Multiscale Geographically Weighted Discriminant Analysis (Short Paper)

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24 – Abstract

This paper describes the novel development and application of a multi-scale geographically weighted 25 discriminant analysis (MSGWDA). This is applied to a case study of survey data of attitudes 26 to a proposed motorbike / scooter ban in Han Noi, Vietnam. It uses discriminant analysis to 27 examine attitudes to the ban in relation to travel purposes, distances, respondent age and so on. 28 The main part of the paper focuses on describing the novel MSGWDA approach, and the results 29 indicate the varying scales of relationship between the different input variables and the categorical 30 responses variable. The paper also reflects on the pervasive logic of the approaches used to fit 31 multiscale geographically weighted bandwidths (for example in regression). These have historically 32 been based on the iterative back-fitting approaches used in GAMs, but risk missing potentially 33 important variable interactions amongst un-evaluated bandwidths because of the sequence of their 34 application. It is argued that although pragmatic in the 1990s, it may be possible to apply more 35 deterministic approaches with increased memory and readily accessible computing power in order to 36 better navigate such highly dimensional search spaces. 37

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⁴³ **1** Introduction

⁴⁴ This paper describes an approach for classification using a novel multi-scale geographically ⁴⁵ weight discriminant analysis (MS-GWDA). Discriminant analysis (DA) or discriminant ⁴⁶ function analysis [6] as generalised by Rao [15], is a commonly used technique for predicting ⁴⁷ membership or class for discrete groups as an alternative to multinomial logistic regression ⁴⁸ [11]. More recently DA has recently gained much attention in the context of machine learning ⁴⁹ [10, 12] and real time analyses [16, 4] because it can be used as an information learning ⁵⁰ technique as well as classification, particularly in the context of pattern recognition.

Conceptually, in DA the independent data used as input to discriminant analysis can be 51 thought of having been drawn from different populations of each class [2]. The discriminant 52 functions are extracted from independent variables and are then used to generate class 53 membership probabilities for each observation. If there are k groups, the aim is to extract k54 discriminant functions. Each observation is assigned to the class i for which value for the 55 discriminant function for the group is the smallest, thereby determining which population 56 each observation is likely to have come from. Under the assumption that the data are 57 multivariate normal, then if \sum_{i} is the variance-covariance matrix for the members of class 58 j, q is the number of predictor variables in \mathbf{x} , μ_j is the mean vector for the observations in 59 class j, and p_j is the prior membership probability of class j, the linear assignment (linear 60 discriminant analysis, LDA) multivariate Gaussian decision rule can be written as: 61

$$_{62} \qquad k = \arg\max_{j \in (1,...,m)} \left[p_j \frac{1}{(2\pi |\Sigma_j|)^{q/2}} exp\left(-\frac{1}{2} (\mathbf{x} - \mu_j)' \sum_j^{-1} \mathbf{x} - \mu_j \right) \right) \right] \tag{1}$$

LDA was extended from the linear to the quadratic case by Marks and Dunn [13]. They and Wahl and Kronmal [17] examined the behaviour of linear and quadratic discriminant function using data with unequal covariances. In cases where the samples are small, the linear DA function has been found to provide more reliable assignment, whereas for large samples, the quadratic DA function may be preferred.

DA was further extended to the spatial case by [2] who proposed a geography weighted 68 DA (GWDA). In a GWDA, the idea is that the decision to allocate an observation to group 69 or population is made whilst taking the geographic location of the observation into account. 70 Whereas a standard DA (LDA and QDA) uses the mean vector and covariance matrix, a 71 GWDA uses geographically weighted means and covariances as described in Brunsdon et al 72 [1] and Fotheringham et al [7]. It uses the same geographical weighted framework as GWR, 73 in which a series of local models are constructed at locations through the study area rather 74 than one global model. In these, observations falling under a moving window or kernel are 75 weighted by their distance to the observation location and used to construct the local model. 76 The key challenge in any geographically weighted model is the determination of the size of 77 the kernel or bandwidth. A standard GWR identifies a single optimal bandwidth or spatial 78 scale over which the process under investigation is assumed to vary. This is usually done 79 through some evaluation of different bandwidths using cross validation or a model parsimony 80 measure such a s AIC. 81

However, thinking around geographically weighted frameworks and specifically geographically weighted regression (GWR) has matured considerably in recent years. This has driven a
number of developments and extensions to the original GWR. Not least of these is multiscale
GWR (MSGWR), which seeks to identify variable specific bandwidths rather than using
a single best on average bandwidth to construct local models. The idea is that individual
response-to-predictor relationships may operate over different spatial scales and the use of

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a single bandwidth in a standard GWR may under- or over-estimate those. As a result, 88 the recommended approach for any GWR is to first undertake a MSGWR to determine 89 these variable specific scales, in order to guide further model choice [5]. This, as is nicely 90 summed up by Oshan et al [14], eliminates the need for predictor-response relationships to 91 vary at the same spatial scale, can reduce over-fitting and bias in the parameter estimates, 92 and can overcome local collinearity. Thus, MGWR has been suggested as the default GWR 93 approach [5]. Such thinking and logic has potential relevance for all geographically weighted 94 frameworks, including geographically weighted discriminate analysis, hence the method 95 proposed in this paper 96

⁹⁷ 2 Multiscale Geographically Weighted Discriminant Analysis

⁹⁸ A GWDA extends QDA and LDA into geographically weighted methods. Here the decision ⁹⁹ population probabilities now depend on the spatial location of the observation – ie the the ¹⁰⁰ variance-covariance matrix \sum_j , the prior membership probabilities of class j, p_j or the μ_j ¹⁰¹ the mean vector for the observations in class j, are assumed to vary with spatial location ¹⁰² **u**. Thus, the probabilities used to derive the decision rules are conditional on **u**, reworking ¹⁰³ Equation 1 above to estimate the local likelihoods for the population models:

¹⁰⁴
$$f_p(\mathbf{x}|\mathbf{u}) = \frac{1}{(2\pi|\Sigma_j(\mathbf{u})|)^{q/2}} exp\left(-\frac{1}{2}(\mathbf{x}-\mu_j(\mathbf{u}))'\sum_j^{-1}(\mathbf{u})(\mathbf{x}-\mu_j(\mathbf{u}))\right)$$
 (2)

MSGWDA extends GWDA but allows the bandwidths for each input parameter to vary individually. The key objective in all multiscale geographically weighted models is to determine the matrix of parameter specific weights. These in this case will be used to weight each input variable at location **u**, as defined by the kernel bandwidth. As an example, Figure 1 shows some of the data from the case study described below, with the shading indicating the different bandwidths and potential scales of relationship between the grouping / classification and different variables, at the location being considered.

3 Case study: Travel Survey in Ha Noi

Ha Noi like many major cities in emerging economies, suffers serious traffic congestion and 113 air pollution due to rapid urbanization rates, increases in private transport. In Ha Noi, 114 motorbikes are the preferred transportation mode: almost everyone in the city owns a 115 motorbike. In 2015, Ha Noi had 4.9 million motorbikes and 0.5 million cars and 11 million 116 motorbikes are projected by 2025. As public transport does not meet the city's requirements, 117 increases in personal traffic are inevitable, resulting in acute welfare problems, especially air 118 quality. Pollution is chronic, with PM2.5 and ozone concentration regularly exceeding safe. 119 As a result the government in Vietnam is exploring the possibility of implementing a 120 ban that will stop motorised scooters from entering the city centre of Ha Noi. A survey has 121 been undertaken to capture data on the travel behaviour and preferences of residents in Ha 122 Noi. This includes information on trips made (origins and destinations), their frequency, 123 the transport modes used for different trips, the reasons for those modal choices as well 124 as demographic information about respondents' home locations, and critically respondent 125 attitudes concerning the proposed travel ban and how they would respond to it. This 126 paper explores the survey responses regarding the ban and the factors associated with those 127 responses in order to illustrate a multiscale geographically weighted discriminant analysis. 128



Figure 1 An illustration of the different adaptive bandwidths, shaded in cyan (30%), yellow (70%), blue (90%) and red (100%), for 4 different variables, for a location marked in black, with an OpenStreetMap backdrop.

Data from some 1191 respondents was obtained and a subset of their responses was used in the analyses as described below. Specifically the aim was to examine create a MSGWDA of attributed to the proposed van on motorised scooters from categorical variables describing:

- ¹³² respondent age group;
- 133 erespondent gender;
- ¹³⁴ the purpose of the main regular journey they make;
- the network distance of that journey, as derived from a shortest path analysis of OSM route data with snap distances.
- ¹³⁷ The resident locations are shown in Figure 2.

To demonstrate the MSGWDA approach combinations of adaptive bandwidth sizes for 138 each variable were defined as sequences running from 20% to 100% in steps of 10%. For 139 4 variables, this resulted in 9^4 bandwidth combinations to evaluate. Each combination of 140 variable specific bandwidths was used to wight inputs into a linear discriminant analysis 141 function (1da part of the MASS R package). For simplicity a boxcar weighting was used, 142 generating weights of 1 for observations underneath the kernel and 0 for those outside. The 143 were used to create a locally weighted LDA at each observation location in the study area, 144 and each local, under each combination of bandwidths model was used to predict make a 145 local classification prediction. The whole map set of classification predictions were then 146 evaluated and metrics describing classification reliability were extracted (including overall 147 accuracy, Kappa etc). The best performing combinations of bandwidths was then identified. 148

¹⁴⁹ 4 Results

Two results are used to illustrate the potential inferential advantages of the MSGWDA: an ordinary global LDA and a novel multiscale GWDA. A geographically weighted LDA was not



Figure 2 The motorbike ban attitudes of the survey respondents, with a heatmap showing the density of respondents, and a Stamen toner backdrop.

undertaken because of the inability of the gwda function in the GWmodel to handle categorical
 predictor variables.

¹⁵⁴ The standard LDA model is relatively weak, with an overall accuracy of 0.548 and a

¹⁵⁵ Kappa statistic of 0.115. The correspondence table is shown in Table 1 and indicates high

¹⁵⁶ specificity (ie good a true negatives) and low sensitivity (ie poor at true positives).

	Observed		
Predicted	agree	disagree	neutral
agree	42	24	24
disagree	222	585	238
neutral	14	16	26

Table 1 The correspondence matrix of the LDA classification of survey responses regarding a proposed motobike ban in the city centre.

The MSGWDA examined combinations of adaptive bandwidths for each variable. For each 157 of these, a geographically weighted LDA model was created at each of the 1191 respondent 158 home locations. At each location weighted LDA model was used to predict the motorbike 159 ban attitude, such that a vector of 1191 predicted ban attitudes were created from 1191 local 160 models. For each set of predictions, a correspondence matrix of predicted against observed 161 ban attitudes was created an evaluated using overall accuracy and Kappa statistics. The best 162 performing combinations were found to be the following sets of bandwidths when evaluated 163 using Overall accuracy and Kappa statistics: 164

 $_{165}$ — Overall accuracy: gender 80%, trip purpose 50%, age 40% and network distance 10%.

¹⁶⁶ Kappa statistic: gender 40%, trip purpose 20%, age 20% and network distance 10%.

¹⁶⁷ These are illustrated in Figure 3 for the same example location as in Figure 2. Here ¹⁶⁸ we can see the different bandwidths indicated by different fit or accuracy measures. The



Figure 3 The best fitting multiscale bandwidths when evaluated using Overall accuracies and Kappa statistics.

correspondences are summarised in Table 2 and result in Overall accuracies and Kappa
 statistics of 0.579, 0.199 and 0.575, 0.207, respectively.

	Overall			Kappa		
Predicted	agree	disagree	neutral	agree	disagree	neutral
agree	59	27	22	65	37	30
disagree	199	573	209	191	556	194
neutral	20	25	57	22	32	64

Table 2 The correspondence matrices of the MSDWDA classifications of survey responses, when evaluated using Overall accuracy and Kappa statistics.

171 **5** Discussion

The MSGWDA approach improves the classification accuracy compared to a standard global 172 LDA. This is to be expected and is a feature of all geographically weighted models. Of more 173 potentially interest and relevance to this specific case study, are the variations in the spatial 174 scale at which categorical data are associated with the outcome: whether evaluated by Kappa 175 or Overall accuracy, the gender variable tends towards the global, with trip purpose, age 176 and distance highly localised in their effect. This understanding of scale will inform future 177 project work in relation to the transport and behaviour simulation models being developed 178 within this project. The MSGWDA results are key to that understanding. 179

There are a number of areas of further work required to exploit the functionality of this
 MSGWDA apprach.

182 1. The bandwidths in this poof of concept were at relatively coarse intervals, evaluating

- different adaptive bandwidth sizes in steps of 10%. This needs to be refined and potentially, potentially using a refined search heuristic and consideration of bandwidth interactions –
- 185 see discussion point below.
- 186 2. Bandwidths will be extended to the fixed distance case.

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The weighting of categorical variables was done using a box car approach, with the response variables in observations falling under the kernel simply weighted to 1. This needs to be explored in more depth, especially if the data variables are ordered in some way.

Whilst the results of the MSGWDA are interesting and potential refinement on both standard approaches top DA and GWDA in terms of inference and understanding, perhaps the major discussion point to arise from this work has been due to the need to unpick the mechanisms of multiscale geographically weighted models. The key question arising from the back-fitting methods they employ is this:

How confident can we be that that potentially important variable interactions are not
being missed by this *fix the first variable bandwidth, then fix the second, then the next, etc, etc...* approach, rather than looking at all possible combinations of bandwidths?

The answer to this is uncertain: the multivariate bandwidth search space to determine the optimal set of weights to be passed to the local model at location on **u** is potentially huge. In the past, pragmatic short-cuts were needed to be able to move through it. But times and computing power have both changed.

The original MSGWR [18, 8] and subsequent refinements in other packages use a back-203 fitting algorithm to determine optimal parameter specific bandwidths and thus weights at 204 each location, for each variable. This was based on the approach taken in generalized additive 205 models (GAMs) [9, 3]. Essentially what these do is to determine the optimal set of bandwidths 206 is to determine the bandwidth for each variable sequentially, using smoothing functions 207 that assume the other terms are known. We suspect that this approach was developed by 208 the GAM team as a pragmatic way overcoming the difficulty in searching through a highly 209 dimension solution space comprised of all possible bandwidths for all possible variables. It 210 was then adopted by the initial work into multiscale geographically weighted regression. The 211 reason is the high dimensionality of the solution search space: given explanatory 5 variables, 212 in a dataset with 2000 observations and an adaptive bandwidth approach (ie based on the 213 number of observations to include rather than a fixed distance), this would potentially require 214 $2000^6 = 6.4 \times 10^{19}$ solutions to be evaluated for a regression (including the intercept) and 215 $2000^5 = 3.2 \times 10^{16}$ for a discriminant analysis 216

In this research, with potentially greater computing power available than at the time the GAM and MSGWR approaches were being developed, a grid of possible combinations of parameter specific bandwidths was used to demonstrate the MSGWDA, as described. Here the aim was to demonstrate how MSGWDA could be undertaken and to explore some of the issues arising from this. Also, this is philosophically preferable: the specification of musicale bandwidths a parameter at a time potentially ignores variable interactions at scales not considered in previously fixed bandwidths.

Future work will definitely explore this in greater detail!

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