GNSS-R Parameter Sensitivities for Soil Moisture Retrieval

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***Abstract*—We consider the problem of retrieving soil moisture based on GNSS-R time series data with incidence angle diversity in the presence of instrument calibration errors, vegetation cover uncertainty, and surface roughness uncertainty. After defining an observation model and a retrieval cost function, we derive a formula for retrieval performance as a function of calibration uncertainty, time series parameters, and prior statistics. Numerical results illustrate relationships among various parameters.**

***Index Terms*—land remote sensing, soil moisture, reflectometry, GNSS-R, CYGNSS, sensitivity analysis**

I. Introduction

Soil moisture (SM) is a fundamental quantity in the study of our planet, providing observability into processes of evapotranspiration and groundwater recharge, which influence cycles of water, energy, and carbon on regional and global scales. Applications supported by SM observations include weather and climate forecasting, flood and landslide prediction, aquifer modeling, drought analysis, crop productivity evaluation, and human health. The advancement of dependable SM retrieval methods is therefore of considerable human interest [1].

In this study, we investigate the theoretical retrieval accuracy for surface SM using time series data from a reflectometer such as NASA's Cyclone GNSS (CYGNSS) mission in the presence of various error sources. We focus on exploring incidence angle diversity since the effect of surface roughness on scattered power is relatively sensitive to incidence angle and also since CYGNSS lacks other modes of diversification such as frequency and polarization. In particular, we consider a given resolution cell on the ground through which multiple specular points pass within a given time interval to provide multi-incidence angle reflectometry data.

In Section II we propose an observation model and a retrieval cost function. Our goal is not necessarily to define complex high-fidelity models but rather only to capture the primary features relevant to sensitivity analysis. We proceed to derive a formula for retrieval performance as a function of calibration uncertainty, time series parameters, and prior statistics. In Section III we give numerical results to illustrate the relationships among the various parameters. In Section IV we discuss limitations of the results and areas for future work.

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II. Statistical Modeling

A. Observation Model

From (S2) of [2], we assume that surface reflectivity can be obtained from received power and various known system parameters. We denote this noisy observation of surface reflectivity by y. In the case of CYGNSS, y is closely related to the Level 1 bistatic radar cross section (L1 BRCS) from the specular bin of the delay-Doppler map (DDM).

Following the approach in [3], which in effect combines (11.2) and (11.11) of [4], we model surface reflectivity by

$$\Gamma_{\rm coh}(\theta; m_{\rm v}, ks, \tau) = A_{\rm vwc}(\theta;\tau)A_{\rm rough}(\theta;ks)\Gamma_{\rm f}(\theta;m_{\rm v}) \quad (1)$$

$$A_{\rm vwc}(\theta;\tau) = e^{-(2\sec\theta)\tau} \quad (2)$$

$$A_{\rm rough}(\theta;ks) = e^{-(2\cos\theta)^2(ks)^2} \quad (3)$$

where θ is incidence angle, $m_{\rm v}$ is volumetric SM, ks is the surface roughness coefficient, τ is approximately $0.1w_c$, w_c is vegetation water content (VWC), $A_{\rm vwc}$ is power attenuation due to VWC, $A_{\rm rough}$ is attenuation of coherent power due to surface roughness under the Kirchhoff approximation [5], and $\Gamma_{\rm f}$ is Fresnel power reflectivity.

Defining geophysical parameter vector

$$\mathbf{x} = [\, m_{\rm v} \;\; ks \;\; \tau \,]^{\rm T} \quad (4)$$

and assuming that $\mathbf{x}$ is constant over the spatio-temporal extent of the time series and expressing $\Gamma_{\rm coh}$ in units of decibels

$$f(\theta;\mathbf{x}) = 10\log_{10}[\Gamma_{\rm coh}(\theta;m_{\rm v},ks,\tau)] \quad (5)$$

then we can write the time series of observed surface reflectivities in vector form as

$$\mathbf{y} = \mathbf{f}(\mathbf{x}) + \boldsymbol{\nu}_{\rm cal} \quad (6)$$

where $y_i = f(\theta_i, \mathbf{x}) + \nu_i$ for observation $i = 1, \ldots, N$. Here, we assume that observation noise $\boldsymbol{\nu}_{\rm cal}$ in decibels comes from instrument calibration error and behaves as multiplicative (speckle-like) noise when (6) is expressed in linear units.

B. Cost Function and Error Covariance Matrix

We assume that the cost function for the retrieval has the following quadratic form

$$J(\mathbf{x}') = [\mathbf{y} - \mathbf{f}(\mathbf{x}')]^{\rm T}\mathbf{C}_{\rm cal}^{-1}[\mathbf{y} - \mathbf{f}(\mathbf{x}')] + (\mathbf{x}_{\rm prior} - \mathbf{x}')^{\rm T}\mathbf{C}_{\rm prior}^{-1}(\mathbf{x}_{\rm prior} - \mathbf{x}') \quad (7)$$

where the prime in $\mathbf{x}'$ serves to distinguish it from truth $\mathbf{x}$, $\mathbf{C}_{\text{cal}}$ is the covariance matrix of $\boldsymbol{\nu}_{\text{cal}}$, $\mathbf{x}_{\text{prior}}$ is the prior mean of $\mathbf{x}$, and $\mathbf{C}_{\text{prior}}$ is the corresponding covariance matrix. We also assume that $\boldsymbol{\nu}_{\text{cal}}$ and $\mathbf{x}_{\text{prior}}-\mathbf{x}$ are zero mean and uncorrelated with each other.

As an aside, (7) remains a valid cost function even if the quantities $\mathbf{C}_{\text{cal}}^{-1}$, $\mathbf{C}_{\text{prior}}^{-1}$, and $\mathbf{x}_{\text{prior}}$ have no statistical meaning attached to them. The following results can be extended to this more general class of retrievals, which includes those based on simplified models [6]. However, for this study we make the statistical assumptions stated in the previous paragraph.

To first order, the error covariance matrix (ECM) for the retrieval is given by

$$\mathbf{C}_{\hat{x}} = \mathrm{E}[(\hat{\mathbf{x}}-\mathbf{x})(\hat{\mathbf{x}}-\mathbf{x})^{\mathrm{T}}] = (\mathbf{F}^{\mathrm{T}}\mathbf{C}_{\text{cal}}^{-1}\mathbf{F} + \mathbf{C}_{\text{prior}}^{-1})^{-1} \tag{8}$$

where the retrieval $\hat{\mathbf{x}}$ is the minimizer of (7) and $\mathbf{F}$ is the Jacobian of $\mathbf{f}(\mathbf{x})$. The first-order approximation in (8) is valid when $\hat{\mathbf{x}}-\mathbf{x}$ is sufficiently small relative to higher-order partial derivatives of $\mathbf{f}(\mathbf{x})$. This, in turn, depends on $\boldsymbol{\nu}_{\text{cal}}$ and $\mathbf{x}_{\text{prior}}-\mathbf{x}$ being sufficiently small [6].

If $\boldsymbol{\nu}_{\text{cal}}$ and $\mathbf{x}_{\text{prior}}-\mathbf{x}$ are jointly Gaussian, then $\hat{\mathbf{x}}$ is the maximum a posteriori probability (MAP) estimator. It is also the minimum mean square error (MMSE) estimator to first order, and therefore the MMSE is given by the trace of (8) to first order [6].

If no prior information is available, i.e. $\mathbf{C}_{\text{prior}}^{-1} = \mathbf{0}$ in (7), and if $\boldsymbol{\nu}_{\text{cal}}$ is Gaussian, then $\hat{\mathbf{x}}$ is the maximum likelihood (ML) estimator. It is also the minimum variance unbiased estimator (MVUE) to first order [6].

If prior information is available for some but not all parameters of $\mathbf{x}$ and if these parameters and $\boldsymbol{\nu}_{\text{cal}}$ are jointly Gaussian, then $\hat{\mathbf{x}}$ is the mixed ML-MAP estimator [6].

Even if the random variables involved are non-Gaussian, the cost function given by (7) may still provide a good retrieval. In any case, (8) always holds to first order under the assumptions of the previous sections regardless of whether the random variables involved are Gaussian [6].

Although not provided here due to space constraints, the partial derivatives in $\mathbf{F}$ are straightforward although somewhat lengthy to calculate. In particular, calculation of $\partial\Gamma_{\mathrm{f}}/\partial m_{\mathrm{v}}$ requires a soil dielectric model such as [7], [8].

We now assume that calibration errors are uncorrelated and homoscedastic with variance σ_{cal}^2 and that prior uncertainties are uncorrelated so that $\mathbf{D}_{\text{prior}}^{-1} = \mathbf{C}_{\text{prior}}^{-1}$ is diagonal. Then, (8) becomes

$$\mathbf{C}_{\hat{x}} = \frac{\sigma_{\text{cal}}^2}{N}(\frac{1}{N}\mathbf{F}^{\mathrm{T}}\mathbf{F} + \frac{\sigma_{\text{cal}}^2}{N}\mathbf{D}_{\text{prior}}^{-1})^{-1} \tag{9}$$

We proceed to derive an expression for the $(1,1)$-element of $\mathbf{C}_{\hat{x}}$, which represents SM retrieval uncertainty.

C. Inner Product Representation

Observing that

$$\frac{1}{N}\mathbf{F}^{\mathrm{T}}\mathbf{F} = \frac{1}{N}\sum_{i=1}^{N}[\boldsymbol{\nabla} f(\theta_i)][\boldsymbol{\nabla} f(\theta_i)]^{\mathrm{T}} \tag{10}$$

has the form of an average, we generalize (10) by defining a matrix of inner products

$$\mathbf{P} = \int [\boldsymbol{\nabla} f(\theta)][\boldsymbol{\nabla} f(\theta)]^{\mathrm{T}} \mathrm{p}_{\Theta}(\theta)\mathrm{d}\theta \tag{11}$$

where the elements of $\mathbf{P}$ are given by

$$p_{lm} = \langle f_l, f_m \rangle = \int f_l(\theta) f_m(\theta) \mathrm{p}_{\Theta}(\theta)\mathrm{d}\theta \tag{12}$$

and where $\mathrm{p}_{\Theta}(\theta)$ is the probability density function of incidence angles and $f_n(\theta) = \partial f(\theta;\mathbf{x})/\partial x_n$. Here, as in the following, indices l, m, and n will refer to the elements of $\mathbf{x}$.

If we take $\mathrm{p}_{\Theta}(\theta) = \sum_{i=1}^{N}\delta(\theta-\theta_i)/N$, then we find that $\mathbf{P} = \mathbf{F}^{\mathrm{T}}\mathbf{F}/N$. In the following, we therefore replace $\mathbf{F}^{\mathrm{T}}\mathbf{F}/N$ by the inner product representation $\mathbf{P}$ and reserve the option to use a general form for $\mathrm{p}_{\Theta}(\theta)$ that is not necessarily tied to specific samples of θ_i or to N.

D. Soil Moisture Retrieval Performance

Since $\mathbf{P}$ is symmetric non-negative definite, it can be factored as $\mathbf{P} = \mathbf{D}_f^{1/2}\mathbf{R}\mathbf{D}_f^{1/2}$ where elements of diagonal $\mathbf{D}_f$ are $\langle f_n, f_n \rangle = \|f_n\|^2$ and elements of correlation $\mathbf{R}$ are given by

$$\rho_{lm} = \frac{\langle f_l, f_m \rangle}{\sqrt{\langle f_l, f_l \rangle \langle f_m, f_m \rangle}} = \frac{\langle f_l, f_m \rangle}{\|f_l\|\|f_m\|} \tag{13}$$

To account for prior information, we define an attenuation-like quantity

$$a_n = \left(1 + \frac{\sigma_{\text{cal}}^2}{N\|f_n\|^2\sigma_n^2}\right)^{-1/2} \tag{14}$$

where σ_n is the uncertainty of the n^{th} prior. We note $0 \leq a_n \leq 1$. Now let

$$\widetilde{\mathbf{P}} = \mathbf{P} + \frac{\sigma_{\text{cal}}^2}{N}\mathbf{D}_{\text{prior}}^{-1} \tag{15}$$

Then, $\widetilde{\mathbf{P}}$ can be factored as

$$\widetilde{\mathbf{P}} = \widetilde{\mathbf{D}}_f^{1/2}\widetilde{\mathbf{R}}\widetilde{\mathbf{D}}_f^{1/2} \tag{16}$$

where the diagonal elements of $\widetilde{\mathbf{D}}_f$ are given by $a_n^{-2}\|f_n\|^2$, the diagonal elements of $\widetilde{\mathbf{R}}$ are unity, and the off-diagonal elements of $\widetilde{\mathbf{R}}$ are given by

$$\tilde{\rho}_{lm} = a_l a_m \rho_{lm} \tag{17}$$

For a matrix $\mathbf{M}$, let $\mathbf{M}(l,m)$ denote the submatrix formed by deleting row l and column m from $\mathbf{M}$. Then, we can factor

$$\widetilde{\mathbf{P}}(1,1) = \widetilde{\mathbf{D}}_f^{1/2}(1,1)\widetilde{\mathbf{R}}(1,1)\widetilde{\mathbf{D}}_f^{1/2}(1,1) \tag{18}$$

and from Cramer's rule the $(1,1)$-element of $\widetilde{\mathbf{P}}^{-1}$ is given by

$$\begin{aligned}\widetilde{\mathbf{P}}_{1,1}^{-1} &= \det[\widetilde{\mathbf{P}}(1,1)]/\det(\widetilde{\mathbf{P}}) \\ &= \|f_1\|^{-2}\det[\widetilde{\mathbf{R}}(1,1)]/\det(\widetilde{\mathbf{R}})\end{aligned} \tag{19}$$

The desired result follows from (19), (15), and (9)

$$\sigma_{\hat{m}_{\mathrm{v}}} = \frac{\sigma_{\text{cal}}}{\sqrt{N}} a_{m_{\mathrm{v}}} \left\|\frac{\partial f}{\partial m_{\mathrm{v}}}\right\|^{-1} \sqrt{\frac{\det[\widetilde{\mathbf{R}}(1,1)]}{\det(\widetilde{\mathbf{R}})}} \tag{20}$$

TABLE I
SOIL PARAMETERS

Frequency	1.575 42	GHz
Water temperature	20	°C
Salinity of water	4	$\mathrm{g_{salt}\,kg_{water}^{-1}}$
Bulk density	1.55	$\mathrm{g\,cm^{-3}}$
Particle density	2.66	$\mathrm{g\,cm^{-3}}$
Mass fraction of sand	40	%
Mass fraction of clay	50	%
Mass fraction of silt	10	%
Water volume fraction m_v	20	%

TABLE II
SENSITIVITY NORMS AND CORRELATIONS

θ (deg)	$\left\lVert \frac{\partial f}{\partial m_\mathrm{v}} \right\rVert$	$\left\lVert \frac{\partial f}{\partial (ks)} \right\rVert$	$\left\lVert \frac{\partial f}{\partial \tau} \right\rVert$	$\rho_{m_\mathrm{v},ks}$	$\rho_{m_\mathrm{v},\tau}$	$\rho_{ks,\tau}$
10–70	12.5	2.9	13.7	–0.893	–0.959	0.735
10–40	12.2	3.7	9.8	–0.990	–0.997	0.977
35–55	12.3	2.7	11.8	–0.968	–0.992	0.929
40–70	12.7	1.6	16.6	–0.912	–0.979	0.813

TABLE III
DETERMINANT FACTOR

Known?			Incidence Angle Range (degrees)			
m_v	ks	τ	10–70	10–40	25–55	40–70
N	N	N	16.0	236.3	75.9	26.5
N	Y	N	3.5	13.7	7.9	4.9
N	N	Y	2.2	7.0	4.0	2.4
N	Y	Y	1.0	1.0	1.0	1.0

The determinant factor in (20) is given explicitly by

$$\sqrt{\frac{1-\tilde{\rho}_{23}^2}{1-\tilde{\rho}_{23}^2-\tilde{\rho}_{12}^2-\tilde{\rho}_{13}^2+2\tilde{\rho}_{23}\tilde{\rho}_{12}\tilde{\rho}_{13}}} \tag{21}$$

It is minimized to unity when $\tilde{\rho}_{12} = \tilde{\rho}_{13} = 0$, i.e. when one or more of the following hold

$$\left\langle \frac{\partial f}{\partial m_\mathrm{v}}, \frac{\partial f}{\partial (ks)} \right\rangle = \left\langle \frac{\partial f}{\partial m_\mathrm{v}}, \frac{\partial f}{\partial \tau} \right\rangle = 0 \tag{22}$$

$$a_{ks} = a_\tau = 0 \tag{23}$$

$$a_{m_\mathrm{v}} = 0 \tag{24}$$

From (14), we see that priors are effective when

$$\sigma_n \ll \sigma_\mathrm{cal}/(\sqrt{N}\|f_n\|) \tag{25}$$

since condition (25) drives a_n to zero. If instead

$$\sigma_n \gg \sigma_\mathrm{cal}/(\sqrt{N}\|f_n\|) \tag{26}$$

holds, then the prior has no benefit to retrieval performance (20) since condition (26) drives a_n to unity.

III. NUMERICAL RESULTS

A. Parameters

Computation of Γ_f and its partials requires specification of transmit/receive polarization and soil dielectric constant. We assume the transmitted signal has right hand circular polarization (RHCP) and the receive antenna has left hand circular polarization (LHCP) to accommodate polarization change on reflection. We use Peplinski's soil dielectric model [7], [8] with soil parameters given in Table I.

B. Sensitivities

Normalized sensitivities are shown in Fig. 1 for $0° \leq \theta \leq 70°$. The corresponding norms and correlations (13) of the sensitivity functions over various ranges of θ are given in Table II. We assume θ has uniform distribution over its corresponding range to compute the underlying inner products (11). We note the values of $\|\partial f/\partial m_\mathrm{v}\|$ and $\|\partial f/\partial (ks)\|$ depend on the assumed values of m_v and ks. Here, $m_\mathrm{v} = 0.20$ by Table I and we take $ks = 0.13$ based on Soil Moisture Active Passive (SMAP) ancillary data [3].

The determinant factor (21) is calculated in Table III for the θ-intervals and ρ-values from Table II. When a parameter n is listed as "known" in Table III, then $\sigma_n = 0$ and thus $a_n = 0$ by (14) and the corresponding values of $\tilde{\rho}$ in (21) are zero by (17). This is equivalent to removing the parameter from $\mathbf{x}$.

C. Calibration Accuracy Requirement

If we solve (20) for σ_cal, then we obtain the calibration accuracy required to satisfy a specified retrieval accuracy $\hat{\sigma}_{m_\mathrm{v}}$ as a function of the time-series parameters and priors. Fig. 2 shows σ_cal as a function of prior surface roughness and prior VWC uncertainties, where we fix $\hat{\sigma}_{m_\mathrm{v}} = 4\%$, $N = 4$, $0° \leq \theta \leq 70°$, and prior $\sigma_{m_\mathrm{v}} = \infty$. Here, the prior uncertainties are expressed in decibels of receive power for nadir incidence, i.e. by $|\partial f_n(\theta = 0)|\sigma_n$ for $n = ks, \tau$. This has the advantage of making $\|f_{ks}\|\sigma_{ks}$ in (14) independent of ks. Otherwise, Fig. 2 would depend on the value of ks. To convert a value on the y-axis to units of σ_{ks} for an assumed true value of ks, divide by 34.7×ks. To convert a value on the x-axis to units of σ_τ, multiply by 0.115 13. To convert an x-axis value to units of $\mathrm{kg\,m^{-2}}$ using the SMAP VWC model, multiply by 1.1513.

For the case where $\sigma_{ks} \to \infty$ in Fig. 2, i.e. when surface roughness is a priori unknown, the corresponding required calibration accuracy is shown as the blue line plotted in Fig. 3. Three other lines are also plotted in Fig. 3 for the three subintervals of incidence angle considered in Tables II and III. As can be seen, requirements are tight for this particular case as compared with the calibration uncertainty of 0.39 dB for the latest CYGNSS Level 1 data [9]. In general, we have found that the requirements become looser for drier soils and tighter for wetter soils due to m_v-dependence of the sensitivity factor $\|\partial f/\partial m_\mathrm{v}\|$ in (20).

IV. DISCUSSION

Equation (20) has not yet been validated with test data. We anticipate performing a validation with version 2.1 of the CYGNSS Level 1 data and with existing SMAP cal/val sites and possible new sites with dry lake beds or salt flats.

The validity of (20) and the numerical results in Section III will depend on the many assumptions stated above. The assumption that coherent power can be measured, e.g. from DDM data, depends on properties of the waveform and the instrument, among others. The simple VWC model (2) may

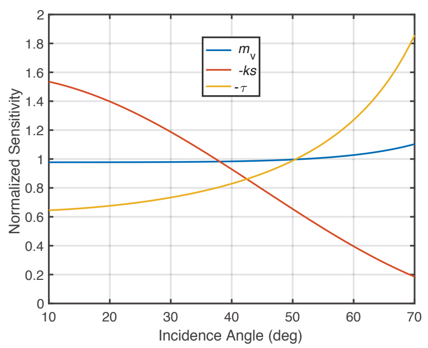

Fig. 1. Normalized sensitivities $f_n(\theta)/\|f_n\| = (\partial f/\partial x_n)/\|\partial f/\partial x_n\|$ as a function of incidence angle θ for $x_n = m_\mathrm{v}, ks, \tau$. As indicated in the legend, the sign of the sensitivity for ks and τ has been reversed for plotting convenience.

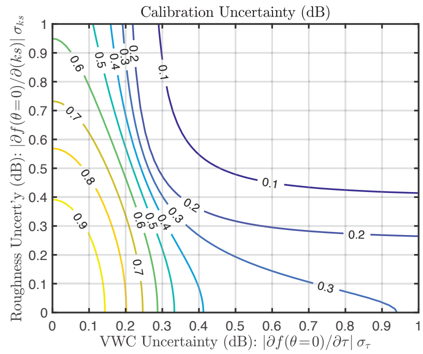

Fig. 2. Calibration uncertainty (dB) as a function of prior surface roughness uncertainty and prior VWC uncertainty that is required to achieve SM retrieval uncertainty of 4% using 4 observations between 0° and 70° of incidence.

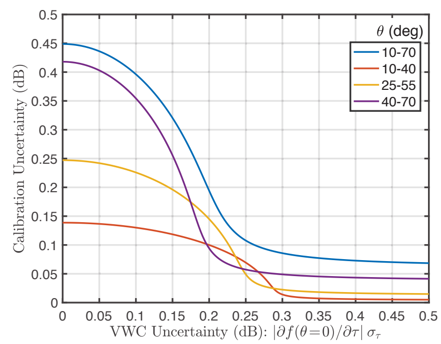

Fig. 3. Calibration uncertainty (dB) as a function of prior VWC uncertainty required to achieve to SM retrieval uncertainty of 4% using 4 observations for various incidence angle intervals when surface roughness is unknown. Multiply x-axis by 1.1513 to convert to $\mathrm{kg\,m^{-2}}$.

need to be developed to account for θ-dependent vegetation structure as in [10]. Validity of the Kirchhoff approximation in (3) depends on properties of the rough surface. Although we assumed perfect knowledge of soil dielectric model and soil texture for computing $\partial\Gamma_\mathrm{f}/\partial m_\mathrm{v}$, our analysis could be extended to include soil texture uncertainty. We also assumed no SM variation with depth. However, such variation may occur and could affect reflected power, e.g. similar to an antireflective coating.

The assumption that geophysical parameters remain constant over the spatial-temporal extent of the time series needs to be investigated. In the case of CYGNSS, the specular region tends to be long and narrow due to the sensor's relatively long noncoherent integration time. Thus, consecutive measurements within a given cell on the ground may not overlap much [2, Fig. S1], giving rise to spatial noise. Furthermore, SM may change during a time series window due to weather events. These variations could be addressed, for example, in the framework of Kalman filtering.

The cost function (7) has desirable optimality properties when the random variables involved are Gaussian as discussed in Section II-B. However, we know that the prior distributions of geophysical parameters cannot be perfectly Gaussian since their values are constrained to lie in closed or half-open intervals. Incorporation of these intervals as constraints in the retrieval may increase its performance and the sensitivity model would need to be updated accordingly.

Although we assumed prior estimates of ks and τ were uncorrelated, if these estimates come from another sensor such as SMAP, then their uncertainties may be correlated and this would need to be accounted for. Additionally, the assumed model of calibration error as uncorrelated homoscedastic multiplicative noise needs to be examined more closely and developed if needed.

While validity of the ECM (8) does not depend on Gaussianity, it does depend on a linear approximation whose validity should be explored. Also, while (8) assumes perfect knowledge of all statistics, it can be extended to account for model mismatch in (7). It is important to understand the effects of such mismatch since statistics are seldom precisely known.

Numerical results in Section III assume that θ is uniformly distributed over a given interval, and we see these results are sensitive to interval size and location. Thus, the assumed uniform distribution should be updated to match the actual θ-distribution, e.g. from orbital simulations or instrument data.

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