Deep learning and Raman spectroscopy - An analysis

Bui Gia Khanh - K68 Physics
Supervisor: Dr. Hoang Chi Hieu

Hanoi University of Science, VNU

Table of contents

1. Introduction and Review

2. Machine learning on Raman

3. Conclusion

Introduction

Preface

It is widely considered for spectroscopy, and **Raman spectroscopy** specifically, to be an important field of study and tools of analysis. The need for accurate detection, material fingerprinting, non-destructive probing, drug detections, medicine and pathological diagnosis, and various on-field examination requires tools of Raman spectroscopy and its properties in major applications.

With that, comes of great importances in understanding Raman scattering itself, for analysis and manipulation of Raman data received from the process and measurements.

Theory of Raman

> *[...] it is only relatively recently [...] discovered that, if light is reunited* **fleetingly** *with matter and then scattered again, it carries with it* **detailed information** *[...] about the structure of matter. It is the purpose [...] for deciphering the information carried by the scattered light.*
>
> *(Claude Monet)*

By that, we are interested in **scattered lights**, in which induces Raman scattering. This is our main character.

Theory of Raman

When **monochromatic radiation** of frequency ω_1 is incident on system of material, most of it is transmitted without change, but some scattering occurs. Those that changes afterward are called **Raman scattering**. [11, 33, 28]

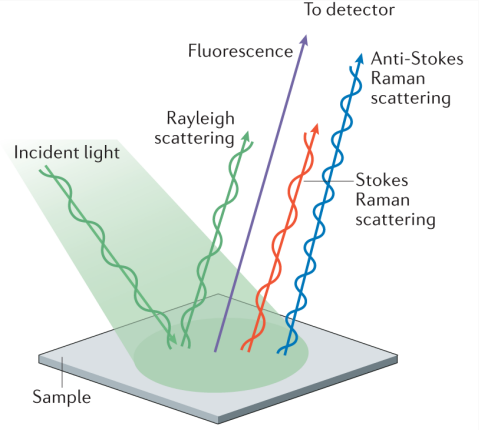


Figure 1: Chain of reaction in a spectroscopic experiment

Theory of Raman

As a scattering effect itself, they have two categorization: either *Stoke* Raman spectroscopy, or *anti-Stoke* Raman spectroscopy. The name is derived from the name Stoke's law, adopting from fluorescent to this. The model used to explain their behaviours is the **energy state transition model**.

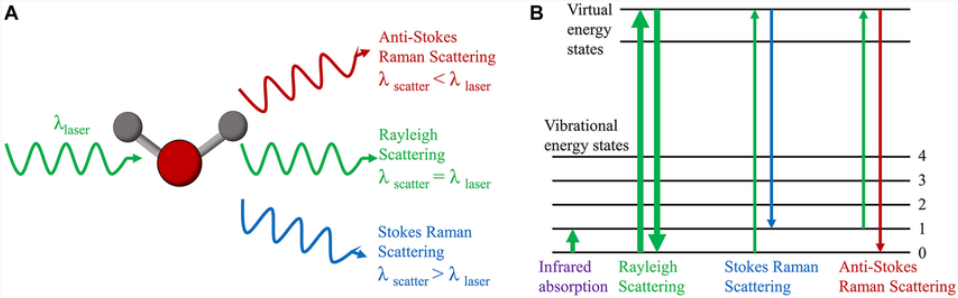


Figure 2: (A) Three types of scattering often encounter and their wavelength condition (B) The *energy state transition model* of scattering interaction. Notice that the received/absorbed energy in transfer classifies Stokes, and anti-Stokes.

Applications

For its scattering patterns are **unique** for materials, its property is applied widely in science. This includes drugs detection, material/mixture purity analysis, pathogen detection, and medical diagnosis - most prominently - **cancer** and Covid-19.

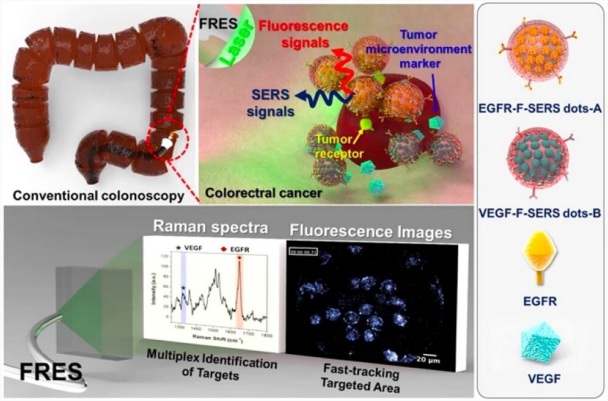


Figure 3: Application of Raman endoscopic system (FRES) for the in vivo multiplex molecular diagnosis of colorectal cancer.

Data representation

So, what does data look like?

Data representation

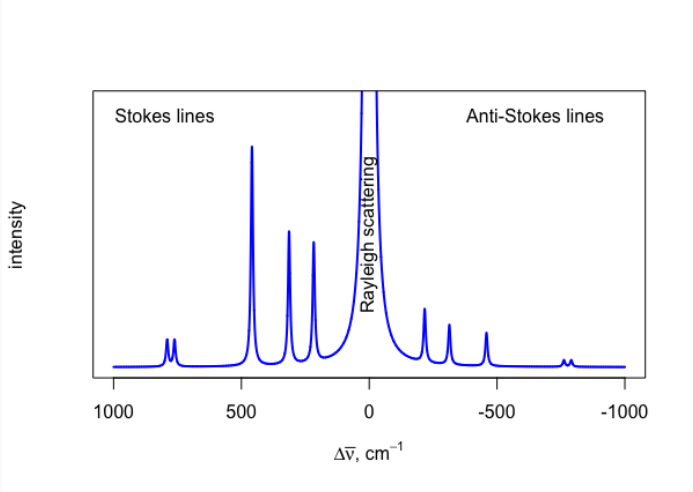


Figure 4: Conventional interpretation of Raman spectra (example for CCl_4). Conventionally, the x-axis is the Raman shift, hence Rayleigh peak at 0. To the left instead, is Stoke Raman region, because Stoke Raman scattering returns positive energy to the incidence matter, thus longer wavelength.

Unit format - wavelength

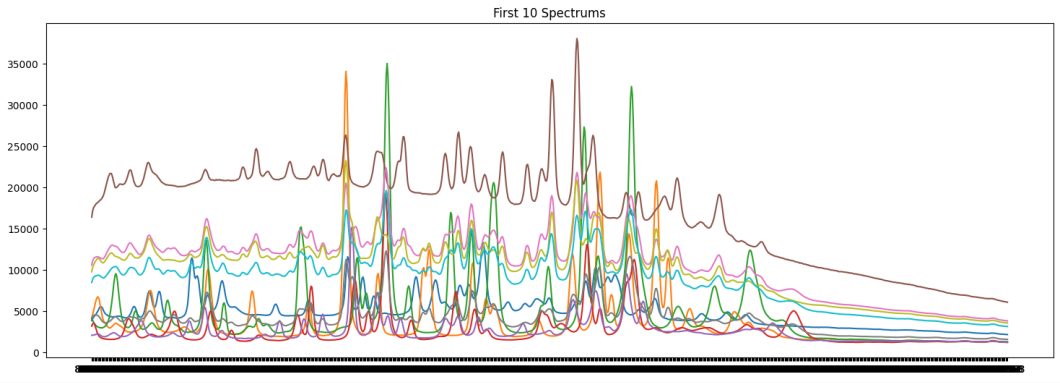


Figure 5: The original wavelength-unit spectral data.

Unit format - wavenumber

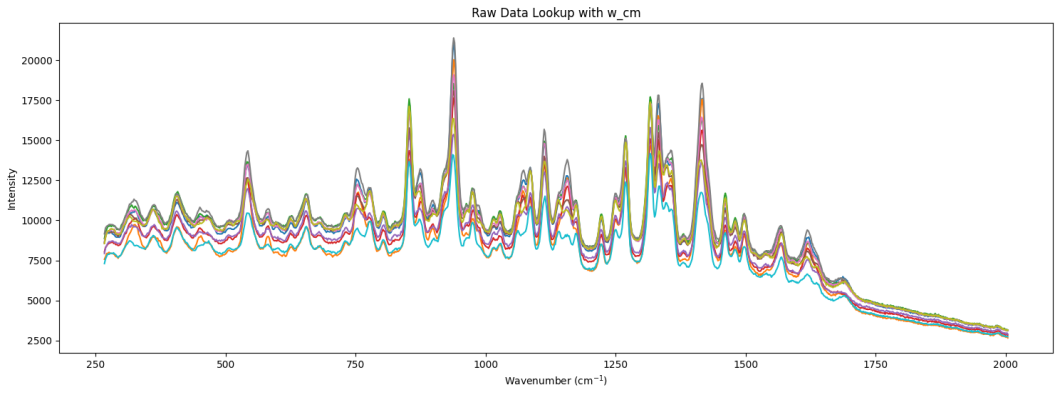


Figure 6: The converted wavenumber spectral data. It is easier to work with, smaller SNR, better proportionality, and nicer numerical values.

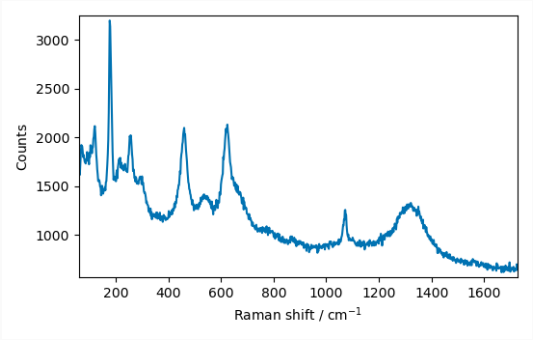
Wavelength to Wavenumber

For [Mahsa et al., 2019], the formula is as:

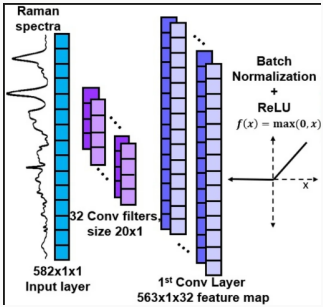
$$\bar{\upsilon} = \frac{1}{\lambda} = \left[\frac{1}{\lambda_e} - \frac{1}{\lambda}\right] \times 10^7 \quad (\mathrm{cm}^{-1}) \tag{1}$$

which use the Raman shift formula, and for λ_e being the excitation wavelength. ([0a], [0b],[0c])

Landscape



(a) An example Raman spectrum data. Taken from RamanSpy.



(b) A CNN pipeline on Raman data. Notice the 1D entry of input data.

Figure 7: Figurative example of the usual formation of data in a machine learning pipeline. In case of classification or feature extraction basis, the intensity values are treated as region of interest, there by wavenumber range are negligible.

Machine learning application

Applications of Machine learning

Based on use cases of Raman spectroscopy, application of machine learning and deep learning [29, 7] is divided into four main categories:

1. Preprocessing data.

Applications of Machine learning

Based on use cases of Raman spectroscopy, application of machine learning and deep learning [29, 7] is divided into four main categories:

1. Preprocessing data.
2. Spectral **classification**

Applications of Machine learning

Based on use cases of Raman spectroscopy, application of machine learning and deep learning [29, 7] is divided into four main categories:

1. Preprocessing data.
2. Spectral **classification**
3. Spectral regression.

Applications of Machine learning

Based on use cases of Raman spectroscopy, application of machine learning and deep learning [29, 7] is divided into four main categories:

1. Preprocessing data.
2. Spectral **classification**
3. Spectral regression.
4. Spectral region **highlighting**

Classical learning model

Details depends on their usage, but most traditional works with the same structure. Most of them, however, utilizes variable primitive analysis types and architectures. Classically, they are:

- Principal component analysis (PCA), SNR denoising, etc. (preprocessing) + partial least square (PLS) model - *regression analysis*
- PCA + SVD for Breast Cancer diagnosis (Manoharan et al.) [7, 24]
- Support vector machine for NIR-Raman (Widjaja et al.) [7]

Modern deep learning

For more recent application of deep learning, a comprehensive list of both usually appearing models are presented. Bottom entries are some of those. [30]

Bayesian	A classification technique based on the Bayes theorem, where the prior probability distribution is selected and then updated to obtain the posterior distribution.
Artificial Neural Network (ANN)	A mathematical model that simulates the brain's neuronal activity as a set of connected input/output units, where each connection has a weight associated with it.
Convolutional Neural Network (CNN)	A class of feedforward neural networks with convolutional computation and deep structures. It is usually applied to analyze visual imagery.
Recurrent Neural Network (RNN)	A class of neural networks with short-term memory, suitable for processing a range of time-series related problems such as text.
Probabilistic Neural Network (PNN)	A neural network technique based on the Bayesian decision rule that is widely used in classification problems.
Generative Adversarial Network (GAN)	A novel adversarial generative model architecture that learns to generate new data with the same statistics as the training set.

Figure 8: A list of recent modern *deep learning* architecture in applications.

Modern deep learning

We focus on the following:

1. Convolutional Neural Network (CNN - and most popular).
2. Bayesian Statistical Model (Most complex, very accurate.)
3. Physics-informed neural network (PINNs - state-of-the-art for physics application).

Convolutional networks (CNN)

Convolutional neural network is the most popular model architecture in papers and projects on Raman spectroscopic analysis ($\approx 57.25\%$) [32, 7, 9, 16].

Most of them are concerned with 1D case, however, from our previous assumption.

Mathematically, a typical 1D CNN operation can be simplified as:

$$y(i) = \sigma\left(\sum_h x(i+h)k(h) + b\right) \tag{2}$$

where x is the 1D input, y is the output, k is the learnable kernel, b is the bias term and σ is a nonlinear operation. Within each layer, we also have the pooling layer for down-sampling spectra:

$$Y_{x',k} = \max_{0 \le m \le s} (X_{x \cdot s + m, k}) \tag{3}$$

where s is the pooling filter size, x and x' are wavenumber indices of the input and output spectra, respectively.

Lastly, usually, there exists a fully connected layer at the end of the convolutional steps:

$$Y_{k'} = b_{k'} + \sum_{x \times k} Fw_{k',x \times k} X_{x \times k}$$

where Fw denotes the weights of the fully connected layer.

Diagrammatical View

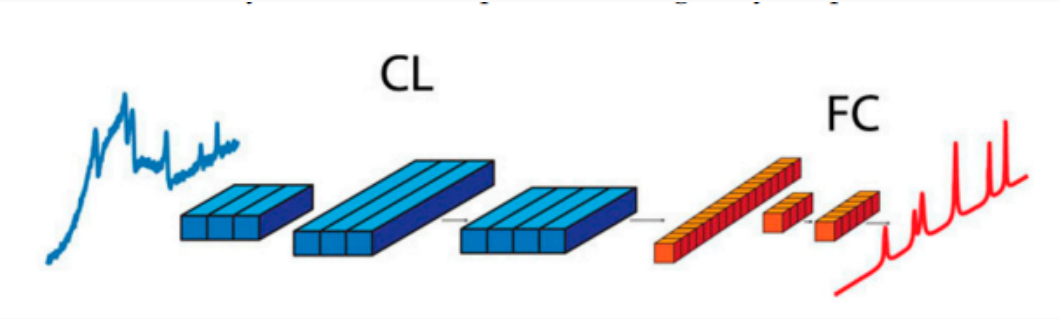


Figure 9: Diagrammatical, simplified view of the underlying structure for the CNN-Raman network. In this case, it is for data preprocessing, such as **baseline correction**. Adopt from **Ruihao** [7]

Usages

CNN is used in all cases of interest mentioned above, from preprocessing to highlighting, which *specifically* utilizes the convolutional logics of the network. Preprocessing also taken large parts of papers regarding CNN application with widespread successes. [7]

Performance

Within various cases, it presents good efficiency, and well-controlled behaviours [7, 9, 12, 30], beats out classical machine learning techniques.

Table 2: Test accuracy of the compared machine learning methods on the baseline corrected dataset

Methods	KNN(k=1)	Gradient Boosting	Random Forest†	SVM(linear)	SVM(rbf)	Correlation	CNN†
Top-1 Accuracy	0.779±0.011	0.617±0.008	0.645±0.007	0.819±0.004	0.746±0.003	0.717±0.006	**0.884±0.005**
Top-3 Accuracy	0.780±0.011	0.763±0.011	0.753±0.010	0.903±0.006	0.864±0.006	0.829±0.005	**0.953±0.002**
Top-5 Accuracy	0.780±0.011	0.812±0.010	0.789±0.009	0.920±0.003	0.890±0.007	0.857±0.005	**0.963±0.002**

Figure 10: Performance evaluation of a typical CNN model on baseline corrected data. Adopt from [21]

Performance

Table 3: Test accuracy of the compared machine learning methods on raw dataset with or without baseline correction methods

Methods	KNN(k=1)	Gradient Boosting	Random Forest†	SVM(linear)	SVM(rbf)	Correlation	CNN†
Raw	0.429±0.011	0.373±0.019	0.394±0.016	0.522±0.011	0.434±0.012	0.310±0.007	**0.933±0.007**
Asym LS	0.817±0.010	0.773±0.009	0.731±0.019	0.821±0.012	0.629±0.016	0.777±0.013	**0.927±0.008**
Modified Poly	0.778±0.007	0.740±0.016	0.650±0.016	0.785±0.014	0.629±0.016	0.734±0.013	**0.920±0.008**
Rolling Ball	0.775±0.009	0.737±0.008	0.689±0.018	0.795±0.011	0.624±0.013	0.730±0.010	**0.918±0.008**
Rubber Band	0.825±0.007	0.792±0.015	0.741±0.009	0.806±0.015	0.620±0.010	0.789±0.010	**0.911±0.008**
IRLS	0.772±0.010	0.710±0.008	0.675±0.007	0.781±0.011	0.614±0.010	0.711±0.011	**0.911±0.008**
Robust LR	0.741±0.009	0.694±0.008	0.667±0.012	0.759±0.013	0.600±0.013	0.696±0.011	**0.909±0.007**

Figure 11: Performance evaluation of a typical CNN model on non-baseline corrected data. Adopt from [21]

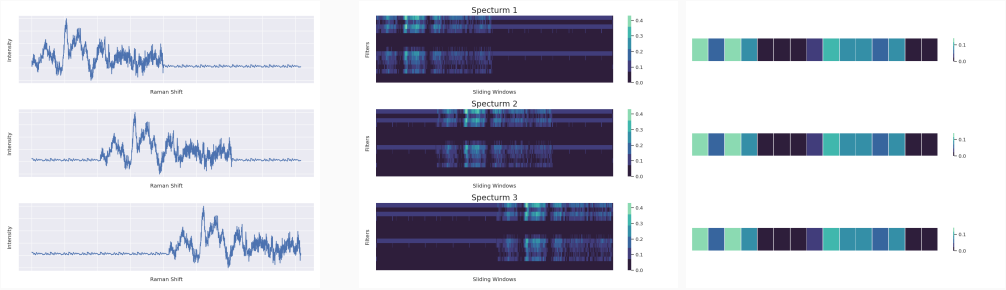
However. . .

From a **visual perception** perspective, Raman spectrum resembles a signal-like waveform. [32, 16]

However, Raman spectra is an energy distribution plot, which might not suitable for normal utilization of CNNs. [16]

Specifically, it discards the time-domain locality of the spectrum, which is crucial for Raman spectra.

However. . .



(a) **(b)** **(c)**

Figure 12: Analysis of CNN for a Raman spectrum input. Reproduced from [16]

Solutions (allegedly)

Several solutions has been proposed to resolve this particular problem, and some else more on-site specific, or situational-specific. The most recent, and can be said, potent, is *RamanNet* [16].

Instead of 2, we have the MLP:

$$y(i) = \sigma(W^T_{f(i)} + b) \equiv \sigma\left[\sum_h x(i+h)k_{f(i)}(h) + b\right] \tag{4}$$

Where $W^T x$ is equivalent to the 1D convolutional operation with proper relation between W and the kernel k. The small index $f(i)$ indicates that they are position-dependent. This is implemented with a **sliding window** in the architecture.

Evaluation

Testing this architecture against classical technique (SVM) shows non-trivial performance boost.

Table 2: Results on COVID-19 Dataset

COVID-19 vs Suspected			
Method	Accuracy	Sensitivity	Specificity
SVM	87 ± 5	89 ± 8	86 ± 9
RamanNet	93 ± 3	97 ± 4	90 ± 6
COVID-19 vs Healthy			
Method	Accuracy	Sensitivity	Specificity
SVM	91 ± 4	89 ± 7	93 ± 6
RamanNet	95	95 ± 4	96 ± 3
Suspected vs Healthy			
Method	Accuracy	Sensitivity	Specificity
SVM	69 ± 5	70 ± 9	66 ± 9
RamanNet	82 ± 6	77 ± 15	87 ± 11

Evaluation

Similarly, on Melanoma Dataset compare to CNN.

Table 3: Results on Melanoma Dataset

	$-NH_2$		$-(COOH)_2$		-COOH		All	
Fold	RamanNet	CNN	RamanNet	CNN	RamanNet	CNN	RamanNet	CNN
1	**100**	97.42	**100**	100	**99.35**	94.19	100	100
2	**99.35**	96.13	**99.35**	98.71	**98.71**	96.12	100	98.71
3	**100**	95.45	**100**	98.05	**99.35**	87.01	100	100
4	**100**	97.40	**100**	98.70	**96.75**	96.10	100	99.35

Evaluation

CNN models have *moderate* accuracy, average size-to-performance, adaptable to various scenarios, and in some way, very *natural* when it comes to adapting Raman interpretation.

Adaptability is best expressed by the *RamanNet* itself - with simple modification comes great improvement and mitigation of earlier issues - very easy to use.

Bayesian system

Another way entirely, is to use Bayesian modelling to instead sample and quantify the Raman spectroscopic system instead. [25, 15, 13].

As the name suggested, those models are highly statistical, and often characterized by certain **statistical processes**, often stochastic, or in the case of [15], it can include a sequential Monte Carlo sampler.

Bayesian system

Performance-wise, it is surprisingly effective:

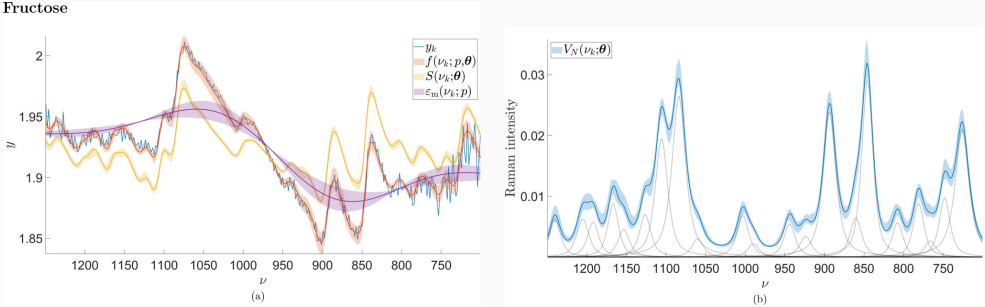


Figure 13: (a) Obtained 95% predictive intervals for y_k, f, S, and ϵ_m shown in blue, red, yellow, and purple respectively for a CARS measurement of a adenosine phosphate sample. (b) Obtained 95% predictive intervals for $V_N(\nu_K, \theta)$ and means of each individual line shape $V(\nu_k, \theta_n)$ for the adenosine phosphate sample. Reproduced from *Teemu et al.* [15]

Bayesian system - disadvantage

The disadvantage however, comes at a cost of:

1. High complexity, less flexibility.
2. Large complex dataset required (multipage prior distributions).
3. Out of trend/fashion in comparison to ANN/DNN.

However, if the need for static, complex settings (or mixture) arises, Bayesian can *squeeze* out the most in many situations.

The PINNs

The last model of discussion is the more recent approach of Physics-informed network - PINNs for Raman spectroscopic setting.

This type of Theory-Trained Network (TTNs) are especially useful for any dynamic physics system, and the scattering phenomena is one of such.

The PINNs

This development is natural, however. PINNs are effective in multi-scattering simulation [26] and was particularly useful in computation of quantum-based spectrums [3].

[5] and [20] explored these options quite thoroughly. However, the most prominent, or at least effective model is the **SRS-Net** [34] (Song et al., 2024), originally intended for *nonlinear* fibre-optic systems' Raman scattering.

This system is inherently difficult, and specialized, customized setting is very much required [34]

The PINNs

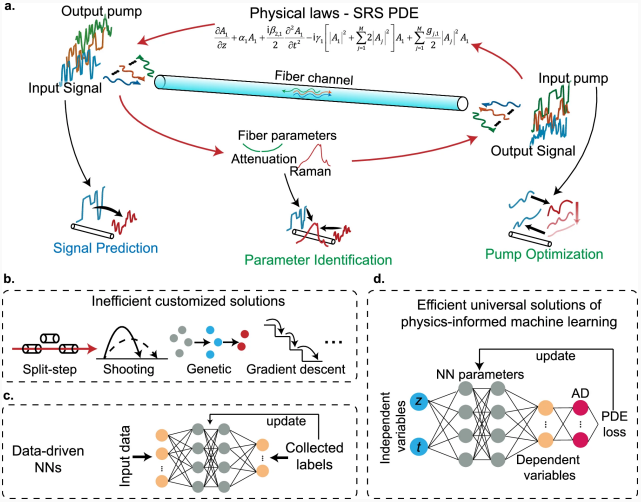


Figure 14: (a) The complex relationships among signals, pumps, and SRS's PDE. (b) Inefficient customized solutions using multiple classical numerical methods. (c) Data-driven NNs trained by collected labels. (d) Efficient universal solutions using physics-informed machine learning and AD.

Performances

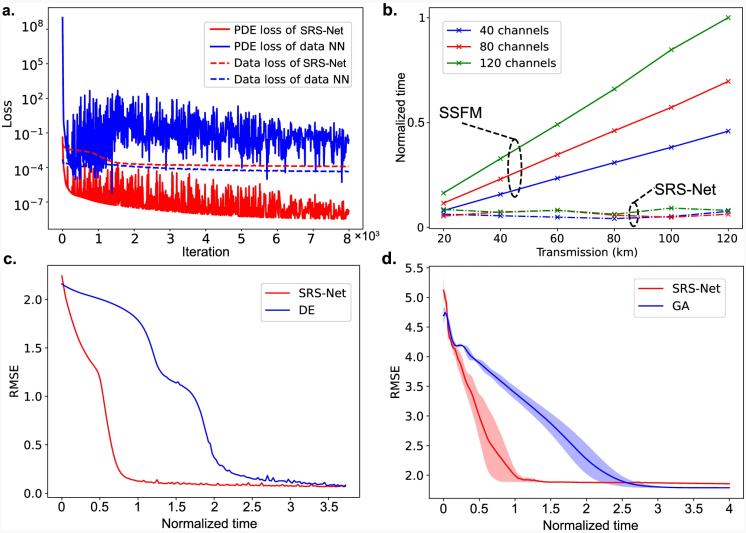


Figure 15: Results of SRS-Net physics consistency, testing speed, and performance comparison to genetic engineering (GA), split-step Fourier method (SSFM), and data NN. Reused from [34]

Remark

PINNs are remarkably optimized and effective in difficult situations (hand-held, on-the-field operations) since it offers relatively specialized and customizable configurations. Most of all, it can be applied to a lot of physical problems, since it was based on PDEs which physics utilized heavily. Additionally, minimal intervention are needed.

Remark

However, PINNs are inherently very restricted (if not outright useless, *for now*) unless it stays in the PDE configuration that it was designed to. **Discontinuous behaviors** are hard to approximated using PINNs, which sometimes fails.

Other drawbacks simply point to the fact that it is **much more expensive, intensive** and less **interpretable** than usual.

Conclusion

In the end

Application Raman spectroscopy and its properties are prominent in modern industry, medical practices, diagnosis of terminal diseases and overall scientific research and experiments. It stands out as a valuable piece of technology for utilization in widescale usages, and with relatively easy data interpretability [4]

In the end

Application Raman spectroscopy and its properties are prominent in modern industry, medical practices, diagnosis of terminal diseases and overall scientific research and experiments. It stands out as a valuable piece of technology for utilization in widescale usages, and with relatively easy data interpretability [4]

Deep learning Utilizing deep learning mostly comes with CNN, Bayesian network, or the state-of-the-art PINNs. Tradeoffs are from ease of use, adaptability, maintainance, complexity, accuracy metric, computational costs, and more, but CNN is still the mainstream choice at-hand.

In the end

Application Raman spectroscopy and its properties are prominent in modern industry, medical practices, diagnosis of terminal diseases and overall scientific research and experiments. It stands out as a valuable piece of technology for utilization in widescale usages, and with relatively easy data interpretability [4]

Deep learning Utilizing deep learning mostly comes with CNN, Bayesian network, or the state-of-the-art PINNs. Tradeoffs are from ease of use, adaptability, maintainance, complexity, accuracy metric, computational costs, and more, but CNN is still the mainstream choice at-hand.

Future works Most directions point to the implementation and employment of PINNs. This might include in the future works related to PINNs system more stable under pertubation analysis, and incorporate CNN components to the network for hybrid interaction. More CNNs designs are also of interest.

Thank you

References

References i

R. Alexander, S. Uppal, A. Dey, A. Kaushal, J. Prakash, and K. Dasgupta.
Machine learning approach for label-free rapid detection and identification of virus using Raman spectra.
Intelligent Medicine, 3(1):22–35, Feb. 2023.

T. W. Bocklitz, S. Guo, O. Ryabchykov, N. Vogler, and J. Popp.
Raman Based Molecular Imaging and Analytics: A Magic Bullet for Biomedical Applications!?
Anal. Chem., 88(1):133–151, Jan. 2016.
Publisher: American Chemical Society.

L. Brevi, A. Mandarino, and E. Prati.
A tutorial on the use of physics-informed neural networks to compute the spectrum of quantum systems.
Technologies, 12(10):174, Sept. 2024.

References ii

G. S. Bumbrah and R. M. Sharma.
Raman spectroscopy – basic principle, instrumentation and selected applications for the characterization of drugs of abuse.
Egyptian Journal of Forensic Sciences, 6(3):209–215, 2016.

Y. Chen, S. V. Pios, M. F. Gelin, and L. Chen.
Accelerating molecular vibrational spectra simulations with a physically informed deep learning model, 2024.

F. W. et al.
A Novel Method to Directly Analyze Dissolved Acetic Acid in Transformer Oil without Extraction Using Raman Spectroscopy.

R. et al.
Deep Learning for Raman Spectroscopy: A Review.

References iii

R. et al.
Machine learning approach for label-free rapid detection and identification of virus using Raman spectra - ScienceDirect.

A. M. Fuentes, A. Narayan, K. Milligan, J. J. Lum, A. G. Brolo, J. L. Andrews, and A. Jirasek.
Raman spectroscopy and convolutional neural networks for monitoring biochemical radiation response in breast tumour xenografts.
Sci Rep, 13(1):1530, Jan. 2023.
Publisher: Nature Publishing Group.

M. Fukuhara, K. Fujiwara, Y. Maruyama, and H. Itoh.
Feature visualization of Raman spectrum analysis with deep convolutional neural network.
Analytica Chimica Acta, 1087:11–19, Dec. 2019.
arXiv:2007.13354 [cs].

M. Grumet, C. v. Scarpatetti, T. Bučko, and D. A. Egger.
Delta Machine Learning for Predicting Dielectric Properties and Raman Spectra, Feb. 2024.
arXiv:2307.10578 [cond-mat].

Y. Gu, K. L. Chiu, A. Muñoz-Jaramillo, A. C. Birkeland, M. Navas-Moreno, and R. Carney.
Abstract B056: Towards a generalized machine learning model for Raman spectroscopy-based liquid biopsy in cancer screening using self-supervised learning.
Clinical Cancer Research, 30(21_Supplement):B056, Nov. 2024.

N. Han and R. J. Ram.
Bayesian modeling and computation for analyte quantification in complex mixtures using raman spectroscopy, 2018.

C. C. Horgan, M. Jensen, A. Nagelkerke, J.-P. St-Pierre, T. Vercauteren, M. M. Stevens, and M. S. Bergholt.
High-Throughput Molecular Imaging via Deep-Learning-Enabled Raman Spectroscopy.
Anal. Chem., 93(48):15850–15860, Dec. 2021.
Publisher: American Chemical Society.

T. Härkönen, L. Roininen, M. T. Moores, and E. M. Vartiainen.
Bayesian Quantification for Coherent Anti-Stokes Raman Scattering Spectroscopy.

J. Phys. Chem. B, 124(32):7005–7012, Aug. 2020.
Publisher: American Chemical Society.

N. Ibtehaz, M. E. H. Chowdhury, A. Khandakar, S. M. Zughaier, S. Kiranyaz, and M. S. Rahman.
RamanNet: A generalized neural network architecture for Raman Spectrum Analysis, Feb. 2023.
arXiv:2201.09737 [cs].

IntechOpen.
Deep Learning Approach for Raman Spectroscopy | IntechOpen.

U. Lab.
Introduction to Raman Spectroscopy Fundamentals, Apr. 2024.

B. Li, M. N. Schmidt, and T. S. Alstrøm.
Raman Spectrum Matching with Contrastive Representation Learning.
Analyst, 147(10):2238–2246, 2022.
arXiv:2202.12549 [cs].

J. Liu, Q. Hou, J. Wei, and Z. Sun.
Esr-pinns: Physics-informed neural networks with expansion-shrinkage resampling selection strategies.
Chinese Physics B, 32(7):070702, jul 2023.

J. Liu, M. Osadchy, L. Ashton, M. Foster, C. J. Solomon, and S. J. Gibson.
Deep convolutional neural networks for raman spectrum recognition: a unified solution.
The Analyst, 142(21):4067–4074, 2017.

O. Malenfant-Thuot.
OMalenfantThuot/ML_calc_driver, July 2024.
original-date: 2019-10-02T17:52:19Z.


O. Malenfant-Thuot, D. S. Kabakiko, S. Blackburn, B. Rousseau, and M. Côté.
Large Scale Raman Spectrum Calculations in Defective 2D Materials using Deep Learning, Oct. 2024.
arXiv:2410.20417 [cond-mat].


R. Manoharan, K. Shafer, L. Perelman, J. Wu, K. Chen, G. Deinum, M. Fitzmaurice, J. Myles, J. Crowe, R. R. Dasarl, and M. S. Feld.
Raman Spectroscopy and Fluorescence Photon Migration for Breast Cancer Diagnosis and Imaging.
Photochemistry and Photobiology, 67(1):15–22, 1998.
_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/j.1751-1097.1998.tb05160.x.


M. Moores, K. Gracie, J. Carson, K. Faulds, D. Graham, and M. Girolami.
Bayesian modelling and quantification of raman spectroscopy, 2018.


S. Nair, T. F. Walsh, G. Pickrell, and F. Semperlotti.
Multiple scattering simulation via physics-informed neural networks.
Engineering with Computers, July 2024.

OMalenfantThuot.
OMalenfantThuot/ml_raman: New repository for the Raman spectra prediction of graphene from machine learning models.

A. Orlando, F. Franceschini, C. Muscas, S. Pidkova, M. Bartoli, M. Rovere, and A. Tagliaferro.
A Comprehensive Review on Raman Spectroscopy Applications.
Chemosensors, 9(9):262, Sept. 2021.
Number: 9 Publisher: Multidisciplinary Digital Publishing Institute.

A. Poppe.
Deep Learning for Raman Spectroscopy: Bridging the Gap between Experimental Data and Molecular Analysis.
phd, University of Kent,, July 2024.

References x

Y. Qi, D. Hu, Y. Jiang, Z. Wu, M. Zheng, E. X. Chen, Y. Liang, M. A. Sadi, K. Zhang, and Y. P. Chen.
Recent Progresses in Machine Learning Assisted Raman Spectroscopy.
Advanced Optical Materials, 11(14):2203104, 2023.
_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/adom.202203104.

Y. Qi, D. Hu, Z. Wu, M. Zheng, G. Cheng, Y. Jiang, and Y. P. Chen.
Deep Learning Assisted Raman Spectroscopy for Rapid Identification of 2D Materials, Dec. 2023.
arXiv:2312.01389 [physics].

P. Ren, R.-g. Zhou, Y. Li, S. Xiong, and B. Han.
Raman ConvMSANet: A High-Accuracy Neural Network for Raman Spectroscopy Blood and Semen Identification.
ACS Omega, 8(33):30421–30431, Aug. 2023.
Publisher: American Chemical Society.

E. Smith and G. Dent.
Modern Raman Spectroscopy A Practical Approach.
unknown, 2005.

Y. Song, M. Zhang, X. Jiang, F. Zhang, C. Ju, S. Huang, A. P. T. Lau, and D. Wang.
SRS-Net: a universal framework for solving stimulated Raman scattering in nonlinear fiber-optic systems by physics-informed deep learning.
Communications Engineering, 3(1):109, Aug. 2024.

F. Wan, L. Du, W. Chen, P. Wang, J. Wang, and H. Shi.
A Novel Method to Directly Analyze Dissolved Acetic Acid in Transformer Oil without Extraction Using Raman Spectroscopy.
Energies, 10(7):967, July 2017.
Number: 7 Publisher: Multidisciplinary Digital Publishing Institute.

V. Yadav, A. K. Tiwari, and S. Siddhanta.
Machine learning driven high-resolution Raman spectral generation for accurate molecular feature recognition, June 2024.
arXiv:2407.01597 [physics].

S. Yu, H. Li, X. Li, Y. V. Fu, and F. Liu.
Classification of pathogens by raman spectroscopy combined with generative adversarial networks.
Science of The Total Environment, 726:138477, 2020.

Y. Zhou, G. Chen, B. Xue, M. Zhang, J. S. Rooney, K. Lagutin, A. MacKenzie, K. C. Gordon, and D. P. Killeen.
Machine Learning for Raman Spectroscopy-based Cyber-Marine Fish Biochemical Composition Analysis, Sept. 2024.
arXiv:2409.19688 [cs].