2nd IOCCG Summer Lecture Series
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Uncertainties in ocean colour remote sensing Computations

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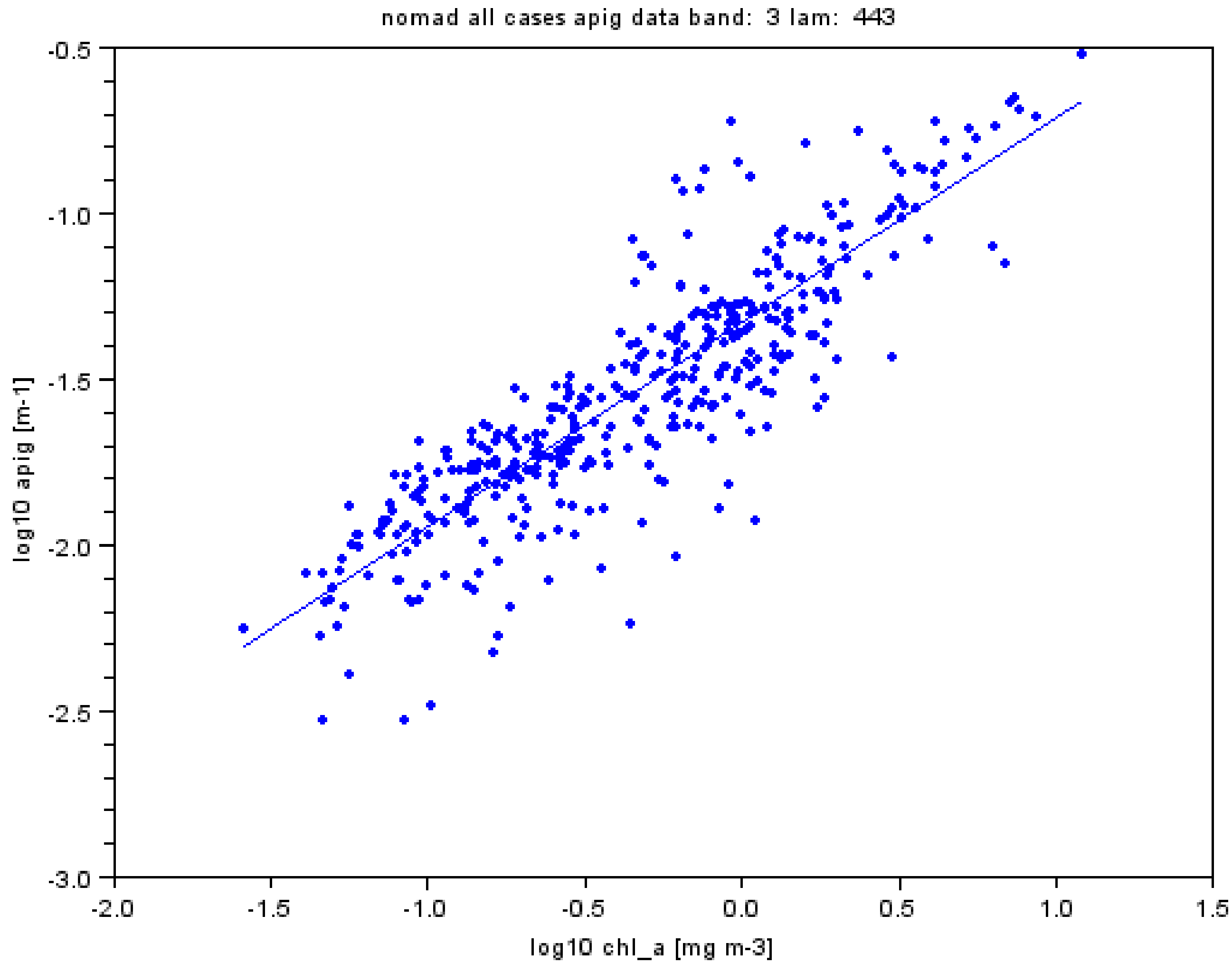
Computation of uncertainties

- Linear model: $\chi 2$ computation
- non-linear models

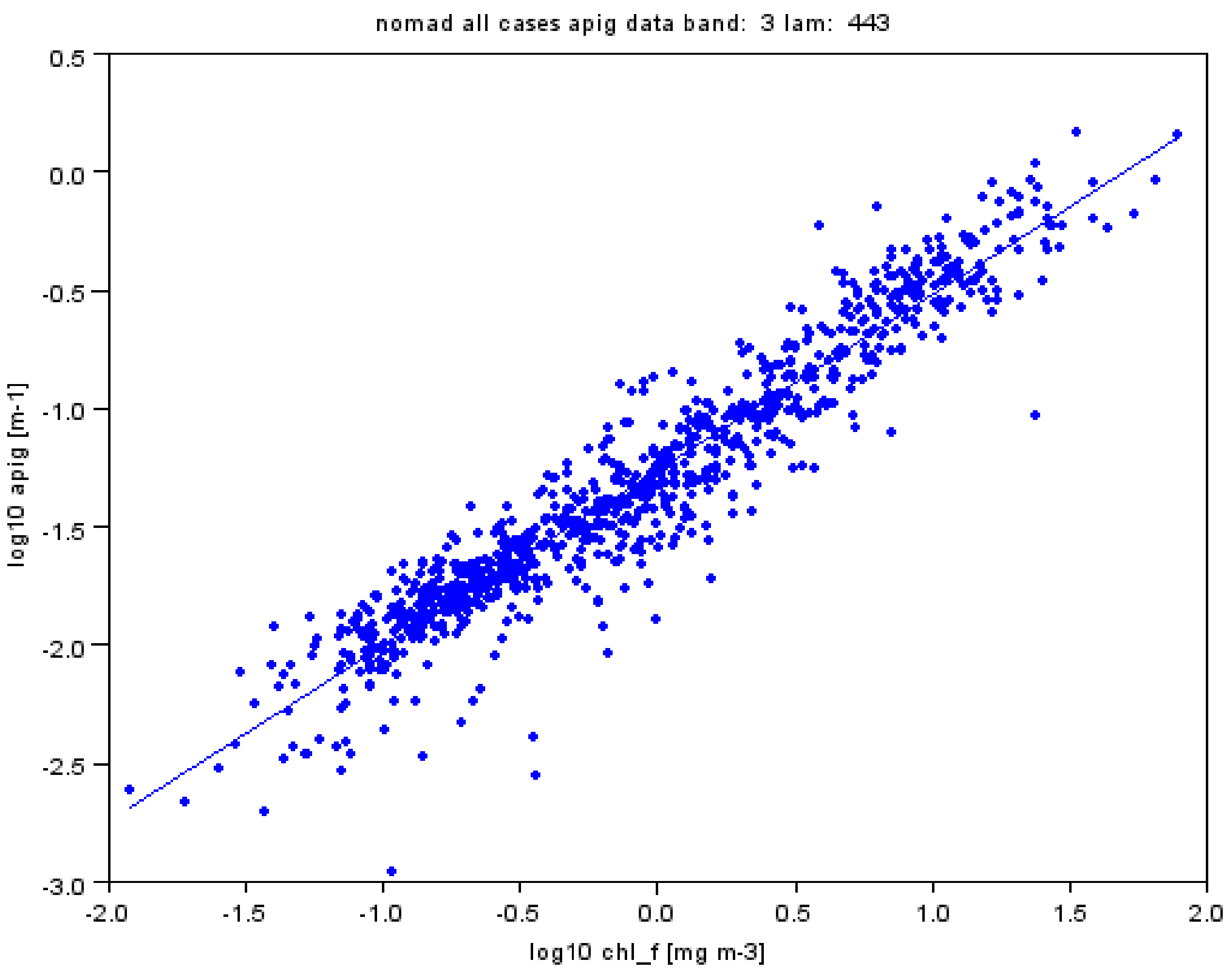
- 1. example chlorophyll concentration and pigment absorption

Bio-optical model: relationship between a_pig and chl_a (443 nm)



443 nm, log10 scale

Bio-optical model: relationship between a_pig and chl_f



443 nm, log10 scale, 920-956 samples for chl_f

The linear model with 2 variables and 2 parameters (also exercise)

one independent variable; chlorophyll concentration
one dependent variable: pigment absorption coefficient

our assumption from the scatter plot is that there is linear relationship between the logarithm of *chl* and the logarithm of *apig*

this relationship will be described by two parameters: *m* and *b*

*log_apig_model = m*log_chl +b*

we have N measurements of apig: *log_apig_meas (y)*, and of *chl (x)* from which want to determine the model parameters m and b, each measurement has also an uncertainty σ (sigma, standard deviation)

The model will probably never fully agree with our measurement, uncertainties remain, the uncertainty will be quantified by X^2 (chi square):

$$X^2 = sum((log\_apig\_meas - log\_apig\_model)\hat{}2 / sig^2)$$

$$X^2 = sum((y - m*chl - b)\hat{}2 / sig^2)$$

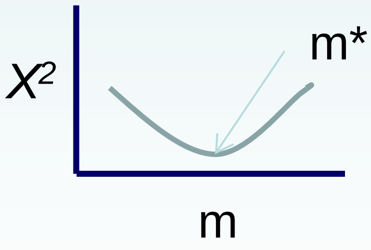
The linear model with 2 variables and 2 parameters (also exercise)

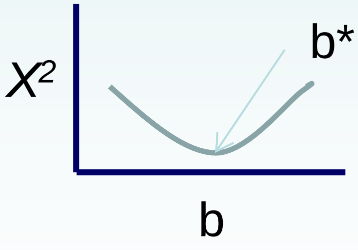
$$X^2(m,b) = sum((y - m*chl - b)^2 / sig^2)$$

The parameters m and b have to set so that the deviation X^2 becomes as small as possible.

If we change m or b away from the *ideal* point, i.e the minimum, m* and b* , then X^2 will increase to both sides.

at m* and b* the first derivative d $X^2 / dm = 0$, and $dX^2 / db = 0$





The linear model with 2 variables and 2 parameters (also exercise)

*$X^2(m,b)$ = sum((y– m*x -b)^2 / sig^2)*

can be transformed into

$$\chi^2 = m^2 \sum x^2 + 2mb \sum x + b^2 \sum 1 - 2m \sum xy - 2b \sum y + \sum y^2$$

this is called a quadratic form

It is a generalization of a quadratic to more than one variable.
It happens to be a “positive-definite'' quadratic form, which means that it has a minimum. Call this point *m = m** and *b = b**. Then it increases in all directions as we vary m and b away from this point.

Think of the two variables m and b as defining a plane and think of X^2 as defining the height of a surface above the plane. The surface then looks like a bowl. The contours of constant elevation are ellipses in *m* and *b*.

The linear model with 2 variables and 2 parameters (also exercise)

$$\chi^2 = m^2 \sum x^2 + 2mb \sum x + b^2 \sum 1 - 2m \sum xy - 2b \sum y + \sum y^2$$

Next task to locate the bottom of the bowl, where *m* = *m** and *b* = *b**.

We do this by setting both partial derivatives of *X2 with respect to m* and b** to zero*:*

we get 2 linear equations:

$$m* \sum x^2 + b* \sum x = \sum xy$$
$$m* \sum x + b* \sum 1 = \sum y$$

these can be written in matrix form:

$$M \vec{a}^* = \vec{c}$$

the vector $\vec{a}^*$ has the elements m* and b* and

$$\vec{c} = \begin{pmatrix} \sum xy \\ \sum y \end{pmatrix}$$

M is a matrix:

$$M = \begin{bmatrix} \sum x^2 & \sum x \\ \sum x & \sum 1 \end{bmatrix}$$

M is twice the Hessian Matrix, which is the matrix of second partial derivatives

$$\frac{\partial^2 \chi^2}{\partial a_i \partial a_j}$$

The linear model with 2 variables and 2 parameters (also exercise)

The solution is: $\begin{bmatrix} m^* \\ b^* \end{bmatrix} = M^{-1} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$

$$m^* = \frac{\sum xy \sum 1 - \sum x \sum y}{\sum x^2 \sum 1 - (\sum x^2)}$$

$$b^* = \frac{\sum x^2 \sum y - \sum x \sum xy}{\sum x^2 \sum 1 - (\sum x)^2}$$

$$\chi_0^2 = \chi^2(m^*, b^*) = \sum y^2 - \vec{a}^* \cdot \vec{c}$$

$$\chi^2(m, b) = \chi_0^2 + (\Delta m)^2 + \sum x^2 + 2(\Delta m)(\Delta b) \sum x + (\Delta b)^2 \sum 1$$

$$\Delta m = m - m^*, \Delta b = b - b^*$$