

Derivation and validation of a new kernel for kernel-driven BRDF models

Xiaowen Li^{a,b}, Feng Gao^{a,c}, Liangzan Chen^a and Alan Strahler^a

^aDept. Geography and Center for Remote Sensing, Boston Univ.,
725 Commonwealth Ave., Boston, MA 02215, USA

^bResearch Center for Remote Sensing, Beijing Normal Univ., Beijing 100875, China

^cNanjing Institute of Geography and Limnology, CAS, Nanjing 210008, China

ABSTRACT

Kernel-driven bidirectional reflectance (BRDF) models have recently been widely used for mapping albedo with multiangle remote sensing data such as ASAS or temporal AVHRR sequences. An Ambrals algorithm will be used to produce global BRDF and albedo products in the coming EOS era using multiangle reflectance data from the MODIS and MISR. Its operational version currently uses a combination of Ross-Thick and Li-Sparse-Reciprocal kernels which has been validated favourably over other kernels or combinations.

To further improve the ability of extrapolation of the Ambrals kernel combination with better physical sense while keeping its data-fitting ability, a new kernel, Li-Transit, is derived and suggested to replace Li-Sparse-Reciprocal kernel in next version of Ambrals. We tested the new kernel combination against the current one and a few alternatives using 29 field collected BRDF data sets. The results show similar data fitting ability and more reliable extrapolation for albedo mapping. A test is also done by using the new combination and the current one to produce temporal albedo change maps of New England of U.S.A. using AVHRR images.

Presented also is our recent study on scaling effect of Helmholtz principle of reciprocity, and discussion on application of a priori knowledge in kernel-driven BRDF model inversion.

Keywords: BRDF, kernel-driven model, inversion, a priori knowledge

1. INTRODUCTION

Albedo is particularly important in the land surface energy balance. Thus accurate representation of surface albedo is necessary for many applications. Albedo can be defined as the ratio of reflected solar shortwave flux from the earth to that incident upon it. Detailed definitions can vary depending upon context, such as spectral albedo, wideband albedo, black-sky albedo (or directional-hemispherical reflectance) and white-sky albedo (synonymous with the bihemispherical reflectance). If incident solar radiation is purely directional, as would happen if there were no scattering atmosphere, it's called black-sky albedo. Alternatively, incident radiation may be isotropic, which case may be called the white-sky albedo. The two cases are unrealistic extremes, but its linear combination weighted by proportions of skylight and direct sunbeam is easier for users to describe temporal change of realistic albedo than using BRDF itself.

Early investigators usually assumed a Lambertian terrestrial surface, a necessity due to the sensors at that time all nadir-viewing only. Most natural surfaces, however, have anisotropic reflectance and the Lambertian assumption can result in errors of up to 45% in the calculation of albedo (Kimes, 1985). Thus in order to accurately retrieve albedo from remotely sensed measurements the directional nature of the reflected radiation needs to be taken into account. The directional reflectance of a surface can be expressed as a function of illumination (i) and viewing (v) geometry, known as the bidirectional reflectance distribution function (BRDF). The black-sky albedo is derived by integrating the BRDF over the observational hemisphere. The white-sky albedo can be obtained by further integrating the black-sky albedo over the illumination hemispheres (Strahler et al., 1994). Unfortunately, the BRDF cannot be directly measured in field as an infinitesimal solid angle and an infinitesimal surface area can hardly be realized. Instead directional radiometers with a finite field of view (FOV) measure bidirectional reflectance factors (BRFs) over the footprint of its FOV. The BRF's limit is related to the BRDF by a scaling factor. Early work in field was performed by Kriebel (1978), Kimes et al. (1986), who measured the BRFs of a variety of bare and vegetated surfaces, Ranson et al. (1985), who studied soybean canopies and Irons (1992) who studied soil surfaces. All of

these studies used ground-based directional radiometers. Deering et al.(1986) developed the PARABOLA directional radiometer which is currently the principal instrument for the ground-based measurement of BRDFs. More recent measurements are obtained by airborne ASAS (Irons, 1992), POLDER simulator (Leroy and Breon, 1994), CAR (Tray, 1998), and few satellite sensors such as temporal sequence of AVHRR (Eidenshink and Faundeed, 1994).

Only with robust physical models, the parameters estimated from a few observations over limited ranges of illumination and viewing directions can be applied to the other parts of bihemispheres. However, these physical models usually are nonlinear, and have many parameters (usually more than 7), and thus are difficult to invert for parameter estimation, especially from sparsely sampled observations.

Following the approach pioneered by Roujean (1992), Wanner et al. (1995) described a reformulation of these physical models through approximations in order to obtain semi-empirical linear combinations of kernels. The model framework, known as AMBRALS, allows a user to fit a three parameter kernel-driven BRDF to the measured BRDF. The values of the three unknowns are determined by the least square fitting. Whether the model can then be used in a forward mode to determine albedos then depends on whether the approximations used for kernel derivation are still valid beyond the range of illumination and viewing geometry at which the observations are sampled. This is a vital point for albedo estimation from kernel-driven BRDF model, since hemispherical and bihemispherical integration may need extrapolations far away from illumination and viewing geometries where the observations were acquired. Moreover, extrapolation is further needed for wideband albedo. Therefore, the ability of extrapolation is the key to claim a kernel-driven model semi-empirical instead of empirical.

2. KERNEL-DRIVEN BRDF MODELS

Linear kernel-driven BRDF models were designed to ease the difficulties in inversion of non-linear physical models, at expense of brutal approximation of original physics. A linear kernel-driven BRDF model has the following form:

$$BRDF = f_{iso} + f_{vol} * k_{vol}(ti, tv, \phi) + f_{geo} * k_{geo}(ti, tv, \phi) \quad (1)$$

where k_* are "kernels", known functions of illumination and viewing geometry (ti: the zenith angle of solar direction, tv: the zenith angle of viewing direction, ϕ : azimuth difference of sun and sensor); f_* are three unknown coefficients to be adjusted to fit observations. With more than 3 uncorrelated multiangular observations, a regression method can get the estimations of the three parameters much more easily than least square error fitting of a nonlinear models.

Original design of AMBRALS includes a collection of different kernels for various landcover types. However, the user community prefers a unique combination of kernels. After extensive effort of validation (Hu, et al., 1997), it's determined that the combination of RossThick (k_{vol}) and LiSparse (k_{geo}) kernels has the best ability fitting BRDF measurements (Privette et al., 1997). RossThick is a volume scattering kernel to describing the BRDF from a homogeneous leaf canopy with very large LAI and spherical LAD; while LiSparse is a geometric kernel to describe strong shadow casting effect of sparsely located crowns, or other opaque clumps. Generally speaking, the RossThick kernel characterizes a hotspot with a "bowl shape" at large zenith angles; while LiSparse kernel characterizes a dune-shape hotspot especially in forward scattering directions.

However, data fitting ability isn't the only important thing for a semiempirical model, more important is its ability of extrapolation. LiSparse kernel was designed for sparsely located clumps and associated shadows, whenever the area proportion of this clump plus shadow is approach the unit, the LiDense kernel should replace LiSparse, since the approximation made for LiSparse is $\exp(-x) = 1-x$, where x is the areal proportion mentioned above, roughly proportional to $\sec(tv)$. It's very clear, whenever x is greater than one, the approximation will be no longer valid in any physical sense. For this reason alone, LiSparse kernel has very poor ability for extrapolation at larger viewing zenith angles, where negative reflectance may appear even the kernel fits the sampled observation very well.

A remedy has been proposed based on the principle of reciprocity, called LiSparseRModis (LiSparseR for short) kernel (Lucht, 1998). Eventhough we have proved that the Helmholtz principle of reciprocity suffers scale effect over heterogeneous landsurface, and thus does not generally apply at the scale of remote sensing pixel (Li, et al., 1999), the remedy improved the kernel's extrapolation ability. The reason can be explained as follows.

We may express the LiSparse kernel as:

$$k_{sparse} = A(ti, tv, \phi) - B(ti, tv, \phi) \quad (2)$$

where $A(ti, tv, \phi) = P(ti, tv, \phi) * sec(tv)$ and $B(ti, tv, \phi) = sec(ti) + sec(tv) - O(ti, tv, \phi)$, where P and O are reciprocal functions regarding ti and tv (details refer to Wanner et al., 1995). Therefore to make the kernel reciprocal, a sec(ti) term is added:

$$k_{sparseR} = P(ti, tv, \phi) * sec(tv) * sec(ti) - B(ti, tv, \phi) \quad (3)$$

As we illustrated above, the poor extrapolation ability of LiSparse comes from the fact that $B(ti, tv, \phi)$ become very large at large zenith angles, an additional sec(ti) in the positive term makes this less likely happen. At the mean time, since solar zenith angle (ti) changes very little for the most of data sets we used to test fitting ability of kernels, this additional term change the kernel's fitting ability very little. For this reason, LiSparseR will be used for operational codes of MODIS BRDF product.

However, at the scale of remote sensing pixels, the physics of reciprocity is weak, Li et al. (1999) pointed out that if there is unsymmetric crosstalking in remote sensing pixel, the principle will break down at that scale. Greffet and Nieto-Vesperinas (1998) also investigated the scale effect of the principle, and found it is still valid as a good approximation at the scale of wavelength, even in case that "lateral shift" (equivalent to cross-talking as we called) exists. In addition, LiSparseR may still make reflectance negative, though less likely than LiSparse does.

In order to solve this problem, we return to the original designs, i.e., whenever the approximation $\exp(-x) = 1-x$ is no longer valid, we should switch to LiDense kernel:

$$k_{dense} = 2 * k_{sparse} / B(ti, tv, \phi) \quad (4)$$

which is stable for full range of sec(tv) or sec(ti). However, there are two problems in actual implementation: 1) after the linearization of the original model, the variable x no longer exists, so we don't know when we should switch from LiSparse to LiDense; 2) in validation, the fitting ability of LiDense is not as good as LiSparse, we don't want such switching to degrade the fitting ability too much.

With these considerations in mind, we designed a new kernel called LiTransit:

$$k_{transit} = k_{sparse}; \text{ if } B(ti, tv, \phi) > 2, k_{transit} = 2 / B(ti, tv, \phi)$$

The transition is natural, i.e., at $B=2$, $k_{sparse} = k_{dense}$, thus it's easy to implement. Though, this transition may not be accurately where the switching should happen. So it needs to be tested using available data sets to know whether this natural seamless transition works.

3. TEST OF THE DATA FITTING ABILITY OF LITRANSIT

Total 29 field measured BRDF data sets were used for testing. Among the 29, 27 sets were used for tests before, and the additional two are also from Deering's Boreas forest measurements (Hu, et al. 1997). RossThick was used as the bowlshape kernel all through the test.

Tests were first done by the LiTransit kernel against LiSparse and LiDense. The results on the square fitting error are:

	LiTransit	LiSparse	LiDense
Least	8	19	2
Mid	21	3	5
Greatest	0	7	22

It is somehow not easy to judge whether LiTransit or LiSparse has the best fit. Among 21 datasets which the LiTransit yields second best fitting, there are 3 categories of cases:

- (1) almost the same good fitting as LiSparse (12 data sets). For example, the corn data set show:

	LiTransit	LiSparse	LiDense
LSE	0.048742	0.048615	0.054245

Thus LiSparse is slightly (0.000127 absolute and 0.3% relative) better in fitting, but the albedo resulted from LiSparse is: 0.021415 (red), 0.105266 (NIR); and the LiTransit gives: 0.0924 (red), 0.2073 (NIR), while the reflectance ranges of the corn dataset are from 0.0497 to 0.2634 for red and from 0.1299 to 0.4981 for NIR. Thus the conclusion is clear, the new kernel is close to what the observations would support, while the old LiSparse suffers a wild extrapolation at large zenith angles.

(2) the LiSparse is clearly fitting the data better than the LiTransit, basically including soil, field, and low cover vegetations (7 in total). For example, the dataset Soil.1 shows:

	LiTransit	LiSparse	LiDense
LSE	0.035740	0.027309	0.042190

But LiSparse gives out an white-sky albedo: 0.147459 (red) 0.207355 (NIR) , which are smaller than all four corresponding black-sky albedo of the same kernel:

VZN	Nadir	30	45	60 (degrees)
Red	0.163225	0.162315	0.161883	0.160044
NIR	0.223696	0.223254	0.223746	0.223453

While the LiTransit kernel gives out similar black-sky albedo:

VZN	Nadir	30	45	60 (degrees)
Red	0.182863	0.172480	0.164256	0.163362
NIR	0.246793	0.235252	0.226725	0.227965

but a more likely white-sky albedo: 0.171636 (red) 0.236552 (NIR).

All 7 datasets in this categories show the similar patterns.

(3) The LiTransit and LiDense have the similar fitting ability while LiSparse is the worst (for mostly dense vegetation).

Therefore, it's concluded that the LiTransit behaves as being designed, i.e., it has the similar fitting ability for moderately vegetation coverage as the LiSparse, slightly better for dense vegetation, but slightly worse for mostly baren sites, but it's constrained reasonably well, thus won't get wild extrapolation.

Eventhough B=2 transition boundary is seamless and natural, we tried to change this bigger or smaller, the results show that whenever by new boundary LiTransit gets a few best fittings from LiSparse, it loses almost equal number to LiDense. So we decide to keep B=2 boundary as the natural transition.

Then we tested LiTransit against LiSparseR and LiTransitR, which is artifitially made by adding another sec(ti) similarly as LiSparseR.

We looked at 1) fitting error difference; 2) black-sky albedo's change with SZN; 3) white-sky albedo.

In 29 data sets, 21(LiTransit) and 22(LiTransitR) behave similarly to LiSparseR, in all regards of the above three criteria. The different behaviors mainly occur for sparsely vegetated datasets: field, grass (very low NDVI), soil.1 to 3, corn (very low NDVI), steppe. All these data show downward black-sky albedo with increasing SZN. How can we judge a data set would show a downward black-sky albedo? Let's again use the corn dataset (red band only) as an example:

	f_{iso}	f_{vol}	f_{geo}	SZN:	0	30	45	60
LiSparse	0.243	0.020	0.088		0.129	0.107	0.074	0.011
LiTransit	0.309	-0.082	0.167		0.172	0.141	0.104	0.055
LiDense	0.417	-0.188	0.200		0.227	0.164	0.116	0.055

The observations has an SZN ranges from 38.2 to 45.1 degrees and the fitting SSE's are 0.0486, 0.0487, and 0.0542 respectively in order.

By looking at these results, we hardly know which set of black-sky albedo we can trust. However, knowing that LiSparse is a sharp downward kernel, RossThick is a bowlshape kernel, and LiTransit and LiDense are milder downward kernels than LiSparse, we can conclude the original data must have a rather sharp downward tendency in SZN range 30-45 degrees, and only LiSparse kernel can model this tendency well, at the expense that going wild near and beyond 60 degrees, while LiDense and LiTransit kernels can hardly fit the downward trend in data and have to turn f_{vol} to negative.

So the downward trend of black-sky albedo (BSA) with SZN should be a real feature in data at the range SZN from 38 to 45 degrees.

Now, we turn to reciprocal version of kernels:

	f_{iso}	f_{vol}	f_{geo}	SZN:	0	30	45	60
LiTransitR	0.263	-0.187	0.168		0.129	0.116	0.102	0.082
LiSparseR	0.226	-0.074	0.100		0.099	0.092	0.081	0.064

The fitting is slightly worse than LiTransit, better than LiDense.

The results are understandable, since R-version of kernels has an additional $\sec(\text{ti})$, so it makes both LiTransitR and LiSparseR have less sharper downward trend, more negative f_{vol} has to be employed to fit the data, and even though, the drop of black-sky albedo seemingly can not be well retrieved.

Worse than that, when the SZN range in the data is larger, the downward tendency of black-sky albedo with SZN in the most of the sparse sites can not be retrieved. For example, the site "field" (red only) has:

	f_{iso}	f_{vol}	f_{geo}	SZN:	0	30	45	60
LiSparse	0.269	0.261	0.063		0.183	0.180	0.178	0.171
LiTransit	0.333	0.078	0.148		0.201	0.189	0.168	0.148
LiDense	0.331	-0.001	0.114		0.221	0.190	0.171	0.153

The SZN ranges from 26 to 45 degrees, and the fitting SSE's are 0.0158, 0.0312, and 0.0416 respectively in order.

This presents a slightly downward trend of black-sky albedo in SZN range 26 to 45 degrees. However, because of the additional $\sec(\text{SZN})$ term, the trends are almost reversed for R-kernels:

	f_{iso}	f_{vol}	f_{geo}	SZN:	0	30	45	60
LiSparseR	0.256	0.186	0.064		0.170	0.178	0.190	0.215
LiTransitR	0.312	0.061	0.154		0.186	0.183	0.185	0.194

The fitting SSE's are between LiSparse and LiTransit respectively in order.

More interesting is the pattern of conifers. Judged from NDVI, they should not be called "sparse", but their black-sky albedo may be slightly downward or slightly upward, hard to judge. For example, the obs.new data set has:

Red band, SZN ranges from 35 to 74 degrees

	f_{iso}	f_{vol}	f_{geo}	SZN:	0	30	45	60
LiTransit	0.059	0.024	0.027		.0357	.0325	.0295	.0274
LiSparse	0.040	0.041	0.009		.0283	.0283	.0284	.0284

The fitting SSE's are .0183 and .0188, the difference is rather small. And the white-sky albedos are .0262 and .0304 respectively. Now interesting question is: which white-sky albedo and which black-sky albedo trend we should trust more.

When we turn to R-version of kernels, as we can expected, both turn the black-sky albedo upward:

	f_{iso}	f_{vol}	f_{geo}	SZN:	0	30	45	60
LiTransitR	0.040	0.011	0.019		.0245	.0247	.0258	.0287
LiSparseR	0.032	0.022	0.007		.0232	.0241	.0256	.0287

The fitting SSE's are .0178 and .0183, and white-sky albedos are .0276, 0.0272 respectively.

Fortunately, the dataset obs.new has almost hemispheric viewing sampling of BRDF at various SZN, so the black-sky albedo can be approximately estimated by average (weighted by $\sin(tv)*\cos(tv)$). Thus we may compare with modeled ones:

SZN	Measured	LiSparse	LiTransit	LiSparseR
35	0.0272	0.0283	0.0315	0.0245
40	0.0277	0.0283	0.0305	0.0250
45	0.0266	0.0284	0.0295	0.0256
50	0.0272	0.0284	0.0287	0.0264
55	0.0269	0.0285	0.0279	0.0274
60	0.0262	0.0284	0.0274	0.0287
65	0.0252	0.0280	0.0271	0.0303
70	0.0261	0.0269	0.0272	0.0325
74	0.0280	0.0247	0.0277	0.0346

The coefficients of correlation with measured BSA are -.3376 for LiSparse, 0.5201 for LiTransit, and -.1487 for LiSparseR. Thus we can see, only RossThick-LiTransit fits the feature, that slightly drops till SZN about 65, and then turn up at larger SZN. Note that because Parabola measurements don't have VZN beyond 75 degrees, so comparison of absolute values is not very meaningful.

4. OTHER TESTS ON CAPABILITY OF LITRANSIT

As being designed, f_{geo} is to have some physical sense to describe how the surface is clumped into shadow-casting stuffs. So we compared classification ability of f_{geo} (both red and NIR) from LiTransit and LiSparseR.

Both kernels show some sense of structure information, major differences occur for only three cases:

- 1) LiTransit makes Irrigated.wheat (NDVI 0.78) very structurally alike to FIFE.July.11 (NDVI 0.81), while LiSparseRModis makes Irrigated wheat very structurally alike to Kimes.corn (NDVI 0.58).
- 2) LiTransit makes Aspen, Pine, and Hardwood well separated, but LiSparseRModis makes all three very alike.
- 3) LiTransit makes Orchard.grass (NDVI 0.61) alike sparsest ones such as Sorg (NDVI 0.61) and Vege (NDVI 0.58), while LiSparseR makes it more alike to denser ones like Old.Jack.Pine (NDVI 0.64) and Irrigated.wheat (0.78).

According to Strugnell and Lucht (SL, 1999), Orchard grass is described as sparse grass-like vegetation, by intuition, irrigated wheat may have more structural similarity with FIFE grassland in July than corn. And Aspen, Pine, and Hardwood may have certain structural difference. However, because we don't have more accurate

information on these different structures and there are some spectral/radiometric differences in instruments, this comparison is inconclusive, we can only say LiTransit looks better than LiSparseR in showing structural difference.

NOAA AVHRR sequence has been used for testing the AMBRALS algorithm (SL, 1999). Test using a poor quality New England AVHRR data (228-243) is done for RossThick-LiTransit against RossThick-LiSparseR, on the frequency of 2 unpleasant cases: inverted white-sky albedo (WSA) negative or greater than one):

(NOL >= 7)		WSA<0	WSA>1		WSA<0	WSA>1
LiTransit	RED	1107	0	NIR	1	0
LiSparseR	RED	1178	0	NIR	1	0

The above results were obtained from direct inversion for all pixels with number of looks (NOL) greater than 7. Eventhough better algorithm can make the inversion less sensitive to noise, the information of poorly sampled and/or noisy observations may still not be enough for three unknowns. In the next section, we illustrate the accumulation of a priori knowledge for more reliable inversion.

5. A PRIORI KNOWLEDGE BASE FOR BRDF OF LAND SURFACE

The earth surface is a very complicated system, and quantitative remote sensing has to rely on the accumulation of knowledge of this surface. Therefore, the 29 datasets will serve as our initial knowledge base, from which we can have some ideas what landsurface's BRDF should look alike. However, BRDF as a function of four variables (t_i, t_v, ϕ , and wavelength) is not easy to display or comprehend or make use as a priori knowledge.

According to Li et al., (1998), a priori knowledge can be represented in different forms: 1) (wide) hard bounded range of parameter values, usually applicable for physical limits, such as albedo must be positive and smaller than one; 2) some parameters or their relations are accurately known or we know they are insensitive to the given observation geometry, then they can be fixed – we may call such knowledge δ -bound; 3) unknown parameters have a priori known joint probability density function (JPDF), we call it a soft-bound range. All three kinds of a priori knowledge can be made of use in inversion depending upon the situations. Here what we need is to accumulate soft-bound knowledge of three f_* , since it's semiempirical nature, we don't have physical limits for them, and a wide hard bound's advantage in inversion is limited. On the other hand, without softbound knowledge, it's unlikely we can have any δ -bound knowledge.

On the other hand, a priori knowledge may be at different levels. We need to know the the JPDF of 3 coefficients for landsurface globally, we also like to know the conditional JPDF for given raw data; or for given landcover type.

The importance of accumulation for such knowledge has been realized for years. It's probably the time to initiate a knowledge base for AMBRALS.

5.1. Initial Knowledge Base

Using AMBRALS inversion capability, we obtained the statistics of three coefficients of the 29 data sets as follows. One problem is, as mentioned previously, is the difference in instruments. Since we don't have good ground to calibrate them, the knowledge is very raw – but still better than nothing. The following statistics of the three coefficients are for LiTransit:

Red	f_{iso}	f_{vol}	f_{geo}	NIR	f_{iso}	f_{vol}	f_{geo}
mean	0.142037	0.043939	0.049334		0.400393	0.189117	0.082912
σ	0.126338	0.044809	0.051687		0.108432	0.158399	0.080192

5.2. Expansion of the Knowledge Base

Strugnell and Lucht collected 68 data sets, among which data sets from Kimes, Ranson, Irons, and some from Deering are the same as those in Hu's collections. First thing we'd like to do before combining two collections together, is to see whether our initial knowledge base can be apply to the SL collection for identifying problem in data compatibility.

We used AMBRALS to invert all new datasets and only 6 data sets have results 'strange' to the a priori knowledge we gained from the above statistics, we have to look into the data and look for reasons.

(1) 1988/chuck.site: It has only one directional observation. Later Strugnell suggests there must be some errors in data transfer, the lose is not recoverable, so we give up this set.

(2) SCAR/forest: It has very fine VZN angular resolution (1 degree in both viewing zenith from 0 to 90, and azimuth from 1 to 360), but only one SZN (56.67). There is a very strong forward scattering from 70 to 90 degrees. The current model combination does not use the specular kernel, so is not able to model this feature. We cut the data beyond 70 degrees of viewing zenith angles.

(3) 1988/dune-flat: Like the chuck.site, there are errors in data transfer, and we don't know how to retrieve the original. We give up this set.

(4) 1987/ifc1-site2: There was error in band information processing. We found corrected the error and then everything is fine.

(5) 1988/snow-on-lake.ice: This is something new to the initial knowledge base, the strange results should be added into knowledge base.

(6) 1989/silt.playa: New, the strange results should be added into knowledge base.

Then, combined with the 29 data sets, we have a expanded knowledge base from total 73 data sets, the global knowledge now include:

Red	f_{iso}	f_{vol}	f_{geo}	NIR	f_{iso}	f_{vol}	f_{geo}
mean	0.15329	0.04148	0.04271		0.39346	0.16249	0.07926
σ	0.14431	0.04297	0.05423		0.12589	0.11993	0.08693

The covariance between the three parameters are:

Red	f_{iso}, f_{vol}	f_{iso}, f_{geo}	f_{vol}, f_{geo}	NIR	f_{iso}, f_{vol}	f_{iso}, f_{geo}	f_{vol}, f_{geo}
	0.00012	-0.00029	0.00403		-0.00556	0.00493	-0.00713

Comparing with the statistics of 29 data sets, the means change very little, while varainces are increased, because the new extremes are now in the knowledge base. So finer grouping is more necessary and feasible. But we would like to illustrate how this raw global knowledge base would be used in inversion first for examples.

6. MAKING USE OF KNOWLEDGE BASE

The principle of applying Bayes inference theory in quantitative remote sensing inversion was illustrated in Li et al., 1998, for example.

6.1. Using a priori knowledge to find and smooth noisy samples

Temporarily we define a failed inversion as its resulted albedo, either BSA or WSA is greater than one or negative. With stable kernel LiTransit, it's now easy to identify the reasons of the failed inversion: poor sampling including insufficient number of looks, and noisy sample(s). For example, one of the above mentioned NIR inversion failure has the following original data (NOL = 8):

	VZN	VAZ	SZN	SAZ	Red	NIR
0	61.300	124.600	28.800	0.000	0.030	0.165
1	27.600	42.000	35.200	0.000	0.055	0.287
2	12.400	42.500	34.300	0.000	0.036	0.298
3	20.200	130.600	32.900	0.000	0.039	0.216
4	33.700	129.200	32.500	0.000	0.037	0.210
5	53.000	126.500	32.000	0.000	0.020	0.195
6	17.000	43.400	37.800	0.000	0.083	0.190
7	1.300	78.300	37.100	0.000	0.072	0.181

Ambrals inversion result for NIR are: $f_{iso} = 0.617029$, $f_{vol} = -0.760900$, and $f_{geo} = 0.395941$. This yields a WSA = -0.004808.

Based on the a priori knowledge in parameter space, it's easy to map the parameter JPDF into data space assuming every PDF is normal and JPDF multivariate normal. Thus we can obtain a priori PDF of observation in each viewing direction. The comparison of true observations and corresponding PDF is as follows:

	NIR.ref	Est.ref	Est.var	Dist
0	0.165	0.290	0.247	0.251
1	0.287	0.347	0.168	0.146
2	0.298	0.331	0.176	0.078
3	0.216	0.285	0.236	0.141
4	0.210	0.278	0.248	0.136
5	0.195	0.282	0.252	0.172
6	0.190	0.326	0.190	0.313
7	0.181	0.300	0.221	0.253

where $Dist = (Est.ref - NIR.ref) / \sqrt{Est.var}$ Then we decide to remove the observations with the largest Dis till the WSA > 0, the looks 6, 7, 0 are removed, inversion using the remaining 5 looks gave the results: $f_{iso} = 0.535270$, $f_{vol} = -0.339929$, and $f_{geo} = 0.292046$. This yields a WSA = 0.118472.

Another failed inversion the section 2.3 has the similar patterns with NOL = 7. The inversion is failed because of a negative BSA at SZN=60 degrees. After removing the two least likely looks, the inversion results are: $f_{iso} = 0.539713$, $f_{vol} = -0.353146$, and $f_{geo} = 0.282723$. This yields a WSA = 0.131668, and a downward BSA from SZN =0, 30 45, to 60 degrees: 0.313777, 0.248728, 0.167710, 0.051598.

The above two inversion after removing the least likely looks are no longer failures, but the result is still problematic, since the NOL is only 5 in both examples and the results both look strange. We define a problematic inversion by the likelihood of inversion results which does not break the hard bound but looks very strange – small a priori likelihood of occurrence based on our knowledge. For example in the above two inversions with 5 looks, inverted coefficients still look strange – unusually negative f_{vol} , and large f_{geo} , comparing to a priori knowledge.

By looking at the scattering plots of inverted parameters for 73 datasets and failed inversions in 3-D parameter space. It's clear that all failed inversions result in coefficients away from and surrounding the known 73 good results. Then we define an inversion is problematic if one or more coefficients fall into the region between the most-likely regions of the a priori JPDF and the least-likely region where failed inversion are distributed.

Again, problematic inversion may be caused by noisy data or poor sampling. We'll continue to deal with noisy data and then the poor sampling.

Knowing some looks may be noisy, instead of dropping them from inversion, we decide to smooth them. Smoothing noisy data as well as dropping outliers are both widely acceptable in practice. However, in hemispheric directions coupled with BRDF, it's very hard to determine how to take average of which directions. We tried to smooth noisy

looks by forward simulations, i.e., take average of NIR.ref and Est.ref in previous tables for noisy looks. Thus the three smoothed looks for example 1 will be: 0.227, 0.258, and 0.240 for the look 0, 6, and 7 respectively.

Adding to unchanged looks, the inversion results are now: $f_{iso} = 0.424$, $f_{vol} = -0.00536$, and $f_{geo} = 0.172$. This yields a WSA = 0.215 and BSA: 0.282, 0.254, 0.222, and 0.184. Similarly after smoothing the two noisy looks for the Example 2, the Ambrals inversion posterior estimates are: $f_{iso} = 0.437$, $f_{vol} = -0.0511$, and $f_{geo} = 0.173$. This yields a WSA = 0.218 and BSA: 0.295, 0.264, 0.228, and 0.183.

Now both inversion results look reasonable, but 3 and 2 simulated data are added into original 8 and 7 respectively. Therefore, we must add remarks into quality flag for "smoothed", "3/8 or 2/7 a priori information added for smoothing". Later in the text we will call this ratio "a priori information ratio".

6.2. Using poorly sampled data to get posterior estimates of unknowns

When sampling is poor, i.e., too few NOL, or directions are poorly located, the inversion matrix may be singular or has a large condition number, or a large noise propagation factor (Gao et. al, 1999), the inversion is underdetermined and there exists no least square solution.

In such case, application of a priori knowledge is a must. Bayes inference theory is the best way to make use of a priori knowledge, but conventional Bayes inversion requires integral in parameter space. Or in case we don't need posterior distribution in parameter space but a simple maximum likelihood estimate, we can get it by minimizing the cost function:

$$Cost(X) = (A * X - Y_{obs})' C_d^{-1} (A * X - Y_{obs}) + (X - X_0)' C_p^{-1} (X - X_0) \quad (5)$$

where Y_{obs} is the vector of BRDF observations, A is the kernel matrix, X is parameter vector f_* , X_0 is the a priori best-guess of the vector X; C_d is noise covariance matrix of data noise and model inaccuracy, and C_p is the covariance matrix of a priori knowledge of X. The total Cost(X) consist of two parts: Cost of data misfitting and cost of parameter deviation from a priori best guess.

For the purpose of illustration, let's assume now we have only single look, then the cost of data misfitting is zero, if and only if

$$f_{iso} + f_{vol} * k_{vol}(ti, tv, \phi) + f_{geo} * k_{geo}(ti, tv, \phi) - y_{obs} = 0 \quad (6)$$

The solution of course is a plane in the 3-parameter space. Everywhere on this plane, the misfitting cost is exact zero, thus we can never find a unique solution for three unknowns on this plane without a priori knowledge. Now assume C_p has a much larger variance (i.e., large uncertainty of a priori knowledg) than noise in the single look, what Bayes inversion does in this extreme case is to get the posterior JPDF over the solution plane of eq (6). And minimizing the eq (5) is actually seeking the peak of this JPDF over the solution plane.

For timely global MODIS BRDF products, integral in 3-D space is not practically possible, and even minimizing eq (5) will cost too much computing time. Therefore, we suggest to map a priori JPDF in 3-D parameter space into data space, to localize the operations, similar to the smoothing we did in the last subsection.

To inject a priori information into poorly sampled data, we simulate more directional BRDF data as:

$$Y_{simu} = A_{simu} * X_0 \quad (7)$$

Pooling these simulation data and real observations together, it can be guaranteed that it will be an overdetermined inversion and thus linear regression can be used to get a least square solution. The problem is how much new information from observation and how much a priori guess is contained in such a solution. We may explicitly write the cost function actually in the linear regression approach as:

$$Cost(X) = [A * X - Y_{obs}]' [A * X - Y_{obs}] + (X - X_0)' [A'_{simu} A_{simu}] * (X - X_0) \quad (8)$$

where A is the kernel matrix for real observations in (5). Now the total cost function consists of two parts, the first is the cost of data misfitting, and the second is again that of parameter deviation. Note that, if A_{simu} is so selected

that $A'_{simu}A_{simu}$ equals to C_p^{-1} , then eq (8) will be equivalent to the eq (5). Since covariance matrix C_p of a priori PDF of three unknowns is positive-determined, we can write it in form:

$$C_p = E * \Lambda * E' \quad (9)$$

where Λ is diagonal matrix of eigenvalues and E is corresponding matrix of column eigen vectors. Then, we can simulate three data points by:

$$A_{simu} = \Lambda^{-1/2} * E' \quad (10)$$

Note A_{simu} need only to be calculated once and stored together with X_0 and C_p .

$$Y_{simu} = \Lambda^{-1/2} * E' * X_0 \quad (11)$$

Note this simulation does not employ the forward model, but directly generates three data points which make their corresponding cost function numerically equivalent to the cost function of parameter deviation. So actually, they are abstract of a large number of random simulation based on a priori JPDF in parameter space.

Now adding the single-look observation together, the conventional LS approach will minimize eq. (8) and get a maximum-likelihood estimate (MLE) of X , which is somewhere between X_0 and the solution plane of (6). For the purpose of illustration, let's imagine that C_p is spherical and very large variance, the above MLE is the perpendicular projection of X_0 onto the solution plane of (6). Such an MLE is better than no solution and is closer to the true value of the unknown than X_0 .

But the cost of misfitting should be weighted by C_d^{-1} . In case that we don't have knowledge on C_d , we may try to add an artificial weight to real observation:

$$Cost(X) = n * [A * X - Y_{obs}]' [A * X - Y_{obs}] + (X - X_0)' [A'_{simu}A_{simu}] * (X - X_0) \quad (12)$$

where the weight n can be easily introduced into the standard linear regression. This weight actually depends on how much we trust on the new observation and how much we trust on the a priori knowledge. The larger the n , the closer the solution X will be drawn to the solution plane of (6), farther from X_0 ; but it will be less stable – since the solution planes of (6) depends on the geometry of the single look. Similar to the case for smoothing, we will call the ratio $3/n$ as "a priori information ratio".

In order to initially determine what a weight n should be used, we subset a single look measurement from one well-sampled set of the 73 sets and apply our algorithm. Their 'true values' of parameters and WSA's are obtained from full dataset. Then we can compare their one-look inversion results with their 'true values' for different a priori information ratio. Then we subset another single look and repeat. Finally, we repeat the above procedure for another well-sampled data set and go on. The same global prior knowledges are used in all cases. The results show that, for single look inversion problem, a priori information ratio $3/4$ can get a rather stable posterior estimates.

Note this approach to use a priori information is by essence the same as being suggested by Jackson (1979), but has been adapted for the use together with Ambrals. Using the algorithm, we run the New England AVHRR albedo map. Compared with the map using the same AVHRR data but standard Ambrals, the improvement is obvious.

7. CONCLUSION AND DISCUSSION

Next to do is to accumulate more a priori knowledge and have a finer grouping of data sets for finer a priori knowledge, based on raw spectral observations or landuse classifications.

The advantage of this algorithm using simulated data is its simplicity for injecting a priori knowledge into Ambral regression. However, the general approach of Bayes linear regression should be applicable to all underdetermined linear inversion problems.

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