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Uncertainty and Sensitivity Matrix of Parameters in Inversion of Physical BRDF Models*

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Abstract Physical BRDF models are usually very complex and difficult to invert. We usually need to employ a priori knowledge in this or that way, fix some parameter values and invert some others. Usually most of us agree that non-sensitive parameters should be fixed, but there has not been any consensus on how to define the sensitivity of a parameter in inversion. Li and Strahler, Li and Wang also suggested that only those the most sensitive and most uncertain parameters should be inverted by using a subset of observations, but they failed to spell out how to determine such "most sensitive and most uncertain" parameters and how to find such a subset of observations. This lacking of consensus and quantitative rules makes inversion of physical BRDF models a case-by-case "trick" or an "art but science".

We tried to develop a general framework for BRDF model inversion. It is based on accumulation of knowledge and an inversion strategy which we called Multi-stage, Sample-direction Dependent, Target-decisions (MSDT).

Our MSDT inversion strategy is based on an Uncertainty and Sensitivity Matrix (USM) of parameters at given directions/bands of observations. Its definition is somehow analogous to the partial derivative matrix used in Newton methods for minimization, but there are three significant differences: 1) the uncertainty of the initial guess is taken into account; 2) It is less dependent on the initial guess; 3) all elements have the same unit and therefore quantitatively comparable. An example of USM from Li-Strahler GOMS model and ASAS sampling will be presented, and it is obvious from the matrix what parameter should be inverted first, and what subset of observations should be used. In order to expressed the USM clearly for more complex sampling patterns, contours may be used.

To demonstrate the MSDT strategy, we used Changping flight data to invert all the 7 parameters in Li-Strahler GOMS model using all the samples at the same time, then invert step by step depending on the USM-based MSDT, the effect is encouraging.

Key words Inversion, BRDF model

1 INTRODUCTION

With the development of multiangular remote sensing (MRS), a lot of instruments for MRS will be launched into the space in next few years, it will provide great opportunities for the quantitative remote sensing (QRS), so it is urgent to improve the methodology of QRS. Inversion of physical BRDF models is a powerful tool to extract the structural and spectral information of the land-cover, and many forward BRDF models have been developed in recent decades, however, forward BRDF models are usually very complex and difficult to invert using limited observations.

We developed the idea of inversion based on accumulation of knowledge and frequent observations[1], by introducing the concept of uncertainty and sensitivity matrix (USM) to be used in the inversion strategy, Multi-stage, Sample-direction Dependent, Target-decisions (MSDT). USM is an objective expression of the prior knowledge, we called it knowledge-based USM. The prior knowledge is the knowledge acquired before inversion or a previous stage in the multi-stage inversion, and MSDT is a inversion strategy depending on the prior knowledge

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and USM.

This paper describes the knowledge—based USM and the MSDT strategy in detail, several examples of USM are clearly presented in contours. Inversion strategy and steps are described using an example of Changping flight data inversion, the field measurement value and inverted value are shown. Finally we discuss on the issues such as uncertainties of inversion results, effects of bias in a prior expectations of parameters, and error analysis of the inversion result of Changping flight data. Some problems remain and should be solved in the future.

2 KNOWLEDGE-BASED UNCERTAINTY AND SENSITIVITY MATRIX(USM)

Presently, our knowledge include: 1) DTM; 2) previous land-cover classification; 3) seasonal change pattern of these land-covers; 4) right model for every type of landcovers; 5) physical limitations (or none) of each parameter in each model; 6) a best guess of each parameter value and the uncertainty of such guess. Where 2) and 3) are the most important prior knowledge to select a suitable physical model, after the model was selected, the physical limitations of each parameter are accepted.

An argument may be about the best guess of each parameter and it's uncertainty. We suggested that the purpose of the inversion is to extract the knowledge (information) about the land-cover as much as possible, and the increase of the knowledge is expressed as the decrease of the uncertainty of such guess[1].

We defined the initial uncertainty of a parameter using both the standard deviation and the physical limitation as:

$$\{\mathbf{P_i} \pm \mathbf{S_i}\}\mathbf{AND}\{\mathbf{Physical\ limit}\}$$

where $\mathbf{P_i}$ and $\mathbf{S_i}$ are the mean and standard deviation of the probability distribution of the values it may take, given the landcover classification and the given model, AND is operation of intersection.

Scientists have realized that the sensitivity of parameters has a direct effect on the inversion, but there has not been any consensus on how to define the sensitivity of a parameter in inversion. Due to the different sensitivities in different sampling direction of each parameter, and the fact that the sensitivity of the same sample can also shows a great diversity among the parameters, we proposed USM to describe the complex situation.

Assuming that a BRDF model has N bands, K structural parameters, L spectral parameters of component materials, $K+N*L$ in total, and the observations have M samples, so the matrix will have $M\times N$ rows and $K+N*L$ columns. This matrix is too big to operate. Because of the spectral parameters of one band are independent of the other band, so we decomposed it into a structural parameters matrix which has $M\times N$ rows, K columns, and N matrix of spectral parameters ($M\times L$) correspond to N bands, total $N+1$ matrix. An element of USM is defined as:

$$\mathbf{USM}[i][j] = \mathrm{Maxdiff}[R(j \mid i)]/R(i) \quad (1)$$

where $\mathbf{Maxdiff}[R(j\mid \mathbf{i})]$ is the maximum difference of BRDF as a function of only the jth parameter within its uncertainty, given the ith geometry of illumination and viewing; $\mathbf{R}(\mathbf{i})$ is BRDF as predicted by the model at the ith geometry, with all parameters at their best guess values.

In the following discussion, we will focus on the Li-Strahler GOMS model[3], which has 4 structural parameters: nR^2, b/R, h/b, $\Delta h/b$; 3 spectral parameters: G, C, Z. nR^2 describes the crown coverage density in the nadir observation; b/R is a crown shape parameter, it has a main effect on the coverage density in the non-nadir direction; h/b is a parameter to describe the height between crown and the ground, mainly affects the outward width of hotspot; $\Delta h/b$ describes the dispersed degree of the distribute of the crown height, it affects the bowl-shape of BRDF, and G, C, Z are the brightness of sunlit background surface, sunlit crown surface and shaded background respectively. After giving the best guesses and associated initial uncertainties of the 7 parameters (Table 1), we obtained the USM under ASAS sampling (Table 2). As an illustration, only red band is used.

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Table 1 Best guesses and uncertainties

	nR^2	b/R	h/b	Δh/b	G	C	Z
Expected	0.177	3.512	2.0	0.5	0.154	0.073	0.01
Uncert.	0～0.78	0.51～8.52	0.09～8.9	0～10.93	0～1	0～1	0～0.073

Table 2 USM of GOMS under given uncertainties and ASAS directions

VZN	nR^2	b/R	h/b	Δh/b	G	C	Z
+60°	1.1683	0.1563	0.1676	0.1533	0.1890	13.1395	0.0855
+46°	1.0643	0.3348	0.1152	0.0268	1.2688	10.9069	0.0614
+30°	2.0645	0.5849	0.2879	0.1861	1.0393	10.2908	0.6476
+15°	3.0440	0.8180	0.2536	0.2139	1.3440	8.5673	1.2235
0°	4.0652	1.1739	0.2332	0.1761	2.0394	5.9914	1.8145
-15°	5.3685	1.5433	0.2334	0.1571	2.0897	4.5142	2.5451
-30°	6.6887	1.7326	0.1747	0.1705	1.5645	4.2235	3.2904
-45°	7.8634	1.7105	0.0963	0.2070	0.8488	4.4417	3.9788
-55°	8.3924	1.5467	0.0476	0.2444	0.4046	4.7447	4.3167

Notes: 1. VZN — Viewing zenith angle on the principal plane.

2. Solar zenith angle is +47.8 degrees, here all the same for 9 geometries.

From the matrix, it is clear that Z is not sensitive near the hotspot. This is obvious, because no shadow can be seen at the hotspot, any information about the shaded area can't be picked up at the hotspot. We can also find out immediately that C is the most sensitive and uncertain at large viewing zenith angle on the side of the illumination. This is due to the fact that the sunlit crown surface is the main factor to determine BRDF at the given samples and best guesses. So, even if we know little about the GOMS model, we can make a decision that the first step is to invert C using large view zenith angle sample on the side of illumination, and the next step is to invert nR^2 and Z using the sample of large view zenith angle on the side of the shadow.

From the matrix, we can also see that despite the large uncertainty, h/b and Δh/b are the most insensitive parameter in these sampling directions, so they should be fixed first when the information is not enough to invert 7 parameters.

For hemispherical uniform sampling, we present the matrix as contours for easier use.

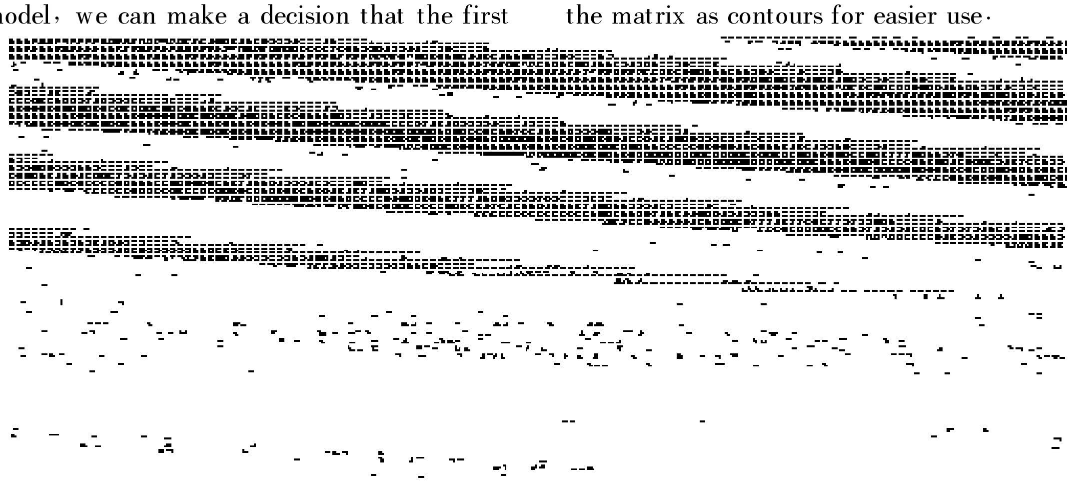

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Fig. 1 USM of hemispherical unifor sampling, Red band

In each of these contours, the brightest present the most sensitive and uncertain samples corresponding to each parameter, the absolute maximum value is shown under the contour to help compare the sensitivity among 7 parameters. From these contours, we can see that the sensitivity and uncertainty matrix in red band is analogous to that in NIR band, but the absolute maximum value is different.

In Fig. 1 and Fig. 2, the sun zenith angle (SZN) is 45 degree, the best guesses and uncertainties are listed in Table 1.

For geometries 's in Changping flight dada, we present the matrix in similar way, the best guesses and uncertainties are listed in Table 3 and Table 4 showed in the following section. But since the SZN changes in one hour flight, the contours are no longer symmetric, as shown in Fig. 3 and Fig. 4 for red and NIR band respectiwely. SZN 's does not show up in the diagrams.

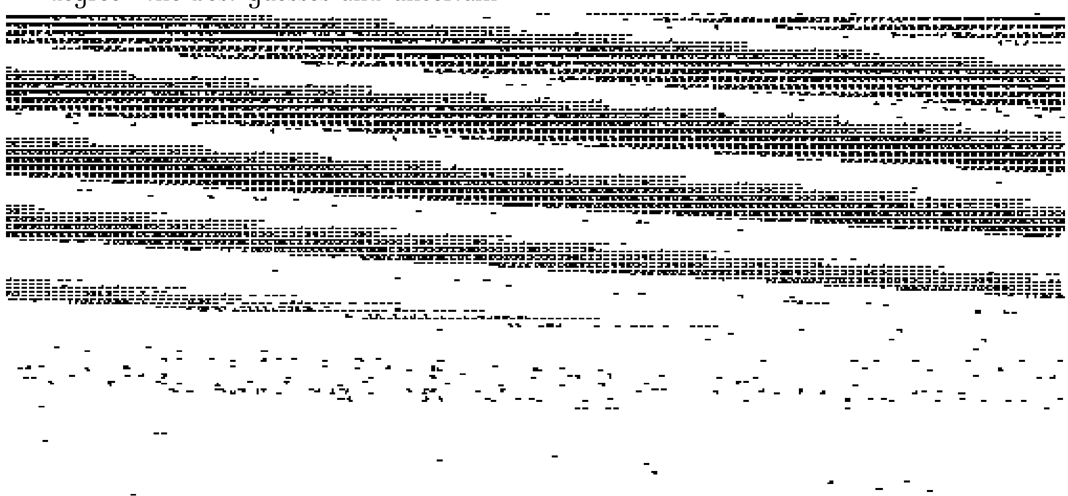

Fig. 2 USM of hemispherical uniform sampling, NIR band

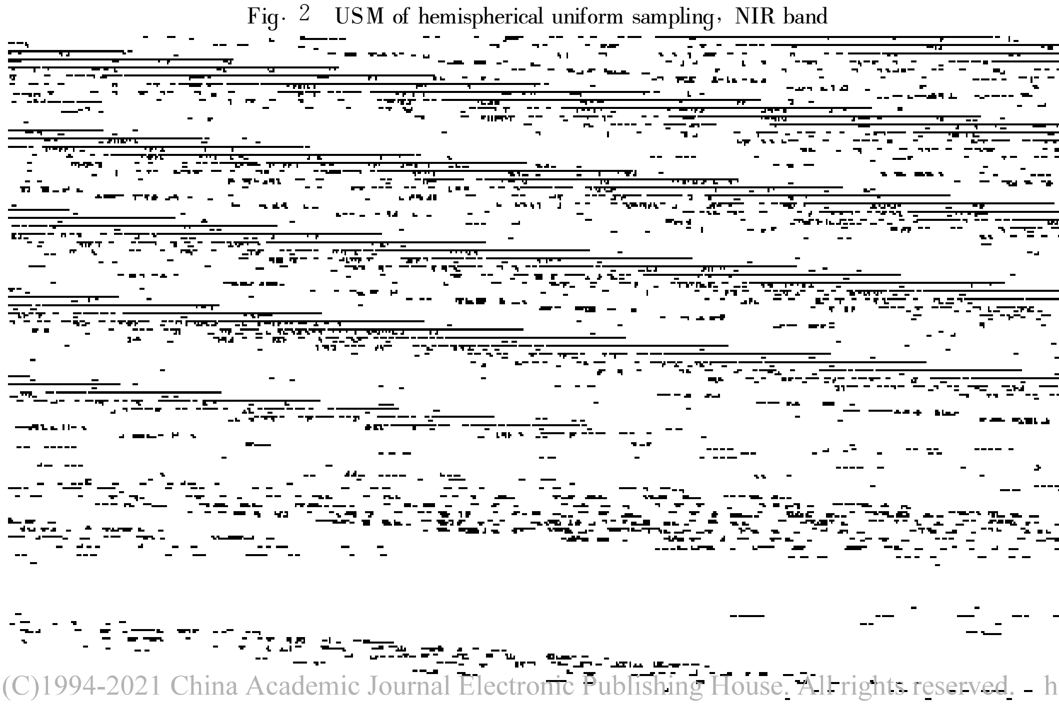

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Fig. 3 USM of Changping flight data in red band

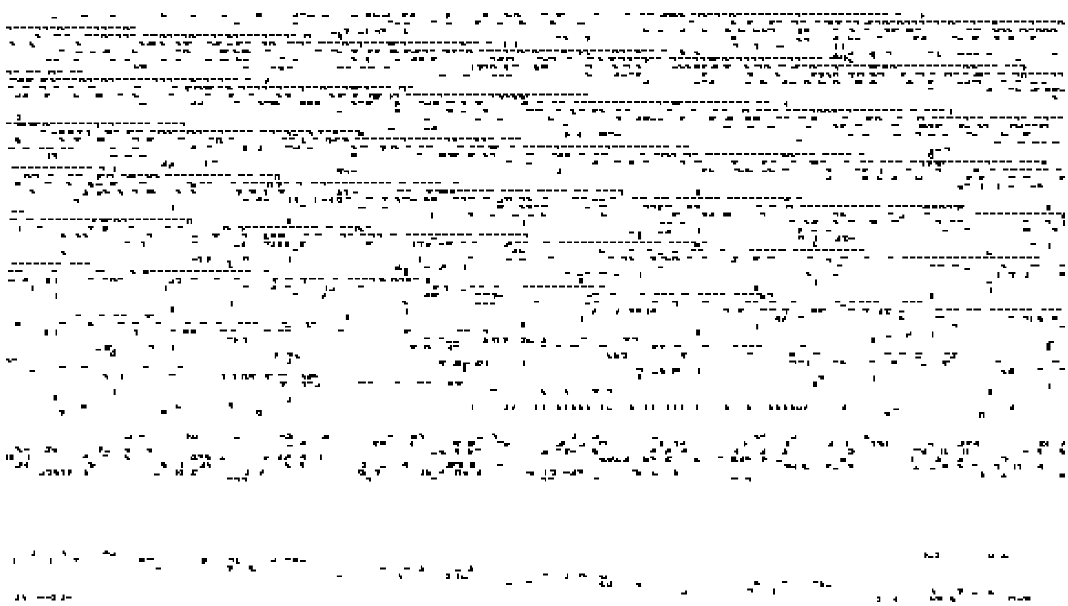

Fig. 4 USM of Changping flight data in NIR band

3 USM-BASED MSDT

Due to the difficulty of inverting BRDF model, people used to fix some parameters in the process of inversion, but there are no quantitative rules for doing so, this makes inversion of physical BRDF models a case-by-case "trick" or an "art but science".

On the basis of USM we mentioned above, we can analyze the inversion process on an objective basis, and selected sensitive samples to invert for selected parameters step by step. We called it Multi-stage, Sample-direction Dependent, Target-decisions (MSDT).

By searching out from the maximum USM[i][j], we can identify $\mathbf{M}_1$ structural parameters and $\mathbf{K}_1$ spectral parameters to be inverted at the first stage of inversion.

Since other less sensitive or less uncertain parameters have been fixed, in fact the original BRDF model has been approximated into a version with only $\mathbf{M}_1 + \mathbf{N} * \mathbf{K}_1$ parameters, if observations have $\mathbf{N}$ wavebands. We call such approximation BRDF_1 model applicable to those observations. Therefore, the least number of direction samples used in this stage of inversion is:

$$\mathbf{L}_1 \geqslant \mathrm{K}_1 + \mathbf{M}_1/\mathbf{N} \tag{2}$$

However, as we have noted from Fig. 1 and Fig. 2, the USM for different bands of structural parameters are very similar in shape, implying a strong correlation. Therefore, presently we prefer to select a single band where the USM elements of a structural parameter larger than other bands for estimating such parameter. Therefore, the least number of required direction samples for that stage will be:

$$\mathbf{L}_1 \geqslant \mathrm{K}_1 + \mathbf{M}_1 \tag{3}$$

In one stage of our MSDT inversion, since the simplied approximation of BRDF has very few sensitive parameters to selected observations, there is little question about whether we can get stable results. But the question is what are the uncertainties of these results.

Currently, we seek the values of parameters by a Powell algorithm by minimizing a Weighted Sum of Square Error With Penalties (WSSEWP):

$$\mathbf{WSSEWP} = \mathbf{exp}\{\boldsymbol{\Sigma}[(\mathrm{p_i} - \mathbf{P_i})^2/\mathbf{S_i^2}]\} * \mathbf{SSE} + \mathbf{Penalty} \tag{4}$$

where SSE and Penalty are the same as in conventional Powell algorithm, and $\mathbf{P_i}$, $\mathbf{S_i}$ are a priori expectation and its uncertainty of the ith parameter, $\mathbf{P_i}$ is the value of the parameter which yields this SSE.

What is the uncertainty of this set of parameters

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which yield this Minimum WSSEWP as correct results? This is an important question to be answered, because such uncertainty will be input to next stage of our MSDT inversion. Currently, we evaluate this uncertainty by two measures.

First, we use the MinWSEEWP, and number of direction samples, i.e., L_1, and number of parameters, i.e., $M_1 + K_1$, to estimate the overall confidence of selection of simplified model $BRDF_1$, and the parameter estimates as well.

Secondly, given that $BRDF_1$ is the best choice, we estimate the new S_i by the p_i deviated from new expectation P_i so that the WSSEWP increases from the MinWSSEWP to 2.72 times of it. This is to guarantee that, if p_i is not sensitive at all, the uncertainty of this parameter will not change after inversion.

The first measure is currently used to select possible candidates of $BRDF_1$. The second one is used as input for the next stage. This is not a robust solution yet, but it works so far.

4 INVERSION USING CHANGPING FLIGHT DATE

To demonstrate the MSDT strategy, Changping flight data are used to invert, First of all, the GOMS model is revised.

4.1 An Improvement on the GOMS Model

When we calculate the initial USM under Changping flight sampling, the uncertain range of h/b is from 0.09 to 8.9, but the Li-Strahler GOMS model (1992) was obtained under assumption that $h/b \geq 1$ (it means that all the spheroid in the model is above the ground), so some formulations are not suitable under a certain condition when $h/b < 1$ (that is a part of the spheroidal envelope of crown is under the ground, this can take place when the widest part of crown is relative low, for example, some conifers, etc.). A set of formulations correspond to the situation have been obtained.

The difference of BRDF which calculated form the old and revised formulations is showed in Fig. 5 and Fig. 6.

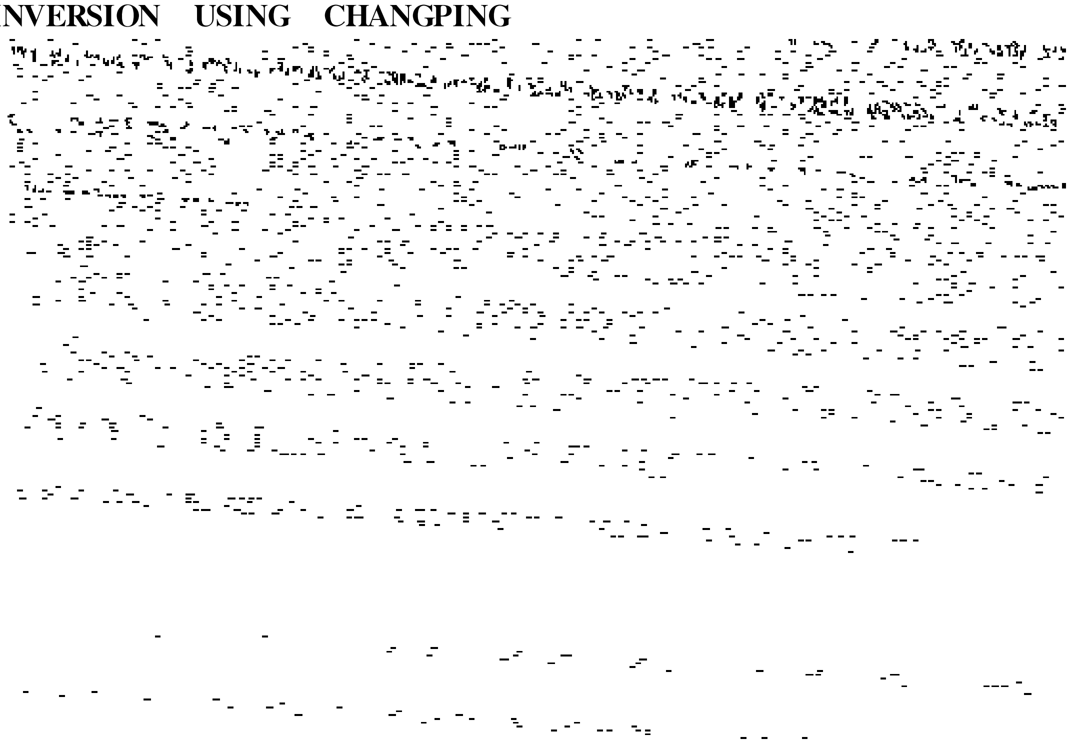

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Fig. 5 BRDF's for conifer (h/b=0.1), SZN=35°

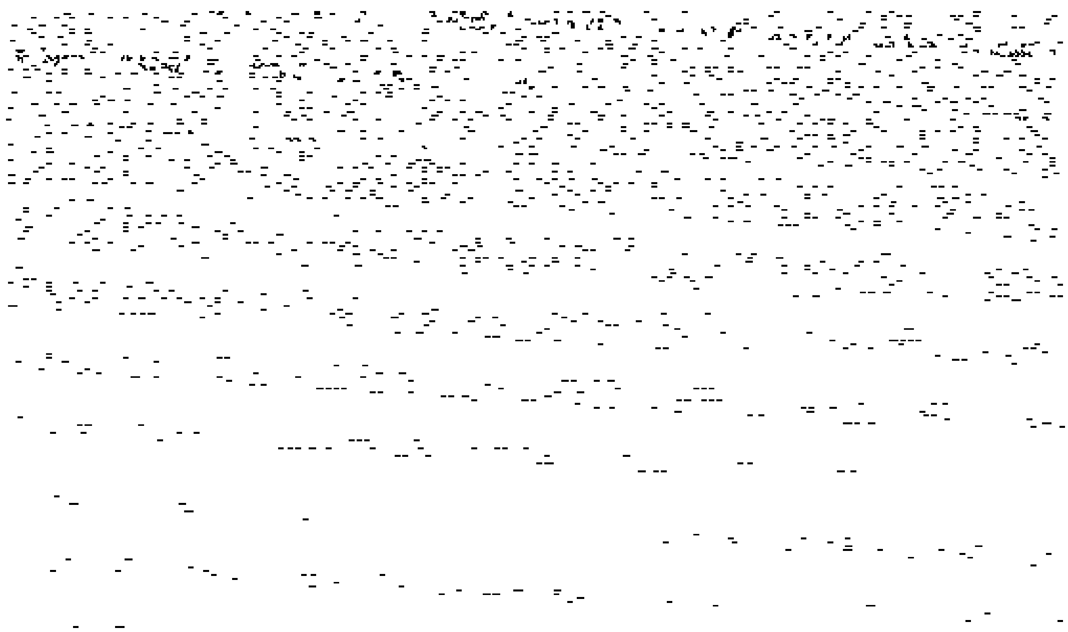

Fig. 6 BRDF's for conifer (h/b=0.1), SZN=45°

In Fig. 5 and Fig. 6, the left (a, c) are calculated from the old formulations, the right (b, d) are obtained from the revised formulations, and (a, b) in the red band, (c, d) in the NIR band.

4.2 USM-based MSDT Inversion

In the Changping flight area, the target are apple trees distributed in a grid of 5m × 6m, through field measurement, we obtained the value of the structural parameters: $nR^2=0.208$; $b/R=0.9$; $h/b=1.222$; $\Delta h/b=0.444$. Before inversion, we give the best guesses and their initial uncertainties as in Table 3 and Table 4.

Table 3 Best guesses and uncertainties of 4 structural parameters

	nR^2	b/R	h/b	Δh/b
Expected	0.177	0.9	2.0	0.5
Uncertain	0~0.78	0.51~8.52	0.09~8.9	0~10.93

Our flight data is obtained in two bands, red and NIR, the best guesses and their initial uncertainties is as the following.

Table 4 Best guesses and uncertainties of 3 spectral parameters in red and NIR bands

	red			NIR		
	G	C	Z	G	C	Z
Expected	0.154	0.073	0.01	0.506	0.225	0.045
Uncertain	0~1	0~1	0~0.073	0~1	0~1	0~0.225

As an illustration, we only use the red band to invert 7 parameters using all the sample at the same time, after it, we invert step by step depending on the USM, the result is encouraging.

The Changping flight data has 75 directional samples in total, despite the sensitivity an uncertainties of the 7 parameters in these sampling directions, all the samples were used to invert all the parameters, the best guesses and their uncertainties are listed in Table 3 and Table 4, the result is listed in Table 5.

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Table 5 Inversion result without MSDT

	nR^2	b/R	h/b	Δh/b	G	C	Z
Inverted	0.148	0.941	1.708	1.014	0.212	0.11	0.007
Uncertainty	0.043～0.204	0.847～1.282	1.113～3	0.129～3.118	0.129～0.253	0.06～0.139	0～0.04

At the given guesses and initial uncertainties listed in Table 3 and Table 4, we obtained the initial USM in the red band, we called it USM_0. It appears that C should be inverted first using 13 samples, then after the other parameters are fixed at the expected value, we obtained :

$$\mathbf{C} = 0.157 \qquad \mathbf{MinSSE} = 0.00026$$

In order to obtain the new uncertainty of C after inversion, we use $2.72 \times$ **MinSSE** as the change range of SSE to find out the maximum and minimum value of C, their difference is taken as the uncertain range of C after inversion. This is the first stage of the whole inversion process, and the next step is to calculate the new USM using the inverted value and new uncertainty of C, we call this new USM USM_1, it is the child of the first stage inversion, from USM_1, we determine to invert nR^2 and b/R using the samples they are most sensitive, and so on, in the end, we obtained the inversion results of the MSDT strategy listed in Table 6.

Table 6 MSDT inversion result

	nR^2	b/R	h/b	Δh/b	G	C	Z
Inverted	0.189	0.898	2.548	0.865	0.174	0.157	0.011
Uncertainty	0.143～0.368	0.878～0.901	1.204～4.618	0.181～1.863	0.173～0.183	0.144～0.161	0.01～0.011

From this table, it is clearly that most of the inverted values are more accurate than which listed in Table 5, and the uncertainties of the inversion are also smaller comparatively.

In this MSDT strategy, we only use the red band for an illustration, because of the USM element of structural parameters are larger than that in the NIR band.

The above MSDT strategy can be sumarrized as:

$$\mathbf{USM_0} \rightarrow \text{invert C} \rightarrow USM_1 \rightarrow \text{invert } nR^2$$
$$\mathbf{b/R} \rightarrow USM_2 \rightarrow \text{invert Z} \rightarrow USM_3 \rightarrow \text{invert h/b, } \Delta h/b$$

5 DISCUSSION AND CONCLUSION

From our practice in physical BRDF model inversion, MSDT appears being a very hopeful approach. The concept of USM is very helpful to decouple a complex BRDF model into a sequence of much simpler approximated models, in which only a small subset of parameters are distinguishingly the most sensitive and uncertain to a subset of observations, and others can be simply omitted or fixed. A typical such first—stage approximation ($BRDF_1$) would be GOMS around the hotsopt. In ideal case, these subsets of parameters may have no intersection, and their union is identical to the set of all parameters. Then we would complete the inversion by a series of first-stage inversions, if each first-stage inversion has enough large subset of observations.

5.1 Uncertainty of Inversion Results

However, it seems that in practice we may not often be able to do so. When there are intersection of parameter sets in $BRDF_1$ approximations or sometimes we can identify only few $BRDF_1$ approximations, we have to invert some $BRDF_1$ approximations, estimate the uncertainties of the inversion results, and apply them to next stage of inversion. Thus correctly estimating uncertainties of inversion results will be more essential, since mis-presentation of a parameter's uncertainty may mislead the later stages of inversion.

A special case of such estimation would be the case when we use only one observation to invert for one parameter. Such inversion would be nothing but

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an indirect measurement, and may result in a zero SSE. The uncertainty of such indirect measurement then could be estimated by noise level, and error analysis of the model approximation about other parameters.

Robust estimation for uncertainty when using $\mathbf{L}_1$ observations to invert for less number of parameters should be developed in future.

5.2 Effects of Bias in a Priori Expectations of Parameters

We claimed that USM is less sensitive to the initial guess of the parameter values than partial derivative matrix. But USM is still sensitive to that, needless to say.

Since a priori guess is based on statistical mean of a land-cover class, such guess is doubtless different from the true value of a certain target. For the parameter active in the first stage of inversion, such bias would result in a bias in the result if the given a priori uncertainty is narrow. A natural suggestion would be to use the same observation to invert but with new expectation and hopefully the iteration may converge to true value. But the danger is that, by doing so we have discarded the priori knowledge and merely depend on the same observations. So we prefer a possibly biased result but with a reasonably wide uncertainty and not too far away from class mean, to an iteration result without new information. However, more studies are needed to minimize the effects of biased initial guess in misleading inversion strategy.

5.3 Stability of MSDT Inversion

Since we always try to invert the most sensitive parameters, the MSDT inversion is quite stable. However, when sensitive parameters are getting less and less uncertain, attention must be paid not to fix sensitive parameters as if they were accurately known. This even applies to the observation's direction measurement in case BRDF has a sharp hotspot, and there are samples around it. If it is desired to use samples around the hotspot, then the limited accuracy of the direction measurements must be taken into account as additional uncertainties in USM, rather than known parameters.

5.4 More a Priori Knowledge

In above USM table for GOMS, the uncertainty of G, C, Z are treated as independent. But in fact even we have little ideas on what their values are, we should know that shadow is darker than sunlit area. We have tried to put this knowledge into USM, and it shows even better ability to decouple BRDF into two simpler approximations.

5.5 Error Analysis of the Inversion Result of Changping Flight Data

As we mentioned above, the noise in the observations can effect the uncertainty of the inversion result, but another important factor is that the bias of the flight position of the plane, it may lead a bigger bias to the inversion result, especially near the hotspot. This should be investigated further in the future.

Because of the Li-Strahler GOMS model is based on the assumption that the crown located on the ground randomly, the apple trees in the Changping flight area distribute regularly in a grid of $5\text{m}\times 6\text{m}$, so it should lead some systematic bias in inversion. However since nR^2, b/R and zenith angles are all small, this bias should be ralatively small comparing to the accuracy we achieved so far in measurements/inversion.

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BRDF 物理模型反演中的不确定性与敏感性矩阵

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摘 要 BRDF 物理模型通常非常复杂，很难反演，一般都要利用先验知识固定其中一些参数来反演其余的参数。通常大多数人认为应该固定不敏感的参数，但就如何定义一个参数在反演中的敏感度的问题至今未达成共识。李小文和 Strahler 以及王锦地也认为只有那些最敏感与最不确定的参数应该参加反演，而且应用全部观测数据的一部分去反演，但他们未能说清楚怎么定义“最敏感与最不确定”的参数以及如何寻找相应的那一部分观测数据。由于缺少对参数敏感性和不确定性定量的描述，使得 BRDF 物理模型的反演成为一种“技巧”或“艺术”。

我们尝试去建立一种 BRDF 模型反演的通用的方法，它基于知识的积累和我们称之为多阶段目标决策（MSDT）的反演策略。

这一反演策略基于给定观测方向/波段下的不确定性和敏感性矩阵（USM)。它有点类似于牛顿最小化方法中的偏微分矩阵，但有 3 个明显的区别：1) 考虑了初始估计值的不确定性；2) 对初始估计值的依赖性小；3) 定义中所有的元素有相同的单位，可定量地比较。文中给出了对于 ASAS 样本利用 Li-Strahler 几何光学模型得出的一个 USM，从中可以很明显地看到应该先反演哪些参数，以及应该用哪部分观测值。在更为复杂的采样模式下，可以用等高线来表示 USM。

为了论证 MSDT 策略，我们先用全部的昌平飞行数据同时反演 Li-Strahler 几何光学模型中的所有的 7 个参数，然后利用基于 USM 的多阶段目标决策去一步步地反演，收到了令人鼓舞的效果。

关键词 反演，BRDF 模型

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