Estimating the uncertainties in the products of inversion algorithms or, how do we set the error bars for our inversion results?

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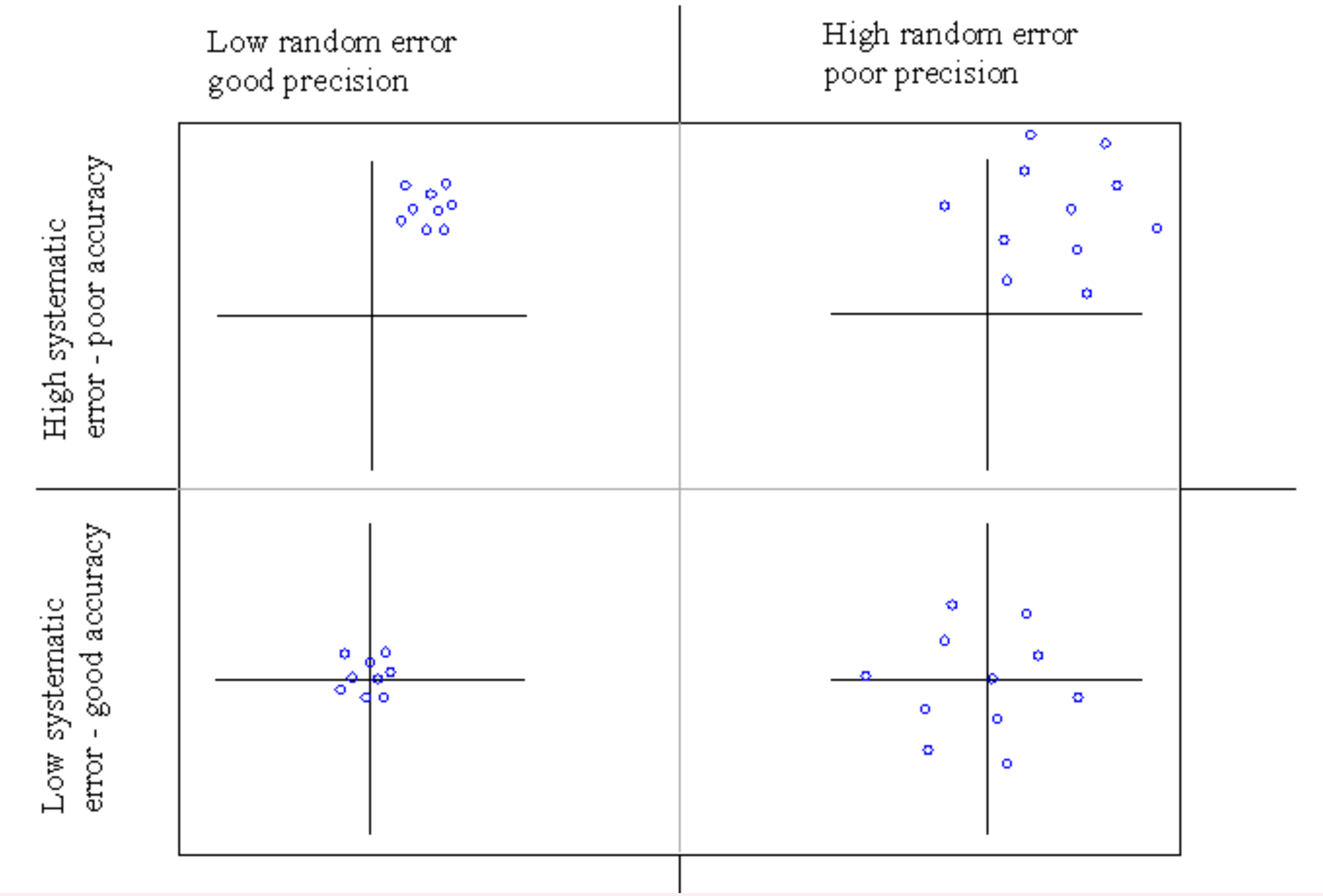
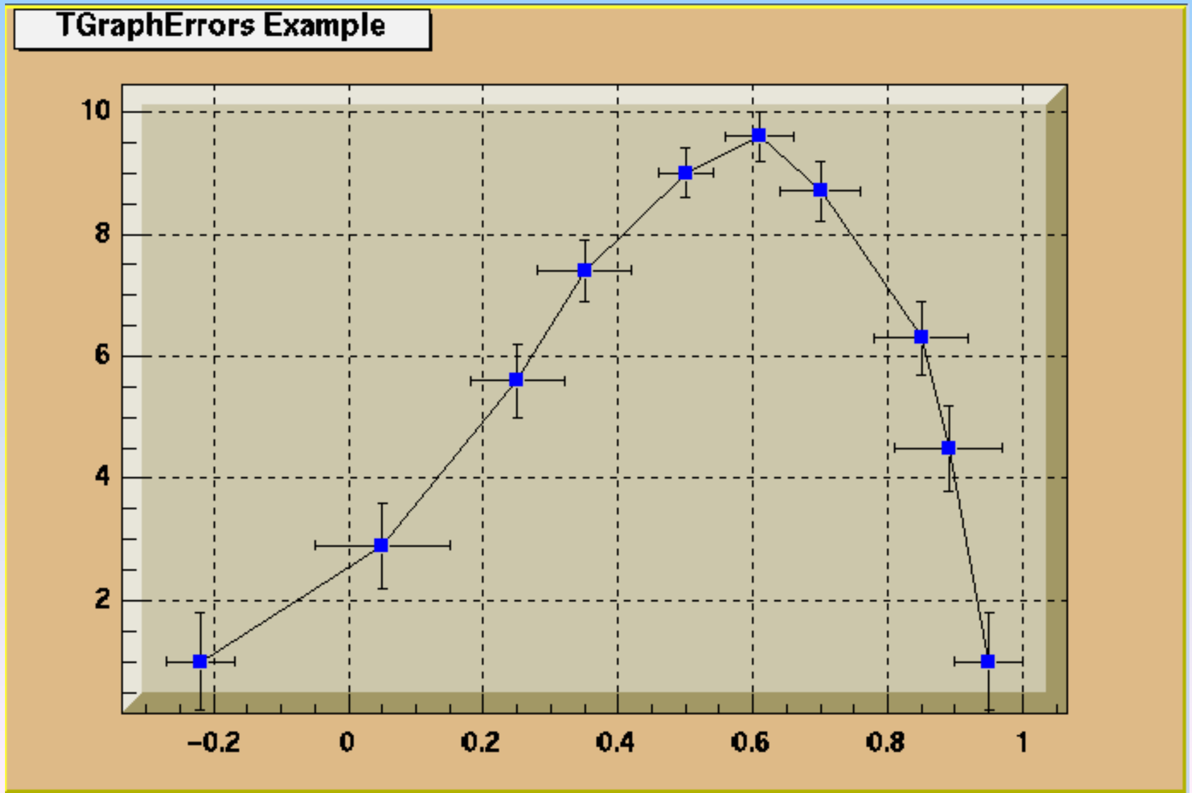


- In science there are no quantities that have no uncertainties associated with them.

- The way we present uncertainties graphically is with error bars.

- Sometimes error bars are either too small to be noticed or simply neglected.

- In the least, uncertainties should be reported so significance in reported relationship can be evaluated.



Sources of uncertainties in empirical inversion algorithms:

- Uncertainties in the training set (e.g. biases in the data set).

- Data inverted not covered by the training set (application of open ocean algorithm in coastal environment).

- Uncertainties in the inverted data (e.g. uncertainties in value of reflectance).

Sources of uncertainties in semi-analytical algorithms:

- Uncertainties in the relationship between Rrs and IOPs (e.g. BRDF, non-elastic scattering).

- Uncertainties in assumed shapes of IOPs (e.g. phytoplankton absorption).

- Uncertainties in the inverted data (e.g. uncertainties in the value of $R_{rs}(\lambda)$).

Quantifying uncertainties in empirical inversion algorithms:

•Use a testing data set collected in the environment of interest to evaluate the likely uncertainties of the inversion algorithm (e.g. how well can we obtain [chl] for the Gulf of Maine in January from SeaWIFS?).

•Quantify the statistics*of the difference between inverted value and measured value to obtain:

- •Bias- how accurate are the inverted values on average? – if a bias exist, re-evaluate the inversion parameters.

- •Precision- what is the absolute (or relative) difference between predicted values and inverted values? – use this as your estimate for error bars.

* If the underlying statistics are not known nonparametric statistics are safest.

What do you do if you don’t have a testing set?

Quantifying uncertainties in semi-analytical algorithms:

Part I: Uncertainties in the relationship between Rrs and IOPs.

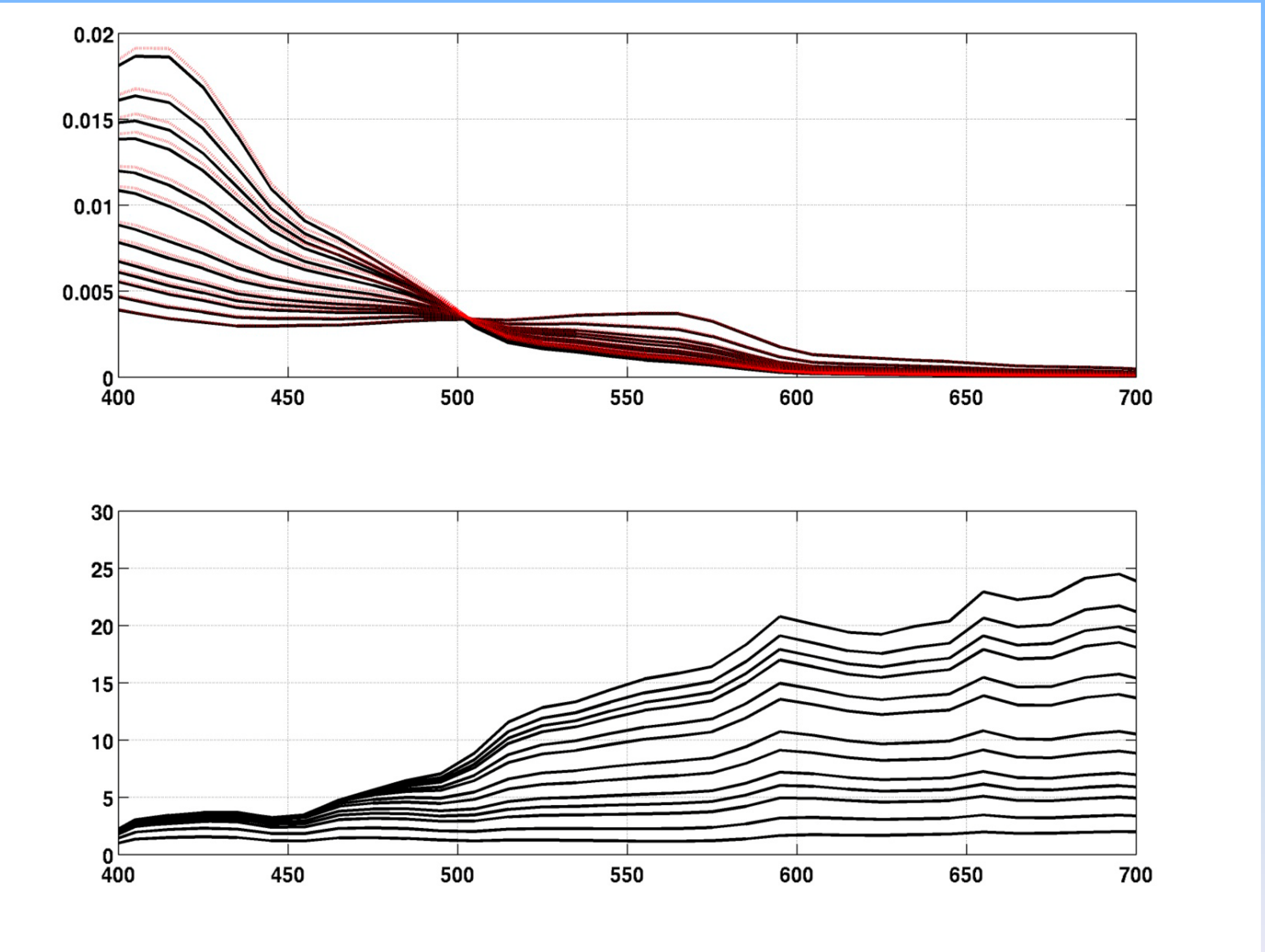
Use a testing set (IOP and Rrs measured closed by) to validate the inversion where Cloud cover/sun angle/surface conditions varied in an area with relatively constant IOP.

Evaluate the contribution of inelastic scattering by incorporating the following iteration (inspired by Pozdnyakov and Grassl, 2003):

1. Once you obtained a_{CDOM} and a_{phyto}, recalculate their likely fluorescence (as well as the contribution of Raman scattering), by e.g., inputing the IOP retrieved into Hydrolight. Note: one needs to choose the fluorescence quantum yields for CDOM and CHL. Residuals will help with estimating Φ_{chl}.

2. Rrs_new=Rrs_inverted-(Rrs_Hydrolight-Rrs_inverted). Invert again, until a convergence criteria is reached (e.g. values change by less than x% between iterations).

Raman effect on semi-empirical inversions



Westberry et al., in press

Raman effect on semi-empirical inversions

$$R_{rs}(\lambda,0^-) = R_{rs,E}(\lambda,0^-) + R_{rs,Raman}(\lambda,0^-)$$

Raman scattering coefficient: $b^R(\lambda_{em}) = \int_{\lambda_{ex}} a^R(\lambda_{ex}) f^R(\lambda_{ex} \to \lambda_{em}) d\lambda_{ex}$

Raman ‘absorption’ coefficient: $a^R(\lambda_{ex}) = 2.7 \times 10^{-4} \left(\frac{\lambda_{ex}}{488}\right)^{-5.3}$ Bartlett et al., 1998

$$L_{u,R}(z_1,\Delta z,\lambda_{em}) = \tilde{\beta}^R(\theta_s \to \pi) \int_{z_1+\Delta z}^{z_1} \int_{\lambda_{ex}} b^R(\lambda_{em}) E_d(z,\lambda_{ex}) e^{-K_d z} d\lambda_{ex}\, dz$$

$$L_{u,R}(0^-,\lambda_{em}) = \frac{\tilde{\beta}^r(\theta_s \to \pi) b_r(\lambda_{em}) E_d(0^+,\lambda_{ex})}{(K_d(\lambda_{ex}) + \kappa_L(\lambda_{em}))}$$

$$R_{rs,Raman}(0^+,\lambda_{em}) = \frac{t}{n^2} \frac{\tilde{\beta}^r(\theta_s \to \pi) b_r(\lambda_{em}) E_d(0^+,\lambda_{ex})}{(K_d(\lambda_{ex}) + \kappa_L(\lambda_{em})) E_d(0^+,\lambda_{em})} \left[1 + \frac{b_b(\lambda_{ex})}{\mu_u (K_d(\lambda_{ex}) + \kappa(\lambda_{ex}))} + \frac{b_b(\lambda_{em})}{2\mu_u \kappa(\lambda_{em})}\right]$$

$$K_d(\lambda) = \frac{a(\lambda) + b_b(\lambda)}{\mu_d} \text{ and } \kappa(\lambda) = \frac{a(\lambda) + b_b(\lambda)}{\mu_u}$$

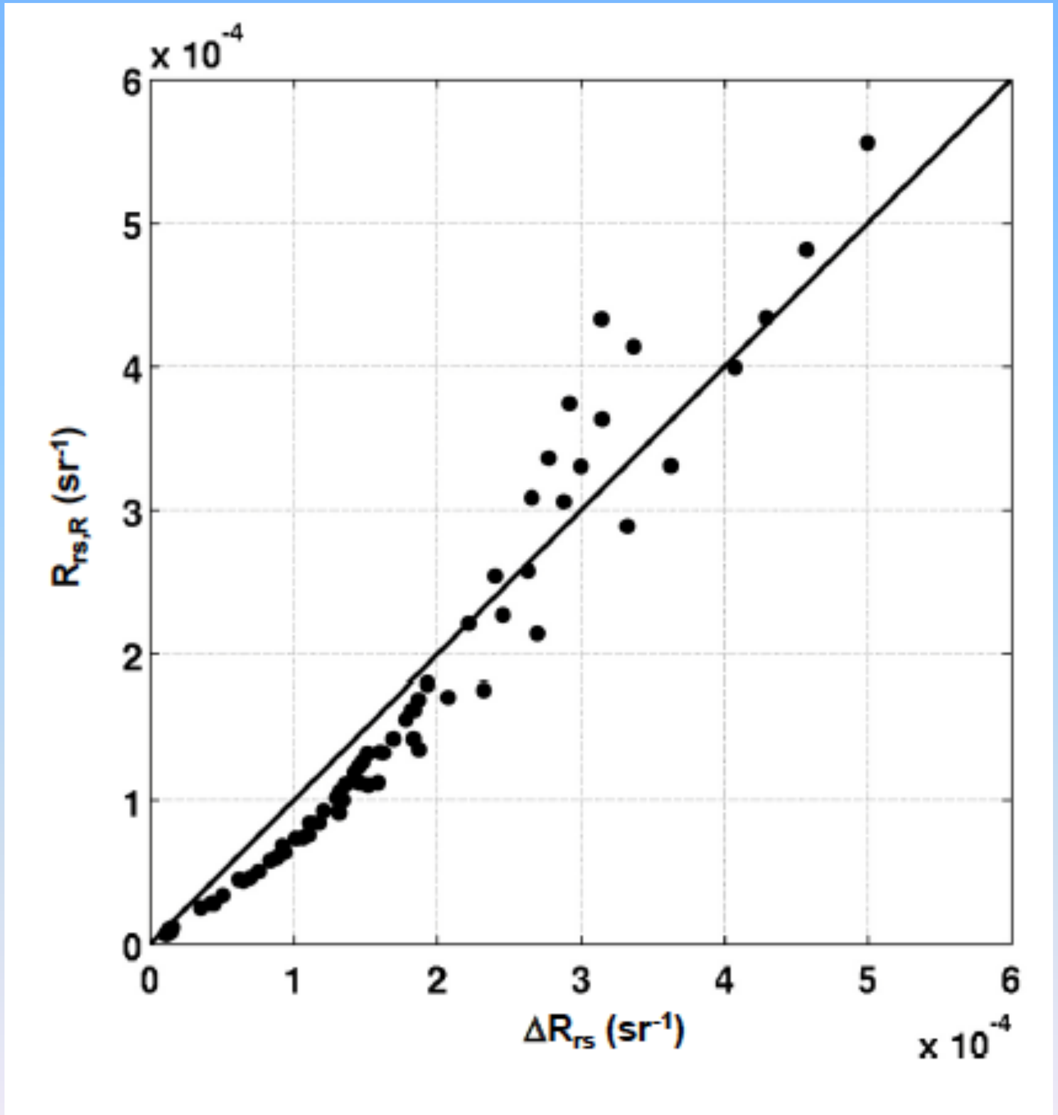
$\mu_d = \cos(\theta_{s,w})$ $\mu_u = 0.5$

IOPs from first iteration w/o Raman

Westberry et al., in press

Raman effect on semi-empirical inversions

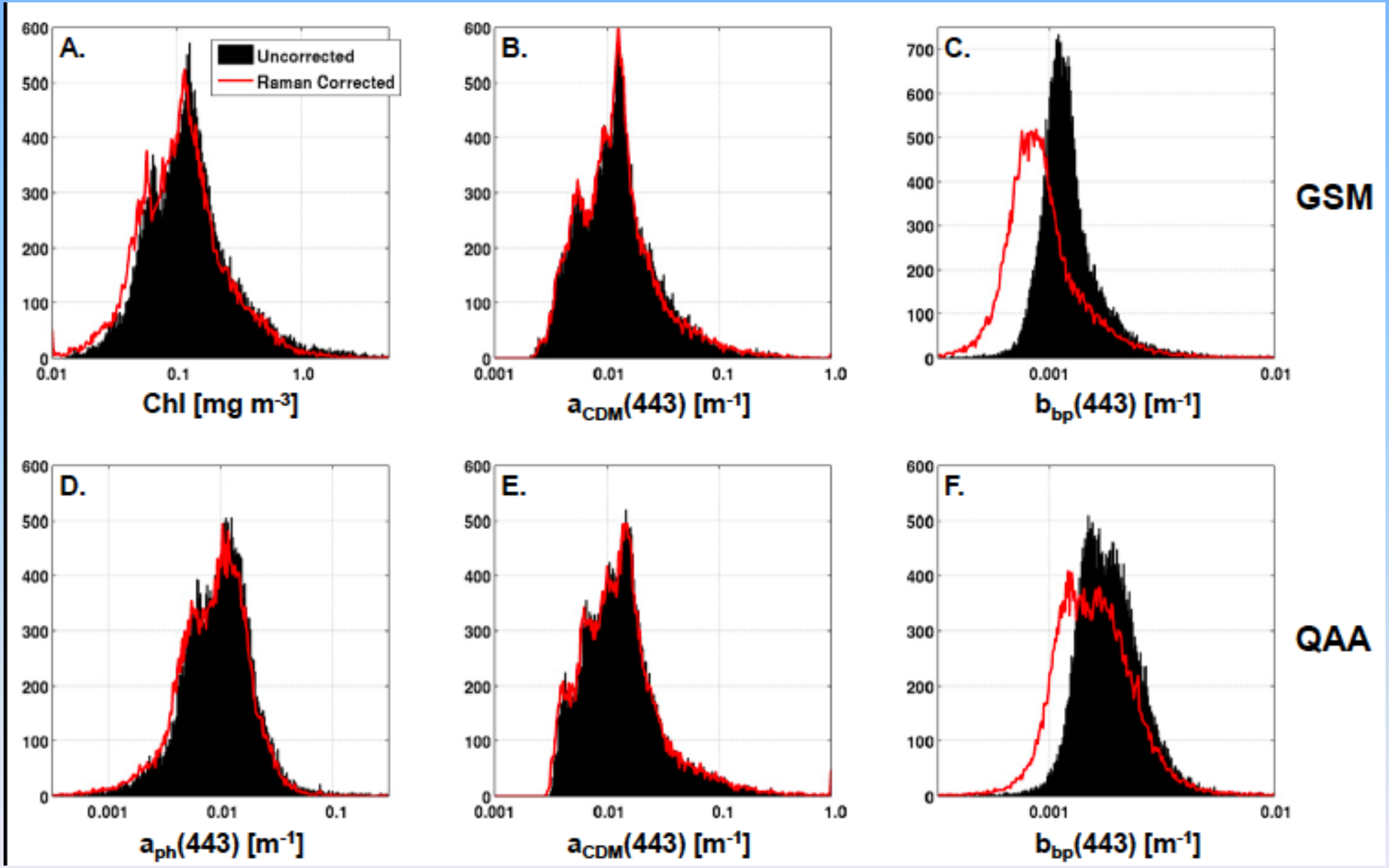
Analytical expression



Hydrolight

Westberry et al., in press

Raman effect on semi-empirical inversions



Westberry et al., in press

Quantifying uncertainties in semi-analytical algorithms:

Part II: Uncertainties in assumed shapes of IOPs (e.g. phytoplankton absorption, spectral slopes of backscattering and a_{CDM}).

A sensitivity analysis is performed looking at how the output varies with shapes of IOPs (e.g. Roesler and Perry, 1995, Lee et al., 1996, Hoge and Lyons, 1996, Garver and Siegel, 1997).

Roesler iterative method for optimizing $a_\phi(\lambda)$: look at the residuals (Rrs_measured-Rrs_modeled). If they look like pigments peaks, modify a_ϕ to include pigment in those wavelengths (e.g. from a library of spectra one has established ahead of time).

Quantifying uncertainties in semi-analytical algorithms:

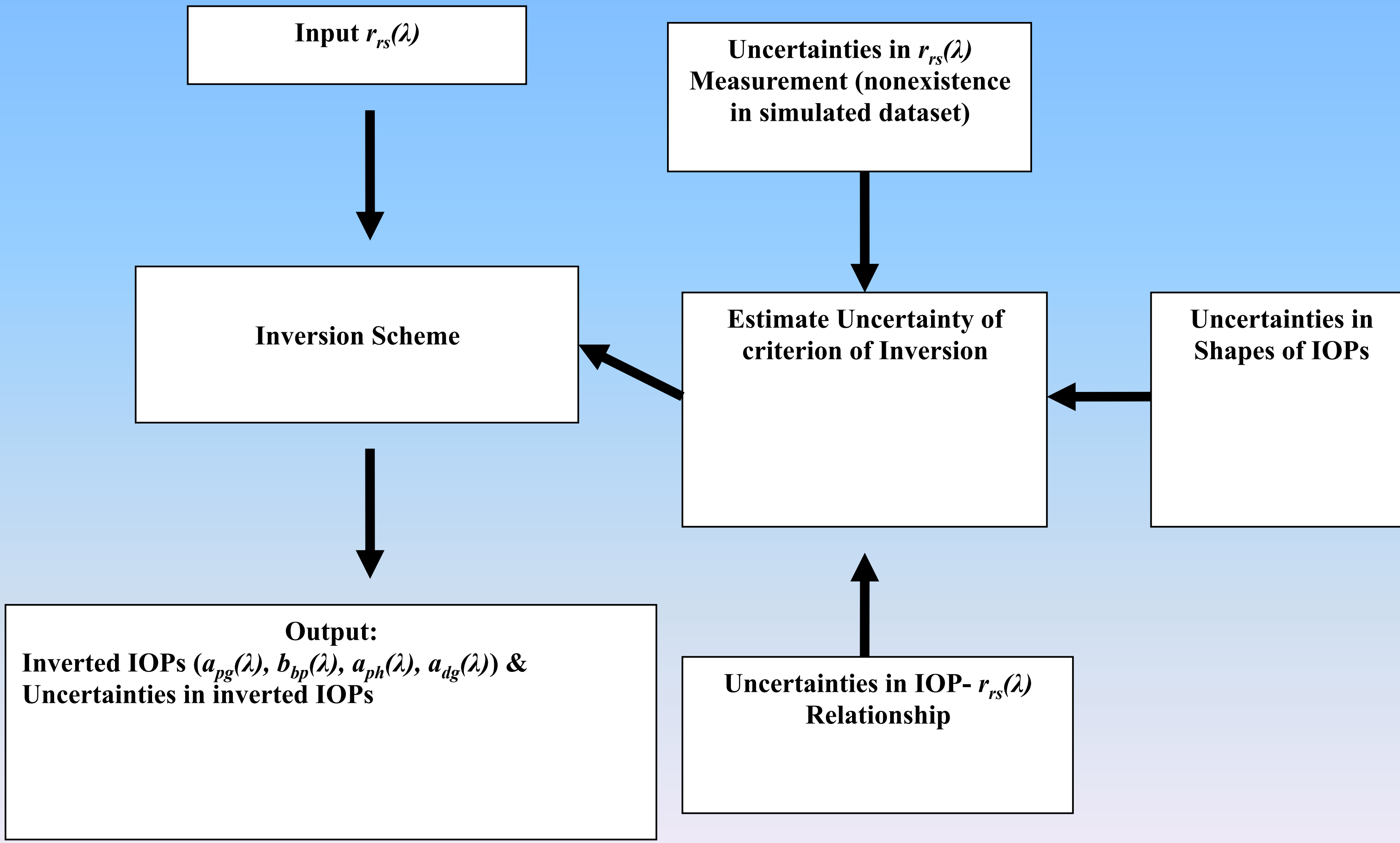
Part III: Uncertainties in the inverted data (e.g. uncertainties in the value of Rrs(λ)).

$$R_{rs} = \frac{L_u}{E_d} \rightarrow \frac{\delta R_{rs}}{R_{rs}} = \sqrt{\left(\frac{\delta L_u}{L_u}\right)^2 + \left(\frac{\delta E_d}{E_d}\right)^2}$$

Note:
For Rrs obtained from a satellite, the uncertainties are very likely to vary spectrally (e.g. due to atmospheric correction).

Quantifying uncertainties in semi-analytical algorithms:

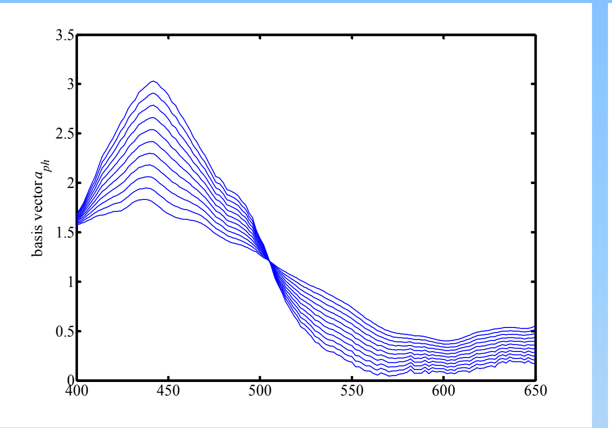
The Wang/Boss/Roesler approach:

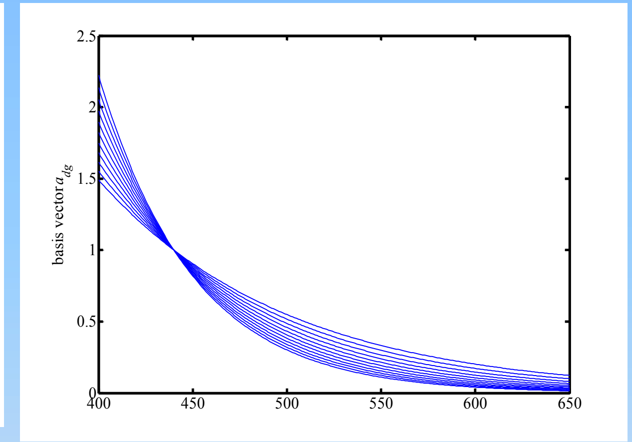


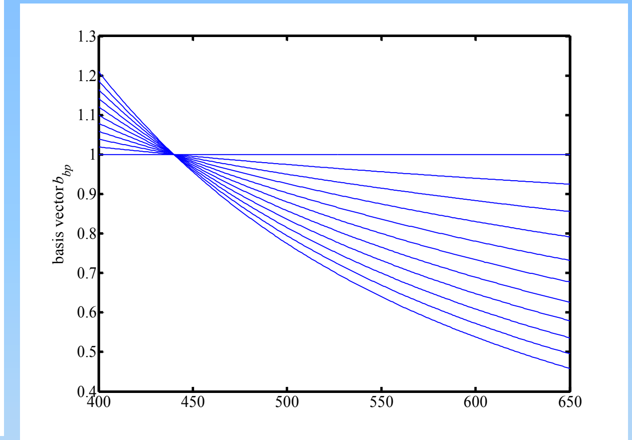
Quantifying uncertainties in semi-analytical algorithms:

The Wang/Boss/Roesler approach:

Shape of component IOPs:







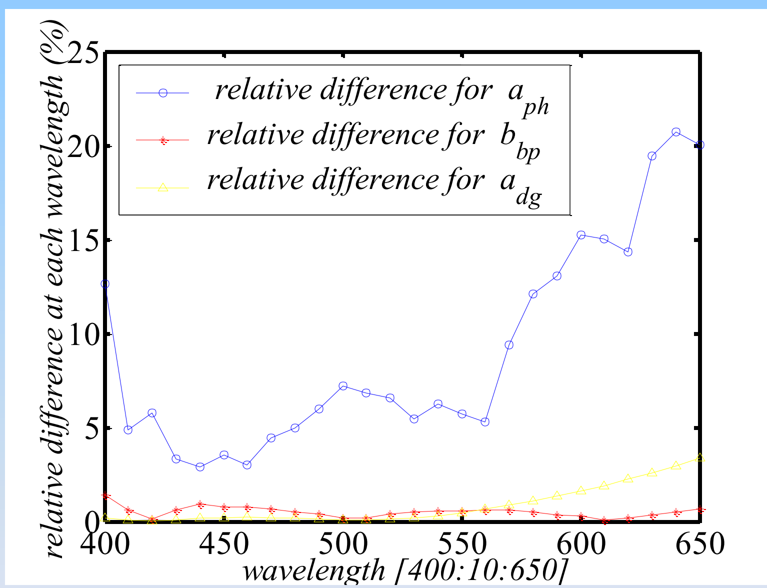
Phytoplankton: Ciotti et al., 2002.
a_{cm} with exponential slope varying from 0.01 to 0.02
b_{bp} with spectral slope varying from 0 to 2.

Choose one combination of shapes and invert linearly (total of 11^3=1331 combinations). Solve for 3 amplitudes (b_{bp}, a_{cm}, a_ϕ), for each choice of 3 shape parameters.

Quantifying uncertainties in semi-analytical algorithms:

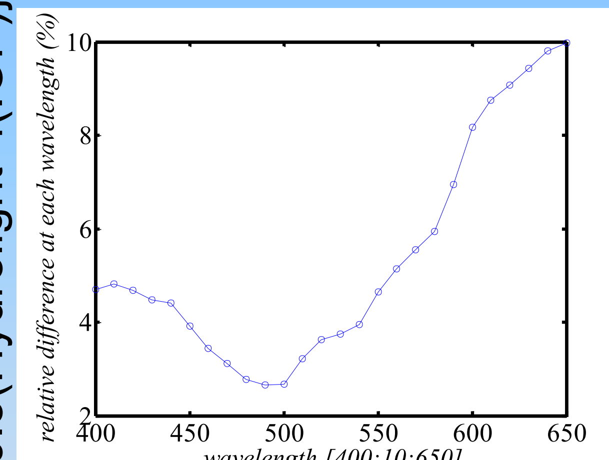
The Wang/Boss/Roesler approach: Evaluating uncertainties

1. Uncertainties in shapes of IOPs (ZP Lee dataset)

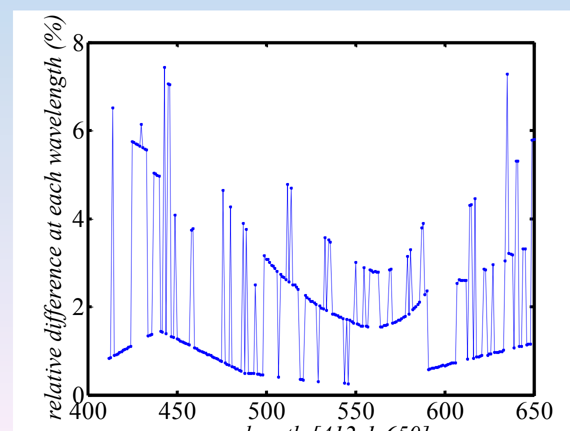


2. Uncertainties in relation of IOPs and r_{rs}.

$$\frac{\{Hydrolight - f(IOP)\}}{\{0.5(Hydrolight + f(IOP))\}}$$



Field: %Diff(r_{rs}) when IOP=const.

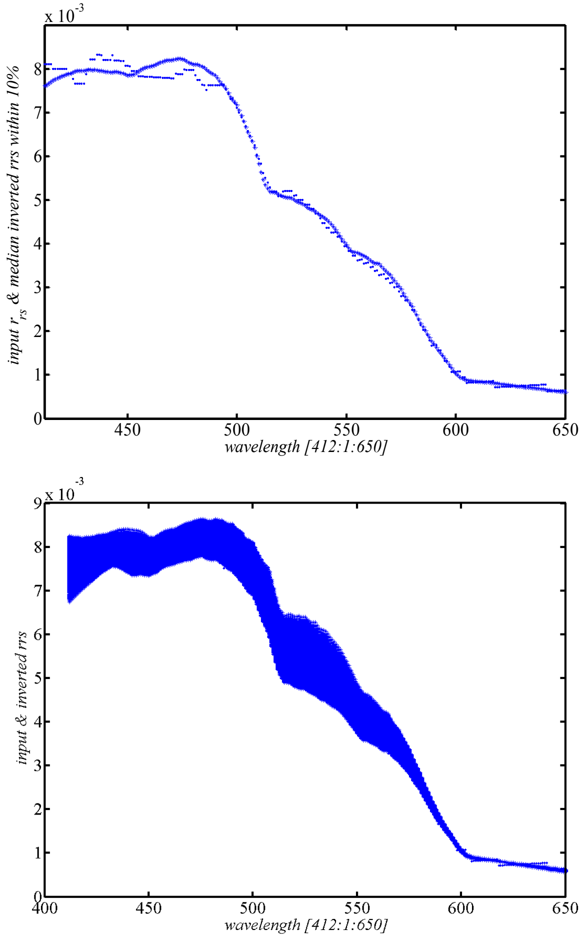


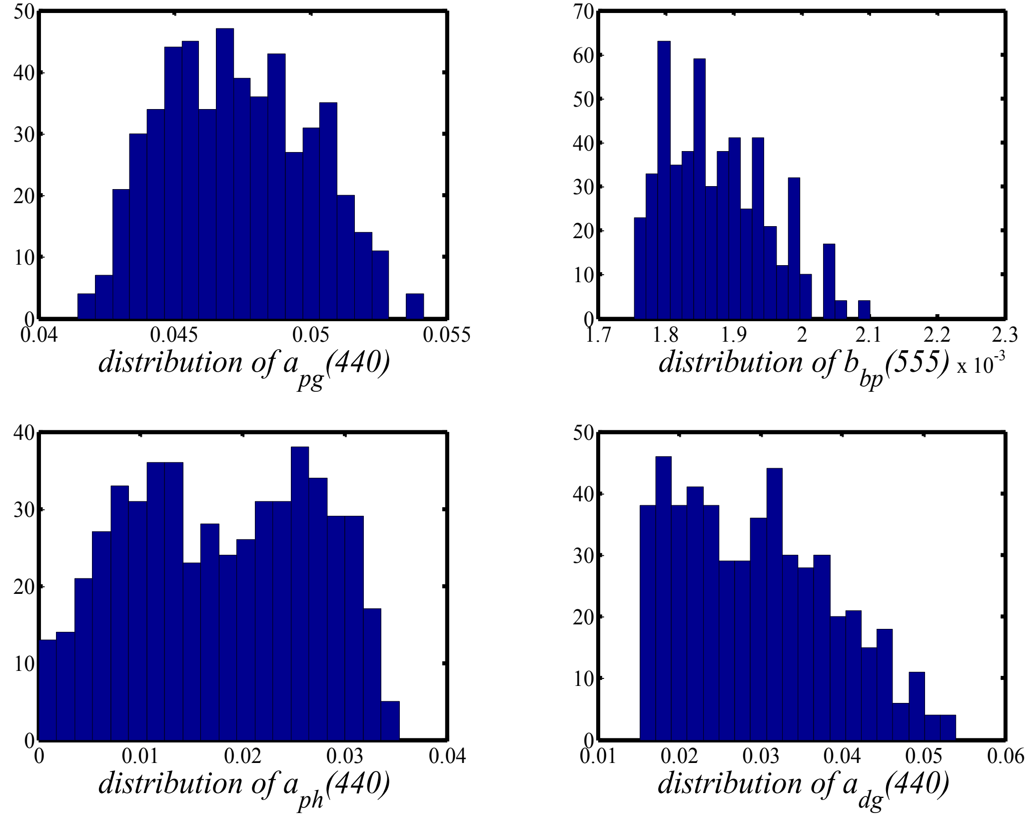
3. Stability of radiometers<2%

→ Any solution within 10% r_{rs} at all λ is kept.

Quantifying uncertainties in semi-analytical algorithms:

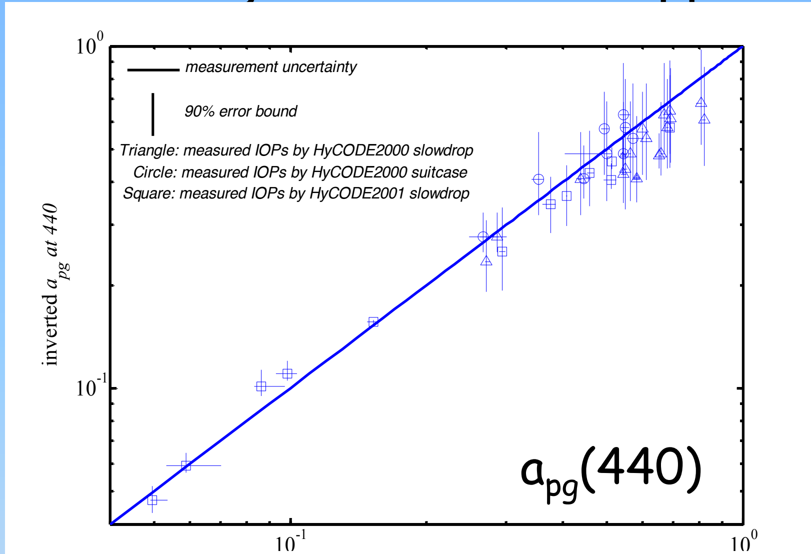
The Wang/Boss/Roesler approach, example:

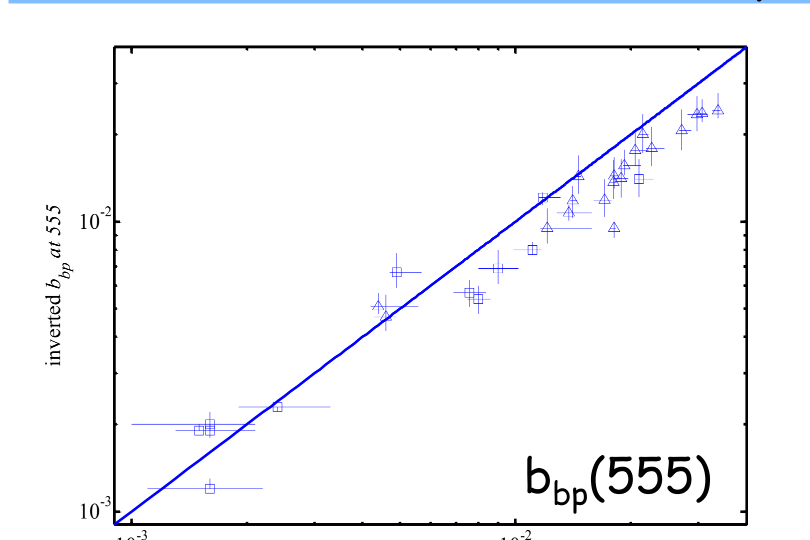




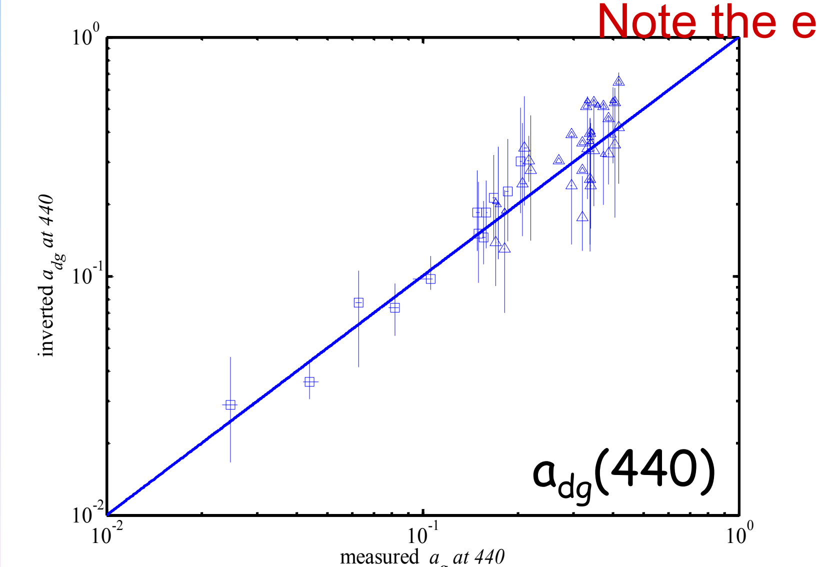
Quantifying uncertainties in semi-analytical algorithms:

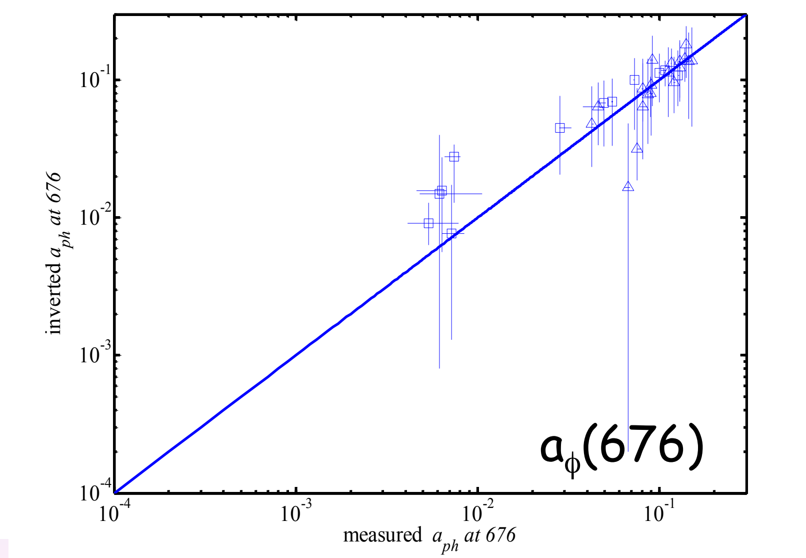
The Wang/Boss/Roesler approach: Results for 31 field matchups





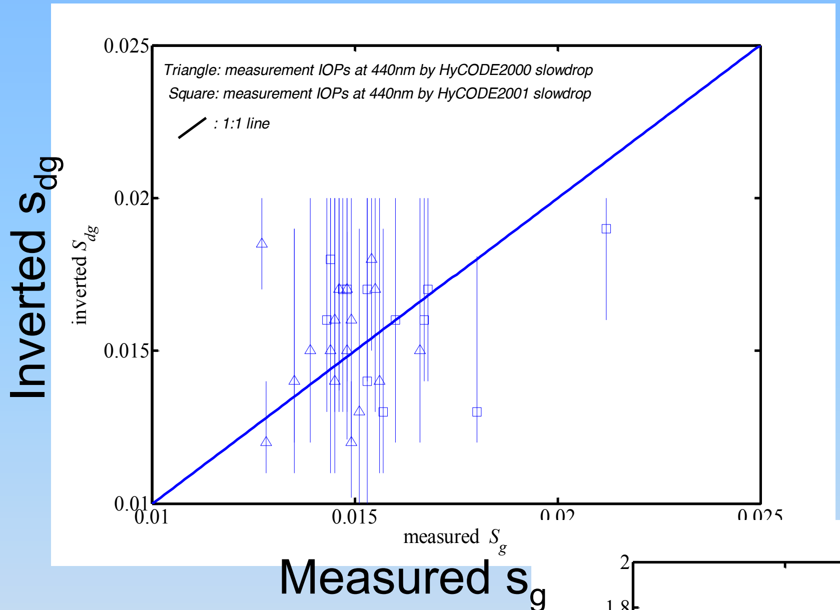
Note the error bars!!!

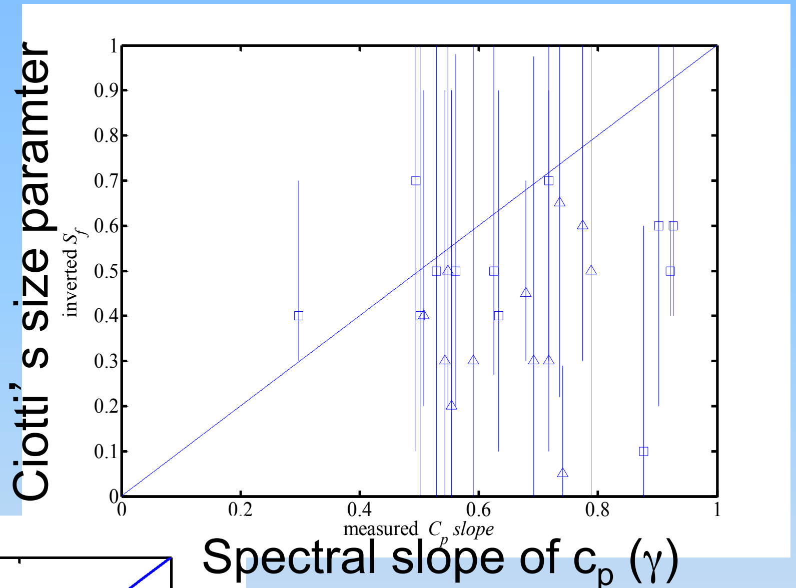


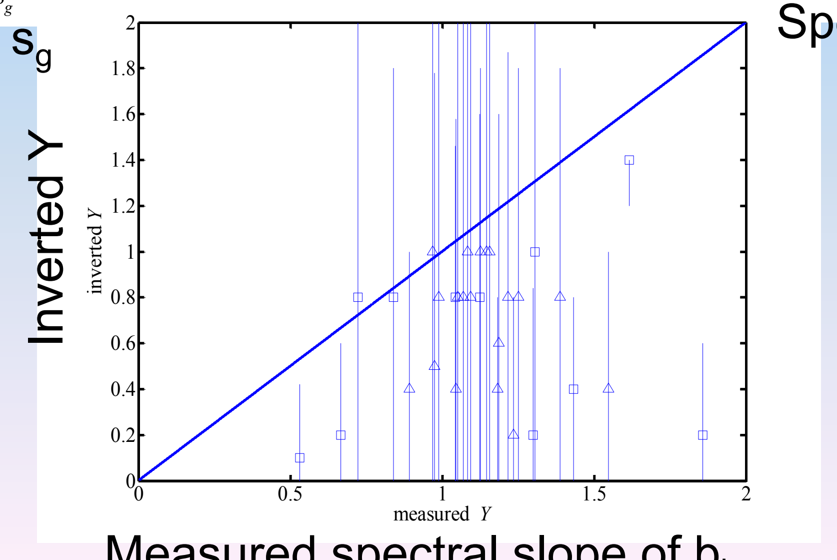


Quantifying uncertainties in semi-analytical algorithms:

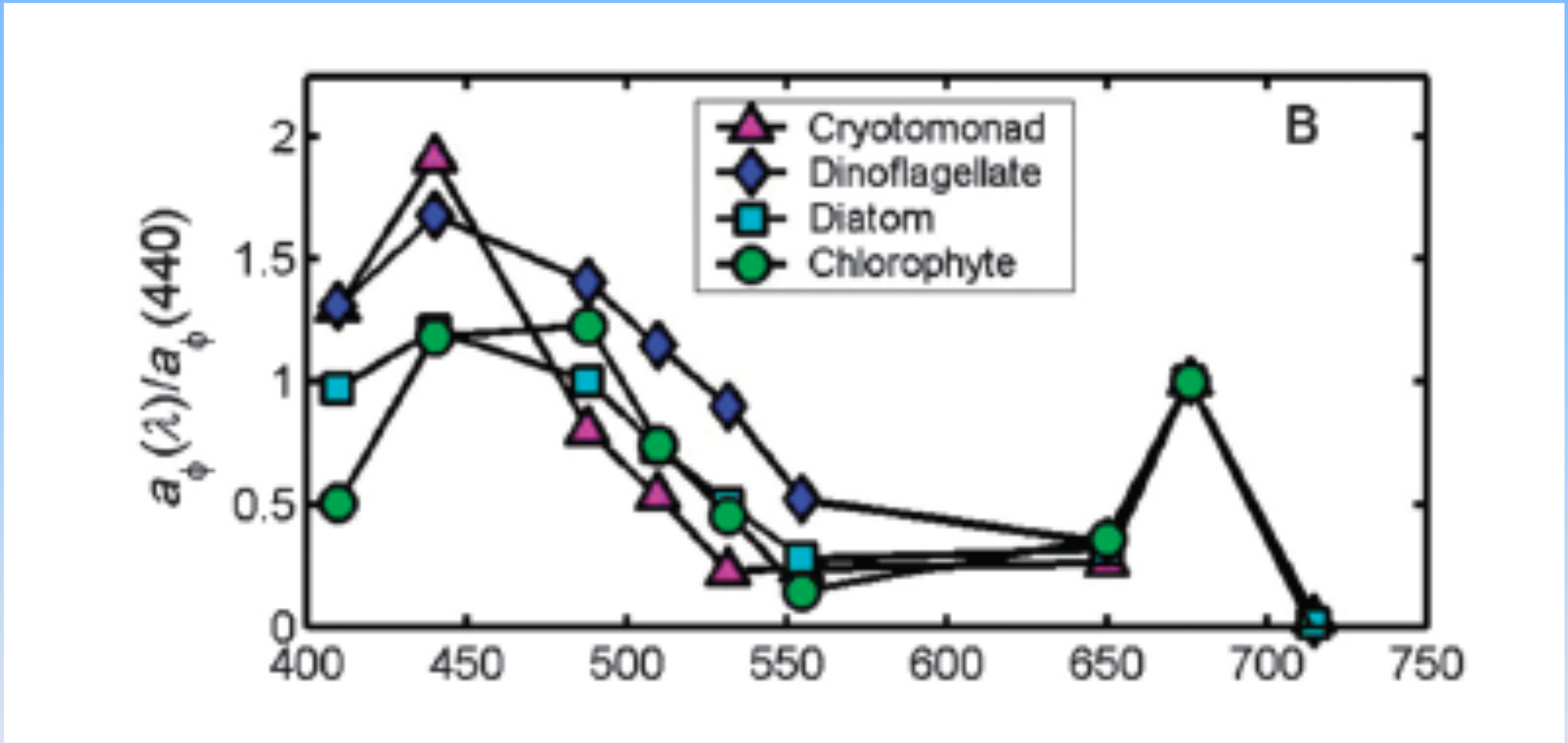
The Wang/Boss/Roesler approach: Results for 31 field matchups







Other possible eigenfunctions:



Roesler and Boss, 2008

Quantifying uncertainties, summary:

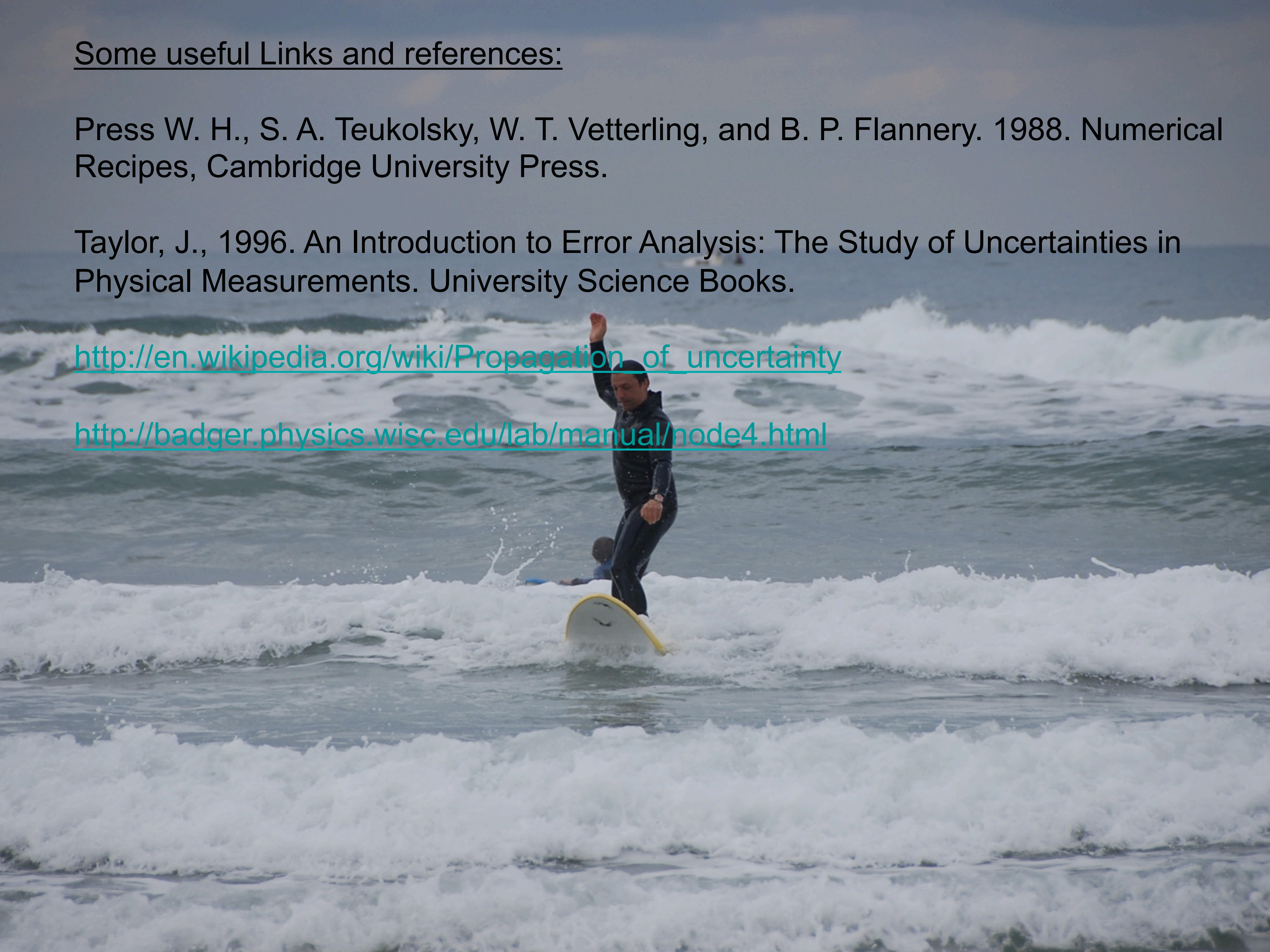
- It is possible to put error bars on inversion products, so lets do it (and on global scales provide maps of uncertainties).

- Error bars will get smaller the more we know about the environment (e.g. limit the shape of the component IOP).

- The magnitude of the uncertainty may make the data useless for some application while still very useful for other.

- Another approach is to use the difference between observed r_{rs} and that from the inverted parameters to derive the uncertainties. This approach fails to take into account the inherent uncertainties in the: 1. measured r_{rs}, 2. IOP-r_{rs} relationships and 3. assumed shapes for IOPs.

- A fundamental difference between the empirical and semi-analytical approaches is that one is a statistical interpolation scheme, while the other is based on the fundamental physics of remote sensing supplemented by empirical knowledge of component IOP shape.



Some useful Links and references:

Press W. H., S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery. 1988. Numerical Recipes, Cambridge University Press.

Taylor, J., 1996. An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements. University Science Books.

http://en.wikipedia.org/wiki/Propagation_of_uncertainty

http://badger.physics.wisc.edu/lab/manual/node4.html