香港中文大學
The Chinese University of Hong Kong

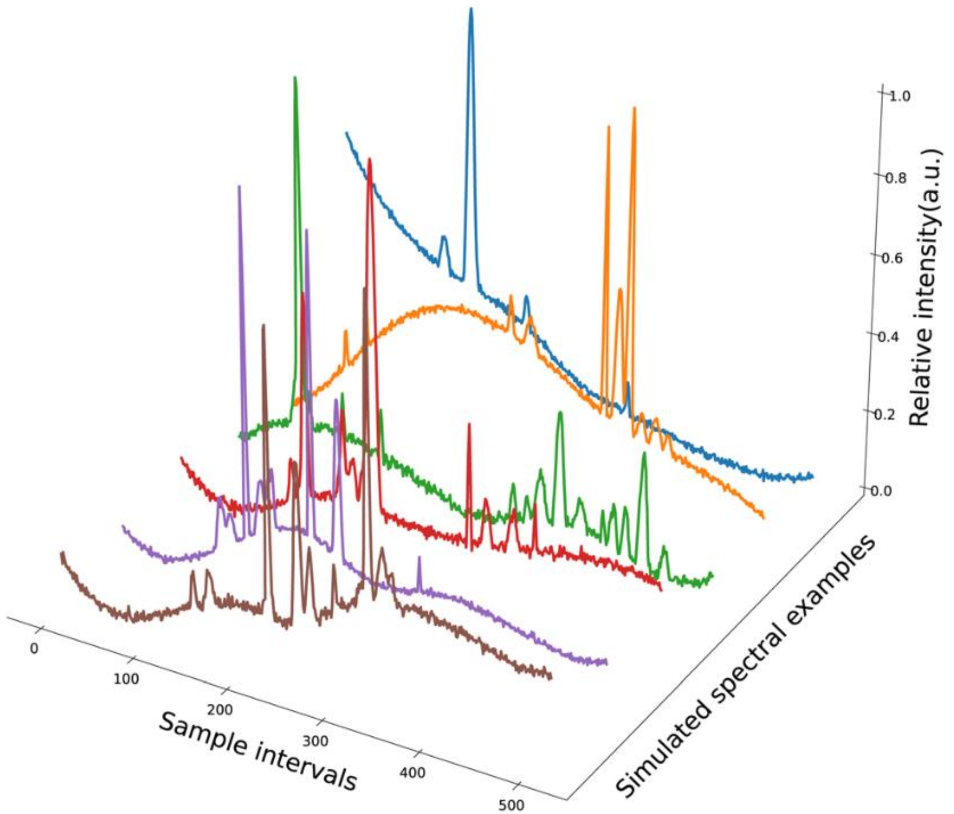
Baseline Correction Using a Deep-learning Model Combining ResNet and UNet

Jingyi Liu

Analyst, 2022, 147, 4285

Outline

1. **Background**
2. **Previous Methods**
3. **Key Challenge**
4. **Proposed Deep Learning Methods**
5. **Results**
6. **Conclusion**



Research Background

Research Background

- Raman spectroscopy has shown to be a versatile analytical technique to obtain physical and chemical information.

- However, raw measured Raman spectra are often disturbed by baseline drifts caused by Rayleigh scattering or fluorescence.

- Accurate corrected baselines are essential for Raman spectra.

Previous Baseline-Correction Methods

Previous Baseline Correction Methods

❖ Wavelet transform

- Baseline -> low frequency; Noise -> high frequency.
- Filters out baseline using a wavelet transform

- Performance greatly depends on the filtering ability of the wavelet transform

❖ Polynomial fitting

- Fits the baseline by continuously and iteratively eliminating the spectral signal peaks

- Prone to overfitting/ underfitting.
- Relies on artificial interventions

❖ Penalized least squares

- Iteratively changes weights by estimating a base-line.
- Efficient, avoid user interventions

- Lack of flexibility

❖Penalized least squares (PLS)

Loss function

Difference matrix

Fitness

$$S(\boldsymbol{z}) = (\boldsymbol{y}-\boldsymbol{z})^T(\boldsymbol{y}-\boldsymbol{z}) + \lambda\, \boldsymbol{D}\boldsymbol{z}^T\boldsymbol{D}\boldsymbol{z}$$

Smoothness

Fitted spectral signal to be identified

A spectral signal of length N
sampled at equal intervals

Balance between fitness and smoothness

$$S(\boldsymbol{z}) = (\boldsymbol{y}-\boldsymbol{z})^T\boldsymbol{W}(\boldsymbol{y}-\boldsymbol{z}) + \lambda\boldsymbol{z}^T\boldsymbol{D}^T\boldsymbol{D}\boldsymbol{z}$$

Weight vector to apply penalty.
Is a matrix with elements w_i

Peak regions: $w_i = 0$

Non-peak regions: $w_i = 1$

❖PLS methods

- ❖ **Asymmetric least squares (AsLS)**
- ❖ **Adaptive iteratively reweighted penalized least squares (AirPLS)**
  - Extra control of smoothness

- Avoid predefining wave regions.
- Boosted-baseline problem

- ❖ **Asymmetrically reweighted penalized least squares (arPLS)**

→ introduced asymmetrical weights to prevent boosted baseline

PLS methods are prone to misjudgment in peak regions!

Key Challenges in Deep Learning Methods

❖Deep learning methods

- Requires numerous labelled datasets
- Costly data collecting and labelling process → simulated spectral data

Convolutional Neural Networks (CNN) based models

❖ Convolutional neural networks (CNN) based models

- **Vanishing-gradient problem**

1. In extremely deep CNN, the gradient values get smaller and smaller when passed back through previous layer.
2. When the gradient is almost zero, the weights will no longer be updated, i.e. CNN stops learning.

⬇

ResNet

Has a better regression and recognition ability compared to the conventional CNN

[1] B.-H. Kung, C.-C. Huang, P.-Y. Hu, S.-y. Lo, C.-C. Lee, C.-Y. Yao and C.-H. Kuan, 2020 Conference on Lasers and Electro-Optics (CLEO), 2020, pp. 1–2.
[2] Y. Liu, Chemometrics and Intelligent Laboratory Systems, 2021, 213, 104317.

❖ Residual Networks (ResNet)

➢ Shortcut connection of the residual learning framework

Identity shortcut

When the input and output have the same dimensions.

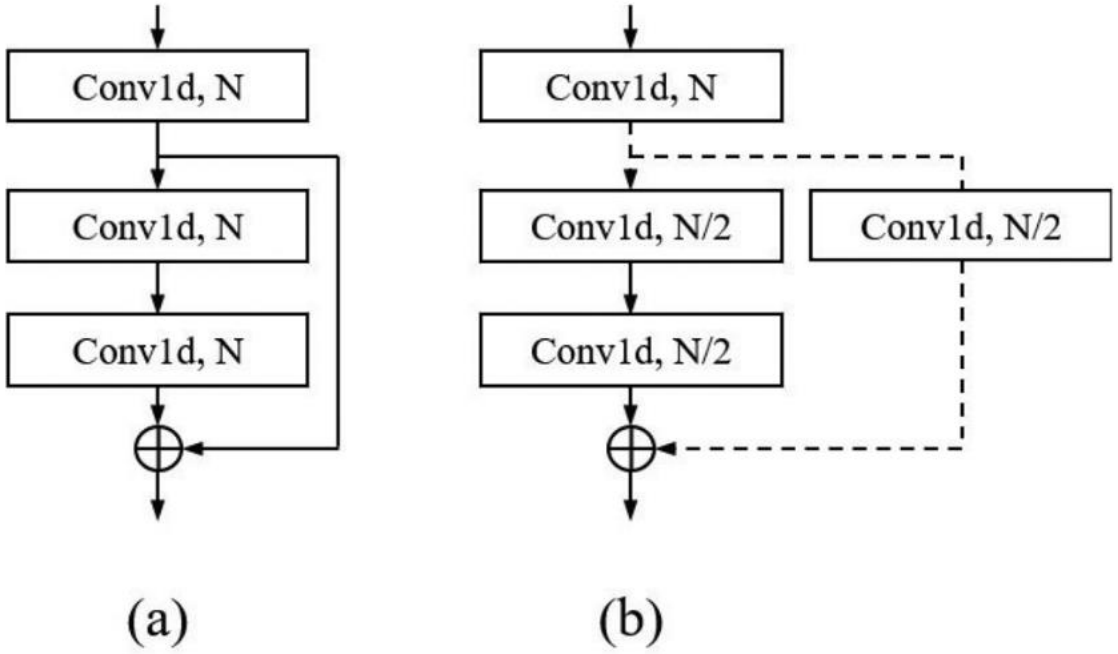


Fig. 1 Structure of the ResNet block. (a) Identity shortcut. (b) Projection shortcut.

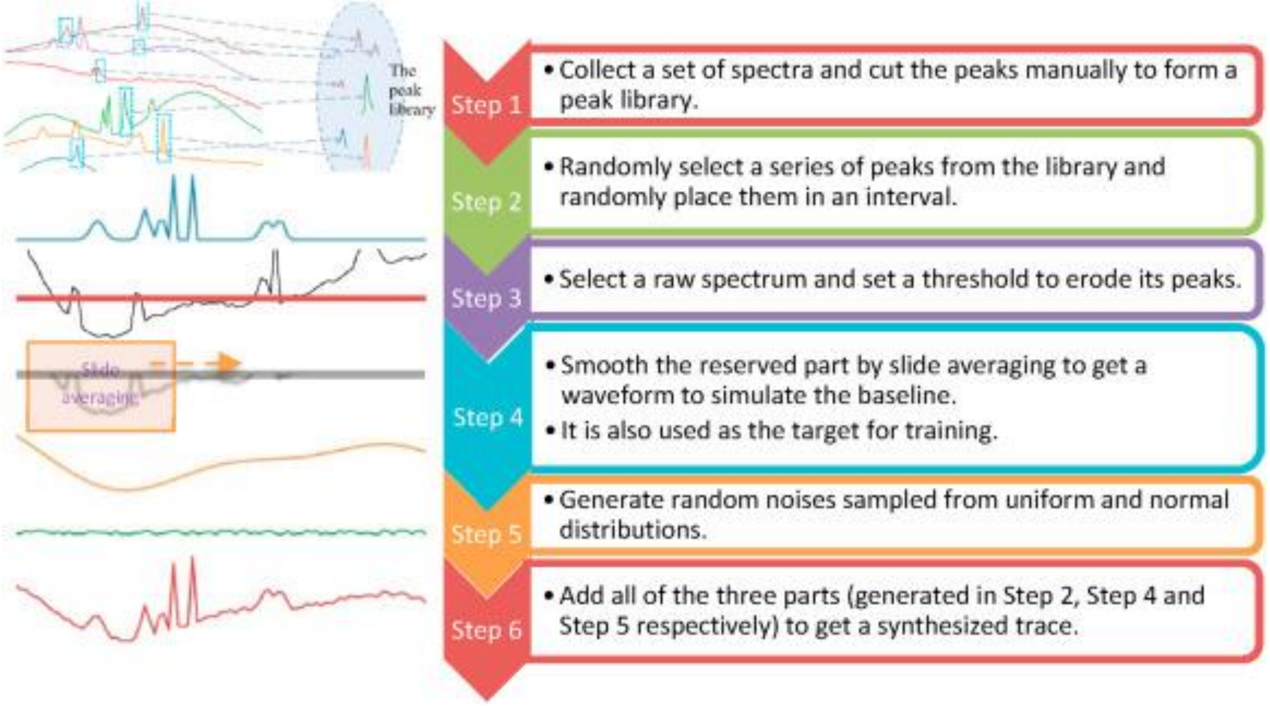
Projection shortcut

Input is projected into the same dimension as the output before adding.

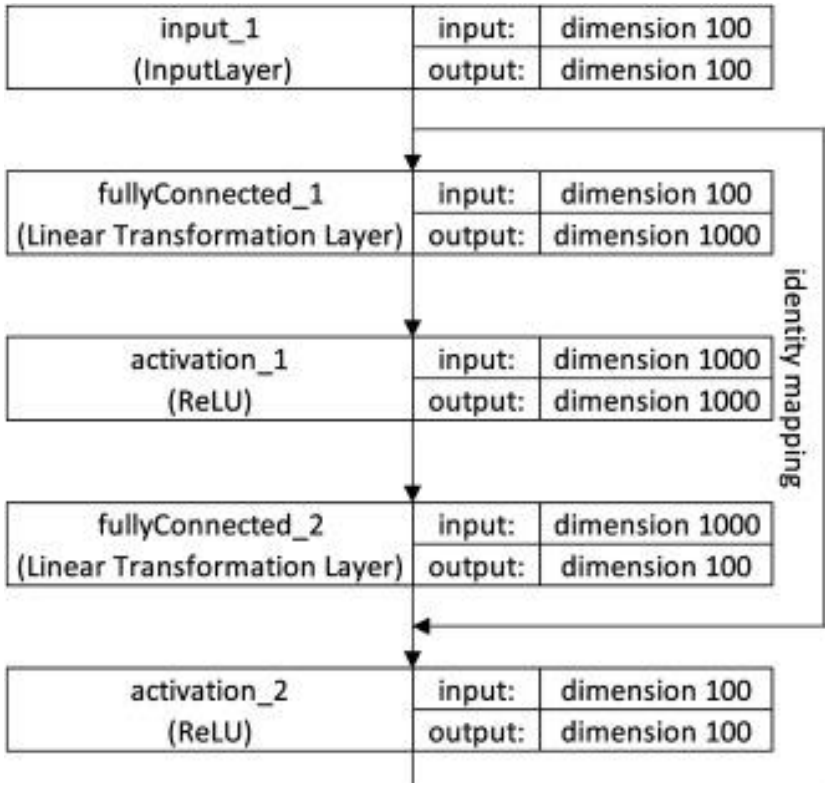
[3] He, Kaiming, et al. "Deep residual learning for image recognition." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

❖ Residual Networks (ResNet)

➢ Baseline Recognition Networks



Data set generated from experimental data

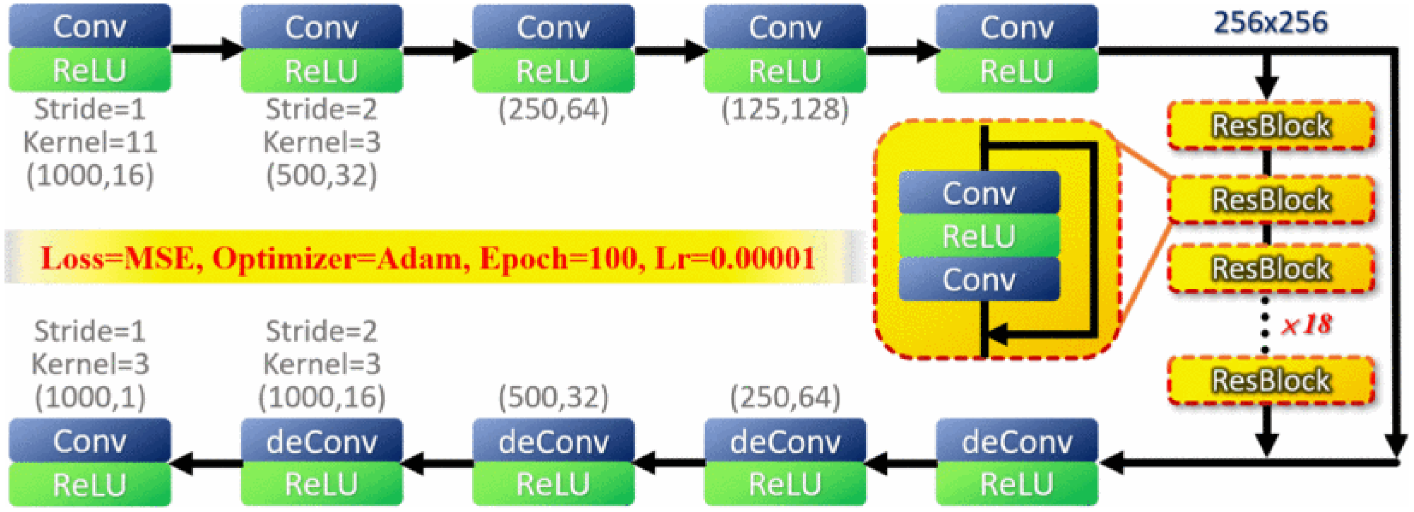


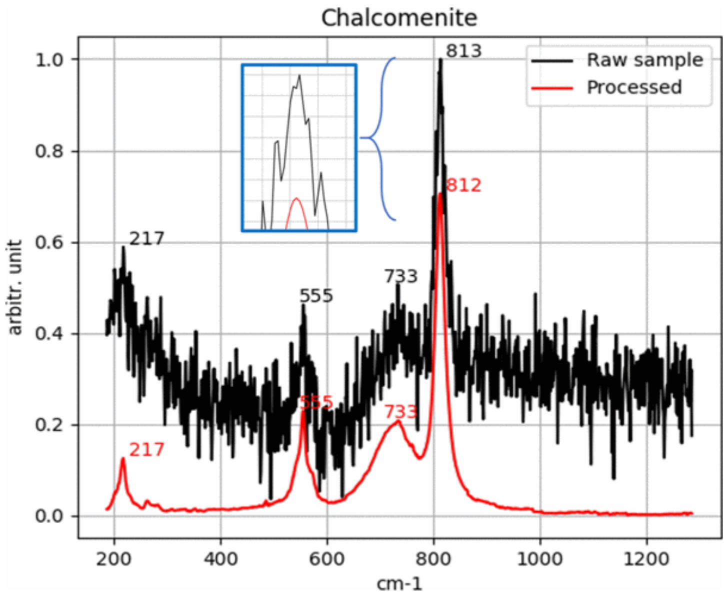
Residual block

[2] Y. Liu, Chemometrics and Intelligent Laboratory Systems, 2021, 213, 104317.

❖ Residual Networks (ResNet)

➢ Deep residual convolutional neural network (DRCNN)





Extract the key information of the spectral peaks from diverse baselines and noises without a priori information of noise levels and baselines.

[1] B.-H. Kung, C.-C. Huang, P.-Y. Hu, S.-y. Lo, C.-C. Lee, C.-Y. Yao and C.-H. Kuan, 2020 Conference on Lasers and Electro-Optics (CLEO), 2020, pp. 1–2.

Proposed Deep Learning Method

❖ **A success deep learning model requires …**

- ➢ The amount and variety of the data set.
- ➢ Structure of the deep learning network
- ➢ Hyperparameter tuning

- A method to generate spectral data set
- **ResUNet:** A new deep learning network combining ResNet and UNet (U-shaped Network)

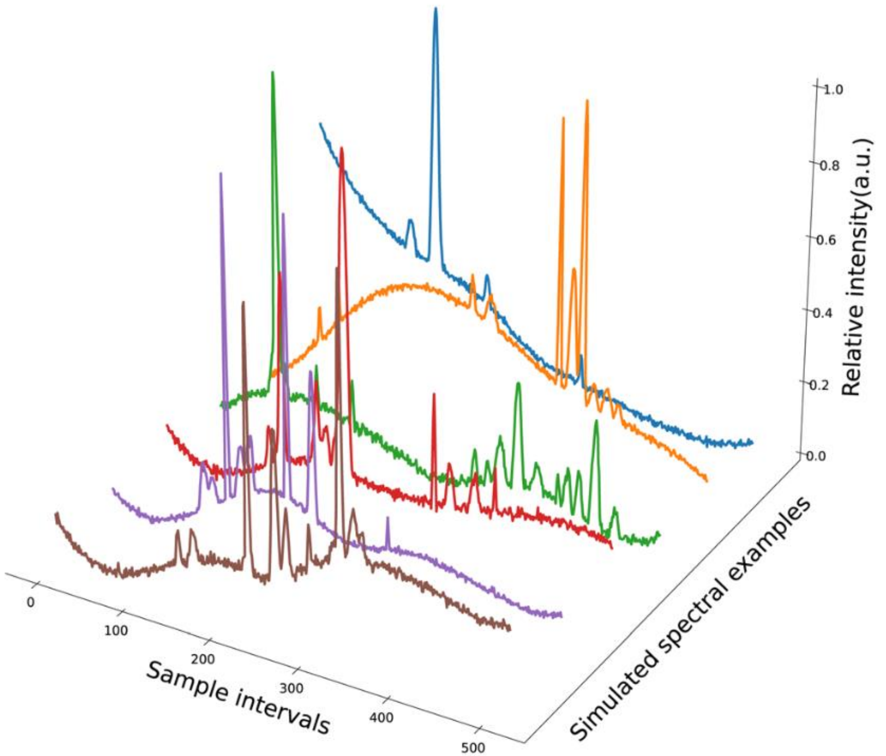


Fig. 3 Simulated data examples with different baseline and additional noise.

❖ Data generation

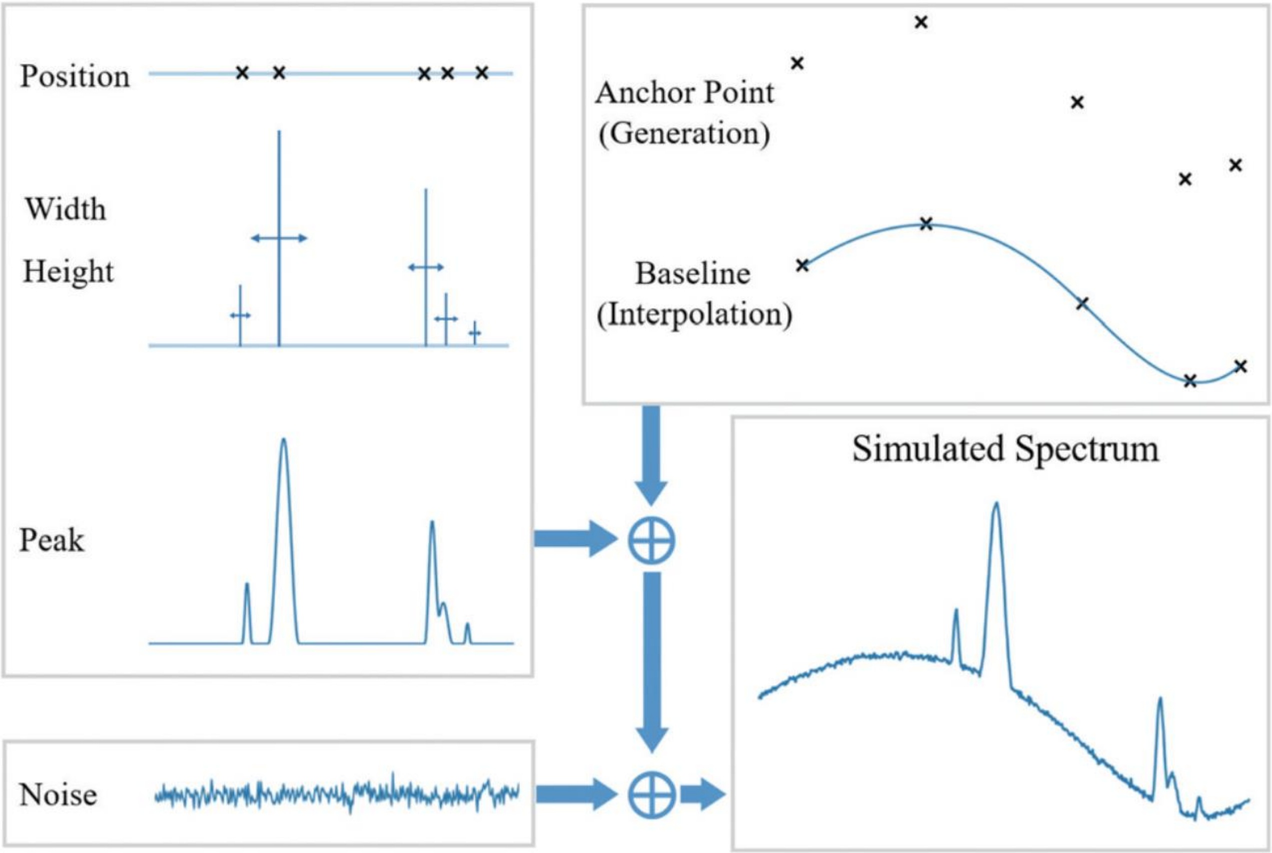


Fig. 2 Procedure for generating simulation data.

❖ UNet (U-shaped Network)

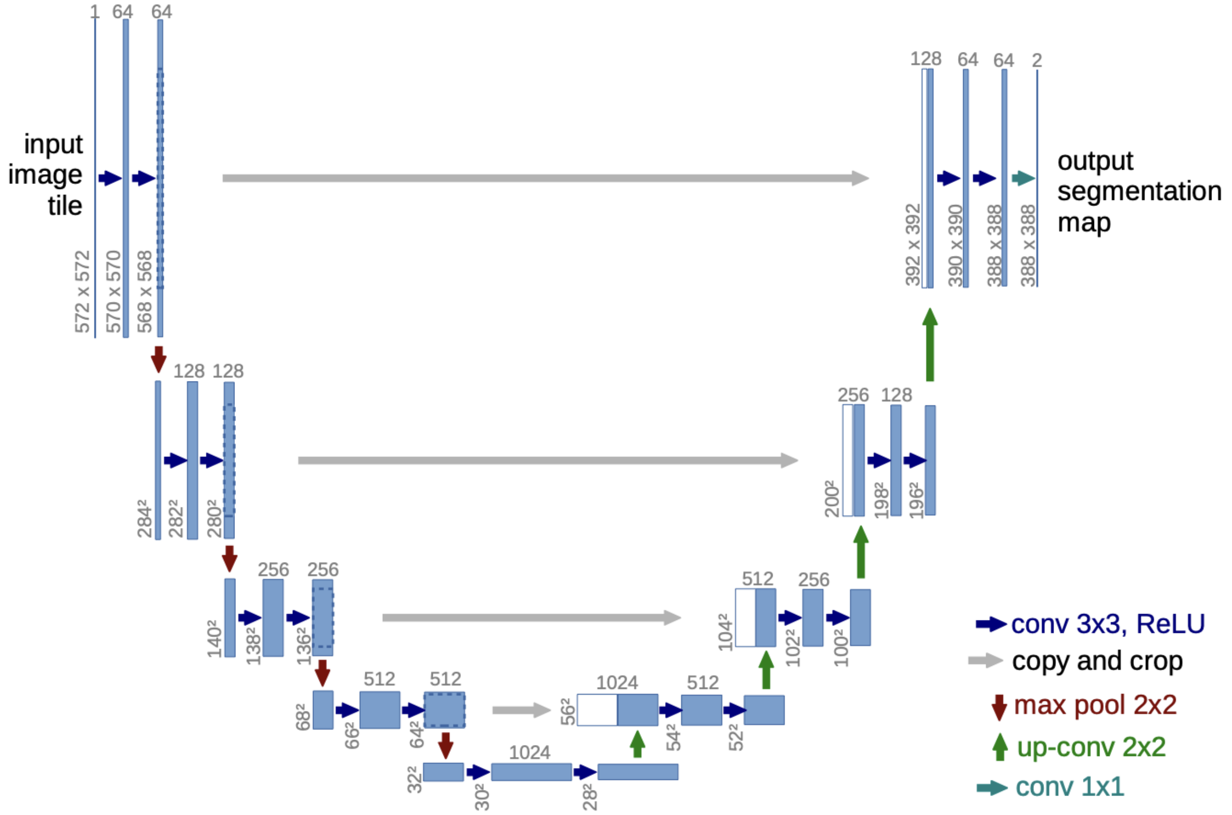


Fig. 1. U-net architecture (example for 32x32 pixels in the lowest resolution). Each blue box corresponds to a multi-channel feature map. The number of channels is denoted on top of the box. The x-y-size is provided at the lower left edge of the box. White boxes represent copied feature maps. The arrows denote the different operations.

- Firstly applied in medical images
- Comprises contracting and expansive paths.
- U-shaped architecture: the size of the data changes from small to large when passing through the contracting and expansive paths.

[4] Ronneberger, Olaf, Philipp Fischer, and Thomas Brox. "U-net: Convolutional networks for biomedical image segmentation." *Medical image computing and computer-assisted intervention–MICCAI 2015: 18th international conference, Munich, Germany, October 5-9, 2015, proceedings, part III 18*. Springer international publishing, 2015.

❖ UNet (U-shaped Network)

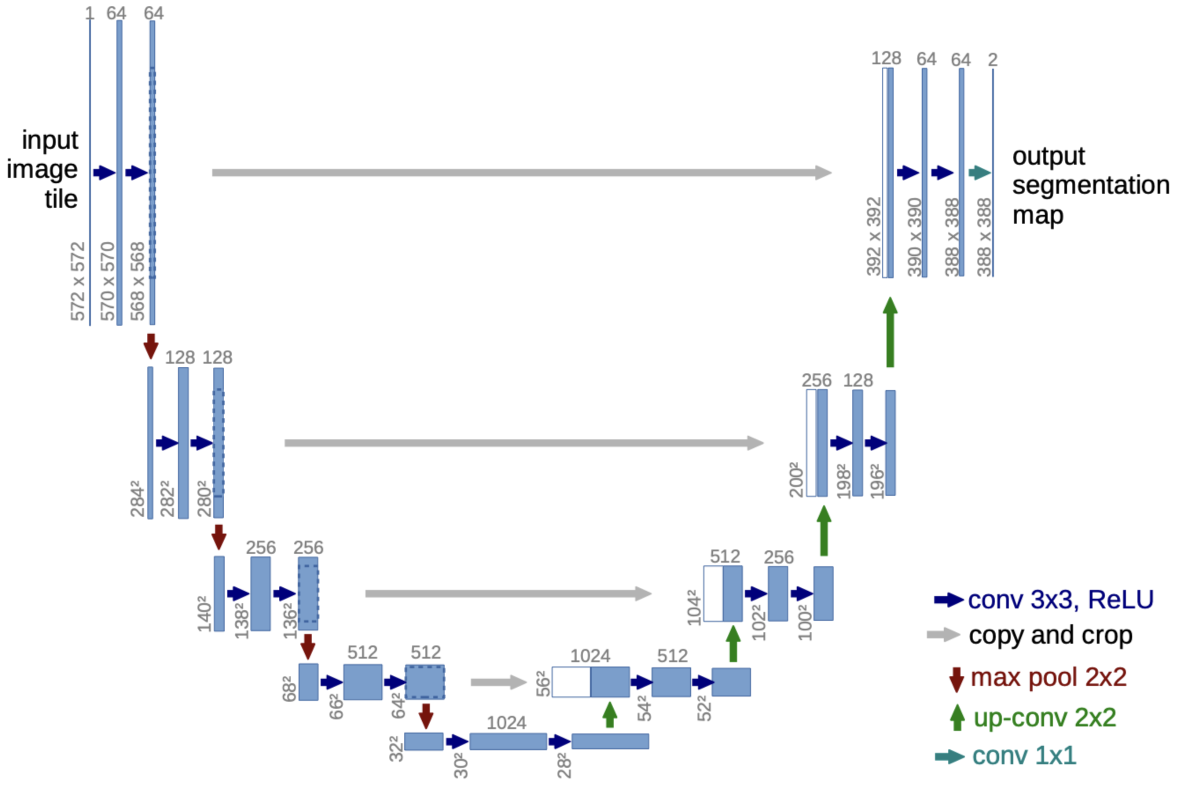


Fig. 1. U-net architecture (example for 32x32 pixels in the lowest resolution). Each blue box corresponds to a multi-channel feature map. The number of channels is denoted on top of the box. The x-y-size is provided at the lower left edge of the box. White boxes represent copied feature maps. The arrows denote the different operations.

- The symmetric structure ensures precise localization while maintaining context.
- Upsample the feature map on the expansive path and combine the context of the feature map captured on the contracting path for more accurate localization.
- Retrieve the lost pixel information

[4] Ronneberger, Olaf, Philipp Fischer, and Thomas Brox. "U-net: Convolutional networks for biomedical image segmentation." *Medical image computing and computer-assisted intervention–MICCAI 2015: 18th international conference, Munich, Germany, October 5-9, 2015, proceedings, part III 18*. Springer international publishing, 2015.

❖ ResUNet

- Uses ResNet for the expansion and contracting paths while maintaining the main structure of UNet

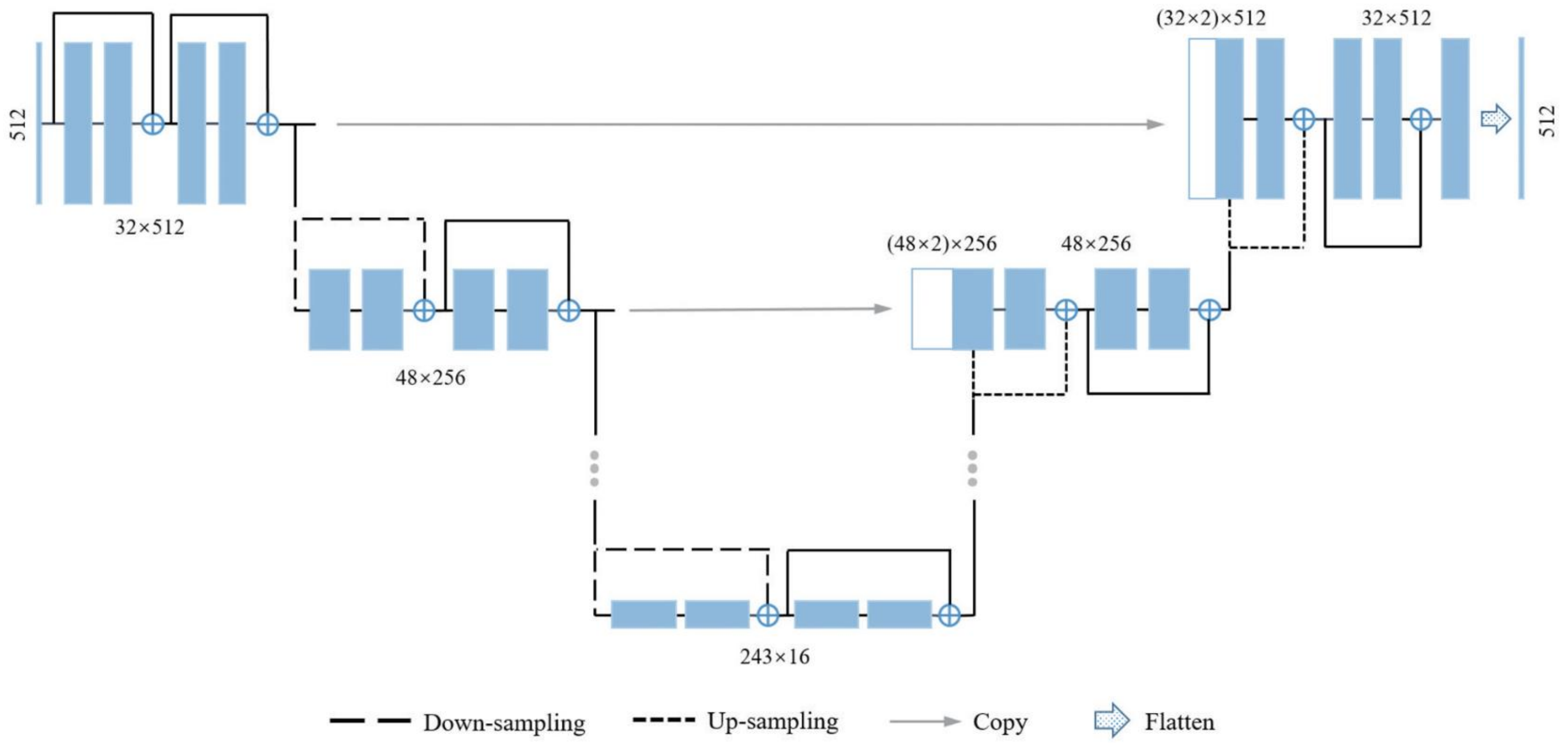


Fig. 4 Structure of the proposed ResUNet.

Results

❖ Preliminary experiments

(1) To select the best smoothness parameter λ of arPLS and asPLS.

Table 2 RMSE ($\times 10^{-4}$) of baseline-corrected spectra for different values of parameter λ

	$\log_{10}\lambda$					
	0	1	2	3	4	5
arPLS	243.74	$\boxed{82.25}$	128.13	577.62	1349.30	1923.00
asPLS	825.87	615.52	242.62	93.21	$\boxed{63.90}$	337.05

$$S(z) = \underbrace{(\boldsymbol{y}-\boldsymbol{z})^T\boldsymbol{W}(\boldsymbol{y}-\boldsymbol{z})}_{\text{Fitness}} + \overbrace{\lambda \boldsymbol{z}^T\boldsymbol{D}^T\boldsymbol{D}\boldsymbol{z}}^{\text{Smoothness}}$$

$$\text{RMSE} = \left[\sum_{i=1}^{N}(y_i - z_i)^2/N\right]^{\frac{1}{2}}$$

❖ Preliminary experiments

(2)To determine the channel size of the deep-learning-based methods.

$$\boxed{C_{i+1}} = \beta C_i, 1 \leq \beta \leq 2.$$

Channel size

Table 3 Results of the preliminary experiments for constructing a deep-learning network

Model	Channel						Parameter	RMSE ($\times 10^{-4}$)
ResNet	16	32	64	128	256	512	6 427 360	6.66
	16	32	64	128	256		3 180 640	7.15
	32	64	128	256	512		8 521 408	7.10
	32	48	72	108	162	243	2 394 762	6.66
UNet	32	48	72	108	162	243	2 070 882	6.20
ResUNet	32	48	72	108	162	243	2 350 457	5.85

- Set appropriate channel size > downsampling or upsampling by a multiple of 2
- Appropriate channel → less number of parameters.

➢ β =1.5

❖ Training strategy

Parameter	Value/Setting
Training Loss Function	Root Mean Square Error (RMSE)
Validation Loss Function	Mean Absolute Error (MAE)
Optimization Method	Adaptive Moment Estimation (Adam)
Batch Size	500
Maximum Learning Epoch	1200
Initial Learning Rate	5×10^{-4}
Learning Rate Decreasing Setting	- Reduced to 4/5 of starting rate if validation loss doesn't improve for 75 epochs
	- Training stops if learning rate reaches 1/8 of original rate
Model Saving Condition	Current model is saved if validation loss is lower than previous

❖ Simulated data: quantitative

➢ 210000 spectra generated.

70000 used for training.

➢ ResUNet shows the lowest RMSE and MAE.

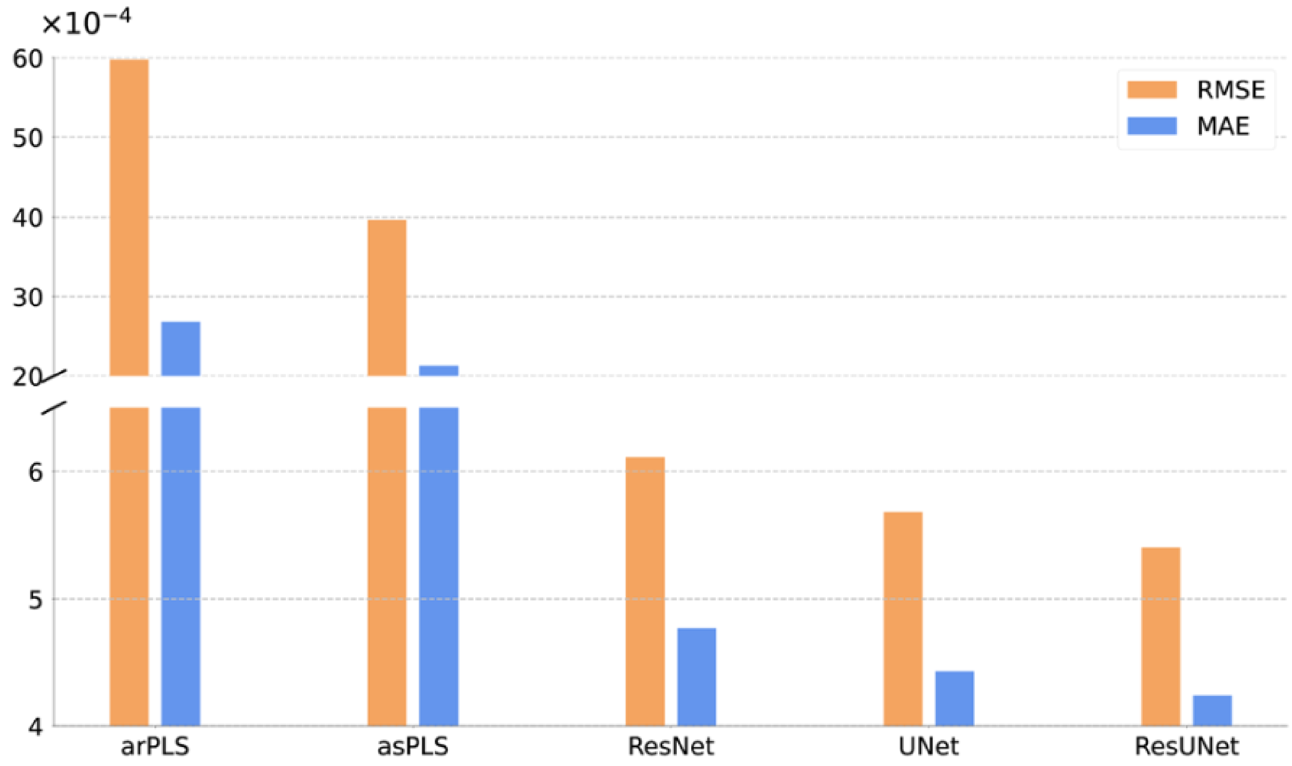


Fig. 5 RMSE and MAE of baseline-corrected spectra obtained by various methods.

❖ Simulated data: qualitative

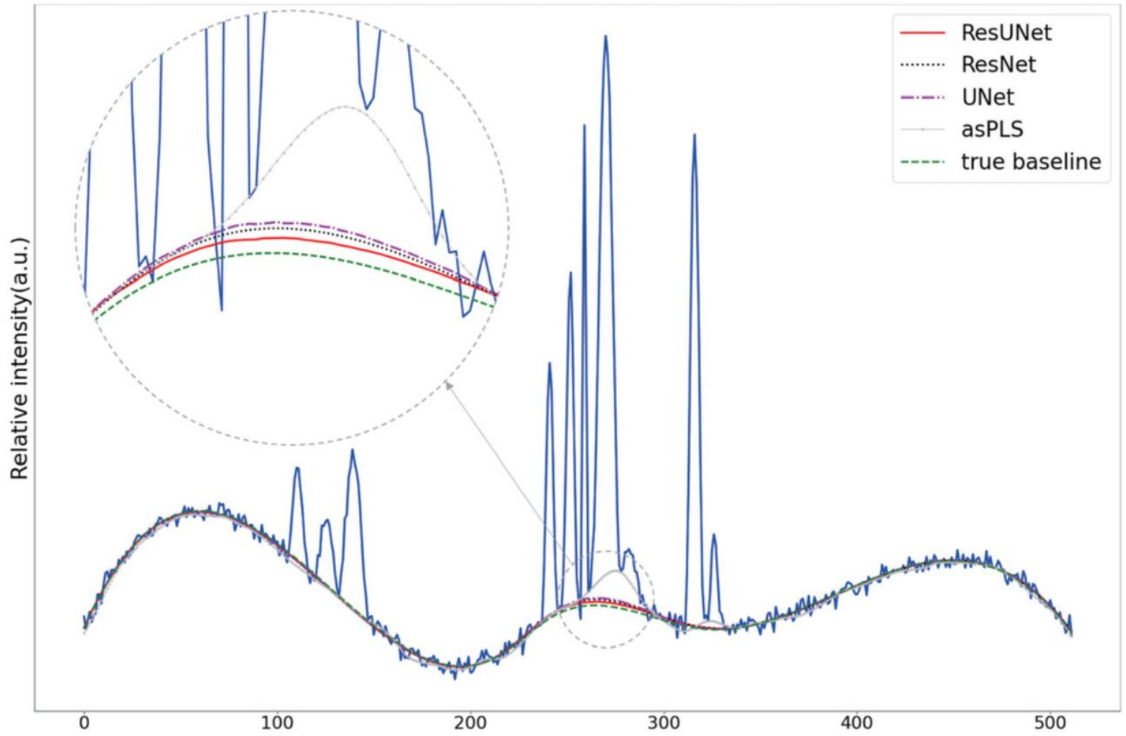


Fig. 6 Baseline-fitting results of the first simulation spectrum.

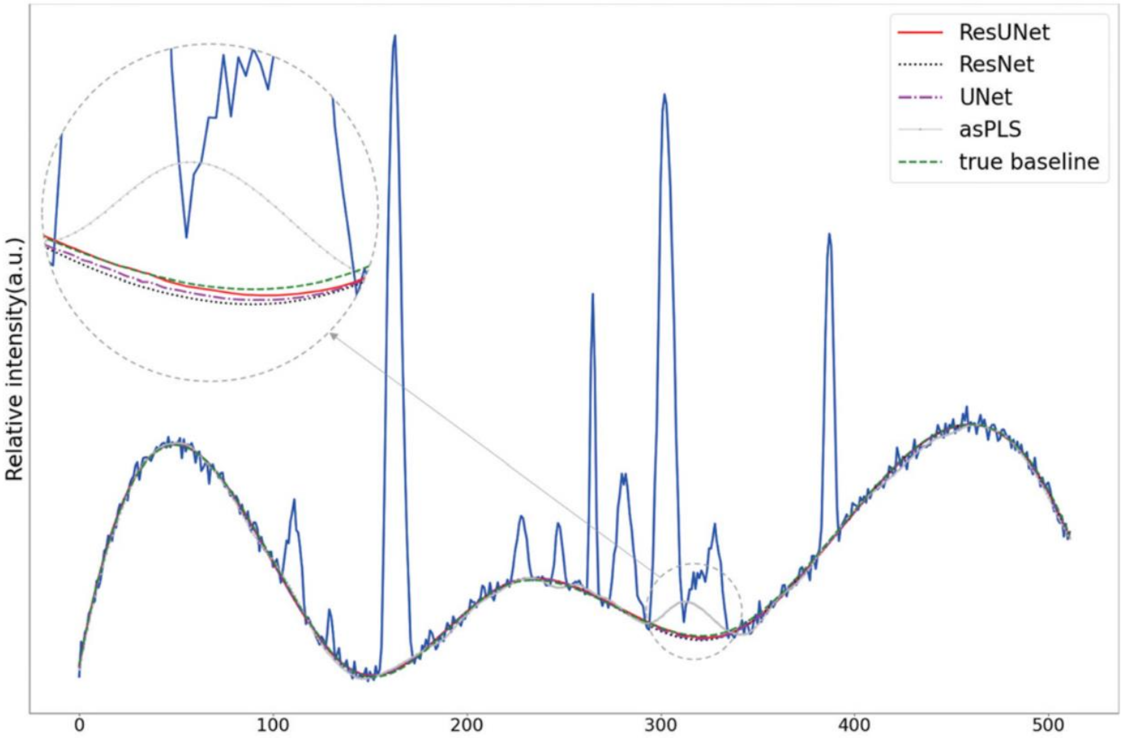


Fig. 7 Baseline-fitting results of the second simulation spectrum.

➢ ResUNet has outperformed the penalized least-squares-based baseline-correction methods and the other two deep learning methods

❖ Experimental Raman Spectrum

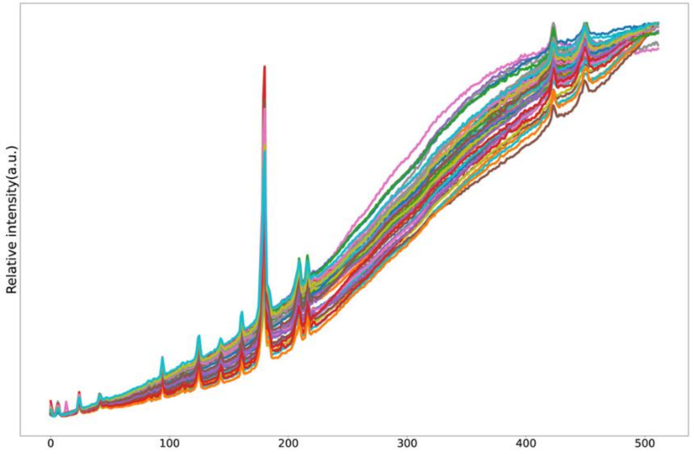


Fig. 8 Measured 35DNT Raman spectra.

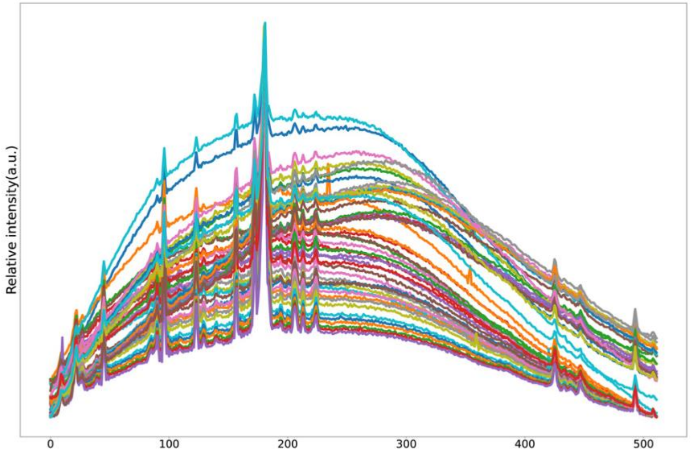


Fig. 10 Measured 4ADNT Raman spectra.

Linear background

Highly curved background

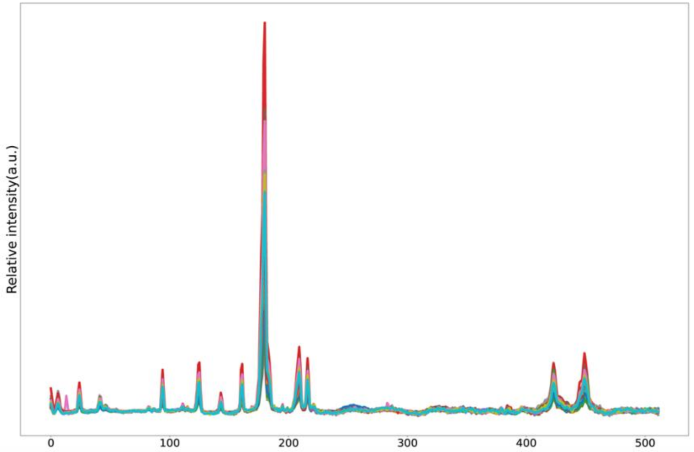


Fig. 9 Baseline-corrected 35DNT Raman spectra.

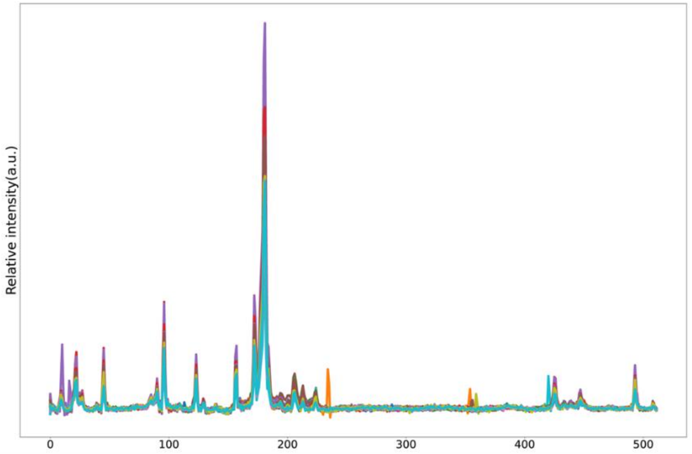


Fig. 11 Baseline-corrected 4ADNT Raman spectra.

- ResUNet has successfully corrected the baselines of the two substances

Conclusions

❖ Conclusion

- A ResNet-based baseline-correction method for spectra was proposed.

- Compared to existing penalized least squares methods, ResUNet does not require subjective parameter estimation and shows better performance.

- Two problems were addressed:
  - Insufficient training data → Simulate spectra by combining randomly generated baseline, peak, and additive.
  - Channel size → for one-dimensional data, an appropriate channel size can reduce the number of model parameters.

- Compared to existing deep-learning-based methods, ResUNet has achieved excellent accuracy without increasing the number of parameters.

- ResUNet gives the smallest standard deviation of the results amongst all the methods that were considered for comparison.

Questions? Comments?

Thank You