

## Reduction of Uncertainties in the USNO Astronomical Refraction Code using Sensitivities Generated by Automatic Differentiation\*

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The ability to accurately estimate and possibly reduce the uncertainties associated with predictions from nonlinear models is a critical component of every scientific and engineering endeavor. At the theoretical level, uncertainties arise from unavoidable simplifications carried out in the modeling process. At the experimental level, they occur due to noise, imperfect conditions and equipment, uncontrollable factors, operational biases, or simply mistakes.

The objective of this paper is to demonstrate the potential reduction of uncertainties that can be achieved by consistently combining model predictions and sensor measurements. This uncertainty reduction is illustrated using a few parameters and responses from the US Naval Observatory (USNO) astronomical refraction code based on the Hohenkerk and Sinclair refraction model.<sup>1</sup> We use automatic differentiation to calculate the sensitivities needed to propagate uncertainties through the model. The real part of the atmospheric index of refraction is a complex nonlinear function of pressure, temperature, elevation, humidity, and wavelength. The index of refraction also depends on atmospheric density and the density of the atmosphere strongly depends on altitude. Therefore, light propagating in the vertical direction is typically bent towards higher density/lower altitude. The density of the atmosphere does not vary significantly in the horizontal direction and hence only the vertical refraction effect needs to be considered. Accurate estimation of this refraction effect is essential for extrapolating the actual position of a target from its observed or apparent position. Significant effort has been expended towards developing accurate algorithms for refraction calculation. These algorithms have been adopted for applications in missile defense, airborne sensor measurement, astronomical observation, and naval research. Atmospheric refraction is divided in three categories: astronomical, terrestrial, and geodesic. Astronomical refraction addresses ray-bending effects for objects outside the earth's atmosphere relative to an observer within the atmosphere. Terrestrial and geodesic cases consider lower altitude refraction. The core of the USNO astronomical code is the evaluation of the refraction integral of Eq. 1.

$$\xi = \xi_t + \xi_s = - \int_{z_0}^{z_t} \frac{rdn/dr}{n + rdn/dr} dz - \int_{z_t}^{z_s} \frac{rdn/dr}{n + rdn/dr} dz \quad (1)$$

The integration is performed using numerical quadrature. The quantity  $\xi$  is the refraction angle,  $z$  is the zenith angle,  $r$  is the vertical distance, and  $n$  is the index of refraction. This integral is evaluated separately for the troposphere and the stratosphere. Many interesting low altitude refractive effects exist because of tropospheric variation in density and water vapor partial pressure as a function of position. Due to the complex dependence of  $n$  on atmospheric parameters, typical variations in the atmospheric conditions cause an uncertainty in refraction correction angles. Furthermore, dispersion of the refractive index causes the refraction correction angle to vary slightly over different frequency ranges. In addition, at infrared through ultraviolet frequencies, refraction depends strongly on the vertical temperature profile. Therefore, sensitivity and uncertainty analysis of the USNO refraction code is crucial for the development of a more accurate refraction model and robust algorithms that, in turn, will aid in the progress of surveillance technology

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*Sensitivities* are defined as the derivatives of computed model results (usually referred to as *system responses*) with respect to intrinsic model parameters and external inputs to the model (referred to as *system parameters*). Sensitivities can be used to determine and rank the importance of system parameters, and to accurately propagate uncertainties from the system parameters to the system responses. Most current efforts in sensitivity analysis have focused on the use of *Automated Differentiation* (AD) tools. In particular, we recently conducted a study in support of the Missile Defense Agency (MDA) that involved very large datasets (over one million parameters) associated with the MODTRAN code<sup>2</sup>. The AD technology produces an enhanced code, which, in addition to computing the nominal outputs of the regular code, also provides the exact local derivatives of the computed results with respect to the code parameters. To enable accurate decisions, a completely general *uncertainty analysis* (UA) must address five key capabilities. First, no important effects should be overlooked, which means that the *complete set of sensitivities* with respect to all system parameters is needed. Second, we require an *efficient computation of the sensitivities*, since, in general, large data sets have to be processed. Large codes can take direct advantage of the efficiency and accuracy of AD technology. Third, since in nature linearity is most often the exception rather than the rule, the methodology should allow for a systematic treatment of *nonlinearities*. The fourth criterion imposes the complete treatment, where relevant, of *full time dependence*; this includes model inputs, parameters, and responses. Finally, one requires a consistent methodology for combining experimental (i.e., sensor-measured) data and model results, the primary goal being to *reduce the uncertainties* of system parameters and responses.

We collect the model parameters and inputs in the vector  $\mathbf{a}$ . The responses calculated by the model are denoted by  $\mathbf{q}$ , and the measured responses by  $\mathbf{r}$ . Bold lowercase letters denote vectors, while bold uppercase letters refer to matrices. The symbol  $\sim$  will denote transposition. The *nominal uncertainties* in the parameters are quantified by specifying their covariance matrix, i.e.,

$$\mathbf{C}_a = \langle \Delta \mathbf{a} \Delta \tilde{\mathbf{a}} \rangle \quad (2)$$

In Eq. (2),  $\Delta \mathbf{a}$  denotes a vector of standard deviations; in particular,  $\Delta a_i$  represents the standard deviation (uncertainty) of parameter  $i$ , and the brackets imply expectation. *Sensitivities* provide a systematic way to propagate uncertainties in complex, non-stationary, nonlinear models. They may be efficiently computed using AD technology. For example, to first order in a stationary system, the sensitivity of calculated response  $n$  to parameter  $i$  evaluated at the nominal parameter values used in the model is given by

$$S_{ni} = \partial q_n / \partial a_i |_{\mathbf{a}} . \quad (3)$$

Using the sensitivity matrix,  $\mathbf{S}$ , we can readily calculate the nominal covariance matrix of the calculated responses.

$$\mathbf{C}_q = \langle \Delta \mathbf{q} \Delta \tilde{\mathbf{q}} \rangle = \mathbf{S} \mathbf{C}_a \tilde{\mathbf{S}} . \quad (4)$$

We now seek *best estimates* for the parameters and responses. We denote these quantities by  $\hat{\mathbf{a}}$  and  $\hat{\mathbf{r}}$ . Their values are related to the current estimates by the sensitivities. To first order,

$$\hat{\mathbf{r}} - \mathbf{r} = \mathbf{q} - \mathbf{r} + \mathbf{S}(\hat{\mathbf{a}} - \mathbf{a}) . \quad (5)$$

To obtain the best estimates, we must *consistently combine* computational results and experimental measurements. We achieve this by optimizing a generalized Bayesian loss function that simultaneously minimizes the differences between (i) the best estimate responses and the measured responses, and (ii) the best estimate and calculated parameters. The optimization process uses the inverse of a generalized total covariance matrix as the natural metric for the computation.

It is convenient to define new variables:  $\mathbf{x} = \hat{\mathbf{a}} - \mathbf{a}$ , and  $\mathbf{y} = \hat{\mathbf{r}} - \mathbf{r}$ . The discrepancy between calculations and measurements is then expressed as  $\mathbf{e} = \mathbf{q} - \mathbf{r}$ . Using the new variables, the local approximated functional relationship assumed in Eq. (5) between the system parameters and responses becomes  $\mathbf{y} = \mathbf{S} \mathbf{x} + \mathbf{e}$ . The loss function is then defined as:

$$\mathcal{Q} = [\tilde{\mathbf{y}} | \tilde{\mathbf{x}} | \dots] \begin{bmatrix} \mathbf{C}_r & \mathbf{C}_p & \dots \\ \tilde{\mathbf{C}}_p & \mathbf{C}_a & \dots \\ \dots & \dots & \dots \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{y} \\ \mathbf{x} \\ \dots \end{bmatrix} . \quad (6)$$

In the above expression,  $\mathbf{C}_r$  represents the covariance matrix of the measured responses,  $\mathbf{C}_p$  the covariance matrix induced by the responses-parameters correlations, and the three-dot patterns denote additional covariance and cross-covariance contributions that may potentially be included, and which may account, for example, for method biases.

The Bayesian loss function  $Q$  must be constrained in terms of the functional relationship between parameters and responses. This relationship is locally approximated above to first order only. However, if the responses are *strongly nonlinear*, an iterative procedure can be implemented. One then constructs an augmented Lagrangian,  $\mathcal{L}$ , in the form

$$\mathcal{L} = Q + \boldsymbol{\lambda}^T [\mathbf{S} \mathbf{x} - \mathbf{y} + \mathbf{e}]. \quad (7)$$

where  $\boldsymbol{\lambda}$  denotes a vector of Lagrange multipliers. The necessary conditions for a locally-optimal solution are obtained by requiring that the partial derivatives of the augmented Lagrangian with respect to  $\mathbf{x}$  and  $\mathbf{y}$  be zero. We solve these equations in conjunction with the constraints satisfaction to obtain the optimal values of  $\mathbf{x}$  and  $\mathbf{y}$ , which determine the best estimates for both the parameters and responses and their associated covariances. For example, assuming no bias contribution to the optimization metric, we find, after some lengthy algebra not shown here, that the covariance matrix corresponding to the best estimates of the system parameters is given by the expression

$$\mathbf{C}_{\hat{\mathbf{a}}} = \mathbf{C}_{\mathbf{a}} - (\tilde{\mathbf{C}}_{\mathbf{p}} - \mathbf{C}_{\mathbf{a}} \tilde{\mathbf{S}})(\mathbf{C}_{\mathbf{r}} - \mathbf{S} \tilde{\mathbf{C}}_{\mathbf{p}} - \mathbf{C}_{\mathbf{p}} \tilde{\mathbf{S}} + \mathbf{S} \mathbf{C}_{\mathbf{a}} \tilde{\mathbf{S}})^{-1} (\mathbf{C}_{\mathbf{p}} - \mathbf{S} \mathbf{C}_{\mathbf{a}}). \quad (8)$$

In a similar fashion, the covariance matrix corresponding to the best estimates of the responses is

$$\mathbf{C}_{\hat{\mathbf{r}}} = \mathbf{C}_{\mathbf{r}} - (\mathbf{C}_{\mathbf{r}} - \mathbf{C}_{\mathbf{p}} \tilde{\mathbf{S}})(\mathbf{C}_{\mathbf{r}} - \mathbf{S} \tilde{\mathbf{C}}_{\mathbf{p}} - \mathbf{C}_{\mathbf{p}} \tilde{\mathbf{S}} + \mathbf{S} \mathbf{C}_{\mathbf{a}} \tilde{\mathbf{S}})^{-1} (\mathbf{C}_{\mathbf{r}} - \mathbf{S} \tilde{\mathbf{C}}_{\mathbf{p}}), \quad (9)$$

Finally, the covariance matrix associated with the model responses recalculated using the best estimates of the system parameters is, to first order, simply

$$\mathbf{C}_{\hat{\mathbf{q}}} = \mathbf{S}_{\hat{\mathbf{a}}} \mathbf{C}_{\hat{\mathbf{a}}} \tilde{\mathbf{S}}_{\hat{\mathbf{a}}}, \quad (10)$$

where the sensitivities must be reevaluated at the new parameter values  $\hat{\mathbf{a}}$ .

In this paper, we combine AD technology with the above mentioned nonlinear uncertainty reduction method to analyze the outputs of the USNO astronomical refraction code as functions of model parameters temperature, wavelength, relative humidity, observer zenith angle, and altitude. The sensitivity and uncertainty analysis presented highlight the approximations/limitations inherent in this model and aid in the design of more accurate refraction algorithms.

## REFERENCES

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