Use of conditional generative adversarial networks to improve representativity of data in optical spectroscopy

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Raman spectroscopy inverse problem

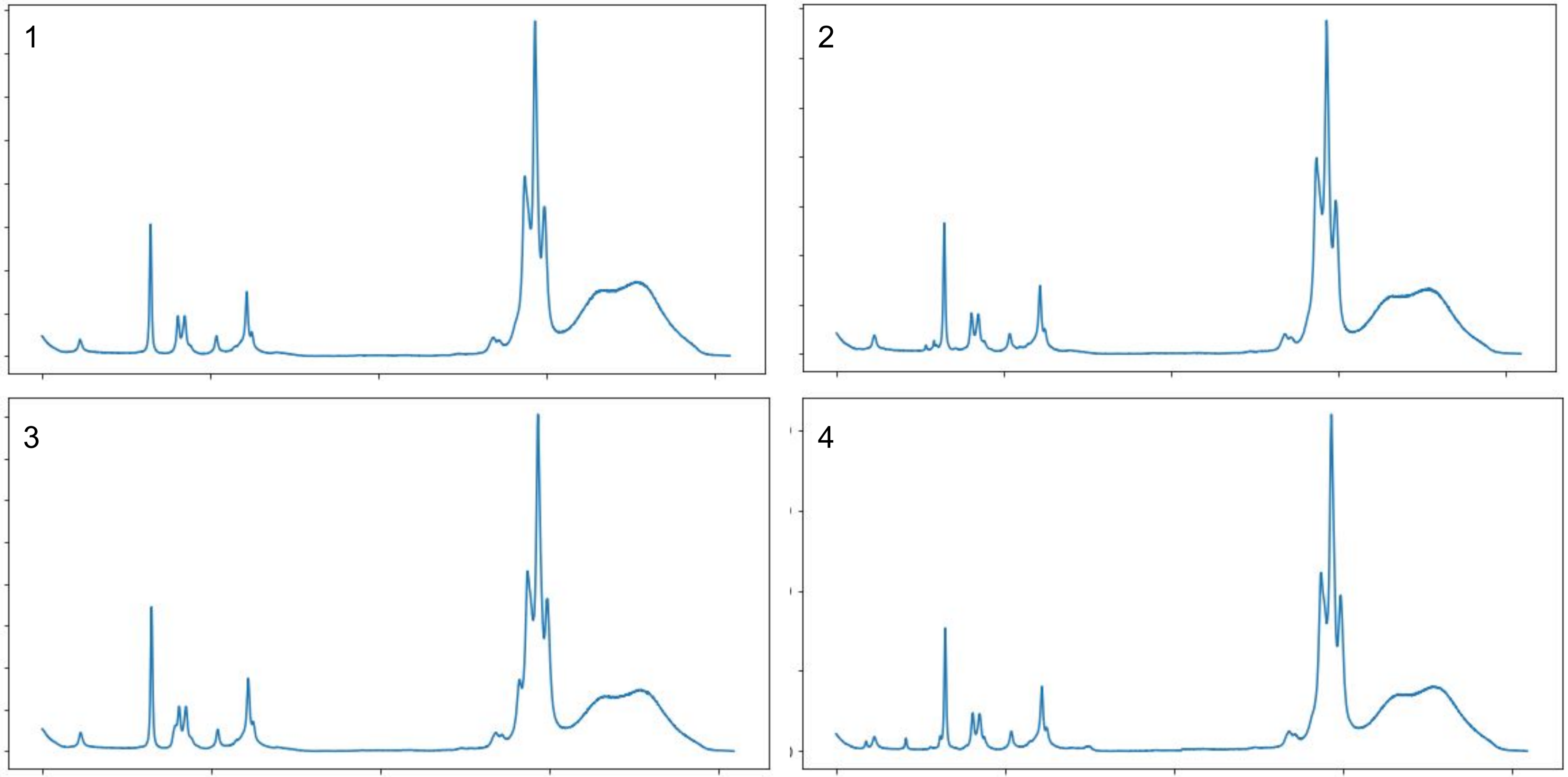
- Main goal: detect dangerous components mixed in ethanol solutions;

- Components of interest:
  - methanol
  - ethyl acetate
  - fusel oil

- Non-invasive observation method based on Raman spectroscopy;

- Inverse problem (multitask classification) solution by machine learning model

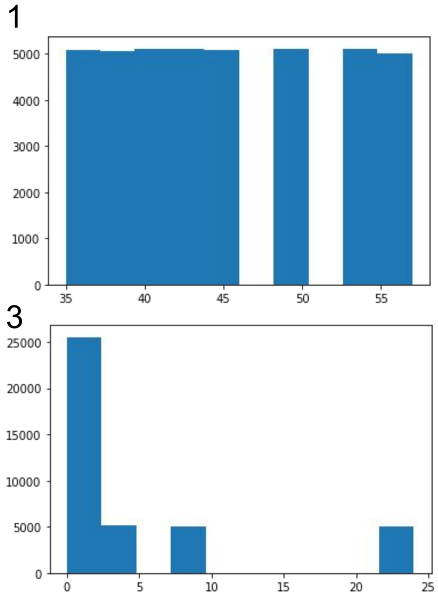
Raman spectra



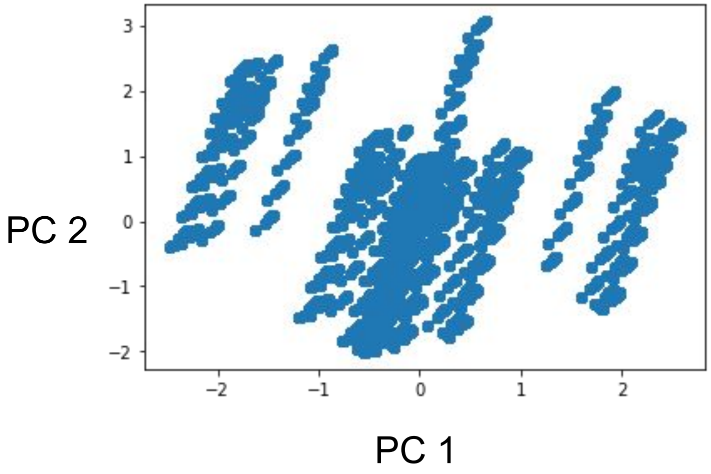
Raman spectra of ethanol (49%) solutions with different component concentrations:
1 - pure ethanol, 2 - fusel oil (5.6%), 3 - methanol (8%), 4 - ethyl acetate (6%)

Components concentrations

- Full dataset: 40710 spectra
- Spectra dimension = 2048 channels
- <u>Problem:</u> wide concentration “gaps” in dataset



Component concentrations (%) at dataset: 1 - ethanol, 2 - fusel oil, 3 - methanol, 4 - ethyl acetate

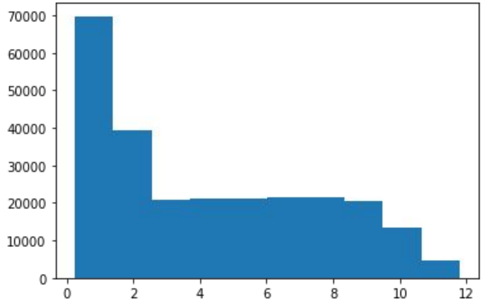


Principal component analysis of component concentrations

Add empty concentrations

- create 2D grid based on PC1\PC2 coordinate space (PC-space);
- fill empty grid cells in PC-space;
- inverse transformation to the original concentrations;
- implement empirical constraints (eliminate negative values, values exceeds max concentrations)
- Component concentrations (%) at generated dataset: 1 - fusel oil, 2 - methanol, 3 - ethyl acetate

1



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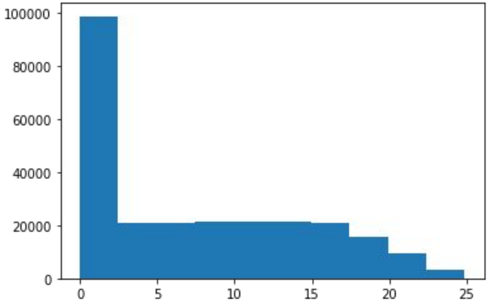

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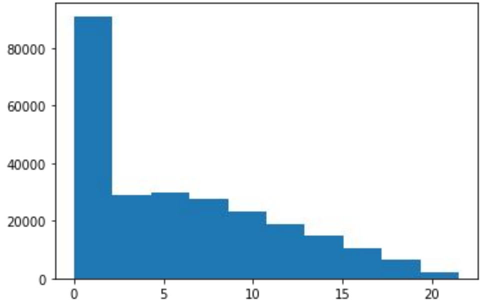


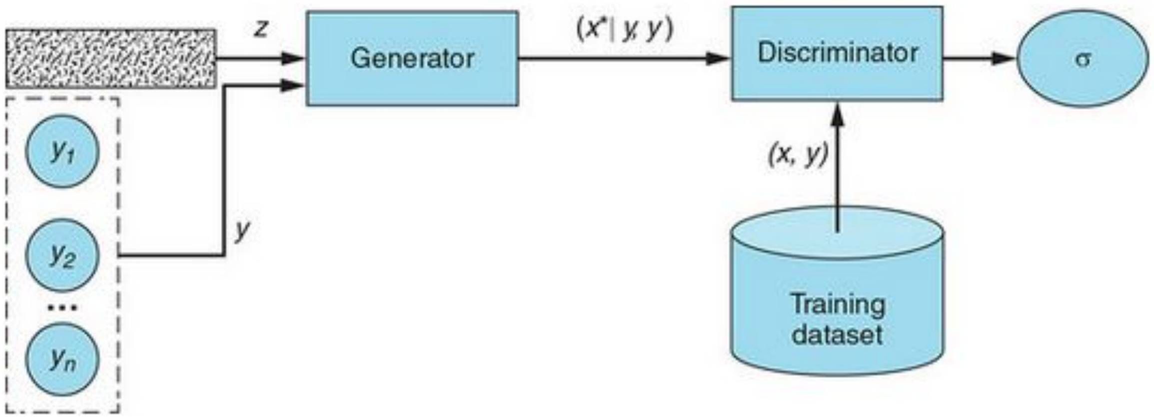
Conditional GAN

Generator

Two inputs of model:

z - random noise

y - label annotation



Discriminator

Loss function minimization in case : {**X (spectra) - real, Y (annotation) - true**}.

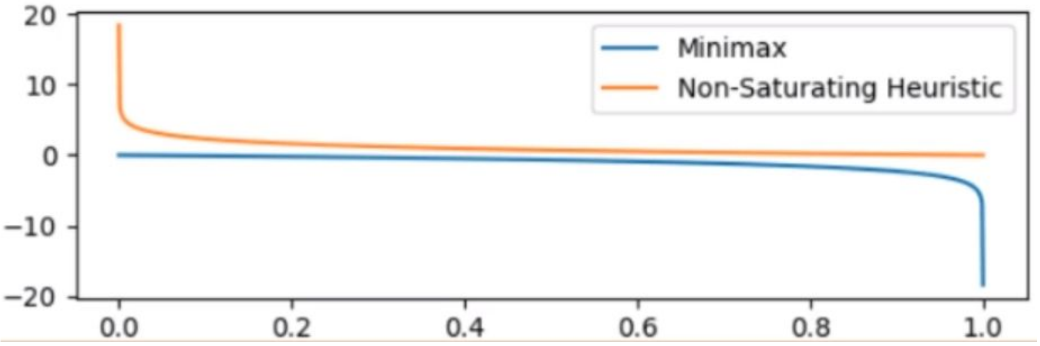
Loss function maximization in cases:

- real spectra [X] - false;
- generated spectra [X*], true;
- generated spectra [X*], false

Non-saturating heuristic

- Non-saturating heuristic - loss function without problem of small gradients;

- Heuristic because there are no theoretical prove*;



$$\frac{d}{dx}\log(1-x) = \frac{-1}{1-x}$$

$$x = 0 \;\rightarrow\; slope = -1$$

$$x = 1 \;\rightarrow\; slope = -\infty$$

*[1701.00160] NIPS 2016 Tutorial: Generative Adversarial Networks

Neural network architectures

Generator network:

- Embedding layer for component vector (size: 256);
- 4 1D-Convolutional layers with LeakyRelu activation;
- Upsampling operation (2x) after each layer;

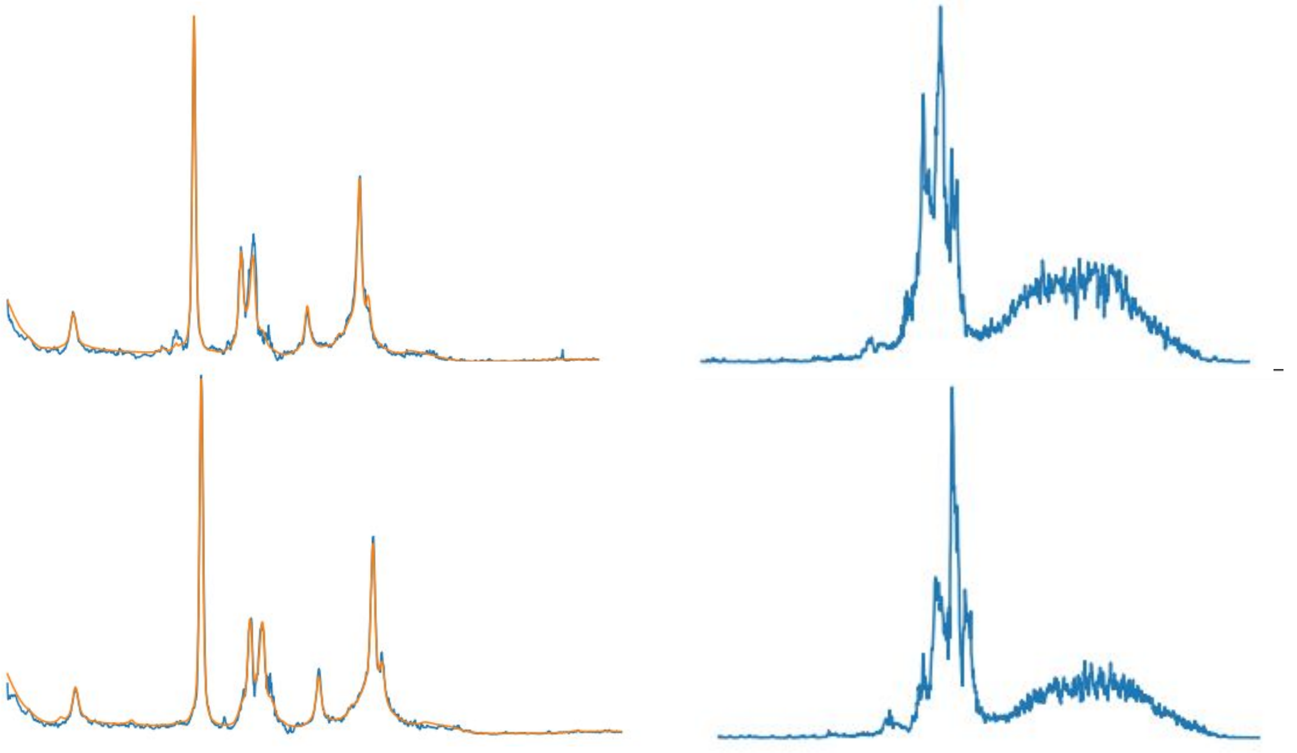
Discriminator network:

- 3 fully connected layers with Relu activation;
- 1 output neuron (real\generated image);

Inverse problem solver network:

- 2 fully connected layers network;
- categorical cross-entropy loss;

Examples of generated spectra



Generated Raman spectra for low frequency band (left) & valence band (right)

Results

		Original spectra	Original spectra + additive noise 10%	Original spectra + multiplicative noise 10%
Low frequency band	original dataset	77.0%	70.2%	55.9%
	cGAN + original data	74.4%	69.3%	54.7%
Valence band	original dataset	67.1%	62.4%	60.1%
	cGAN + original data	67.4%	63.0%	57.5%
Full spectra	original dataset	72.8%	69.7%	59.1%
	cGAN + original data	75.4%	70.7%	60.4%

The accuracy of the multiclass classification problem solution by neural networks model based on original and generated spectra

Conclusions

- The Raman spectroscopy inverse problem was solved by neural network model;
- Conditional generative adversarial networks were implemented to improve representativity of data;
- The proposed approach demonstrates results improvement for full spectra data and noisy data

Thank you for your attention!

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