Assessing Errors

Janet W. Campbell
Ocean Color Climate Data Records
August 11, 2005
Corvallis, Oregon
Outline

• Points from “Climate Data Records from Environmental Satellites: Interim Report” (CRC, 2004)

  Definition of a CDR
  Fundamental CDRs vs. thematic CDRs
  Assessing errors: FCDR
  Assessing errors: TCDRs

• Including the CZCS record as part of the Ocean Color CDR
• Merging data from concurrent missions
• Assessing errors: semi-analytic algorithms (Maritorena & Siegel, 2005)
• Assessing errors: empirical chlorophyll algorithms
• Beware of statistics based on log-log regressions!
• Algorithms can yield very different results even if they seem to be comparable
A climate data record is a time series of measurements of sufficient length, accuracy, and stability to determine climate variability and change.

“Climate Data Records from Environmental Satellite: Interim Report”

Committee on Climate Data Records from NOAA Operational Satellites, NRC, 2004

The report outlines key elements to consider in designing a program to create climate-quality data from satellites. It examines historical attempts to create climate data records, provides advice on steps for generating, re-analyzing, and storing satellite climate data, and ...

A climate data record is a time series of measurements of sufficient length, accuracy, and stability to determine climate variability and change.
The goal “to determine climate variability and change” implies that we can differentiate real trends or variability from spurious trends in the data due to sensor differences, sensor or orbit drift over time, ....

**FIGURE 3-3** Example of satellite intercalibration from monthly global Microwave Sounding Unit (MSU) Channel 2 anomalies. If sensors on different platforms are not calibrated with one another, spurious trends can appear. SOURCE: NASA Global Hydrology and Climate Center.
FIGURE 1-2 Thematic CDRs (TCDRs) related to different themes will be generated from the fundamental climate data records (FCDRs); for example, the calibrated antenna signals from a series of satellites (e.g., AVHRR, MODIS, VIIRS) will be used to generate a variety of TCDRs. A major effort should focus on creating and managing the FCDRs. The process of calibrating the FDCR generally involves the use of in situ measurements and critical feedback resulting from assessments of the TCDRs. Arrows might be shown in two directions. SOURCE: J. Campbell, University of New Hampshire.
The FCDRs (TOA calibrated radiances) require a continuing program of vicarious (post-launch) calibration. The sensor input data errors (uncertainty) must be rigorously characterized.

SeaWiFS Lunar Calibrations

Normalized Total Lunar Radiance / 555nm vs. Days since first image.
Validated TCDRs must have known levels of uncertainty.
The process of validating a TCDR derived from satellite measurements is not simply a matter of “ground truthing” a satellite-derived product. It is the process of establishing rigorously derived uncertainties … using independent correlative measurements. The identification, quantification, and minimization of biases and errors helps users understand … how much of a trend can be detected with the record.

A rigorous and detailed understanding of the measurement error structure is critical. Error propagation from raw data to the final derived product must be understood. Instruments and data processing will introduce systematic artifacts in the data. Error sources are not necessarily Gaussian, nor are errors uncorrelated spatially and temporally. The steps involved in deriving a geophysical variable (e.g., geo-location, calibration, correction for atmospheric effects, etc.) must be explicitly identified. Each of these requires algorithms specific to the task and will introduce uncertainties in the geophysical product.

… Quantitative estimation of uncertainties requires both a theoretical framework and empirical evidence of the differences between “truth” and satellite-derived estimates.
“A climate data record is a time series of measurements of sufficient length, accuracy, and stability to determine climate variability and change”

Do we include the CZCS record as part of our Ocean Color CDR?
Bridging ocean color observations of the 1980’s and 2000’s
in search of long-term trends.

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In press, JGR, March 2005
A complete re-processing of CZCS and SeaWiFS was undertaken in order to make the data sets as consistent as possible.

It would be worthwhile doing a similar reprocessing of MODIS Aqua data to extend this time series, but the resulting MODIS “CZCS-type” chlorophyll data will not be the best chlorophyll.

So question is: will the chlorophyll data in the long-term time series be same as our best contemporary product?
Antoine et al. 2005 (in press, JGR)
Abstract

A comprehensive revision of the “Coastal Zone Color Scanner” (CZCS) data-processing algorithms has been undertaken to generate a revised level-2 data set from the near 8-year archive (1979-1986) collected during this “proof-of-concept” mission. The final goal of this work is to establish a baseline for a global, multi-year, multi-sensor, ocean color record, to be built from observations of past (i.e., CZCS), present, and future missions. To produce an internally consistent time series, the same revised algorithms also have been applied to the first five years of the SeaWiFS ocean color observations (1998-2002). Such a data base is necessary in order to determine whether or not the ocean biogeochemistry has evolved in the past years and if so, to be able to detect near future trends. Algorithmic and calibration aspects, along with validation results presented in this paper, are tailored towards the identification of long-term trends, which mandated this reprocessing effort. The analysis of decadal changes from the CZCS to the SeaWiFS era shows an overall increase of the World ocean average chlorophyll concentration by about 25%, mainly due to large increases in the inter-tropical areas, where the seasonal cycles also substantially changed over the past two decades. Increases in higher latitudes, where seasonal cycles did not change, contribute to a lesser extent to the general trend. In contrast, oligotrophic gyres display declining concentrations.

Bridging ocean color observations of the 1980’s and 2000’s in search of long-term trends.
Plummeting plankton linked to warmer oceans

August 14, 2002 Posted: 10:50 AM EDT (14:50 GMT)

By Richard Stengel
CNN

(CNN) -- Concentrations of microscopic plants that comprise the foundation of the ocean's food supply have fallen during the past 20 years as much as 30 percent in northern oceans, according to a satellite checkup of planetary health.

2002 Results by Watson Gregg …
NASA Satellite Shows Ocean Plants Increasing Along Coasts
Phytoplankton help regulate atmosphere, health of ocean ecosystems

NASA researchers have used NASA satellite data from 1998-2003 to show that amounts of tiny free-floating ocean plants called phytoplankton have increased globally by more than 4 percent, mainly along coasts. … According to a March 3, 2005, NASA press release, this is important because phytoplankton help regulate Earth’s atmosphere and the health of ocean ecosystems. They produce half of the oxygen generated by plants on Earth and can soften the impacts of climate change by absorbing carbon dioxide, a heat-trapping greenhouse gas. …

"The ocean deserts are getting bluer and the coasts are getting greener," said Watson Gregg, an oceanographer at NASA's Goddard Space Flight Center (GSFC) in Maryland. "The study suggests there may be changes occurring in the biology of the oceans, especially in the coast regions."

"We don't know the causes of these coastal increases," said Gregg. "The trends could indicate improved health of the ecosystems as a whole, or they could be a sign of nutrient stress." … Gregg and coauthors caution that the length of time the data cover is too short to answer questions about long term trends, but for the time being the phytoplankton declines in the global oceans observed between the 1980s and 1990s appear to have subsided.

Co-authors on the study include Nancy Casey of Science Systems Applications, Inc., who works at NASA GSFC, and Charles McClain, also a researcher at NASA GSFC.
The purpose of this workshop is to help NOAA move forward with plans for creating Ocean Color CDRs …

Meanwhile NASA and/or NOAA could begin to create the Ocean Color CDRs using CZCS, SeaWiFS, MODIS, MERIS … before the launch of NPP and NPOES.

The recent papers by Antoine et al. (2005), Gregg et al. (2005) present models for how this can be done … and newsworthy results based on decadal scale changes in the chlorophyll concentration.
Let’s consider now the uncertainty in chlorophyll. How do we assess the uncertainty?.

The “errors,” “uncertainty,” and “accuracy” are typically expressed as a percentage.

The specifications for VIIRS ocean color products (RDRs, SDRs, and EDRs) is given as an “accuracy” ranging from 5% to 30% depending on the range of chlorophyll.

Historically, specification for chlorophyll was 35% -- and some claims have been made even with CZCS that these specs have been met!

Have they?

What is meant by a 35% accuracy?
NASA has just released a new data set (Werdell and Bailey, 2005) called NOMAD for evaluating algorithms. We’re planning a workshop at UNH in September to consider whether we can improve the Chlorophyll algorithm.
Fig. 6a - Comparison of the algorithm fitted to the HPLC data vs. the OC4.v4 algorithm.

The equation fitted to the data is:

\[ y = 1.2581x^4 - 3.2062x^3 + 2.8997x^2 - 2.7659x + 0.3158 \]

The coefficient of determination is:

\[ R^2 = 0.9013 \]
Measured Chlorophyll (NOMAD)

Derived Chlorophyll (OC4v4 algorithm)

one-to-one

all data

HPLC

R²=0.84

R²=0.90 (HPLC)
Table 1. Polynomial fits to the NOMAD data. Coefficients are defined based on equation (1). Error statistics based on the samples of size N where errors are defined by equation (4).

<table>
<thead>
<tr>
<th>Variable</th>
<th>OC4</th>
<th>all data</th>
<th>HPLC</th>
<th>fluoro</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>2230</td>
<td>2230</td>
<td>1350</td>
<td>880</td>
</tr>
<tr>
<td>$a_0$</td>
<td>0.366</td>
<td>0.373</td>
<td>0.316</td>
<td>0.405</td>
</tr>
<tr>
<td>$a_1$</td>
<td>-3.067</td>
<td>-2.496</td>
<td>-2.766</td>
<td>-2.403</td>
</tr>
<tr>
<td>$a_2$</td>
<td>1.930</td>
<td>1.827</td>
<td>2.810</td>
<td>1.437</td>
</tr>
<tr>
<td>$a_3$</td>
<td>0.649</td>
<td>-1.979</td>
<td>-3.206</td>
<td>-1.539</td>
</tr>
<tr>
<td>$a_4$</td>
<td>-1.532</td>
<td>0.801</td>
<td>1.258</td>
<td>0.661</td>
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</table>

Error Statistics (log-log)

<table>
<thead>
<tr>
<th></th>
<th>bias</th>
<th>RMSE</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>OC4</td>
<td>-0.047</td>
<td>0.255</td>
<td>0.86</td>
</tr>
<tr>
<td>all data</td>
<td>0.000</td>
<td>0.245</td>
<td>0.86</td>
</tr>
<tr>
<td>HPLC</td>
<td>0.000</td>
<td>0.216</td>
<td>0.90</td>
</tr>
<tr>
<td>fluoro</td>
<td>0.000</td>
<td>0.256</td>
<td>0.84</td>
</tr>
</tbody>
</table>
What is the relationship between errors expressed as bias or RMS values in units of log and the percentage or relative error?

Beware: statistics based on calculated percentage errors can be misleading. They are \( \sim \) lognormally distributed.

You can never have greater than a -100% error whereas positive errors can be arbitrarily large.
Relative error = \[ 100\% \cdot \left( \frac{\hat{C} - C}{C} \right) = 100\% \cdot \left( \frac{\hat{C}}{C} - 1 \right) \]
<table>
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</tr>
</thead>
<tbody>
<tr>
<td>mean</td>
<td>6%</td>
<td>16%</td>
<td>13%</td>
<td>18%</td>
</tr>
<tr>
<td>median</td>
<td>-7%</td>
<td>4%</td>
<td>-1%</td>
<td>5%</td>
</tr>
<tr>
<td>std dev</td>
<td>66%</td>
<td>67%</td>
<td>60%</td>
<td>74%</td>
</tr>
</tbody>
</table>

Table 2. Statistics of the percentage errors associated with the polynomials fitted to the NOMAD data.

<table>
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<tbody>
<tr>
<td>mean</td>
<td>6%</td>
<td>17%</td>
<td>13%</td>
<td>19%</td>
</tr>
<tr>
<td>median</td>
<td>-10%</td>
<td>0%</td>
<td>0%</td>
<td>0%</td>
</tr>
<tr>
<td>std dev</td>
<td>67%</td>
<td>72%</td>
<td>60%</td>
<td>77%</td>
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Error Statistics (log-log)

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<tbody>
<tr>
<td>bias</td>
<td>-0.047</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>RMSE</td>
<td>0.255</td>
<td>0.245</td>
<td>0.216</td>
<td>0.256</td>
</tr>
<tr>
<td>$R^2$</td>
<td>0.86</td>
<td>0.86</td>
<td>0.90</td>
<td>0.84</td>
</tr>
</tbody>
</table>

Statistics based on lognormal assumption (eq. 7-9)

<table>
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<td>std dev</td>
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Linear Statistics

$R^2=0.510$

$R^2=0.523$ (HPLC)
Fig. 9 – Histograms of chlorophyll data. NOMAD data distribution (blue) is compared with global SeaWiFS distribution (red) over its lifetime (1997-2005).
Ocean color CDRs will be derived by merging data from concurrent satellite missions....

Consistent merging of satellite ocean color data sets using a bio-optical model

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Received 19 April 2004; received in revised form 26 August 2004; accepted 29 August 2004
Fig. 1. Schematic of the input data and output products of the GSM01 merging model.
Frequency (histogram) of the ratio of confidence intervals
Merged Chlorophyll: SeaWiFS Chlorophyll
Fig. 8. Comparison the SeaWIFS and MODIS Terra $L_{\text{sw}}(\lambda)$ data at 443 and 490 nm for pixels with reduced confidence intervals in the Chl product (left panels) and for the pixels where the Chl confidence intervals are higher in the merged data set (right panels). Terra and SeaWIFS daily level 3 $L_{\text{sw}}(\lambda)$ data (Dec. 4, 2000).
Recommendations

1. Recognize that chlorophyll is lognormally distributed on a range of scales. Thus accuracy or uncertainty should be expressed in terms of biases and RMS errors of log(Chl).

2. Uncertainty in the log(Chl) can be converted to an uncertainty in Chl but you won’t like the answers!

3. Uncertainty should be allowed to vary – improving over time from CZCS to SeaWiFS to MODIS to VIIRS.

4. Finally, given the budgetary constraints within NOAA to create CDRs, given the history of what’s considered news worthy, and the challenges of getting the Chlorophyll right … I recommend that the Ocean Color TCDR be chlorophyll concentration, and that the FCDRs be nLw’s.