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Chemometrics Methods with

Applications to Environmental and Quantitative

Structure-Activity Relationship Studies3

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mohd zuli bin jaafar

(max 2 lines)

Dissertation submitted in partial fulfillment
of the requirements for the degree of

Master of Education

(Educational Management and Leadership)

Faculty of Education

July 2018

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ABSTRACT

The lack of management data and not knowing what level of park quality local authorities are trying to deliver is becoming a growing concern. The problem of urban landscape cannot be solved simply by providing more parks and spending more money on development and management. There is an urgent need for innovation, for better understanding of the current and potential role of the park to meet the needs in modern urban life. Thus, the adoption of a strategic approach is needed to planning and managing that urban landscape to carry out its function and roles. This research aim is to study the factors of park attributes that influence the development, planning and management of successful urban park in Kuala Muda. It specifically studies on Taman Tasik Cini as the sole representative of urban park in the context of Kuala Muda Structure Plan 2020. This research is based on data obtained from survey questionnaire that polled public attitudes regarding the factors of park attributes based on visitor’s perception and Harris’s (2008), park success factors. The data was analysed to evaluate and determine the park attributes and its level of preferences that influence the strategic approach to the planning and management of successful urban park. The research suggested that successful urban park as are linked to the physical and functional qualities of the park; security and comfort; visitors’ preferences and needs of the place. The results of the study also suggested that a holistic strategic approach is needed for the local authority to successfully managing the urban park. It is hope that the study can contribute to the improvement of urban park planning and management in Kuala Muda.

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*Note:*

*Master – minimum 200 words*

*PhD – minimum 250 words*

*Limit to one (1) page only*

*No Paragraph*

*Font: Times New Roman - 12*

ACKNOWLEDGEMENT

Firstly, I wish to thank God for giving me the opportunity to embark on my PhD and for completing this long and challenging journey successfully. My gratitude and thanks go to my supervisor Assoc Prof Datuk.

My appreciation goes to the Captain and crewmembers of the MMC who provided the facilities and assistance during sampling. Special thanks to my colleagues and friends for helping me with this project.

Finally, this thesis is dedicated to the loving memory of my very dear late father and mother for the vision and determination to educate me. This piece of victory is dedicated to both of you. Alhamdulilah.

*--please delete--*

*Must include all supervisors names*

*Limit to one (1) page only*

*Font: Times New Roman - 12*

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LIST OF SYMBOLS

|  |  |
| --- | --- |
| Symbols |  |
| A | Number of PLS or PCA components in the model and the number of selected latent variable in the model |
| a | Number of the PLS or PCA component |
| b | PLS regression coefficient  |
| b | Number of blocks (b=1,2,3.....,K) |
| C | Coarse APM block |
|  | Pooled covariance matrix for the two classes |
|  | Covariance matrix for class g |
|  |  |
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LIST OF ABBREVIATIONS

|  |  |
| --- | --- |
| Abbreviations |  |
| PCA | Principal Component Analysis |
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LIST OF NOMENCLATURE

|  |  |
| --- | --- |
| Nomenclatures |  |
| A | Amplitude Ratio, (No Units) |
| C | Centroid of pipe, inches |
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# INTRODUCTION

## Research Background

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Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

## Motivation

Themes and styles also help keep your document coordinated. When you click Design and choose a new Theme, the pictures, charts, and SmartArt graphics change to match your new theme. When you apply styles, your headings change to match the new theme. Themes and styles also help keep your document coordinated. When you click Design and choose a new Theme, the pictures, charts, and SmartArt graphics change to match your new theme. When you apply styles, your headings change to match the new theme.

## Problem Statement

Video provides a powerful way to help you prove your point. When you click Online Video, you can paste in the embed code for the video you want to add. You can also type a keyword to search online for the video that best fits your document as shown in Table 1.1.

To make your document look professionally produced, Word provides header, footer, cover page, and text box designs that complement each other. For example, you can add a matching cover page, header, and sidebar. Click Insert and then choose the elements you want from the different galleries.

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On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages,

Table 1.1
The Title for This Table is Here

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| --- | --- | --- |
| Title | Title | Title  |
| To change the overall look of your document | To change the overall look of your document | To change the overall look of your document |
| To change the overall look of your document | To change the overall look of your document | To change the overall look of your document |
| Source: World Bank report 2016 |

Table 1.2
The Statistical Information of APM Dataset

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Batch | No of samples | Average per month | Percentage of LoD (Coarse APM) | Percentage of LoD (Fine APM) |
| 1 | 100 | 8 samples | 1.70% | 6.48% |
| 2 | 102 | 9 samples | 9.29% | 9.09% |
| 3 | 176 | 9 samples | 2.65% | 4.34% |

Table 1.3
The Title for This Table is Here

|  |  |  |
| --- | --- | --- |
| Chemical CComposition | Surface Area (m2g-1) | Porosity(cm3g-1) |
| Neutral clay 0.68 0.68 | Neutral clay 0.68 0.68 | Neutral clay 0.68 0.68 |
| Bleaching clay | Bleaching clay | Bleaching clay |
|  |  |  |
| 0.80  | 0.89 | 0.99 |
| Note: Influence of the physical chemistry properties of an acid activated bentonite in the bleaching of olive oil. (Pradas et.al., 1993, p. 23) |

Themes and styles also help keep your document coordinated. When you click Design and choose a new Theme, the pictures, charts, and SmartArt graphics change to match your new theme. When you apply styles, your headings change to match the new theme as shown in equation (1.1).

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|  | (1.1) |

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## Objectives

To make your document look professionally produced, Word provides header, footer, cover page, and text box designs that complement each other. For example, you can add a matching cover page, header, and sidebar. Click Insert and then choose the elements you want from the different galleries.

###### To perform data pre-processing and exploratory analysis by using PCA, SOMs and Class Separation Indices.

###### To analysis analysis Multiblock methods and regression analysis of environmental dataset.

###### To find the trend using pattern recognition in method QSAR with the application of SOMs and PLSDA.

###### To test model validity using data Splitting Methods for Regressions and Classifications.

## Significance of Study

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Plate 1.1 A Picture of Light

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Figure 1.1 The Spectrum of Cooking Oil On

#### Univariate Regression

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#### Multivariate Regression

##### Principal Components Regression

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##### Multivariate Regressions using PLS Method

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###### You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

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# LITERATURE REVIEW

## Introduction

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Table 2.1
The Temperature Infomation

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Variable | Minimum | Maximum | Average | Standard deviation |
| Minimum temperature over 24 hours preceding 0300 GMT (0C) | 0.0 | 30.0 | 15.33 | 7.06 |
| Maximum temperature over 24 hours preceding 1200 GMT (0C) | 12.5 | 44.7 | 29.85 | 6.93 |

Table 2.2
The Environmental Dataset Infomation

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Variable | Minimum | Maximum | Average | Standard deviation |
| Average relative humidity (%) | 31.0 | 97.0 | 63.70 | 14.80 |
| Average pressure (hPa) | 994.37 | 1022.43 | 1009.04 | 6.48 |
| Average wind speed (Knot) | 0.0 | 9.0 | 0.79 | 1.43 |
| Average rainfall (mm) | 0.0 | 140.0 | 3.82 | 14.05 |

#### Data Pre-Processing and Data Drift: The Utility of Principal Component Analysis, Self-Organizing Maps and Class Separation Indices

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. The sample of equation is given in (2.1). On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look as shown in equation (2.2).

|  |  |
| --- | --- |
|  | (2.1) |
|  | (2.2) |

#### Multivariate Linear Regression

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

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## Environmental Studies

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Table 2.3
Summary of the Meteorological Parameters

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Variable | Minimum | Maximum | Average | Standard deviation |
| Minimum temperature over 24 hours preceding 0300 GMT (0C) | 0.0 | 30.0 | 15.33 | 7.06 |
| Maximum temperature over 24 hours preceding 1200 GMT (0C) | 12.5 | 44.7 | 29.85 | 6.93 |
| Average relative humidity (%) | 31.0 | 97.0 | 63.70 | 14.80 |
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| Average rainfall (mm) | 0.0 | 140.0 | 3.82 | 14.05 |

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#### Airborne Particulate Matter Datasets

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Table 2.4
Title for Third Table in Chapter 2

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| To change the overall look of your document | To change the overall look of your document | To change the overall look of your document |
| Source: World Bank report 2016 |

Table 2.5
The Statistical Information of APM Dataset

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Batch | No of samples | Average per month | Percentage of LoD (Coarse APM) | Percentage of LoD (Fine APM) |
| 1 | 100 | 8 samples | 1.70% | 6.48% |
| 2 | 102 | 9 samples | 9.29% | 9.09% |
| 3 | 176 | 9 samples | 2.65% | 4.34% |

#### Meteorological Dataset

##### Data Pre-Processing and Data Drift

###### You Can Use These Galleries To Insert Tables, Headers, Footers, Lists, Cover Pages, And Other Document Building Blocks. When You Create Pictures, Charts, Or Diagrams, They Also Coordinate With Your Current Document Look.

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## Quantitative Structure Activity Relationships Studies on the Active and Inactive Antimalarial Compounds

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Plate 2.1 A Sample of Grass and Bamboo 2

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Table 2.6
The Sample of the Table with More Than One Page Items

| No | Molecular Descriptors | Abbreviation | Groups | Amount | Description |
| --- | --- | --- | --- | --- | --- |
| 1 | Constitutional descriptors | Con | 0D | 48 | 0D-descriptors, independent from molecular connectivity and conformations. Atom and bonds counts, molecular weight, sum of atomic properties, etc |
| 2 | Topological descriptors | Topo | 2D | 119 | Molecular descriptors obtained from the molecular graph (usually H-depleted), i.e 2D-descriptors conformationally independent. |
| 3 | Walk and pathcounts | Wap | 2D | 47 | Molecular descriptors obtained from the molecular graph, counting paths, walk and self returning walks of different lengths. |
| 4 | Connectivityindices | Coni | 2D | 33 | Topological Molecular descriptors calculated from the vertex degree of the atoms in the H-depleted molecular graph. |
| 5 | Informationindices | Info | 2D | 47 | Molecular descriptors calculated as information content of molecules, based on the calculation of equivalences classes from the molecular graph. Among them, the indices of neighbourhood degree and edge multiplicity. |
| 6 | 2Dautocorrelations | 2D | 2D | 96 | Molecular descriptors calculated from the molecular graph by summing the products of atom weights of the terminal atoms of all the paths of the considered path length (the lag) |
| 7 | Edge adjacency indices | Edge | 2D | 107 | Topological Molecular descriptors derived from the edge adjacency matrix which encodes the connectivity between graph edges. |
| 8 | Burdeneigenvalues | Bur | 2D | 64 | Molecular descriptors contained from the positive and negative eigenvalues of the adjacency matrix, weighting the diagonal element with atom weight. |
| 9 | Topologicalcharge indices | Topoc | 2D | 21 | First 10 eigenvalues (absolute values) obtained from a corrected adjacency matrix. |
| 10 | Eigenvalue-based indices | EiG | 2D | 44 | Topological descriptors calculated by the eigenvalues of the square(usually symmetric) matrix representing a molecular graph. |
| 11 | Randic molecular profiles | Ran | 3D | 41 | Molecular descriptors derived from the distance distribution moments of the geometry matrix, defined as the average row sum of its entries raised at the k-th power, normalized by the factor k. |
| 12 | Geometrical descriptors | Geo | 3D | 74 | Different kinds of conformationally dependent descriptors based on the molecular geometry. Reliable values are obtained if reliable conformations were previously calculated. |
| 13 | RDF descriptors | RDF | 3D | 150 | Molecular descriptors obtained by radial basis functions centred on different interatomic distances (from 0.5A to 15.5A) |
| 14 | 3D-MoRSE descriptors | 3D | 3D | 160 | Molecular descriptors calculated by summing atom weights by different angular scattering function. |
| 15 | WHIMdescriptors | WHIM | 3D | 99 | Molecular descriptors obtained as statistical indices of the atom projected onto the 3 principal components obtained from weighted covariance matrices of the atomic coordinates. |
| 16 | GETAWAY descriptors | GATE | 3D | 197 | Descriptors calculated from the leverage matrix obtained by the centred atoic coordinates (molecular influences matrix,MIM). The first four descriptors are calculated as information content and connectivity indices. HATA and H descriptors are 3D-autocorrelation descriptors obtained from MIM; R and R+ descriptors obtained from the leverage. Geometry matrix. |
| 17 | Functional group counts | Funct | Others | 152 | Molecular descriptors based on the counting of chemical functional groups. They are calculated by knowing the molecular composition and atom connectivities. |
| 18 | Atom-centred fragments | Atom | Others | 120 | Molecular descriptors, based on the counting of 120 atom-centered fragments, as defined by Ghose-Crippen. Some fragments are undefined by the authors. They are calculated by knowing the molecular composition and atom connectivities. |
| 19 | Charged descriptors | charged | Others | 14 | Fourteen charge descriptors which are reliable only when charge are estimated by quantum molecular methods |

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Figure 2.1 A Sample of Formatting Method



Plate 2.2 The View of the Tuanku Syed Sirajuddin Building, UiTM from the Dataran Tengku Fauziah

# RESEARCH METHODOLOGY

## Introduction

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## Data Pre-Processing for Classifcation

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Figure 3.1 Compressive strength of Rice Husk Ash (RHA) concrete of Grade 30

#### Individual Transformation

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|  |  |
| --- | --- |
|  | (3.1) |
|  | (3.2) |

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template. On The Insert Tab, The Galleries Include Items That Are Designed To Coordinate With The Overall Look Of Your Document.

Save time in Word with new buttons that show up where you need them. To change the way a picture fits in your document, click it and a button for layout options appears next to it. When you work on a table, click where you want to add a row or a column, and then click the plus sign.

Reading is easier, too, in the new Reading view. You can collapse parts of the document and focus on the text you want. If you need to stop reading before you reach the end, Word remembers where you left off - even on another device.

#### Row Scaling

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.nYou Can Use These Galleries To Insert Tables, Headers, Footers, Lists, Cover Pages, And Other Document Building Blocks.

When you create pictures, charts, or diagrams, they also coordinate with your current document look. You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab.

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#### Column Scaling

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“You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.”

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

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## Exploratory Data Analysis Principal Component Analysis

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Figure 3.2 Typical Steps Involved in QSAR Methodology



Nilore

Figure 3.3 A Map Showing the Sampling Location in Islamabad, Pakistan

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## Quantitative Structure Activity Relationships Studies on The Active and Inactive Antibacterial Compounds

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|  |  |  |
| --- | --- | --- |
|  |  |  |
| 1. Pre-process data: A1, R1 and C1
 | 1. Pre-process data: A1, R1 and C2
 | 1. Pre-process data: A1, R1, C3
 |
|  |  |  |
| 1. Pre-process data: A1, R2 and C1
 | 1. Pre-process data: A1, R2 and C2
 | 1. Pre-process data: A1, R2, C3
 |

Figure 3.4 A PCA Plots for Data Processing Strategy

Table 3.1
The QSAR Dataset the Sources in This Thesis for Regression and Classification

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| No | Name | Dimension | Classes/ Types | Reference |
| 1 | Blood Brain Barrier | 406 × 926 | Non-penetrating (class 1), 136 compoundsPenetrating (class 2), 270 compounds | [150] |
| 2 | Antimalarial | 57 × 1661 | Regression  | [151] |
| 3 | Skin | 131 × 926 | Strong skin sensitizers (Class 1), 67 compoundsNon- strong skin sensitizers(class 2), 64 compounds | [152] |

# RESULTS AND DISCUSSION On the Pattern Recognition and Data Mining Methods in Chemometrics.

## Introduction

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On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document.

You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks.

When you create pictures, charts, or diagrams, they also coordinate with your current document look.

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## Chemometrics

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## PCA and PLS

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APPENDICES

APPENDIX 1

Example of the Codes in PLS Algorithms

APPENDIX 2

Table of Parameters Used in Data Processing for PLS Testing Precuders on the Classification of Biological Activity

|  |  |  |
| --- | --- | --- |
| Type | Formula | Description |
| C1 |  | Mean centring |
| C2 |  | Standardisation |
| C3 |  | Range scaling  |

AUTHOR’S PROFILE

|  |  |  |
| --- | --- | --- |
|  | C:\Users\MohdZuliDell\Dropbox (MZJ Word for Thesis)\Zuli PHOTO.png |  |

Mohd Zuli Jaafar obtained Bachelor of Science in Chemistry (Hons.) in 1996 from University Malaya, Kuala Lumpur, MSc in Chemistry (2002) from Universiti Teknologi Malaysia and PhD in Chemometrics (2011) from the University of Bristol, United Kingdom. His PhD thesis involves several methods in Chemometrics and Pattern Recognition includes Data Preprocessing, Regression, Classification and Variable Selection. Currently he is working on several scientific dataset i.e. Fourier Transform Infrared Spectroscopy, Near Infrared, Particle-Induced X-Ray Emission and Quantitative Structure-Activity Relationship.

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