UNIVERSITY OF TECHNOLOGY SYDNEY

A Study on Stable Feature Representations for Artificial Olfactory System

by Taoping Liu

Thesis submitted in fulfilment of the requirements for the degree of

Doctor of Philosophy

under the supervision of Steven Su

University of Technology Sydney
Faculty of Engineering and Information Technology

March 2021

Certificate of Original Authorship

I, *Taoping Liu* declare that this thesis, is submitted in fulfilment of the requirements for the award of *Doctor of Philosophy*, in the *School of Biomedical Engineering*, *Faculty of Engineering and Information Technology* at the University of Technology Sydney.

This thesis is wholly my own work unless otherwise referenced or acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis.

This document has not been submitted for qualifications at any other academic institution.

This research is supported by the Australian Government Research Training Program.

Production Note:
Signature removed prior to publication.

SIGNATURE: ______________________

[Taoping Liu]

DATE: 1st March, 2021

Dedication

To Mom and Dad

To My Wife, Chaoran

Acknowledgments

I would like to express my most sincere gratitude to my principal supervisor, A/Prof. Steven Su, for his continued support and wise guidance throughout my Ph.D. study. His knowledge, expertise, understanding, and insights greatly expanded my knowledge and skills in many areas. His patience and optimism helped me though the ups and downs of the Ph.D. life. Without his persistent help, the goal of this research would not have been achieved.

I would also like to show my great appreciation to my co-supervisor, Dr. Jun Li, for his solid support and skilful guidance. His expertise, intelligence, and encouragement enlarged my vision to a broader field and steered me to dive deeper into my research.

I am grateful to the UTS NOS.E Team members, Prof. Shari L. Forbes (University of Quebec in Trois-Rivières, Canada), A/Prof. Steven Su, Dr. Maiken Ueland, Dr. Wentian Zhang, and Amber Brown, for their selfless help. It is a great honour for me to be part of the team.

I am also grateful to the BeFAQT Team, especially to Prof. Ren Ping Liu, Mr. Peter Loneragan, A/Prof. Steven Su, A/Prof. Qiang Wu, A/Prof. Jian Zhang, Dr. Xu Wang, Mr. Erik Poole (Sydney Fish Market, Australia), and Dr. Zongjian Zhang for giving me the opportunity to further research in this amazing project.

I would like to thank all stuff in the School of Biomedical Engineering, especially to Prof. Joanne Tipper and Prof. Gyorgy Hutvagner, for all the suggestions, advice, and help they have given me. Special thanks to Prof. Gyorgy Hutvagner for his effort in letting us feel a sense of connectedness and belongingness, especially in this tough year.

I would like to acknowledge the assistance from my colleagues, Dr. Tao Zhang, Dr. Lin Ye, Dr. Wenhui Chen, Dr. Hairong Yu, Yao Huang, Hanjie Wu, Yujiao Wu, Palayil Baby Jephil, *etc.*.

I would like to recognize the help that I received from my friends Dr. Miao Zhang, Li Wang, Chen Wang, Yanhao Zhang, Dr. Ye Shi, Dr. Huan Yu, Dr. Wenwei Mo, Kairui Guo, Lingmeng Li, and Mingjian Wang.

I must also thank Prof. David Huang (Western Sydney University, Australia) and

Mrs. Sarah Huang for their warm help.

My deepest gratitude goes to my parents for their immeasurable support and encouragement throughout my Ph.D. life.

I would like to sincerely thank the love of my wife, Chaoran, for her accompany and encouragement.

Finally, I would like to thank the sponsors for the scholarships, including China Scholarship Council (CSC), University of Technology Sydney (UTS), and Food Agility Cooperative Research Centre (Food Agility CRC).

Abstract

The electronic nose (e-nose) is an artificial olfactory system, consisting of a gas sensor array, a control system, and algorithms, designed to detect and identify the single or mixtures of odours. Owing to the boom of gas sensor technology and machine learning algorithms, e-noses have found wide applications in many different fields. However, the performance of e-noses in real applications has been challenged due to the 3D issue (i.e. the discreteness issue, the drift issue, and the disturbance issue). This thesis mainly focuses on the discreteness issue, especially the instability in feature representations caused by sensor noises.

A kernel regularization modelling-based method is proposed to provide stable representations for target odours. This method regards the e-nose as a whole system. The estimated parameters of the system are applied as features to represent the odour. The use of a smooth and stable kernel in the regularization term helps to overcome the ill-posed problem existing in deconvolution. The performance of the proposed method is verified by the experiment of classifying six target perfumes measured under a relatively stable environment.

However, the above-proposed method requires an accurate setting of the initial time (time of gas-on). In order to avoid a laborious searching of this time point, an improved method based on multiscale wavelet kernel regularization is proposed. The multiscale wavelet kernel inherits the advantage from wavelet function in approximating arbitrary signals and equips the method with the ability in resistance to random noise. The performance of the proposed method is verified by the experiment of classifying four target whiskies. The training and testing samples were obtained from two environments. Accordingly, a framework of "feature extraction – domain adaptation" is proposed in the experiment.

Aiming at the instability of traditional transient-state features extracted from the noise-contaminated signal, a novel kernel Tikhonov regularization-based numerical differentiation algorithm is proposed. The proposed method can improve such features by directly estimating accurate high-order derivatives from noisy signals. The performance

of the proposed method is verified by the experiment of identifying four target whiskies. The training and testing set were collected from two different environments. Moreover, samples of two new whiskies were added to the testing set as disturbances. Accordingly, a framework of "feature extraction – domain adaptation – one-class classification" is proposed in this experiment.

In addition, on the basis of stable feature representations, we also proposed two frameworks for food freshness monitoring and evaluation. Monitoring is realized by one-class classification. A single hidden Markov model (HMM) trained only by fresh samples is applied to track the change in freshness. For freshness evaluation, an HMM-based decoding algorithm is proposed to cluster the freshness level when the whole life-span data of meat stored in a specific storage condition is available. Then, HMM for each freshness level is trained and applied in parallel as freshness evaluation models to classify the tested meat samples.

List of Publications

Related to the Thesis :

[1] T. Liu, W. Zhang, L. Ye, M. Ueland, S. L. Forbes, and S. W. Su, *A novel multi-odour identification by electronic nose using non-parametric modelling-based feature extraction and time-series classification*, Sensors and Actuators B: Chemical, 298 (2019), pp. 126690.

[2] T. Liu, W. Zhang, M. Yuwono, M. Zhang, M. Ueland, S. L. Forbes, and S. W. Su, *A data-driven meat freshness monitoring and evaluation method using rapid centroid estimation and hidden Markov models*, Sensors and Actuators B: Chemical, 311 (2020), pp. 127868.

[3] T. Liu, W. Zhang, J. Li, M. Ueland, S. L. Forbes, W. X. Zheng, and S. W. Su, *A multiscale wavelet kernel regularization-based feature extraction method for electronic nose*, Submitted to IEEE Transactions on Systems, Man, and Cybernetics: Systems. (*Under Review*)

[4] T. Liu, W. Zhang, L. Wang, M. Ueland, S. L. Forbes, W. X. Zheng, and S. W. Su, *Numerical differentiation from noisy signals: a kernel regularization method to improve transient-state features for electronic nose*, Submitted to IEEE Transactions on Industrial Electronics. (*Under Review*)

Others :

[5] T. Liu, W. Zhang, P. McLean, M. Ueland, S. L. Forbes, and S. W. Su, *Electronic nose-based odor classification using genetic algorithms and fuzzy support vector machines*, International Journal of Fuzzy Systems, 20 (2018), pp. 1309-1320.

[6] W. Zhang, T. Liu, M. Zhang, Y. Zhang, H. Li, M. Ueland, S. L. Forbes, R. X. Wang, and S. W. Su, *NOS.E: a new fast response electronic nose health*

monitoring system, in 2018 40th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC), IEEE, 2018, pp. 4977-4980.

[7] W. Zhang, T. Liu, L. Ye, M. Ueland, S. L. Forbes, and S. W. Su, *A novel data pre-processing method for odour detection and identification system*, Sensors and Actuators A: Physical, 287 (2019), pp. 113-120.

[8] W. Zhang, T. Liu, M. Ueland, S. L. Forbes, R. X. Wang, and S. W. Su, *Design of an efficient electronic nose system for odour analysis and assessment*, Measurement, 165 (2020), pp. 108089.

[9] M. Zhang, H. Li, S. Pan, T. Liu, and S. Su, *One-shot neural architecture search via novelty driven sampling*, in Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence Yokohama, Japan: International Joint Conference on Artificial Intelligence Organization, 2020, pp. 3188-3194.

Table of Contents

List of Publications ix

List of Figures xv

List of Tables xxv

1 Introduction 1

1.1 Motivation and Scope 1
1.2 Applications of Electronic Nose 4
1.2.1 Auxiliary Disease Diagnosis 4
1.2.2 Food Safety Control 5
1.2.3 Hazardous Gas Detection and Localization 6
1.3 Algorithmic Challenges and Solving Strategy 7
1.3.1 Discreteness Issue 7
1.3.2 Drift Issue 7
1.3.3 Disturbance Issue 8
1.3.4 Solving Strategy 10
1.4 Thesis Contribution 11
1.5 Thesis Outline 14

2 Literature Review 19

2.1 Introduction 19
2.2 Review of Signal Processing Algorithms 20
2.2.1 Linear Transformation Algorithms 20
2.2.2 Smoothing Algorithms 22
2.3 Review of Feature Extraction Algorithms 26
2.3.1 Traditional Hand-Crafted Features 26
2.3.2 Curve Fitting-Based Features 28

2.3.3 Learning-Based Features 29
2.3.4 Frequency-Domain Features 30
2.3.5 Other Features 31

3 Feature Extraction Based on Non-Parametric Modelling 33
3.1 Introduction 33
3.2 Methodology 35
3.2.1 Kernel-Based Model Estimation 36
3.2.2 Parameter Optimization 37
3.3 Field Experiment Setup 38
3.3.1 Material Preparation and Instrument Settings 38
3.3.2 Experiment Process 41
3.4 Results and Discussion 43
3.4.1 Automatic Initial Time Detection 43
3.4.2 Result of Parameter Selection 44
3.4.3 Comparison of Resistance to Noise 49
3.4.4 Comparison of Different Feature Extraction Methods 51
3.4.5 Comparison of Different Multiclass odour Identification Methods . 53
3.5 Conclusion 56

4 Feature Extraction Based on Multiscale Wavelet Kernel Regularization 59
4.1 Introduction 59
4.2 Methodology 61
4.2.1 Multiscale Wavelet Kernel 62
4.2.2 Feature Extraction Using Kernel-Based Modelling 63
4.3 Numerical Experiment 65
4.3.1 Experiment Setup 66
4.3.2 Comparison of Different Kernel-Based Modelling Methods 66
4.4 Field Experiment 68
4.4.1 Experiment Setup 68
4.4.2 Comparison of Different Feature Extraction Methods 73
4.4.3 Comparison in Resistance to Noises 76
4.5 Conclusion 77

5 Numerical Differentiation Based on Kernel Regularization to Improve Transient-State Features 79

5.1 Introduction 79
5.2 Methodology 81
5.2.1 Derivative Estimation for Electronic Nose Signals 81
5.2.2 Boundary Distortion Reduction Using Polynomial Extension 83
5.2.3 Derivative Estimation for Arbitrary Differentiable Functions . . . 85
5.3 Numerical Experiment 85
5.3.1 Experiment Setup 85
5.3.2 Comparison of Different Numerical Differentiation Methods 86
5.4 Field Experiment 88
5.4.1 Experiment Setup 88
5.4.2 Comparison of Different Feature Extraction Methods 91
5.5 Conclusion 91

6 Data-Driven Meat Freshness Monitoring and Evaluation Using Electronic Nose 93
6.1 Introduction 93
6.2 Methodology 96
6.2.1 Preliminary of HMMs 96
6.2.2 Segmental RCE-Based Training 97
6.2.3 HMM-Based Meat Freshness Monitoring 97
6.2.4 HMM-Based Meat Freshness Grading and Evaluation 98
6.3 Field Experiment Setup 102
6.3.1 Material Preparation 102
6.3.2 Instrument Settings 103
6.3.3 Data Pre-Processing and Feature Extraction 103
6.4 Results and Discussion 104
6.4.1 Meat Freshness Monitoring 104
6.4.2 Meat Freshness Grading 108
6.4.3 Meat Freshness Evaluation 111
6.5 Conclusion 117

7 Conclusion and Future Work 119
7.1 Conclusion 119
7.2 Limitations 121
7.3 Future Work 121

Bibliography **123**

List of Figures

Figure **Page**

1.1 An intuitive comparison between two olfactory systems (a) Human olfactory system. Odorant molecules entered the nasal cavity by inhalation to touch olfactory sensory neurons. Once the molecules are caught, they will interact with specific reactors on the surface of olfactory sensory neurons. Then, action potentials are activated and transmitted via the neuron axons to the olfactory bulb. In the olfactory bulb, the potentials are further processed by glomerulus and mitral cells, and finally interpreted by the brain [70, 188]. (b) Artificial olfactory system. Odorant molecules are sniffed in to the sensor chamber by air intake/exhaust system. Once the odorant molecules are perceived by the sensor, the sensor's resistance will change. Then, this change is reflected by the voltage over the load resistor. After analog-to-digital (A/D) conversion, the sensor's reading is further processed by signal processing and feature extraction algorithms, and finally interpreted by pattern recognition algorithms. 3

1.2 Representative example of the discreteness issue. The example displayed is responses of TGS 2602 sensors to the Chanel Chance perfume sample. (a) Odour concentration variation. The concentration of the target odour decreases as the number of measurements increases. Concentration variation causes the difference in response curves. (b) Sensor manufacturing discrepancy. Two identical sensors produce different response curves under the same environmental conditions. 8

1.3 Representative example of the drift issue. The example displayed is responses of TGS 2602 gas sensor to the Chanel Chance perfume sample. The blue and red lines represent the samples measured at UTS CB11 and UTS CB04, respectively. The change in temperature and humidity causes the difference in response curves. 9

1.4 Illustrative example of the disturbance issue. (a) Continuous disturbance. (b) Contingent disturbance. (c) Changing from target odour to non-target odour. T_i denotes the i^{th} target odour. D denotes disturbance. $T_i + D$ represents the mixture of target and disturbance odour. 9

1.5 The solving strategy to the 3D issue. 12

2.1 Typical response curve of MOS-type gas sensors. The example displayed is responses of TGS 2602 gas sensor to the Chanel Chance perfume sample. . . 20

2.2 Representative example of linear transformations. The example displayed is responses of TGS 2602 sensors to the Chanel Chance perfume sample. (a) Original response curves. (b) Differential conductance. (c) Fractional conductance. (d) Normalization. (e) Standardization 21

2.3 Basic elements for hand-crafted features. The example displayed is responses of TGS 2602 sensors to the Chanel Chance perfume sample. The blue solid line is the estimation result of our proposed method Chapter 5. The gray dashed line is the filtering result of WTDF. 27

2.4 Representative example of polynomial curve fitting-based feature extraction. The example displayed is responses of TGS 2602 sensors to the Chanel Chance perfume sample. (a) Curve fitting in the absorption stage. (b) Coefficients of 2^{nd}-degree polynomials. (c) Coefficients of 3^{rd}-degree polynomials. (d) Coefficients of 4^{th}-degree polynomials. 29

2.5 Representative example of SAE-based feature learning. 30

2.6 Illustrative example of modulation system. (a) Temperature modulation module. (b) Flow rate modulation module 31

3.1 Schematic diagram of experimental setup 39

3.2 Representative example of the measurement circuit. Inside the e-nose, two pairs of sensors are connected to two dual-channel amplifiers (OP2177) respectively, and the single rest sensor is connected to one single-channel amplifier (OP1177). The representative example shows the measurement circuit using a dual-channel amplifier. The heater voltage (VCC_5V) is applied to the integrated heater to make the gas sensor work at a specific temperature that is most suitable for gas sensing. The VCC_5V DC voltage is also applied as sensor circuit voltage to allow measurement of the voltage across the load resistors (R4, R5 and R7, R8) which are connected in series with the sensor. Once the sensor detected the target gas, the measurement voltage is changed due to the variation of the sensor resistance. The measurement voltage is sent to the non-inverting amplifier (OP2177) before transmitting to the analogue to digital module of the microcontroller for further processing. 39

3.3 The basic structure of hidden Markov Models. HMM contains two processes: the unobserved discrete first-order Markov process, where the current state, Q_d, only depends on the previous state, Q_{d-1}, and the observed stochastic process, where the current observation, O_d, is only dependent on the current hidden state, Q_d. 42

3.4 Flowchart of GMM-HMM-based odour classification. (a) Training procedure: Model parameters for both feature extraction and classification algorithms should be decided first. Next, send the normalized sensor array's responses to the feature extraction models and obtain finite impulse responses. Then, the classification model is learned based on these finite impulse responses. This procedure is repeated for every perfume class. (b) Testing procedure: sensor array's responses to an unknown odour is first normalized and then processed by the feature extraction method. Then, log-likelihood of the extracted feature sequence is evaluated by each trained classification model, λ_n. The label of the model that reaches the highest value is regarded as the label of the unknown odour. 43

3.5 Representative example of sensor initial time detection. The real initial time is 37s for this sensor. When the selected initial time is set to 20s, its kernel-based estimation generates negative values on the interval $(20, 37)$. 44

3.6 Illustration of SS kernel parameter optimization. (a) Contour plot of parameter optimization for Perfume 1. $\beta = 0.9825$, $c = 7$. (b) Contour plot of parameter optimization for Perfume 2. $\beta = 0.9800$, $c = 8$. (c) Contour plot of parameter optimization for Perfume 3. $\beta = 0.9850$, $c = 5$. (d) Contour plot of parameter optimization for Perfume 4. $\beta = 0.9850$, $c = 8$. (e) Contour plot of parameter optimization for Perfume 5. $\beta = 0.9900$, $c = 2$. (f) Contour plot of parameter optimization for Perfume 6. $\beta = 0.9825$, $c = 2$. 45

3.7 Representative example of the finite impulse responses to one sensor. The number of impulse responses, D, is selected as 200, at which the amplitude is much close to zero. When c is set to 1, the IE equals 4.1932. The IE decreases to 4.1096, when c increases to 100. However, the NMSE reduces from 0.12% to 0.06%. 46

3.8 BIC for Gaussian mixtures. The results are Perfume 1: $Q = 8$, Perfume 2: $Q = 15$, Perfume 3: $Q = 9$, Perfume 4: $Q = 8$, Perfume 5: $Q = 9$, Perfume 6: $Q = 13$. 47

3.9 Boxplot of classification sensitivity 48

3.10 ROC curves for considered methods. (a) Perfume 1: AUC4 > AUC1 > AUC3 > AUC2 > AUC6 > AUC5; (b) Perfume 2: AUC1 > AUC4 > AUC3 > AUC5 > AUC2 > AUC6; (c) Perfume 3: AUC1 > AUC4 > AUC6 > AUC5 > AUC3 > AUC2; (d) Perfume 4: AUC3 > AUC1 > AUC4 > AUC6 > AUC5 > AUC2; (e) Perfume 5: AUC1 = AUC6 > AUC4 > AUC3 > AUC2 > AUC5; (f) Perfume 6: AUC1 > AUC3 > AUC4 > AUC6 > AUC5 > AUC2. 57

4.1 Representative example of sensor's response. The example displayed here is TGS2600's response to one sample of Ardbeg whisky. The operating parameters representing the presence or absence of the target odour divide the sensor response into a baseline stage, an absorption stage, and a desorption stage. Feature extraction is usually performed at the first two stages. The curve of operation parameters is regarded as the ideal input of the e-nose system from the view of modelling-based feature extraction. 61

4.2 Basic measuring circuit of Figaro TGS MOS sensor. The integrated heater (R_{heat}) provides an optimal temperature for the sensing element (R_{sensor}). The sensor's reading is the voltage across the load resistor (R_{load}) connected in series with the sensor. Both of the V_{cc} and V_{heat} are constant voltage sources. 67

4.3 Simulated TGS MOS sensor's response. The blue line denotes the simulated response, and the red dashed line denotes the noised observation. The features are extracted from the noised observation. The experiment parameters were set as: $V_{cc} = 5$ V, $R_{\text{load}} = 0.45$ kΩ, $R_0 = 4$ kΩ, $k = 100$, and $\beta = 0.4$. The concentration of odour is ranged from 0 to 40 mol·dm^{-3}, and the initial time $t_{\text{gas-on}} = 20$ s. 67

4.4 Experiment setup. (a) Field experiment on CeBIT Australia 2019. (b) Diagram of material measurement. Firstly, ambient air is drawn into the sealed sensor chamber through the input port II for 10 s to obtain a baseline for each sensor. Next, the target odour is inhaled by a sampling needle through the input port I for 10 s. Then, the sensor chamber is cleaned by the ambient air for 40 s. The flow rate is kept constant at 1.1 L/min. The sampling rate of the e-nose is set as 10 Hz. After one measurement, the collected data is sent to a laptop for further processing via the Wi-Fi. 71

4.5 Flow diagram of experiment process. (a) Training procedure. (b) Testing procedure. 72

4.6 Confusion matrix for the field experiment (the testing procedure). (a) Proposed features. Sensitivity (Sen.) for each label: 100%, 85.96%, 87.10%, and 100%; Specificity (Spe.) for each label: 100%, 94.41%, 94.20%, and 100%. (b) Handcrafted features. Sen.: 97.50%, 77.19%, 72.58%, and 97.56%; Spe.: 99.38%, 90.91%, 87.68%, and 99.37%. (c) Polynomial curve fitting-based features. Sen.: 92.50%, 73.68%, 80.65%, and 82.93%; Spe.: 98.12%, 89.51%, 91.30%, and 95.60%. (d) Sparse auto-encoder features. Sen.: 100%, 85.96%, 79.03%, and 100%; Spe.: 100%, 94.41%, 90.58%, and 100%. (e) Time series (no feature extraction). Sen.: 87.50%, 68.42%, 56.45%, and 53.66%; Spe.: 96.88%, 87.41%, 80.43%, and 88.05%. 74

4.7 Boxplot of different features in resistance to Gaussian white noises 76

5.1 Illustration of polynomial extension. $\boldsymbol{y} \in \mathbb{R}^N$ is the input signal. $\boldsymbol{y}_L \in \mathbb{R}^m$ ($\boldsymbol{y}_R \in \mathbb{R}^m$) represents the first (last) m points of $\boldsymbol{y}$ used to training polynomial function $p_L(t)$ ($p_R(t)$). $\boldsymbol{y}_{LE} \in \mathbb{R}^m$ ($\boldsymbol{y}_{RE} \in \mathbb{R}^m$) represents the related extension. $\boldsymbol{y}_E$ denotes the polynomial extension. $y_{[0]}$ ($y_{E[0]}$) denotes the first point of $\boldsymbol{y}$ ($\boldsymbol{y}_E$). 84

5.2 Framework of experiment process to tackle the 3D issue. (a) Training procedure. (b) Testing procedure. 88

5.3 Representative example of feature extraction. Six transient-state features are extracted, including: $z_1 = dy_{max}$, $z_2 = d2y_{max}$, $z_3 = d2y_{min}$, $z_4 = \Delta t_1$, $z_5 = \Delta t_2$, and $z_6 = \Delta t_3$. 90

5.4 Confusion matrix for the field experiment (the testing procedure @ICC Sydney). (a) Traditional transient-state features (proposed method). Accuracy (Acc.): 86.36%; Averaged sensitivity (A. Sen.): 87.29%; Averaged specificity (A. Spe.): 96.50% (b) Traditional transient-state features (wavelet filter). Acc. 73.14%; A. Sen.: 73.66%; A.Spe.: 93.18%. (c) Polynomial curve fitting-based features. Acc.: 60.33%; A. Sen.: 60.49%; A.Spe.: 89.97%. (d) Sparse auto-encoder features. Acc.: 83.47%; A. Sen.: 84.43%; A. Spe.: 95.75%. 92

6.1 Flowchart of HMM-based meat freshness monitoring. Sensor array's responses of meat samples are first pre-processed before extracting features. In the training procedure, only the feature vectors extracted from fresh meat samples (i.e. $t = 0$) can be sent to segmental RCE algorithm to learn the monitoring model, λ_0. In the monitoring procedure, the monitoring result can be achieved by evaluating the feature vector of an incoming sample (i.e. $t > 0$) via the forward algorithm. 100

6.2 Representative example of a N-state no-jump left-right HMM. In such HMMs, the current state is restricted to transit only to itself and the following state. Jumps of more than one state are not allowed. 100

6.3 Flowchart of HMM-based meat freshness grading. Sensor array's responses of the whole life-span meat samples are first pre-processed before extracting features. Feature vectors are arranged from the first test to the last test. In the training procedure, the arranged dataset is sent to segmental RCE algorithm to learn a stable grading model, λ_{life}. In the decoding procedure, the most probable state path is calculated according to λ_{life} via the Viterbi algorithm to illustrate the grading result. 101

6.4 Flowchart of HMM-based meat freshness evaluation. The pattern of each freshness level is trained based on its corresponding samples. In evaluating procedure, log-likelihood of the sample to be evaluated is evaluated by all trained models. Its specific freshness level is determined by the model that achieves the highest log-likelihood. 102

6.5 (a) Experiment setup. The odour of the tested meat sample was pumped to the sensor chamber through the input port II by sampling needle. After one measurement, fresh air was pumped to clean odour molecules from the sensor array. Meanwhile, the sensors' responses were sent to and stored in a tablet PC (Pad). (b) Control logic of the NOS.E system. Connect the meat sample to input port II. At the baseline setting stage, open Valve I, III, IV and Pumps I, II and keep the flow rate at 1.1L/min for 30 seconds letting the fresh air to wash the sensor chamber. The baseline of each sensor can be obtained. At the testing stage, keep Valve III, IV and the Pump I, II open, and control the flow rate at 1.1L/min. Then, close Valve I while opening Valve II. This state would last for 90 seconds, during which the sensor's response would increase and reach the steady value. At the recovery stage, keeping the state of Valve III, IV and the Pump I, II unchanged, close Valve II while opening Valve I. This state would last for 300 seconds, during which the sensor's response would return to its baseline. After the measurement, remove the meat sample from input port II. Open all valves and pumps, and set the flow rate at 2.2L/min letting the fresh air clean the residual odour molecules in the gas circuit for 80 seconds. Meanwhile, the sensor's response were converted into digital signal at a 1-Hz sampling rate and sent to the Pad via the Wi-Fi module. 105

6.6 Boxplots of HMM-based meat freshness monitoring. (a) Fish monitoring result. During the first 48 hours of storage at 4°C, log-likelihood values remained at a very similar level around -0.52. The monitoring index began to decrease gradually after 56 hours, and then dropped sharply after 112 hours. After 136 hours of storage, the log-likelihood values began to fluctuate from -13.45 to -10.12 until the end of the experiment. (b) Beef monitoring result. For samples stored at 4°C, the log-likelihood value decreased slightly from 0 to -2.31 during the first 40 hours of storage. Then, it dropped obviously to an average of -17.28 after 96 hours, and eventually fluctuated from -18.01 to -21.64. For samples stored at 25°C, the log-likelihood values dropped directly to the final fluctuation range of the counterparts stored in the refrigerator, within 36 hours of storage. (c) Chicken monitoring result. For samples stored at 4°C, the log-likelihood values remained at around -0.70 during the first 48 hours of storage. After 88 hours of storage, it falls rapidly to an average of -11.30. And then, the log-likelihood value fluctuated from -15.71 to -11.62 until the end of the experiment. For samples stored at 25°C, the log-likelihood value dropped directly to the final fluctuation range of the counterpart stored in the refrigerator, within 24 hours of storage. 106

6.7 Representative example of real-time monitoring. This figure compares HMM- and PCA-based monitoring algorithms in tracking the real-time freshness change of the salmon stored at 4°C. (a) to (e) are the results of monitoring obtained for five consecutive days. Subplot (f) shows the result of the last day. Blue symbols denote the samples obtained from the first day. Red represents the newly obtained data, and gray the historical data. Symbol "•", "×" and "+" represent data in group A, B and C, respectively. The number (i.e.: $8, 16, 24, \ldots, 288$) in PCA score plots represents the storage time. 107

6.8 BIC index for selection of the number of hidden states. The selection results are: Fish, $N = 4$; Beef, $N = 3$; Chicken, $N = 3$. 109

6.9 Representative example of HMM-based freshness grading. (a) Hidden path for fish. Fish samples stored at 4°C from 8 to 48 hours were generated by State I, from 56 to 80 hours by State II and from 88 to 120 hours by State III. The rest samples were generated by State IV. (b) Hidden path for beef. Beef samples stored at 4°C from 8 to 40 hours were generated by State I, from 48 to 88 hours by State II. The rest samples were generated by State III. (c) Hidden path for chicken. Chicken samples stored at 4°C from 8 to 48 hours were generated by State I, from 56 to 80 hours by State II. The rest samples were generated by State III. 110

6.10 Voronoi diagram of meat freshness clustering based on PCA + RCE. (a) Clustering result for fish. Fish samples stored at 4°C from 8 to 48 hours were classified in Cluster I, from 56 to 80 hours in Cluster II and from 88 to 120 hours in Cluster III. The rest samples were classified in Cluster IV. (b) Clustering result for beef. Beef samples stored at 4°C from 8 to 40 hours were classified in Cluster I, from 48 to 88 hours in Cluster II. The rest samples were classified in Cluster III. (c) Clustering result for chicken. Chicken samples stored at 4°C from 8 to 56 hours were classified in Cluster I, from 64 to 80 hours in Cluster II. The rest samples were clustered in Cluster III. 113

List of Tables

Table **Page**

2.1 Representative traditional hand-crafted features 28

3.1 Gas sensors used for perfume identification 40
3.2 Perfume Information 40
3.3 Comparison result of resistance to noise 50
3.4 Comparison result of resistance to noise 52
3.5 Classification result of proposed method 53
3.6 Classification result of modelling-based features with DHMM 54
3.7 Classification result of modelling-based features with KNN 54
3.8 Classification result of traditional features with SVM (1 v 1) 54
3.9 Classification result of traditional features with SVM (1 v Rest) 55
3.10 Classification result of traditional features with Softmax regression 55

4.1 Simulated signal reconstruction by kernel-based modelling with different kernels 69
4.2 Whisky information (four targets) 70
4.3 Classification Results Via Different Feature Representations 75

5.1 Normalized root mean square error in derivative estimation (SNR=15 dB) . . 87
5.2 Whisky information (four targets and two disturbances) 89

6.1 Gas sensors used for meat freshness monitoring and evaluation 104
6.2 Comparison result of algorithm stability 112
6.3 Comparison result of fish freshness evaluation (mean% ± std%) 114
6.4 Comparison result of beef freshness evaluation (mean% ± std%) 115
6.5 Comparison result of chicken freshness evaluation (mean% ± std%) 116