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1 A Satellite-based Model for Estimating PM_{2.5}
2 Concentration in a Sparsely Populated Environment
3 Using Soft Computing Techniques

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25 **Highlights**

- 26 • We used comprehensive satellite-based, meteorological and geographical data to develop
27 a satellite-based model for estimating the PM_{2.5} concentration.
- 28 • Representative animations are created to visualize the spatiotemporal variation of the
29 predictors.
- 30 • We applied the adaptive neuro-fuzzy inference system (ANFIS) for the first time as a
31 core model to estimate the spatiotemporal variation of PM_{2.5} concentration.
- 32 • We compared ANFIS with support vectors machine and back-propagation artificial
33 neural network.
- 34 • Adaptive model identification technique has been used to identify the optimal predictive
35 model.

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44 **Abstract**

45 We applied three soft computing methods including adaptive neuro-fuzzy inference system
46 (ANFIS), support vectors machine (SVM) and back-propagation artificial neural network
47 (BPANN) algorithms for estimating the ground-level PM_{2.5} concentration. These models were
48 trained by comprehensive satellite-based, meteorological, and geographical data. A 10-fold
49 cross-validation (CV) technique was used to identify the optimal predictive model. Results
50 showed that ANFIS was the best-performing model for predicting the variations in PM_{2.5}
51 concentration. Our findings demonstrated that the CV-R² of the ANFIS (0.81) is greater than that
52 of the SVM (0.67) and BPANN (0.54) model. The results suggested that soft computing methods
53 like ANFIS, in combination with spatiotemporal data from satellites, meteorological data and
54 geographical information improve the estimate of PM_{2.5} concentration in sparsely populated
55 areas.

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58 **Keywords:** PM_{2.5}; Aerosol optical depth; ANFIS; SVM; BPANN; Australia.

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63 **Data availability**

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65 The type and source of the data set considered in this study.

Name of the data set	Data source (Developer) (All websites accessed on Jan 2016)	Data format	Software required	Data availability
OMI Near-UV AOD	Aura OMI AOD product via NASA Giovanni interface http://giovanni.sci.gsfc.nasa.gov/giovanni/?instance_id=omil2g	HDF / NetCDF files	ArcGIS	Freely available
Major road	PSMA Australia Transport and Topography product https://www.pdma.com.au/products/transport-topography	ESRI shape files	" "	Price depends on the area of interest
Minor road	" "	" "	" "	" "
Industrial point source PM_{2.5} emissions	Australia National Pollutant Inventory http://www.npi.gov.au/reporting/industry-reporting-materials	xml files	Microsoft Excel / R	Freely available
Australia population density	Australian Bureau of Statistics http://www.abs.gov.au/ausstats/abs@.nsf/mf/1270.0.55.007	PNG ESRI Grid GeoTIFF	ArcGIS	" "
Australia land use classification	Australian Bureau of Statistics http://www.abs.gov.au/websitedbs/ce/nsushome.nsf/home/meshblockcounts	Excel spreadsheets / CSV files	Microsoft Excel / R / ArcGIS	" "
Elevation	U.S. Geological Survey https://www.usgs.gov/products/maps/topo-maps	PNG GeoTIFF	ArcGIS	" "
Normalized difference vegetation index	Terrestrial Ecosystem Research Network http://www.auscover.org.au/node/9	NetCDF files	" "	" "
Temperature Rainfall Humidity Solar exposure	Australian Bureau of Meteorology http://www.bom.gov.au/climate/maps/#tabs=Maps	ESRI Grid GIF	" "	" "

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67 **Software availability**

68 The following software has been used in this study for statistical analysis, spatial data processing
69 and map creation:

- 70 • R v.3.2.3 (R Foundation for Statistical Computing, Vienna, Austria)
- 71 • MATLAB R2014b (MathWorks Inc., Natick, USA)
- 72 • ArcGIS version 10.2 (ESRI Inc., Redlands, USA)

73 **Note:** No specific software component has been developed for this study.

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83 **1. Introduction**

84 Exposure to fine particulate matter (PM_{2.5}, particles with aerodynamic diameter less than 2.5
85 µm) is a leading environmental risk factor associated with respiratory and cardiovascular
86 morbidity and mortality (Franklin et al., 2007) and it is the twelfth-ranked contributor to the
87 global burden of diseases (Forouzanfar et al., 2015).

88 Urbanisation increases the risk of being exposed to PM_{2.5} (Han et al., 2015), and Australia, as
89 one of the most urbanised countries in the world, is faced with adverse health effects of PM_{2.5}.
90 To date, very little attention has been paid to the health effect of exposure to PM_{2.5} in Australia.
91 Some studies consistently suggest that PM_{2.5} is associated with respiratory diseases and has
92 significant effects on mortality (Barnett et al., 2005; Simpson et al., 2005), while conflicting
93 results have been reported on cardiovascular health effects (Hinwood et al., 2006). These
94 inconsistent results could be due to difficulties in assessing the Australian population exposure to
95 PM_{2.5}.

96 Ground level aerosol measurement has been historically provided by ground monitoring
97 networks, but there are high establishing and maintaining expenses associated with these
98 measurements (Wu et al., 2012). The sparse ground PM_{2.5} measurement network in Australia
99 makes it difficult to evaluate the spatiotemporal variability of PM_{2.5} and has significantly
100 restrained the epidemiological studies on PM_{2.5} health effects. Australia is the sixth largest
101 country in the world by area while its population is quite small compared to the land size
102 (Australian Government, 2015). Australia is one of the 10 least dense populated countries in the
103 world (United Nations, 2015). The majority of the Australian population is living in the east and
104 west coasts (Lunn et al., 2002). The population within these areas is concentrated in urban
105 centres, particularly the capital cities (Australian Bureau of Statistics, 2012; Lunn et al., 2002).

106 Therefore, limited monitoring stations were established only in populated areas due to population
107 distribution in Australia. Had such monitoring networks existed, there would have been no
108 guarantee of an effective measurement of the spatiotemporal variation of PM_{2.5}, since it is
109 changing on scales much smaller than monitoring networks density.

110 Estimates of air pollution exposure have been traditionally provided by assigning
111 measurements derived from one (Chen et al., 2006) or several air pollution monitors (Barnett et
112 al., 2005; Brook et al., 2010; Chan et al., 2006), allocating exposure using the nearest monitoring
113 station (Lee et al., 2014) or using different proxies to estimate a local population's exposure
114 (Hoffmann et al., 2007; Salam et al., 2008; Samet, 2007). There is potential for over-smoothing
115 the exposure estimation and the results are likely to be biased with all these approaches (Jerrett et
116 al., 2005a).

117 Satellite imagery is another important tool rapidly gaining interest in air pollution monitoring
118 as it provides sequential observations over a broad area. Satellite sensors can be coupled with
119 ground-based sensors at different spatiotemporal scales to reduce the limitations of surface
120 monitoring station (Reis et al., 2015). Aerosol Optical Depth (AOD) is the most common
121 parameter derived from satellite observations and applied to estimate PM_{2.5}. AOD describes the
122 level of which aerosols attenuate the electromagnetic radiation at a given wavelength by
123 absorption or scattering in an atmospheric column (Chudnovsky et al., 2012; Kaufman et al.,
124 2002; NASA, 2013). The availability of satellite-derived AOD has helped to overcome the
125 problems associated with sparse monitoring networks by providing observations where
126 previously there were none (Hoff and Christopher, 2009; Reis et al., 2015).

127 A variety of methods have been used to investigate the quantitative relationship between
128 satellite-derived AOD and ground-level PM_{2.5} measurements. These studies mainly fall into two

129 major classes: numerical-based methods and empirical observation-based methods (Lin et al.,
130 2014).

131 Numerical-based models, including dispersion and chemical transport models, are still under
132 development due to the uncertainties regarding the definition of source inventories, and chemical
133 and dynamical processes of aerosols in atmosphere (Gupta and Christopher, 2009b; Kondragunta
134 et al., 2008). Empirical observation-based methods rely on the relationship between air quality
135 measurements and different observations (Maciejewska et al., 2015). Several techniques have
136 been used to describe this relationship including simple regression (Chu et al., 2003), multiple
137 regression (Dirgawati et al., 2015; Gupta and Christopher, 2009b; Li et al., 2011), geostatistical
138 methods (Jerrett et al., 2005b; Kunzli et al., 2005), generalized additive models (GAM) (Strawa
139 et al., 2013), land use regression (Henderson et al., 2007; Kloog et al., 2011; Knibbs et al., 2014;
140 Liu et al., 2009), and hybrid approaches (Beckerman et al., 2013b; Lindstrom et al., 2011). Soft
141 computing refers to computational techniques which are able to achieve optimal solutions for
142 analysing complicated phenomena at reasonable costs (Carnevale et al., 2016; Kruse et al., 2013;
143 Ovaska, 2004). In recent years, soft computing techniques such as support vector machine
144 (SVM) (Moazami et al., 2016; Reid et al., 2015; Yeganeh et al., 2012), Bayesian models (Corani
145 and Scanagatta, 2016; McBride et al., 2007), *k*-nearest neighbours (kNN) (Reid et al., 2015), and
146 artificial neural network (ANN) (Al-Alawi et al., 2008; Gupta and Christopher, 2009a; Ordieres
147 et al., 2005; Wu et al., 2012) have been gaining popularity in air quality modelling because of
148 their high flexibility and well documented prediction abilities. However, other soft computing
149 methods like adaptive neuro-fuzzy inference system (ANFIS), which is accepted as an efficient
150 and robust method for multivariate analysis, have not been used for modelling the spatiotemporal
151 variations of PM_{2.5} concentrations.

152 Although most of the aforementioned methods can be applied to determine the relationship
153 among AOD and PM_{2.5}, imposing a specific method could make it difficult to select the best
154 predictive model. Hence, adaptive model identification approach is used to choose the most
155 efficient model by using cross-validation technique rather than fitting a specific model to the
156 dataset (Reid et al., 2015; Syed, 2011).

157 Few studies have investigated the relationship between PM_{2.5} and satellite-based AOD in
158 Australia (Gupta et al., 2007; Gupta et al., 2006; Meyer et al., 2008). While other studies have
159 recommended the meteorological and geographical factors incorporation to the AOD–PM_{2.5}
160 relationship to improve models' performance (Chudnovsky et al., 2014; Liu et al., 2009), there is
161 a clear need to conduct an Australian study to develop a satellite-based model investigating
162 significant geographical and meteorological factors including humidity, planetary boundary
163 layer, and wind speed and direction.

164 In this study, we aimed to improve the estimate of PM_{2.5} concentration by using remotely-
165 sensed AOD in conjunction with comprehensive meteorological and geographical data. Three
166 different soft computing algorithms were applied to estimate the monthly average exposure to
167 PM_{2.5} in the South-east Queensland (SEQ) region of Australia, from 2006 to 2011. In turn, an
168 adaptive model identification approach was used to choose the optimal model from ANFIS and
169 other soft computing methods: SVM and BPANN, by using 10-fold cross-validation (Pandey et
170 al., 2013; Syed, 2011). We ultimately used the model with the best predictive ability to estimate
171 spatiotemporal variation of PM_{2.5} in this sparsely populated area with dense vegetation cover.

172 **2. Materials and Methods**

173 **2.1. Study location and ground-level PM_{2.5} measurements**

174 SEQ is a region in the state of Queensland, Australia, which covers 22,420 km² and is home to
175 3.05 million people out of the state's population of 4.58 million based on the 2011 Australian
176 census (Australian Bureau of Statistics., 2012). The study area consists of Brisbane, the state's
177 capital city, as well as other urban and rural centres including Ipswich, Logan City, Gold Coast,
178 Sunshine Coast, and the Lockyer Valley. Motor vehicle emissions and industrial boilers are
179 identified as major sources of PM_{2.5} in SEQ (Queensland Government., 2014). The Queensland
180 government and other agencies are responsible for regulatory aerosol monitoring in SEQ. We
181 obtained quality-assured 24 h ground-level PM_{2.5} measurements from January 2006 to December
182 2011. During the study period, PM_{2.5} was measured at 8 monitoring sites across SEQ
183 (supplement, page S3). We used monthly averages of the daily measured PM_{2.5}, and the
184 inclusion criteria for a given month was that less than 5% of the daily measurements were
185 missing.

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187 **2.2. Land use data**

188 We obtained data on anthropogenic and natural land use variables as spatial predictors that
189 were possible predictors of measured PM_{2.5} concentrations. The selected land use variables,
190 summarised in Table 1, were examined to discover which ones improved the prediction of PM_{2.5}
191 (Knibbs et al., 2014). They included proxies for emissions from traffic, point sources and
192 changing land cover conditions.

193 The impacts of vegetation cover and its phenological state on the relationship between the
194 PM_{2.5} and satellite AOD were also examined in the present study. Normalized difference
195 vegetation index (NDVI) is used to provide a measure of greenness and vegetation cover. NDVI

196 was found to be an effective predictor for pollutant concentrations in previous studies
197 (Chudnovsky et al., 2014; Dirgawati et al., 2015; Su et al., 2009). The monthly mean NDVI data
198 were derived from an Advanced Very High Resolution Radiometer (AVHRR) sensor carried on
199 the National Oceanic and Atmospheric Administration (NOAA) satellite and processed by the
200 Australian Bureau of Meteorology (BoM) at a spatial resolution of 1 km (Bureau of
201 Meteorology, 2015).

202 **2.3. Satellite data**

203 Daily global gridded observations of AOD at a resolution of 0.25 degrees latitude and
204 longitude are derived from the Ozone Monitoring Instrument (OMI) aboard the Aura satellite
205 (Levelt et al., 2006). Aura crosses the equator in a sun-synchronous polar orbit for the daylight
206 ascending orbit (Torres et al., 2007), and it passes over SEQ at approximately 14:00 local time.
207 We download the monthly average OMI AOD level 2 Near-UV AOD and single Scattering
208 Albedo product (OMAERUVG.003 at 342.5 nm) from NASA Giovanni interface for each month
209 from 2006–2011.

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219 Table 1. Independent variables included as potential predictors of PM_{2.5}

Variables (units)	Spatial resolution	Point or buffer	Data source
OMI Near-UV AOD	0.25 degrees Lat/Lon	Point	Aura OMI AOD product via NASA Giovanni interface
Distance to coast (m)	-	Point	ArcGIS geoprocessing tools
Distance to port (m)	-	Point	" "
Distance to airport (m)	-	Point	" "
Distance to nearest major road	-	Point	" "
Distance to nearest minor road	-	Point	" "
Airport (present/not present)	-	Buffer	" "
Major road (m)	-	Buffer	PSMA Australia Transport and Topography product
Minor road (m)	-	Buffer	" "
Industrial point source PM_{2.5} emissions (kg/yr)	-	Buffer	Australia National Pollutant Inventory
Time (Julian month)	-	Point	ArcGIS geoprocessing tools
Population density (person/km²)	1 × 1 km ²	Point	Australian Bureau of Statistics
Land use by type (% area)^b	Mesh block ^c	Buffer	Australian Bureau of Statistics
Elevation (m)	30 m	Point	U.S. Geological Survey
Normalized difference vegetation index	1 × 1 km ²	Point	Terrestrial Ecosystem Research Network, Australian Bureau of Meteorology, AusCover project and NASA NOAA satellite
Mean daily maximum temperature (°C)	5 × 5 km ²	Point	Australian Bureau of Meteorology
Mean daily minimum temperature (°C)	5 × 5 km ²	Point	" "
Rainfall (mm)	5 × 5 km ²	Point	" "
Humidity (hPa)	5 × 5 km ²	Point	" "
Solar exposure (MJ/m²)	6 × 6 km ²	Point	" "
Planetary boundary layer height (m)	3 × 3 km ²	Point	Derived from Weather Research and Forecasting model
U-component of wind speed (m/s)	3 × 3 km ²	Point	" "
V-component of wind speed (m/s)	3 × 3 km ²	Point	" "
Wind speed (m/s)	3 × 3 km ²	Point	" "
Wind direction (Degrees)	3 × 3 km ²	Point	" "

220 ^a 22 Circular buffers were generated with radii of 50 m, 100 m, 200 m, 300 m, 400 m, 500 m, 600 m, 700 m, 800 m, 900 m, 1000 m, 1200 m,
221 1500 m, 1800 m, 2000 m, 2500 m, 3000 m, 3500 m, 4000 m, 5000 m, 7500 m, and 10,000 m (Novotny et al., 2011).

222 ^b Four different land use classes were investigated including industrial, commercial, residential, and open space (which contains the
223 agricultural land, parks, and water bodies (Rose et al., 2010)).

224 ^c Mesh Block is the smallest geographic unit defined by the Australian Statistical Geography Standard for which the Census data is available
225 (Australian Bureau of Statistics, 2011), and can be variable in size.

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228 **2.4. Meteorological Data**

229 We obtained surface meteorological parameters including mean maximum and minimum
230 temperature, rainfall, and humidity from high-quality spatial climate data-sets developed by
231 BoM which provides gridded climatological maps for each month of the year (Jones et al.,
232 2009). In addition, monthly solar exposure maps are also obtained from BoM during the study
233 period.

234 Planetary boundary layer height (PBLH), wind direction (WD) and wind speed (WS) can play
235 a critical role in the transport and dilution of PM_{2.5} (Harrison et al., 1997); hence, special
236 attention was paid to these parameters in this study. The Weather Research and Forecasting
237 model (WRF) was used to calculate these parameters as at 2:00 pm local time at a spatial
238 resolution of 3 km to match the over-pass time of the Aura satellite. Details on the WRF
239 configuration are provided in the supplement (page S3-S7).

240 **2.5. Modelling approach**

241 Following similar studies (Knibbs et al., 2014; Novotny et al., 2011), 22 circular buffers were
242 created around each monitoring site to obtain local and more remote sources of PM_{2.5} (Table 1).
243 Certain variables were calculated within a buffer (e.g., land use type, road length) while others
244 were extracted at each monitoring site (e.g., wind speed, humidity, temperature). In total, 194
245 independent variables were obtained including 18 point variables and 176 buffer variables (8
246 variables calculated at 22 buffers each).

247 **2.6. Statistical analysis**

248 In this study, there were 194 predictor variables to choose from, hence choosing the optimum
249 subset was a complicated process and needed to be carefully conducted. In many soft computing
250 and data mining tasks, there can be some irrelevant variables which may affect the derived
251 statistical relationship between the dependent variable and the other relevant predictors. A
252 common solution to overcome this problem is to use a variable selection process which can help
253 to select a subset of the most relevant and representative predictors from input predictors. The
254 Least Absolute Shrinkage and Selection Operator (Lasso) is a well-known method which is
255 widely used to suppress or shrink variables to select the most relevant predictor variable set.
256 Lasso-type variable selection method was used in this study since it was successfully adopted in
257 many applications (Hu et al., 2015; Li and Shao, 2015; Tibshirani, 2011).

258 Following Beelen et al. (2013), we only included potential predictor variables with less than
259 10% null values and centred and standardised some independent variables to improve model
260 convergence and make the parameter estimates more interpretable. Subsequently, all remaining
261 predictor variables were evaluated, and variables with p-value greater than 0.10 or variance
262 inflation factor (VIF) greater than 6 were removed in order to avoid multicollinearity (see Table
263 S2). As suggested by other studies (Beelen et al., 2013; Henderson et al., 2007; Novotny et al.,
264 2011; Vienneau et al., 2013), if two buffer sizes of a particular variable were found to be
265 collinear, donut ring buffers (so called concentric adjacent rings) were replaced with original
266 circular buffers and the analysis was redone. Ring buffers (i.e., annulus) were calculated by
267 differencing the circular buffers.

268 In this study, we employed the soft computing techniques ANFIS, BPANN and SVM. The soft
269 computing techniques employed here are explained in the supplement, page S8-S17. The input
270 variables were composed of different types of data, including land use, meteorological, and

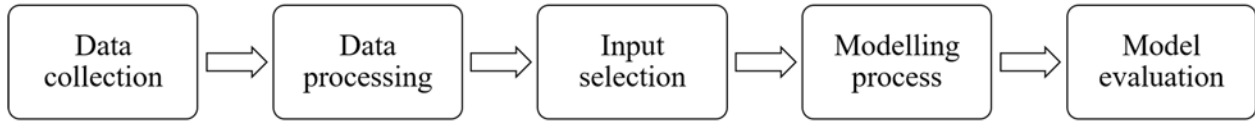
271 satellite data. We matched the selected variables with the PM_{2.5} measurements at 8 monitoring
272 sites during the study period (72 months) which resulted in more than 550 observation sets in
273 total. These observations were divided into training, validation, and test subsets. The majority of
274 the observations (70%) were used for training the models. In order to avoid over-training, 15%
275 of the observations were used for validation and checking the model's generalisation (Wu et al.,
276 2012). Finally, the remaining 15% of the observations were employed as the test subset to
277 estimate the PM_{2.5} concentration by the models.

278 In this study, 10-fold cross validation (CV) method was applied to evaluate the performance of
279 the BPANN, ANFIS, and SVM models and identify the optimal model for estimating the PM_{2.5}
280 concentration. This method has the ability to examine the model's predictive ability (Beckerman
281 et al., 2013a). This examination was accomplished by randomly splitting the data into 10 equal-
282 sized folds. Subsequently, one of the folds was used to test the model and the remaining 9 folds
283 were used to train the model (Kim, 2009; Refaeilzadeh et al., 2009). This process was repeated
284 10 times for each candidate model while all folds were used as the test subset and the 10 results
285 were averaged to obtain the overall CV-R² and CV-RMSE. The best predictive model was
286 selected from those with the smallest CV-RMSE and highest CV-R² (Dirgawati et al., 2015).

287 Bland-Altman plot was also used to examine the agreement between the observations and
288 predictions. In this plot, X axis shows the average of the model predictions and observations, and
289 Y axis represents the difference between these values. Bland-Altman plot also provides statistical
290 limits by calculating the average and mean and the standard deviation (*sd*) of the differences
291 between observations and predictions (Giavarina, 2015). These limits were used to evaluate the
292 agreement between observations and model predictions. For more explicit information on Bland-

293 Altman plot see Giavarina (2015). Figure 1 illustrates the overall research process used in this
294 study.

295



296 Figure 1. General research process for estimating PM_{2.5} concentration.

297 We used R v.3.2.3 (R Foundation for Statistical Computing, Vienna, Austria) and MATLAB
298 R2014b (MathWorks Inc., Natick, USA) for all statistical and soft computing analyses and
299 ArcGIS version 10.2 (ESRI Inc., Redlands, USA) for spatial data processing and map creation.

300 3. Results

301 3.1. Modeling results and evaluation

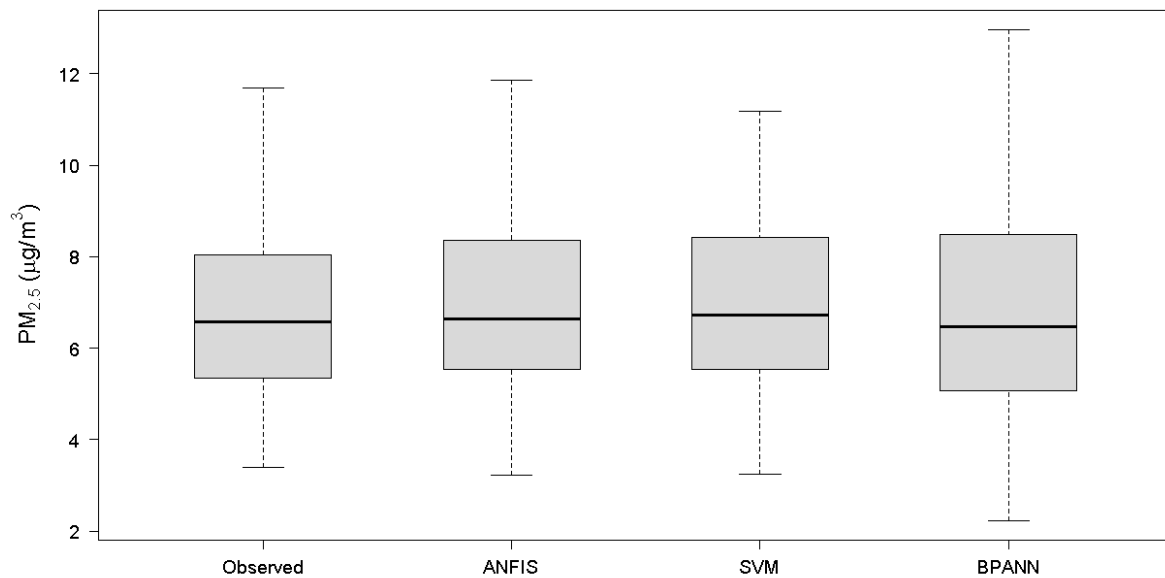
302 In this study, a wide range of ground-based PM_{2.5} measurements, land use, meteorological, and
303 remotely-sensed AOD data were employed to estimate the PM_{2.5} concentration using soft
304 computing techniques. In following section, the agreement between predicted and observed
305 PM_{2.5} concentration is evaluated. 10-fold cross validation is also used to compare the potential of
306 different algorithms for estimating PM_{2.5} concentration.

307 The variable selection results showed that 16 variables were the most effective predictors of
308 PM_{2.5} concentration. The variables most correlated with the outcome were firstly humidity,
309 followed by maximum temperature, AOD and then the length of the major roads. The results of
310 the variable selection process are provided in the supplement (Table S2).

311 Using the testing dataset for each of the developed models, PM_{2.5} concentrations were then
312 predicted. A summary of the observed and predicted PM_{2.5} concentrations is presented in Fig. 2.

313 The mean observed $PM_{2.5}$ concentration for the testing dataset is $6.77 \mu\text{g}/\text{m}^3$. All three models
 314 approached this value within a numerical range of -0.02 to $+0.38 \mu\text{g}/\text{m}^3$. The non-parametric
 315 Wilcoxon test was performed to check if there was any significant difference between the
 316 predicted and observed mean $PM_{2.5}$ concentrations of each model. The test on all models yielded
 317 p-values greater than 0.01, showing an insignificant difference between the predicted and
 318 observed $PM_{2.5}$ concentration at 1% significant level. A comparison of the predicted values
 319 demonstrated that the ANFIS model predicted values were slightly closer to the full range of the
 320 observed monitoring data than the SVM and BPANN models. In general, Fig. 2 shows that all
 321 models reliably calculated the average and range of $PM_{2.5}$ concentration; therefore, predicted-
 322 observed plots are used to evaluate the predictive abilities of the models (Fig. 3).

323

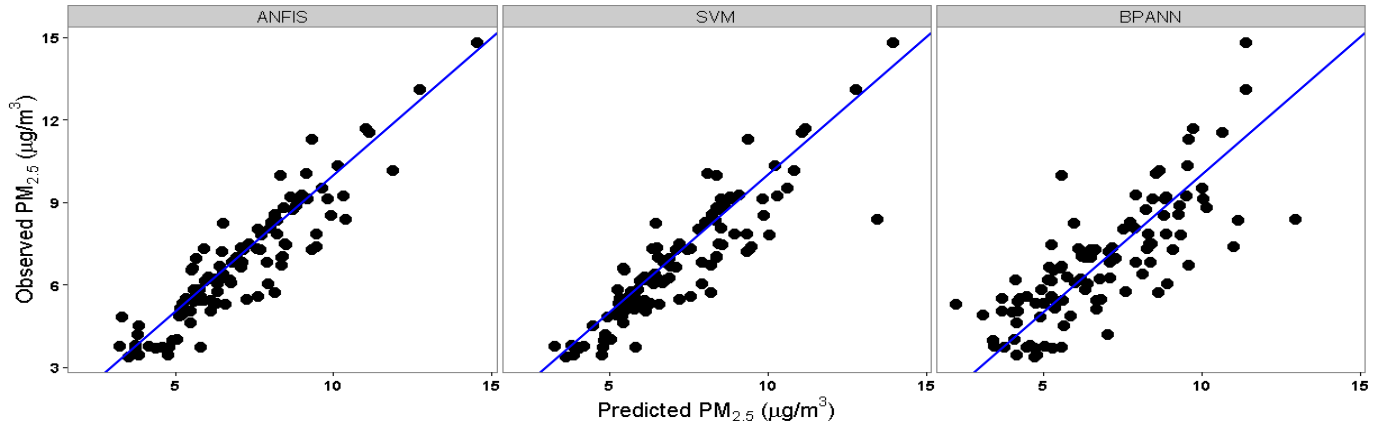


324

325 Figure 2. Summary of $PM_{2.5}$ model predictions on the testing dataset.

326 We compared the observed $PM_{2.5}$ concentrations to the predicted values of the ANFIS, SVM,
 327 and BPANN models. The ANFIS's predicted-observed plot indicates that the values are more
 328 equally scattered across the line of agreement at the low and high $PM_{2.5}$ concentrations whereas

329 the SVM model under-predicts and over-predicts these values, respectively. In addition, the
330 predicted-observed plot shows relatively weak correlation between the BPANN's predictions and
331 actual observations.



332
333 Figure 3. Scatter plots of observed vs. predicted PM_{2.5} for the optimal model fitting on the testing
334 dataset using ANFIS, SVM, and BPANN, respectively. Blue line indicates the line of agreement
335 ($y = x$).

336 Table 2 compares the R^2 and RMSE for model fitting and cross validation. For the model fit
337 the R^2 values are 0.61, 0.73, and 0.84 for the BPANN, SVM and ANFIS models, respectively.
338 The RMSE values are $1.57 \mu\text{g}/\text{m}^3$, $1.36 \mu\text{g}/\text{m}^3$, and $0.94 \mu\text{g}/\text{m}^3$ for the BPANN, SVM, and
339 ANFIS models, respectively. Comparing the model fittings and cross validation, CV-R^2
340 decreases by just 0.03 and CV-RMSE increases by $0.85 \mu\text{g}/\text{m}^3$ for the ANFIS model indicating
341 negligible model overfit. The CV-R^2 of the SVM and BPANN decreased by 0.06 and 0.07,
342 respectively indicating both models overfit more than ANFIS.

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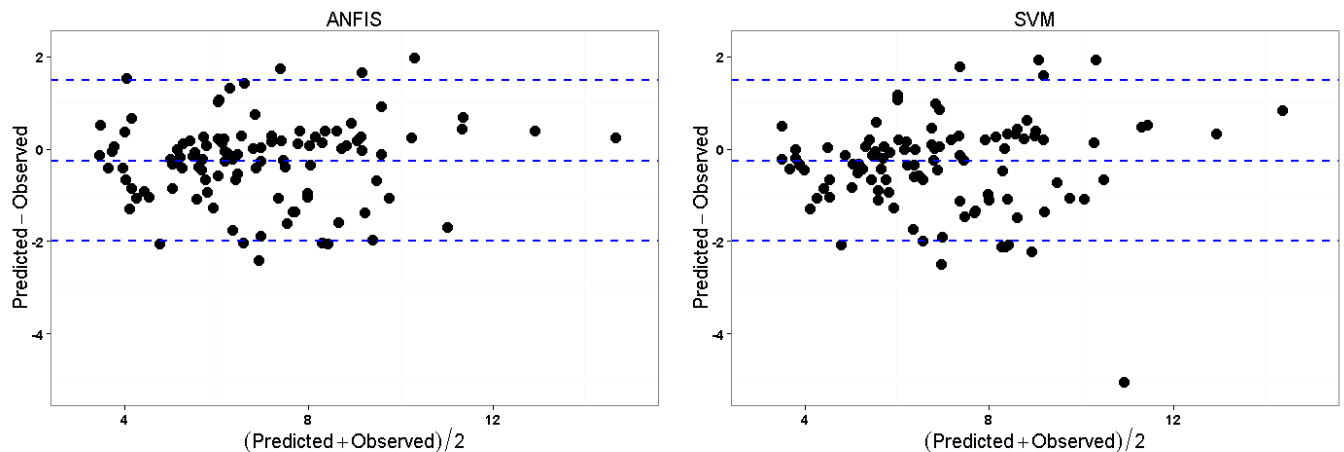
347 Table 2. R-squared and RMSE for model fittings vs. cross validation

	R²	RMSE ($\mu\text{g}/\text{m}^3$)	CV- R²	CV-RMSE ($\mu\text{g}/\text{m}^3$)
ANFIS	0.84	0.94	0.81	1.79
SVM	0.73	1.36	0.67	2.02
BPANN	0.61	1.57	0.54	2.11

348

349 Our findings demonstrated that the CV-R² of the ANFIS (0.81) was higher than that of the
 350 SVM (0.67) and BPANN (0.54) model. Also, the CV-RMSE of the ANFIS model (1.79 $\mu\text{g}/\text{m}^3$)
 351 was lower than that of the SVM (2.02 $\mu\text{g}/\text{m}^3$) and BPANN (2.11 $\mu\text{g}/\text{m}^3$) model. Compared to
 352 SVM and BPANN models, the ANFIS model had higher accuracy without causing more overfit.

353 Bland-Altman analysis was used to evaluate the agreement between the observation and
 354 predictions of ANFIS and SVM since both models showed promising performance in the testing
 355 stage (Figure 4). The Bland-Altman plots demonstrated low bias in both models; however, the
 356 ANFIS model had slightly tighter agreement than the SVM with fewer large residuals.



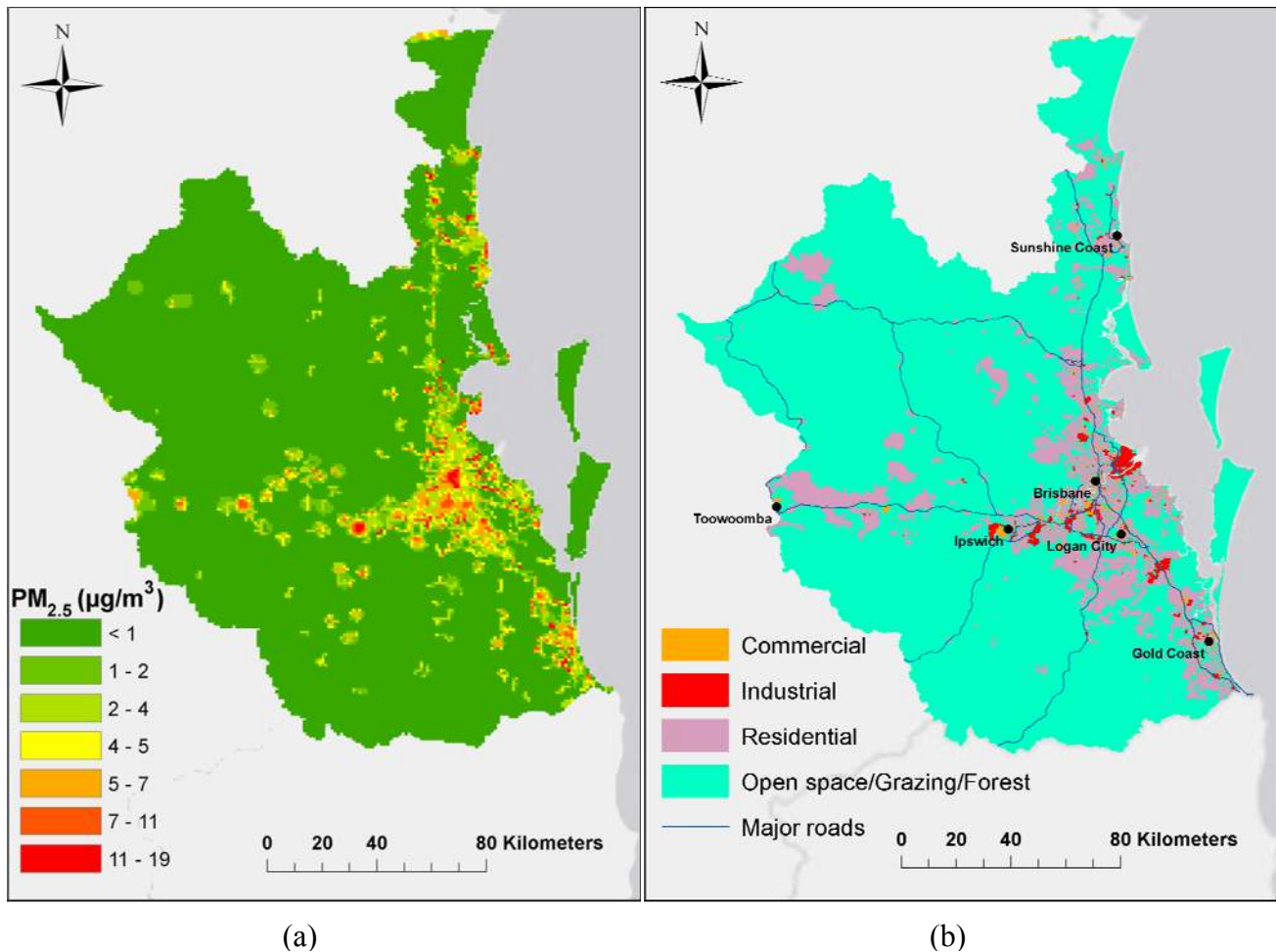
357

358 Figure 4. Bland-Altman plots of predicted and observed PM_{2.5} concentrations ($\mu\text{g}/\text{m}^3$)

359

360 **3.2. Application of the model**

361 The predicted values of PM_{2.5} concentration in September 2011, selected from the 6-year study
362 period, using ANFIS model for the study area 1 km grid is presented in Figure 5a.
363



364 Figure 5. a) Monthly average PM_{2.5} concentration in September 2011 predicted by ANFIS model
365 b) land use map of SEQ

366 Figure 5b illustrates land use map of SEQ. Concentrations ranged from less than 2 to 19 µg/m³.
367 Areas with higher concentrations (7 to 19 µg/m³) corresponded to cities and major towns. Higher
368 concentrations were predicted in locations with extensive adjacent industrial areas and major
369 roads. This pattern was observed in all 6 cities of the study area. The highest levels were

370 predicted for the three largest cities: Brisbane (with 1.977 million people), Gold Coast (494,500)
371 and Logan (287,474).

372 **4. Discussion**

373 We employed soft computing techniques to improve concentration estimates for PM_{2.5} using
374 satellite, meteorological and land use predictor variables in South-east Queensland, Australia.
375 The ANFIS model utilized in this work was the first attempt to apply it for spatiotemporal
376 modelling of PM_{2.5}. Using cross validation technique, the ANFIS model was found to have the
377 best performance compared to SVM and BPANN models, and better agreement with the
378 observed data. The results provide estimates of monthly PM_{2.5} concentrations for SEQ from 2006
379 to 2011.

380 ANFIS is a hybrid system that combines the strengths of fuzzy logic and artificial neural
381 network (Jang, 1993; Lin and Lee, 1991), which provides a robust and accurate method for
382 predicting PM_{2.5} concentration over the range of observations used in this study.

383 In this research, WRF used to calculate PBLH, and WS. Both parameters were highly
384 associated with PM_{2.5} concentration across ANFIS runs. In addition, daily maximum temperature
385 had higher importance compared to the daily minimum temperature. This might be because daily
386 maximum temperature is temporally coincident with the Aura satellite overpass time for the
387 study area.

388 Prior studies mostly considered land use parameters mainly focused on roadways and
389 population-related data. We also evaluated industrial point source emissions, port and airport
390 locations as potential land use predictors. Land use parameters used in our study, may not be

391 important predictors for short term events (e.g. bush fire episode) but our findings revealed that
392 they are of the strong predictors for PM_{2.5} estimation in a long term period.

393 Data sets with different spatial resolutions have been used in our study. The resolution of NDVI
394 and WRF outputs for example are finer than the OMI sensor data. Individually, OMI AOD data
395 are not spatially fine enough for estimating the PM_{2.5} exposure in epidemiological studies.
396 However, method of combining different buffer sizes of land use parameters with meteorological
397 and satellite-based data enabled the model to integrate fine and more spatially coarse data sets to
398 estimate PM_{2.5} concentration and provide more informative results for epidemiological studies.

399 Our results also corroborated with Reis et al. (2015) who suggested that the incorporation of ‘big
400 data’ derived from different sources provides new opportunities for data-intensive models to
401 improve the estimates of population exposures to air pollution. Another important finding was
402 that the highest concentrations (10 to 20 µg/m³) were estimated in the Brisbane, Gold Coast and
403 Logan City which have the highest population density in SEQ (Fig. 5); hence, the increased risk
404 of population expose to higher concentration of PM_{2.5}. Although the average PM_{2.5} concentration
405 was below the WHO guideline (25 µg/m³), epidemiological studies have demonstrated that PM_{2.5}
406 exposure to even lower concentrations is associated with high health risks (Burnett et al., 2014).
407 Based on the shape of the PM_{2.5} exposure-response curves derived by Burnett et al. and used in
408 the Global Burden of Disease studies (Burnett et al., 2014), characterizing with a steep slope for
409 concentrations ranging from 10 to 20 µg/m³, exposure to PM_{2.5} concentration between 10 to 20
410 µg/m³ highly increases the relative risk of stroke and chronic obstructive pulmonary disease;
411 therefore, even PM_{2.5} concentration below the WHO guideline could not be considered safe.

412 Different methodologies make it difficult to compare our results to other studies, however we
413 have attempted to compare our results with two studies which have demonstrated the ability of

414 remotely sensed AOD and meteorological data to predict PM_{2.5} concentration (Gupta and
415 Christopher, 2009a; Wu et al., 2012). Both studies used BPANN method to estimate the
416 spatiotemporal variation of PM_{2.5}, and reported R² lower than 0.61. Our model exhibited better
417 correlations than these models, which could be due to either: (1) the comprehensive input
418 variables used or (2) the more robust modeling algorithms used. We also compared our
419 methodology with a study of the global burden of disease 2013 conducted by Brauer et. al.
420 (2016) which combined ground measurements, chemical transport model outputs, and satellite-
421 based data to provide global estimates of PM_{2.5} concentration. Although, chemical transport
422 model simulations were unavailable for our study area, our model was still able to capture 81%
423 of PM_{2.5} variations.

424 Previous research demonstrated that PBLH and WS significantly affect the PM_{2.5}-AOD
425 relationship. Our results support these findings, but also demonstrate that incorporating other
426 spatial and spatiotemporal data as well as road density, land use types, NDVI, and industrial
427 point sources improves the model's performance.

428 **5. Conclusions**

429 Three different soft computing methods were applied to develop a satellite-based model for
430 estimating the spatiotemporal variation of PM_{2.5}. ANFIS performed very well compared to SVM
431 and BPANN. It exhibited satisfactory performance with CV-R², and CV-RMSE equals to 0.81,
432 and 1.79 µg/m³, respectively. It provides estimates of monthly PM_{2.5} concentrations during 2006-
433 2011. The modelling approach used in this study is highly applicable to similar settings
434 anywhere in the world assuming that researchers have access to data sets equivalent to these used
435 in our study. WRF, and its underlying boundary condition data, is a community model available

436 to the world research fraternity. The NASA Giovanni data is available to anyone in the research
437 community who can be registered with NASA as a data user. It is expected that researchers will
438 have access to all other similar data sets or proxies in their own national research and
439 information collection institutions, hence this method could be applied in other regions that
440 experience PM_{2.5} exposure. We hope that our approach will be beneficial for epidemiological
441 studies and other researches seeking spatially accurate estimates of PM_{2.5} with few monitoring
442 stations. It is certainly feasible to develop a model with higher spatial resolution which is a
443 direction of our future research. Further analysis such as global sensitivity and uncertainty
444 analyses (GSUA) can also be done to assess input factor importance and interaction (Lüdtke et
445 al., 2008; Saltelli et al., 2008). Recently developed Unified-Weather Research and Forecasting
446 model (NU-WRF) can be employed to obtain more accurate estimates of meteorological
447 parameters compared to WRF model (Peters-Lidard et al., 2015). Data management remains a
448 major challenge for empirical modelling as it requires to store, process and analyse large data
449 sets containing different types of data from multiple sources. Recently, new information models
450 have been developed to facilitate the data management and validation in observation-based
451 studies (Horsburgh et al., 2016; Shu et al., 2016).

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