Peak Detection and Baseline Correction using a Convolution Neural Network

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In memory of Prof. Jan Larsen, 1965–2018

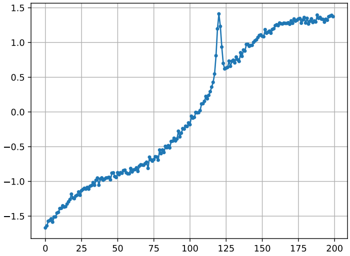
Honory special session Friday 8.30–10.30, organized by
Professor Tülay Adali, University of Maryland Baltimore
Professor Zheng-Hua Tan, Aalborg University

Abstact

- *Peak detection* and *baseline suppression* in a noisy signal with an unknown baseline.
- In practical applications, one of the most *successful* approaches to *joint* baseline suppression and peak localization is based on the *continuous wavelet transform*.
- Reformulate this as a *convolutional neural network*.
- Demonstrate that with sufficient training data, the approach consistently *compares* to (and often outperforms) the *optimized continuous wavelet method*.

Peak detection problem

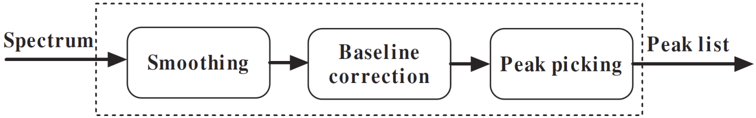
- Peak finding – detect the existence of peak and locate the position.
- Baseline suppression – carry out this task robustly in the presence of a baseline.



Background

Study by Yang et al[1] – compares:

- 7 smoothing methods.
- 5 baseline correction methods.
- 8 peak finding criterions.



- Alternative – joint baseline correction and peak detection/localization.
- "*Results show that CWT provides the best performance*".

[1] Chao Yang, Zengyou He, and Weichuan Yu. "Comparison of public peak detection algorithms for MALDI mass spectrometry data analysis". In: BMC Bioinformatics 10 (2009). DOI: 10.1186/1471-2105-10-4.

Signal model

$$s(f) = b(f) + v(f - f_0) + s \cdot e(f)$$

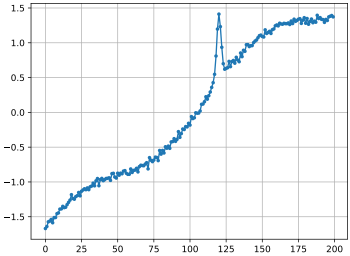
where

$s(f)$: Measured spectrum

$b(f)$: Baseline

$v(f)$: Peak line-shape

$e(f)$: i.i.d Gaussian noise



Continuous wavelet peak localization

The mexican hat wavelet

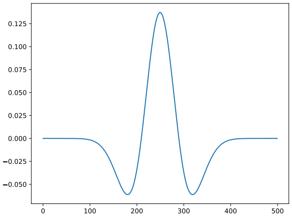
$$\psi_a(f) = \frac{2}{\sqrt{3a}\pi^{1/4}}\left(1 - \frac{f^2}{a^2}\right)\exp\left(-\frac{f^2}{2a^2}\right)$$

Write as a convolutional sum

and pick $c[j]$

$$c[j] = \sum_{f=1}^{W} s[f+j]\psi_a[f]$$

Mexican hat example:



Suppressing the baseline

The continuous wavelet peak localization scheme suppresses a locally smooth baseline, i.e. baseline is modelled as constant plus an odd signal:

$$b(f) = \delta + g(f), g(f) = g(-f)$$

The convolution with the baseline then vanishes:

$$(b * \psi)(f) = \int_{-\infty}^{\infty} b(f')\psi_a(f' - f)\mathrm{d}f' = 0$$

This is due to the CW begin a zero–mean symmetric function.

As a convolution network

1–d convolutional layer:

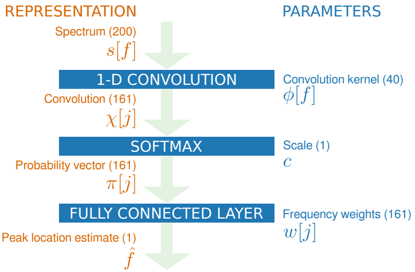
$$\chi[j] = \sum_{f=1}^{W} s[f+j]\phi[f]$$

Softmax layer:

$$\pi[j] = \frac{\exp(c \cdot \chi[j])}{\sum_{k=0}^{F-W} \exp(c \cdot \chi[k])}$$

Linear readout layer:

$$\hat{f} = \sum_{j=0}^{F-W} \pi[j] w[j]$$

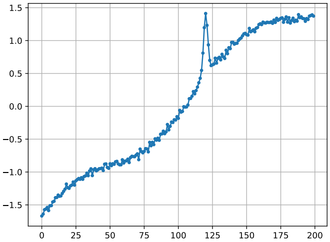


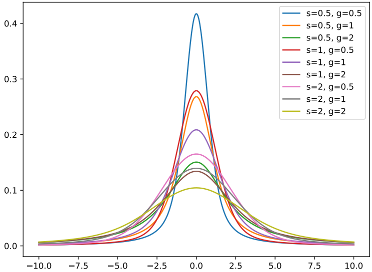
Formulation enables *end–to–end learning*

Data generation

Generate spectra according to our model:
$s(f) = b(f) + v(f - f_0) + s \cdot e(f)$

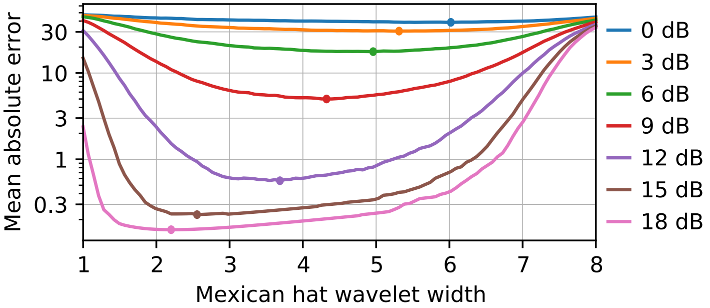
1. Baseline is generated using smoothed Gaussian random walk.
2. Add Voigt shaped peak:
   $v(f) = \frac{1}{\sigma\sqrt{2\pi}} \mathrm{Re}\left[w\left(\frac{f+i\gamma}{\sigma\sqrt{2}}\right)\right]$
3. Add i.i.d Gaussian noise.





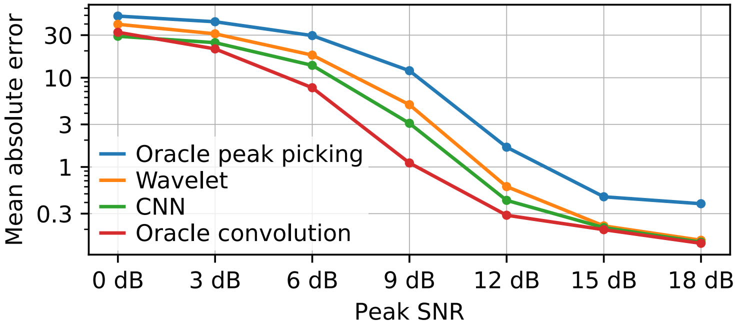
Mexican hat wavelet width

$$\psi_a(f) = \frac{2}{\sqrt{3a}\pi^{1/4}} \left(1 - \frac{f^2}{a^2}\right) \exp\left(-\frac{f^2}{2a^2}\right)$$



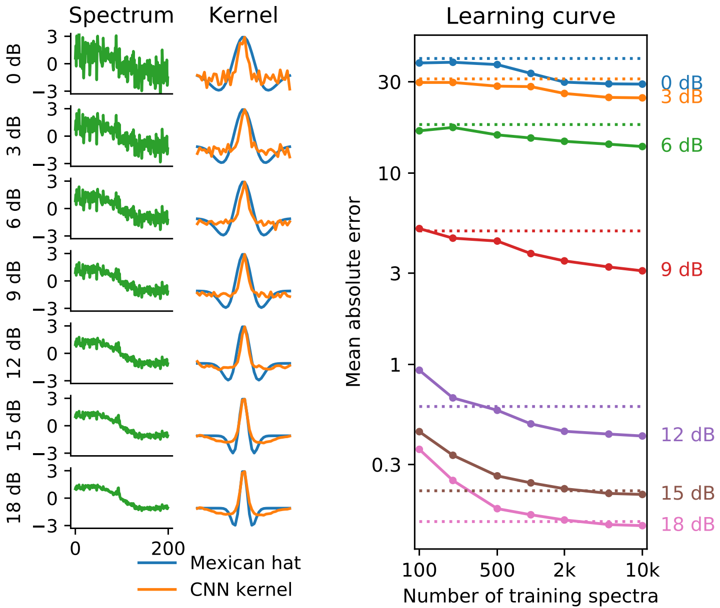
$$\text{Error} = \sum_{i=1}^{N} |f_i - \hat{f}_i|$$

Peak localization



Oracle peak picking: No baseline – pick maximum value.
Oracle convolution: No baseline – convolve with true peak lineshape – pick maximum value.

Learning curves and learned kernels



Limitations and possible extensions

Limitations:

- Spectral peak shape assumed constant.
- Peak signal–to–noise ratio was held constant in any given training.
- It was assumed that a single peak always exists.

Possible extensions:

- Have multiple peak location estimators and endow them with an attention mechanism so that each estimator will focus on a sub-range of frequencies.

Conclusions

The CNN approach to peak localization shows great promise, as it can more *efficiently leverage data* to outperform the current state of the art, and can readily be extended and *incorporated as a module in a larger neural network architecture*.

Thank you