# Generative adversarial network for robust Raman spectra identification

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## 1. Introduction

Generative adversarial network (GAN) is a reinforcement machine learning technique where two machines contest in learning abilities. This algorithm was often realized by constructing two neural networks (NN) where one evaluates data (discriminator) and the other generates confusing data (generator) to deceive the other one. Recently, the effects of GAN on discriminators have incurred some attentions due to its efficacy to improve the network robustness.<sup>1</sup>

Raman spectroscopy is a highly promising technique for explosives detection due to its label-free and stand-off nature.<sup>2</sup> However, as few as 1 in  $10^6-10^8$  photons scatters as Raman signal, which makes Raman detections susceptible to fluorescence and environmental noises. This problem deteriorates in situations of distant detection, which is indispensable in Raman detection of explosives.

In this work, a semi-supervised GAN classifier was constructed to classify the Raman spectra of the most prevalent explosive, TNT, and its precursor, 24-DNT. With highly resembling Raman spectra accompanied by severe noises, these chemicals were often hard to be distinguished through Raman detections. Herein, the GAN classifier with better network robustness was adopted which outperformed its supervised counterparts due to superior network robustness.

### 2. Result and Discussion

3 classifiers (A, B and C) with identical NN structures were trained to identify Raman spectra of the positive group of TNT and 24-DNT and a negative group of non-TNT/24-DNT data. The standard ranks for Raman spectra of TNT, 24-DNT and the negative group were [1,0], [0,1] and [0,0], respectively. While the same positive group was used to train each classifier, negative data of randomly distributed noises, Raman spectra from other chemicals and Raman spectra generated from generator were used, respectively, for A, B and C classifiers.

In the GAN classifier, C, the discriminator tried to correctly classify each category while the generator tried to deceive the discriminator by mimicking real data (Fig. 1). However, the generated data was constantly ranked as [0,0] by the discriminator. This prompted the generator to be a craftier counterfeiter to pursue a higher score. Meanwhile, discriminator became a more meticulous detective to distinguish fakes from reals.

The robustness of C classifier is demonstrated in Fig. 2. While the ranks of the test data in Fig. 2(a) and (b) for A and B classifiers, respectively, were of large variances, ranks in (c) for C classifier were uniformly distributed in the proximities of ideal scores except for few outliers. The testing errors shown in Fig. 2 for A, B and C classifiers were 0.095, 0.144 and 0.026, respectively.

#### 3. Conclusion

According to Fig. 2(a) and (b), the Raman spectra of TNT are rather difficult to be identified for NN classifiers and were often misidentified as fake data. This issue was overcome by the GAN classifier indicating a superior network robustness. In sum, both classifying accuracy and robustness were refined by modifying the NN into a GAN-assisted one.



Figure 1. Given the commands of [1,0], [0,1] and [0.5,0.5], which correspond to the Raman spectra of TNT, 24-DNT and 0.5 TNT+0.5 24-DNT, respectively, to the generator, the evolution of generated Raman spectra after 0, 50, 100, and 150 rounds of training shows the learning of the generator.



Figure 2. The ranks of testing data for (a) A, (b) B and (c) C classifiers, where the ranks of Raman spectra for TNT and 24-DNT are marked as T and D, respectively, and the corresponding ideal scores are [1,0] and [0,1], respectively.

#### Acknowledgements

The work was supported by the Ministry of Science and Technology, Taiwan under Contract no. MOST 107-2221-E-002-013.

#### References

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