Supplementary Information

Contents

Title

Exploring AdaBoost and Random Forests machine learning approaches for infrared pathology on unbalanced data sets

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Data and source code availability

The data and MATLAB source code used in this study, and to generate this document, is freely available from the Zenodo data repository here: http://doi.org/10.5281/zenodo.4730312

This document uses *ChiToolbox* to pre-process data and generate figures. ChiToolbox is available here: http://bitbucket.org/AlexHenderson/chitoolbox

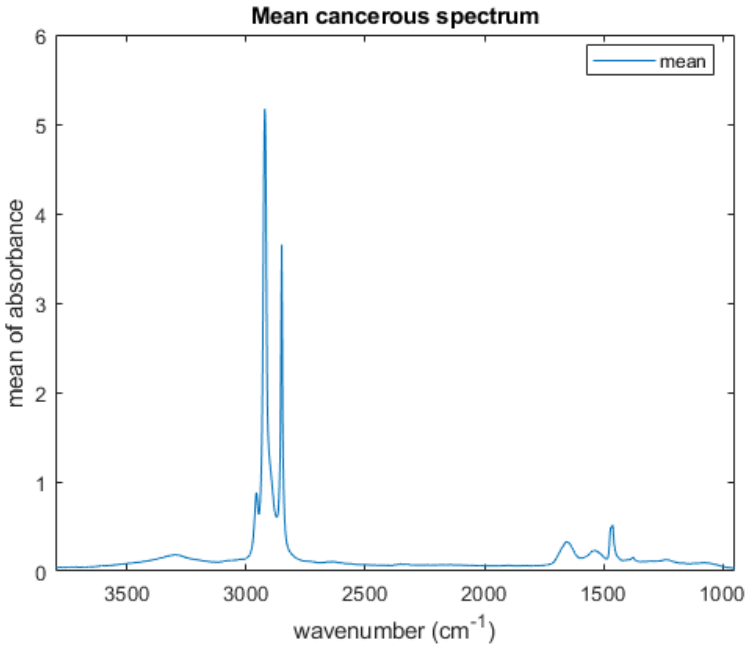
Define plotting options

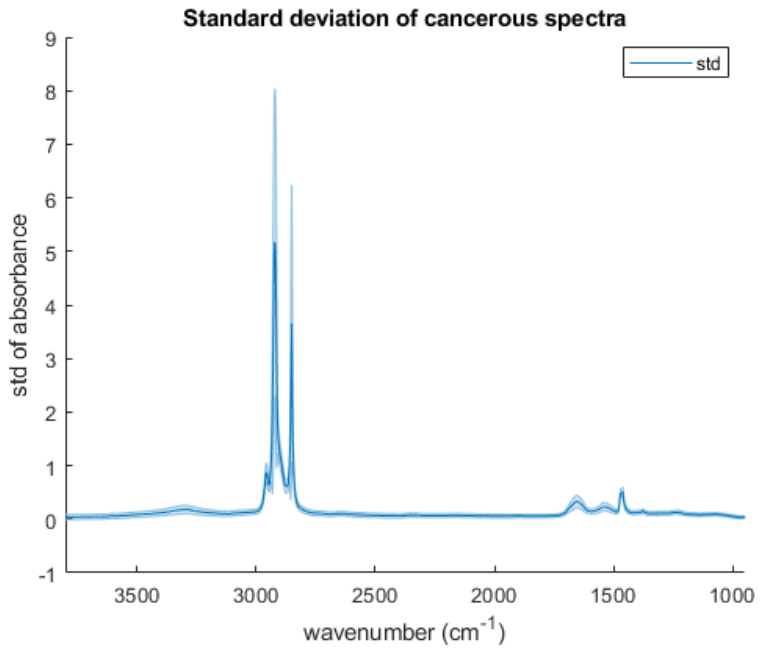
```
showplots = true;
```

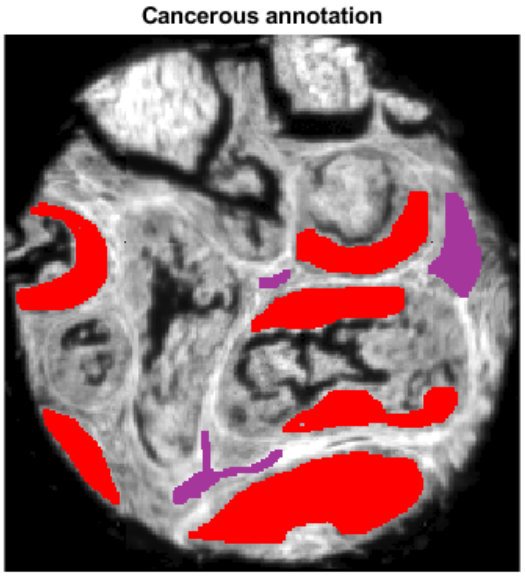
File D8.mat contains FTIR spectra from core id D8 and corresponds to a cancerous tissue core

```
% Read cancerous core spectra into memory
d8mat = load('D8.mat');

% Create a ChiIRSpectralCollection object containing the core's data
d8spectra = ChiIRSpectralCollection(d8mat.wavenumbers,d8mat.spectra);

% Read cancerous core tissue annotation into a ChiImageFile object
d8png = ChiImageFile('D8.png');

% Make space in memory for 3D array of cancerous core data
d8data = zeros(d8png.height * d8png.width, d8spectra.numchannels);

% Insert cancerous spectra into correct locations in the 3D array
d8data(d8mat.indices,:) = d8spectra.data;

% Convert 3D array into a ChiIRImage hyperspectral image object
d8image = ChiIRImage(d8mat.wavenumbers,d8data,d8png.width,d8png.height);


% Define colour of a 'red' pixel
redpixel = [255,0,0]; % RGB

% Identify 'red' pixels in the annotation
d8redmask = d8png.createmask(redpixel);

% Extract 'red' pixel spectra into a ChiIRSpectralCollection object
d8redspectra = d8image.applymask(d8redmask);


% Define colour of a 'purple' pixel
purplepixel = [165,55,156]; % RGB

% Identify 'purple' pixels in the annotation
d8purplemask = d8png.createmask(purplepixel);
```

```
% Extract 'purple' pixel spectra into a ChiIRSpectralCollection object
d8purplespectra = d8image.applymask(d8purplemask);

% Show plots if requested
if showplots
    % Mean spectrum
    d8spectra.plot('mean', 'title','Mean cancerous spectrum')

    % Standard deviation of spectra
    d8spectra.plot('std', 'title','Standard deviation of cancerous spectra')

    % Annotation
    d8png.display('title','Cancerous annotation')
end
```

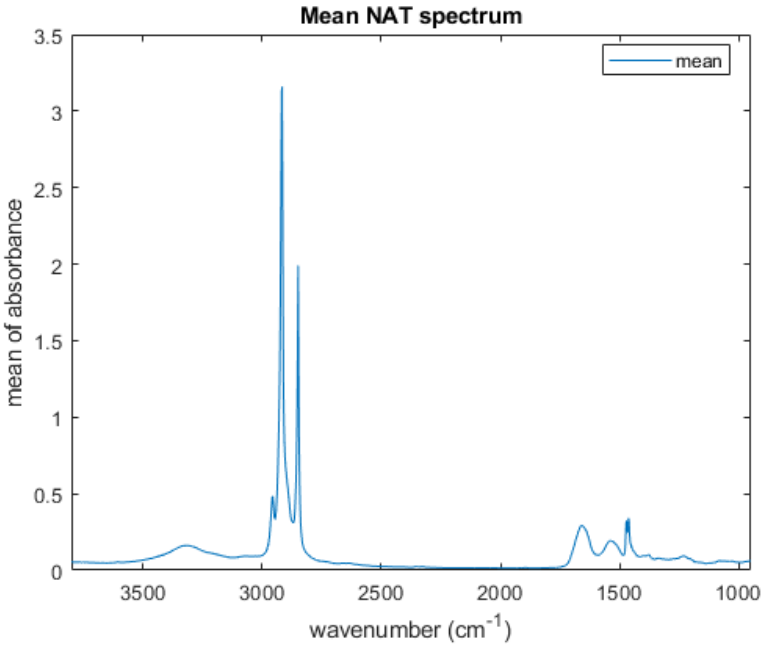


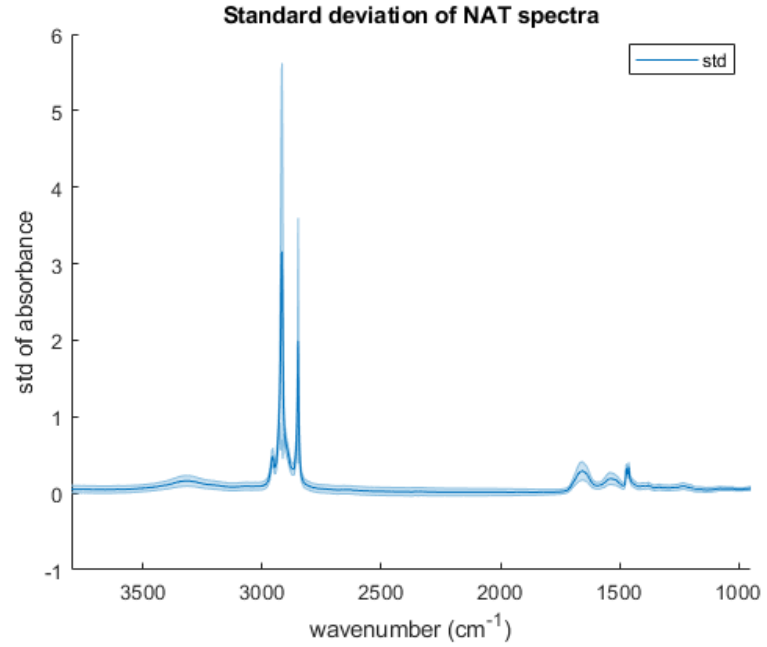


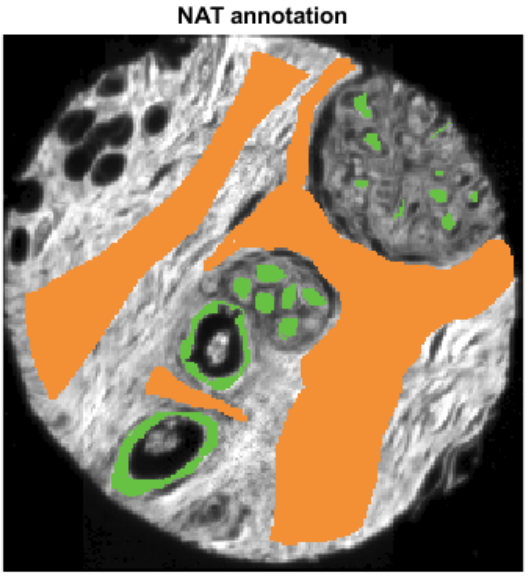


File M4.mat contains FTIR spectra from core id M4 and corresponds to a normal associated tissue core

```
% Read NAT core spectra into memory
m4mat = load('M4.mat');

% Create a ChiIRSpectralCollection object containing the core's data
m4spectra = ChiIRSpectralCollection(m4mat.wavenumbers,m4mat.spectra);

% Read NAT core tissue annotation into a ChiImageFile object
m4png = ChiImageFile('M4.png');

% Make space in memory for 3D array of NAT core data
m4data = zeros(m4png.height * m4png.width, m4spectra.numchannels);

% Insert NAT spectra into correct locations in the 3D array
m4data(m4mat.indices,:) = m4spectra.data;

% Convert 3D array into a ChiIRImage hyperspectral image object
m4image = ChiIRImage(m4mat.wavenumbers,m4data,m4png.width,m4png.height);

% Define colour of a 'green' pixel
greenpixel = [103,193,66]; % RGB

% Identify 'green' pixels in the annotation
m4greenmask = m4png.createmask(greenpixel);

% Extract 'green' pixel spectra into a ChiIRSpectralCollection object
m4greenspectra = m4image.applymask(m4greenmask);

% Define colour of an 'orange' pixel
orangepixel = [243,143,53]; % RGB

% Identify 'orange' pixels in the annotation
m4orangemask = m4png.createmask(orangepixel);

% Extract 'orange' pixel spectra into a ChiIRSpectralCollection object
m4orangespectra = m4image.applymask(m4orangemask);

% Show plots if requested
if showplots
    % Mean spectrum
    m4spectra.plot('mean', 'title','Mean NAT spectrum')

    % Standard deviation of spectra
    m4spectra.plot('std', 'title','Standard deviation of NAT spectra')

    % Annotation
    m4png.display('title','NAT annotation')
end
```

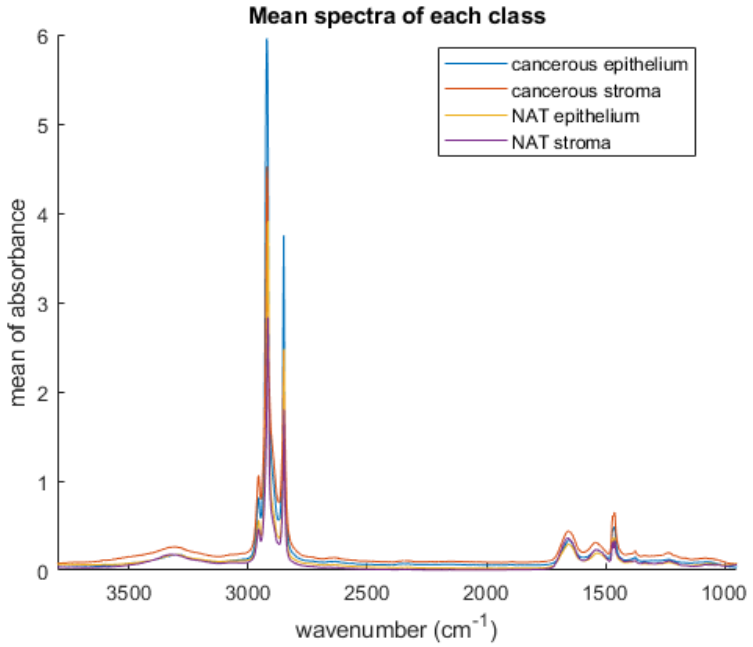

Mean NAT spectrum
mean
mean of absorbance
wavenumber (cm-1)
3500
3000
2500
2000
1500
1000
0
0.5
1
1.5
2
2.5
3
3.5

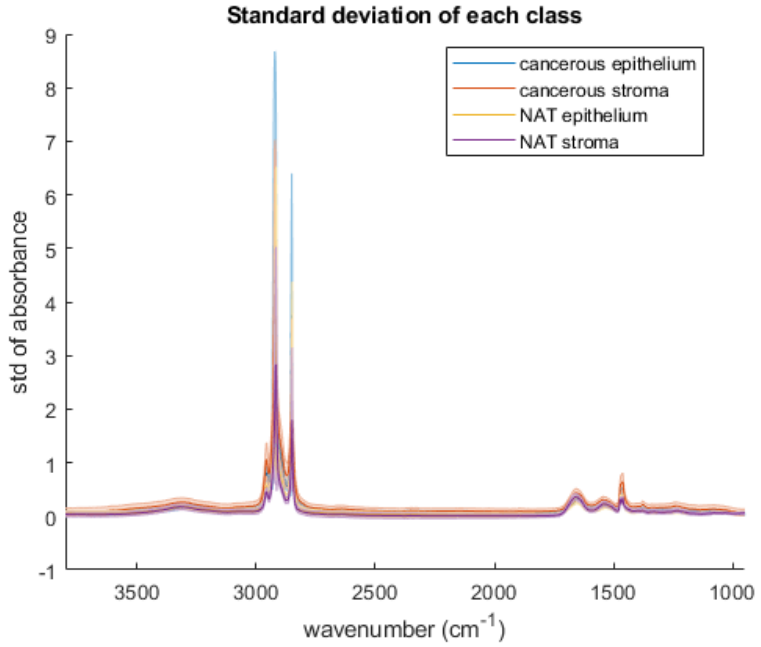

Standard deviation of NAT spectra
std
std of absorbance
wavenumber (cm-1)
3500
3000
2500
2000
1500
1000
-1
0
1
2
3
4
5
6



Pool data

```
% Create a ChiIRSpectralCollection ojbect to hold the pooled data
annotatedpixels = ChiIRSpectralCollection;

% Append each annotated region to this object
annotatedpixels.append(d8redspectra);
annotatedpixels.append(d8purplespectra);
annotatedpixels.append(m4greenspectra);
annotatedpixels.append(m4orangespectra);

% Generate a ChiClassMemberhip object containing labels for each spectrum
labels = ChiClassMembership('annotation', ...
                        'cancerous epithelium',d8redspectra.numspectra, ...
                        'cancerous stroma',d8purplespectra.numspectra, ...
                        'NAT epithelium',m4greenspectra.numspectra, ...
                        'NAT stroma',m4orangespectra.numspectra);

% Attach the labels to the data
annotatedpixels.classmembership = labels;

% Show plots if requested
if showplots
    % Mean spectra of each class
    annotatedpixels.plot('mean', 'byclass', 'title','Mean spectra of each class')

    % Standard deviation of each class
    annotatedpixels.plot('std', 'byclass', 'title','Standard deviation of each class')
end
```

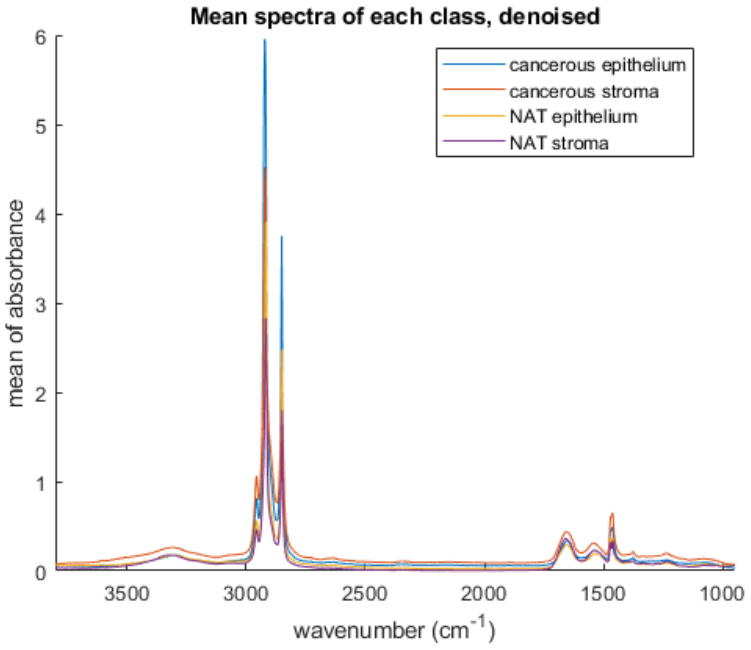


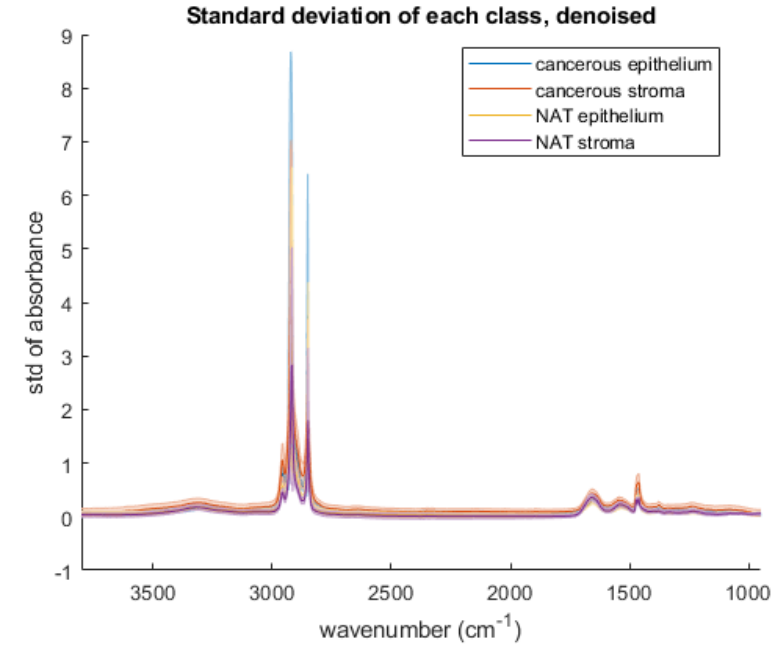


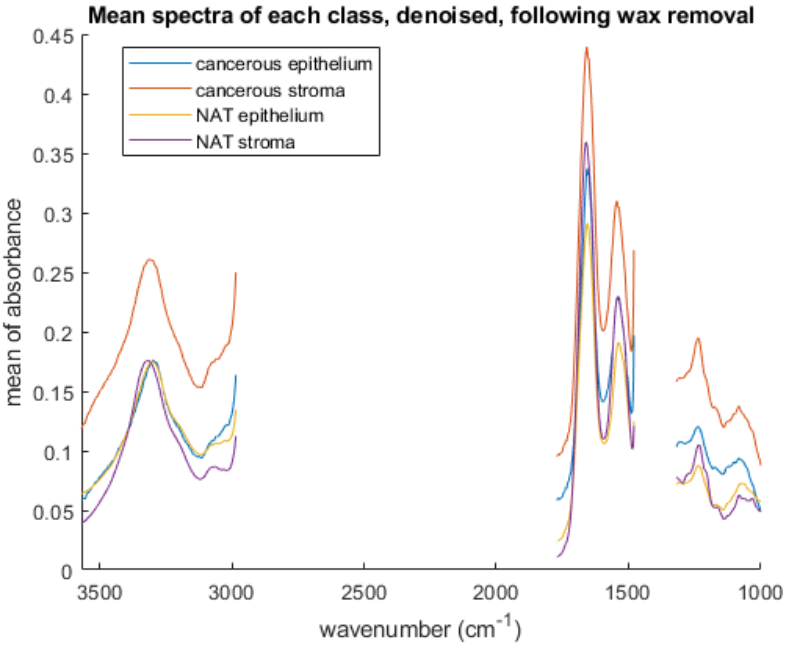
Pre-processing

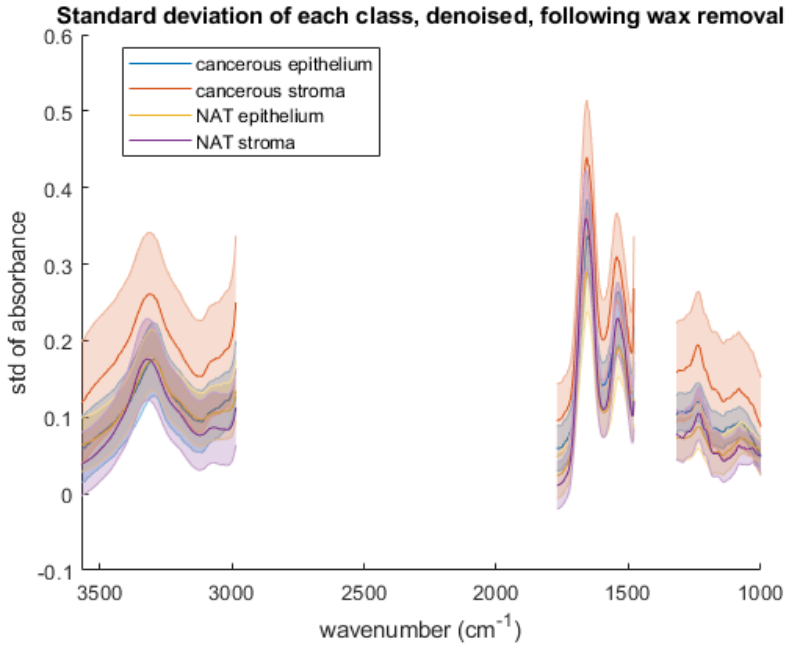
```
% Perform PCA denoising, retaining 80 principal components
annotatedpixels.denoise(80);

% Show plots if requested
if showplots
    % Mean spectra of each class, denoised
    annotatedpixels.plot('mean', 'byclass', 'title','Mean spectra of each class, denoised')

    % Standard deviation of each class, denoised
    annotatedpixels.plot('std', 'byclass', 'title','Standard deviation of each class, denoised')
end

% Remove spectral regions heavily influenced by the paraffin wax embedding
% material
annotatedpixels = annotatedpixels.keeprange(1000,1319, 1481,1769, 2986,3569);

% Show plots if requested
if showplots
    % Mean spectra of each class, denoised, following wax removal
    annotatedpixels.plot('mean', 'byclass', 'title','Mean spectra of each class, denoised, following wax removal')

    % Standard deviation of each class, denoised, following wax removal
    annotatedpixels.plot('std', 'byclass', 'title','Standard deviation of each class, denoised, following wax removal')
```

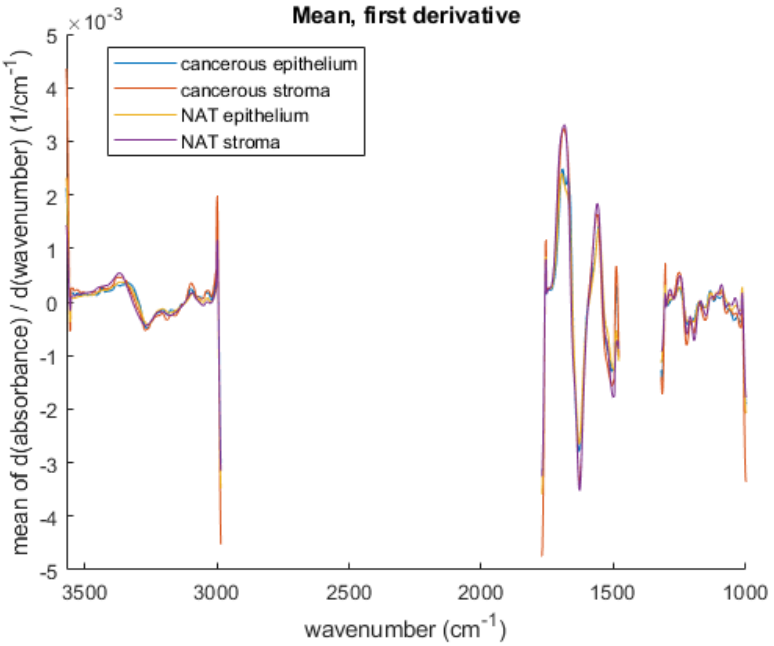
```
end

% Perform fourth-order polynomial Savitzky-Golay first derivative with
% window size of 19
annotatedpixels.firstderiv(19);

% Show plots if requested
if showplots
    % Mean spectra of first derivative of each class, denoised, following
    % wax removal
    annotatedpixels.plot('mean', 'byclass', 'title','Mean, first derivative')

    % Standard deviation of first derivative of  each class, denoised,
    % following wax removal
    annotatedpixels.plot('std', 'byclass', 'title','Standard deviation, first derivative')
end

% Remove regions of the spectra influenced by the ends of the spectral
% regions
annotatedpixels = annotatedpixels.keeprange(1019,1300, 1500,1750, 3005,3550);

% Show plots if requested
if showplots
    % Mean spectra of first derivative of each class, denoised, following
    % wax removal, with end regions removed
    annotatedpixels.plot('mean', 'byclass', 'title','Mean, first derivative, trimmed')

    % Standard deviation of first derivative of  each class, denoised,
    % following wax removal, with end regions removed
    annotatedpixels.plot('std', 'byclass', 'title','Standard deviation, first derivative, trimmed')
end
```

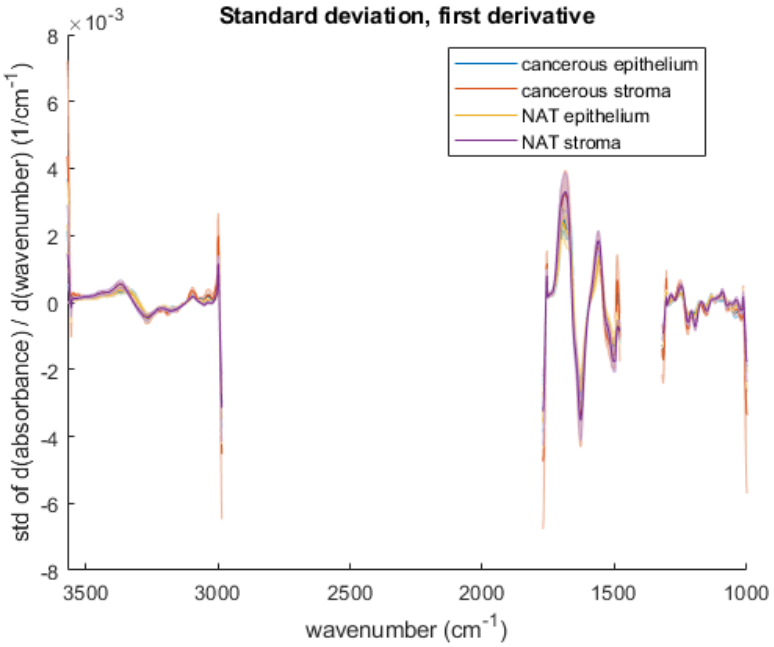


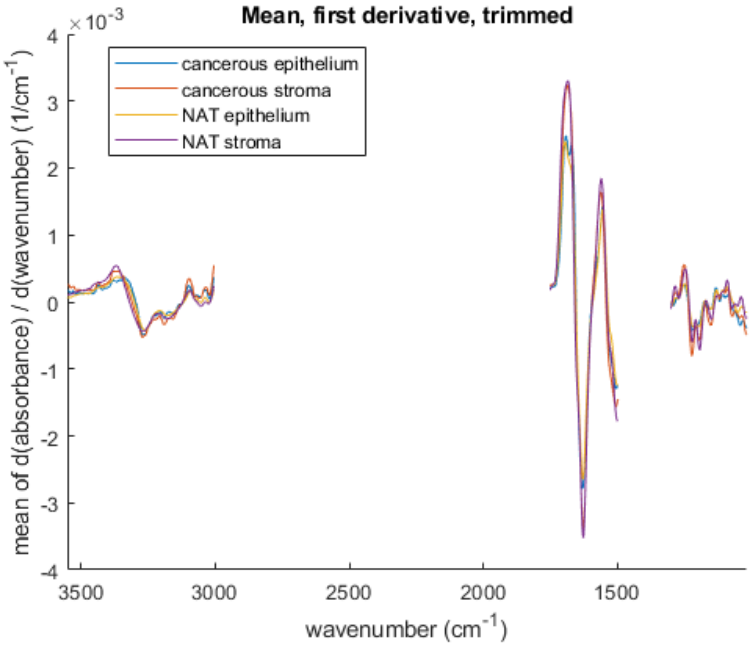

Standard deviation of each class, denoised
cancerous epithelium
cancerous stroma
NAT epithelium
NAT stroma
std of absorbance
wavenumber (cm-1)

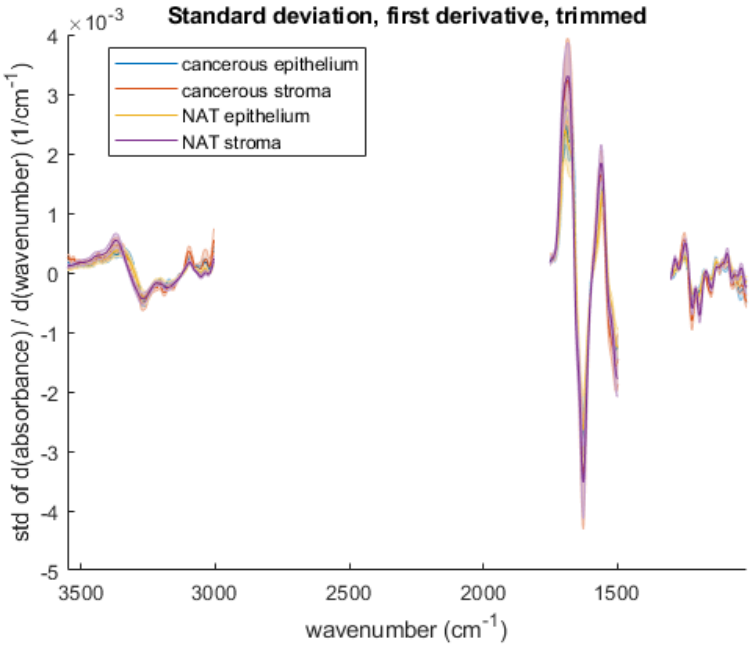

Mean spectra of each class, denoised, following wax removal
cancerous epithelium
cancerous stroma
NAT epithelium
NAT stroma
mean of absorbance
wavenumber (cm-1)


Standard deviation of each class, denoised, following wax removal
cancerous epithelium
cancerous stroma
NAT epithelium
NAT stroma
std of absorbance
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
3500
3000
2500
2000
1500
1000
wavenumber (cm-1)


Mean, first derivative
×10-3
cancerous epithelium
cancerous stroma
NAT epithelium
NAT stroma
mean of d(absorbance) / d(wavenumber) (1/cm-1)
5
4
3
2
1
0
-1
-2
-3
-4
-5
3500
3000
2500
2000
1500
1000
wavenumber (cm-1)


Standard deviation, first derivative
×10^-3
8
6
4
2
0
-2
-4
-6
-8
std of d(absorbance) / d(wavenumber) (1/cm^-1)
cancerous epithelium
cancerous stroma
NAT epithelium
NAT stroma
3500
3000
2500
2000
1500
1000
wavenumber (cm^-1)


Mean, first derivative, trimmed
×10^-3
4
3
2
1
0
-1
-2
-3
-4
mean of d(absorbance) / d(wavenumber) (1/cm^-1)
cancerous epithelium
cancerous stroma
NAT epithelium
NAT stroma
3500
3000
2500
2000
1500
wavenumber (cm^-1)



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