



Using a deep neural network to detect methane point sources and quantify emissions from PRISMA hyperspectral satellite images

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| 4 | Peter Joyce ^{1,2,3} , Cristina Ruiz Villena ^{4,5} , Yahui Huang ^{2,3} , Alex Webb ^{4,5} , Manuel Gloor ¹ , Fabien H. |
| 5 | Wagner ^{6,7} , Martyn P. Chipperfield ^{2,3} , Rocío Barrio Guilló ⁴ , Chris Wilson ^{2,3} , and Hartmut Boesch ^{4,5} |
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| 7 | ¹ School of Geography, University of Leeds, Leeds, United Kingdom |
| 8 | ² National Centre for Earth Observation, University of Leeds, Leeds, United Kingdom |
| 9 | ³ School of Earth and Environment, University of Leeds, Leeds, United Kingdom |
| 10 | ⁴ University of Leicester, Leicester, United Kingdom |
| 11 | ⁵ National Centre for Earth Observation, University of Leicester, Leicester, United Kingdom |
| 12 | ⁶ Institute of Environment and Sustainability, University of California, Los Angeles, CA, USA |
| 13 | ⁷ Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove, Pasadena, CA 91109, USA |
| 14 | Correspondence to: Hartmut Boesch (hb100@leicester.ac.uk) |
| 15 | Abstract. Anthropogenic emissions of methane (CH ₄) make up a considerable contribution towards the Earth's radiative |
| 16 | budget since pre-industrial times. This is because large amounts of methane are emitted from human activities and the global |
| 17 | warming potential of methane is high. The majority of anthropogenic fossil methane emissions to the atmosphere originate |
| 18 | from a large number of small (point) sources. Thus, detection and accurate, rapid quantification of such emissions is vital to |
| 19 | enable the reduction of emissions to help mitigate future climate change. There exist a number of instruments on satellites |
| 20 | that measure radiation at methane-absorbing wavelengths, which have sufficiently high spatial resolution that can be used for |
| 21 | detecting highly spatially localised methane 'point sources' (areas on the order of km ²). Searching for methane plumes in |





22 methane sensitive satellite images using classical methods, such as thresholding and clustering, can be useful but are time-23 consuming and often inaccurate. Here, we develop a deep neural network to identify and quantify methane point source 24 emissions from hyperspectral imagery from the PRecursore IperSpettrale della Missione Applicativa (PRISMA) satellite with 25 30-m spatial resolution. The moderately high spectral and spatial resolution as well as considerable global coverage and free 26 access to data make PRISMA a good candidate for methane plume detection. The neural network was trained with simulated 27 synthetic methane plumes generated with the Large Eddy Simulation extension of the Weather Research and Forecasting 28 model (WRF-LES), which we embedded into PRISMA images. The deep neural network was successful at locating plumes 29 with F1-score, precision and recall of 0.95, 0.96 and 0.92, respectively, and was able to quantify emission rates with a mean error of 24%. The neural network was furthermore able to locate several plumes in real-world images. We have thus 30 31 demonstrated that our method can be effective in locating and quantifying methane point source emissions in near real time 32 from 30-m resolution satellite data which can aid us in mitigating future climate change.

33 1 Introduction

34 Methane (CH₄) is a powerful greenhouse gas with a warming potential which per unit mass emitted is 84 times larger than 35 for carbon dioxide over a 20-year period (Stocker et al., 2013). Emissions of methane as a result of human activities have 36 contributed one quarter of climate warming since preindustrial times (Etminan et al., 2016). A large proportion of 37 anthropogenic methane from industrial sources originates from point sources such as coal mines and oil and gas production 38 facilities (Saunois et al., 2020). Furthermore, these emissions are generally underestimated by inventory-based approaches 39 (Alvarez et al., 2018; Karion et al., 2013; Zavala-Araiza et al., 2015). A large proportion of these anthropogenic emissions 40 originates from a small number of strong point sources due to oil and gas production equipment malfunction (Brandt et al., 41 2016; Duren et al., 2019; Zavala-Araiza et al., 2017). Consequently, much of the methane emitted from such sources could 42 be reduced at no net cost (IEA, 2017; Ocko et al., 2021). Acting to reduce methane emissions in this sector can be one of the most cost-effective methods of mitigating against further climate change. 43

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45 Methane point sources from oil and gas production are typically small in extent and emissions difficult to quantify and variable in time (Allen et al., 2013; Frankenberg et al., 2016). The primary challenge faced when estimating methane emissions from 46 47 point sources from satellite data comes from the relatively low spatial resolution (in the order of kilometres) of satellite imagery from dedicated sensors such as the Greenhouse Gases Observing SATellite (GOSAT) (Kuze et al., 2009) and the 48 49 TROPOspheric Monitoring Instrument (TROPOMI) (Levelt et al., 2006). These sensors typically have high spectral resolution of methane absorption bands in the shortwave infrared (SWIR) range of the electromagnetic spectrum to provide 50 accurate measurements with high precisions of around 10-20 parts per billion (ppb) (Lorente et al., 2021; Parker et al., 2020). 51 52 SWIR bands can also be effectively utilised to detect and quantify point sources from lower spectral-resolution sensors (Jacob 53 et al., 2016; Duren et al., 2019). Recent hyperspectral spaceborne imaging spectrometers contain hundreds of spectral





54 channels in the visible-shortwave-infrared range with spectral resolution typically around 10 nm and spatial resolutions of 55 tens of m. Due to their spatial and spectral resolution, they have been identified as useful new tools for identifying and 56 quantifying methane point source emissions. PRecursore IperSpettrale della Missione Applicativa (PRISMA), developed and 57 operated by the Italian Space Agency (ISA) since 2019, is the first hyperspectral mission where the satellite imagery has been 58 openly released to the scientific community. The satellite consists of a panchromatic camera and an advanced hyperspectral 59 instrument that measures radiances in approximately 250 bands between 400 and 2500 nm. The instrument has a spatial resolution of 30 m, a swath of 30 km, and a 12-nm spectral resolution (Galeazzi et al., 2008). How to best extract information 60 on the location and extent of methane plumes is not yet fully established. Successful detection of methane point sources from 61 PRISMA using a matched-filter retrieval technique has been reported by Guanter et al. (2021), albeit with a strong dependence 62 63 of detection accuracy on surface type. In particular, brightness and homogeneity of the satellite images were identified to significantly influence the accuracy of methane detection techniques. 64

Current approaches for detecting methane point sources and quantifying emission rates are time-intensive, laborious, and 66 67 prone to errors owing to the substantial human intervention required. They typically involve a spectral analysis to infer methane column mean mixing ratios (Thorpe et al., 2014) followed by a methane plume detection method (often based on 68 thresholding and clustering) and finally the integrated mass enhancement (IME) method to estimate the emission (Varon et 69 70 al., 2018). Previous efforts utilising spaceborne imaging spectrometers to quantify methane point source emission rates have 71 proved successful, but often with large errors of source detection and emissions estimates. The IME method yielded errors 72 between 5-12% using 50-m resolution Greenhouse Gas Satellite - Demonstrator (GHGSat-D) imagery (Varon et al., 2018). However, this uncertainty estimate does not include errors from unknown wind speed and direction, which are both highly 73 uncertain, thus uncertainties are effectively much larger. The multi-band multi-pass (MBMP) method was successful in 74 75 quantifying methane point source emissions from Sentinel-2 multispectral instrument (MSI) imagery with precision between 76 30% and 90% (Varon et al., 2021). The primary limitation of this approach is surface interference (Cusworth et al., 2019) 77 which leads to artefacts and false anomalies, which can be mistakenly attributed to emission plumes. This is a major disadvantage for multi and hyperspectral missions because the better the resolution (and the greater the number of channels), 78 79 the better the discrimination between the surface and methane absorption. Thus, producing a model that minimises such errors 80 and can automatically locate methane sources would make emission monitoring from space faster, more reliable, and more 81 scalable, thus providing an invaluable tool to aid mitigation. A first effort has also been made to estimate emission rates from 82 AVIRIS-NG data using a neural network and without utilising wind speed and direction data. These estimates were subject 83 to an error of roughly 30% of the emission rates (Jongaramrungruang et al., 2019). It is apparent that the noise in the satellite 84 data, the lack of accurate wind data, and the complex structures of methane plumes make it difficult to model emission rates 85 accurately via traditional approaches.

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87 In recent years, deep neural network methods have improved rapidly. LeNet (Lecun et al., 1989) was one of the earliest 88 convolutional neural networks (CNNs) and was used successfully to identify handwritten digits. This work laid the foundations for using artificial intelligence to obtain meaningful information from image data (known as *computer vision*). 89 90 Deep learning models entered the mainstream following considerable reductions in model training time through the utilisation 91 of graphics processing units (GPUs) (Oh and Jung, 2004). Deep learning was then revolutionised for image classification 92 with the introduction of AlexNet (Krizhevsky et al., 2012). CNNs have since been applied to self-driving cars (e.g., Nugraha 93 and Su, 2017), discovering new drug treatments (e.g. Wallach et al., 2015), facial recognition (e.g. Matsugu et al., 2003), and 94 many other applications. The ease with which deep neural networks can be trained and deployed has also improved 95 considerably in recent years, partially due to the development of application programming interfaces (APIs) such as Keras (Chollet, 2015). This has been supplemented by the increasing ubiquity and decreasing costs of GPUs and cloud computing 96 97 servers, which together have enabled deep learning models to be trained rapidly and at a relatively low cost. Currently, work utilising deep neural networks has already proven to be considerably more effective than classical methods to detect point 98 99 source emissions of nitrogen dioxide (NO₂) (Finch et al., 2021).

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101 More recently, a deep neural network has been used to quantify methane point source emissions using the airborne AVIRIS-102 NG instrument (Jongaramrungruang et al., 2022). In this study, a CNN was trained on synthetic plumes inserted into real images to extract features present in plumes of varying intensities and with differing wind speeds to locate and quantify the 103 104 emission rates of the point sources. Jongaramrungruang et al. (2022) estimated emission rates of plumes with a mean absolute 105 error of 17% for emissions larger than 40 kg hr⁻¹. The classification accuracy (determining whether a plume is present in an image) was 90% when testing plumes with emission rates above 100 kg hr⁻¹, however, the accuracy dropped to 50% for 106 107 emission rates around 50-60 kg hr⁻¹. The spatial and spectral resolution of the aircraft data used in this study (AVIRIS-NG) 108 has far higher spatial and spectral resolution than PRISMA, thus making methane detection prone to lower errors. However, 109 PRISMA data is publicly available and covers a far larger spatial range with regular repeat measurements, thus making it a 110 superior resource for rapid detection of methane point source emissions across many regions on earth. Thus, a deep neural 111 network that is capable of utilising PRISMA data to detect methane emissions could be very effective in our efforts to mitigate 112 future climate change.

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In this study, we produced pseudo-observations of simulated synthetic methane plumes generated with the Large Eddy Simulation extension of the Weather Research and Forecasting model (WRF-LES). These simulated plumes were then embedded into an array of PRISMA images and used as training data for a novel neural network architecture that aimed to produce masks of the locations of methane plumes and estimate their emission rates from PRISMA satellite imagery. The effectiveness of this model was then tested on images of real-world plumes. The techniques utilised here can be adapted to locate and quantify emission rates using any satellite imagery with suitable shortwave-infrared bands, or applied to detecting other greenhouse gases, such as carbon dioxide (CO₂).





121 **2 Methods**

122 **2.1 Simulating methane plumes with WRF-LES**

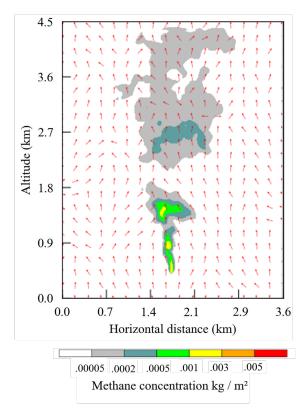
123 The Weather Research and Forecasting (WRF) model system has comprehensive and multiple capabilities for studying 124 atmospheric phenomena from global down to large eddy scales. The default large eddy simulation case (LES) of the WRF 125 V4.2.2 was used and modified to simulate methane plumes for a single point source with a releasing rate of 1000 kg hr⁻¹. The default LES case does not consider clouds, radiation, or topography, but includes surface physics and 1.5-order TKE 126 127 (Turbulent Kinetic Energy) prediction scheme (WRF model User's Guide: https://www2.mmm.ucar.edu/wrf/users/). A constant thermal flux of 100 W m⁻² was applied at the surface to drive the turbulence. Two nested domains with one-way 128 nesting were deployed in the simulations. The outer domain had a size of 5.4 km x 6.3 km with 90 m horizontal resolution 129 and periodic boundary conditions. The inner domain had a size of 3.6 km x 4.5 km with 30 m horizontal grid spacing and 30 130 131 m vertical resolution, and flow-dependent boundary conditions for scalars. The plume was only released in the inner domain after a 3-hour spin-up run. The total running time is 5 hours, and the final 2-hour run was considered for the training, test, 132 133 and validation data.

134

We designed 15 scenarios consisting of 5 different southerly wind speeds ranging from 1 m s⁻¹ to 9 m s⁻¹, each of which was 135 uniformly applied from the surface to the model top, and 3 different patterns of potential temperature vertical profiles (Figure 136 137 S1). The potential temperature in the scenarios is specified as 290 K from the surface to one of the 3 different mixing depths 138 of 500 m, 800 m, and 1100 m (Figure S2). Above the mixing depth, there is an inversion layer of 700 m with a vertical 139 gradient of potential temperature of 0.009 K m⁻¹ applied from the top of the mixing layer to the model top. For each simulation, 140 the CH₄ distribution is saved once every minute and thus there are 120 different scenes for a two hour simulation. Altogether there are 1800 scenes for the 15 simulations in the data, where the plume was integrated over vertical columns. Figure 1 141 shows one snapshot of a plume with initial conditions of 3 m s⁻¹ southerly wind and 800 m mixing depth 30 minutes after 142 143 release.







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Figure 1: Snapshot of a simulated plume 30 minutes after release for initial conditions of 3 m s⁻¹ southerly wind and 800 m mixing
depths. Red arrows indicate wind direction at the moment of the snapshot.

147 **2.2 Satellite data retrieval**

Methane absorbs solar radiation at a set of shortwave-infrared wavelengths that are well known and documented in spectroscopic databases. The absorption of light by methane in the atmosphere therefore alters the reflected sunlight measured by the satellite in a very predictable way that allows us to quantify the amount of methane along the light path. Here we use a data-driven retrieval algorithm to estimate the methane enhancements from reflected sunlight using statistical methods based on the work by Thorpe et al. (2014). This type of simple and fast retrieval method is commonly used for instruments with comparably low spectral resolutions, for which a more sophisticated, so-called full-physics approach provides no extra benefit.

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156 The relationship between the spectral intensity at each point in the satellite spectra and the column enhancement of methane 157 in the scene is represented by a methane Jacobian vector, which describes the change in the logarithm of the intensity I_k in

band k with respect to the column enhancement of methane C_{CH4} . The spectral variation of the background of the scene (i.e.

159 outside of the plume) is approximated by a number of Principal Components of all measured spectra combined derived using





the Principal Component Analysis (PCA) method. We perform the PCA on the logarithm of measured spectra of the scene and select the singular vectors (principal components) that best describe the spectral variability of the scene. The optimal number of singular vectors was determined by trial and error, and was found to be the first three. We then concatenate these vectors with the methane Jacobian to construct the matrix **J** with dimension 4x number of PRISMA bands, which we use along with the logarithm of the measured radiances, **y**, to find a vector **W** that minimises the cost function in a linear least squares fit for each pixel:

- 166 $||y JW||^2$, (1)
- 167

170

173

168 The modelled radiance **F** is calculated from **J** and **W** as follows:

$$169 F = JW (2)$$

171 We can then rewrite Eq. (2) as the sum of the background (k) and CH4
$$(c+1)$$
 components of the radiance:

172
$$F(W,J) = \sum_{k=1}^{c} J_k \cdot W_k + J_{c+1} \cdot W_{c+1}, \qquad (3)$$

where *c* is the number of singular vectors used. Thus, the modelled logarithmic radiance F(W, J) is a linear combination of the singular vectors, J_k , the CH₄ Jacobian, J_{c+l} , and their weights, W_k and W_{c+l} , respectively. This method is described in more detail in Thorpe et al. (2014). Since the wavelengths scale for each across-track pixel of a PRISMA image are different, it is necessary to infer the Principal Components for each column in the across-track direction separately.

178 **2.3 Training data generation**

We generated synthetic datasets to train the machine-learning model by combining PRISMA images with the synthetic plumes simulated with WRF-LES (described in section 2.1). We use the SWIR spectral radiance from PRISMA Level-1b data as well as the RGB bands. These datasets come with pixel quality and cloud mask information, which we apply in our data preparation process. We selected 36 different PRISMA background images to cover a wide range of scenes representative of places where methane plumes might be expected (Table S1). These images also cover a range of different dates throughout the \sim 3 years of PRISMA data available in the archive, to account for different illumination conditions. All the selected scenes have less than 1% cloud cover, and any pixels flagged as cloudy in the PRISMA product were excluded from the analysis.

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A total of 9700 image tiles were generated for training, each tile with a size of 256 x 256 pixels. The tile size was deliberately selected as a power of two to optimise the model performance. Each tile was selected at random from one of the 36 1000x1000-pixel PRISMA background scenes, and a synthetic methane plume subsequently embedded in it. The synthetic plume was also selected randomly from the WRF-LES simulations, with the following parameters also randomised following

a uniform distribution:





192

193 - **Time step**: between 1 and 120 seconds (Figure S3).

- Plume origin: any point within the background scene tile, excluding the areas near the edges to avoid missing parts
 of the plume.
- Emission rate: all simulated plumes have a 1000 kg hr⁻¹ emission rate, so we applied a scaling factor between 0.1
 and 10 to have a range of emissions between 100 and 10,000 kg hr⁻¹ (Figure S4).

The synthetic plumes from WRF-LES are first converted into maps of methane vertical column densities in molecules cm⁻². 198 The original plume simulations are all carried out for an emission of 1000 kg hr⁻¹ and the scenarios for different emission 199 rates are obtained by scaling the simulated concentrations. Each plume is inserted into the background PRISMA image tile 200 201 by modifying the PRISMA SWIR radiances according to the Beer-Lambert law for absorption. Methane columns are converted into optical depth for each band using a representative methane absorption cross-section for each band computed 202 203 from the HITRAN database (Gordon et al., 2022) for a temperature of 293K and pressure of 1 atmosphere. Each of the 9700 204 training datasets contain: 38 PRISMA radiance bands (3 RGB, and 35 SWIR (2100 - 2365 nm) channels) and the synthetic 205 plume (i.e., the "true" methane enhancements to be used as labels in the model).

206 **2.4 Training data processing**

Each PRISMA sub-image (256 x 256-pixel tile) was normalised by subtracting the mean and dividing by the standard deviation (std) of the whole collection of training images such that the mean of all the images was 0 and the std was 1 for each band. This data normalisation step is standard when using deep neural networks as it is understood to optimise the training time. Following on from this, the undefined (NaN) values present in the images were changed to equal the mean value of each band in the respective image. These NaN values correspond to either invalid (e.g., saturated) or cloudy pixels.

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Every time an image was retrieved during the training process, data augmentations were randomly applied. The augmentations were as follows: rotation by a multiple of 90°, and horizontal and vertical flipping. No brightness and contrast augmentations were made because the quantification of methane plumes relies on the specific band information inside the plume region. The purpose of data augmentation was to increase the data volume, to reduce overfitting, and improve the ability of the model to produce accurate results with data that is different to the training data.

218

To predict the methane concentration, it was first necessary to model the methane plume mask (binary classification of plume/non-plume) because the vast majority of pixels in the training images did not contain a plume (zero-inflated data). An initial methane concentration threshold of 8×10^{18} molecules cm⁻² was chosen as it was the cut-off point where the plumes were no longer visible. Furthermore, training the model with a lower threshold resulted in non-convergence. After the model was trained at the 8×10^{18} molecules cm⁻² threshold, it was possible to continue training the model at a lower threshold. Thus,





we tested training the model at 5×10^{17} molecules cm⁻² increments until the validation loss dropped substantially. The lowest threshold where this was the case was 4×10^{18} molecules cm⁻². This final step is important because it increases the range for which the model can locate and quantify methane emissions.

227 **2.5 Deep neural network architecture and training process**

228 The training of the neural network was split into 4 steps. First, the model was trained to locate the regions of the image 229 containing a plume via binary semantic segmentation. Next, the column enhancements of methane were predicted inside the 230 region of the estimated plume mask from the first stage. Following on from this, the emission rate of the plume in the image 231 was estimated. To ensure that the emission rate estimates would equal zero when no plume was present, an intermediate prediction layer was included where a binary classification was made regarding whether a plume was present in the image or 232 233 not. At each stage of the model, the input was a concatenation of the input satellite image and all the previous outputs (Figure 234 2). To optimise the training of the model weights, each portion of the model was trained alone such that the weights in all the 235 other parts were not being updated. The parts of the model were trained in order moving downwards across the models depicted in Figure 2. The loss function to predict the plume mask was as follows: 236

$$237 \quad \text{Loss}_{\text{mask}} = 1 + BC - SDC \quad , \tag{4}$$

238

241

239 Where *BC* is binary cross entropy, *SDC* is the Sørensen-dice coefficient defined as follows:

$$240 \qquad SDC = \frac{2TP}{2TP + FP + FN},\tag{5}$$

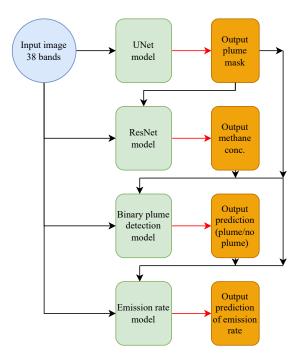
242 where TP is true positive, FN is false negative, and FP is false positive. This loss function was chosen because of the large number of non-plume pixels present in the image. The loss function for the mask concentration was mean squared error 243 244 (MSE), a standard choice for regression modelling. For the binary classification part of the model, binary cross-entropy was 245 chosen, which is common for solving 1-dimensional binary problems. Finally, for the emission rate part of the model, MSE was chosen as the loss function until the validation error started to plateau, after which, the model was only trained on images 246 247 containing plumes and mean absolute percentage error was given as the loss function. This was done to ensure that the 248 proportion error was minimised rather than the absolute error. Mean absolute percentage error was not used throughout the 249 whole training process because it was important that the model was trained on some images with no plumes (so an emission 250 rate of zero could be possible) and mean absolute percentage error produced very high loss values when false positives were 251 made by the model.

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The two encoder CNNs have identical architectures except the activation function at the end of the binary classification model has sigmoid activation because the predictions are constrained between 0 and 1, and the emission rate estimator has a ReLU activation function.







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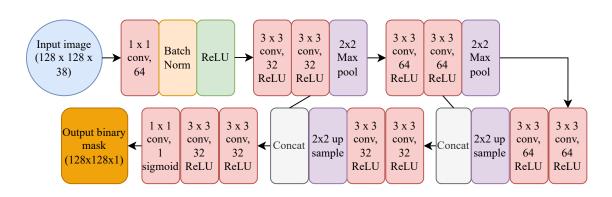
Figure 2: Structure of the neural networks used in this study. Green boxes indicate portions of the neural network, orange boxes indicate predictions made by each stage of the neural network. Black lines indicate flow of data into models, and red lines indicate predictions resulting from a model.

260 **2.5.1 Estimating plume masks**

261 Estimating the mask of a methane plume involved using a similar architecture to a UNet model (Ronneberger et al., 2015) 262 (Figure 3). UNet models consist of two paths; the first is the encoder, which captures the context in the image and is composed of convolutional and max pooling layers. The second path is the decoder, which enables localisation of the features captured 263 264 by the encoder and consists of convolutional and upsampling layers (Ronneberger et al., 2015). In our model architecture, there is an additional 1×1 convolutional layer with 64 filters at the beginning because methane plumes are associated with 265 anomalies in certain SWIR bands of the PRISMA imagery. Methane is not absorbed in the visible bands; thus, their inclusion 266 267 helps the neural network to distinguish between plume and non-plume by providing information on the background of the 268 image. Methane plumes can be identified based on the typical spatial structures that form as a result of turbulence and 269 advection in the atmosphere, as well as the variations in methane-absorbing bands compared with the background landscape. 270 It is the latter reason why an additional 1×1 convolutional layer was deemed to be helpful in improving the accuracy of the 271 model.







273

Figure 3: Architecture of the deep neural network for the UNet portion of the model. 1 × 1 conv, 64 refers to a convolutional filter with kernel size 1 × 1 and 64 filters. Batch Norm refers to a batch normalisation layer, Concat refers to a concatenation between the inputs to that layer, 2 x 2 Max pool refers to a max pooling layer with pool size 2, and 2 x 2 up sample refers to upsampling layer with size 2. ReLU and sigmoid refer to the Rectified Linear Unit and sigmoid activation functions respectively.

278 **2.5.2 Estimating methane column enhancements inside plumes**

279 Estimating the methane column enhancement within the plumes predicted in section 2.4.1 uses a concatenation of the input 280 image and the mask predictions. This step to aid the estimation of methane concentrations is necessary because the vast 281 majority of pixels do not contain a plume (a zero-inflated regression problem). Such problems often have the issue that the 282 model will converge at predicting zeros everywhere. Thus, the inclusion of the mask prediction helps to prevent this. The 283 ensuing model is composed initially of a 1×1 convolutional layer for a similar reason as its inclusion in the UNet model (see 284 section 2.4.1). Following on from this are 2 ResNet layers (He et al., 2016), which are characterised by double-layer skip 285 connections, ReLU activation functions, and batch normalisation (Figure 4). A ResNet architecture was selected for this 286 portion of the model as it is known to be lightweight and powerful at regression predictions in computer vision.

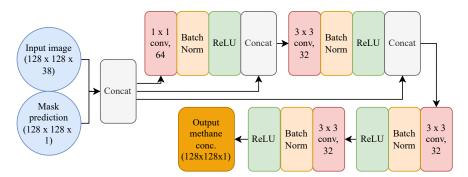


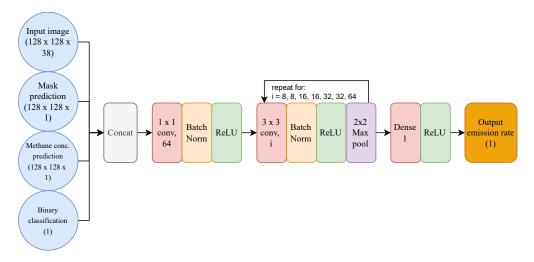
Figure 4: Architecture of the deep neural network for the ResNet portion of the model. 1 × 1 conv, 64 refers to a convolutional filter with kernel size 1 × 1 and 64 filters. Batch Norm refers to a batch normalisation layer and Concat refers to a concatenation between the inputs to that layer. ReLU refers to the Rectified Linear Unit activation function.





291 **2.5.3 Estimating emission rate of plumes**

292 The prediction of the binary classification of plume/not plume involved an architecture identical to the one presented in this section (except the final activation layer was sigmoid, not ReLU). The inputs to the emission rate portion of the model are 293 294 the outputs from all the previous stages of the model concatenated with the input image. This is to ensure that more 295 information is available to the model to accurately estimate emission rates. Following on from this is the 1×1 convolutional 296 layer, which was included for the same reason as in the previous stages of the model (see section 2.4.1). This is followed by 297 the decoder part of the model, in which a convolutional layer is followed by batch normalisation, ReLU activation, and max pooling, which is done 7 times with increasing filters every 2^{nd} loop. These layers encode features about the methane plumes 298 299 and reduce the dimensionality of the tensors. Finally, there is a dense layer and ReLU activation to collect all information 300 obtained and output a single floating-point number as the predicted emission rate (Figure 5).



301

Figure 5: Architecture of the deep neural network for the emission rate prediction of the model. 1 × 1 conv, 64 refers to a convolutional filter with kernel size 1 × 1 and 64 filters. Batch Norm refers to a batch normalisation layer, Concat refers to a concatenation between the inputs to that layer, and 2 x 2 Max pool refers to a max pooling layer with pool size 2. ReLU refers to the Rectified Linear Unit activation function.

306 3 Results

307 **3.1 Application of neural network to simulated plumes**

The total training/validation dataset consisted of 9700 images, 80% of which were reserved for training and the remaining 20% for validation. After each iteration of the model through the training dataset (known as an *epoch*), the model was tested on the validation dataset. If the loss of the model when tested on the validation dataset was lower than the lowest loss





previously recorded, the weights of the model were updated. Thus, at the end of the training procedure, the best model was saved. Each of the stages of the model depicted in Figure 2 were trained separately in descending order, where the weights of the other stages did not vary. This was done so that the most accurate predictions were being produced from the earlier layers so that no errors from insufficient training would propagate through the model because the outputs are concatenated with the satellite data in later parts of the model.

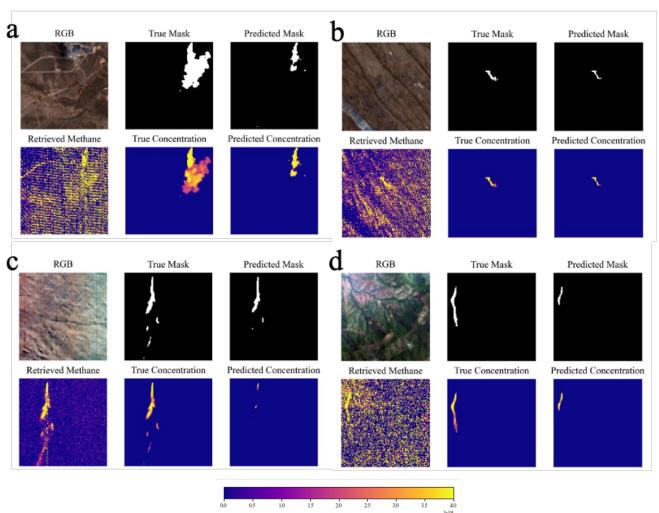
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- 317 Once training was complete, the model was tested on an additional 2000 images not seen during training sampled randomly
- from a uniform distribution of emission rates from 500 to 10 000 kg hr⁻¹. 36/2000 of the images had a maximum methane
- 319 concentration under the 4×10^{18} molecules cm⁻² threshold imposed during training, however they were still included in the
- 320 testing to determine if they can still be detected by the model. The model is able to accurately locate and identify the shape
- 321 of methane plumes in the test dataset (Figure 6).





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- 324
- 325
- 323



Methane concentration (molecule cm⁻²)

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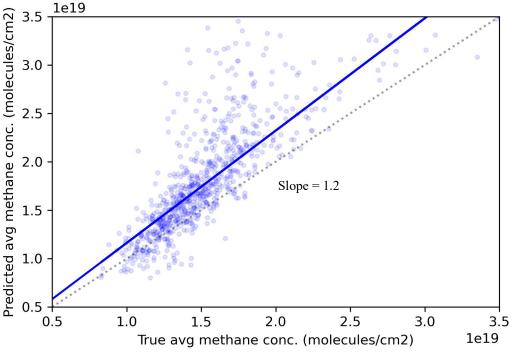
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Figure 6: Example images and predictions taken from the test dataset. Images are 3840x3840m composed of 128x128-pixel tiles. True emission rates and initial wind speeds are (a) 8068 kg hr⁻¹, 1 ms⁻¹, (b) 1484 kg hr⁻¹, 1 ms⁻¹, (c) 7673 kg hr⁻¹, 5 ms⁻¹, (d) 6270 kg hr⁻¹, 4 ms⁻¹. Retrieved methane comes from the retrieval described in section 2.2. RGB image courtesy of PRISMA © (Italian Space Agency).

The total methane column enhancement in the images was well estimated, where total estimated methane was closely correlated with the ground truth (Figure 7) with a tendency to slightly overestimate column values.







334 Figure 7: Scatter Plot of mean methane concentration predicted vs true.

335

In the binary classification part of the model, we assess its success using the F1-score, precision and recall, which are defined

337 as follows:

| 338 | F1 = TP/(TP+0.5*(FP+FN)), | (6) |
|-----|---------------------------|-----|
| 339 | Precision = TP/(TP+FN), | (7) |
| 340 | Recall = $TP/(TP+FP)$, | (8) |

341

In the binary classification part of the model, the F1-score, precision, and recall were 0.95, 0.96 and 0.92, respectively (Table
1). These statistics come from predictions made on the 2000 images with plumes in, as well as an additional 1533 images
with no plumes.

- 345
- Table 1: Confusion matrix of binary classification portion of the model broken down per image.

| | Plume present | No plume present |
|--------------------|---------------|------------------|
| Predicted plume | 1846 | 51 |
| Predicted no plume | 154 | 1482 |





The distributions of the scene noise and methane concentrations in the cases where no plume was predicted but a plume was present (false negative) reveal slightly lower than average scene noise and much lower than average maximum methane concentration (Table S2). However, in the cases where a plume was predicted but no plume was present (false positive), scene noise is not noticeably different (Table S2).

351

The actual vs predicted emission rate has a slope of 0.83 with a relatively small spread about the line of best fit (std = 1447)

- kg hr⁻¹). This means that there is a tendency for underestimating emissions with a mean absolute percentage error in emission
- rate of 23.7% (Figure 8). This bias in the slope is possibly a result of training the model on images without plumes as well as
- those containing plumes.

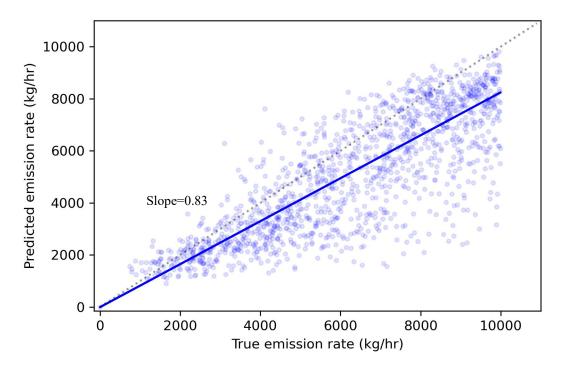




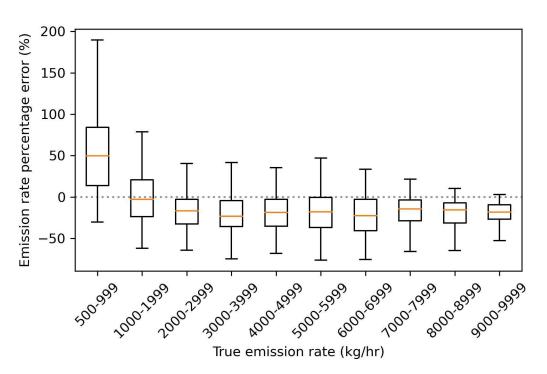
Figure 8: Actual vs predicted emission rate using the deep learning model. Line of best fit calculated using Huber loss so outliers
 do not have an inordinate influence on the slope.

The absolute emission rate error increased in magnitude as the emission rate increased (Figure 8), as one might expect. The percentage error was largest in magnitude for the smallest emission rates (500-999 kg hr⁻¹), but the distribution remained relatively consistent above 2000 kg hr⁻¹, with a median error of 25% and interquartile range of 40% error (Figure 9). The error in percentage emission rate had a positive bias for emission rates under 1000 kg hr⁻¹ and a negative bias for emission rates over 2000 kg hr⁻¹ (Figure 9).





364



365

Figure 9: Error in emission rate predictions from the deep learning model as a function of true emission rate. Positive values indicate predicted emission rates being larger than true emission rates. Top panel shows absolute emission rate error and bottom panel shows percentage emission rate error.

369 **3.2 Application to real-world images**

370 **3.2 Application to real-world images**

371 The model was then tested on 40 PRISMA scenes obtained during 2020-2022 in the Korpeje oil field, Turkmenistan (37.9°N,

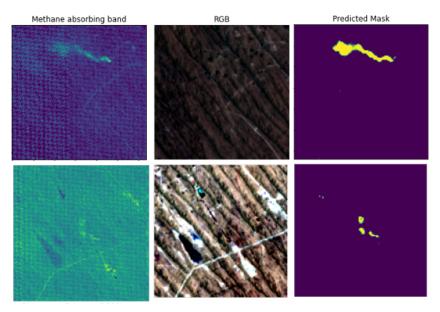
53.2°E - 39.4°N, 55.2°E), a well-studied area with frequent methane point source emissions plumes (Irakulis-Loitxate et al.,

373 2022). The images were normalised in the same way that the training, test, and validation images were. 21 plumes were

identified from 15 different scenes with predicted emission rates ranging from 1112-7615 kg hr⁻¹ (Figure 10; Table S3).







375

Figure 10: Images of plumes detected by the neural network in the Korpeje oil field, Turkmenistan. Left panels depict methane retrievals, middle panels depict the RGB of the image, and the right panel depicts the mask prediction by the neural network. The predicted emission rates are (top) 7615 and (bottom) 2370 kg hr⁻¹. RGB image courtesy of PRISMA © (Italian Space Agency).

379

Methane plume detection capability using the neural network was compared with using clustering and thresholding techniques (see section 2.2). Out of the 21 plumes, 14 were found using this approach. The neural network model took roughly 1 minute to make predictions of plume masks, methane concentrations, and emission rates of located plumes in an image of 1000x1000 pixels (900km² area) without the need for time-consuming human inspection typically needed for classical clustering approaches.

385 4 Discussion

386 Identification and reduction of methane emissions can have a considerable influence over the Earth's surface radiation budget 387 and hence our efforts to mitigate climate change. Methods utilising classical approaches have had some success in detecting 388 fossil fuel methane point sources and estimating their emissions, but the errors are high (roughly 50% error for emission rate 389 predictions) if no accurate local wind speed information is available and often time-consuming human judgement is necessary 390 to separate plumes from surface effects. Within the pseudo-observation dataset produced in this study, only one quarter of 391 the images were deemed suitable to be analysed via clustering algorithms, which demonstrates its limitation for detecting 392 methane point source emissions. In comparison, only 7.7% of the pseudo-observations were undetected by the neural network 393 (Table 1). The neural network presented in this study was able to accurately locate simulated methane point source plumes





with a precision and recall of 0.96 and 0.92, respectively. The estimates of emission rate did not require wind speed information, which is a major source for uncertainty in emission estimates in conventional approaches such as the IME method, and had an average error of 23.7%, which is considerably lower than that obtained from classical methods. The emission rate prediction error could possibly be further reduced with training on a larger dataset.

398

399 The approach used in this study differs from the approach by Jongaramrungruang et al. (2022), who directly predicted the 400 emission rate from the satellite data without first estimating the plume mask. However, we found that excluding these stages 401 dramatically worsened the model prediction, where the error in emission rate was greater than 50%. The model architecture 402 presented here utilises the maximum amount of information available from the training data. Possible explanations for why 403 the model from Jongaramrungruang et al. (2022) was nevertheless successful could include the large training data volume available in their study (in the order of hundreds of thousands of images), which is an order of magnitude larger than that 404 405 available in this study. This larger training volume may have enabled the neural network to make the link between plume 406 shapes and emission rates. In addition, the spectral and spatial resolution of the aircraft imagery used in their study (AVIRIS-407 NG) is substantially higher than that of PRISMA. Finally, the input bands for this study totalled 38, whereas in the study of (Jongaramrungruang et al., 2022), only 1 band was sufficient due to the low noise in the signal in the AVIRIS-NG data and 408 409 high methane absorption in that band. Thus, it may have been easier for their neural network to learn features in the image 410 due to lower noise present.

411

When producing the training data labels for plume masks, a constant threshold was chosen for what methane concentration constitutes a plume. However, the minimum methane concentration that is detectable likely varies depending on scene noise and brightness. Thus, more work is necessary to quantify the most appropriate threshold. However, precise estimates of the edges of a plume are of lesser importance than the initial identification of a plume and its corresponding emission rate.

416

417 There is a noticeable bias present in the emission rate prediction errors (Figure 8; Figure 9) which was also evident in the 418 study by Jongaramrungruang et al. (2022). This bias should be rectified, and future work is needed in fine tuning the neural 419 network training procedure to do so. Such adjustments could include modifying the emission rate loss function or the model 420 architecture. The model was trained only on images with a single methane point source; thus, the model is not able to 421 discriminate between emissions from different sources within a single 128x128-pixel image. The solution to this would be to 422 add in training data with multiple sources and solve the instance segmentation problem using an appropriate architecture, 423 such as Mask-RCNN (He et al., 2020). It is likely that the errors would be larger in general when using this approach owing 424 to the increased noise present.





425 5 Conclusions

426 In this study, we present a novel deep neural network model for identifying and quantifying methane point source emissions 427 from PRISMA satellite data. PRISMA data has sufficient spectral and spatial resolution to identify methane plumes, while 428 still having considerable spatial coverage and is still in operation today. These factors make PRISMA an ideal tool for methane 429 detection and the deep neural network developed here has great potential to impact climate mitigation efforts. The model 430 proved to be more successful with both identification and quantification than previous efforts using classical approaches. 431 Rapid identification and quantification of methane point sources is a vital contribution to climate change mitigation, and the 432 approach outlined here opens the door to the capability to automate methane plume detection. Our model was able to produce 433 predictions on an area of 900 km² over real PRISMA images in less than a minute. Such a capability would vastly reduce the time and costs associated with reducing anthropogenic methane emissions. 434

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