Progressive metaheuristics for high-dimensional radiative transfer model inversion
Application to New Horizons LEISA data

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Pluto as seen by LEISA

Figure: Local average reflectance factor spectra of the surface of Pluto extracted for a few typical regions (Schmitt et al., 2017)

New Horizons LEISA hyperspectral data:

- Complex spectra showing the presence of many components (CH$_4$, N$_2$, CO, H$_2$O, organics...)
- Qualitative maps from PCA and integrated band depths
- Real abundances and proportions?
Surface modeling

Figure: Schematic representation of the various materials present on Pluto and their possible mixing states (Schmitt et al., 2017)

- 6 components with corresponding grain sizes
- 4 mixing modes (areal, vertical, granular, molecular)

\[ \text{approx. 45-dimensional problem} \]

- A quantitative map has been made using a simplified 8-dimensional model (Protopapa et al., 2017), but a more accurate map cannot be produced with the same methods
Search strategies

- Lowest-resolution exhaustive computation time of all the spectra = 1500 years on 1000-core cluster
- Simple iterative optimization e.g. gradient descent not possible: too many local minima

What are metaheuristics?
High-level heuristics designed to find a sufficiently good global solution to a complex problem.

Simulated annealing
An algorithm inspired by annealing in metallurgy, which combines gradient descent with stochastic perturbations (slowly decreasing in probability over time) to escape local minima.

Figure: Schema showing the concept behind simulated annealing (Ghasemalizadeh et al., 2016)
Application to spectral fitting

Classic probability acceptance function: \( P = \exp \left( -\frac{\text{new err} - \text{old err}}{T} \right) \)
Complications inherent to this problem:

• Magnitude of effect on spectrum varies between parameters $\rightarrow$ finer-scale optimization gets lost amid big shifts
• Complex interplay and "ruggedness" of parameter landscape $\rightarrow$ lots of local minima/"false positives"

Solutions:

• Common-sense constraints on parameter space, e.g. number of simultaneous components
• Fit the derivative of the spectrum
• Sort the parameters by magnitude of effect, and optimize in that order
Current algorithm

15 dimensions (neglecting areal and vertical mixing), 2 simultaneous components out of 6

3 fitting phases:

1. Fit the derivative of the spectrum
2. Fit only the strong-magnitude parameters
3. Fit only the weak-magnitude parameters

Iteration: Algorithm is run for a time $t$ for all possible pairs of components; the ones with a low RMSE are kept for the next iteration. $t$ increases exponentially as we iterate.
Does it work?

- Naïve fitting, with all components permitted simultaneously, frequently converges to incorrect results.
- The progressive 3-phase fitting algorithm is much more efficient at finding the correct components than unsorted fitting: the correct set is found within 1-3 iterations.
- In testing, a good spectral fit is obtained in under 24 hours on a laptop.
Synthetic fitting

**Granular two-component mix**

<table>
<thead>
<tr>
<th></th>
<th>Composition</th>
<th>Proportion</th>
<th>Grain size</th>
<th>g</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Pure CO</td>
<td>87.4%</td>
<td>53 mm</td>
<td>0.033</td>
</tr>
<tr>
<td>2</td>
<td>N₂-rich ice + dilute CH₄ (1%) + dilute CO (3%)</td>
<td>12.6%</td>
<td>11 mm</td>
<td>0.033</td>
</tr>
</tbody>
</table>

**BEST FIT**

<table>
<thead>
<tr>
<th></th>
<th>Composition</th>
<th>Proportion</th>
<th>Grain size</th>
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</thead>
<tbody>
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<td>1</td>
<td>Pure CO</td>
<td>85%</td>
<td>95 mm</td>
<td>0.033</td>
</tr>
<tr>
<td>2</td>
<td>N₂-rich ice + dilute CH₄ (1%) + dilute CO (1%)</td>
<td>15%</td>
<td>26 mm</td>
<td>0.033</td>
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**RMSE=0.24%**

**Figure**: Simulated annealing fit of synthetic two-component mix after 20 hours
Pluto LEISA test case

Figure: SA fit of LEISA North Pole data (potential CH$_4$-rich endmember)

Areal two-component mix

<table>
<thead>
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<th>Composition</th>
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<th>Grain size</th>
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<tbody>
<tr>
<td>1</td>
<td>Pure CH$_4$</td>
<td>72%</td>
<td>2.7 mm</td>
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<td>2</td>
<td>N$_2$-rich ice + dilute CH$_4$ (5%)</td>
<td>28%</td>
<td>0.6 mm</td>
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RMSE=7%
Conclusions

• Metaheuristics in general, and simulated annealing in particular, are an extremely promising tool for high-dimensional inverse problems such as modeling complex spectra

• The multiplicity of solutions means common-sense constraints need to be applied

Future work:

• Add dynamic differentiation between 1, 2 or 3 components
• Add areal and vertical mixing
• Progressively build up a compositional map, using spatial continuity to constrain the model complexity for individual pixels