

# SPARSE PARTICLE MODELS FOR DATA ANALYSIS AND ASSIMILATION



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## Introduction

Sparse aerosol representations include sectional, modal, and moment models whereby the aerosol is classified into a basis consisting of a typically small number of size sections, modes, or moments. For our purposes, the term “sparse” will refer to the replacement of an essentially continuous particle size/composition population by a (typically small) set of delta functions or abscissas and weights.

This poster describes a class of sparse particle models derived from linear programming (LP). The widely used quadrature method of moments (QMOM) [1] is shown to fall into this class. Here it is shown that a wider class of sparse aerosol models can be constructed, which are not required to be based on the moments of the particle distribution function.

## Linear Programming

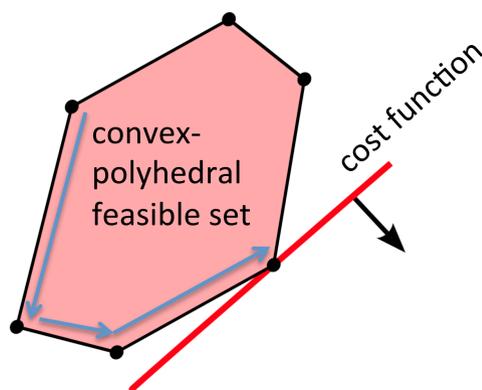
The linear programming problems treated here are all of the same general form:

$$\begin{aligned} &\text{Minimize cost function: } \mathbf{c} \cdot \mathbf{w}^T \\ &\text{Subject to equality constraints: } \mathbf{a}_k \cdot \mathbf{w}^T = \mathbf{M}_k \\ &\text{Together with: } w_i \geq 0 \end{aligned} \quad (\text{LP})$$

Here  $\mathbf{w} = \{w_1, w_2, \dots, w_n\}$  is a vector of variable amplitudes such as the number of particles at grid location  $r_i$ , and  $n$  is the number of grid locations.  $\mathbf{c} = \{c_1, c_2, \dots, c_n\}$  is the vector of cost function coefficients. Each of the equality constraints takes the form shown in (LP) for some specified moment or measurement  $\mathbf{M}_k$ :

$$M_k = \int_0^\infty \sigma_k(r) f(r) dr \approx \sum_{i=1}^N \sigma_k(r_i) w_i \quad (1)$$

where  $\sigma_k(r)$  is a known kernel function, such as a light extinction kernel, and  $r_i$  ( $w_i$ ) are abscissas (weights).  $f(r)$  is the, generally unknown, radial size distribution. For  $\sigma_k(r) = r^k$ ,  $\mathbf{M}_k$  recovers the ordinary radial moments. The linear programming problem (LP) is solved using the simplex method of Danzig, illustrated below.



Simplex method schematic

## Recovery of the QMOM from LP

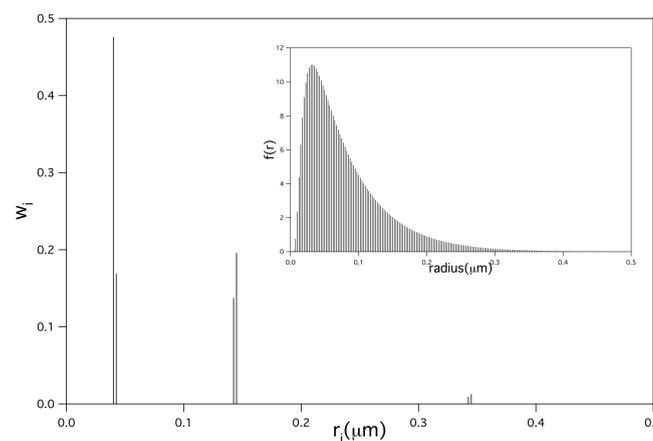


Figure 1. Quadrature abscissas and weights obtained by constraining the first 6 integral moments to those of the normalized test aerosol distribution shown in the insert. The test distribution is from Hoppel et al. [2] and is their distribution #4. The three quadrature points are each split among neighboring grid points due to limited resolution of the grid. Otherwise perfect agreement with QMOM matrix-based moment inversion is obtained.

## Rigorous Nested Bounds on Optical Extinction

Minimizing, instead, the negative of the cost function (LP) maximizes the cost function, yielding a second sparse solution and a pair of bounds. Because the feasible set either stays constant or shrinks as new constraints are added to a previously existing set, nested bounds are obtained as illustrated in Fig. 2. The extent to which the bounds are refined through a doubling and then quadrupling of the number of sections provides a quantitative measure of information achievable through sub-grid resolution.

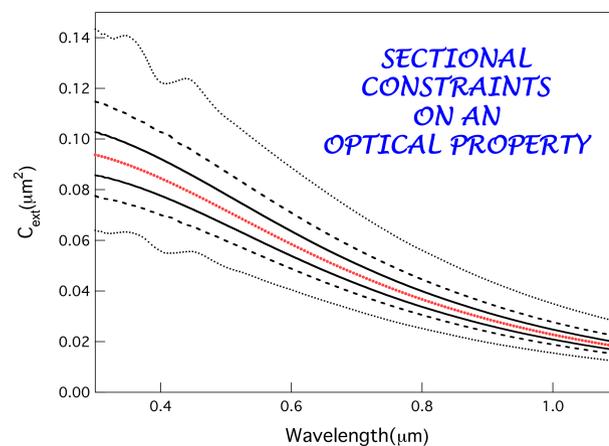


Figure 2. Nested pairs of upper and lower bounds to the extinction coefficient. Obtained by partitioning the Hoppel test distribution into various numbers of equally-spaced radial size sections between 0 and 0.5 microns and using the known particle number concentrations in each section as LP constraints. Dotted, dashed, and solid bounds result from partitioning into 10, 20, and 40 sections, respectively. The center (red) curve gives the extinction coefficient for the test distribution itself as a function of wavelength from Mie theory.

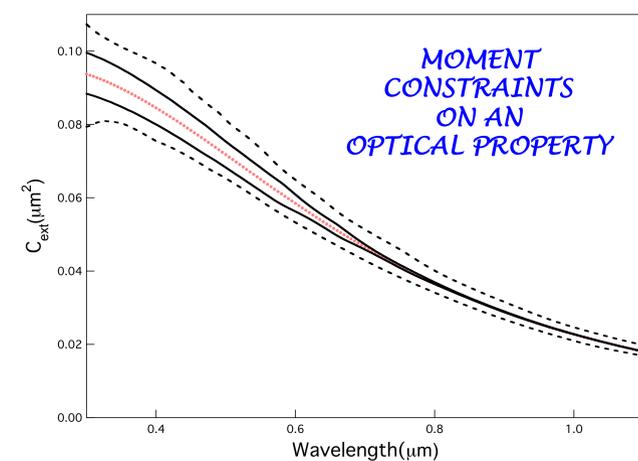


Figure 3. Similar to Fig. 2 except that the sectional constraints are replaced by moment constraints. Dashed and solid bounds derive from the first 6 and first 20 integral radial moments, respectively.

Because of their similar structure, the cost function and any one of the equality constraint vectors are interchangeable. Thus one can bound extinction coefficient at a given wavelength from moment constraints (Fig. 3) or bound a moment from extinction measurements as shown below.

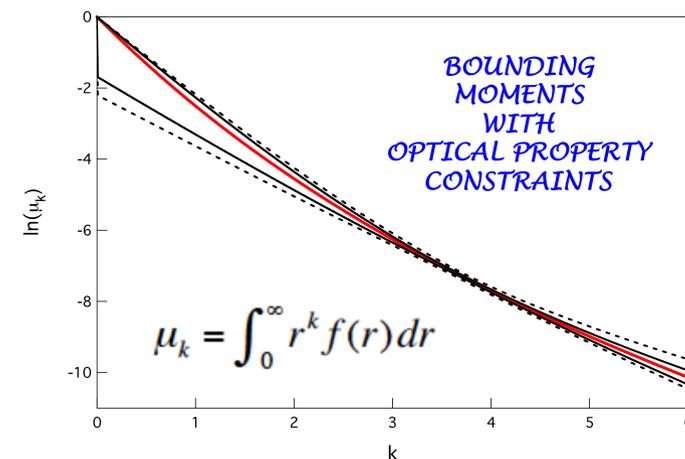


Figure 4. The inverse problem: bounding moments from extinction simulated measurements. Following [3] we use the Sage II wavelengths (0.385, 0.525, and 1.02 microns), dashed bounds. Solid bounds result from a random set of 20 wavelength constraints selected from the spectral range of Figs. 2. and 3. A particle number (normalization) constraint, necessary to get reasonable upper bounds for small  $k$ , has been added.

## Acknowledgments and References

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[1] McGraw, R. (1997), Description of aerosol dynamics by the quadrature method of moments, *Aerosol Sci. and Technol.* **27**, 255-265.

[2] Hopper, W. A., Fitzgerald, J. W., Frick, G. M., and Larson, R. E. (1990), Aerosol size distributions and optical properties found in the marine boundary layer over the Atlantic ocean, *J. Geophys. Res.* **95**, 3659-3686.

[3] Livingston, J. M., and Russell, P. B. (1989), Retrieval of aerosol size distribution moments from multiwavelength particulate extinction measurements, *J. Geophys. Res.* **94**, 8425-8433.