Rapid determination of bulk composition and quality of marine biomass in mass spectrometry

Doctoral proposal seminar

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assets/island-bay.jpg

PSO [1] inspired by social behaviour of animals

assets/school_of_fish.png

Topics

1. Problem Statement
2. Mass Spectrometry
3. Motivations
4. Goals
   - identification
   - Quantitative contaminant analysis
   - Traceability
5. Preliminary Work
6. Proposed contributions, thesis outline, timeline
   - Proposed contributions
   - Thesis outline
   - Timeline

Fish + AI + Business

Paul the octopus

Have you been catfished? [?]

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Popular restaurant accused of serving cheap Vietnamese catfish to customers who thought they were getting Australian dory

- **A Melbourne restaurant has been accused of serving catfish to customers**
- **Hunky Dory has allegedly been selling frozen fillets of basa as dory**
- **Owner Greg Robotis has denied allegations he is misleading customers**
- **The City of Port Phillip is investigating Hunky Dory's Port Melbourne store**

By HARRY PEARL FOR DAILY MAIL AUSTRALIA
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A Melbourne restaurant has been accused of serving a Vietnamese catfish to customers who believe they are ordering Dory.

A whistleblower has alleged that Hunky Dory outlets have been selling frozen fillets of basa, a species of catfish native to the Mekong basin, as fish-of-the-day dory, **The Age** reports.

Owner Greg Robotis has denied the claims and said inexperienced staff may have been calling the fish the wrong name.

Aussies! No surprises there...

Catfishing [?], Mislabelling [2], and Quality Assurance [?]

Nutrition Facts

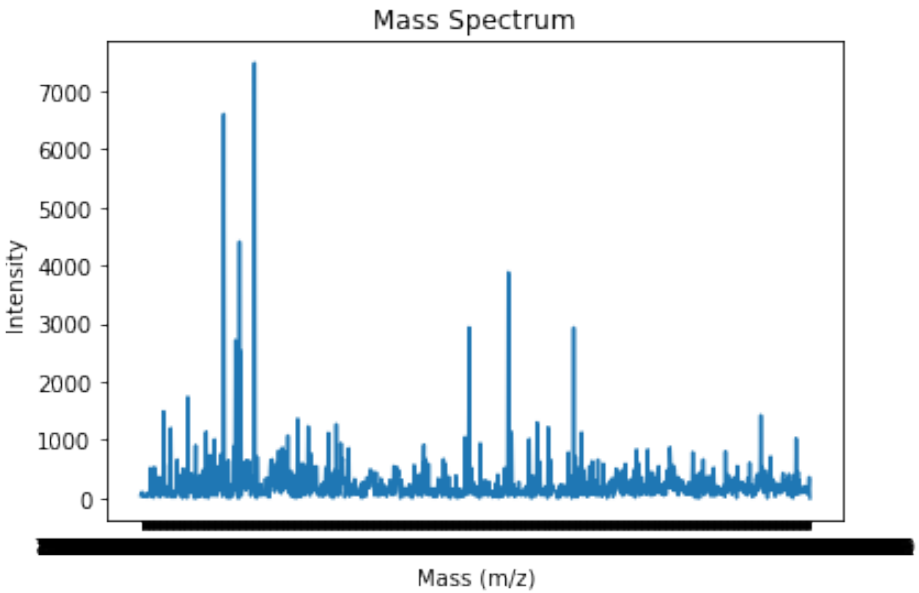
6 servings per container
Serving size **4-5 ounces(187g)**

Amount per serving
Calories **200**

	% Daily Value*
Total Fat 5g	**6%**
Saturated Fat 0.5g	**3%**
Trans Fat 0g	
Cholesterol 80mg	**27%**
Sodium 610mg	**27%**
Total Carbohydrate 10g	**4%**
Dietary Fiber 0g	**0%**
Total Sugars 3g	
Includes 0g Added Sugars	**0%**
Protein 27g	
Vitamin D 2mcg	10%
Calcium 79mg	6%
Iron 3mg	15%
Potassium 519mg	10%

*The % Daily Value tells you how much a nutrient in a serving of food contributes to a daily diet. 2,000 calories a day is used for general nutrition advice.

Mass Spectrometry [?] ≈ Chemical Fingerprint



Fish oil is brain food! [?, ?]

Fish oil analyzed with Gas Chromatography! [3]

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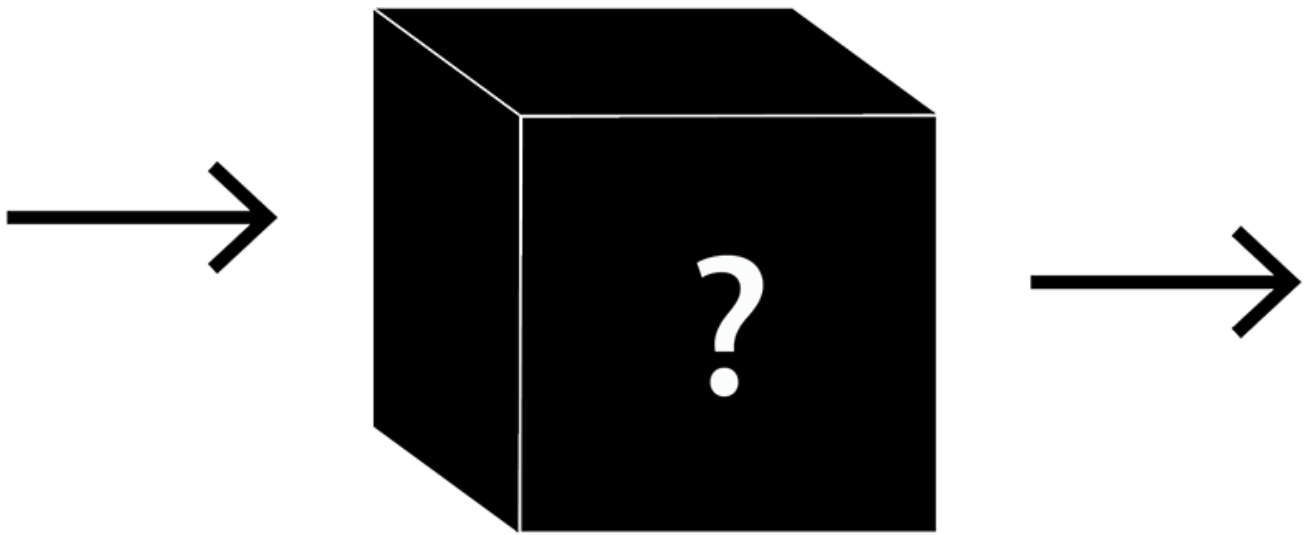
Fish oil analysis can't be blackbox! [?, 4]



Fish identification

Fish species identification

Fish body parts identification

Contamination detection

Contamination analysis

Contamination quantification

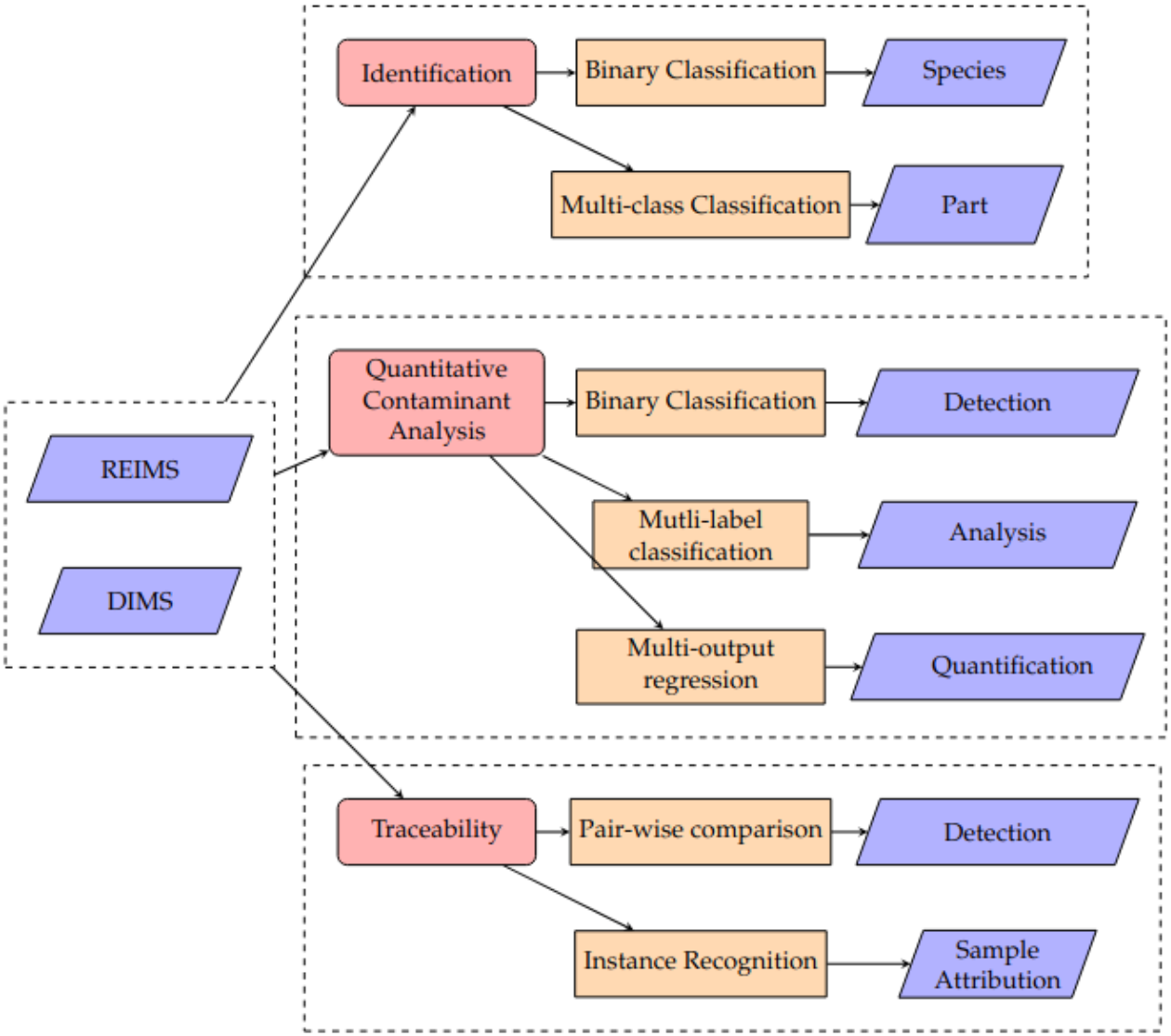
Detection - pair-wise comparison

Sample attribution - instance recognition

Evolutionary Computation for gas chromatography

Exploratory data analysis for rapid mass spectrometry

Proposed contributions



Aussies! No surprises there...

Thesis outline

Timeline

TLDR;

Novel AI variable-width input multi-scale resolution-invariant pre-trainied analysis algorithms for rapid mass spectrometry datasets of marine biomass.

1. fish **species** & body **part identification** $\rightarrow$ multi-scale resolution-invariant binary & multi-class classification, respectively;
2. **quantitative contaminant analysis** $\rightarrow$ multi-label classification & multi-output regression & out-of-distribution outlier thresholding; and
3. **traceability** $\rightarrow$ few-shot similarity-based contrastive learning for pair-wise comparison & instance recognition.

[1] J. Kennedy and R. Eberhart, "Particle swarm optimization," in *Proceedings of ICNN'95-international conference on neural networks*, vol. 4. IEEE, 1995, pp. 1942–1948.

[2] M. Á. Pardo, E. Jiménez, and B. Pérez-Villarreal, "Misdescription incidents in seafood sector," *Food Control*, vol. 62, pp. 277–283, 2016.

[3] C. Black, O. P. Chevallier, K. M. Cooper, S. A. Haughey, J. Balog, Z. Takats, C. T. Elliott, and C. Cavin, "Rapid detection and specific identification of offals within minced beef samples utilising ambient mass spectrometry," *Scientific reports*, vol. 9, no. 1, pp. 1–9, 2019.

[4] D. D. Matyushin and A. K. Buryak, "Gas chromatographic retention index prediction using multimodal machine learning," *Ieee Access*, vol. 8, pp. 223 140–223 155, 2020.