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Spectral Image Analysis for Medical Imaging

Part II Computer Science Tripos

Churchill College, 2016

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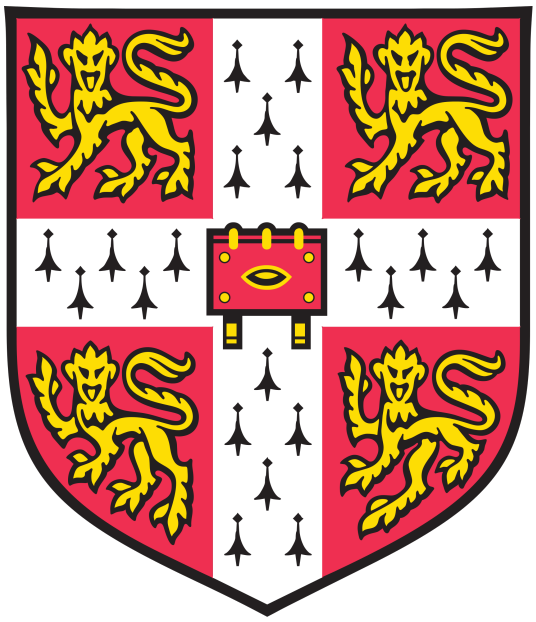

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Declaration

I, Michael Painter of Churchill College, being a candidate for Part II of the Computer Science Tripos, hereby declare that this dissertation and the work described in it are my own work, unaided except as may be specified below, and that the dissertation does not contain material that has already been used to any substantial extent for a comparable purpose.

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Chapter 1

Introduction

In this chapter we introduce the problem: what sort of data are we given and what would we like to do with it? We begin by introducing new terminology, and specifically by defining terms that might otherwise be ambiguous. We briefly discuss the motivation behind the implementation of this system, then suggest some possible methods that could be used to implement a solution. We decide on one solution to explore and identify what we might hope to discover by exploring said solution.

1.1 Terminology and preliminary definitions

It is sensible to start by introducing some terminology and preliminary definitions, as they will be used frequently throughout the dissertation, including even the rest of the introduction chapter.

Firstly let $\mathbb{N}_k$ where $k \in \mathbb{N}$ denote the set $\{n \in \mathbb{N} \mid n < k\} = \{0, 1, ..., (k-1)\}$. And let $\mathbb{B}$ denote the set $\{0, 1\} = \mathbb{N}_2$, which will be used for boolean choices.

Typically, the word *spectral* refers to use of the Fourier domain; for example *spectral methods* refers to the use of Fourier domain to solve differential equations. For our purposes the *spectrum* of some signal is the Fourier transform of the time-domain signal and more specifically, referring to a quantised spectrum. The word *spectrum* refers to either a continuous or quantised spectrum, for which the context should make it obvious which one is intended.

The term *spectral bin* will be used to refer to an interval of wavelengths. Typically, this will be with respect to the case where we are dealing with quantised spectra, where the term spectral bin refers to the range of wavelengths some bar in the histogram represents. For example, consider (c) in Figure 1.1.

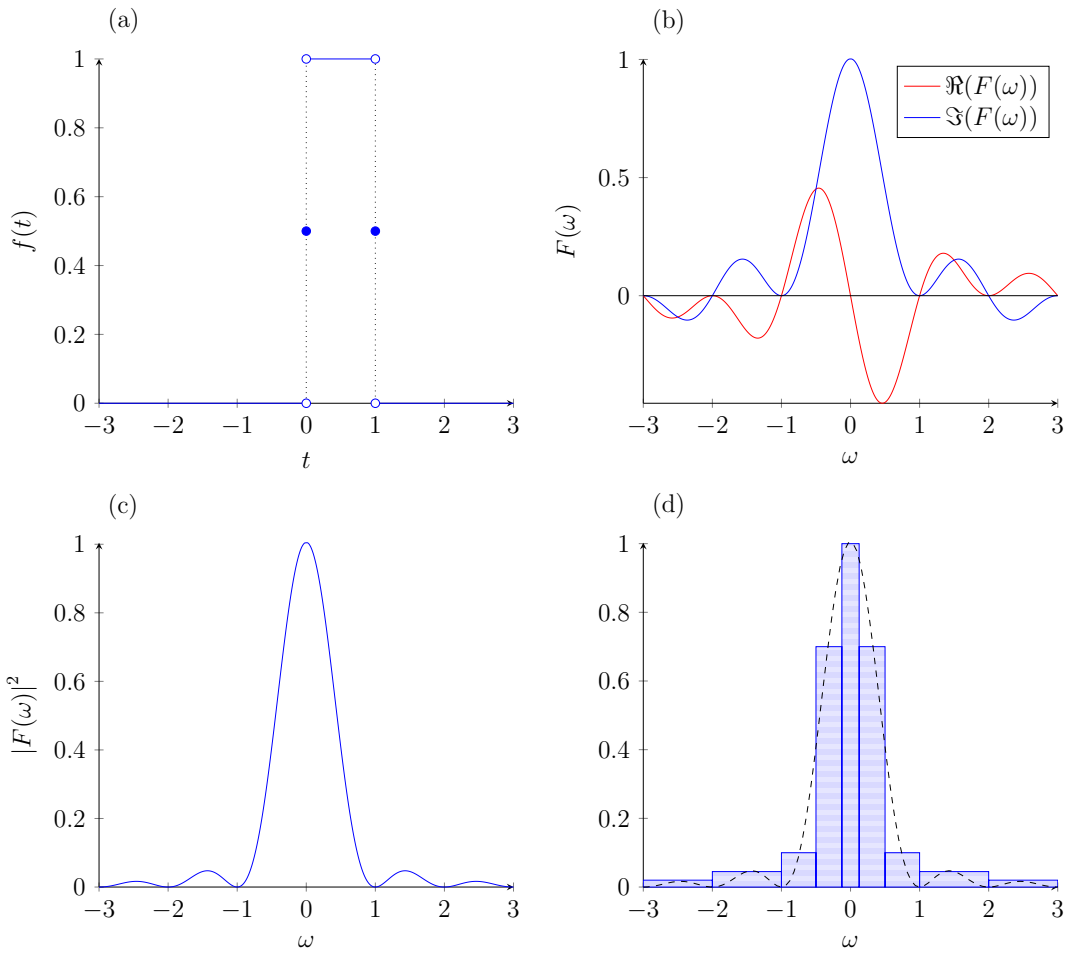


Figure 1.1: Examples of (a) a time-domain signal $f(t)$, (b) it's Fourier transform $F(\omega)$, (c) it's power spectrum $|F(\omega)|^2$ and (d) a quantisation of c.

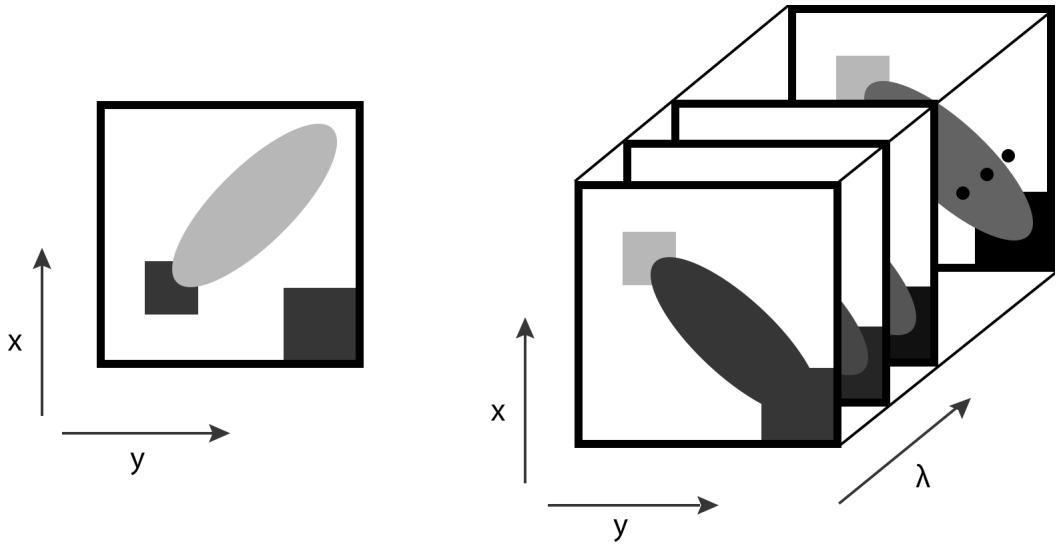


Figure 1.2: Examples of a monochrome image (left) and a spectral image (right).

Spectral image to refer to an image with an arbitrary number of frequency components. More formally we define an *image* as a function $I : \mathbb{N}_w \times \mathbb{N}_h \to \mathbb{N}$, where w is the width, h is the height. An image is simply a function of two spatial values. For a *spectral image* I', the concept is extended to a function $I' : \mathbb{N}_w \times \mathbb{N}_h \times \mathbb{N}_f \to \mathbb{N}$, where w is the width, h is the height and f is the number of spectral bins. We call this a spectral image, because at each 'pixel' (coordinate), we have a spectrum of values, that is we can define the spectrum s_{xy} of the pixel (x, y) by $s_{xy}(\cdot) = I'(x, y, \cdot)$. An intuitive way to think of a *spectral image* is a cube of values, so a spectral image is commonly referred to as a *data cube* (as in [18] and [3]) and we will use this interchangeably with the term *spectral image*.

An "RGB" image can be considered spectral, where we have $f = 3$, with a spectral bin for the red, green and blue regions of the visible spectrum.

Finally some literature refer to *multispectral* and *hyperspectral* images (which may be referenced such as in [19] and [3]), which are simply special cases of a spectral image. A multispectral image refers to a small number of spectral bands (such as 5) and a hyperspectral image refers to a large number of spectral bands (such as 50). Intuitively, we can think of the difference between multispectral and hyperspectral in terms of their spectra: a multispectral image should be thought of as having quantised spectra (histograms), whereas a hyperspectral image can be thought of as attempting to approximate the continuous spectra.

1.2 Aims of the project

Nowadays computer vision techniques are used in abundance to aid medical diagnosis, and they are used by doctors to help provide more accurate and earlier diagnoses. This is clearly an area of interest, as such tools may help improve, or even save lives where we wouldn't have been able to do so in the past.

In this project we consider using spectral images (recall that this includes RGB images) for medical purposes and we wish to segment the image to indicate different regions of interest, typically which would indicate some form of disease or abnormality. The problem can easily be described mathematically: given an arbitrary spectral image $I : \mathbb{N}_w \times \mathbb{N}_h \times \mathbb{N}_f \to \mathbb{N}$ and a set of possible classes $\mathcal{C}$, we want to output a *pixel labelling* $\mathcal{P} : \mathbb{N}_w \times \mathbb{N}_h \to \mathcal{C}$ that correctly identifies regions of the image according to $\mathcal{C}$. Succinctly put, we want to perform *image segmentation*, on (noisy) medical (spectral) images.

The motivation for this project comes from use of a the hyperspectral imager for use with contrast agents [19]. The aim is that the imager can be used to identify the presence of fluorescent contrast agents, some of which have a negative binding response to cancerous cells in the oesophagus, thus allowing cancerous tissues to be identified. The Biological and Soft Systems group from the physics department at Cambridge have kindly given me some images taken with the imager used by Luthman et al [19], which we will refer to as "the BSS dataset".

To summarise, we wish to produce a system capable of producing a pixel labelling from a spectral image. The pixel labelling will depend highly on the data and so we would likely wish to learn from some examples.

1.3 Possible solutions

As we will be looking to segment images, we will need to identify regions of the image based on the data available. One approach that we might take is to try and identify some properties manually, For example one possible solution in the BSS dataset is to explicitly find the spectra of *endmembers* (the fluorescents) in the images, then use a *spectral unmixing* algorithm [15] such as constrained least squares. The output of a spectral unmixing algorithm will identify the proportions of endmembers present at each given point [19].

An alternative would be to utilising machine learning methods, where one might hope to learn relationships within the data through supervised learning. Such a system may be more versatile, be able to solve many similar problems and may not be constrained to a specific problem. For example, the spectral unmixing solution above requires the endmembers to be measurable, requiring

significant work prior to putting the data through the algorithm. We would hope by using machine learning that we can avoid such additional work, and even solve problems where the 'endmembers' are not separable with explicitly measurable spectra.

1.4 Related work

Medical imaging is an active research area and will likely be for a long time. Medical imaging is ubiquitous in hospitals and an essential tool to aid doctors in diagnosing a patient. Along with medical imaging comes medical image analysis, where image processing methods are used to give more information to doctors which they may not be able to see with the naked eye. The task of image segmentation is important in medicine: illnesses and viruses are commonly localised, only affecting parts of tissues and identification of which parts of tissues are healthy or not is important to successful treatment.

Plenty of work and research that has gone into image segmentation, and it is a common technique used in medical imaging. It can be implemented using a variety of methods such as classifiers, thresholding and region growing [21]. However traditional (non machine learning) methods seem to be loosing traction, with few papers written in this decade readily available, paling in comparison to the vast number of machine learning based literature.

Recently neural networks have seen a major dominance with regards to machine learning; within medical imaging other areas of machine learning are still finding success, with whole books still dedicated to the topic [6]. True to the current trend, there is plenty of current work utilising neural networks in medical imaging. For example they have been successfully applied to segment different regions of the brain, such as 'white matter', 'gray matter', and 'cerebrospinal fluid' [28], and similarly for segmentation of brain tumours [29].

However, other machine learning methods are still of interest and random forests are still an active area of research within medical imaging and computer vision [4], especially because of their simplicity and lack of complexity, which can potentially make them very efficient [7].

SegNet [2] is a deep convolutional neural network architecture built on top of Caffe [14] for pixel wise labelling, and provides some inspiration for the project. SegNet uses supervised learning to train the neural network using known labelled images. In normal operation it takes some image as input and outputs a pixel labelling. Bayesian SegNet which is an extension to SegNet, includes an additional output image, which is a mapping of uncertainty in each pixel labelling, some-

thing that is desirable in our own system. The Caffe implementation includes support for OpenCL (an open source GPU programming language), allowing for an efficient implementation. This is realised by applying it to run on a real-time video stream, with 360 by 480 resolution. Whilst this implementation isn't necessarily geared towards medical purposes, it could certainly be utilised for a medical application, and is a good example of a system solving the more general problem of image segmentation/pixel labelling.

Chapter 2

Preparation

In this section we will introduce the area of image segmentation and how we may perform segmentation. Then we introduce decision trees and explain the supervised learning method of random forests. Since many medical imaging techniques tend to require short exposure times they frequently exhibit visible noise, leading to grainy images. Thus we then discuss how we may want to model the noise and how we can deal with this. In the second half of the chapter we outline the design with a requirements analysis, pipeline overview, what tools we will use and a backup strategy to avoid loosing any work.

From a list of machine learning algorithms: State Vector Machine [16], [17], Hidden Markov Models [26], k Nearest Neighbour [8], Random Forests [6], and Neural Networks [12], we decided on two algorithms that would be useful in our case, Random Forests and Neural Networks. So a Random Forests library will be implemented and the Encog library will be employed for Neural Networks in Java [13].

2.1 An introduction to image segmentation

Image segmentation concerns splitting an image into connected subsets, in some meaningful way. Despite being an ill-posed problem with no 'best' segmentation, we often have some desired segmentation that we would like our system to perform. The term 'ground truth' is used to refer to a hand labelled image, in which an accuracy of 100% is assumed. When training a supervised learning system we will provide some number of ground truth images.

More formally if we let Ω be the set of pixels in some image, a valid image segmentation is $(S_1, ..., S_n)$ for some $n \in \mathbb{N}$ which satisfy the following:

$$\Omega = \bigcup_{i=1}^{n} S_i \tag{2.1}$$

$$S_i \cap S_j = \emptyset \qquad \text{for all } i \neq j \tag{2.2}$$

where each S_i is connected, which means that there is a path between any two pixels of S_i. A path may take steps of one pixel up, left, down or right [20].

There are a number of ways that we may try to perform an image segmentation. One such method consists of finding the edges present in an image, by using the zero crossings of a gradient operator, such as the Laplacian. Furthermore, we may want to look at edges at different scales, which suggests blurring the image before taking the gradient operator, leading to the Laplacian of Gaussian operator, as discussed by Pal et al [20]. An even simpler method would be to use grey level threshold, where we segment images depending on whether they fall above or below some threshold, also discussed by Pal et al [20].

Finally, the method that we will use is to generate some pixel labelling $\mathcal{P} : \Omega \to \mathcal{C}$ as described in section 1.2. This implicitly defines a segmentation of an image via regions of similarly classed pixels.

2.2 Supervised learning for classification

Before discussing any machine learning methods we first need to define some terminology that we will be using. In classification we are given a *feature vector* (or *instance*) $\mathbf{x} = (x_1, x_2, ..., x_d) \in \mathbb{R}^d$ and a set of classes $\mathcal{C} = \{C_1, C_2, ..., C_n\}$. We want to *learn* some hypothesis $h : \mathbb{R}^d \to \mathcal{C}$ which maps instances to their classification. To learn what hypotheses are appropriate we rely on a *training sequence* $\mathbf{s} = ((\mathbf{x}_1, c_1), (\mathbf{x}_2, c_2), ..., (\mathbf{x}_m, c_m))$, which makes the method *supervised*. We usually assume that the training sequence is noisy, which can be sufficiently represented by noise solely attributed to the classes of $\mathbf{s}$ (that is $c_1, ..., c_m$). So we can consider each of the c_i to be a random variable, and hence consider $\mathbf{s}$ to be a random variable. Two sensible approaches that we might take to choosing some hypothesis h either picking

$$h_{\mathrm{ML}} = \arg\max_{h \in \mathcal{H}} \Pr(h|\mathbf{s}) \tag{2.3}$$

or picking

$$h_{\text{MAP}} = \arg\max_{h \in \mathcal{H}} \Pr(\mathbf{s}|h) \Pr(h) \tag{2.4}$$

where ML stands for *maximum likelihood* and MAP stands for *maximum a-posteriori*. The MAP hypothesis allows the prior $\Pr(h)$ to be used (indicating some prior knowledge about the hypothesis), however if $\Pr(h)$ is uniform, then the ML and MAP hypothesis are easily shown to be equivalent using Bayes' theorem. These two methods of picking a hypothesis are referred to as Bayesian learning methods; as we look to maximise likelihoods. We will see that this is not the only way of picking a suitable hypothesis. [25]

We often also see that some hypothesis will take the form of $h' : \mathbb{R}^d \to (\mathcal{C} \to [0, 1])$, that is it gives a probability distribution over classes. We can then simply set

$$h(\mathbf{x}) = \arg\max_{c \in \mathcal{C}} h'(\mathbf{x})(c) \tag{2.5}$$

which is 'the most likely class'.

2.3 Decision trees and random forests

This section defines what a decision tree is, how it can be used in supervised learning and then extend it to the concept of random forests. As mentioned in section 2.2 we opt for a hypothesis which outputs a probability distribution over classes as opposed to a single class, which can be used to give a single class.

2.3.1 Introduction to decision trees

Decision trees consist of a simple binary tree structure. Intuitively, we think about asking a question at each node, making a decision on which child node to traverse to and eventually reach some conclusion at a leaf node, such as in figure 2.1. We can use this model for the situation described in section 2.2, where we are allowed to 'ask a question' about the feature vector at each decision node and leaf nodes consider

More formally we can define a decision tree T for classification, which has a set of states $Q \subseteq \mathbb{N}$, such that if $i \in Q$ is a decision node, then it has children $2i, 2i + 1 \in Q$.

For our model we specify some function $f : \mathbb{R}^d \times \mathcal{T} \to \mathbb{B}$, where $\mathcal{T}$ is some parameter space and is used to specify a function from $\mathbb{R}^d$ to $\mathbb{B}$ at each decision

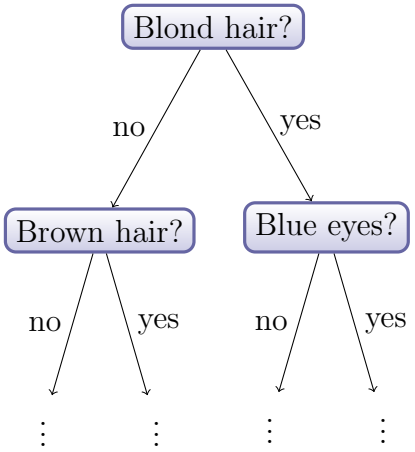


Figure 2.1: Example of (part of) a tree used to classify humans.

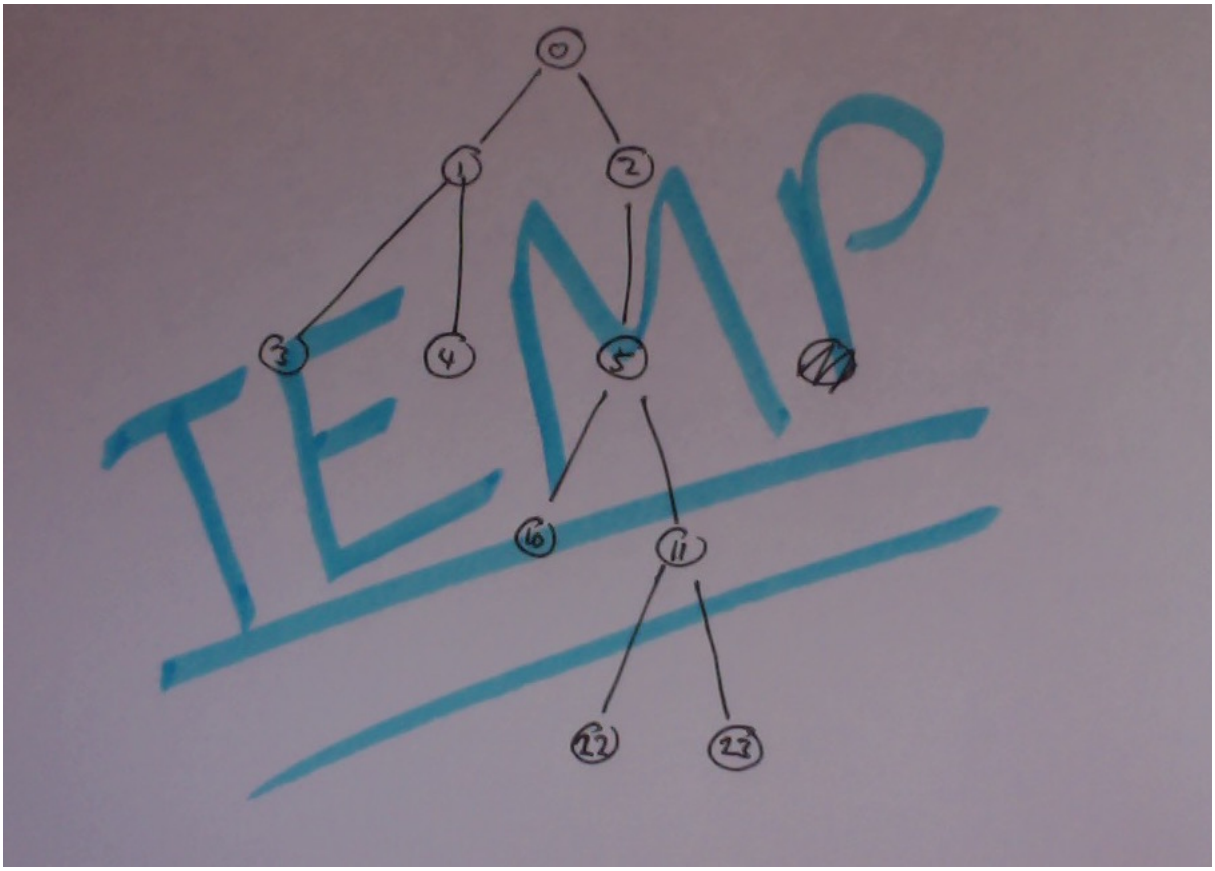


Figure 2.2: Example of node numberings in a decision tree.

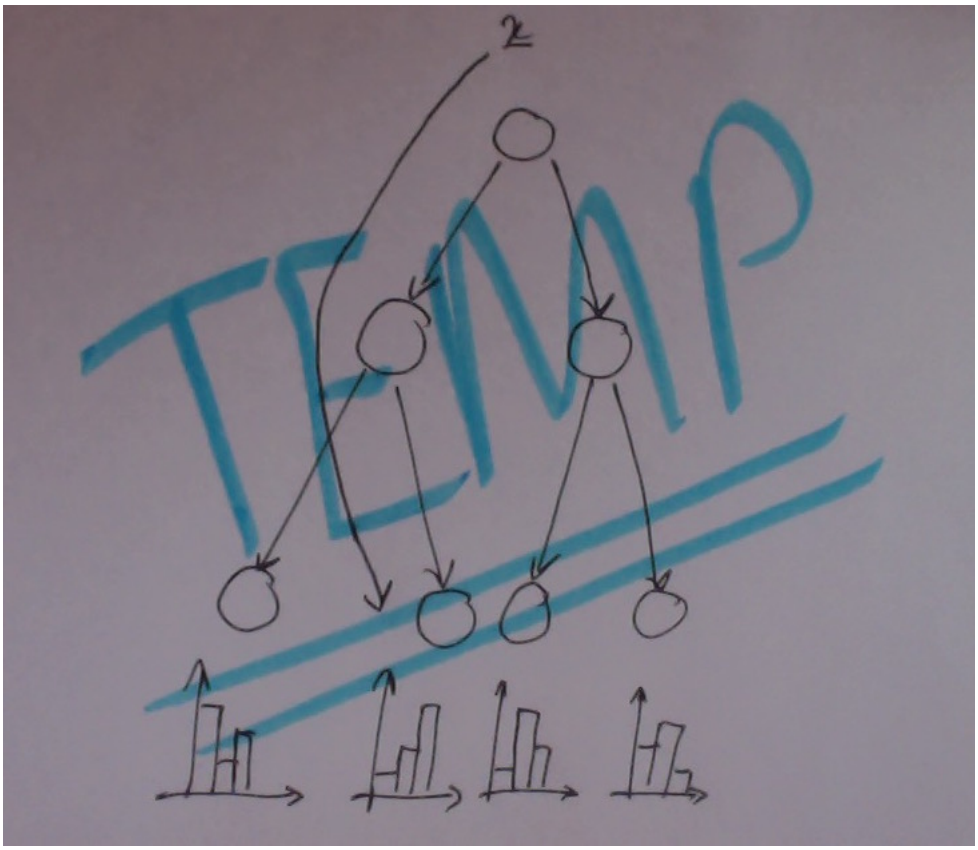


Figure 2.3: Example of how some instance $\mathbf{x}$ would be classified using a decision tree.

node. f is called a *weak learner* or a *split function*. In a decision tree for each state $i \in Q$ we have some associated $\theta_i \in \mathcal{T}$ called a *split parameter*, used to specify $f_i(\mathbf{x}) = f(\mathbf{x}; \theta_i)$. The function $f_i : \mathbb{R}^d \to \mathbb{B}$ is then used to make a decision to traverse to either state $2i$ or $2i + 1$ next. Finally when we hit a leaf node $j \in Q$ we need to specify some probability distribution $p_j : \mathcal{C} \to [0, 1]$ where:

$$p_j(c) = \Pr(\mathbf{x} \in c | \mathbf{x} \text{ traversed to } j \text{ in } T). \tag{2.6}$$

As it can be seen in Figure 2.3 to classify some instance $\mathbf{x}$ using a decision tree T we simply traverse T using f_i at each node $i \in Q$ to make a decision whether to traverse to $2i$ or $2i + 1$ next. We usually use the following rule: if $f_i(\mathbf{x}) = 0$ then traverse to $2i$, otherwise if $f_i(\mathbf{x}) = 1$ then traverse to $2i + 1$. [6]

2.3.2 Training a decision tree

When training a decision tree we use a greedy approach, to train at each node optimally. A greedy approach is necessary because optimising over all possible trees is a computationally infeasible task (it is an NP-complete problem to decide if a tree is optimal). So consider having a set of states Q and for each state $i \in Q$ we want to learn the split parameter $\theta_i \in \mathcal{T}$. Let $\mathbf{s}_i$ be the training sequence that i is trained on. It is sensible to set $\mathbf{s_0} = \mathbf{s}$.

We first define the *entropy* of a training sequence:

$$H(s) = -\sum_{c \in \mathcal{C}} p(c) \log_2(p(c)). \tag{2.7}$$

We assume feature vectors in s to be unique for ease of notation and let:

$$p(c) = \frac{|\{\mathbf{v} \mid c' = c \wedge (\mathbf{v}, c') \in S\}|}{|S|}, \tag{2.8}$$

which is the empirical probability of a training sample vector in s being classified as c. Now we define a left and right split of $\mathbf{s}$, using some split parameter $\theta \in \mathcal{T}$ according to our weak learner f as follows:

$$L(\mathbf{s}, \theta) = \{(\mathbf{x}, c) \in s | f(\mathbf{x}, \theta) = 0\} \tag{2.9}$$

$$R(\mathbf{s}, \theta) = \{(\mathbf{x}, c) \in s | f(\mathbf{x}, \theta) = 1\}. \tag{2.10}$$

Consider the *information gain* I for performing a split according to θ of

$$I(\mathbf{s}, \theta) = H(\mathbf{s}) - \frac{1}{|\mathbf{s}|} \left(|L(\mathbf{s}, \theta)| H(L(\mathbf{s}, \theta)) + |R(\mathbf{s}, \theta)| H(R(\mathbf{s}, \theta)) \right). \tag{2.11}$$

We now have a way of picking θ_i at each node

$$\theta_i = \arg\max_{\theta \in \mathcal{T}} I(\mathbf{s}_i, \theta). \tag{2.12}$$

Once we have found a θ_i we then set $s_{2i} = L(\mathbf{s}_i, \theta_i)$ and $s_{2i+1} = R(\mathbf{s}_i, \theta_i)$, which allows us to begin training at node 0 with $\mathbf{s}_0 = \mathbf{s}$ and then recursively train down the tree. [6]

2.3.3 Moving swiftly on to random forests

Decision trees have a couple major disadvantages, which are solved by extending the concept to random forests. The first problem is that we learn θ_i using

$$\theta_i = \arg\max_{\theta \in \mathcal{T}} I(\mathbf{s}_i, \theta), \tag{2.13}$$

which is a problematic because $|\mathcal{T}|$ may be infinite. We resolve this by randomly sampling $\mathcal{T}$ with ρ values, so let $\mathcal{T}_\rho = \{\theta_i^{(1)}, ..., \theta_i^{(\rho)}\} \subseteq \mathcal{T}$. So we instead set

$$\theta_i = \arg\max_{\theta \in \mathcal{T}_\rho} I(\mathbf{s}_i, \theta), \tag{2.14}$$

when training at node i, where ρ *fresh* samples are taken from $\mathcal{T}$ per node. This optimisation is called the *random node optimisation*. The second problem with decision trees is that we can easily over fit and also we cannot solve some XOR/parity problems [6]. We can address this by using a *forest* of decision trees. A forest F is a set of trees, that is $F = \{T_1, T_2, ..., T_k\}$, where each T_ℓ is trained separately with training sequence $\mathbf{s}$. As we randomly train each tree on the same data, it is reasonable to say that the probability of any given tree in F to be 'correct' tree is equally likely. Hence we set $\Pr(T_\ell) = 1/k$ for each ℓ. Finally, when we wish to classify some instance $\mathbf{x}$ using a random forest we output

$$\begin{aligned} p(c) &= \Pr(\mathbf{x} \in c) && (2.15)\\ &= \sum_{\ell=1}^{k} \Pr(\mathbf{x} \in c, T_\ell) && (2.16)\\ &= \sum_{\ell=1}^{k} \Pr(\mathbf{x} \in c | T_\ell) \Pr(T_\ell) && (2.17)\\ &= \frac{1}{k} \sum_{\ell=1}^{k} \Pr(\mathbf{x} \in c | T_\ell) && (2.18) \end{aligned}$$

where each $\Pr(\mathbf{x} \in c|T_\ell)$ is the probability obtained by traversing each tree. [6]

Therefore, to classify using a forest, we just take an average of the outputs from the trees.

2.4 Neural Networks

We now move on to describe a second method of supervised learning, neural networks. We begin by defining a single neuron and how it operates, then develop the idea into a neural network. Then the general idea of how to train a neural network is explained.

TODO

2.5 Imaging and image noise

We now consider image sensor arrays, to understand how images are captured and what might cause image noise at a high level. We will then define the quantum noise and discuss its suitability to many cases of medical imaging.

2.5.1 Image sensor arrays

All forms of digital imaging involve some form of sensor array. Two common technologies are used in image sensors, Charge-Coupled Devices (CCD) and Complementary Metal-Oxide Semiconductors (CMOS). These devices are laid out in a grid, which are typically combined with (colour) wavelength filters.

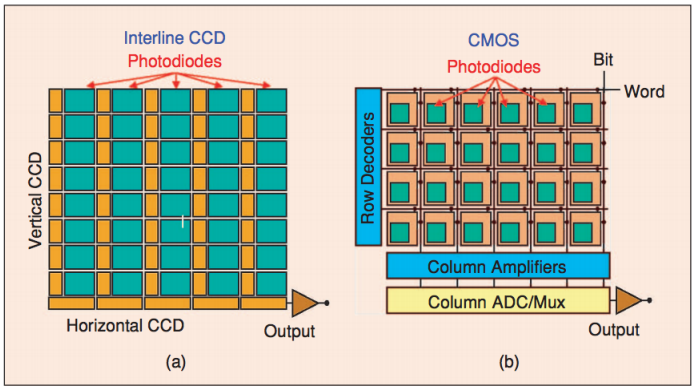


Figure 2.4: CCD and CMOS sensor arrays. Reproduced from Gamel et al [10].

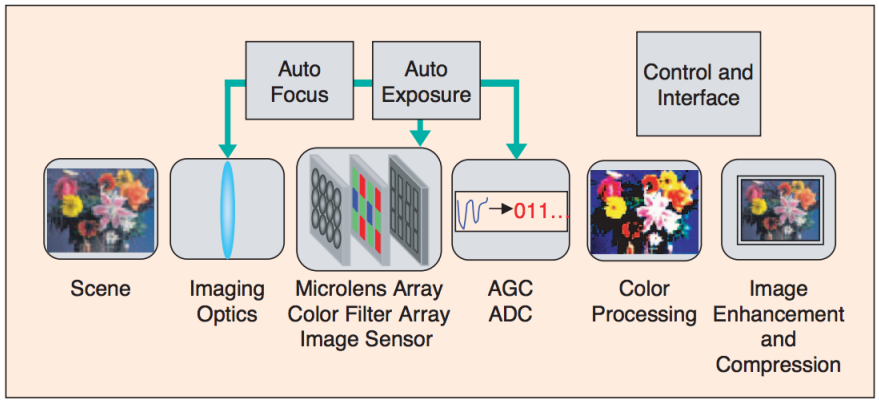


Figure 2.5: Overview of an imaging 'pipeline'. Reproduced from Gamel et al [10].

In a camera we have a focussing lens, followed by wavelength filters and then sensors. In many medical imagers there is a collimator, so it is appropriate to consider a model where we have parallel streams of photons hitting each sensor.

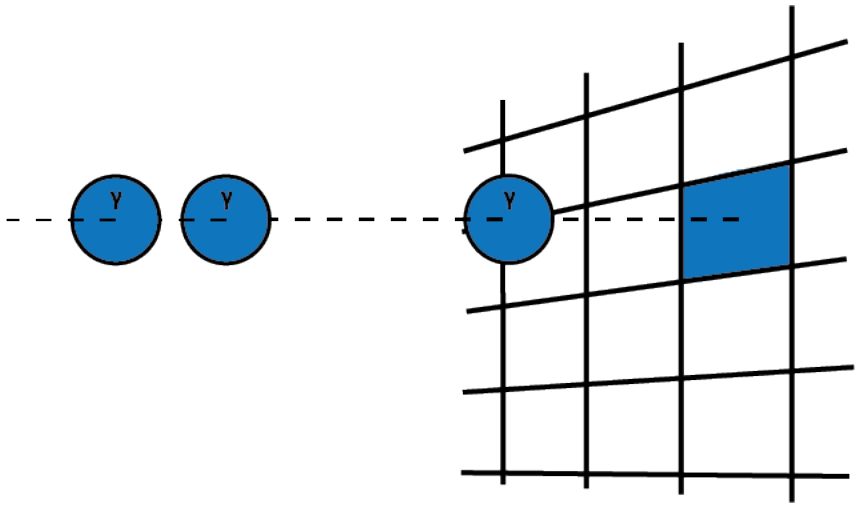


Figure 2.6: Parallel stream of photons incident on one sensor in a sensor array.

We consider that a stream of photons, will be hitting some photodiode (the part of a sensor that generates a current upon absorbtion of a photon), causing charge to collect on a connected capacitor, which will increase linearly with respect to time at a rate proportional to the rate of photons incident on the photoreceptor (the photocurrent), until it hits some maximum value. [10]

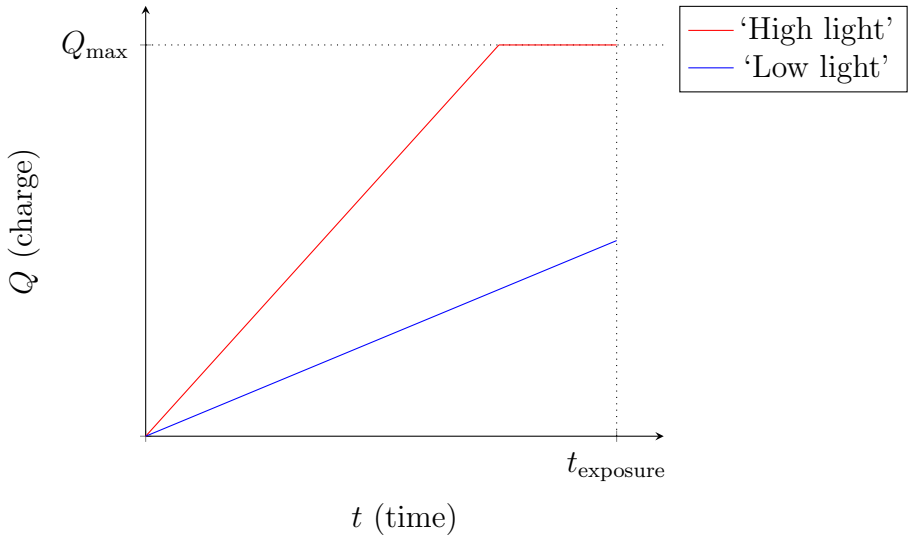


Figure 2.7: The charge held on a capacitor is linear with respect time, until it hits some maximum [10].

2.5.2 Quantum noise

Quantum noise, *Photon noise* or *Poisson noise* can be thought of as a uncertainty associated with the measurement of light, due to the quantised nature of electromagnetic waves and the independence of photon detections [11]. More mathematically suppose we have some noiseless image $I(x, y)$, then we define an image corrupted by photon noise $\tilde{I}$ by

$$\tilde{I}(x, y) \sim \text{Poisson}(I(x, y)). \tag{2.19}$$

So we have

$$\Pr(\tilde{I}(x, y) = k) = \begin{cases} e^{-I(x,y)} \frac{I(x,y)^k}{k!} & 0 \leq k \\ 0 & \text{otherwise} \end{cases} \tag{2.20}$$

$$\mathbb{E}\left[\tilde{I}(x, y)\right] = I(x, y) \tag{2.21}$$

$$\text{Var}\left[\tilde{I}(x, y)\right] = I(x, y). \tag{2.22}$$

It is appropriate to consider a procvess such as the one in Figure 2.6 as a Poisson process, where each event is a photon hitting the photoreceptor. Suppose the exposure time to the sensor is t_{exposure}, the average rate of events is ϕ and that $N(t)$ is the number of events that occur in the interval $[0, t]$, then we have

$N(t) \sim \text{Poisson}(\phi t)$ [24]. Thus we have $N(t_{\text{exposure}}) \sim \text{Poisson}(\phi t_{\text{exposure}})$. From figure 2.7 we can justifiably say that if ϕ is the flux (rate) of photons hitting sensor at index (x, y) in the array, then $I(x, y) \propto N(t_{\text{exposure}})$.

The model is easily and obviously extended to spatial images by including spectral bin indices

$$\tilde{I}(x, y, \lambda) \sim \text{Poisson}(I(x, y, \lambda)). \tag{2.23}$$

Because of the filters (shown in Figure 2.5) being spatially separated we can consider each value in the datacube to be an independent random variable. This means that

$$(x, y, \lambda) \neq (x', y', \lambda') \Rightarrow \Pr(\tilde{I}(x, y, \lambda), \tilde{I}(x', y', \lambda')) = \Pr(\tilde{I}(x, y, \lambda)) \Pr(\tilde{I}(x', y', \lambda')). \tag{2.24}$$

However, in images the values are constrained to a finite range, typically we have that for each x, y, λ that $I(x, y, \lambda) \in \mathbb{N}_{256}$, but this however doesn't restrict the value of $\tilde{I}(x, y, \lambda)$ to $\mathbb{N}_{256}$. By considering Figure 2.7 we see that the charge becomes *saturated* at the upper limit, that is for $\phi > \phi_{\text{crit}}$ (from Figure 2.7) we achieve Q_max, but for $\phi < \phi_{\text{crit}}$ we don't achieve this before t_{exposure}. Thus for any $\phi > \phi_{\text{crit}}$ the maximum value is recorded in the image values. To deal with this it makes sense to define a *Saturated Poisson* distribution. So we say $X \sim \text{SPoisson}(\mu, n)$ if

$$\Pr(X = k) = \begin{cases} e^{\mu} \frac{\mu^k}{k!} & 0 \leq k < n - 1 \\ \sum_{i=n-1}^{\infty} e^{\mu} \frac{\mu^i}{i!} & k = n - 1 \\ 0 & \text{otherwise.} \end{cases} \tag{2.25}$$

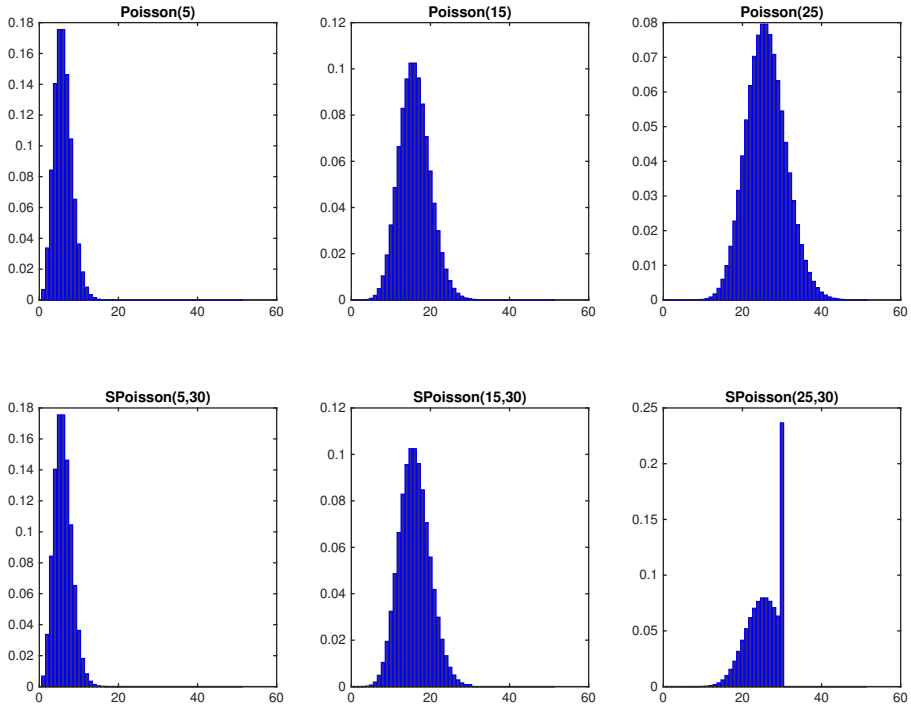


Figure 2.8: Example of Poisson(μ) and SPoisson(μ, 30) distributions, for $\mu = 5, 15, 25$.

2.5.3 Additive White Gaussian Noise

A more general noise model that should also be considered is *additive white Gaussian Noise*. We will 'saturate' values with similar reasoning to section 2.5.2. The general model will add a value sampled from a Gaussian distribution with some constant power. That is if we have a 'true spectral image' I, then the image corrupted by noise is:

$$\tilde{I}(x, y, \lambda) = I(x, y, \lambda) + X_{ij\lambda} \tag{2.26}$$

where for each i, j, λ we let $X_{ij\lambda} \sim N(0, \sigma^2)$. The noise is parametrised by σ and $\mathbb{E}[X_{ij\lambda}] = \sigma^2$ is the *power* of the noise.

2.5.4 Medical imaging noise

This section ends by considering how our noise models could be used in medical imaging. For many methods of medical imaging we use ionising radiation that

would be considered harmful given extended exposure times [22]. As a consequence there is an inherent trade off between exposure time (for greater image clarity) and risk of causing damage [27]. Since we may potentially use shorter exposure times, or we may be imaging something in low light we find that often the quantum noise model is more appropriate and also cannot be approximated by Gaussian noise. However, there are many cases such as ultrasound where we may want to consider more sophisticated noise models [5], but for the purpose of this dissertation we will restrict ourselves to the above.

2.6 TVMM Image De-Noising

- A method developed for additive white Gaussian noise [9], which even when produced is outperformed by wavelet methods, outperforms algorithms developed for Poisson noise [23].
- Definition of total variation
- Definition of the optimisation problem and the Q function used
- Some properties of the Q function, that allow us to find the optimal solution to the optimisation problem
- Outline of the procedure
- Requires solution of linear equations. Can be done using conjugate gradients (appendix B).
- Trying to solve an inherently ill-posed problem

2.7 Requirements analysis

Now that the relevance in context has been discussed, we move onto the design of the system. Firstly we carefully consider the requirements of the system. This is important to begin identifying the work that needs to be undertaken and where potential risks lie.

Goal Requirement	Priority	Risk	Difficulty
Build a random forests machine learning library	High	Low	Medium
Incorporate a neural network library (Encog)	High	Medium	Medium
Image segmentation via pixel labelling	High	Low	Low
Suitably model and account for image noise	Medium	High	High
Train the pixel labelling system on real data	High	High	Low
Build an aid to help create training sets	Medium	Low	Low
Model uncertainty and output in a certainty map	Medium	Medium	Medium

Table 2.1: High level goals and desired outcomes for the project.

2.8 System Design

This section outlines the overview of the whole system, where we begin with a work flow diagram comprising of files and system components. The system is then divided into its separate components and used to define an interface, along with a brief description of each module in addition to defining inputs and outputs. The formats of the files that the user should input can be found in appendix A.

2.8.1 Pipeline/Overview

An overview of what we want the system to do (the pipeline of the system) is illustrated in terms of the files input and output by different modules of the system. In the system overview in Figure 2.9, blue boxes are code modules and red boxes represent files.

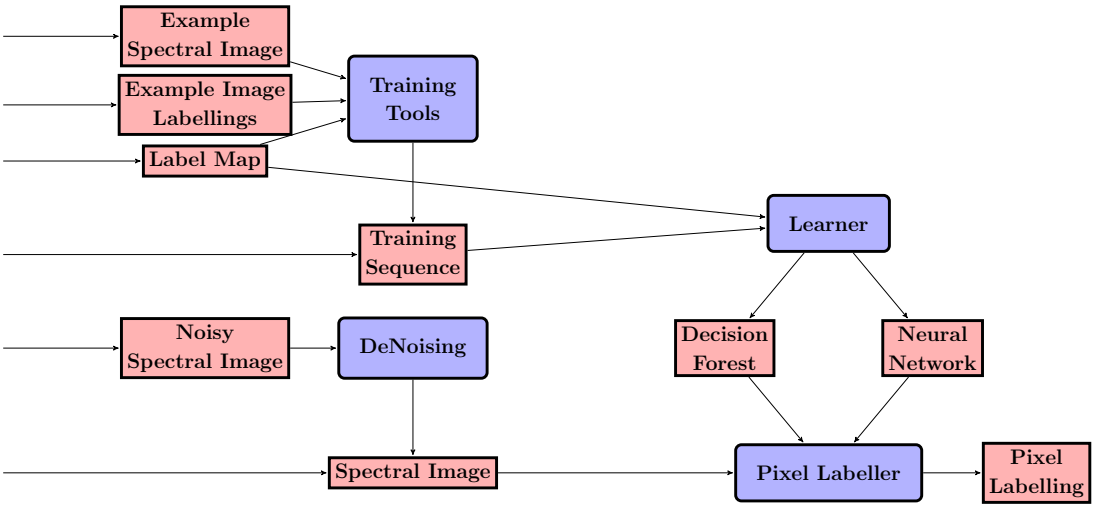


Figure 2.9: Overview of the system and its intended use.

2.8.2 Interface/Usage

We will not only allow usage for each module separately, but also for combined steps that will avoid unnecessary intermediate files to be produced. For our interface the diagrams that consisted of red boxes for files and blue boxes for code modules are extended to denote files/modules unused in a given function by a faded/duller colour. An intermediate file that isn't saved during some function is marked by a regularly bright, but dashed border. It should be assumed that an intermediate file need not be provided by the user.

2.8.2.1 Training Tools

The training tools' function is to take an example class map, pixel labelling and spectral image (see appendix A for how their formats). From this 'ground truth' we will output a training sequence as specified in appendix A. The use of this function is to generate vast quantities of training data with minimal effort.

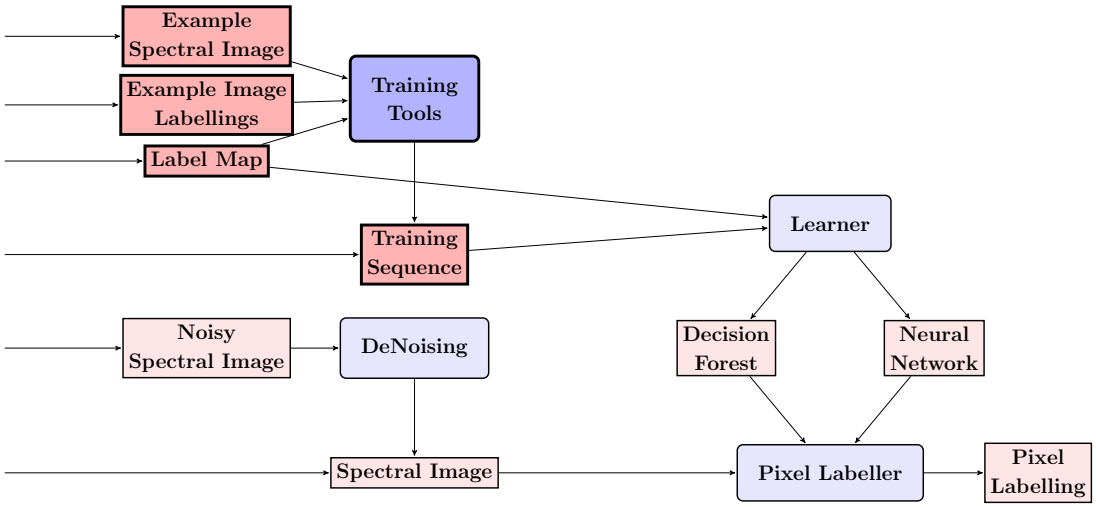


Figure 2.10: Overview of the training tools function.

2.8.2.2 Train

The train function will take a training sequence and then produce either a forest file or a neural network file. These files will be output to be used later by the pixel labeller.

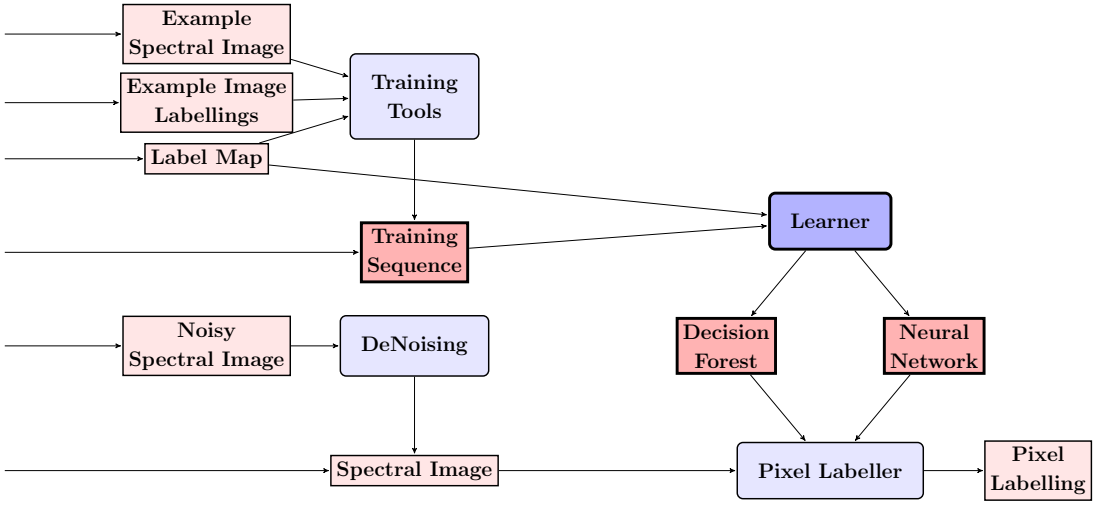


Figure 2.11: Overview of the train function.

2.8.2.3 Learn From Example

The *learn from example* function is a composite of the training tools and train functions. This will take the same inputs as the training tools function, but

instead will immediately use the training sequence produced to train a random forest or neural network. The training sequence is not saves in the process.

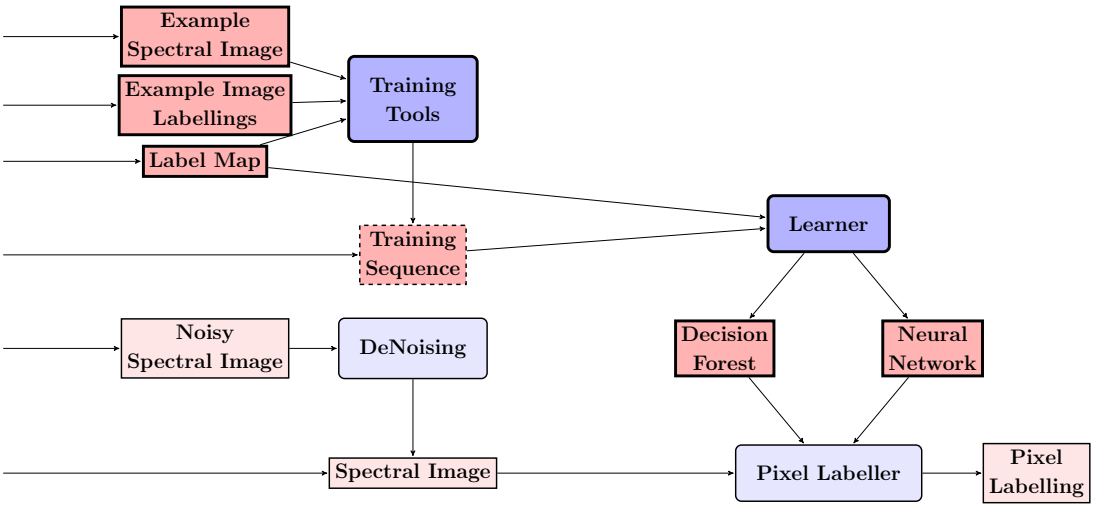


Figure 2.12: Overview of the *learn from example* function.

2.8.2.4 Pixel Labeller

The pixel labeller could be considered the primary part of the system. It uses the pixel labeller module to label a spectral image using a trained forest/neural network.

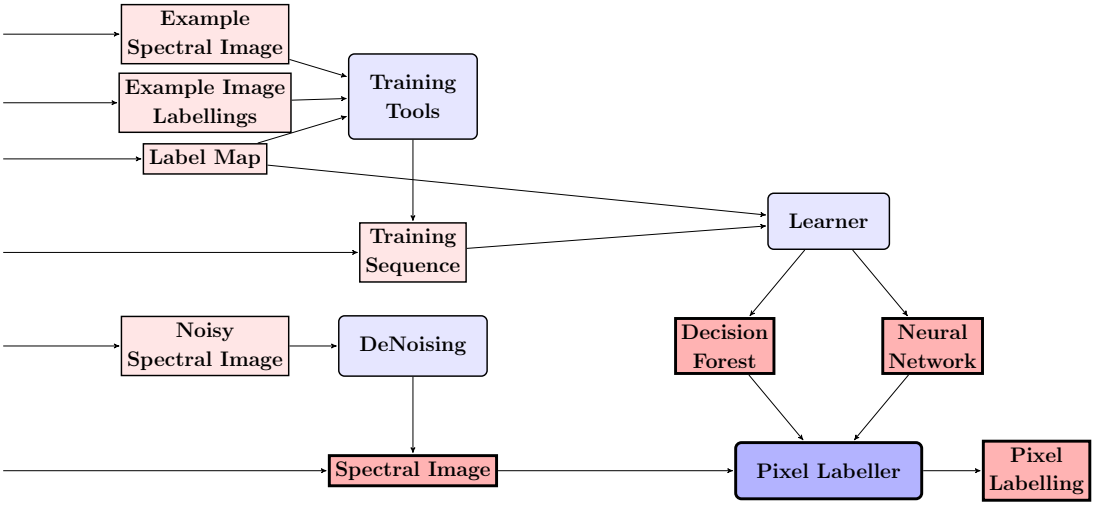


Figure 2.13: Overview of the pixel labeller function.

2.8.2.5 De-Noiser

The de-noiser function attempts to reduce the effect of noise on the image. It takes a spectral image as input and outputs the de-noised spectral image.

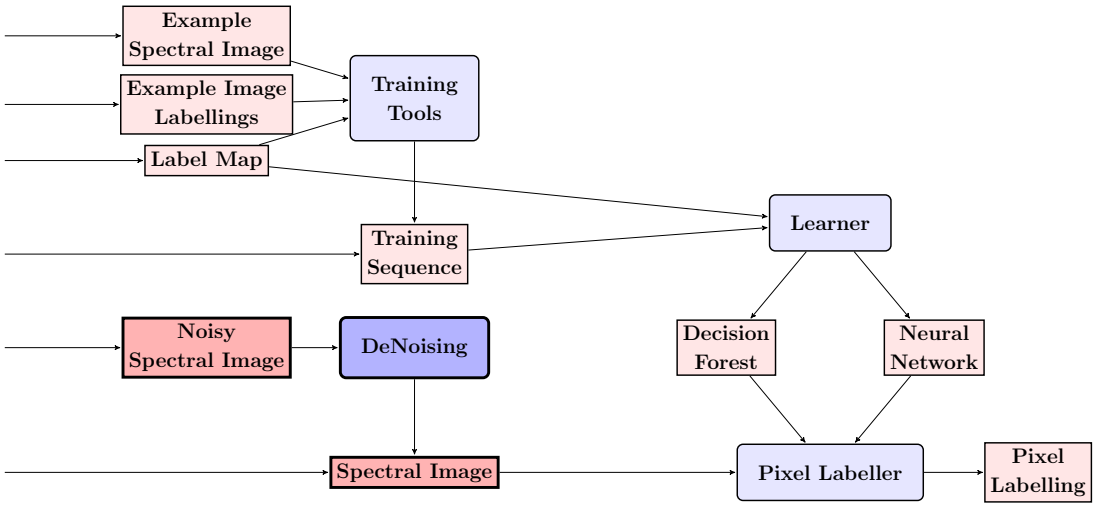


Figure 2.14: Overview of the de-noiser function.

2.8.2.6 Noisy Pixel Labeller

The noisy pixel labeller is a composite of the de-noiser and pixel labeller functions. We take a noisy spectral image as input, along with a trained forest or neural network. De-noising is run on the image before feeding the spectral image to the pixel labeller.

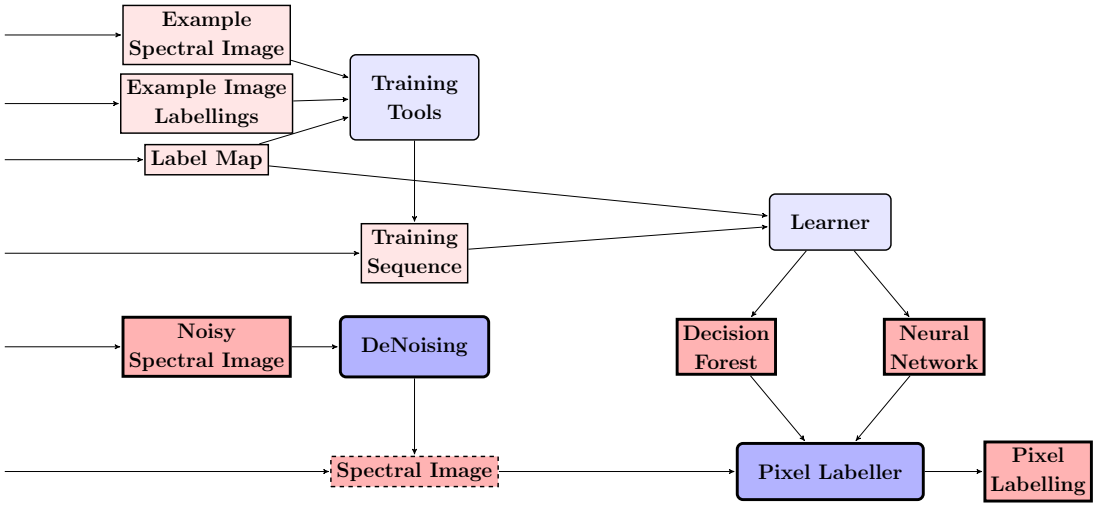


Figure 2.15: Overview of the noisy pixel labeller function.

2.9 Languages and tools

In this section we briefly describe the languages, libraries and tools that we used for the project.

Programming Languages and Libraries

Java: provides an OS independent language and is object oriented to allow for modular design.

JUnit: a Java library used for unit testing, used for white box and black box testing throughout the development of the system. Unit tests are essential to find bugs and prevent their re-introduction.

Encog: an easy to use neural networks library in Java/C# written by Heaton research [13].

Integrated development environment

Eclipse: allows for rapid development in Java and integrates easily with libraries and tools such as JUnit and Git.

EclEmma: an Eclipse plug-in compatible with JUnit which highlights lines to indicate code coverage of unit tests.

ObjectAid: another Eclipse plug-in, used to create UML class diagrams.

Statistical analysis and visualisation

Matlab: an easy to use, extensible statistical package used for producing graphs.

Document preparation

LaTeX: used for typesetting this dissertation in a precise manor allowing control over most aspects of document layout and style.

Tikz: a LaTeX library useful for producing diagrams, such as Figure 2.9.

Listings: a LaTeX library allowing colour formatted code for a plethora of languages.

Adobe Photoshop: image editing software used to produce some diagrams.

Version Control

Git: allows code to be developed systematically and rollback if necessary, as well as providing the ability to fork my core repository to try different strategies.

Backup

DropBox and Google Drive: repositories were kept in both DropBox and Google Drive folders, which synced every time a file was changed.

Github: provides a remote Git repository to store code, so also helps in provision of version control. The repository was updated every time a stable commit was made.

Time machine: Apple's automatic backup system, allowing for hourly backups of the whole hard drive to be taken.

2.10 Software engineering techniques

2.10.1 Development model

The design of the system calls for a mixture of iterative and waterfall models to be employed in this project. The system is split into well defined modules (as can be seen in Figure 2.9). Each module then needs to be implemented and tested rigorously before moving onto the next, important because of the dependencies between modules. For each module it is possible to produce manually suitable files for testing.

Once a working system was produced, tested and deemed to be correct with some confidence, additional features and improvements to the system were added in an iterative manner, similar to a spiral model. Unit tests were used to make sure that any new additions do not break the existing, working parts of the system.

2.10.2 Testing

Development was test driven by necessity, as a large amount of work was required to reach a *minimum viable product*. If it were not tested thoroughly throughout development could have lead to nasty and difficult to find bugs. All tests were written as unit tests so that they could be reused later to make sure that the system still works. The following methodologies were employed:

Black box testing: When the internal system design is not taken into account, black box testing is used to ensure that the system works as a 'black box', in terms of the expected input/outputs we specified in the design. To assure that internal system design wasn't taken into account these were written *before* any code was written.

White box testing: When the internal system design is taken into account, tests are designed so that every line of code is checked using the unit tests. This is difficult to check manually, so Eclipse plug-in EclEmma was used, a code coverage tool that works with JUnit.

Input sanitisation testing: Additional unit tests were written to make sure that erroneous inputs were handled correctly.

Incremental integration testing: This refers to using a bottom up approach, testing functionality as it is implemented.

Usability testing: A few users were asked to try use the system given only instructions in a readme file. The feedback was vital in shaping the design of the training tools module.

2.10.3 Backup Plan

It is important to make sure that we have an effective backup plan to avoid any software, hardware or user error that may result in a loss of work, which is important to ensure that we do not lose a year's worth of work.

To make sure that no work was lost a number of systems were set in place to not only regularly back up any work but also provide rollback if necessary. Google Drive and DropBox were employed to keep shadow copies of the project directory, GitHub was used as a remote repository which was pushed to regularly. Finally Apple's time machine software was also used to automatically take backups of the whole local file system every hour.

[1]Image modified from: apple.com, google.com, dropbox.com, github.com, clipart-panda.com.

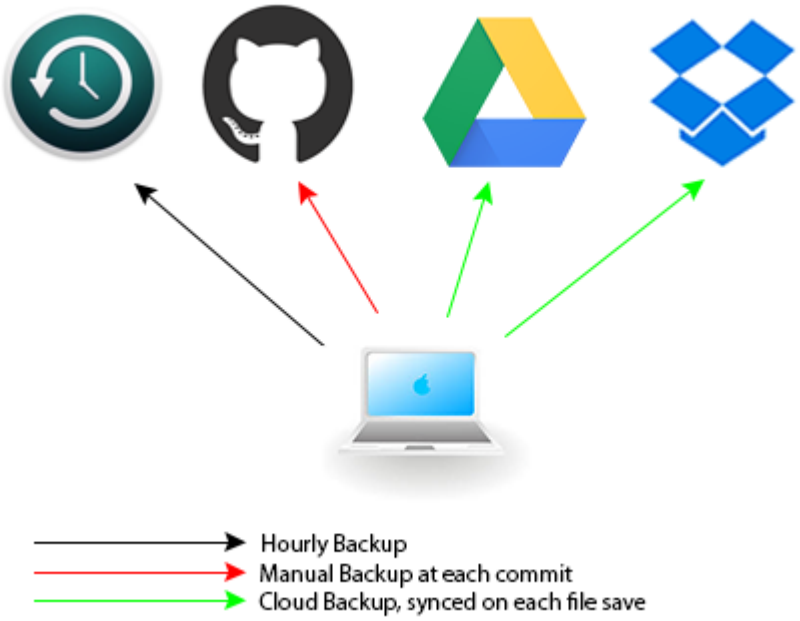


Figure 2.16: Overview of the backup strategy employed[1].

Chapter 3

Implementation

This chapter by elaborates on the implementation of the Random Forests algorithm and the use of the Encog, a neural network library for Java. We then proceed to use the supervised learning methods to build a procedure for producing a pixel labelling from a spectral image. We initially set aside the problems of how we will produce training data for the supervised learning methods, as these likely need to be extracted from an example labelling, a problem that will be addressed in section 3.4, along with the treatment of image noise in section 3.5.

The project is modularised into a number of packages, each building on top of another. Dependencies can be visualised in Figure 3.1. We will use UML class diagrams[1] to show the overview of classes within each package.

Add dependency from NN to RF because of use of ProbabilityDistribution class

[1] As defined in http://www.uml-diagrams.org/class-reference.html

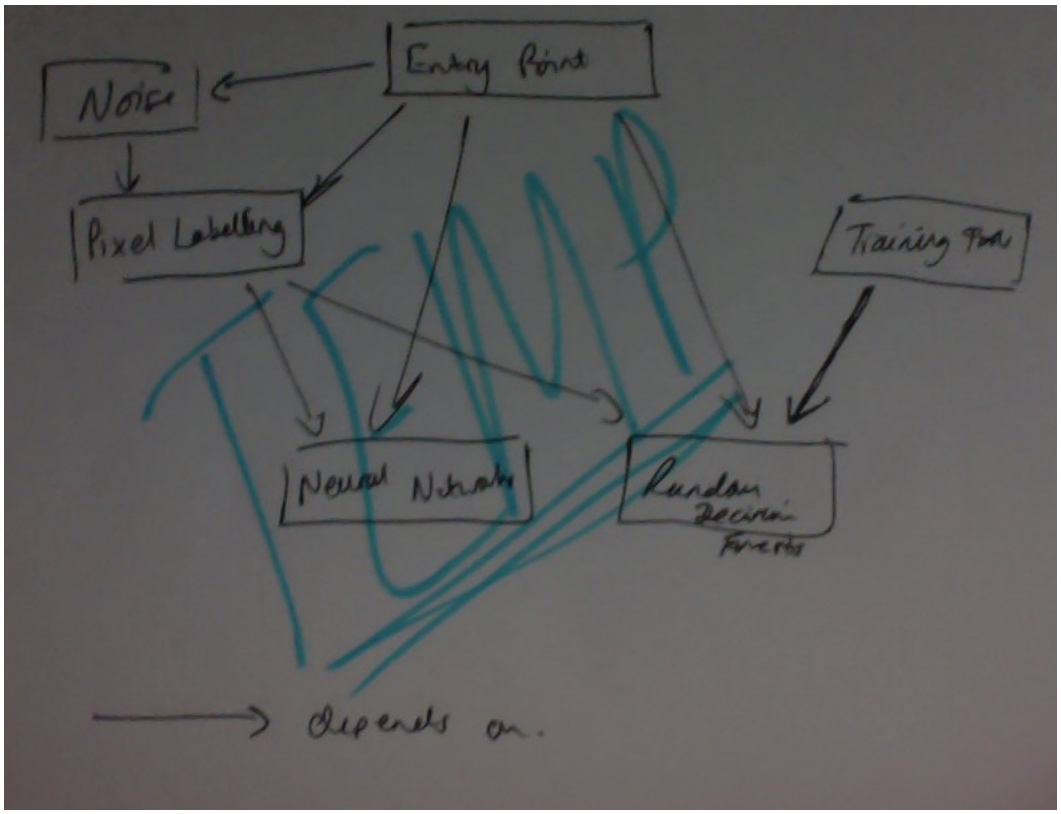


Figure 3.1: The dependencies between different packages/modules in the system. Although the TrainingTools package is capable of producing training sequence files for both the NeuralNetworks and RandomDecisionForests, it only *depends* on RandomDecisionForests as it uses the class `TrainingSequence`.

3.1 Random Forests Library

We begin by describing our implementation of random forests, looking specifically at critical design choices that were made. A generic and easily extensible random forests library is implemented, which can be specialised for many applications, then specialising subclasses are written that utilise the library for our purpose of providing a pixel labelling.

Figure 3.2: An overview of classes in the RandomDecisionForest package, from which relevant sections will be looked at closer when appropriate.

3.1.1 Data structures

A number of important data structures are used throughout the library, each requiring an efficient implementation and providing necessary abstraction. Before we move onto the more complicated issues regarding supervised learning, we need to describe the structures used. This subsection describes the main classes that are used in the RandomDecisionForest package, providing a table of functions defined with corresponding English descriptions of what they do and some small code listings where necessary.

3.1.1.1 ClassLabels

Our first class, `ClassLabels`, abstracts classification labels into its own class. As can be seen in Figure 3.3 `ClassLabels` groups together a class name and its corresponding colour, both of which should be unique, and we note that `classId` is only used internally. The colour will be used sections 3.2 and 3.4 to indicate its corresponding class in a pixel labelling, where the pixel labelling is either input in a "ground truth" image or output by our system.

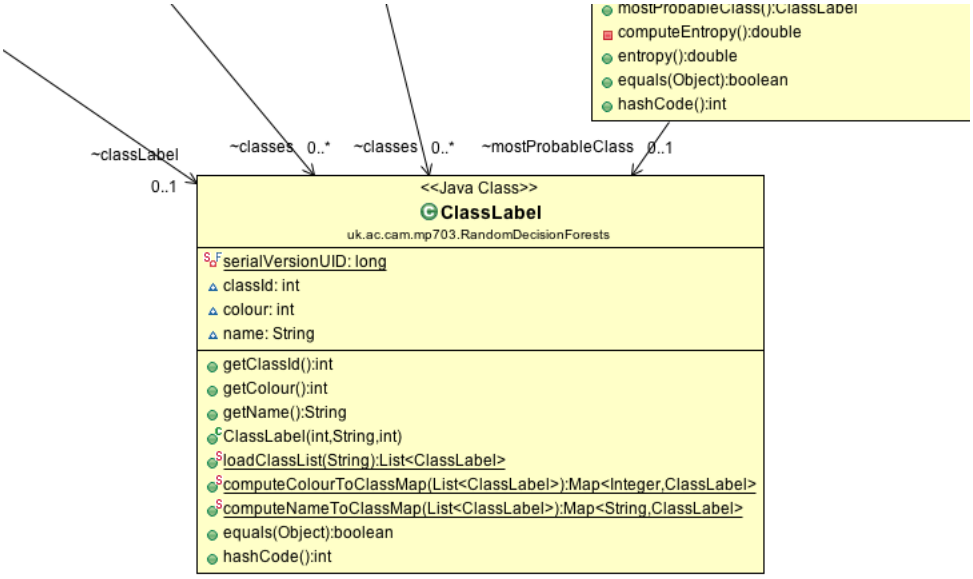


Figure 3.3: A closer view of `ClassLabel` in Figure 3.2.

Function Name	Function Description
`loadClassList`	A `static` function that returns a value of type `List<ClassLabel>` given a filename specifying "class colour map" as in appendix A, of classes specified in the file. In this function we make sure that we preserve the uniqueness of class names their associated colours.
`computeColourToClassMap`	Returns a value of type `Map<Integer, ClassLabel>`, a mapping from a class colours to their corresponding `ClassLabel` objects.
`computeNameToClassMap`	Returns a value of type `Map<String, ClassLabel>`, a mapping from a class names to their corresponding `ClassLabel` objects.
`equals`	An override of `Object`'s equality function. This is needed as we will frequently use `ClassLabel` as the key to a map structure, and might not use the same instance as a key. The function checks that the class name's, class colour's and class id's are identical.
`hashCode`	Similarly to `equals` this is overridden for a correct implementation when `ClassLabel` is used as the key in a (hash) map structure.

Table 3.1: Important methods implemented in the `ClassLabel` class.

3.1.1.2 Instances

The `Instance` class is used to specify a feature vector, or some instance of our problem. We define an interface to represent the base structure of an instance.

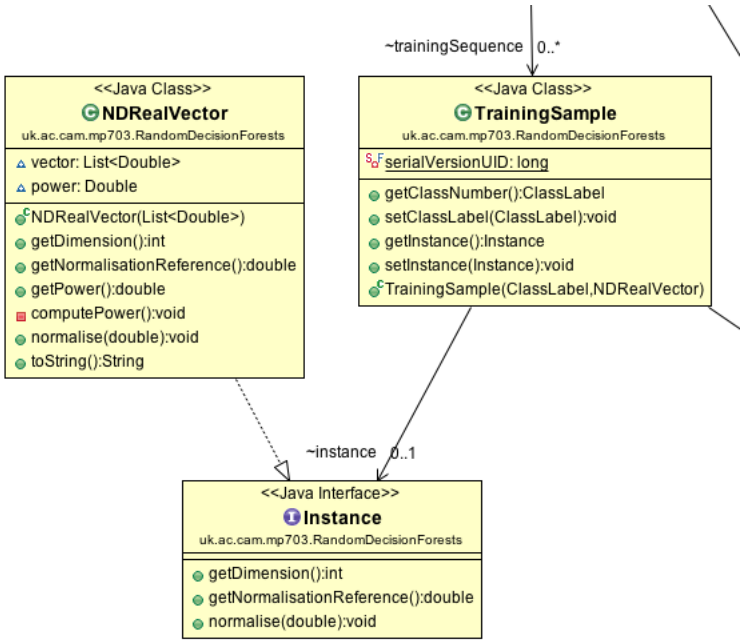


Figure 3.4: A closer view of `Instance` in Figure 3.2.

A feature vector will have some finite number of 'features' that we use and the `getDimension` function that should return the number of features (i.e. the dimension) in the instance. The functions `getNormalisationReference` and `normalise` are used for normalisation of instances. During classification we may want to normalise so that small changes in data with low variance have the same weighting as larger changes in data with low variance. This is explored more in section 4.2.6. Intuitively we define some sort of 'power' value for each instance and use normalisation so that all `Instance`s have the same power. It is optional to use normalisation in the learning (and therefore classification) algorithms in sections 3.1.2 and 3.1.3.

Let `NDRealVector` be a concrete implementation of `Instance` which can also be seen in Figure 3.4. We use `NDRealVector` to represent spectra in spectral images, that is, values in $\mathbb{R}^N$. We can simply think of this as a wrapper for a list of values. We also store the power of the spectrum, and use this as our "normalisation reference" value. The *power* of a spectrum (or vector) is the sum of squared values in the list.

Function Name	Function Description
`getDimension`	This returns n if there are n values in `vector`, our list of doubles.
`getPower`	This returns the power of the spectrum of values. If we consider the list of values to be $\mathbf{v}$ then we return $\|\|\mathbf{v}\|\|^2$.
`getNormalisationReference`	This function returns the power of the spectrum.
`normalise`	Normalisation of vectors can be implemented by scalar division of the vector with the power. I.e. we divide all values in the spectrum by the power.
`toString`	We override `Object`'s `toString` method. This is used later in section 3.4 when we wish to print a training sequence to a text file. It simply returns a comma separated list of values.

Table 3.2: Important methods implemented in the `NDRealVector` class.

3.1.1.3 Probability Distributions

As discussed in section 2.3 probability distributions are associated with each node, and is the effective output from the classification algorithm. Thus any implementation of Random Forests needs to have some way to represent probability distributions over possible classifications. Although we can represent a probability distribution as `Map<ClassLabel, Double>`, we choose to encapsulate this in its own class `ProbabilityDistribution` so that we can perform validation on the properties of a probability distribution, that is each probability is a value in $[0, 1]$ and the probabilities sum to a 1 and we also cache some frequently used values such as `entropy`.

The *entropy* of a probability distribution $p : \Omega \to [0, 1]$ can be defined as:

$$H(p) = \sum_{x \in \Omega} -p(x) \log_2(p(x)) \tag{3.1}$$

which is consistent with the definition of entropy given in equation 2.7.

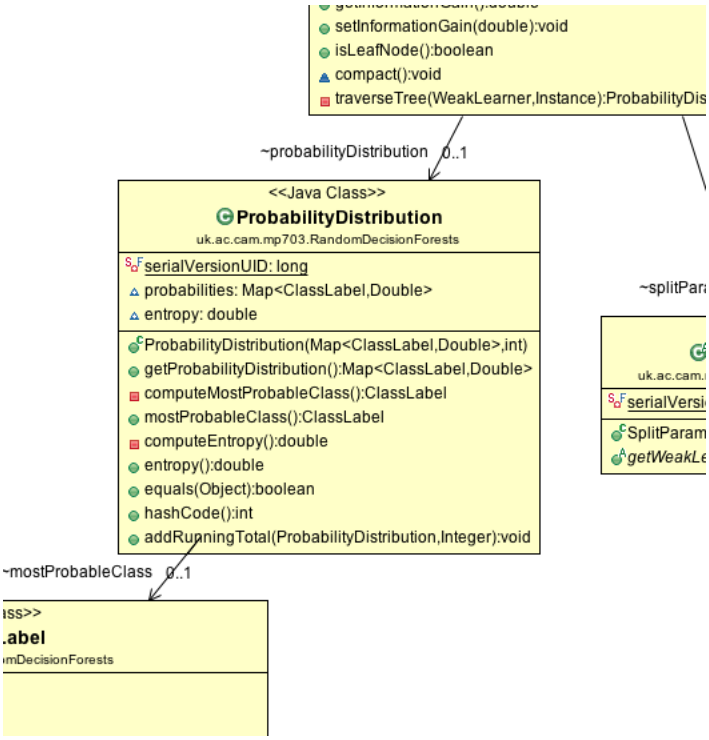


Figure 3.5: A closer view of `ProbabilityDistribution` in Figure 3.2.

The class is immutable so that we cannot accidentally modify the distribution into something invalid. Therefore we make each variable `final` and remove any setter functions. We also make use of the `unmodifiableMap` function in the `Java.Collections` package, when setting the `probabilities` variable. This gives a reference to a `Map` where no entries can be added, nor removed, which prevents someone from getting a reference to the map `probabilities` and altering it.

Also in the implementation of the class constructor we allow for a small error in the sum, this is because we will often have small errors from rounding in floating point numbers. The checks that are made in the constructor of `ProabilityDistribution` are:

- each value is in the range $[0, 1]$;
- the sum of values is in the range $[1 - \epsilon, 1 + \epsilon]$, for some $0 < \epsilon \ll 1$.

Another implementation problem is found in the computation of entropy, as $-y \log_2(y)$ isn't defined for the value of $y = 0$. Mathematically we solve this problem by setting

$$-y\log_2(y)|_{y=0} \stackrel{\text{def}}{=} \lim_{y\to 0} -y\log_2(u) \tag{3.2}$$
$$= 0. \tag{3.3}$$

When computing entropy according to equation 3.1 we try to sum with $p(x) = 0$ for some x. In this case we would accidentally set the sum to a `NaN` value

$$\texttt{sum} = \texttt{sum} + 0.0 * \log(0.0) \tag{3.4}$$
$$= \texttt{sum} + 0.0 * -\infty \tag{3.5}$$
$$= \texttt{sum} + \texttt{NaN} \tag{3.6}$$
$$= \texttt{NaN}, \tag{3.7}$$

where ∞ is the floating point representation of infinity, and we have

$$\log(0.0) = -\infty, \tag{3.8}$$
$$0.0 * \infty = \texttt{NaN}. \tag{3.9}$$

in accordance with the IEEE 754 standard [1]. We hence need to skip over updating the accumulating `sum` variable when $p(x) = 0$ otherwise we will accidentally set `sum` to a `NaN` value.

When classifying a using a decision tree we need to take an average over many probability distributions. Consider the problem of numerically computing an average

$$\overline{x}_n = \frac{1}{n}\sum_{i=1}^{n} x_i. \tag{3.10}$$

Then a naïve implementation would first compute the value of $\sum_{i=1}^{n} x_i$ and then divide by n, however for very large n this can lead to numerical instability, introducing a large rounding error. We know that the following relation holds

$$\overline{x}_n = \overline{x}_{n-1} + \frac{x_n - \overline{x}_{n-1}}{n} \tag{3.11}$$

and is easily verified by substituting equation 3.10 in the right hand side of equation 3.11. This can be used to compute $\overline{x}_n$ accurately for large n and we

```
1  public class ProbabilityDistribution implements Serializable {
2
3    ...
4
5    public ProbabilityDistribution(
6      Map<ClassLabel, Double> distribution, int noClasses)
7        throws MalformedProbabilityDistributionException {
8
9      ...
10
11     // Check that the sum is 1, allowing for a small floating
12     // point error
13     double eps = 1e-10;
14     if (sum < 1.0-eps || 1.0+eps < sum) {
15       throw new MalformedProbabilityDistributionException;
16     }
17
18     // Assign the values (so they are immutable)
19     this.probabilities =
20       Collections.unmodifiableMap(distribution);
21     this.mostProbableClass = computeMostProbableClass();
22     this.entropy = computeEntropy();
23   }
24
25   ...
26 }
```

Listing 3.1: Part of the `ProbabilityDirstribution` constructor, where we set $\epsilon = 2^{-10}$.

should provide a method to perform the equivalent procedure to equation 3.11 over probability distributions.

Function Name	Function Description
`computeMostPorbableClass`	Returns the `ClassLabel` with the highest probability in the distribution. This function is labelled private and is only used in the constructor.
`mostProbableClass`	Getter for the `mostProbableClass` value.
`computeEntropy`	Computes the entropy and returns the value. This function is labelled private and is only used in the constructor.
`entropy`	Getter for the `entropy` value.
`equals`	Override of `Object`'s function `equals`, returns true if the variable `probabilities` are equal in the two objects. We want this when comparing probability distributions rather than referential equality.
`hashCode`	Override of `Object`'s function `equals`, as we have overridden the `equals` function.
`addRunningTotal`	Add a probability to a running average distribution to avoid numerical instability problems as discussed above, using equation 3.11.

Table 3.3: Important methods implemented in the `ProbabilityDistribution` class.

3.1.1.4 Training Sequences

The `TrainingSample` object is a pairing between a `ClassLabel` and an `Instance`. There are no other functions in this class other than the getters, setters and constructor.

A `TrainingSequence` consists of a list of `TrainingSample`s, and we keep a list of `ClassLabel`s for reference. A number of convenience functions are defined in the class and are listed in table 3.4, which are used to compute useful values, such as entropy and information gain from equations 2.7 and 2.11 respectively.

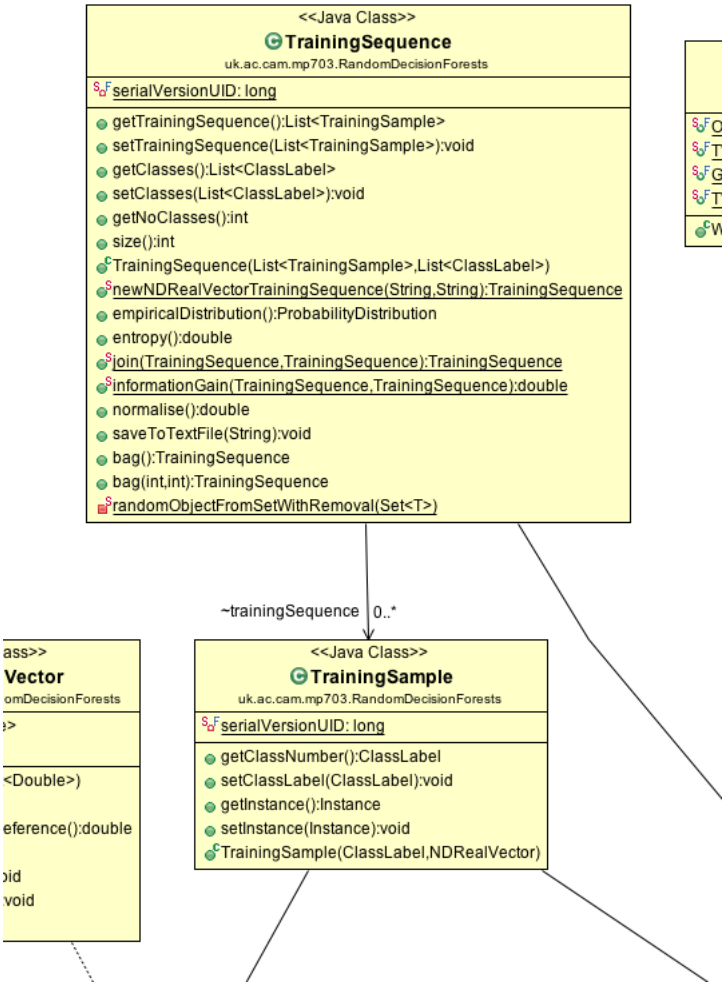


Figure 3.6: A closer view of `TrainingSequence` and `TrainingSample` in Figure 3.2.

Function Name	Function Description
`newNDRealVector-TrainingSequence`	`newNDRealVectorTrainingSequence` is a `static` function taking two file names: one specifying a "class colour map" file and one specifying a training sequence. Both these files should be of the format described in appendix A. This function parses the files and returns a `TrainingSequence` instance generated from it, with instances of the type `NDRealVector`.
`empericalDistribution`	Returns a `ProbabilityDistribution` that represents the empirical distribution of the training sequence, as defined in equation 2.8.
`entropy`	This returns the entropy of the empirical distribution. It is essentially just a shorthand for calling `empiricalDistribution().entropy()`.
`join`	A `static` function that takes two `TrainingSequence`s, and joins them together. This simply appends the lists of `TrainingSample`s from two `TrainingSequence`s into a new `TrainingSequence` instance.
`informationGain`	A `static` function that takes two `TrainingSequence`s `ts1` and `ts2`. The function returns the information gain for splitting the training sequence `join(ts1,ts2)` into the training sequences `ts1` and `ts2` according to equation 2.11.
`normalise`	This parses all of the `Instance`s in the training sequence and computes an average "normalisation reference" (see `getNormalisationReference` in table 3.2). It then returns a new training sequence where every sample has been normalised to this average value.
`saveToTextFile`	This `static` function writes out a training sequence file with the data from the given `TrainingSequence` instance, in accordance with the file format specified in appendix A.
`bag`	This performs bagging on a training sequence, and returns a bagged training sequence. The concept of *bagging* is discussed in section 3.1.2.

Table 3.4: Important methods implemented in the `TrainingSequence` class.

3.1.1.5 Split Parameters

We define an abstract class `SplitParameters`, which is used as a common superclass for any implementation of a split parameter, as defined in section 2.3.1. We make this an abstract class so that it can implement `Serializable`, forcing any implementing classes to also implement this `Serializable`. Which is necessary to be able to save decision forests to a file in section 3.1.1.8. We also mention that each split parameter needs to be able to specify what weak learner it is for, because we only save the split parameters in decision trees and we need some way to determine which `WeakLearner` subclass to use from a `SplitParameter` instance.

We also consider a concrete implementation of `SplitParameters`, in particular `OneDimensionalLinearSplitParameters` which specifies a "dimension" and a threshold as needed for the `OneDimensionalLinearWeakLearner` in section 3.1.1.6.

The `SplitParameter` classes are simple and only include getters, setters and constructors.

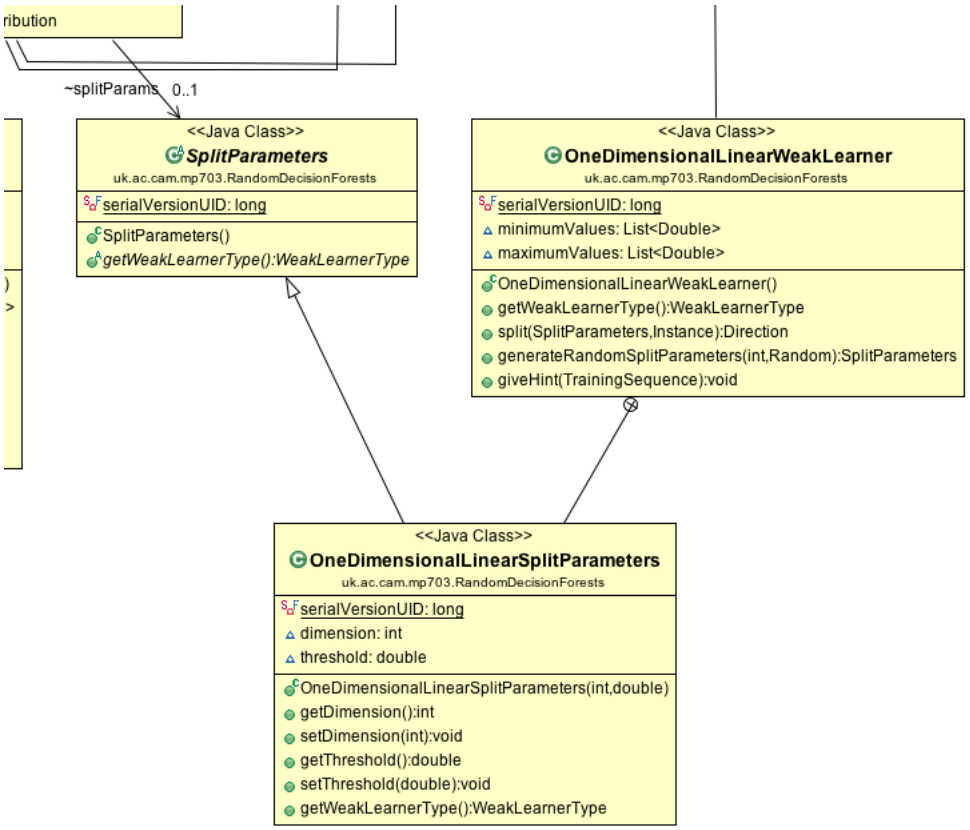


Figure 3.7: A closer view of `SplitParamter` and `OneDimensionalLinearSplitParameter` in figure 3.2.

3.1.1.6 Weak Learners

`WeakLearner` is implemented as an abstract class, because it provides a partial implementation. Any common code between subclasses can be put directly into the `WeakLearner` abstract class, such as helper functions for generation of randomised parameters. The function of each abstract method is explained in table 3.5. The function `uniformRandomDoubleInRange` is a simple convenience method that is used to generate a value uniformly in some range `[lowerBound,highBound]`, and uses Java's implementation of generating a uniform random variable in the range `[0,1]`. To identify the type of each weak learner with some tag we define an `enum` type `WeakLearnerType`, seen in Figure 3.8.

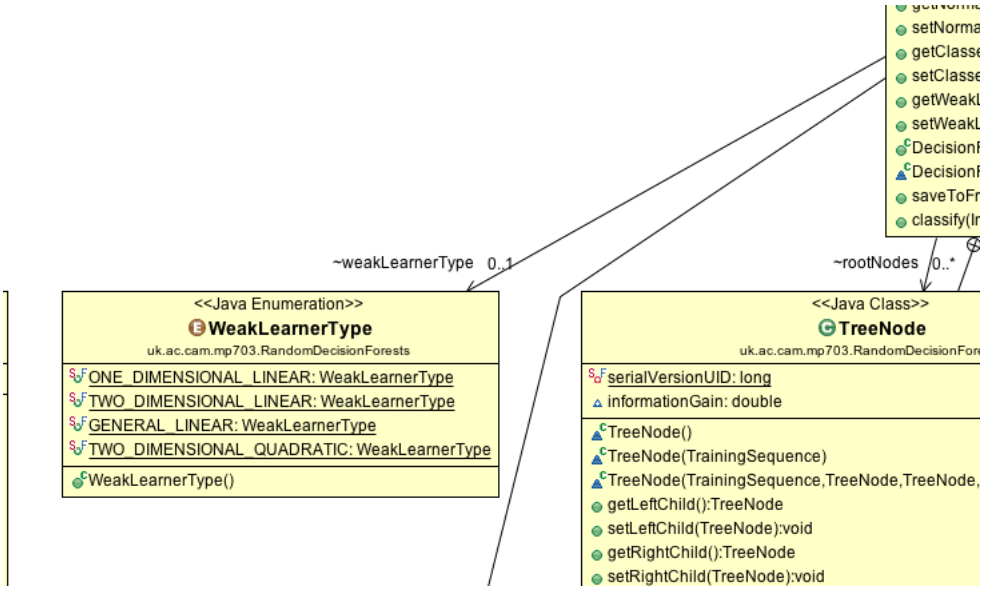


Figure 3.8: A closer view of the `WeakLearnerType` enum in Figure 3.2.

We also consider a concrete implementation `OneDimensionalLinearWeakLearner` of the `WeakLearner` class. This is the most simple weak learner function that we could use and has the simplest parameters, when we are considering `NDRealVector` instances. We note that subclasses of `WeakLearners` are specific to particular subclasses of `Instance`. The `OneDimensionalLinearWeakLearner` picks one value in the feature vector/instance, compares it to some threshold and then makes a decision based on this. For example, consider an instance $\mathbf{v} \in \mathbb{R}^n$. In this case our split parameters are $\theta = (i, \tau) \in \mathbb{Z}_n \times \mathbb{R}$, and the split function/weak learner is

$$f(\mathbf{v}; \theta) = f(\mathbf{v}; (i, \tau)) = \begin{cases} 1 & \text{if } v_i \geq \tau \\ 0 & \text{otherwise.} \end{cases} \tag{3.12}$$

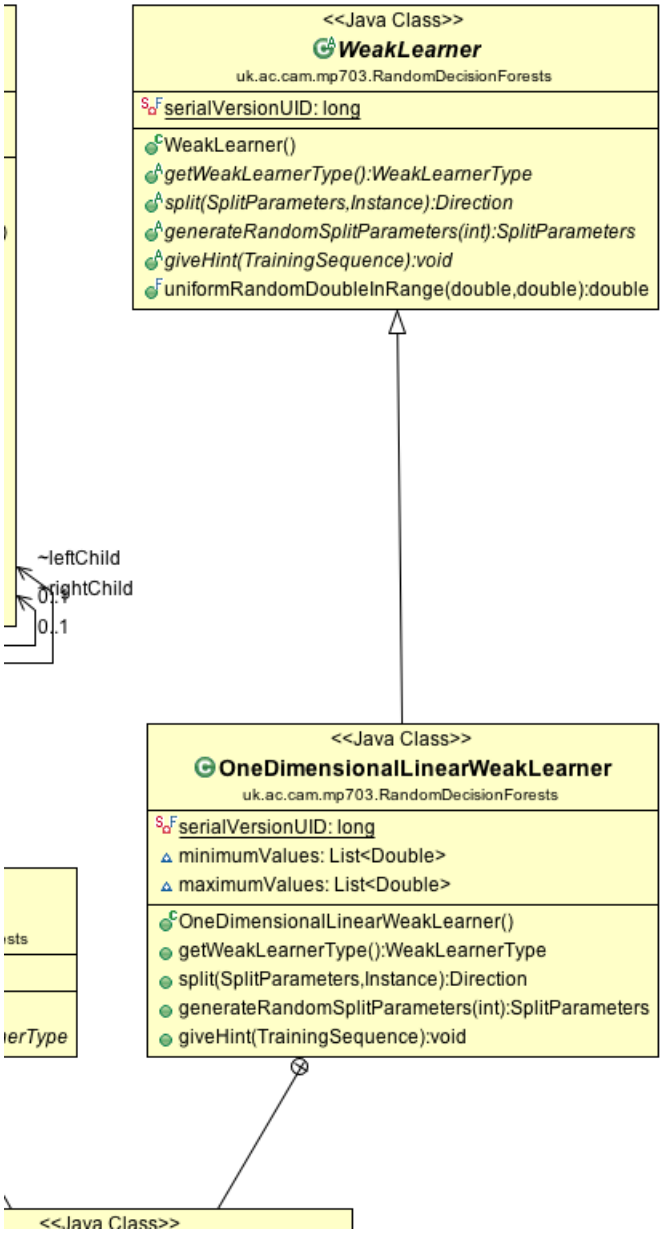


Figure 3.9: A closer view of `WeakLearner` and `OneDimensionalLinearWeakLearner` in Figure 3.2.

These split parameters for the `OneDimensionalLinearWeakLearner` class are represented by the `OneDimensionalLinearSplitParameters` class as described in section 3.1.1.5. This is an example that each subclass of `WeakLearner` should have a corresponding subclass of `SplitParameters` which it uses to represent

its split parameters. We note that `OneDimensionalLinearSplitParameters` is implemented as a nested class within `OneDimensionalLinearWeakLearner`, to make this relationship obvious.

The `split` function is of particular interest in table 3.5 as it implements equation 3.12.

Function Name	**Function Description**
`getWeakLearnerType`	A function that is used to identify what type of weak learner an instance is. This is useful when a subclass is cast to `WeakLearner` and we want to cast it back to the subclass without causing an exception.
`split`	This function takes a split parameter and an instance, it is the concrete implementation of the split function. It returns an enum of type `Direction`, which specifies if we should traverse to the left or right child of a decision tree node.
`giveHint`	In this function we are passed the training sequence prior to training a decision tree. It is used as a chance to look at the data to give a hint to what split parameters we might want to generate, or more specifically not generate.
`generateRandomSplitParameters`	This function provides a routine for generating a random split parameter to be tried in the split function during training a decision tree.

Table 3.5: Important methods implemented in the `OneDimensionalLinearWeakLearner` class.

The `OneDimensionalLinearWeakLearner` makes use of the `giveHint` function by iterating through all `NDRealVector` instances in the training sequence and recording a minimum and maximum value for each dimension in the lists `minimumValues` and `maximumValues`. This allows us to avoid picking particularly bad `OneDimensionalLinearSplitParameters`. For any of the features/dimensions in the `NDRealVector` that are chosen, if we pick a threshold value outside

the range between the minimum and maximum we know that the split function will split the training sequence with zero information gain. Using the notation from equations 2.9 and 2.10 it means that one of $L(\mathbf{s}, \theta)$ or $R(\mathbf{s}, \theta)$ will be empty, leading to an information gain of zero ($I(\mathbf{s}, \theta) = 0$ in equation 2.11).

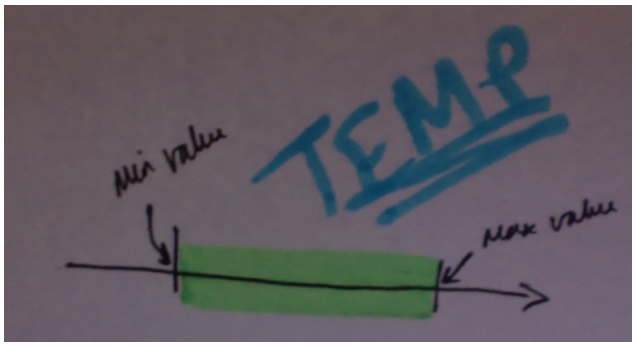


Figure 3.10: Knowing the minimum and maximum values in each dimension allows us to make an informed choice on split parameters to pick, which in this case is the green zone of values.

3.1.1.7 Decision Tree Node

Finally we move onto defining our decision tree, implement the `TreeNode` class nested in `DecisionForest` to show that their behaviour is tightly coupled. Each node has a reference to a left and right child node, which are set to `null` in a leaf node. Every node caches a probability distribution, even if it is a decision node, and the probability distribution that is cached is the empirical distribution of the training sequence that is passed to it. Each decision node has a reference to a `SplitParameters` instance, which it uses with a weak learner to make decisions for tree traversal as in section 2.3.1. We then cache the information gain, computing it according to the equation 2.11 during the training algorithm.

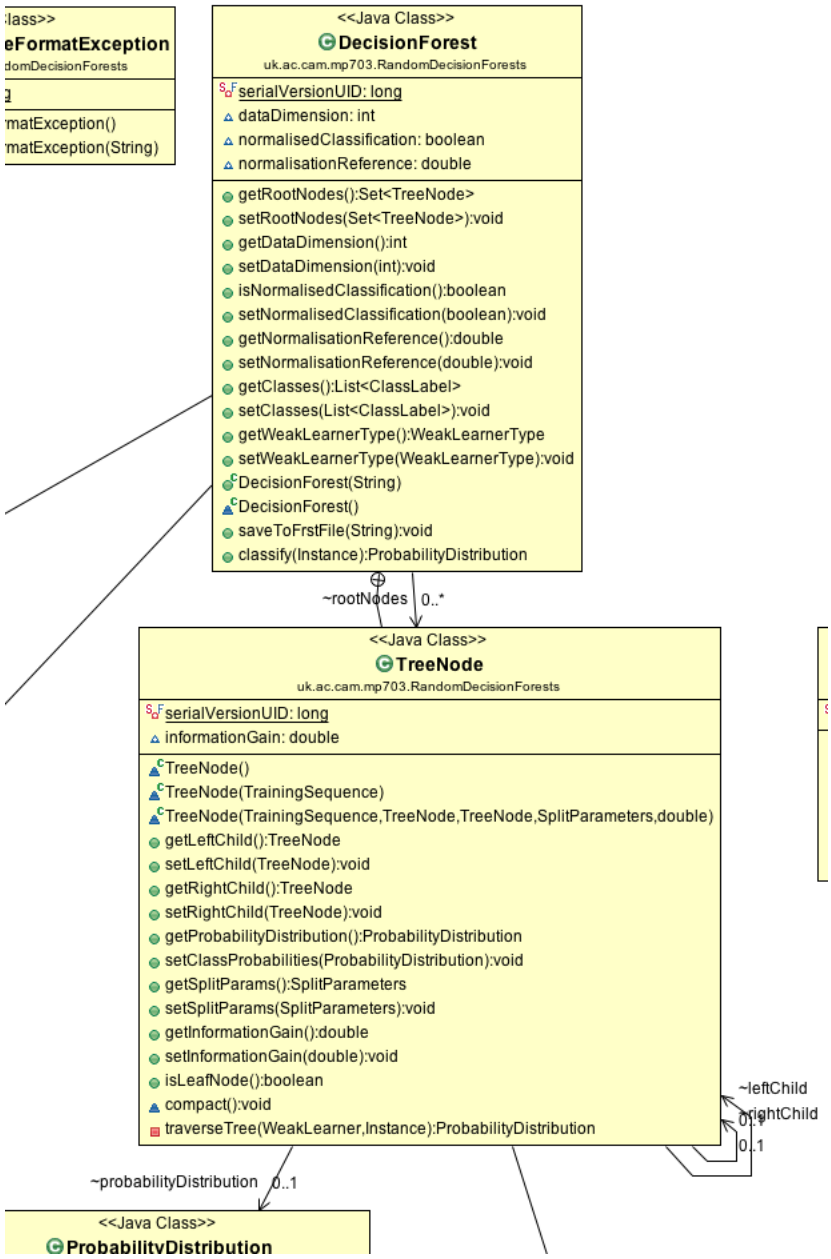


Figure 3.11: A closer view of `TreeNode` and `DecisionForest` in Figure 3.2.

The function `compact` is seen in listing 3.2. This is an optimisation used to eliminate unnecessary nodes from the tree after its construction. If we are at some decision node and it has two children which are leaf nodes with identical distributions, then we can replace this decision node by a single leaf node with the same distribution. The implementation performs `compact` recursively on the left and right children of a decision node first, and `compact` does nothing in the base case (a leaf node), after we try to compact at the given node. Essentially,

compaction is performed from the bottom of the tree upwards.

We also note that the `TreeNode` class implements the `Serializable` interface, which is again necessary to be able to use `ObjectOutputStream` in section 3.1.1.8, when saving forests to a file.

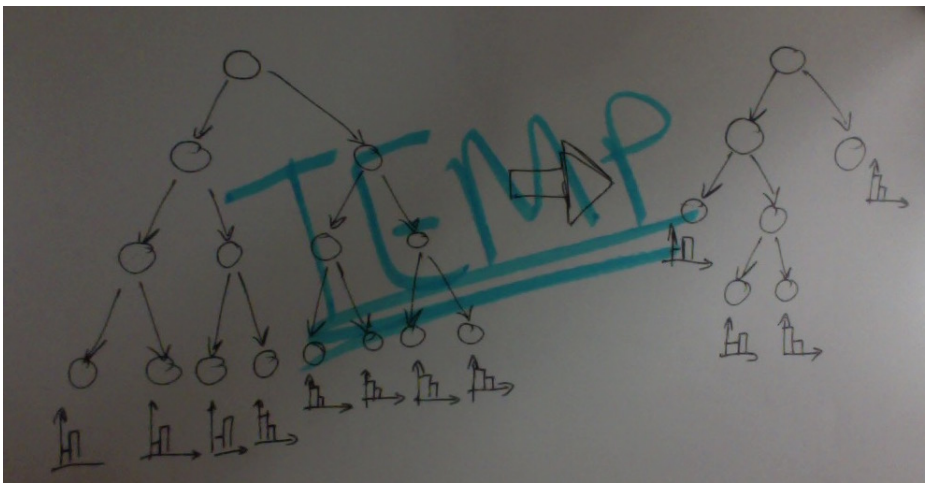


Figure 3.12: An example of how `compact` could be used to reduce the size of a decision tree.

Function Name	**Function Description**
`isLeafNode`	Checks if the `leftChild` and `rightChild` have a value of `null`. If they do then the node is a leaf and this functions returns a true value. If only one of the nodes has a value of `null` then the tree is invalid and an exception is raised. Otherwise it returns a false value.
`compact`	As described above, this compacts the tree to an equivalent tree, replacing any unnecessary decision nodes with a leaf node.
`traverseTree`	A method that given an instance of a `WeakLearner` and an `Instance` will traverse the tree and return a probability distribution for that instance. As described in section 2.3.1 and visualised in figure 2.3. The algorithm this method implements is covered in more detail in section 3.1.3.

Table 3.6: Important methods implemented in the `TreeNode` class.

```
1  void compact() throws MalformedForestException {
2    if (this.isLeafNode()) {
3      return;
4    }
5
6    this.leftChild.compact();
7    this.rightChild.compact();
8
9    if (!this.isLeafNode() &&
10       leftChild.isLeafNode() &&
11       rightChild.isLeafNode() &&
12       probabilityDistribution.equals(leftChild.↩
             probabilityDistribution) &&
13       probabilityDistribution.equals(rightChild.↩
             probabilityDistribution)) {
14
15     // Make this node a leaf node
16     leftChild = null;
17     rightChild = null;
18   }
19 }
```

Listing 3.2: The `TreeNode` declaration, found as a static class within the `DecisionForest` class.

3.1.1.8 Decision Forest

The `DecisionForest` class is basically a set of `TreeNode`s, which also includes additional metadata, that which can be seen in Figure 3.11. We have made sure that `TreeNode`, `WeakLearner`, `WeakLearnerType`, `SplitParameters` and `ClassLabel` (which are all composite in the forest data structure) implement the interface `Serializable` so that a concise "save to file" method can be implemented. We use an instance of `ObjectOutputStream` in the `Java.Io` package to write the object to a binary file in a single line "`out.writeObject(this);`".

`dataDimension` keeps track of the dimension of data this forest classifies, while the `weakLearnerType` specifies what weak learner our forest is related to, and implicitly the type of data that it classifies. The `DecisionForest` keeps a reference to all the possible classification labels in the variable `classes` of type `List<ClassLabel>`. `DecisionForest` uses `normalisedClassification` and `normalisationReference` to perform normalisation during classification, if we specified that normalised values should be used during training.

Function Name	Function Description
`DecisionForest`	We have a `default` access default constructor, which is used to construct forests in the training algorithm. The other allows the forest to be loaded from a file using an `ObjectInputStream` from the `Java.Io` package.
`saveToFrstFile`	This function saves a forest to a persistent ".frst" file.
`classify`	This takes an `Instance` and returns a probability distribution for it, according to the forest. The algorithm implementation is discussed in more detail in section 3.1.3.

Table 3.7: Important methods implemented in the `DecisionForest` class.

3.1.2 Training

The concept of training was discussed in section 2.2 and an overview of how we can train decision trees and decision forests in section 2.3. This section provides some simple psuedocode to generate trees given a training sequence, then extends it for training a decision forest. We then discuss some design choices for an implementation of the algorithm, problems that may be encountered and some possible solutions to those problems.

```
1  TreeNode generateTree(trainingSequence, depth, ↩
       randomnessParameter) {
2    // Base (terminating) case
3    if (depth <= 0) {
4      return new TreeNode(trainingSequence);
5    }
6
7    // Remember the best split
8    bestInfoGain = 0.0;
9    bestLeftSplit = null;
10   bestRightSplit = null;
11
12   // Try [randomnessParameter] number of times
13   for (int i = 0; i < randomnessParameter; i++) {
14
15     // Split
16     splitParameter = generateRandomSplitParameter();
17     for (sample in trainingSequence) {
18       // 'split' is our split function
19       if (split(sample, splitPerameter) == 0) {
20         leftSplit.add(sample);
21       } else {
22         rightSplit.add(sample);
23       }
24     }
25
26     // Update best if necessary
27     infoGain = informationGain(leftSplit, rightSplit)
28     if (infoGain > bestInfoGain) {
29       bestInfoGain = infoGain;
30       bestLeftSplit = leftSplit;
31       bestRightSplit = rightSplit;
32     }
33   }
34
35   // Recurse
36   leftChild = generateTree(bestLeftSplit, depth-1, ↩
       randomnessParameter);
37   rightChild =  generateTree(bestRightSplit, depth-1, ↩
       randomnessParameter);
38
39   // Return the tree
40   return new TreeNode(leftChild, rightChild)
41 }
```

Listing 3.3: Psuedocode to train a decision tree.

The full code listing for training a decision tree is given in listing B.1. The value `randomnessParameter` is the value ρ from section 2.3.3. The algorithm abstracts away from using a single weak learner and the `WeakLearner` class specifies functions synonymous to the `generateRandomSplitParameter` and `split` used in listing 3.3. This allows the algorithm for training to be written in a generic way and allowing for high code re-usability.

There are a number of things to consider when implementing this algorithm if we wish to return useful and efficient trees. Firstly, deep trees (specified by a high depth) may be necessary to provide correct classifications in large multi-class problems, however as we get deeper into the tree, decision nodes could be adding little information. I.e. consider when we have a empirical distribution at depth 3 which is almost identical to the distribution found at depth 20, in this case the decisions made at depths 3 to 20 have made very little difference to the output and effectively waste computation time. To ameliorate the problem we can provide a threshold value for the information gain, which if not surpassed at some node causes the training to terminate. This is included in the implementation seen in listing B.1 with the parameter `informationGainCutoff`.

Secondly we consider the generation of split parameters. Sometimes with prior information, or even analysis of the training sequence, a more informed choice of split parameter can be made. We talk about this at the end of section 3.1.1.6, when we discuss optimising `OneDimensionalWeakLearner` parameter selection. The optimisation discussed is included in the `OneDimensionalWeakLearner` implementation.

Lastly, in listing 3.3 we see a depth first traversal of the tree as we train it, alternatively a breadth first approach can be imagined, as in Figure 3.13, where we train all nodes at some depth at the same time and the collective information gain is what we optimise over. In the implementation B.1 we decide to implement a depth first algorithm as it is easier to parallelise (and distribute if wanted), because each of the child nodes are trained independently.

The algorithm for training a decision forest extends easily from training a decision tree and psuedocode is given in listing 3.4.

In listing 3.4 the training sequence is 'bagged' for each tree, which yields a subsequence of the training sequence, which is used to train each tree. The term *bagging* refers to taking a subsequence of the training sequence and using that for training. Here it is used as a way to introduce randomness and is a way to reduce over-fitting. One problem which is commonly encountered and leads to over-fitting is when on class of data is abundantly in the training sequence, and another class of data isn't. In this case the abundant data will have a large influence on the information gain from equation 2.11. We can deal with this

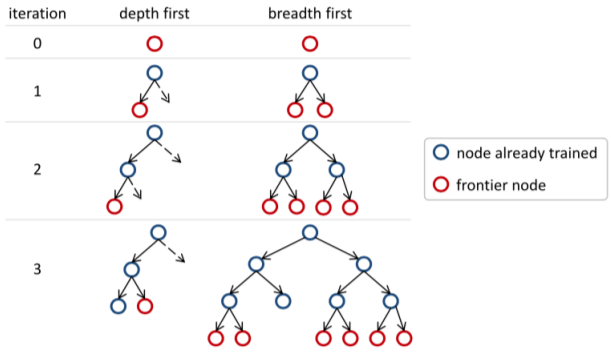


Figure 3.13: Visualisation of breadth first vs depth first. Optimisation of information gain takes place over all of the nodes in the frontier. Recreated from Criminisi et al [6].

```
1  DecisionForest train(trainingSequence, noTrees,
2    depth, randomnessParameter) {
3
4    rootNodes = [];
5    for (int i = 0; i < noTrees; i++) {
6      subSequence = trainingSequence.bag();
7      treeNode =
8        generateTree(subSequence, depth, randomnessParameter);
9      rootNodes.add(treeNode);
10   }
11
12   return new DecisionForest(rootNodes);
13 }
```

Listing 3.4: Psuedocode to train a decision forest.

```
ProbabilityDistribution traverseTree(instance) {
  currentNode = this;
  while (!isLeaf(currentNode)) {
    direction = split(currentNode.splitParams, instance);
    if (direction == LEFT) {
      currentNode = currentNode.leftChild;
    } else {
      currentNode = currentNode.rightChild;
    }
  }

  // When we get here we are a leaf node
  return currentNode.probabilityDistribution;
}
```

Listing 3.5: Psuedocode for traversing a decision tree.

problem either by weighting the influence of each class inversely by its size in equation 2.11 or by bagging in such a way that each tree is trained on a sequence with equal numbers of samples from each class. In our implementation in listing B.2 we take the later approach.

Another trick that can be used to reduce over-fitting is to increase the randomness of our choice of split parameters. By this we mean using a low value for ρ or `randomnessParameter`. One option is to start with a low value of ρ at high depths in the tree and increase it at lower depths. This is not included in our implementation.

Finally there is some obvious parallelism to exploit again, where each tree can be independently trained in it's own thread. This is a feature of the actual implementation and can be seen in listing B.2.

3.1.3 Classification

As discussed in section 2.3.3 we classify by walking along each tree and averaging over the different distributions. Psuedocode for traversing the tree is given in listing 3.5 and psuedocode for classification is given in listing 3.6.

Similar to the learning algorithm, parallelism can be exploited from traversing each tree in a separate thread, and again is in the implementation found in listing 3.6. We make use of the `addRunningTotal` function that we defined in section 3.1.1.3 so that we sum in a numerically stable fashion. There is not much

```
1  public ProbabilityDistribution classify(instance) {
2    for (node in rootNodes) {
3      if (accumulatingDistr == null) {
4        accumulatingDistr = node.traverseTree(instance);
5        treesTraversed++;
6      } else {
7        leafDistr = node.traversTree(instance);
8        accumulatingDistr.addRunningTotal(leafDistr, ++↩
             treesTraversed);
9      }
10   }
11   return accumulatingDistr;
12 }
```

Listing 3.6: Psuedocode for classification using a decision tree.

more that can be said about the classification algorithm for random forests, its simplicity is one of its major advantages.

3.2 Neural Networks

For our neural network solution we use a standalone Java neural network library, Encog. Following Encog's quickstart guide[2] it is very easy to set up a simple neural network. Then using Encog's user guide[3] gives us a better understanding of Encog's architecture and how it can be manipulated into what we want.

To load a dataset, we

3.3 Pixel Labelling

- We've given the overview of two supervised machine learning techniques
- Assume for now that we have appropriate training data - dealt with later
- We now need to use that to provide a pixel labelling
- Listing for the datacube, and listing that implements the pixel labelling

[2]https://s3.amazonaws.com/heatonresearch-books/free/encog-3_3-quickstart.pdf
[3]https://s3.amazonaws.com/heatonresearch-books/free/Encog3Java-User.pdf

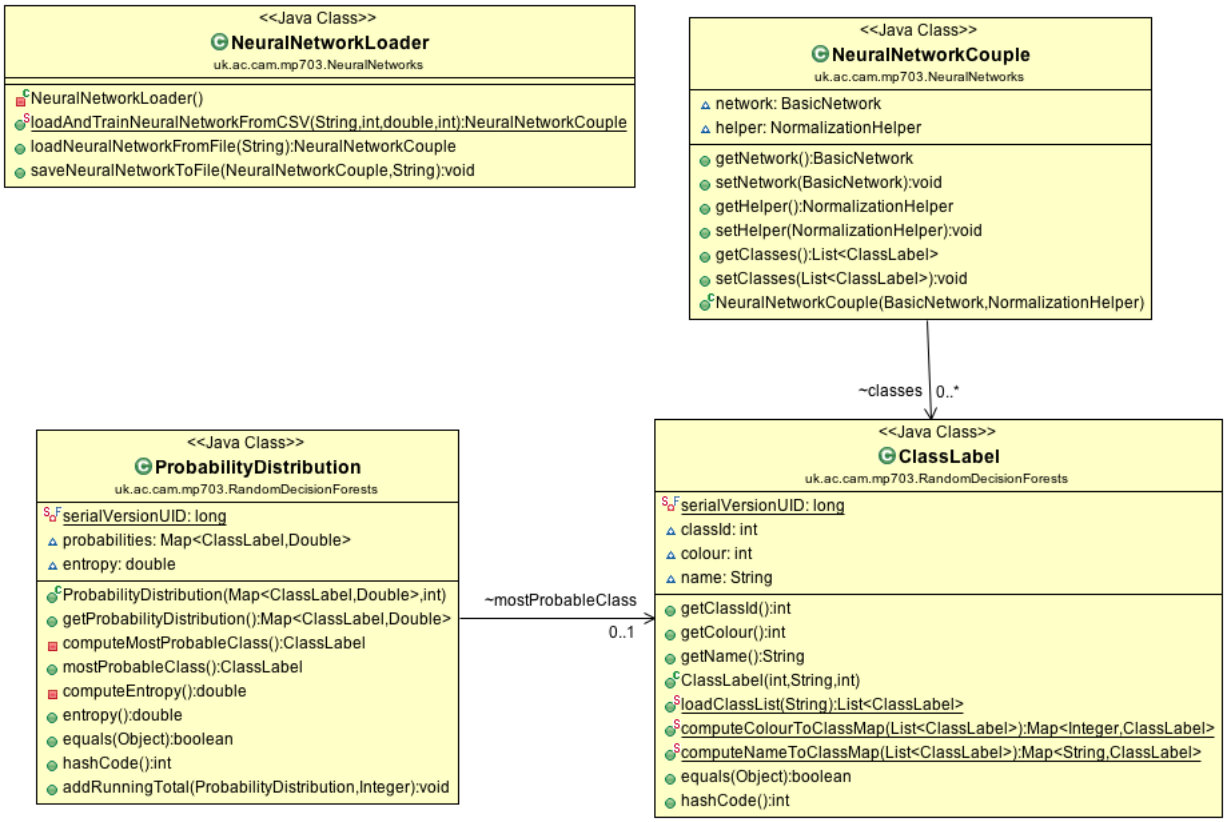


Figure 3.14: The UML diagram for the training tools, consisting of a single class with a single static method.

- Assuming we have appropriate training data, and non-noisy images we are now done! Unfortunately not the case.

3.4 Training Tools

At this point we now have a system capable of producing pixel labellings. This section is concerned with making the task of generating a training sequence feasible, as it is certainly not by hand. It would be preferable to have some way of taking a "ground truth" pixel labelling and transforming it into a training sequence. This is precisely what the training tools module does.

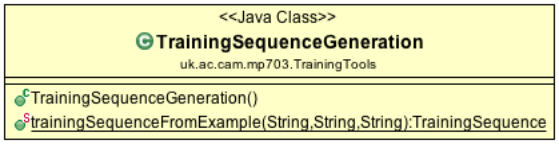


Figure 3.15: The UML diagram for the training tools, consisting of a single class with a single static method.

The function `trainingSequenceFromExample` performs the following sequence of actions:

1. Load the list of classes into a `List<ClassLabel>` object and uses `computeColourToClassMap` in `ClassLabel` to compute a map from colours to classes.

2. Load in the ground truth pixel labelling and the spectral image into the `DataCube` object from section 3.2.

3. For each pixel (x, y):

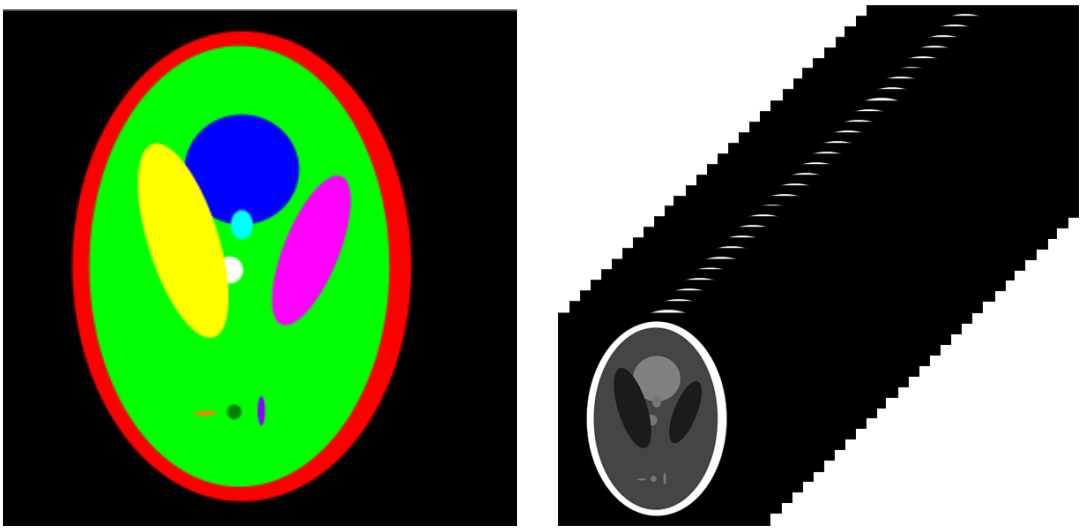
   3.1. Put the spectrum at (x, y) into a `NDRealVector` instance.

   3.2. Lookup the correct `ClassLabel` object from the map computed in step 1, using the colour in the ground truth image at (x, y).

   3.3. Pair the `ClassLabel` and `NDRealVector` together in a `TrainingSample` and put it into an accumulating training sequence.

4. Return the accumulated training sequence.

When using the training tools module through the `.jar` file, the interface adds an extra step to the end, using the `saveToTextFile` function of the



```
Skeleton, 0xFF0000,
Tissue, 0x00FF00,
LeftOrgan, 0xffff00,
CentreOrgan, 0x0000ff,
RightOrgan, 0xff00ff,
Artifact1, 0x00ffff,
Artifact2, 0xffffff,
Artifact3, 0xff7f00,
Artifact4, 0x008100,
Artifact5, 0x8c00ff,
Background, 0x000000
```

Figure 3.16: An example input to the training tools module: a ground truth pixel labelling, a spectral image and a class to colour mapping file (as defined in appendix A).

```
...
Artifact3, 140.0, 140.0, 141.0, 141.0, 140.0, 139.0, 145.0,
148.0, 148.0, 149.0, 148.0, 150.0, 147.0, 145.0, 143.0, 140.0,
140.0, 141.0, 141.0, 140.0, 140.0, 140.0, 141.0, 139.0, 140.0,
139.0, 140.0, 140.0, 139.0, 139.0;
Tissue, 91.0, 92.0, 90.0, 91.0, 91.0, 92.0, 95.0, 94.0, 100.0,
104.0, 105.0, 104.0, 100.0, 99.0, 96.0, 95.0, 94.0, 95.0, 91.0,
89.0, 89.0, 91.0, 90.0, 90.0, 91.0, 91.0, 92.0, 90.0, 91.0,
90.0;
...
```

Figure 3.17: Example of part of the output file (2 training samples) from the training tools module. (The actual file is over 88000 lines long).

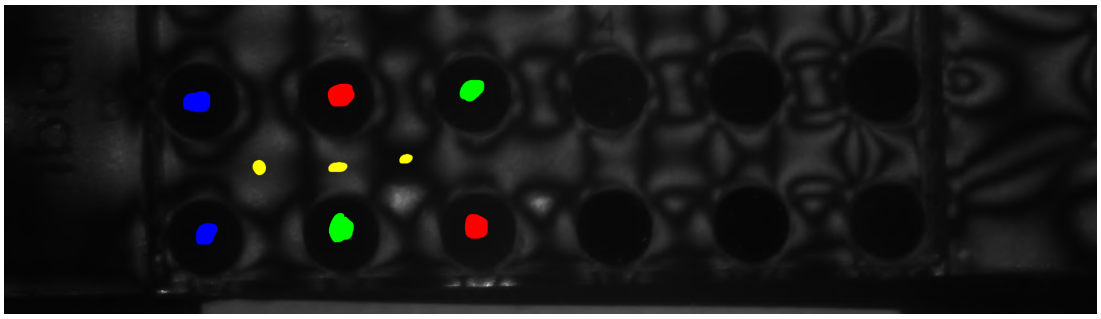


Figure 3.18: An example of a pixel labelling we might want to provide, when we wish to ignore large regions of the image.

`TrainingSequence`, which saves and formats the sequence to a text file. We can also use the `.jar` to pass the generated `TrainingSequence` directly to the one of the training functions specified in sections 3.1.2 and 3.2.

If an 'invalid' colour is encountered in the example labelling we have two reasonable options, either raise an exception or just ignore the spectrum for that pixel. Our implementation we decide to opt for the latter, as it provides greater flexibility to use the system when input data isn't perfect, for example in figure 3.18.

3.5 De-noising

- Explain total variation

- Minimising gradients, can think of this as removing high frequency components
- Listing for overview of

3.6 Application on example data sets

- We've build a system, but we need to actually apply it to some problems!

3.6.1 Siri's data

- TODO: Come up with a better title for this subsection
- Explanation of how produced training data
- Example pixel labellings

3.6.2 Teng's data

- TODO: Come up with a better title for this subsection
- Explanation of how produced training data
- Example pixel labellings

Chapter 4

Evaluation

In this section we will look at the performance of the different components of the system based on a number of metrics.

4.1 Performance measures for classifiers

- Briefly say about the different measures as described at the end of AI II.
- Justify what might be the most informative here.

4.2 Evaluation of the Random Forests library

- Define a standard training set, this can actually be independent of pixel labelling and similar to the Chriminsi forests paper.

4.2.1 Training time

4.2.2 Classification time

4.2.3 The effect of the number of trees

4.2.4 The effect of the depth of trees

4.2.5 The effect of the randomness of trees

4.2.6 The effect of normalisation

4.3 The effect of the de-noising component

- Use a couple images with added noise
- Compare the SNR for the method with respect to different noise models (does it handle any other types of noise?)
- Plot SNR as a function of the parameter lambda in the TVMM method
- Plot SNR as a function of noise power (for different types of noise)

Chapter 5

Conclusion

5.1 Summary

- Overview and summary of work undertaken - re describe system overall
- What was achieved, what was different
- What did the evaluation show?

5.2 Further Work

- Implement a convolutional neural network solution to allow local spatial data to influence the labelling of a pixel. This may allow the model to incorporate image de-noising and could compact two stages of the pipeline into one.
- Implementation of the random forests library to support GPU processing. We could use a language such as OpenCL. Parallelism could be exploited either in the random forest implementation OR/AND the inherent parallelism from performing image processing.

5.3 Lessons Learned

- When using machine learning, use someone else's library, they probably spent a long time on it and it will save a lot of work. It took one day to implement the NN solution, whereas a long time was spent on the RF solution. Even if it did a lot better, it was a lot more pain and effort. "Stand on the shoulders of giants".

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Appendix A

File formats

Here we define the file formats that a user might be expected to input into the system, an explanation of the files that are output by the system and how to interpret them.

A.1 (Example/Noisy) Spectral Image

...

A.2 Example Image Labelling

...

A.3 Label Map

```
typewriter .txt file eg here
```

A.4 Training Sequence

```
typewriter .txt file eg here
```

A.5 Output Files

...

Appendix B

Code for training a decision forest

```
1  private static TreeNode generateTree(
2    TrainingSequence trainingSequence,
3    WeakLearner weakLearner,
4    int depth,
5    int randomnessParameter,
6    double informationGainCutoff)
7      throws MalformedProbabilityDistributionException {
8
9    // Check for the training sequence being 0 in size, that
10   // should never happen
11   if (trainingSequence.size() == 0) {
12     throw new IllegalArgumentException(
13       "Can't generate a tree from an empty sequence.");
14   }
15
16   // If the depth is zero or there is only one sample in
17   // the training sequences, then we need to create a leaf
18   // node, take the class as the majority vote from the
19   // training sequence.
20   if (depth <= 0 || trainingSequence.size() == 1) {
21     return new TreeNode(trainingSequence);
22   }
23
24   // Give the weak learner the training sequence as a hint
25   // for what subspace of the split parameter space it
26   // should search
27   weakLearner.giveHint(trainingSequence);
28
```

```
29    // We will generate split paramters, and we will keep
30    // track of the best split. Initialise best information
31    // gain to -1.0 so we have a check that it was explicitly
32    // set at least once in the loop
33    double bestInformationGain = -1.0;
34    TrainingSequence bestLeftSplit = null;
35    TrainingSequence bestRightSplit = null;
36    SplitParameters bestSplitParameters = null;
37    int dataDimension = trainingSequence.trainingSequence.
38        get(0).instance.getDimension();
39
40    // Try "randomnessParameter" number of random split
41    // parameters
42    for (int i = 0; i < randomnessParameter; i++) {
43      SplitParameters splitParameters =
44        weakLearner.generateRandomSplitParameters(
45          dataDimension);
46      List<TrainingSample> leftList = new ArrayList<>();
47      List<TrainingSample> rightList = new ArrayList<>();
48
49      // Split the training sequence into a left and right split
50      for (TrainingSample sample :
51          trainingSequence.trainingSequence) {
52
53        if (weakLearner.split(splitParameters, sample.instance)
54              == Direction.LEFT) {
55          leftList.add(sample);
56        } else {
57          rightList.add(sample);
58        }
59      }
60
61      // See what information gain this leads to
62      TrainingSequence leftSplit = new TrainingSequence(
63        leftList, trainingSequence.classes);
64      TrainingSequence rightSplit = new TrainingSequence(
65        rightList, trainingSequence.classes);
66      double informationGain =
67        TrainingSequence.informationGain(leftSplit, rightSplit);
68
69      // If its the best information gain found so far,
70      // remember it!
71      if (informationGain > bestInformationGain) {
72        bestInformationGain = informationGain;
73        bestLeftSplit = leftSplit;
74        bestRightSplit = rightSplit;
75        bestSplitParameters = splitParameters;
```

```
76      }
77    }
78
79    // We make a greedy choice using the best split that we
80    // found, and recursively build our child nodes.
81    // N.B. If the split doesn't gain enough information, then
82    // just try again, (so we've used up "one depth").
83    // N.B.B. informationGainCutoff >= 0.0, and if one of the
84    // sequences is empty, then there is and information gain of
85    // 0.0, hence if one of the sequences is empty we don't EVER
86    // pass the information gain cutoff. Hence any split that
87    // actually causes a recursion will have two non empty
88    // subsequences.
89    TreeNode node = null;
90    if (bestInformationGain <= informationGainCutoff) {
91      node = generateTree(trainingSequence, weakLearner, depth-1,
92          randomnessParameter, informationGainCutoff);
93    } else {
94      TreeNode leftChild =
95        generateTree(bestLeftSplit, weakLearner, depth-1,
96          randomnessParameter,informationGainCutoff);
97      TreeNode rightChild =
98        generateTree(bestRightSplit, weakLearner, depth-1,
99          randomnessParameter, informationGainCutoff);
100     node =
101       new TreeNode(trainingSequence, leftChild, rightChild,
102         bestSplitParameters, bestInformationGain);
103   }
104
105   // We have trained a tree! Return it
106   return node;
107 }
```

Listing B.1: The implementation code for tree generation.

```
1  public static DecisionForest trainDecisionForest(
2      final TrainingSequence trainingSequence,
3      final WeakLearner weakLearner,
4      final int maxTrees,
5      final int maxDepth,
6      final int randomnessParameter,
7      final double informationGainCutoff,
8      final boolean normaliseInstances,
9      final boolean bagging)
10     throws MalformedForestException,
```

```
11        MalformedProbabilityDistributionException,
12        InterruptedException {
13
14    // If we are given nonsensical input, throw an exception
15    if (trainingSequence == null || trainingSequence.size() == 0
16      || trainingSequence.classes.size() == 0) {
17      throw new IllegalArgumentException("We need a non-empty, "
18          + "non-null training sequence to train a tree.");
19    } else if (weakLearner == null) {
20      throw new IllegalArgumentException("We need a non-null "
21          + "weak learner to be able to train a tree.");
22    } else if (maxTrees <= 0) {
23      throw new IllegalArgumentException("A non-positive "
24          + "number of trees doesn't make sense for a forest.");
25    } else if (maxDepth <= 0) {
26      throw new IllegalArgumentException("A non-negative depth "
27          + "doesn't make sense for a tree. A tree consisting "
28          + "of a single node has depth 0. If we limit trees to "
29          + "be just leaves then there is no decisions being "
30          + "made - the tree does nothing.");
31    } else if (randomnessParameter <= 0) {
32      throw new IllegalArgumentException("We need a positive "
33          + "randomness parameter, it doens't make sense to "
34          + "have a negative quantity.");
35    } else if (informationGainCutoff < 0.0) {
36      throw new IllegalArgumentException("Information gain is "
37        + "a strictly non-negative value, so must have a cutoff "
38        + "of more than or equal to zero.");
39    }
40
41    // Normalise the training sequence if we want that
42    // Remember the reference value (power)
43    double normalisationReference = 0.0;
44    if (normaliseInstances) {
45      normalisationReference = trainingSequence.normalise();
46    }
47
48    // Create a DecisionForest instance
49    DecisionForest forest = new DecisionForest();
50    forest.setDataDimension(trainingSequence.trainingSequence.
51      get(0).instance.getDimension());
52    forest.setClasses(trainingSequence.classes);
53    forest.setWeakLearnerType(weakLearner.getWeakLearnerType());
54
55    // Use a new thread to build each tree
56    final Set<DecisionForest.TreeNode> rootNodes =
57      new HashSet<>();
```

```
58    Set<Thread> workers = new HashSet<>();
59    for (int i = 0; i < maxTrees; i++) {
60
61      // Train the new tree in its own thread
62      Thread thread = new Thread() {
63        public void run() {
64          // Perform bagging of the training sequence if we want
65          TrainingSequence ts = trainingSequence.bag();
66          if (bagging) {
67            ts = trainingSequence.bag();
68          }
69
70          // Generate the tree node
71          TreeNode node = generateTree(ts, weakLearner, maxDepth,
72              randomnessParameter, informationGainCutoff);
73          node.compact();
74          synchronized(rootNodes) {
75            rootNodes.add(node);
76            System.out.println("Tree number " + rootNodes.size()
77              + " trained.");
78          }
79        }
80      };
81      thread.start();
82      workers.add(thread);
83    }
84
85    // Wait for the threads to finish
86    for (Thread thread : workers) {
87      thread.join();
88    }
89
90    // Add the root nodes to the forest structure
91    forest.setRootNodes(rootNodes);
92
93    // Add normalisation variables to the forest structure
94    forest.setNormalisedClassification(normaliseInstances);
95    forest.setNormalisationReference(normalisationReference);
96
97    // Return the constructed forest
98    return forest;
99  }
```

Listing B.2: The implementation code for training a decision forest.

Appendix C

Code for classifying using a decision forest

```
1  private ProbabilityDistribution traverseTree(
2    WeakLearner splitter,
3    Instance instance)
4      throws MalformedForestException {
5
6    try {
7      // Use the split function to traverse the tree until we
8      // hit a root node
9      TreeNode currentNode = this;
10     while (!currentNode.isLeafNode()) {
11       Direction splitDirection =
12         splitter.split(currentNode.splitParams, instance);
13
14       if (splitDirection == Direction.LEFT) {
15         currentNode = currentNode.leftChild;
16       } else {
17         currentNode = currentNode.rightChild;
18       }
19     }
20
21     // Return the class associated with the root node
22     return currentNode.probabilityDistribution;
23
24   } catch (NullPointerException ex) {
25     // If we get a null pointer, then we must have a
26     // malformed tree
27     throw new MalformedForestException("Failed traversing a "
28       + "tree due to null pointer exception.");
```

```
29    }
30  }
```

Listing C.1: The implementation code for tree traversal.

```
1   public ProbabilityDistribution classify(
2     final Instance instance) {
3
4     // Create a splitter depending on our weak learner type
5     final WeakLearner splitter;
6     switch (weakLearnerType) {
7       case ONE_DIMENSIONAL_LINEAR:
8         splitter = new OneDimensionalLinearWeakLearner();
9         break;
10      default:
11        throw new MalformedForestException("No weak learner for "
12          + "the type given, unable to classify.");
13    }
14
15    // If we are using normalised labeling, then normalise
16    if (normalisedClassification) {
17      instance.normalise(normalisationReference);
18    }
19
20    // Define a wrapper for the accumulator distribution
21    // We use this as a closure in the threads, so we get past
22    // the restriction of only using final variables in threads
23    final class AccumulatorDistributionWrapper {
24      ProbabilityDistribution accDistr;
25      int distributionsSummed;
26    }
27
28    // Define the accumulator distribution we use
29    final AccumulatorDistributionWrapper wrapper =
30      new AccumulatorDistributionWrapper();
31
32    // Compute the trees votes in parallel, and then add them
33    // together in an accumulating probability distribution
34    Set<Thread> threads = new HashSet<>();
35    for (final TreeNode node : rootNodes) {
36
37      // Run the traversal in a new thread
38      Thread thread = new Thread() {
39        public void run() {
40        // Traverse to the leaf distribution, then add it to the
```

```
41        // accumulating
42        ProbabilityDistribution leafDistr =
43          node.traverseTree(splitter, instance);
44
45          synchronized(wrapper) {
46            if (wrapper.distributionsSummed == 0) {
47              wrapper.accDistr = leafDistr;
48            }
49            else {
50              wrapper.accDistr.addRunningTotal(
51                leafDistr, wrapper.distributionsSummed+1);
52            }
53            wrapper.distributionsSummed++;
54          }
55        }
56      };
57      threads.add(thread);
58
59    }
60
61    // Wait for the threads to finish
62    for (Thread thread : threads) {
63      thread.join();
64    }
65
66    // Return the probability distribution
67    return wrapper.accDistr;
68  }
```

Listing C.2: The implementation code for classification using a decision forest.

Appendix D

Project Proposal

Computer Science Project Proposal

Spectral Image Analysis for Medical Imaging

M. Painter, Churchill College

Originator: Dr. Pietro Lio'

Project Supervisor: Dr Pietro Lio', Dr Gianluca Ascolani

Director of Studies: Dr John Fawcett

Project Overseers: Prof John Daugman & Dr David Greaves

Introduction and Description of the Work

The core idea of the project is to use spectral algorithms and machine learning to analyse biomedical images. I will explore the use of multiple learning techniques (namely Random Decision Forests and Neural Networks) and compare them via a number of metrics, described later.

The aim of the project will be to build a classifier that is capable of handling a wide variety of noisy medical images. Different types of medical images will present different challenges such as contrast between tissues and amount and type of noise. It will classify images per pixel into classes (dependent on the image), using the spectral analysis.

During the implementation I will start by implementing something for a toy problem, by which I mean an artificially produced, noiseless image. From this solution I will move onto solving the same problem with the introduction of artificial noise, at which point I will explore the use of de-noising techniques to improve the accuracy of the classifier. Finally after this I will move onto an implementation for real images.

For the real images I will use MRI images from Zhongzhao Teng from the Department of Radiology, Engineering, which include fatty tissues from patients with atherosclerosis (the build up of fatty tissues in arteries). In this case I can train the classifier to recognise regions of calcium, lipids, haemorragic tissue, and mixtures of these.

To demonstrate the versatility of the tool I will also use another set of images obtained in a completely different way, so will present a different set of challenges including the nature of noise in the image. The images are from Siri Luthman of the BSS group in the Department of Physics, and are obtained using a hyper-spectral camera with 72 spectral bins. The images use contrast agents with various spectral profiles, each of which has a negative binding response or neutral binding response for cancerous cells. By ‘negative binding response’ I mean that the contrast agent binds to only non-cancerous cells, and ‘neutral’ means that it binds to both cancerous and non-cancerous cells. Here the classes will be cancer cells, non-cancerous cell, and a mixture of both.

Starting Point

I will use Java for the implementation of my algorithms and use libraries provided for Java. I will also use OpenCV's machine learning library as a benchmark to test my implementations against.

Resources Required

I will use my own computer to code on as I am more comfortable with it than the MCS machines.

I will also need example (spectral) image sets to be used in training and testing. I have kindly been provided with some MR images by Zhongzhao Teng of the Department of Ragiology and some hyperspectral images from Siri Luthman of the BSS group in the Department of Physics, as mentioned in the introduction.

Backup Plan

I will be using a git repository for my project, which will be a private repository on GitHub. I will have two branches (at least, more if necessary) one 'master' for completed features and one 'in progress'. The in progress branch will be to push regularly any unfinished/in progress work onto so that my work is always backed up, and I don't loose any work in progress.

The local folder will also be in my Google Drive folder and so will be automatically synced to the Google servers, and I also have a time machine set up, which will take backups of the whole file system every hour.

Work to be done

I can break down the project into the following stages:

1. Implement the infrastructure (data structures etc) and reading in of the raw data.
2. Create a tool used to indicate areas of interest on the teaching data to be used with the training data.

3. Implement the main machine learning algorithm(s), and implement an out the box solution, initially to solve the 'toy problem'.

4. Extend the implementation to work for noisy images and then real images.

Success Criterion for the Main Result

I will use an 'out the box' solution (such as OpenCV's machine learning libraries) as a benchmark to compare my implementation(s) against. I will provide each machine learning algorithm with the same inputs for training and the same inputs for testing and will use the following metrics to compare the performance of the systems and which has 'learnt' better:

- Overall run time (of classifying a single image);
- Accuracy of classifier (percentage images correctly identified).

Possible Extensions

- *Image Segmentation.*

  It would be useful to be able to segment the images given into separate regions of interest. (For example if we want to classify an image with cancer cells present, we indicate the regions containing cancerous cells). This is opposed to just returning the output per pixel, and would provide a more useful output for users.

- *Dimensionality Reduction.*

  If I finish the core of my project then one of the additional tasks that I could look at would be to implement a data reduction (learning) algorithm. In a spectral image with a high number of spectral bands it would be useful to identify which spectral bands are important to the classification and which are not.

  This problem more generally is called "dimensionality reduction" as we are looking to reduce the dimension of data input to the algorithm.

Timetable: Workplan and Milestones to be achieved.

Michaelmas weeks 3–4 (26th Oct to 4th Nov)

In preparation for the main implementation I will read about many machine learning algorithms. For example I will use the book "Decision Forests for Computer Vision and Medical Image Analysis" to learn about Random Forests. I will similarly research about Neural networks, and I will also research some other forms of learning algorithm.

Deliverables:

- A small description/overview of random forests and how they work, and a similar description for any other learning algorithms researched. This should be written up in LaTeX for easy embedding into the preparation chapter of the dissertation.

Milestones:

- Preparation reading completed, so that I am sufficiently able to implement the learning algorithm(s) and handed in description of reading to project supervisor for review - 4th Nov.

Michaelmas weeks 5–6 (5th Nov to 18th Nov)

I will spend this block familiarising myself with any technologies that I will possibly use. This will include the OpenCV library. I will also design a simple UI that will be used for the supervised learning. I will also familiarise myself with OpenCL and GPU programming.

Deliverables:

- A sketch of the UI for the tool which will be used for the supervised learning.
- A small overview of what OpenCV, GPU programming (or other technology(s) I have looked at), and a description of why/where they will be useful. This should again be written up in LaTeX for easy embedding into the preparation chapter of the dissertation.

Milestones:

- Handed in the UI design to supervisor for review - 9th Nov

- Handed in the description of familiarisation of technologies to supervisor for review - 18th Nov.
- Demonstrated any small programs written for familiarisation to supervisor - 18th Nov.

Michaelmas weeks 7–8 (19th Nov to 2nd Dec)

Implementation block 1. Implement the infrastructure that will be used for the project. This will include loading the raw data into the appropriate data structures and do so efficiently as possible.

Deliverables:

- A bullet point list indicating what has been implemented during this block. Written up in LaTeX and to be used as a basis for the implementation portion of the dissertation. To be handed in for review.

Milestones:

- Have the framework that I will use completed, including unit tests, and demonstrate the tests to supervisor to check that this has been done - 2nd Dec.

Christmas vacation weeks 1–2 (3rd Dec - 16th Dec)

I will be on holiday during this period and so I will work on little bits when I can, this may be catching up on any work that I got behind on in Michaelmas term (effectively making this a 'slack' block), and I will begin some work on the next block if up to date.

Christmas vacation weeks 3–4 (17th Dec - 30th Dec)

Implementation block 2. Write the tool that will be used to indicate which images (or image regions) belong to a given class to be used for the supervised learning.

Deliverables:

- A bullet point list indicating what has been implemented during this block. Written up in LaTeX and to be used as a basis for the implementation portion of the dissertation.

Milestones:

- Sent the completed tool to my supervisor as proof of completion. (As it is the vacation I will not be in Cambridge and so will not be able to demonstrate in person). - 30th Dec

Christmas vacation weeks 5–6 (31st Dec - 13th Jan)

Implementation block 3. Implement the machine learning algorithm(s) chosen, and also write the 'out of the box' solution using the OpenCV library. At this stage I will only aim to have

If this block is delivered on time then I am close to having a completed project. I have purposely stacked more of the work in the holiday compared to term time, as I have other commitments in term than out of term, such as lectures and supervisions.

Deliverables:

- A bullet point list indicating what has been implemented during this block. Written up in LaTeX and to be used as a basis for the implementation portion of the dissertation.

Milestones:

- Finished writing the machine learning algorithm, and demonstrated it classifying some 'toy images' to supervisor - 13th Jan. (I will be back in Cambridge by this time).

Lent weeks 1–2 (14th Jan - 27th Jan)

The progress report needs to be given up by noon on the 29th Jan, and so should be written in this block.

This rest of this block will be kept free for 'slack'. This slack should include incorporating any feedback from my supervisor.

If I am up to date and there is no additional feedback that needs to be resolved, then I will proceed to work a block ahead. This will give me an additional block at the end of lent to implement any extensions.

Deliverables:

- Progress report.

- Item written in LaTeX which begins with the supervisors comments/feedback and ends with how that was incorporated into the system.

Milestones:

- Demonstration of any features added made to supervisor - 27th Jan

Lent weeks 3–4 (28th Jan - 10th Feb)

Implementation block 4. In this block I will finish implementing my solution, and extend my simple solution to a more complex one capable of handling 'toy images' with artificial noise, and then real images. This will require implementing de-noising of the images.

Also after the progress report a small presentation needs to be prepared. I will use the beginning of this time block to do this.

Deliverables:

- A bullet point list indicating what has been implemented during this block. Written up in LaTeX and to be used as a basis for the implementation portion of the dissertation.

Milestones:

- Hand in progress report (completed in the previous block) - 29th Jan.
- Perform a small mock presentation/interview with supervisor - 3rd Feb.
- Made progress presentation to overseer group - 5th Feb.
- Finished implementing any de-noising algorithms, and have a working solution for real images, including a demonstration to supervisor - 10th Feb.

Lent weeks 5–6 (11th Feb - 24th Feb)

Evaluation of the system. This will require writing tests that will gather the quantitative data (run time and accuracy of classification) to be used in the comparison required to satisfy the success criteria.

I will generate graphs from data in this phase using MATLAB, so that I can decide if the data is useful or not. This will prevent me from realising that the data isn't good at too late a stage in the project and when there is not enough time to re-evaluate the system. This has the advantage that the graphs will be ready to be exported directly into the dissertation.

Deliverables:

- Table for any qualitative data evaluated and spreadsheet of quantitative data, which must include values for accuracy of the system (in a specific test case) and timings for how long classification takes (on my home machine).
- Generated meaningful graphs using MATLAB with data gathered from evaluation.

Milestones:

- Table/spreadsheet completed and filled out with all data required for a good write up. Spreadsheet and graphs sent to supervisor for reviewing - 24th Feb.

Lent weeks 7–8 (25th Feb - 9th Mar)

I will use my last block of work in lent as another 'slack' block for if I get behind on any work for any reason such as a high load of supervision work through the term. This should also be used to incorporate any final feedback from my supervisor.

If am up to date at this point I will work on implementing some of the extension tasks outlined in this document.

Milestones:

- System complete, success criterion met and demonstrated these to supervisor - 9th Mar.

Easter vacation weeks 1–2 (10th Mar - 23rd Mar)

Set up the dissertation document and write introduction and preparation chapters of the dissertation.

Deliverables:

- Introduction and preparation chapters of dissertation.

Milestones:

- Completed first draft of introduction chapter and given to supervisor - 17th Mar.
- Completed first draft of preparation chapter and given to supervisor - 23rd Mar.

Easter vacation weeks 3–4 (24th Mar - 6th Apr)
Write up the implementation and evaluation chapters of the dissertation.

Deliverables:

- Implementation and evaluation chapters of dissertation.

Milestones:

- Completed first draft of implementation chapter and given to supervisor - 31st Mar.
- Completed first draft of the evaluation chapter and given to supervisor - 6th Apr.

Easter vacation weeks 5–6 (7th Apr - 20th Apr)
Complete dissertation by completing the conclusion section and any appendices. I will also re-iterate through dissertation see if anything can be improved.

Deliverables:

- Draft of complete dissertation.
- 2nd draft of complete dissertation.

Milestones:

- Full first draft of dissertation handed into supervisor for review - 11th Apr.
- Hand in second draft of completed dissertation to supervisor - 18th Apr.

Easter term weeks 1–2 (21st Apr - 5th May)
Final 'slack' block for the dissertation. If the dissertation is completed then I will proof read multiple times. I would like to have the dissertation 'finished' by now to focus on revision for the exam and on learning any of the Easter term courses.

Milestones:

- System complete and success criterion met - 5th May.

Easter term week 3 (6th May - 13th May)
Final proof read and then an early submission so that I can focus on exam revision for the remainder of the term.

Deliverables:

- Dissertation.

Milestones:

- Hand in dissertation on time. (Project finished). - 13th May.

Appendix E

Glossary