Progressive metaheuristics for high-dimensional radiative transfer model inversion

Application to New Horizons LEISA data

Leila Gabasova [1] Nicolas K. Blanchard [2] Bernard Schmitt [1] Will Grundy [3] New Horizons COMP team

[1] Université Grenoble Alpes, CNRS, IPAG, Grenoble, France

[2] IRIF, Université Paris-Diderot, Paris, France

[3] Lowell Observatory, Flagstaff AZ, USA

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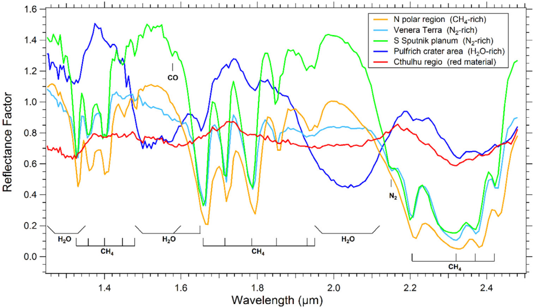


Figure: Local average reflectance factor spectra of the surface of Pluto extracted for a few typical regions (Schmitt et al., 2017)

New Horizons LEISA hyperspectral data:

- Complex spectra showing the presence of many components (CH_4, N_2, CO, H_2O, organics...)
- Qualitative maps from PCA and integrated band depths
- Real abundances and proportions?

Surface modeling

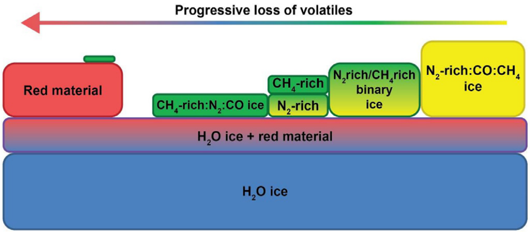


Figure: Schematic representation of the various materials present on Pluto and their possible mixing states (Schmitt et al., 2017)

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

↪ 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

- 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.

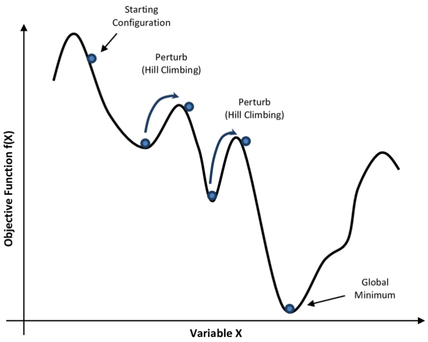
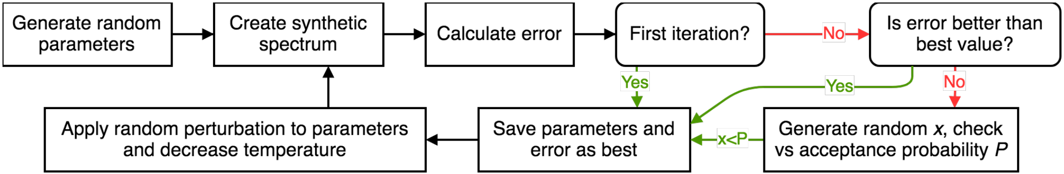


Figure: Schema showing the concept behind simulated annealing (Ghasemalizadeh et al., 2016)



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

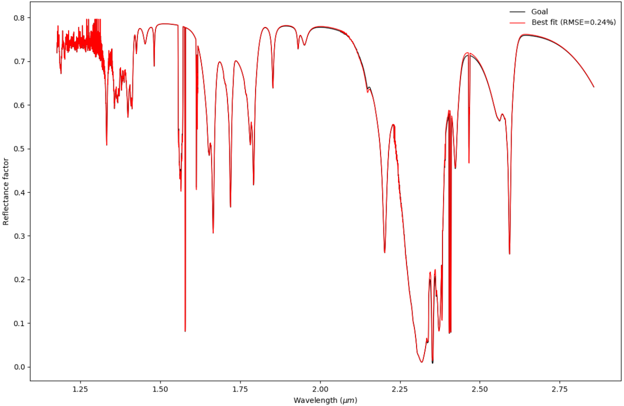


Figure: Simulated annealing fit of synthetic two-component mix after 20 hours

RMSE=0.24%

Granular two-component mix

	Composition	*Proportion*	*Grain size*	*g*
	TARGET			
1	Pure CO	87.4%	53 mm	0.033
2	N_2-rich ice + dilute CH_4 (1%) + dilute CO (3%)	12.6%	11 mm	0.033
	BEST FIT			
1	Pure CO	85%	95 mm	0.033
2	N_2-rich ice + dilute CH_4 (1%) + dilute CO (1%)	15%	26 mm	0.033

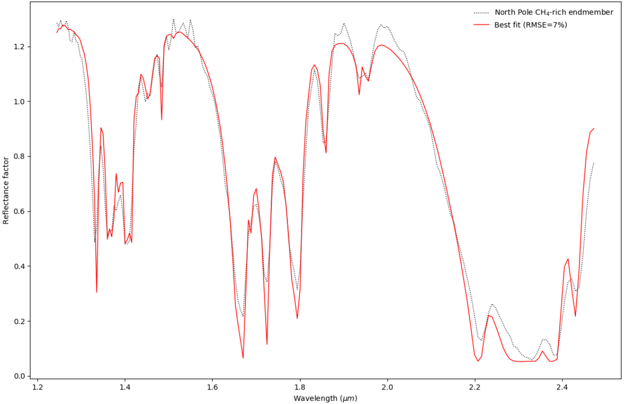


Figure: SA fit of LEISA North Pole data (potential CH_4-rich endmember)

RMSE=7%

Areal two-component mix

	Composition	Proportion	Grain size	*g*
1	Pure CH_4	72%	2.7 mm	0.734
2	N_2-rich ice + dilute CH_4 (5%)	28%	0.6 mm	0.734

- 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