Deep learning of data cubes: From human hearts to galaxies.

Michael Smith, James Geach

University of Hertfordshire

Introduction

Deep learning with a two-channel three dimensional Convolutional Neural Network (CNN) has been used to successfully diagnose and locate artefacts in simulated 3D two channel Single Photon Emission Computed Tomography (SPECT) heart scans. Transferability of diagnosis has been demonstrated between simulated and real SPECT scans.

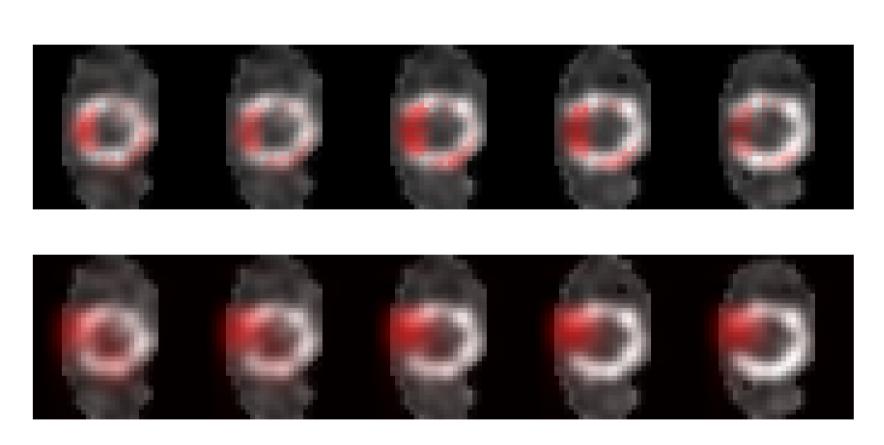


Figure 1: Detection of an artefact site performed via occlusion mapping (top), and Class Activation Mapping (CAM, [Zhou et al., 2016]) (bottom).

The SPECT scans used share a lot of similarities with astronomical Integral Field Unit (IFU) and spectral data cubes, and so the techniques used here can be generalised to classification problems in three dimensional astronomical data. For example, automatic classification of dynamical systems and blind source detection could be achieved through a simple replacement of the medical training data with labelled astronomical training data.

CNN architecture

The CNN used for SPECT scan diagnosis has:

- A three dimensional, dual-channel architecture. One channel carries a scan of the heart when the patient is at rest. The other carries a scan of the patient's heart when they they are performing a cardiac stress test.
- A global average pooling layer in place of traditional dense layers, with the added benefits of fewer parameters, and easy, computationally cheap attention visualisation (through CAM, [Zhou et al., 2016]).

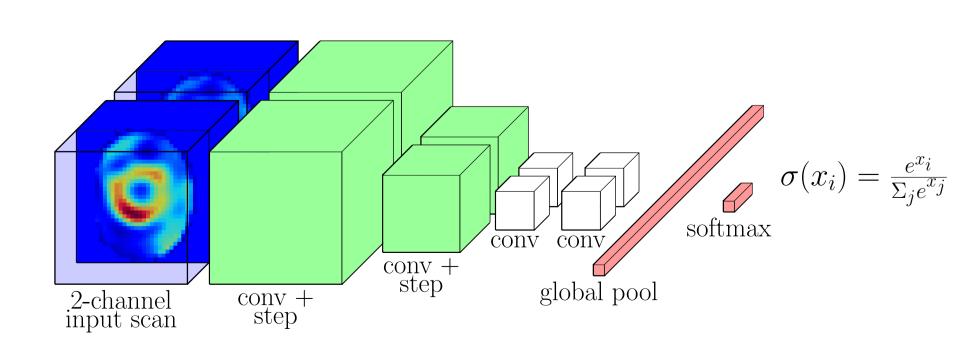


Figure 2: Green convolutional layers have a kernel size of [4,4,4], and a step size of 2. White convolutional layers have a kernel size of [2,2,2], and a step size of 1. A global average pool is used to merge the two channels together and feed them forward to the softmax diagnosis layer.

SPECT CNN training method

- 1. Cut and interpolate incoming SPECT scans so that they have a shape of [32,32,32,1]. Concatenate "rest" and "stress" scans together along the fourth axis, resulting in an array of shape [32,32,32,2].
- 2. Train the CNN on simulated scans, with 10,000 simulations per class of illness. The classes chosen were: Infarcted, ischaemic, artefacted, mixed, and healthy. The simulations were generated through a parametric method.
- 3. Finetune the CNN on available real data by holding all but the final two layers static, and continuing training on the real data. Finetuning reduces the chances of overfitting, always a problem when training on small (in this case, 29 healthy, and 29 ischaemic scans) datasets.
- 4. **Highlight artefact sites** with the fully trained classifier through either CAM, or occlusion mapping.

SPECT CNN results

Table 1 summarises the diagnostic ability of the CNN on simulated scans. Figure 3 shows the ROC curves for both the CNN trained on simulated scans, and the finetuned CNN.

Normal	Ischaemic	Infarcted	Mixed	Artefact	Avg
0.45	0.51	0.37	0.47	0.51	0.46

Table 1: Performance of multi-diagnosis CNN at 30 epochs of 50,000 total scans evenly distributed over all diagnoses. The first five values are the accuracies found from an unseen validation set of 5,000 total scans, with 0.2 being the accuracy if the diagnosis is chosen randomly.

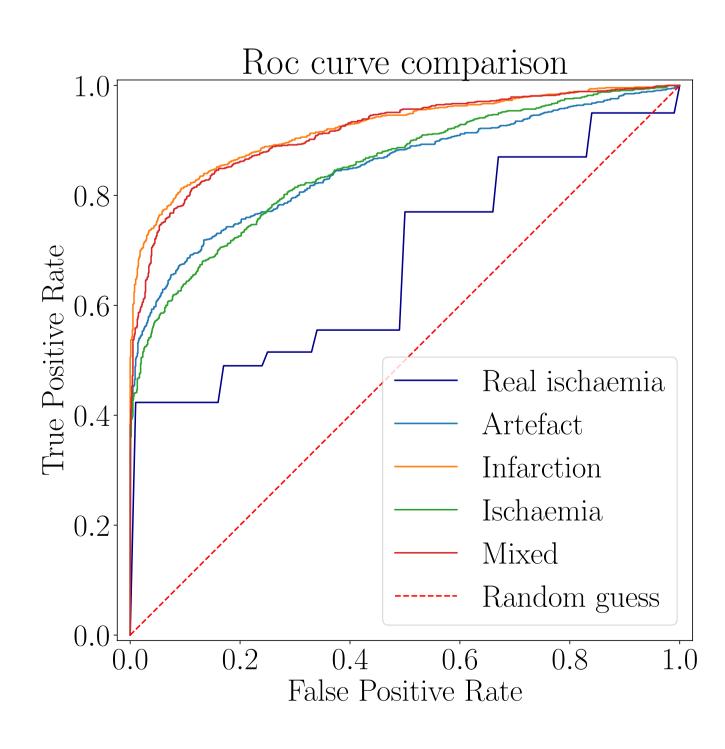
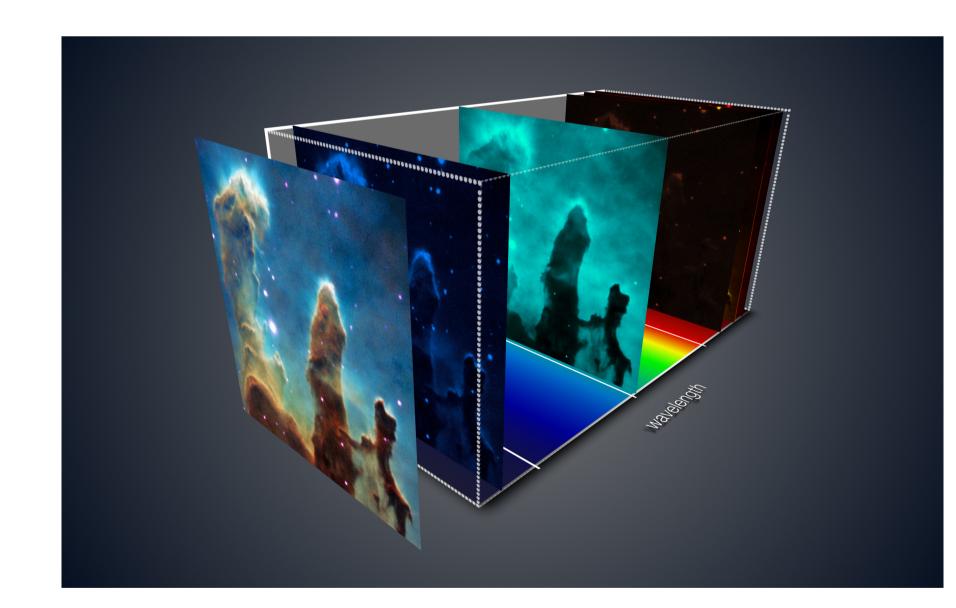


Figure 3: ROC curves of all possible ill/healthy combinations of simulated data diagnosis pairs, and mean ROC curve of the real data healthy/ischaemia pair over k = 5 folds.

Adaptation to astronomical data cubes

- The SPECT CNN can easily be adapted for training (and categorising) astronomical integral field unit (IFU) or interferometric data cubes, where one may wish to automatically identify and classify sources of line or continuum emission, or detect specific spectral features (e.g. absorption systems).
- We aim to train our CNN on simulated Atacama Large Millimetre/submillimetre Array (ALMA) 'mock observations' of cosmological volumes to generate 1000s of data cubes with and without realistic noise and astronomical signal. The underlying simulation provides the ground truth that will allow us to test how well the CNN can be used to rapidly identify real sources of emission in interferometric blank fields (e.g. http://www.mpia.de/~ASPECS/).
- Figure 4 shows some schematic examples of astronomical IFU cubes. It can be seen that their shapes are similar to our SPECT data.



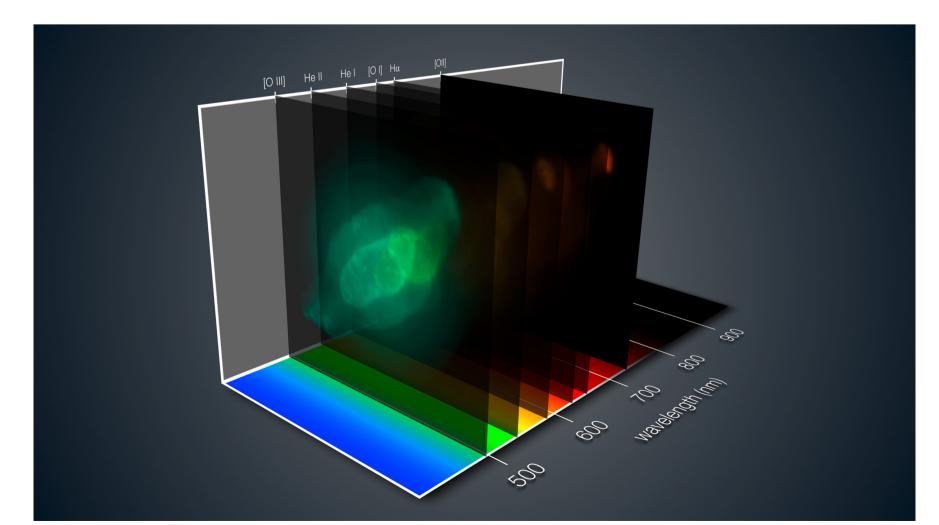


Figure 4: IFU cube examples of the Pillars of Creation (top [ESO, 2015]) and the Saturn Nebula (bottom [ESO, 2017]), observed by the European Southern Observatory's (ESO) Very Large Telescope (VLT) multi unit spectroscopic explorer.





Conclusions

- Figure 3 shows that the SPECT CNN works well on simulated SPECT scans, and has some diagnosis transferability to the very small real SPECT scan sample. With enough real scans (or more accurate simulations) we can expect a greatly improved diagnostic capability.
- The CNN developed for SPECT scan classification can be easily adapted for use with astronomical IFUs or interferometric data cubes, for rapid identification of emission sources in blank fields. Far more of this astronomical data is available compared to the SPECT data, so we can expect better classification results.

Forthcoming research

- GAN data augmentation: Since our SPECT data sample is small, the addition of more data would almost certainly result in greater classification accuracy. An unsupervised data augmentation method, trained with classically augmented data may produce more convincing simulations than the current parametric method. Generative Adversial Networks (GANs) are good candidates for carrying out this augmentation, since the latest generation has been shown to generate very convincing large images [Goodfellow et al., 2014, Jolicoeur-Martineau, 2018]. This unsupervised augmentation can also be applied to astronomical data cubes.
- Massively parallel computing: Writing the CNN in TensorFlow allows us to leverage the many distributed computing libraries available for Tensor-Flow [Abadi et al., 2015]. Currently, Horovod is being used to parallelise training over many GPUs, resulting in a significantly faster computation time [Sergeev and Balso, 2018]. Since astronomical data can be on the order of petabytes in size, this increase in computational power will prove crucial when training and evaluating IFU data cubes.
- This project is currently in heavy development; a link to the git repo is embedded in the QR code at the top of this page!

Acknowledgements

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