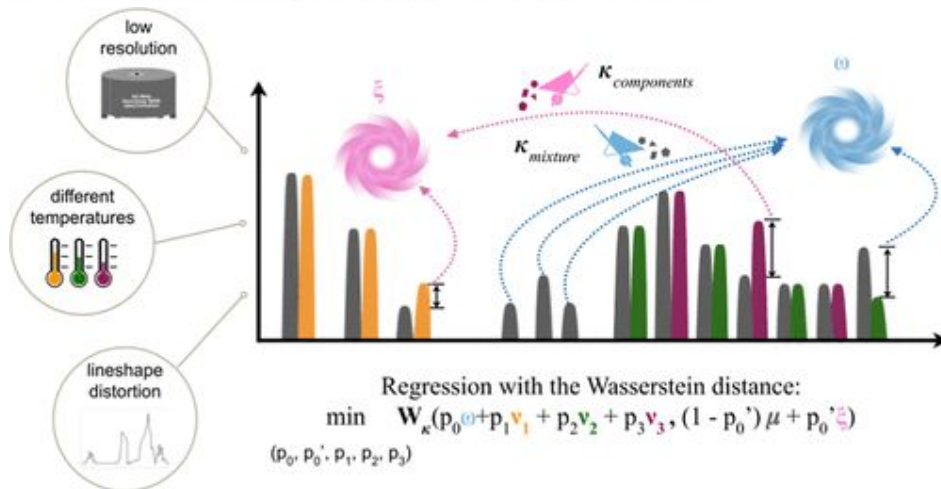


# ***Visualization package for Magnetstein***

Zofia Kozaryna, Ko Natoński

# Introduction to the project

## Magnetstein: An Open-Source Tool for Quantitative NMR Mixture Analysis Robust to Low Resolution, Distorted Lineshapes, and Peak Shifts



The Magnetstein project addresses a key challenge in NMR-based mixture analysis: how to decompose complex spectra into their molecular components. While algorithms based on the optimal transport theory can estimate proportions with removing noise detected in spectra, interpreting and validating these results visually remains difficult—especially for non-specialist users.

Thus, **we developed a dedicated visualization package** to bridge this gap by turning computational outputs into clear, informative, and interactive spectral plots.

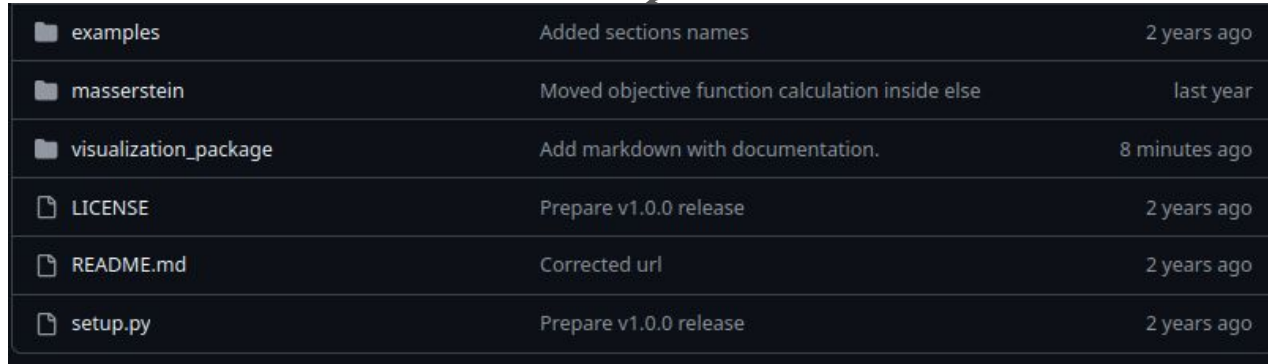
# Objectives

The primary goals of the visualization module were:

- **Visual Clarity:** To provide intuitive spectral plots for mixtures, components, and decompositions.
- **Decomposition Insight:** To illustrate how a mixture is decomposed into components and how much each contributes.
- **Noise Interpretation:** To show what signal parts were considered "noise" and removed during normalization.
- **Transport Interpretation:** To visualize the transport plan — the optimal way intensities are shifted between mixture and components.

# Github repository

official Magnetstein repository



examples	Added sections names	2 years ago
masserstein	Moved objective function calculation inside else	last year
visualization_package	Add markdown with documentation.	8 minutes ago
LICENSE	Prepare v1.0.0 release	2 years ago
README.md	Corrected url	2 years ago
setup.py	Prepare v1.0.0 release	2 years ago

Branch: visualization\_package

Name	Last commit message	Last commit da...
..		
documentation.md	Add markdown with documentation.	9 minutes ago
utils.py	Add one function retrieving transport plan and one which shifts and s...	yesterday
visualization_examples.ipynb	Update the notebook.	7 hours ago
visualization_module.py	Add function to visualize stacked spectra.	yesterday

# Results

The visualization package now supports the following core features:

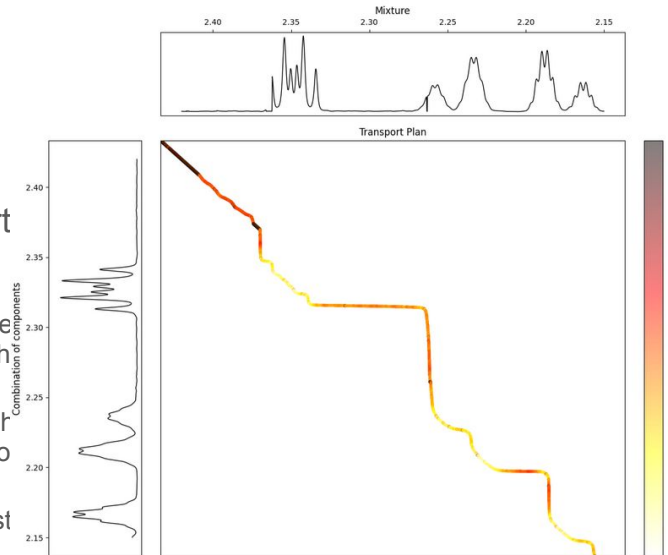
- **Transport Plan Matrix**
  - Visualizes how mass (in this case intensity) is transported between the mixture and optimal combination of components in the spectral domain, optionally scaled logarithmically for clarity.
- **Distance Distribution Plot**
  - Generates a histogram showing how much spectral mass was transported across different distances (in ppm). This helps assess the kappas required for decomposition, and whether the components align well with the mixture or need significant shifting.
- **Cumulative Decomposition Plot**
  - Displays how a mixture is reconstructed from weighted, shifted, and smoothed components using `fill_between`—revealing the additive nature of the decomposition.
- **Stacked Spectra Plotting**
  - Plots multiple spectra (e.g., components + mixture) stacked with proper vertical offsets, customizable labels, colors, and regions of interest.
- **Noise Visualization**
  - Highlights what parts of the spectra were removed as noise from both mixture and component sides. This helps evaluate the decomposition quality and residual signal.
- **Integration with Internal Data Models**
  - Works seamlessly with `NMRSpectrum` objects and `.confs` structure used internally in Magnetstein.

```
visualize_transport_plan(transport_df, mix_confs, wsom_confs, experiment_name=None, lower_lim=None, upper_lim=None)
```

# Results

The visualization package now support

- **Transport Plan Matrix**
  - Visualizes how mass (in this case domain, optionally scaled logarithmically) is distributed across the components required for decomposition.
- **Distance Distribution Plot**
  - Generates a histogram showing the distribution of distances (kappas) required for decomposition.
- **Cumulative Decomposition Plot**
  - Displays how a mixture is reconstructed as a function of the number of components, showing the additive nature of the decomposition.
- **Stacked Spectra Plotting**
  - Plots multiple spectra (e.g., components + mixture) stacked vertically for comparison.
- **Noise Visualization**
  - Highlights what parts of the spectra were removed as noise during decomposition, showing decomposition quality and residual signal.
- **Integration with Internal Data Models**
  - Works seamlessly with NMRspectrum objects and .conf files.



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```
visualize_transport_plan(transport_df, mix_confs, wsom_confs, experiment_name=None, lower_lim=None, upper_lim=None,
figures_path=None, variant=None, cmap='hot_r', point_scaling=20, show_colorbar=True, save=True, figsize=(14, 12),
title='Transport Plan', *args, **kwargs)
Visualizes the transport plan using scatter and line plots.
```

```
Args:
transport_df (pd.DataFrame): Transport matrix (2D) to visualize.
mix_confs (np.ndarray): Coordinates of mixture components.
wsom_confs (np.ndarray): Coordinates of WSOM components.
experiment_name (str, optional): Prefix for saving the plot.
lower_lim (int, optional): Lower limit index for region label in filename.
upper_lim (int, optional): Upper limit index for region label in filename.
figures_path (str, optional): Directory to save the figure.
variant (int, optional): Variant index to include in filename.
cmap (str): Matplotlib colormap name.
point_scaling (int): Scaling factor for point size in scatter plot.
show_colorbar (bool): Whether to display the colorbar.
save (bool): Whether to save the figure.
figsize (tuple): Size of the entire figure.
title (str): Title of the visualization.
*args, **kwargs: Additional args passed to 'scatter()'.
```

```
Returns:
None
```

# Results

The visualization package now supports the following core features:

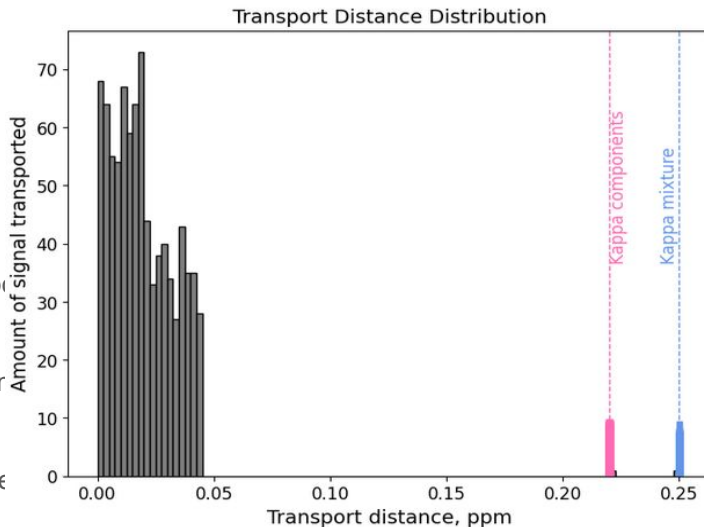
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  - Works seamlessly with `NMRSpectrum` objects and `.confs` structure used internally in Magnetstein.

```
visualize_transport_distance_distribution(distances, kappa_comp, kappa_mix)
```

# Results

The visualization package now supports the following

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  - Displays how a mixture is reconstructed from weights
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  - decomposition quality and residual sig
- **Integration with Internal Data Models**
  - Works seamlessly with NMRspectrum



```
visualize_transport_distance_distribution(distances, component_kappa=None, mixture_kappa=None, component_label='Kappa components', mixture_label='Kappa mixture', component_color='hotpink', mixture_color='cornflowerblue', bins=100, figsize=(8, 6), title='Transport Distance Distribution', save_path=None)
```

Plots a histogram of transport distances with optional markers for specific kappa values.

Args:

distances (list or np.ndarray): List of transport distances.  
component\_kappa (float, optional): Value for a component kappa to highlight.  
mixture\_kappa (float, optional): Value for a mixture kappa to highlight.  
component\_label (str): Label for the component kappa line.  
mixture\_label (str): Label for the mixture kappa line.  
component\_color (str): Color for the component kappa markers.  
mixture\_color (str): Color for the mixture kappa markers.  
bins (int): Number of histogram bins.  
figsize (tuple): Size of the figure.  
title (str): Title of the plot.  
save\_path (str, optional): Path to save the plot. If None, plot is not saved.

Returns:  
None



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The visualization package now supports the following core features:

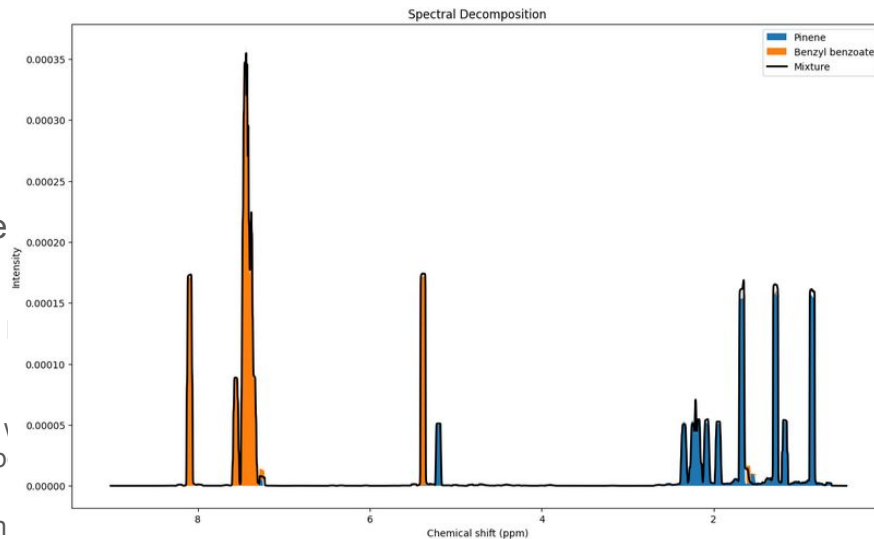
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- **Integration with Internal Data Models**
  - Works seamlessly with NMRspectrum objects and .co

```
visualize_spectra(mix_spectrum, spectra_objects, probs, components_names, 500, shifts)
```



```
visualize_spectra(mixture, spectra_object, probs, components_names, window, shift=None, cumulate=True, figsize=(15, 9),
title='Spectral Decomposition', save_path=None)
Visualizes the spectral decomposition of a mixture into its component spectra.
```

Supports both cumulative plotting using 'fill\_between' and standard stack plotting, with optional spectral shifting and moving average smoothing.

Args:

mixture: An object representing the mixture spectrum, with a '.confs' attribute, where each element is a (x, y) tuple.  
spectra\_object (list): List of component spectrum objects, each with '.confs'.  
probs (list of float): Scaling factors (e.g., probabilities or weights) for each component.  
components\_names (list of str): Names of each component for the legend.  
window (int): Window size for moving average smoothing.  
shift (list of float, optional): Horizontal shift (e.g., ppm offset) for each component.  
cumulate (bool): If True, plot a cumulative filled spectrum using 'fill\_between'. If False, plot standard stacked spectra using 'stackplot'.  
figsize (tuple of int): Figure size in inches.  
title (str): Title of the plot.

Returns:  
None

# Results

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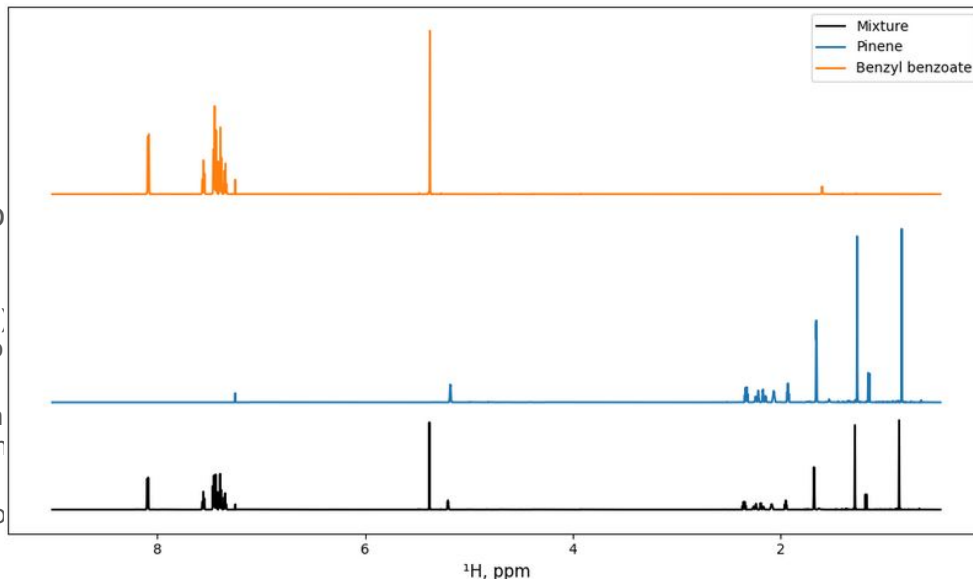
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  - Works seamlessly with NMR

```
visualize_stacked_spectra(spectra, colors=colours, labels=["Mixture", 'Pinene', 'Benzyl benzoate'])
```



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itive

```
visualize_stacked_spectra(spectra, colors=None, labels=None, scale_factor=1.2, figsize=(10, 6), xlim=None, title=None)
Plot stacked NMR spectra with vertical offsets based on each spectrum's max intensity.
Spectra must have a '.confs' attribute with (ppm, intensity) pairs.
```

Args:

spectra (list): List of spectral objects with '.confs' attribute.  
colors (list of str, optional): Plot color per spectrum.  
labels (list of str, optional): Labels for the legend.  
scale\_factor (float): Vertical spacing multiplier between spectra.  
figsize (tuple): Size of the matplotlib figure.  
xlim (tuple, optional): x-axis (ppm) limits.  
title (str, optional): Plot title.

Returns:

None

# Results

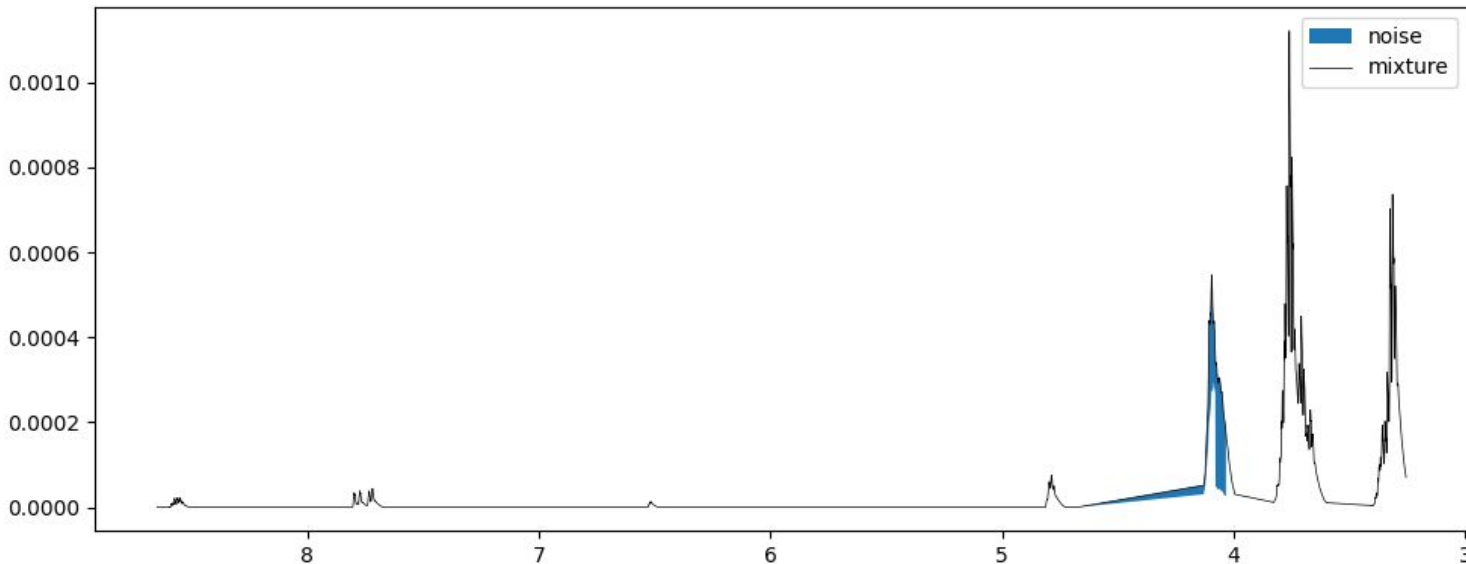
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```
...
plot_removed_noise(estimation, mix, linewidth=0.5)
    Plots an NMR mixture spectrum and highlights the estimated noise that was removed.

    Visualizes the full mixture spectrum and shades the region corresponding to the removed noise,
    as estimated by `estimate_proportions()`.

    Args:
        estimation (dict): Output dictionary from `estimate_proportions()` containing a "noise" key,
                           which holds the noise intensity values for each spectral point.
        mix: NMRspectrum object representing the full mixture, with a `.confs` attribute of (ppm,
        intensity) tuples.
        linewidth (float): Line width for the plotted mixture spectrum.

    Returns:
        None
...

```

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# Conclusions & possible directions for the future

## Conclusions

The visualization module has proven essential for understanding and communicating the results of spectral decomposition in Magnetstein. It allows users to:

- Validate decomposition quality visually.
- Identify noise patterns and transport mismatches.
- Generate high-quality figures for publication and presentations.

## Possible directions for the future

- Interactive Plots (e.g., via Plotly or Bokeh) for zooming, highlighting transport lines, or toggling components on/off.



Thank you for your attention!