and roads/pavements). Similarly, Belluco et al. (2006) use the technique to assist in mapping vegetation based on remotely-sensed spectral imaging, although they find that which method performs best depends on the type of imaging and field data. On a much smaller scale, Dunning et al. (2009) use K-means and other clustering algorithms to extract discontinuity orientations from

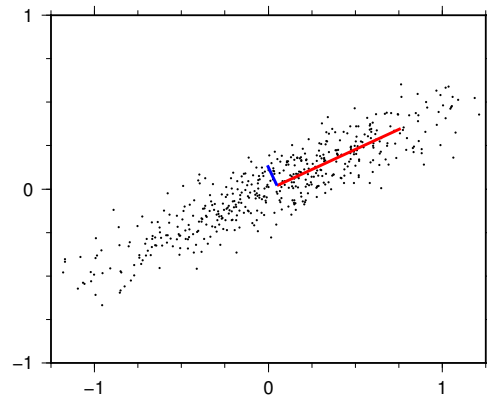


Figure 3. Principal component analysis of a simple dataset. Dominant principal component shown in red; secondary principal component shown in blue. Line lengths are proportional to the weight attached to each component. It is apparent that the principal components align with the directions in which the dataset shows most variance.

laser-derived observations of landslide scarps, which help constrain the mechanism behind the slope failure.

3.3 Principal component analysis

Often, the different observations comprising a given data vector are correlated, and thus not fully independent: for example, topographic heights at adjacent sites are likely to be reasonably similar to one another, and an imprint of topography will often be found in other datasets such as soil thickness or temperature. For analysis purposes, it is often desirable to identify the patterns common to multiple data elements, and to transform observations into a form where each parameter, or component, is uncorrelated from the others. Principal component analysis (PCA) provides one of the most common techniques for doing so, and has its roots in the work of Pearson (1901). Essentially the same mathematical operation arises in a variety of other contexts, and has acquired a different name in each: for example, ‘singular value decomposition’, ‘eigenvector analysis’, and the

concept of ‘empirical orthogonal functions’ are all closely-related to PCA.

Numerical algorithms for performing PCA are complex, and there is usually little need for the end-user to understand their intricacies. In general terms, PCA involves finding the ‘direction’ in which the elements of a dataset exhibit the greatest variation, and then repeating this with the constraint that each successive direction considered must be at right angles (orthogonal) to those already found. Although easiest to visualise in two or three dimensions (see [Fig. 3](#)), the principle works in the same way for data vectors with more elements: for a set of data vectors with M elements, it is possible to construct up to M perpendicular directions.

Thus, the outcome of PCA is an set of orthogonal directions (referred to as principal components) ordered by their importance in explaining a given dataset: in a certain sense, this can be regarded as a new set of co-ordinate axes against which data examples may be measured. [The principal components may be regarded as a set of weighted averages of different combinations of the original parameters, chosen to best describe the data.](#) Often, much of the structure of a dataset can be expressed using only the first few principal components, and PCA can therefore be used as a form of dimensionality-reduction (see [Fig. 4](#)). In a similar vein, it can form a useful precursor to other forms of analysis, such as clustering, by virtue of its role in unpicking the various signals contributing to a dataset: often, each component will exhibit sensitivity to particular physical parameters. [However, particularly where the original data is composed of a variety of different physical data types, the results of PCA may not be straightforward to interpret: each principal component may be influenced by a number of disparate measurements.](#)

One example of this can be found in Cuadrado and Perillo (1997), where PCA is performed on a dataset consisting of bathymetric measurements for a given region repeated over several months. The first principal component is then found to describe the mean bathymetry of the period, while the second provides information about the general trend of change in bathymetry over time, highlighting areas of deposition and erosion. Another typical application occurs in Baeza and Corominas (2001), where PCA is used to identify the observable parameters that best serve as predictors of landslide hazard. [A more recent example is Tamene et al. \(2006\), who use PCA to identify which observable parameters best explain variability in sediment yield between different river catchments in Ethiopia. This example also shows how a single principal component may be a combination of observables: their first component, which explains about 50% of the variability, is dominated by a combination of topographic variables, such as height difference, elongation ratio, and catchment area. The second component, which explains approximately 20% of the variability, is dominated by variables associated with lithology and land use/vegetation cover.](#)

3.4 Neural Networks

Perhaps the most varied and versatile class of algorithm discussed in this paper is the neural network. As their name suggests, these were originally developed as a model for the workings of the brain, and they can be applied to tackling a wide range of problems. It has been shown (e.g. Hornik, 1991) that neural networks can, in principle, be used to represent arbitrarily complex mathematical functions, and their use is widespread in modern technology—with applications including tasks such as voice recognition or automatic language translation. They may be used to tackle problems falling in all three of the classes discussed in Section 2. A comprehensive introduction to neural networks may be found in Bishop (1995); the aforementioned book by Mackay (2003) also discusses them at some length. Some readers may also be interested in a review by Mas and Flores (2008), targeted at the remote sensing community.

A neural network is constructed from a large number of interconnected ‘neurons’. Each neuron is a processing unit that takes a number of numerical inputs, computes a weighted sum of these, and then uses this result to compute an output value. The behaviour of the neuron can therefore be controlled by altering the weights used in this computation. By connecting together many neurons, with the outputs from some being used as inputs to others, a complex system—or network—can be created, as in [Fig. 5](#). The weights associated with each neuron are unique, so that the behaviour of the network as a whole is controlled by a large number of adjustable parameters. Typically, these are initially randomised; then, a ‘training’ procedure is used to iteratively update the weights until the network exhibits the desired behaviour for a given training set.

Such a brief description glosses over the richness of approaches within ‘neural networks’: choices must be made regarding how individual neurons behave, how they are connected together (the ‘network architecture’), and how the training algorithm operates. These are generally somewhat application-dependent, and may dictate how effectively the network performs. The simplest form of neural network, sometimes called a ‘multi-layer perceptron’ (MLP), consists of neurons arranged in two or three ‘layers’, with the outputs from neurons in one layer being used as the inputs for the next layer (see [Fig. 5](#)). Traditionally, these are trained by ‘back-propagation’ (Rumelhart et al., 1986), which involves calculating how network outputs are influenced by each individual weight. The canonical use for such a network is as a classifier (e.g. Lippmann, 1989; Bischof et al., 1992), although they are exceptionally versatile: for example, Ermini et al. (2005) demonstrate that MLPs can be used for landslide susceptibility prediction. They may also be used to model a wide variety of physical relationships between observables, for example, in interpolation problems such as estimating ~~difficult to measure~~ surface properties from satellite observations (e.g. Krasnopolsky and Schiller,

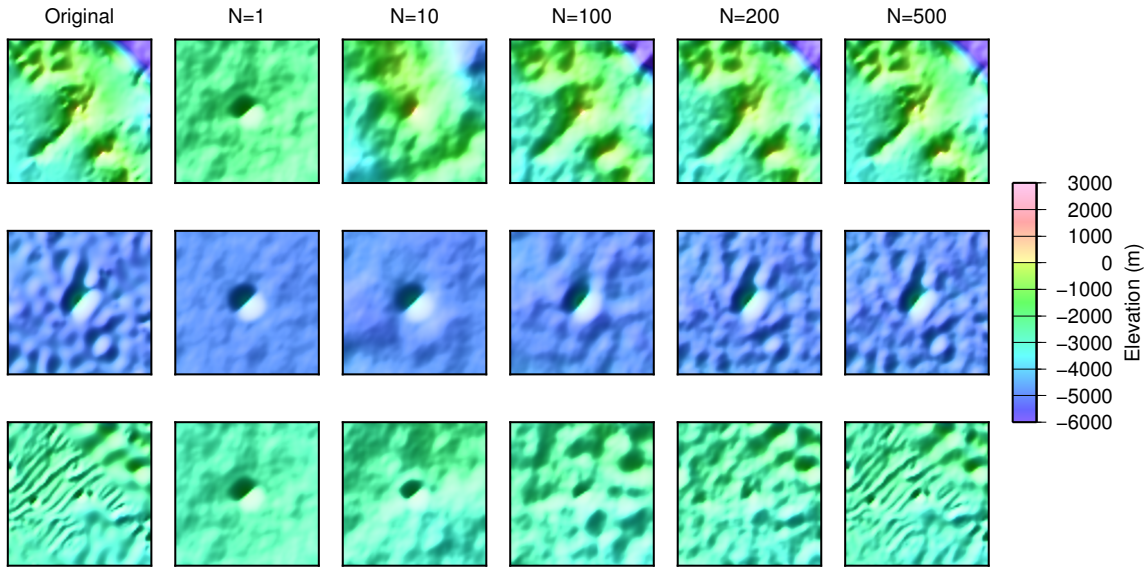


Figure 4. Image reconstruction using principal components. PCA has been performed on a dataset containing 1000 square ‘patches’ of bathymetric data, each representing an area of dimension 150×150 km, and centred upon a seamount (the ‘training set’ used in Valentine et al., 2013). Each patch is comprised of 64×64 samples—thus, each can be seen as a 4096-dimensional object. Three examples from this set are shown here (one per row). In the left-most column we show the original bathymetry for each; then, we present reconstructions of this bathymetry using only the N most significant principal components, for $N = 1, 10, 100, 200$ & 500 . It is apparent that **much of the information—large-scale structures** within this dataset can be represented using only 100–200 dimensions, **rather than 4096**; while around 500 dimensions are required to allow some of the fine-scale structure to be represented, particularly in the third example. This still represents almost an order of magnitude reduction, in comparison to the original, 4096-dimensional, data.

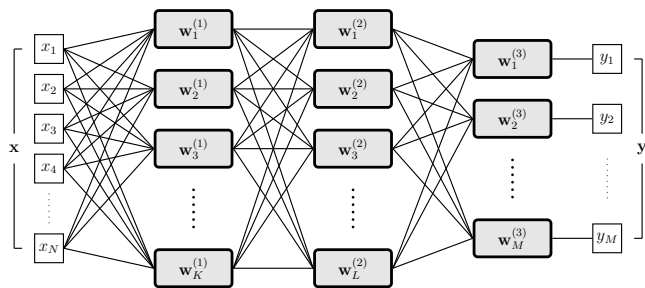


Figure 5. Schematic of a simple neural network (a ‘multi-layer perceptron’). The network takes an N -dimensional vector, \mathbf{x} , on the left side and transforms it into an M -dimensional vector \mathbf{y} on the right side. Each grey box represents a ‘neuron’, and is a simple mathematical operation which takes many inputs (lines coming in from the left), and returns a single output value which is sent to every neuron in the next ‘layer’ (lines coming out from the right). The neuron’s behaviour is governed by a unique set of ‘weights’ (\mathbf{w}): one common mathematical relation has a neuron in a layer with K inputs return $y = \tanh(w_0 + \sum_{i=1}^K w_i x_i)$, where the single output element y will become part of the inputs for the next layer.

2003), and to detect unusual or unexpected features within datasets (e.g. Markou and Singh, 2003).

In recent years, attention has increasingly focussed on ‘deep learning’, where many more layers of neurons are used. This has proven effective as a means to ‘discover’ structure in large, complex datasets, and represent these in a low-dimensional form (Hinton and Salakhutdinov, 2006). Typically, these require specialised training algorithms, since the number of free parameters in the network is exceptionally large. Such systems are particularly useful for applications in cluster analysis and dimension reduction, and these properties can be exploited to enable cataloguing of geomorphological features in large datasets, as in Valentine et al. (2013).

3.5 Support Vector Machines

The modern concept of the Support Vector Machine (SVM) stems from the work of Cortes and Vapnik (1995), although this builds on earlier ideas. The approach is targeted towards classification problems, framed in terms of finding, and then utilising, ‘decision boundaries’ that separate one class from another. In the simplest case, linear decision boundaries can be found—that is, any two classes can always be separated by a straight line when two-dimensional slices through the dataset are plotted on a graph. The SVM method provides an algorithm for constructing linear decision boundaries that

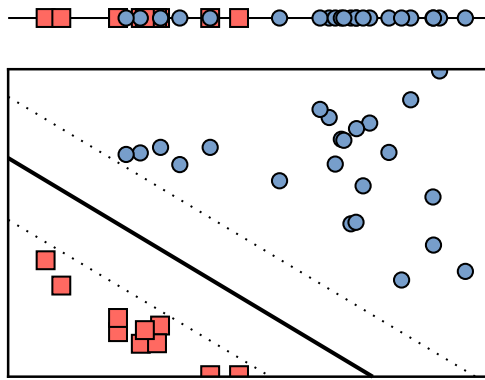


Figure 6. Segmenting datasets with linear decision boundaries. In [the original](#) one dimension ([bottom](#)[top](#)), it is not possible to separate red squares from blue circles. However, by mapping this dataset into [two dimensions](#)[an artificial second dimension](#), it becomes possible to draw a linear ‘decision boundary’ that distinguishes the two classes. The support vector machine provides a technique for achieving this in such a way that the ‘margin’ between the boundary and the nearest data points is maximised (as shown by the dotted lines).

maximise the ‘margin’ between boundary and adjacent data points, as shown in Fig. 6.

However, in most realistic cases, the dataset cannot be cleanly categorised using linear boundaries: all possible linear decision boundaries will misclassify some data points. To handle this scenario, the SVM approach uses a mathematical trick to create nonlinear decision boundaries in a way that is computationally tractable. Data is first mapped into a higher-dimensional ‘feature space’ (the opposite of dimensionality reduction); in this space, the data can then be separated using linear boundaries (see Fig. 6). This mapping, or transformation, may be nonlinear, so that lines in the feature space may correspond to curves in the original data space. Various extensions to this approach exist that allow for a less-than-perfect division of the dataset, to reflect the presence of classification errors or observational noise. Once boundaries have been determined, the SVM may then be used for classification of new examples. SVMs have some similarities in structure to simple neural networks, although the ‘training’ or optimisation procedure is quite distinct.

Again, landslide susceptibility assessment offers one aspect of geomorphology where SVMs have found significant application (e.g. Brenning, 2005; Yao et al., 2008; Marjanović et al., 2011; Peng et al., 2014). They have also been used to differentiate between fluvial and glacial river valleys (Matías et al., 2009). Another similar use can be found in Beechie and Imaki (2014): there, the authors use an SVM to classify river channel morphologies based on geospatial data including DEMs, precipitation, and geology. This can then be used in river conservation and restoration to infer the natural patterns that existed in areas that have been subject to extensive human intervention.

3.6 Self-Organising Maps

The concept of the Self-Organising Map (SOM) stems from the work of Kohonen (1990), and it can be viewed as a particular class of neural network. The SOM implements a form of dimensionality reduction, and is generally used to help identify clusters and categories within a dataset. The basic premise is to take a (usually) two dimensional grid and, through training, create a mapping between that 2D space and a higher-dimensional dataset (see Fig. 7). The 2D representation can then be used to help visualise the structure of the data. The SOM is also typically designed to be significantly smaller than the training set, spanning the same data space with fewer points, and is thus easier to analyse.

To create an SOM, we start with a map consisting of a number of ‘nodes’, often arranged as a regular grid, so that it is possible to define a ‘distance’ between any two nodes, and hence identify the set of nodes that lie within a certain radius of a given node, known as its ‘neighbourhood’. Each node is associated with a random ‘codebook vector’ with the same dimensionality as the data (Fig. 7a). During training, we iteratively select a data example at random from the training set, identify the node with the closest-matching codebook vector, and then adjust this vector, and those of neighbouring nodes, to better match the training example (Fig. 7b). Given sufficient training, the codebook vectors come to mirror the distribution of data in the training set (Fig. 7c). Typically, the extent to which codebook vectors are updated and the radius used to define the neighbourhood of a given node are reduced as training proceeds, to promote fine-tuning of performance.

Once the SOM is trained, various approaches exist to enable visualisation of the codebook vectors, with the goal of highlighting any underlying structure within the dataset. One common approach is to try to identify clusters in the dataset by examining the distances between the codebook vectors for neighbouring nodes, often by plotting the SOM grid coloured according to these distances (sometimes described as depicting the ‘U-matrix’). Alternatively, a method can be used to distort the grid in such a way that when plotted in 2D, the distance between nodes is proportional to the distance between their codebook vectors; one common technique for this is ‘Sammon’s mapping’ (Sammon, 1969). Another visualisation approach, sometimes called ‘component plane analysis’, looks for correlations between input parameters, e.g. between rainfall and elevation or slope orientation and landslide risk. Here, the SOM grid is coloured according to the values of particular elements of the codebook vectors, with each element corresponding to an input parameter. Correlated parameters can then be identified by their similar colour patterns.

Potential applications in geomorphology are numerous. Marsh and Brown (2009) use an SOM-based method to analyse and classify bathymetry and backscatter data, allowing near-real-time identification of regions with particular seafloor characteristics, e.g. for benthic habitat map-

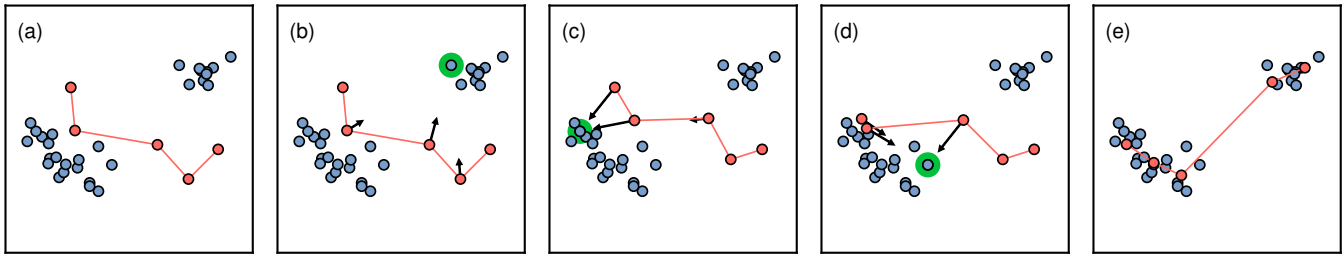


Figure 7. The self-organising map (SOM). A dataset consists of numerous data points (blue), and is to be represented by an a one-dimensional SOM (red). The SOM contains of a number of nodes, organised spatially so that ‘neighbouring’ nodes can be identified with a well-defined spatial relationship (as represented here using a line, depicted by lines connecting points). Initially the, all SOM is randomised nodes are associated with random locations in data space (a). Then a During training procedure (b, c, d) involves selecting a datum is selected at random (highlighted in green), identifying the nearest. The closest SOM node is identified, and moving this and its nearest neighbours towards are adjusted so as to be closer to the chosen point (arrows), with the scale of adjustment proportional to the separation. Eventually After many iterations of this procedure, the distribution of SOM nodes mirrors that of the dataset (e). For ease of illustration, this figure depicts a two-dimensional dataset and a one-dimensional SOM; in practice, the dataset will usually have much higher dimensionality, and the SOM is usually arranged organised as a two-dimensional grid.

ping. Similarly, Ehsani and Quiel (2008) demonstrate that SOMs can be used to classify topographic features, identifying characteristic morphologies contained within DEMs such as channels, ridge crests, and valley floors. One of
 5 In a third example, Friedel (2011) uses SOMs to assess post-fire hazards in recently burned landscapes. Both PCA and K-means clustering are then used to divide the 540 areas studied into 8 distinct groups, which the author suggests could be used for focusing future field research and development of empirical models. As illustrated by these examples, one of the key strengths of the SOM method is that learning is unsupervised, and does not rely on the user having any prior knowledge of the ‘important’ structures contained within the dataset.

3.7 Bayesian inference

To conclude this section, we mention the concept of Bayesian inference. This is a much broader topic than any of the methods discussed so far; indeed, in many cases these methods are themselves formally derived from Bayesian concepts.
 20 Bayes’ theorem (Bayes, 1763) underpins a significant fraction of modern statistical techniques, and explains how new observations can be used to refine our knowledge of a system. It tells us that the probability that the system is in a certain state, given that we have made a particular observation (‘obs.’), $P(\text{state}|\text{obs.})$, can be expressed in the form

$$P(\text{state}|\text{obs.}) = \frac{P(\text{obs.}|\text{state})P(\text{state})}{P(\text{obs.})}. \quad (2)$$

Here, $P(\text{state})$ represents our prior knowledge—that is, our assessment of the probability that the system is in the given state without making any measurements—while $P(\text{obs.})$
 30 represents the probability with which we expect to obtain the exact measurements we did, in the absence of any knowledge about the state of the system. Finally, $P(\text{obs.}|\text{state})$

expresses the probability that we would get those measurements for a system known to be in the relevant state.

In many cases, it is possible to estimate or compute the various probabilities required to implement Bayes’ theorem, and thus it is possible to make probabilistic assessments. This is often useful: for example, hazard assessment is generally better framed in terms of the chance, or risk, of an event, rather than attempting to provide deterministic predictions.
 40 An extensive discussion of Bayesian analysis can be found in Mackay (2003). Sivia (1996) is another useful reference, and a paper by Griffiths (1982) provides some geomorphological context. A wide range of computational techniques have been developed to enable Bayesian calculations in various settings, for which a review by Sambridge and Mosegaard (2002) may be a good starting point. It does not appear that explicitly Bayesian techniques have found widespread adoption in geomorphology to date, although some examples can be found in related fields such as sediment transport modelling (e.g. Schmelter et al., 2011).

As a simple example, suppose we are interested in classifying land use from satellite imagery. Grassland will appear as a green pixel 80% of the time, although it may also be brown: thus, $P(\text{green}|\text{grass}) = 0.8$. On the other hand, desert environments appear as brown in 99% of cases. A particular region is known to be mainly desert, with only 10% grassland—so an image of the area will consist of 8.9% green pixels ($= ((0.01 \times 0.9) + (0.8 \times 0.1))$). If we look at one specific pixel, and observe that it is green, Bayes’ theorem tells us there is a 90% chance that the location is grassland: $P(\text{grass}|\text{green}) = P(\text{green}|\text{grass})P(\text{grass})/P(\text{green}) = 0.8 \times 0.1 / 0.089 \approx 0.899$. On the other hand, if a pixel is seen to be brown, we can classify it as desert with 98% certainty. This illustrates a property that emerges from the Bayesian formalism: unusual observations convey more information than routine ones. Before we obtained any satellite imagery, we could have guessed with 90% accuracy that a particular

location in the region was desert; observing a brown pixel leads to only a relatively modest increase in the certainty of this determination. However, if we were to observe a green pixel, the chance that the location is a desert drops markedly, to only 10%.

Most examples in geomorphology again come from landslide susceptibility: Lee et al. (2002) and Das et al. (2012) use Bayesian techniques to assess landslide susceptibility in Korea and the Himalayas, respectively. In a similar application, Mondini et al. (2013) map and classify landslides in southern Taiwan using a Bayesian framework. Examples from other areas of geomorphology include Gutierrez et al. (2011), who use a Bayesian network to predict shoreline evolution in response to sea-level change, and Schmelter et al. (2011), who use Bayesian techniques for sediment transport modelling.

4 Practical considerations

Each of the techniques discussed in the previous section—and the wide variety of alternatives not mentioned here—have their strengths and weaknesses, and a number of practical issues may need to be considered when implementing a solution to a particular problem. Here, we discuss some topics that may be relevant across a range of different approaches, and which may affect the viability of a learning algorithm solution in any case.

4.1 Constructing a training set

Unsurprisingly, the training data used when implementing a learning algorithm can have a major impact upon results: everything the system ‘knows’ is derived entirely from these examples. Any biases or deficiencies within the training data will therefore manifest themselves in the performance of the trained system. This is not, in itself, necessarily problematic—indeed, the landform cataloguing system introduced by Valentine et al. (2013) relies upon this property—but it must be borne in mind when tools are used and results interpreted. In particular, the If training data is low-quality or contains artefacts, glitches and other observational ‘noise’, results will suffer. In general, time invested in properly selecting and processing datasets will be well-spent. However, it is also important that training data remains representative of the data that will be used during operation.

One particular issue that can arise stems from the fact that the learning algorithm lacks the trained researcher’s sense of context: it has no preconception that certain structures in the data are more or less significant than others. For example, suppose a system is developed to classify valley profiles as being formed by either a river or a glacier. The training data for this system would consist of a sequence of hand-classified valley profiles, each expressed as a vector of topographic measurements. If, for the sake of example, all glacial

examples happen to be drawn from low-elevation regions, and all riverine examples from high-elevation regions, it is likely that the system would learn to treat elevation as an important factor during classification.

A second potential pitfall arises from the statistical basis underpinning most learning algorithms. Typically, the extent to which a particular feature or facet of the dataset will be ‘learnt’ depends on its prevalence within the training examples as a whole. This can make it difficult for a system to recognise and use information that occurs infrequently in the training data, since it gets ‘drowned out’ by more common features. Again, considering the problem of valley classification: if 99% of training examples are glacial, the system is likely to learn to disregard its inputs and simply classify everything as glacial, since this results in a very low error rate; for best results, both types should occur in roughly equal proportions within the training set. As before, this should be regarded as a natural property of the learning process, rather than as being inherently problematic; indeed, it can be exploited as a tool for ‘novelty detection’, allowing unusual features within a dataset to be identified (for a review, see e.g. Marsland, 2002). Nevertheless, it is a factor that ought to be borne in mind when a system is designed and used.

To avoid problems, it is important to choose training data with care, and to develop strategies for evaluating and monitoring the performance of the trained system. It is often beneficial to invest time in finding the best way to represent a given data type, so as to accentuate the features of interest, and remove irrelevant variables. This process is sometimes referred to as ‘feature selection’ (e.g. Guyon and Elisseeff, 2003). Thus, in the situation mentioned above, the valley profiles might be more usefully represented as variations relative to their highest (or lowest) points, rather than as a sequence of absolute elevations. In line with our comments in Section 3.2, it is often helpful to ‘de-mean’ and normalise the data: using the training set, it is straightforward to compute the mean input vector, and the standard deviation associated with each component of this. Then, all examples—during training, and during operation—can be standardised by subtraction of this mean, and rescaling to give unit standard deviation. Clearly, the inverse of these transformations may need to be applied before results are interpreted. For more complex applications, specialist representations such as the ‘geomorphons’ developed by Jasiewicz and Stepinski (2013) may be beneficial, providing and provide a targeted route to encoding geomorphological information. Training examples should be chosen to cover a spread of relevant cases, perhaps including different regions or measurements made at different times of year, to avoid introducing unintended biases into results.

4.2 Assessing performance

For ‘supervised’ learning algorithms, where a pre-defined relationship or structure is to be learnt, it is possible to assess

performance using a second set of user-selected data—often referred to as a ‘test’ or ‘monitoring’ dataset. This test data intended to provide an independent set of examples of the phenomena of interest, allowing quantitative measures of effectiveness to be evaluated; this strategy is sometimes referred to as ‘cross-validation’. It is important to do this using examples separate from the training set, to ensure that the system’s ‘generalisation performance’ is measured: we want to be sure that the algorithm has learned properties that can be applied to new cases, rather than learning features specific to the particular examples used during training. (As an analogy, a dog may learn to respond to particular commands, but only when issued in a very specific manner: it cannot then be said to properly understand a spoken language.)

The metric by which performance is assessed is likely to be situation-dependent. In general, a supervised learning algorithm will be designed to optimise certain ‘error measures’, and these are likely to provide a good starting point. Nevertheless, other statistics may also prove useful. For classification systems, analysis of ‘receiver operating characteristics’ (ROCs) such as hit and false positive rates may be instructive (e.g. Fawcett, 2006). More difficult to quantify, but still potentially valuable, is the experienced researcher’s sense of the plausibility of a system’s predictions: do results exhibit geomorphologically reasonable patterns? For example, does a prediction of landslide risk seem plausible in its relationship with the topography and underlying bedrock?

Assessing performance in unsupervised learning is more challenging, as we may not have prior expectations against which to measure results: fundamentally, it may be challenging to define what ‘good performance’ should signify. In many cases, application-specific statistics may be helpful—for example, in cluster analysis it is possible to calculate the standard deviation of each cluster, quantifying how tightly each is defined—and again, the researcher’s sense of plausibility may provide some insight. It may also prove instructive to repeat training using a different subset of examples, to assess how stable results are with respect to variations in the training data: a structure or grouping that appears consistently is more likely to be real and significant than one that is very dependent on the precise examples included in the training set.

4.3 Overtraining and random noise

The phenomenon of ‘overtraining’ or ‘overfitting’, which typically arises in the context of supervised learning algorithms, has already been alluded to. It occurs when an iterative training procedure is carried out for too many iterations: at some point, the system usually begins to learn information that is specific to the training examples, rather than being general. This tends to reduce the performance of the system when subsequently applied to unseen data. It can often be detected by monitoring the algorithm’s generalisation performance using an independent set of examples as train-

ing proceeds: this enables the training procedure to be terminated once generalisation performance begins to decrease. In certain cases, post-training strategies can be used to reduce the degree of over-fitting: the example of ‘pruning’ decision trees has already been mentioned. It has also been shown that ‘ensemble methods’ may be useful (indeed, ‘random forests’ provide one example of an ensemble method), whereby multiple instances of the same learning algorithm are (over-)trained, from different randomised starting points, and their outputs are then somehow averaged (e.g. Dietterich, 2000). Because each instance becomes sensitive to distinct aspects of the training data, due to their different initialisation conditions, each performs well on a subset of examples, and poorly on the remainder. However, the overall performance of the ensemble (or ‘committee’) as a whole is typically better than that of any individual member.

Another strategy that is adopted is to add random noise to the training data. The rationale here is that training examples typically exhibit an underlying pattern or signal of interest, overprinted by other processes and observational errors. In order to learn the structure of interest, we wish to de-sensitise our training procedure to the effects of this overprinting. If we can define a ‘noise model’ that approximates the statistical features of the unwanted signal, adding random realisations of this to each training example allows us to limit the extent to which the algorithm learns to rely on such features: by making their appearance random, we make them less ‘useful’ to the algorithm. Returning again to the example of valley classification, local variations in erosion and human intervention might be modelled as correlated Gaussian noise on each topographic measurement. During training, each example is used multiple times, with different noise on each occasion; in theory, this results in only the gross features of the valley profile being taken into account for classification purposes. However, it may be challenging to identify and construct appropriate noise models in many realistic cases.

It is worth noting here that a similar strategy may prove useful in other cases where it is desirable to desensitise systems to particular aspects of the data. For example, spatial observations are typically reported on a grid, aligned with geographic coordinates. However, natural phenomena typically do not display any such alignment, and orientation information may be irrelevant in many cases. If 2D spatial information is used in a particular case, it may be desirable to make use of multiple, randomly-rotated copies of each training set example. This allows an effectively-larger training set to be created, and reduces the chance that features are treated differently depending on their alignment.

4.4 Operational considerations

As with any analysis technique, results obtained using learning algorithms can be misleading if not treated carefully. This is especially true where a technique invites treatment as a ‘black box’, and where the mechanism by which it op-

erates is not always easily understood. The great strength of artificial intelligence is that it enables a computer to mimic the experienced researcher—but this is also a potential drawback, tending to distance the researcher from their data. In some sense, this is an inevitable consequence of the ever-increasing quantity of data available to researchers—but there is a risk that it leads to subtleties being missed, or results interpreted wrongly due to misapprehensions surrounding computational processing. To minimise the risk of these issues arising, it is important that researchers develop heuristics and procedures that enable ‘intelligent’ systems to be monitored. For example, users of automated data classification systems should monitor the statistical ~~distribution of the various classification distributions of classification outputs~~, and investigate any deviations from the norm; it is also desirable to spot-check classifications. This is particularly true in settings where there is a risk that new examples lie outside the scope of the training set—perhaps where data ~~is~~ are drawn from new geographic regions, or ~~was~~ were collected at a different time of year.

Learning algorithms have immense potential in enabling exploration of large, complex datasets and in automating complicated tasks that would otherwise have to be done manually. However, developing a learning algorithm system—especially those targeted at classification, regression, or interpolation—can also be time-consuming and resource-intensive. Computational demands may also be significant: although many applications require no more than a standard laptop or desktop computer, some may only be viable with access to large-scale parallel computing resources. By way of an illustration for the more computationally-intensive end of the spectrum: training the learning algorithm used to catalogue seamounts in Valentine et al. (2013) currently requires a few hundred CPU-hours on a 1.9 GHz machine, in addition to considerable computational demands for processing the raw bathymetric data. Thus, learning algorithms do not currently present an economic solution to all problems—although this balance will undoubtedly change as technology and algorithms continue to evolve.

5 Outlook

In this paper, we have attempted to provide a general survey of the field of learning algorithms, and how they might be useful to researchers working in the fields of geomorphometry and Earth surface dynamics. These fields benefit from extensive, large-scale, feature-rich datasets, bringing opportunities and challenges in equal measure. Although currently dominated by a few specific topics in the field, such as landslide hazard assessment, the use of artificial intelligence to help explore, process and interpret geomorphological data is almost certain to be an increasingly significant aspect of research in coming years.

An increased use of learning algorithms in geomorphological communities is likely to require developments in computational infrastructure. There are obvious requirements for access to appropriate hardware and software resources, as well as skill development. In particular, larger problems or more complex algorithms may make use of parallel computing and other high performance computing techniques essential. In addition, in light of the potentially substantial development cost of implementing some of the more complex learning algorithms, it is worth trying to plan for a flexible implementation. Most of these approaches can, in principle, be implemented in a fairly general framework, allowing the same underlying algorithm to be applied to many problems.

The computational implications of both parallelisation and generalisation are beyond the scope of this review, but one area of particular relevance to the geomorphology community concerns data input and output, and hence data format: The ability to reuse an algorithm across multiple data types is a key element of flexibility in a field with such a diversity of measurements. The ability to handle large file sizes and support efficient data access, potentially in parallel, is also an important consideration. As these techniques develop, this places increasing importance on the development and use of robust community standards for data formats. File frameworks, which allow the development of multiple specialist file formats all adhering to a common set of rules, may be particularly valuable in combining consistency from an algorithmic point of view with flexibility to accommodate varied data.

However, learning algorithms are not a panacea. ‘Traditional’ approaches to data analysis will remain important for the foreseeable future, and are well-suited to tackling many problems; we do not advocate their wholesale replacement. In addition, it is important that the use of more advanced computational techniques is not allowed to become a barrier between researchers and data; it is almost certain that the nature and practice of ‘research’ will need to evolve to accommodate increasing use of these technologies. Some interesting perspectives on these issues may be found in—for example—an issue of *Nature* dealing with ‘2020 Computing’ (e.g. Muggleton, 2006; Szalay and Gray, 2006), and in work aimed at developing a ‘robot scientist’ (e.g. King et al., 2009). Nevertheless, artificial intelligence opens up many new possibilities within the fields of geomorphology and Earth surface processes—particularly given the common scenarios of large datasets; complex, interacting processes; and/or natural variability that make many geomorphological situations difficult to classify or model using conventional techniques. Learning algorithms such as those discussed here thus represent a powerful set of tools with the potential to significantly expand our capabilities across many branches of the field.

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