Dimensionality reduction of MALDI Imaging datasets using non-linear redundant wavelet transform-based representations

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- The problem of meaningful reduction
- The sparse representation problem
- Iterative hard thresholding algorithm
- Avoiding local minima
- Results on data compression
- Conclusions
- Future Work

Meaningful reduction

- Mass Spectrometry Imaging (MSI) experiments very often need a reduction in dimensionality
- Meaningless vs. meaningful reduction:

Original message

What your compression algorithm does

Meaningful reduction

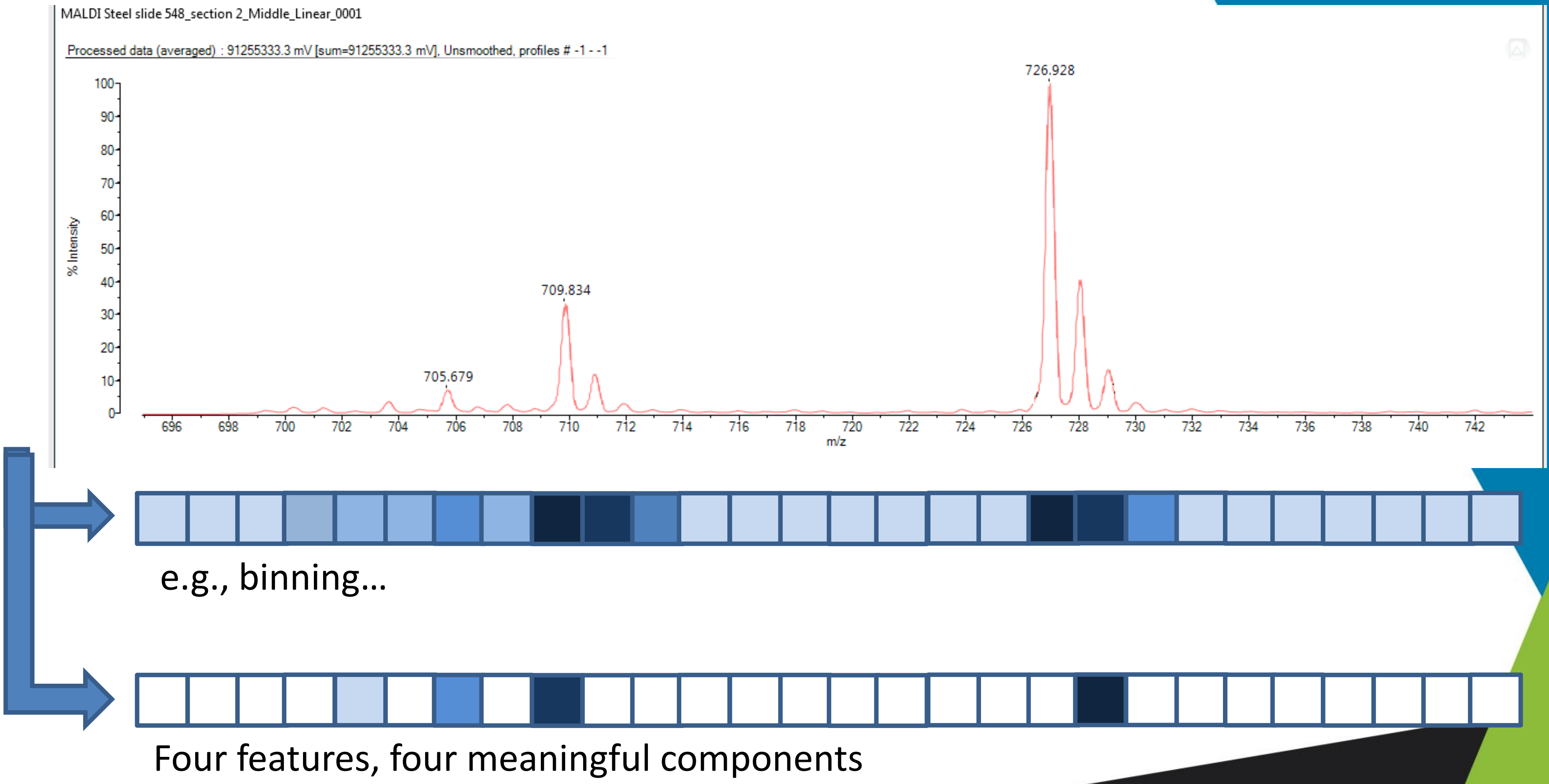
- Mass Spectrometry Imaging (MSI) experiments very often need a reduction in dimensionality
- Meaningless vs. meaningful reduction:

Original message

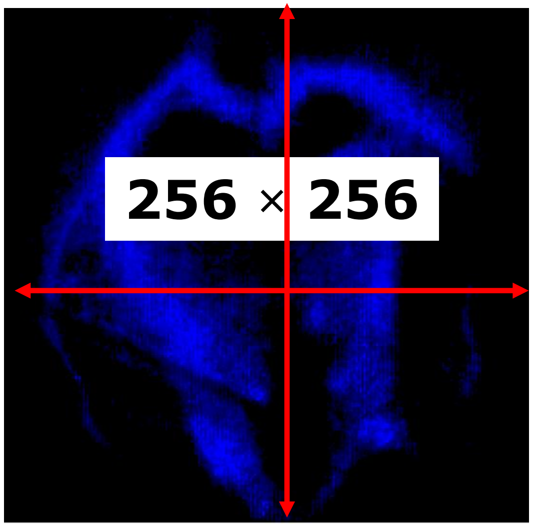
Meaningful compression

Meaningful reduction

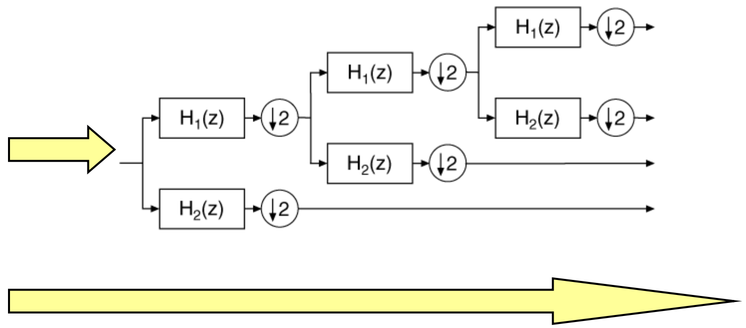
- The target is to have a *sparse* representation

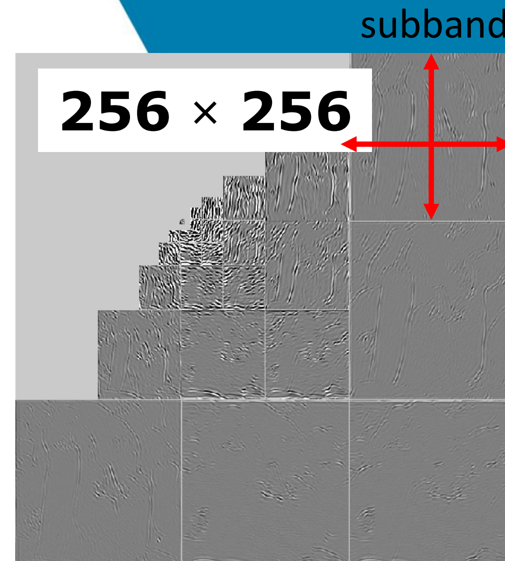


Redundant wavelets



A MALDI image





Wavelet [Mallat 89]*:*

- Well adapted to represent some typical features of the images (scale invariance, local orientations)
- Band-pass, multi-scale, multi-orientation

X-lets** (Redundancy)**:

- Invariance to translation
- Better orientation selectivity
- Better compaction of energy
- Curvelets [Candes *et al* 99], DT-CWT [Kingsbury 01], Steerable Pyramid [Simoncelli et al 92],...

The sparse representation problem

x: A spectrum as a vector of N elements

Φ^T: A MxN linear transformation

M > N
range(Φ^T) = N
Φ^T is a Parseval frame

Are there any solutions in **a** to the equation:

$$\Phi \boldsymbol{a} = \boldsymbol{x} \quad \Rightarrow$$

YES, INFINITE

Solving the **sparse representation problem** means looking for the sparsest solution:

$$\widehat{\boldsymbol{a}} = \min_{a \in R^M} \|\boldsymbol{a}\|_0 \; s.t. \, \Phi \boldsymbol{a} = \boldsymbol{x}$$

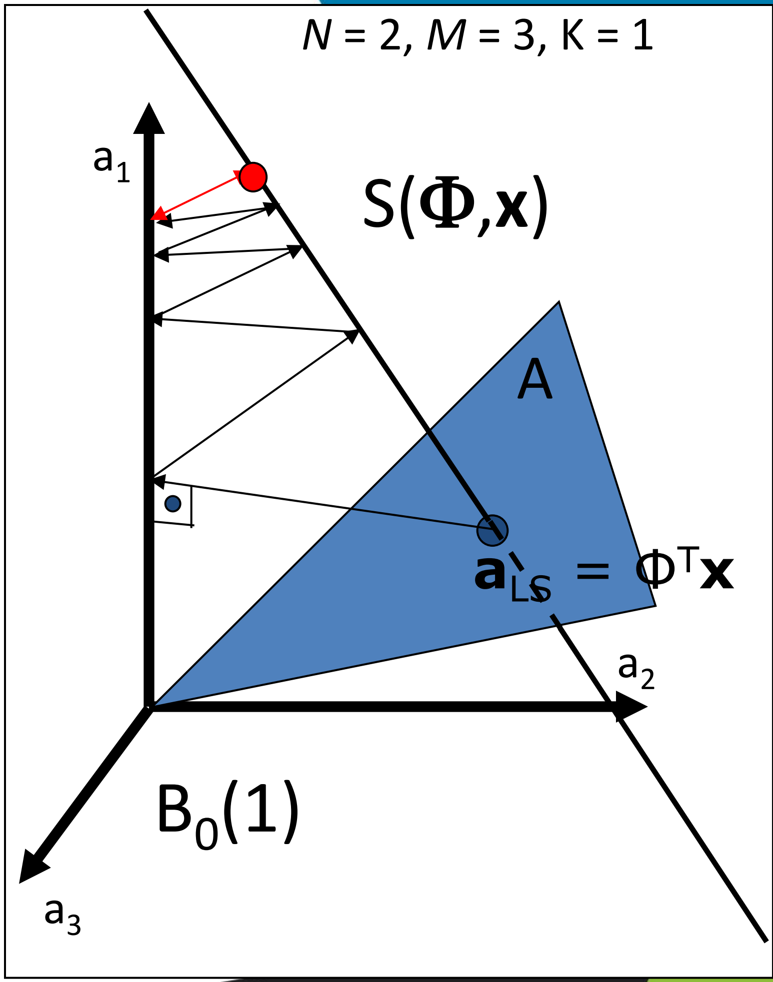
The l0-norm counts the number of non-zero elements in a vector

The sparse representation problem in MSI

- 3 approaches for MSI experiments:
  - **Spectrum-based**
    - Each single spectrum gets compressed independently
  - **Image-based**
    - Each single MALDI image from a selected mass list gets compressed independently
  - **Dataset-based**
    - The whole dataset is represented as a 2D matrix with pixels as rows and selected masses as columns
    - This dataset is compressed as a whole
    - Advantage: Takes into account dependencies across all directions

Iterative hard thresholding

- Example using:
  1. $B_0(1)$: *L*0-ball of dimension 1. All those vectors with just one non-zero element
  2. $S(\mathbf{\Phi},\mathbf{x})$: set of perfect reconstruction



- Alternated orthogonal projections: local minimum of the distance from $B_0(K)$ to $S(\mathbf{\Phi},\mathbf{x})$
  - Convergence can be proved [Blumensath & Davies, 09]

- The solution provides a perfect representation of the input as close as possible to the limits of the *L*0-ball of radius K.

Iterative Hard Thresholding algorithm

1. Set a level of sparseness K
   This is equivalent to setting a threshold Θ

2. Get the minimum energy solution $\mathbf{a}^{(0)} = \mathbf{a}_{LS} = \Phi^T\mathbf{x}$

3. Repeat until convergence:

   1. $\mathbf{b}^{(k+1)} =$ Project $\mathbf{a}^{(k)}$ onto $B_0(K)$:

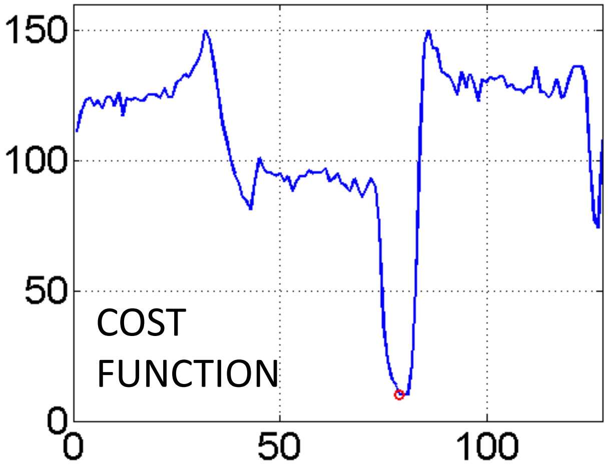
      Set to zero all elements with intensity lower than Θ

   2. Project $\mathbf{b}^{(k+1)}$ onto $S(\mathbf{\Phi},\mathbf{x})$:

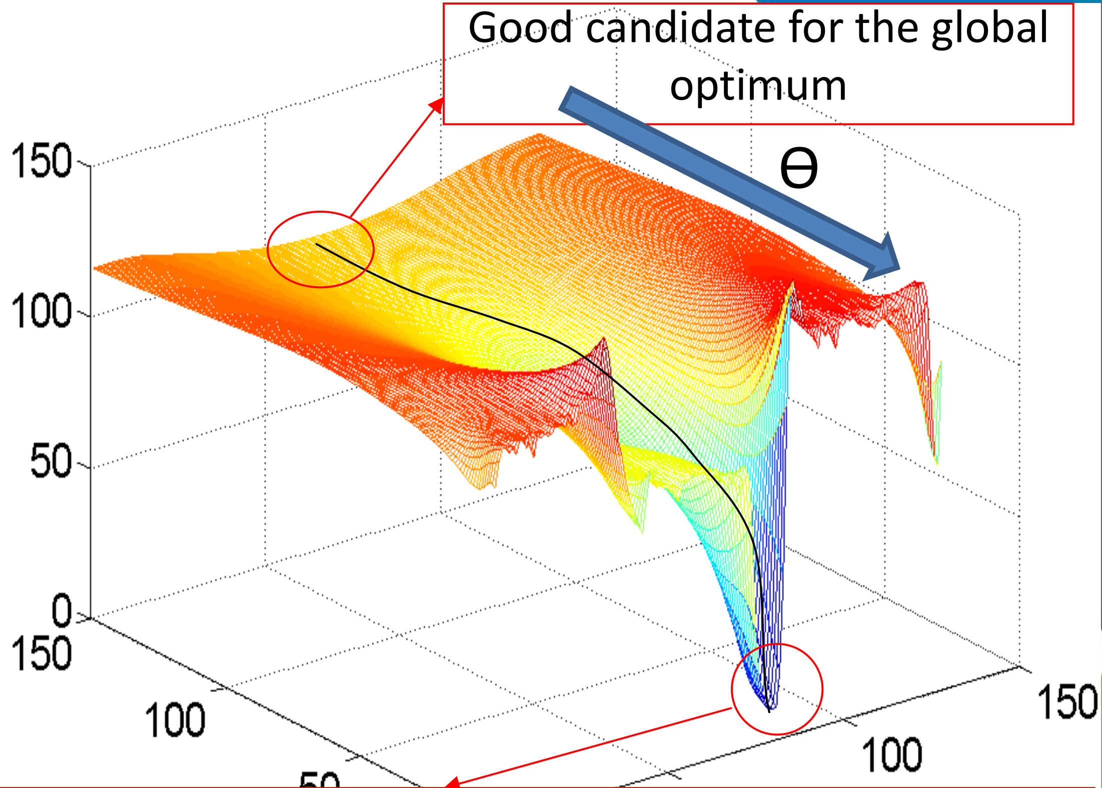
      $\mathbf{a}^{(k+1)} = \mathbf{b}^{(k+1)} + \Phi^T(x - \Phi\, \mathbf{b}^{(k+1)})$

Using dynamic thresholding

Intuitive justification of dynamic thresholding:



Multiple minima:
Difficult global
optimization



Find favourable optima searching from good candidates at higher θs

Compressing single spectra

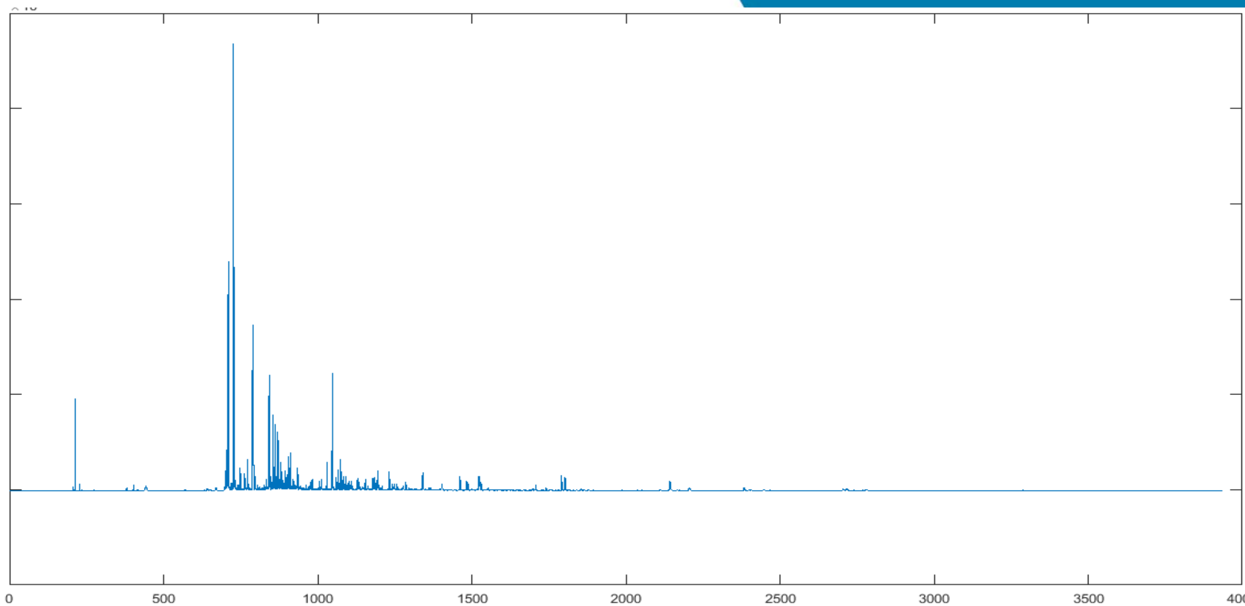
- β = 0.9, Dual-Tree Complex Wavelets, 8 levels, x2 redundancy factor

- Basepeak spectrum from a mouse brain tissue
  - Basepeak spectrum chosen for illustration because it typically shows more number of peaks and is typically more noisy than the ROI spectrum

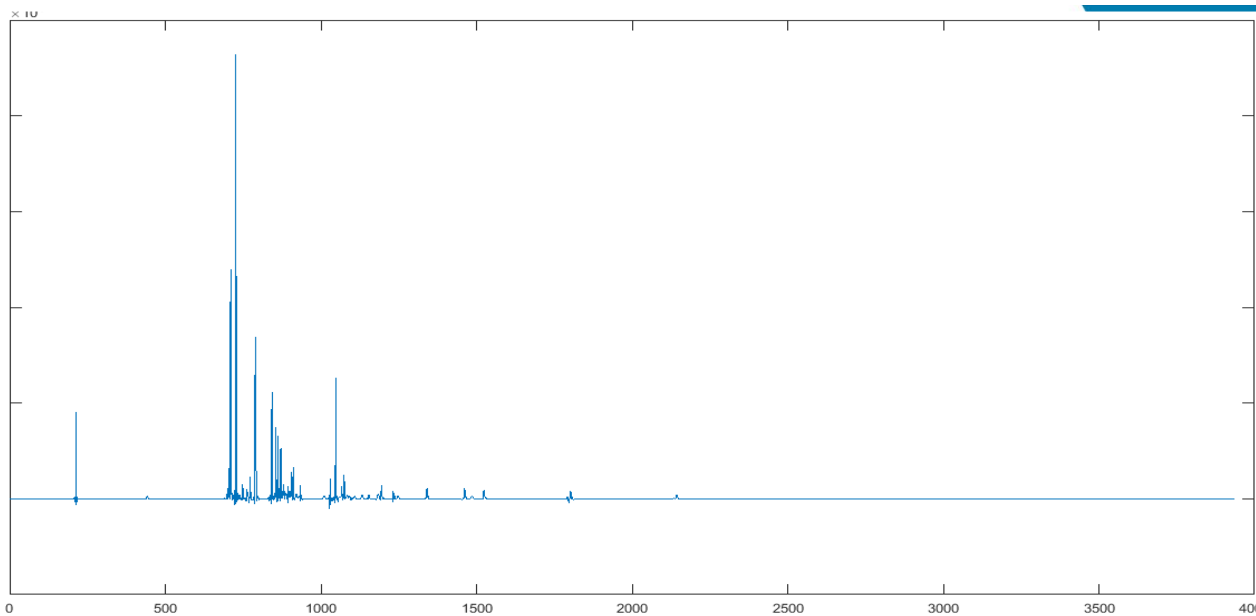
- Results obtained using Matlab™ R2016a on an Intel® Core™ i5-3230 @ 2.60 GHz

Compressing single spectra

Original (179200 data points)

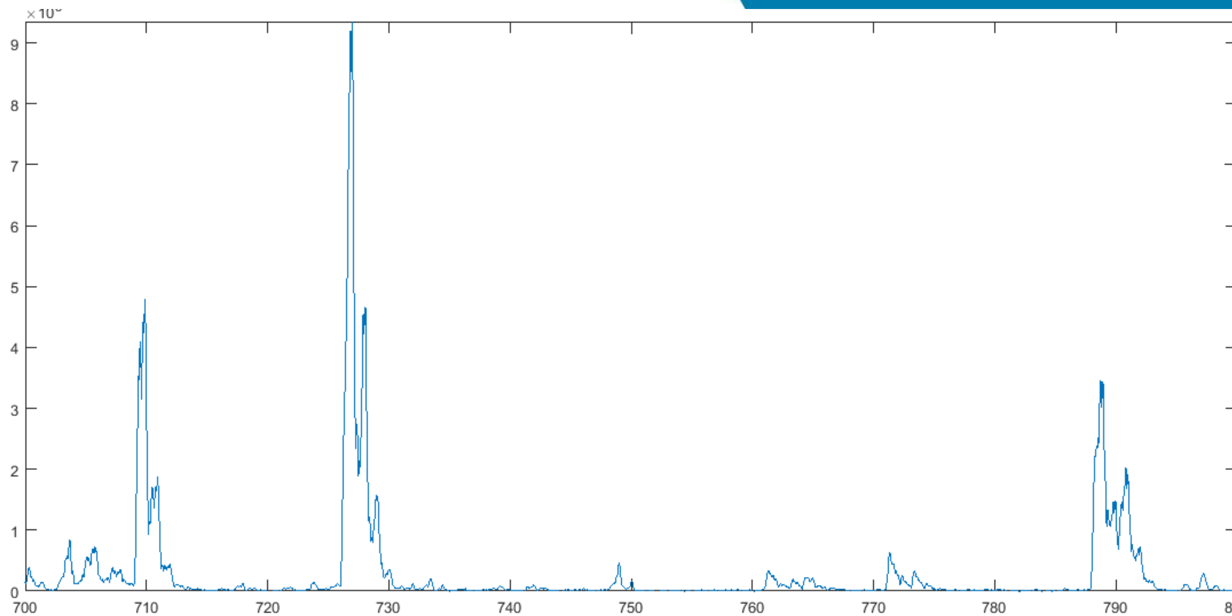


From top 230 wavelet coeffs
(99.87% reduction)



Compressing single spectra

Original (zoomed in to 700-800 Da)



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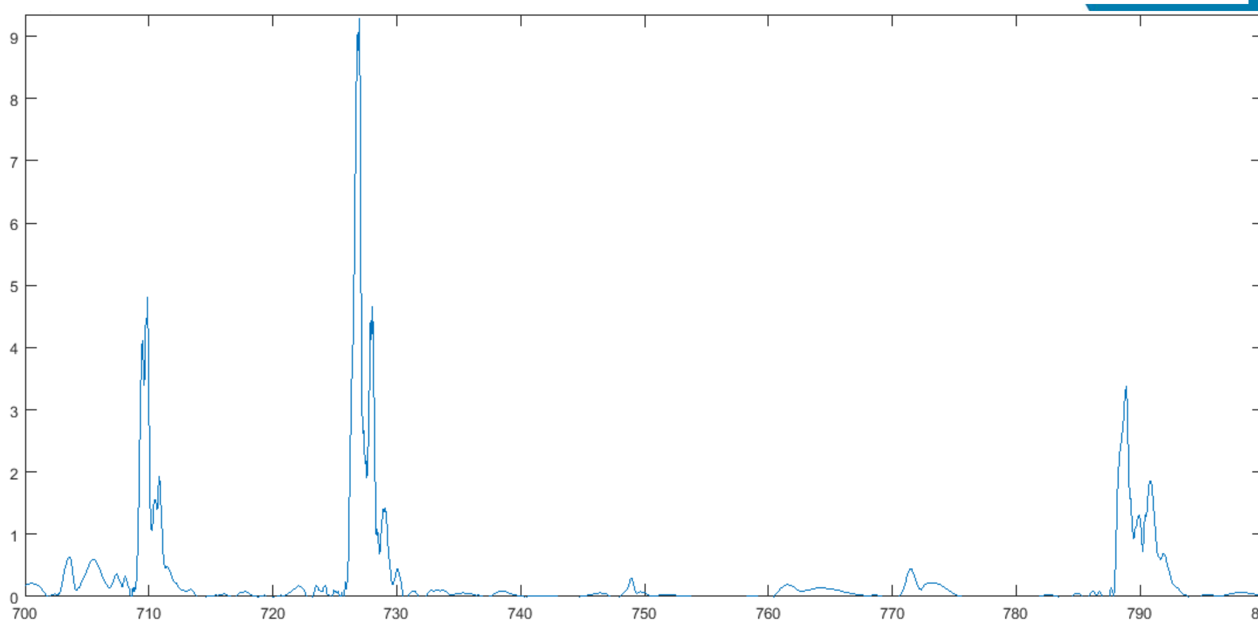

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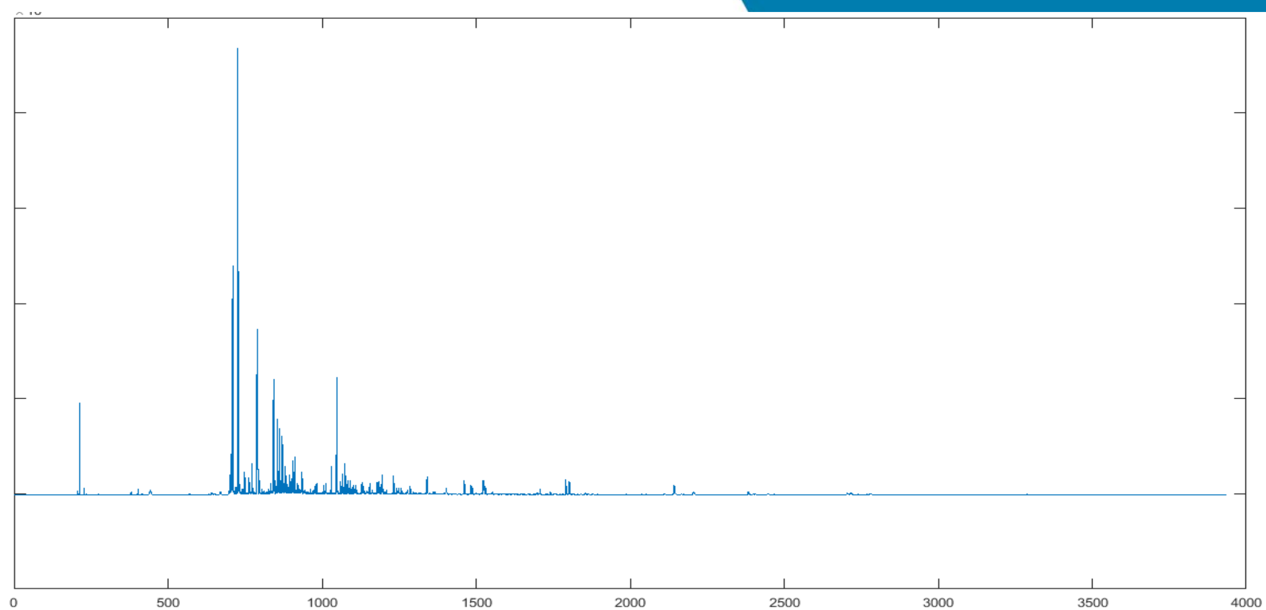
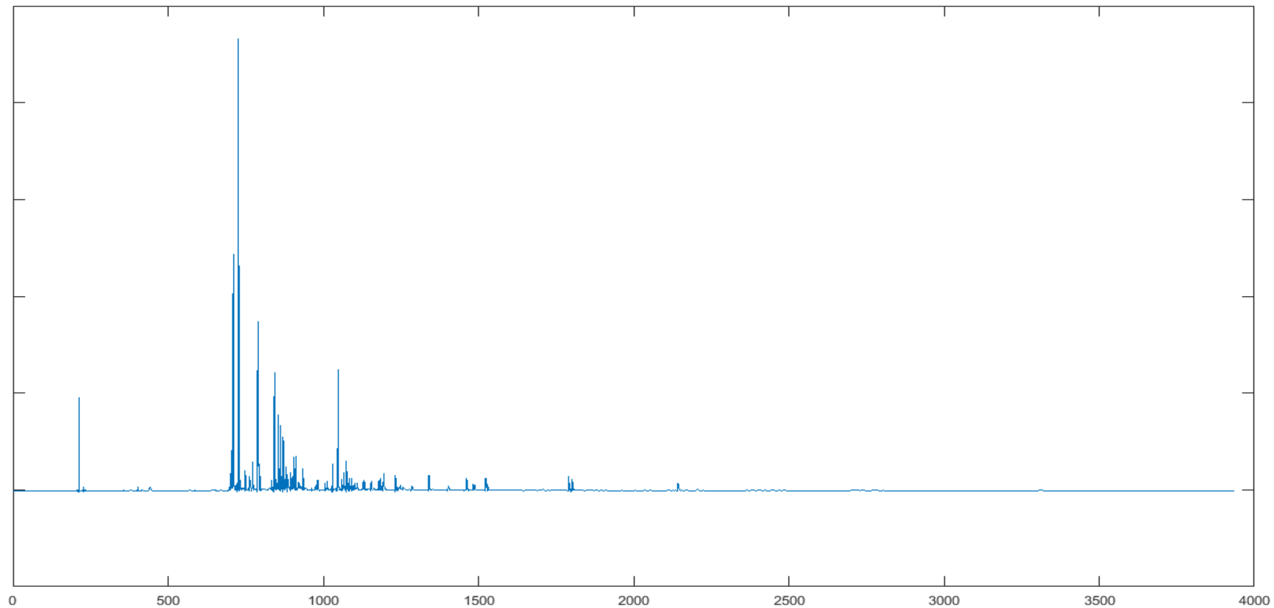


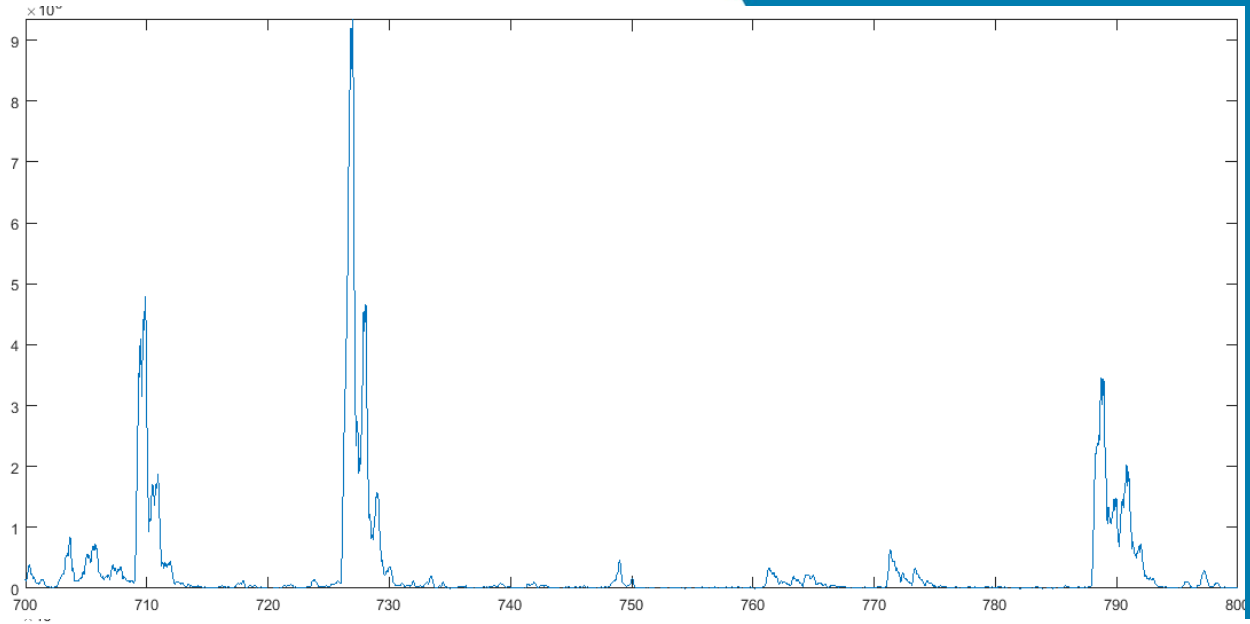
From top 1432 wavelet coeffs

(99.20% reduction)



Compressing single spectra

Original (zoomed in to 700-800 Da)



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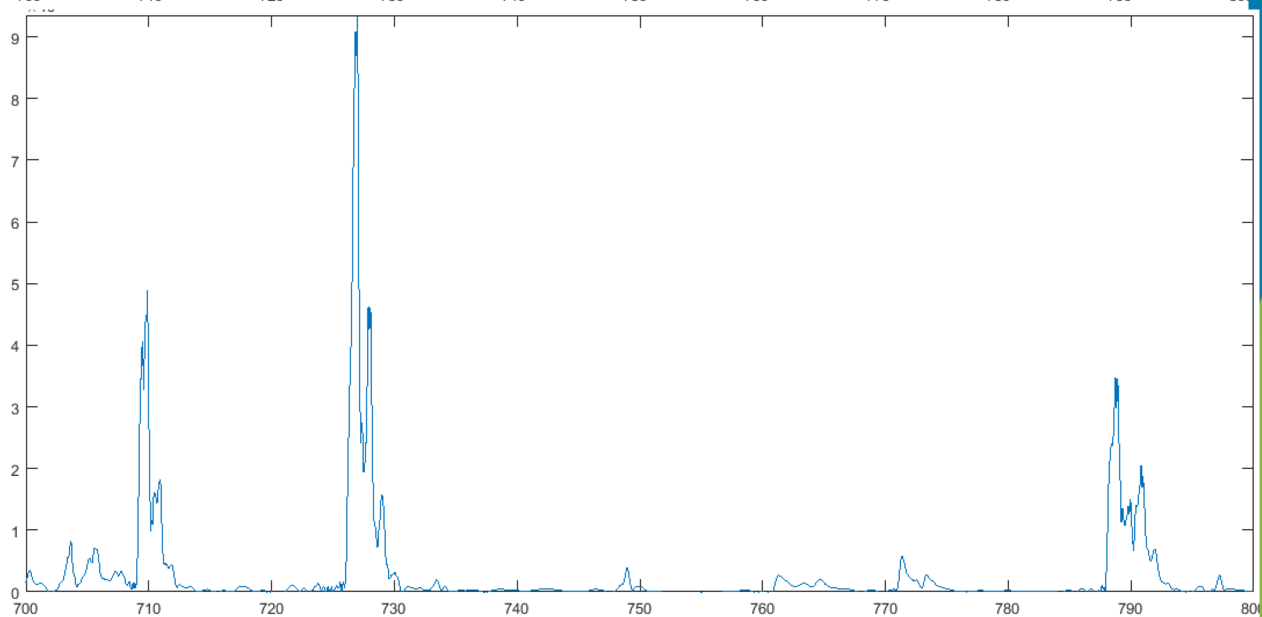
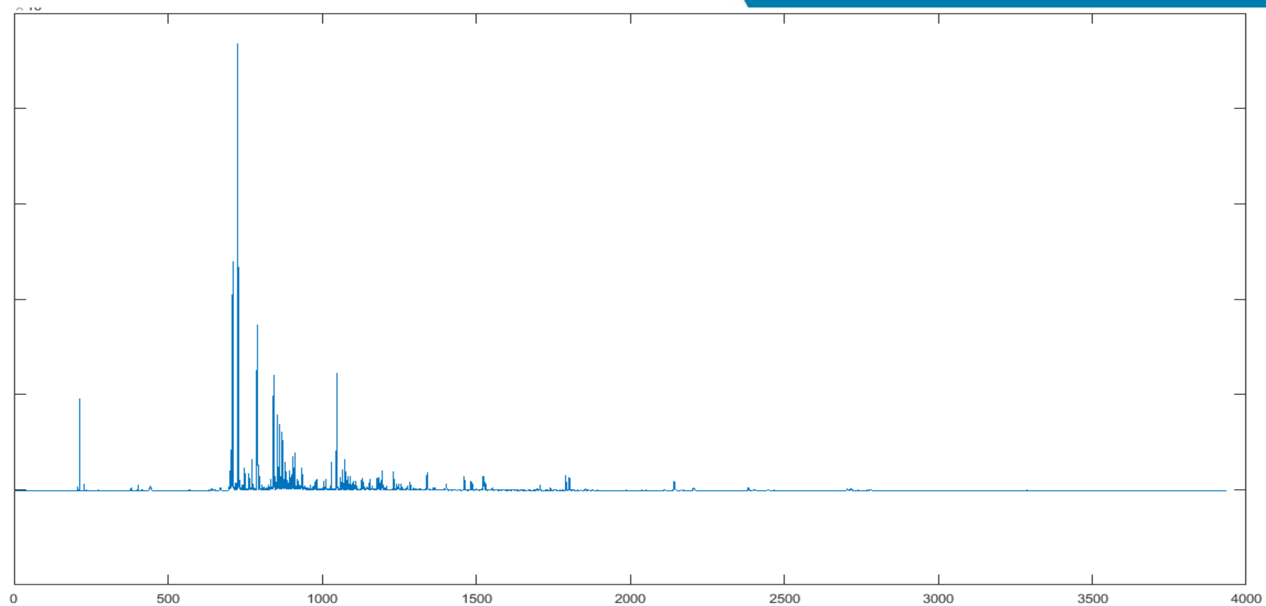


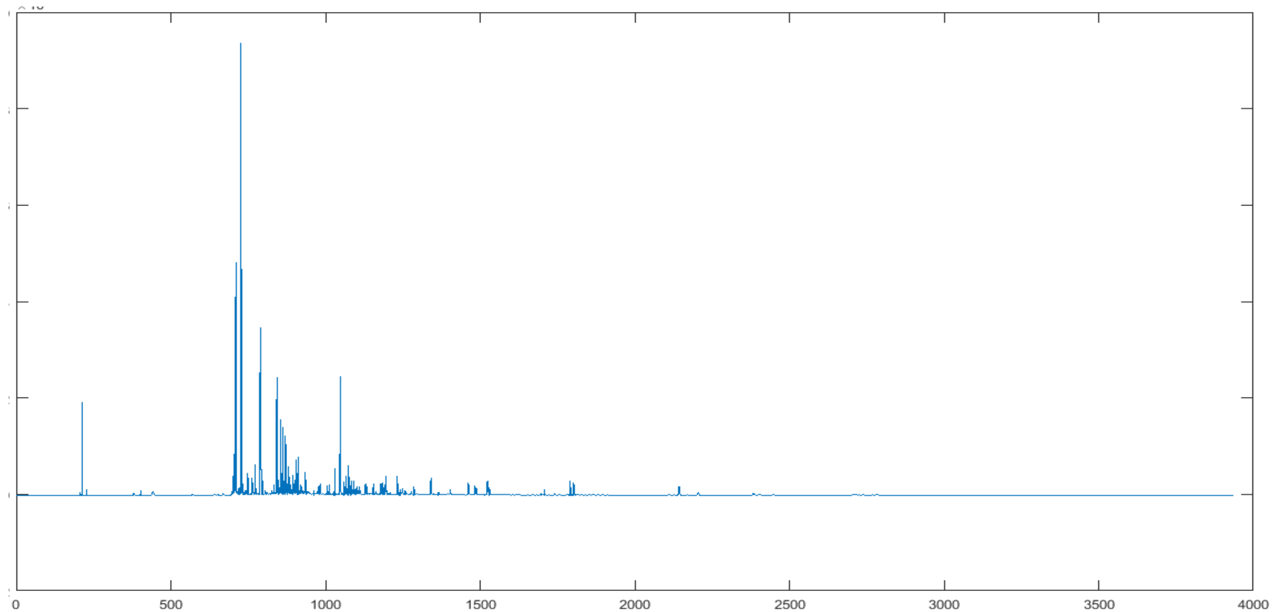
Compressing single spectra

Original (179200 data points)



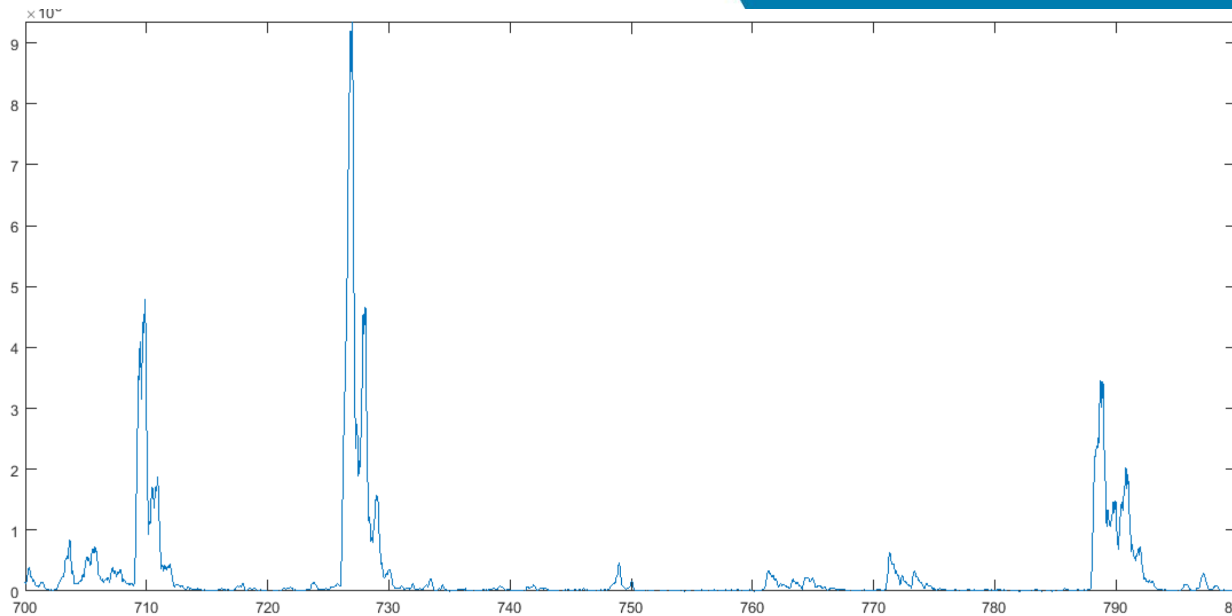
From top 2214 wavelet coeffs

(98.76% reduction)



Compressing single spectra

Original (zoomed in to 700-800 Da)



From top 2214 wavelet coeffs
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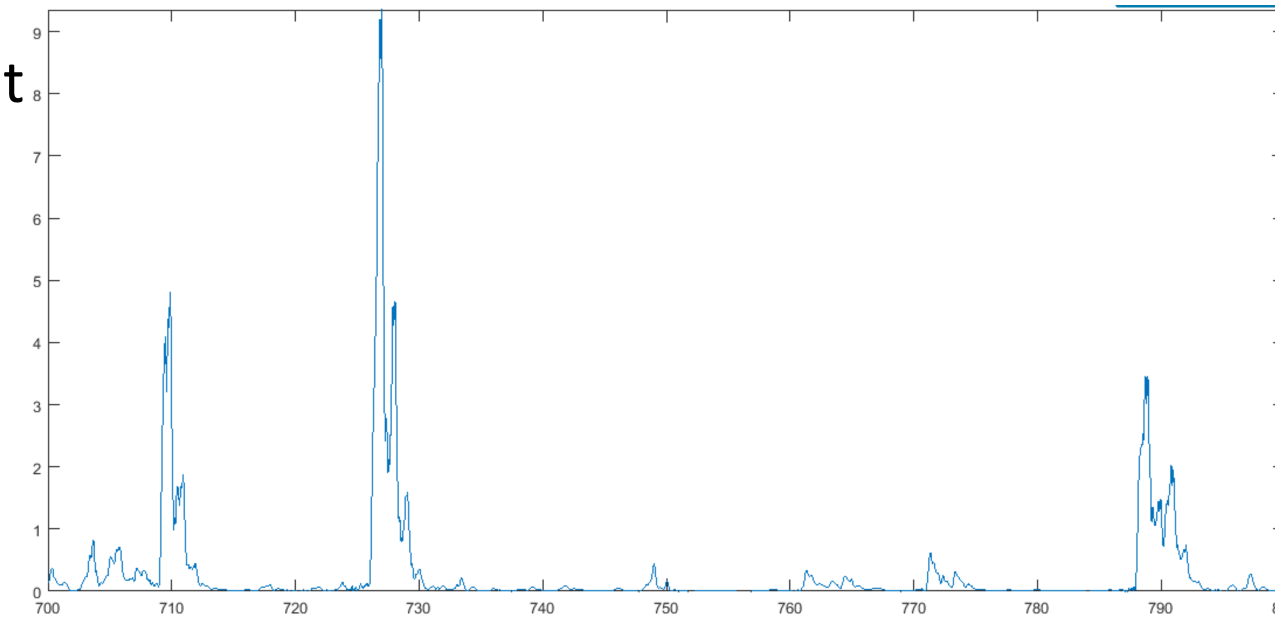
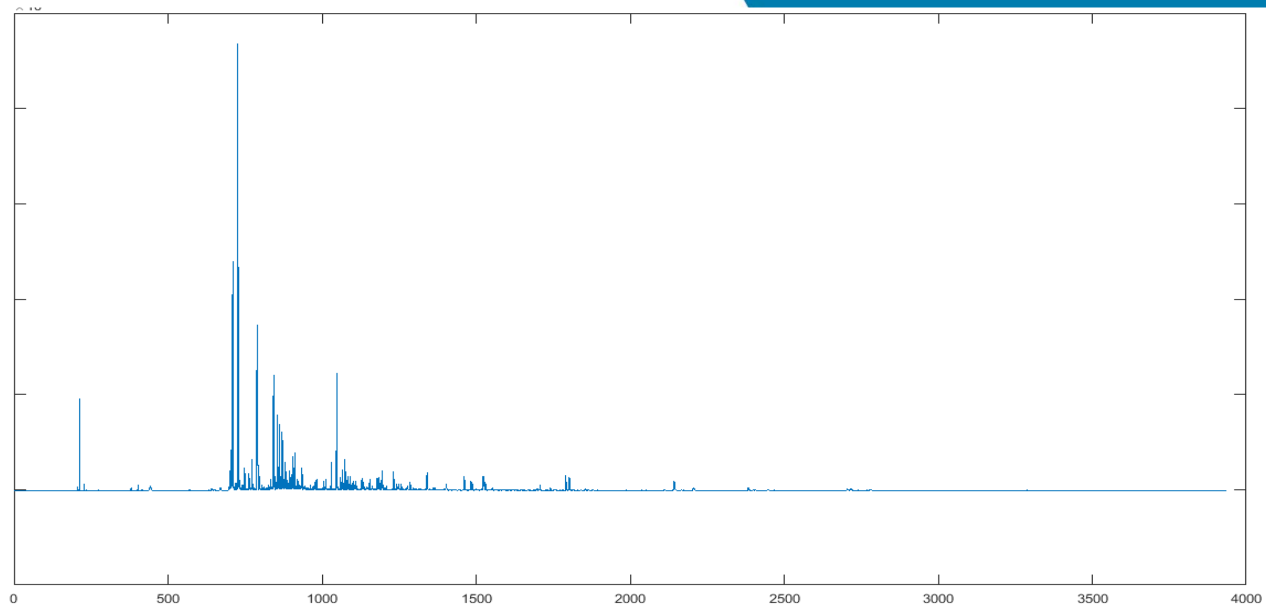


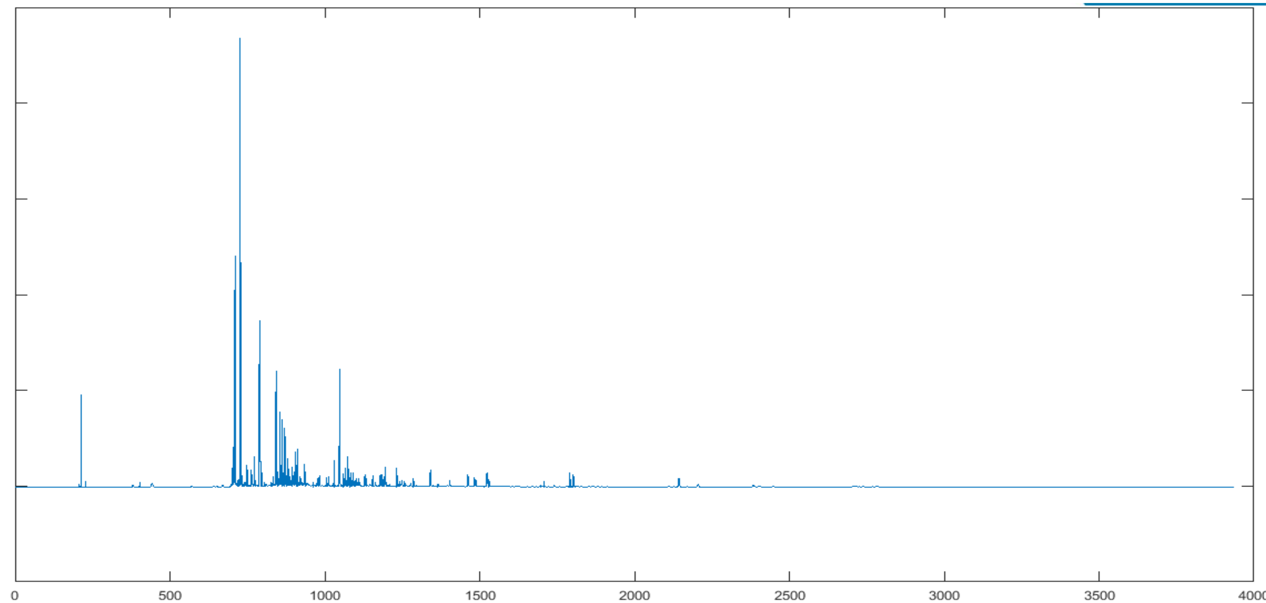
Compressing single spectra

Original (179200 data points)



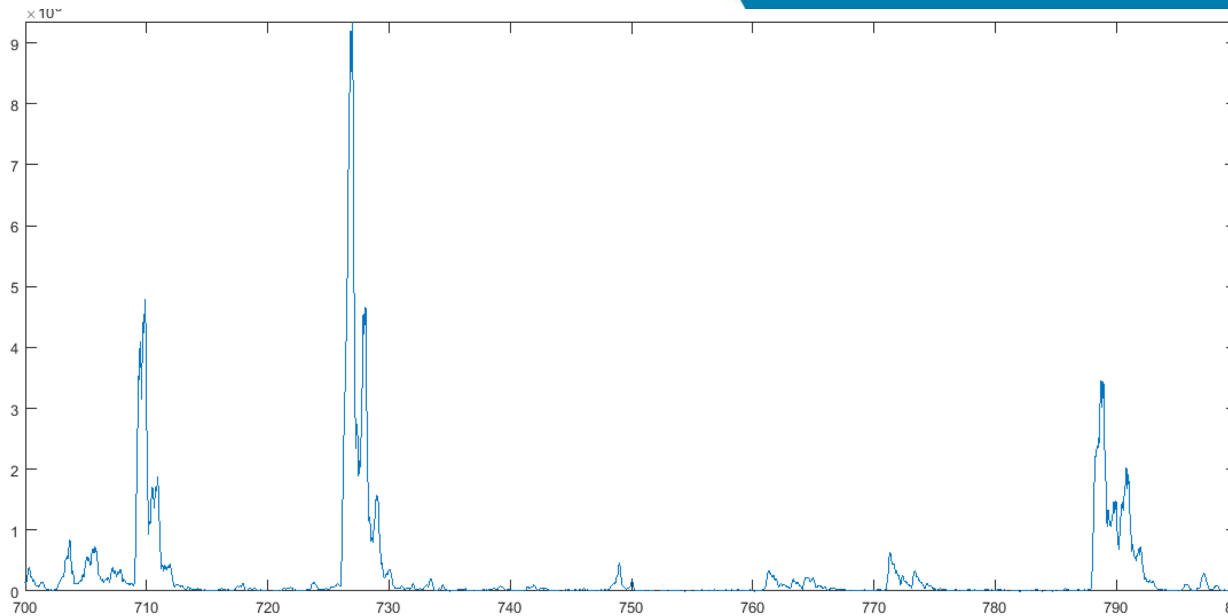
From top 3672 wavelet coeffs

(97.95% reduction)



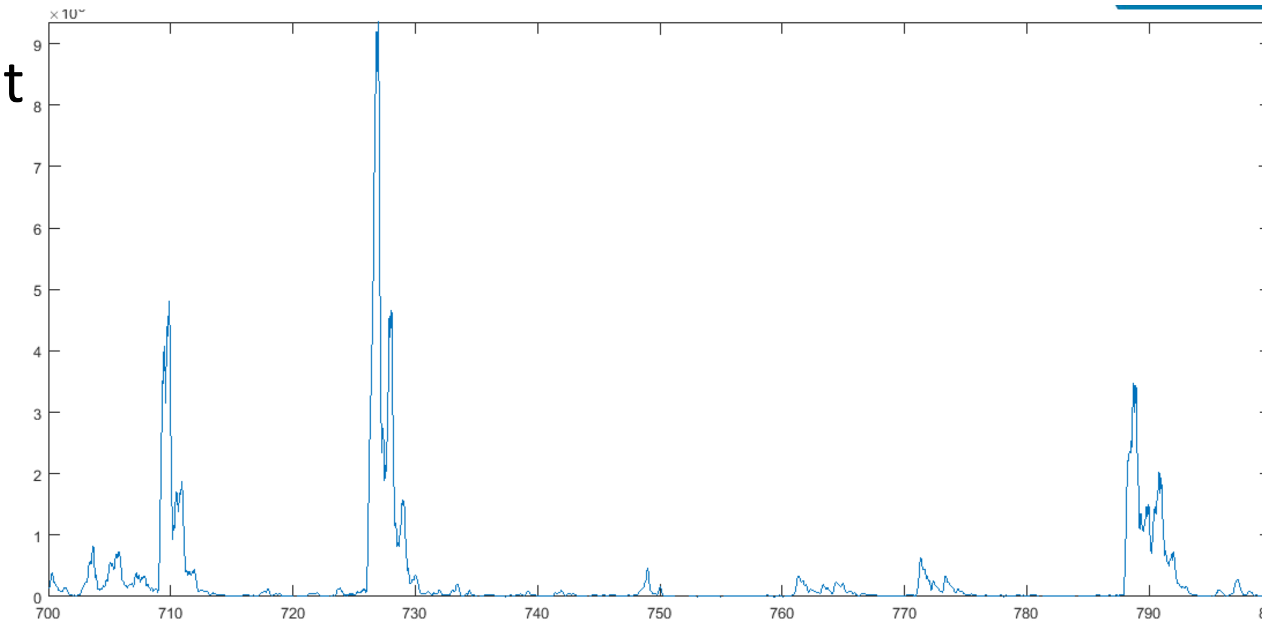
Compressing single spectra

Original (zoomed in to 700-800 Da)



From top 3672 wavelet coeffs

(97.95% reduction)



Compressing all spectra in a dataset

Dataset (ROI)	Number of pixels	Number of data points per pixel	Size in disk (ASCII)	Avg. num of reduced data points	Reduced size in disk (ASCII)	Avg. % of reduction	Avg. accuracy of the representation (MSE)
Mouse brain 1	10397	292,864	35.4 GB	13,718	2.49 GB	92.97%	$2.8 \cdot 10^{-2}$
Mouse brain 2	11976	179,200	24.95 GB	7,780	1.62 GB	95.66%	$2.4 \cdot 10^{-2}$
Mouse brain 3	8976	154,300	16.10 GB	10,452	1.64 GB	93.23%	$1.99 \cdot 10^{-2}$
Averaged	**10450**	**208,788**	**25.48 GB**	**10,650**	**1.91 GB**	**93.95 %**	$\mathbf{2.4 \cdot 10^{-2}}$

Compressing single spectra

- Further compression with traditional algorithms is possible
- Alternative convex relaxation algorithm provides a total average of 89.54%
- Execution time averaged approx. 9 seconds per spectrum on a non-optimised script in Matlab™
  - Win64 Intel® Core™ i5-3230M CPU @ 2.60 GHz
  - Most of the time spent on Analysis/Synthesis operations
- The average compression done image-wise is lower, averaging roughly **75%** for images showing “some” structure

Application to other problems

- Application to other problems need to reformulate the problem to look for the sparsest approximation

- Many applications might also need to redefine the concept of *perfect reconstruction* to that of *compatibility to the observation*

Conclusions

- We have presented a method to find sparse (*compressible*) representations of imaging datasets using redundant wavelet transformations
- The large dictionary forming a redundant wavelet basis provides **meaningful representation** of features in relatively few number of coefficients
- We have applied the **Iterative Hard Thresholding algorithm**, shown previously to be superior to other alternatives to find sparse representations [Blumensath & Davies 08, Mancera & Portilla 08]
- We have used a technique inspired by simulated annealing to **avoid local minima** of the non-convex quasi-norm used in the cost function and remove the need to estimate the level of sparsity required
- Results show **high compression ratios**, with increasingly better approximations as more coefficients are used

Future work

- Need to speed up the iterations
  - Approaches to reduce the number of iterations needed
  - Code optimisation
- Adaptive threshold strategy
  - Deal differently with different mass range
- Potential applications include:
  - Spectra smoothing
  - Peak detection
  - Image denoising
  - Restoration after vector quantization
  - Improving image resolution
  - Mutivariate analysis
  - …

Thanks for your attention!

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