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Fourier transform near infrared spectroscopy of otoliths coupled with machine learning to improve fish age predictions

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Study Objective and Presentation Outline

Study objective:

Explore advanced technologies using FT-NIR spectroscopy of fish otoliths coupled with deep machine learning models to estimate fish age more rapidly and with greater efficiency than traditional approaches.

Presentation outline:

- Fish ageing methods
 - Traditional microscopic method
 - FT-NIR spectroscopy method
- Deep learning approach
- Results
- Conclusions



Traditional Ageing Method







Otoliths:

- Small calcified structures in the inner ear of fish.
- Continue to grow throughout the life of a fish.
- Composed of alternating protein-rich and mineral-rich bands.
 - Lay down an annulus (year mark) once per year.



NOAA Professional Paper NMFS 13

Age determination manual of the Alaska Fisheries Science Center Age and Growth Program

Mary Elizabeth Matta and Daniel K. Kimura (editors)

February 201



Traditional Ageing Method

Fish age determination:

- Counting visible annual growth rings under a microscope.
- Labor-intensive particularly for longlived species (3-10 minutes per age).
- Can be subject to poor repeatability.













Diffuse Reflectance Spectroscopy



Fundamental Principles of FT-NIR Spectroscopy

- Spectra in the NIR region result from energy absorption by organic molecules.
- NIR region absorption bands include overtones and combinations of overtones originating from fundamental bond vibrations (stretching or bending).





- Due to the overtone and combination modes, FT-NIR spectra are complex (consist of many overlapping peaks).
- Multivariate calibration is needed to find relationships between spectral measurements and reference measurements.

Predicting Fish Age from Otolith Spectra



General Chemometrics Approach

- Partial least-squares regression (PLS) predicts target feature using small set of intermediate linear latent variables.
- PLS exhibits good results for fish ageing.
- Rely on users having advanced skills to deal with non-selectivity and non-linearity problems.



Canadian Journal of Fisheries and Aquatic Sciences

A transformative approach to ageing fish otoliths using Fourier transform near infrared spectroscopy: a case study of eastern Bering Sea walleye pollock (*Gadus chalcogrammus*)



Ageing fish at the molecular level using Fourier transform near infrared spectroscopy (FT-NIRS): A case study of Pacific cod

ICES JOURNAL OF MARINE SCIENCE JOURNAL DU CONSEL

Age estimation of red snapper (*Lutjanus campechanus*) using FT-NIR spectroscopy: Towards a feasibility for fisheries management



MARINE & FRESHWATER RESEARCH

Rapid age estimation of longnose skate (*Raja rhina*) vertebrae using near infrared spectroscopy

Calibration Problems

Non-linearity:

• Differences in sample absorbance variations and light scattering.

Non-selectivity:

- Each spectrum contains thousands of wavenumbers that are highly correlated.
- Difficulty to find exact wavenumbers for the chemical constituents in the sample.

Existing chemometric techniques:

- Often effective dealing with these issues.
- Introduce many adjustable parameters.
- Increase difficulty of analysis and may not lead to an optimal model.



Deep Learning

- Recent developments of deep learning in speech recognition, object detection, and image processing.
- Can automatically learn features in data.
- Efficient way to process and extract features of high-dimensional data (automated wavenumber selection).
- Neural networks (NN) used for overcoming the effects of non-linearity.





First Neural Network



Convolutional Neural Network

- Convolutional neural networks (CNN) are based on the <u>study of the brain's visual cortex</u> and have been applied for RGB (2D) and hyperspectral (3D) image recognition since the 1980s.
- CNN algorithms were found to be useful for spectral data (<u>spectra</u> can be represented as <u>1D</u> image data).
- CNN is more <u>robust to overfitting</u> because it relies on the <u>spatial relationship</u> in the spectral data and has fewer parameters than traditional neural networks.



Modern practical convolutional neural networks for multivariate regression: applications to NIR calibration

Chenhao Cui and Tom Fearn

Department of Statistical Science, University College London, London, WC1E 6BT, U.K.

The Proposed Multi-Input Neural Network

Most fundamental unit used to build a neural network is perceptron.

Simple computational unit that have weighted input signals and produce an output signal using an activation function.

Convolutional layer consists of a kernel that slides along our data and applies its weights to the data values.



Convolutional kernels can lower data complexity and capture features (i.e. identify important spectral regions).



Activation function governs the threshold at which neuron is activated.



Non-linear activation functions introduce non-linear properties into network.



Case Study: shorter-lived species



Relative feature importance

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aggregated aggregated aggregated aggregate aggregate	gear_ ed by 3,000 l by 10,000 ed by 8,000 gear ed by 9,000 l by 11,000	depth - cm^{-1} - cm^{-1} - cm^{-1} - temp - cm^{-1} - cm^{-1} -		3S surv 'ears: n = 8,6 No oto	vey da 2014 - 17 lith w	ta 2018 cights	
		0.00	0.25 0.5 Averag	0 0.75 e Impact o	1.00 on Model	1.25	
lodel	Number of otoliths			R ²		RMSE	
	Train	Test	Outliers*	Train	Test	Train	Test
IN				0.93	0.92	0.83	0.91
LS with all bectral avenumbers	6866	1751	12	0.89	0.87	0.99	1.14
LS with selected bectral avenumbers				0.90	0.87	0.97	1.12

Neural Networks | Results | Conclusions Ageing methods

The future of fish age estimation: deep machine learning oupled with Fourier transform near infrared spectroscopy of otoliths

Model Performance









Model Uncertainty



Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning

2016

Yarin Gal Zoubin Ghahramani University of Cambridge • Established connection between dropout networks and approximate Bayesian interference.

• Monte Carlo Dropout is a good measure of the model's uncertainty.



probability of the prediction sample set not being contained within the interval

Case Study: long-lived species

Red Snapper (*Lutjanus campechanus*)

- Long-lived reef fish (50+ years)
- Ecologically and economically important
- Estimated to be recovering in US Gulf of Mexico waters



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Relative feature importance



Ageing methods | Neural Networks | Results | Conclusions

Case Study: long-lived species

Northern Rockfish (Sebastes polyspinus)



• Commercially important rockfish in the Gulf of Alaska and the Aleutian Islands fisheries management areas.







Ageing methods | Neural Networks | Results | Conclusions

Conclusions

- Deep learning models are capable of accepting and learning information from <u>multiple feature types</u>, extracting <u>important spectral features</u> automatically, and handling <u>non-linearity</u> in data better than traditional chemometrics approach.
- FT-NIR spectroscopy of otoliths coupled with deep machine learning can predict fish ages more <u>rapidly</u>, with <u>greater efficiency</u>, and with <u>comparable precision</u> to traditional microscopic ageing method.



- Working with UW Information Processing Lab (Prof. Hwang) to develop <u>more sophisticated model</u>.
 Collecting otolith images and otolith weights for walleye pollock (AFSC) and red snapper (SEFSC).
- Evaluating FT-NIR age data performance in <u>stock assessments</u>.
- Evaluating trade offs between <u>traditional ageing (double reads</u>, outliers, issues specimens, model updating) and <u>FT-NIR efficiency gains</u>.
- Establishing decision rules for <u>model updating</u> important for future predictions.

Acknowledgements



NOAA FISHERIES





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- Jon Short manages data and creates tools to improve data export efficiencies.
- Ajith Abraham (AFSC) and Giovanni Marchetti (Google) introduced us to the deep machine learning possibilities.
- Jason Erickson (Bruker) provides application support.

Thank you.

Take a picture to find out more information on fish age and growth research in Alaska



CNN Building Blocks

<u>Convolutional layer</u> consists of a kernel that slides along our data and applies its weights to the data values.



Deep learning networks have multiple kernels and will produce multiple output arrays.

<u>Pooling layer</u> reduces the amount of parameters and computation in the network.



Maximum pooling reduces the spatial size of a layer keeping just the maximum values.

Core Processing Unit of NN



Perceptron:

- Most fundamental unit used to build a neural network.
- Resembles a neuron in the human brain.
- Simple computational unit that have weighted input signals and produce an output signal using an activation function.



Activation function governs the threshold at which neuron is activated.



Non-linear activation functions introduce non-linear properties into network.

Model 1.2 test data set predictions plus 2019 and 2021



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NOAA Fisheries

- Alaska Fisheries Science Center, Age and Growth Program
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