Analysis Methods in Atmospheric and Oceanic Science

# AOSC 652

# Least Squares Analysis, Statistical Regression, and Spline Fitting: Day 1

### 26 Sep 2016

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#### Assignment 4a: Integer Sorting

Only 9 or 15 students turned in code that was working: output to file fort.99 designed to *let you check* if your code worked

If you know your code is not working, please ask me, Jeff, or Walt for help

We had hoped that the answers to the functional dependence of the timing would be drawn from the readings: please try to do the readings

#### **Review Mon:**

```
Call to piksrt in our code:
```

```
call piksrt(iarray_in,iarray_out,npts)
```

New subroutine piksrt to comply with our call statement

```
subroutine piksrt(arr_in,arr_out,n)
integer n,i,j
real a,arr_in(n),arr_out(n)
do i=1.n
  arr out(i)=arr in(i)
enddo
                        ! Pick out each element in turn
do j=2,n
   a=arr_out(j)
   do i=j-1,1,-1
                          ! Look for the place to insert it
      if(arr out(i).le.a) goto 10
      arr out(i+1)=arr out(i)
   enddo
   i=0
                              ! Insert it
  arr out(i+1)=a
enddo
return
end
```

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integer a, arr_in(n), arr_out(n)
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#### Assignment 4a: Integer Sorting

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Reading: piksrt speed varies as N<sup>2</sup>  $\Rightarrow$  sort of 1 million points would take 10×10×speed of 100,000 point sort or ~100 min

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Ratio of run times either:

 $N^2 / N \log_2 N = 10^6 / \log_2 (10^6) = ~50,000$  (theory)

\*or\*

 $100 \min \times 60 \sec / \min / 2.6 \sec = \sim 2300$  (observation)

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Assignment 4a: Integer Sorting

It is remarkable that, for a little bit more effort (~30 min for most students, hopefully), we can obtain an algorithm thousands of times more efficient for sorting a million numbers than a "brute force" method

There are many times in your research life you may need to make a choice between "clock time" in getting a computation started and "run time" on the computer

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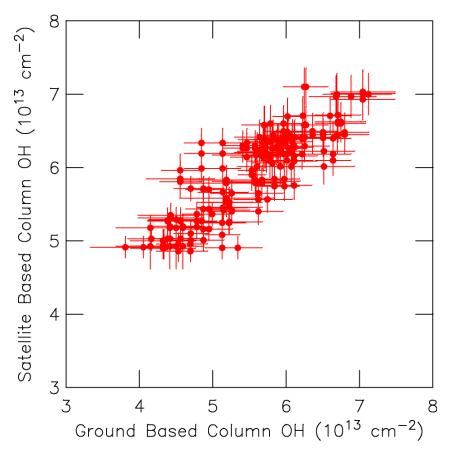
Please take Assignment 4B, check your numbers, and return on Wed at start of class

Name: \_\_\_\_\_

Year	Temperature	Year	Temperature
1951		1967	
1952		1968	
1953		1969	
1954		1970	
1955		1971	
1956		1972	
1957		1973	
1958		1974	
1959		1975	
1960		1976	
1961		1977	
1962		1978	
1963		1979	
1964		1980	
1965		Baseline Hand	
1966		Baseline Code	

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Suppose you have two sets of measurements (or data and model) that you'd like to relate.



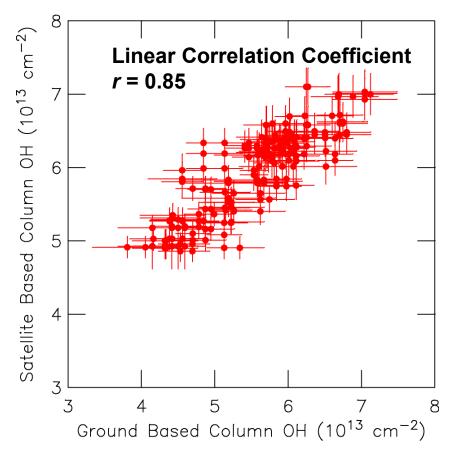
#### What are some aspects of the data that are typically examined?

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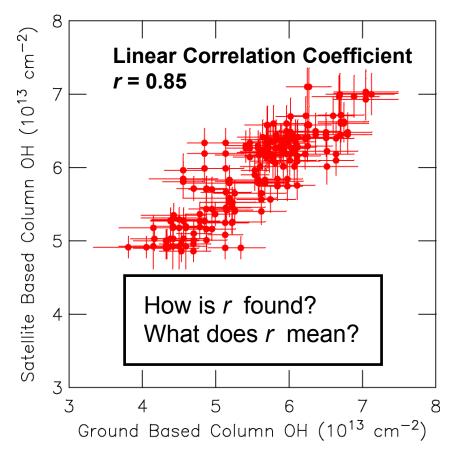
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**Linear Correlation Coefficient:** 

$$r = \frac{\sum_{i=1}^{N} (x_i - \overline{x}) (y_i - \overline{y})}{\sqrt{\sum_{i=1}^{N} (x_i - \overline{x})^2} \sqrt{\sum_{i=1}^{N} (y_i - \overline{y})^2}}$$

r must lie between -1 and 1

If r = 1, the data are said to have a *complete positive correlation* r = 0, the data are said to be *uncorrelated* 

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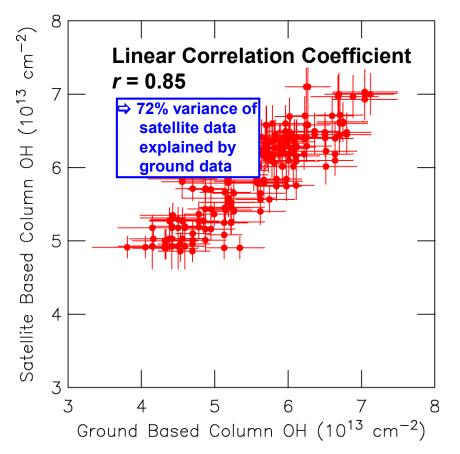
If r = 1, the data are said to have a *complete positive correlation* r = 0, the data are said to be *uncorrelated* 

 $r^2 \ge 100$  = percent of variance in common between *x* and *y* 

See <a href="http://www.mega.nu/ampp/rummel/uc.htm#C2">http://www.mega.nu/ampp/rummel/uc.htm#C2</a> for a nice explanation

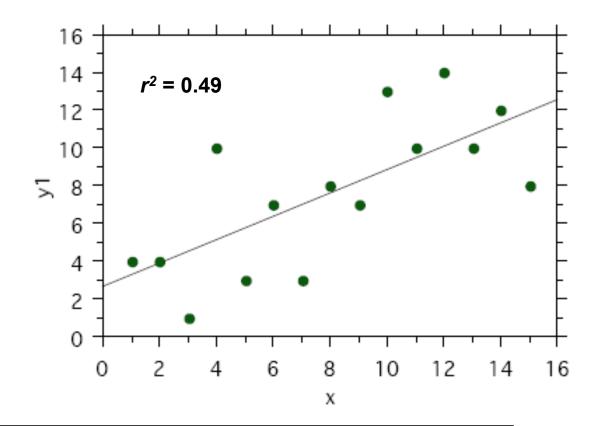
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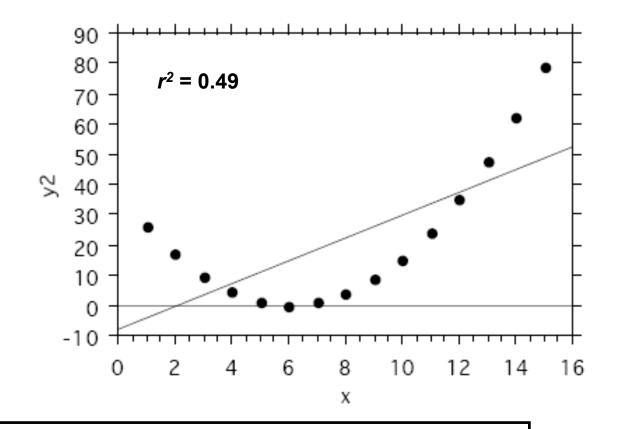
#### Visualization of data is vital



From Dennis Hartmann's class notes: http://www.atmos.washington.edu/~dennis/552\_Notes\_3.pdf

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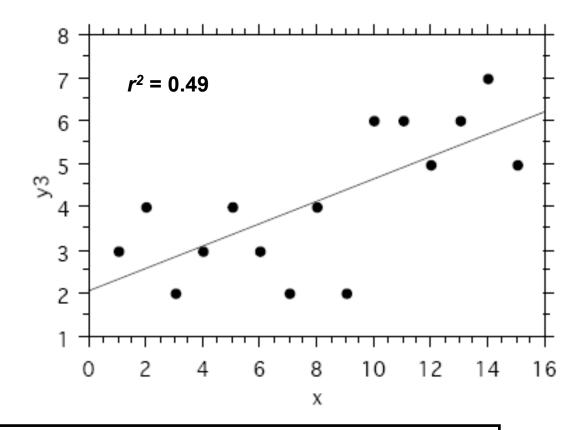
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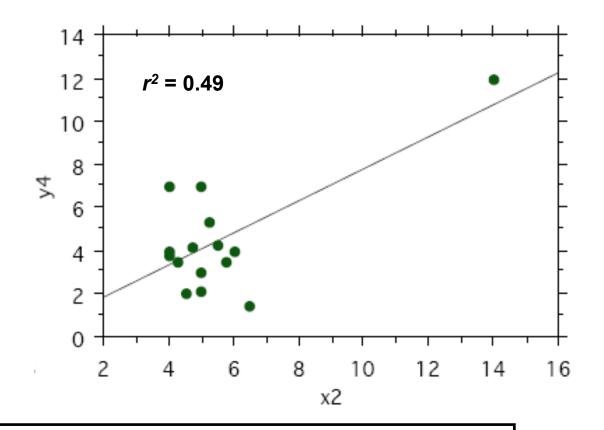
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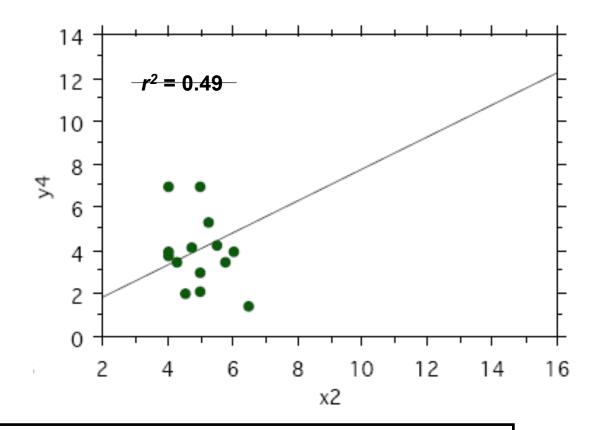
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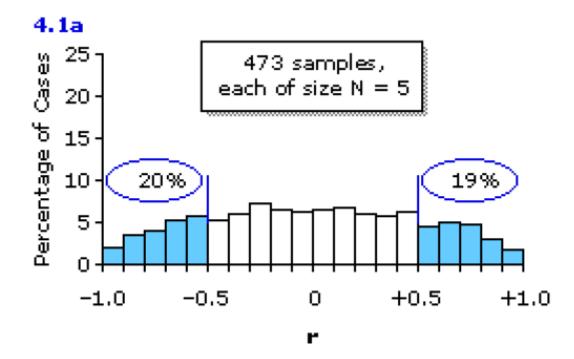
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### Test for statistical significance of correlation vital

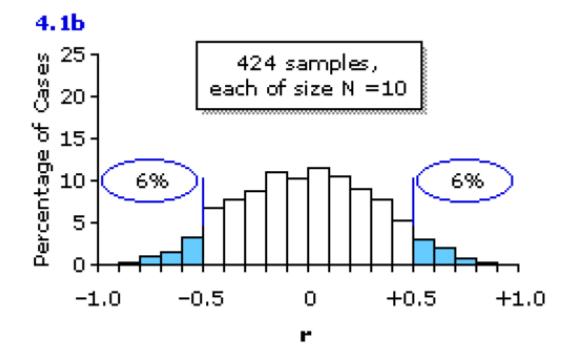


Practice: Linear Correlation Coefficient for 5 throws of a pair of dice, done 473 times

From Richard Lowry's class notes: <a href="http://www.vassarstats.net/textbook/ch4pt1.html">http://www.vassarstats.net/textbook/ch4pt1.html</a>

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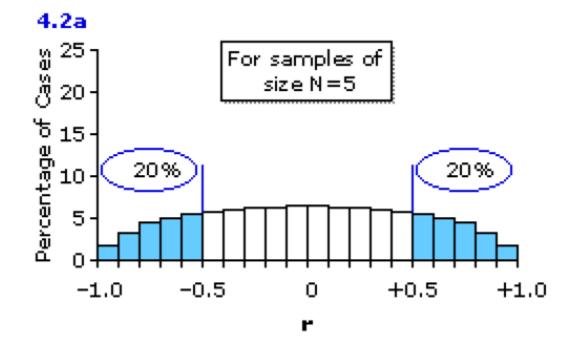


Practice: Linear Correlation Coefficient for 10 throws of a pair of dice, done 424 times

From Richard Lowry's class notes: http://www.vassarstats.net/textbook/ch4pt1.html

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### Test for statistical significance of correlation vital

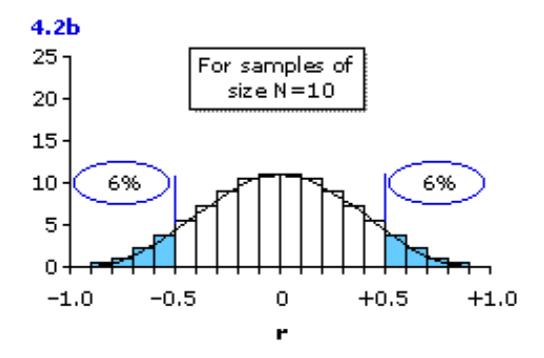


Theory: Correlation Coefficient for 5 throws of a pair of dice, done infinite # of times

From Richard Lowry's class notes: <a href="http://www.vassarstats.net/textbook/ch4pt1.html">http://www.vassarstats.net/textbook/ch4pt1.html</a>

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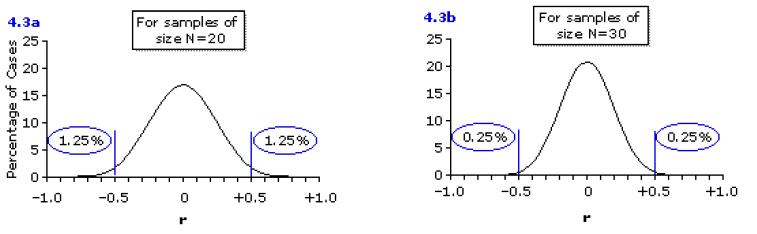


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#### Test for statistical significance of correlation vital



Theory: Correlation Coefficient for 20 throws (left) and 30 throws (right) of a pair of dice (left)

From Richard Lowry's class notes: http://www.vassarstats.net/textbook/ch4pt1.html

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#### Test for statistical significance of correlation vital

Absolute value of r needed to show two quantities bear a statistically significant relation at the 95% confidence interval, as a function of sample size

N	Directional	Non-Directional
5	0.81	0.88

From Richard Lowry's class notes:

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Absolute value of r needed to show two quantities bear a statistically significant relation at the 95% confidence interval, as a function of sample size

N	Directional	Non-Directional
5	0.81	0.88
10	0.55	0.63
15	0.44	0.51
20	0.38	0.44
30	0.30	0.35

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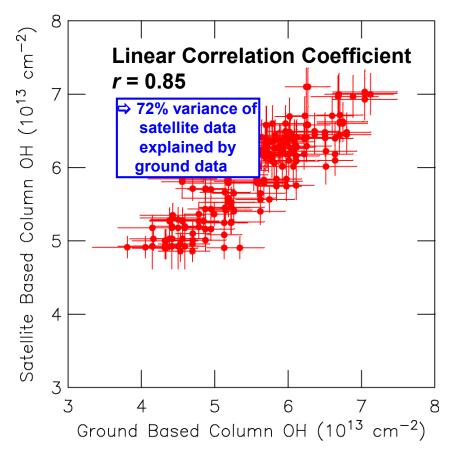
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30	0.30	0.35

See Section 8.4 of von Storch and Zwiers, *Statistical Analysis of Climate Research* for methodology for assessing statistical significance of a linear correlation

http://www.leif.org/EOS/vonSt0521012309.pdf

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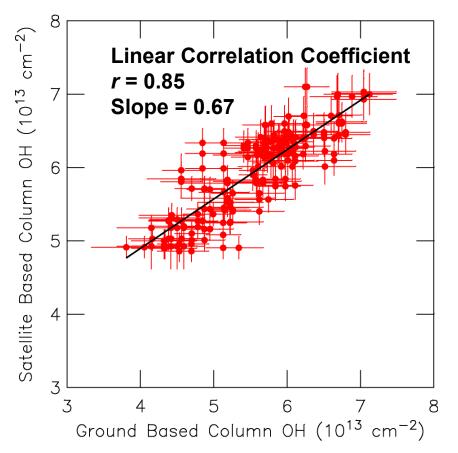
Suppose you have two sets of measurements (or data and model) that you'd like to relate.



#### What else might we want to know?

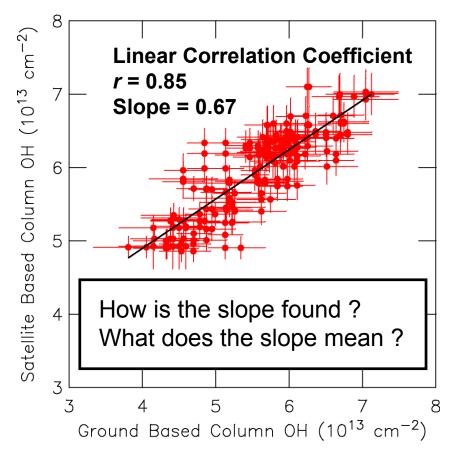
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### **Linear Least Squares Fitting:**

y = a + b x

Minimize:

$$\sum_{i=1}^{N} (a+b x_i - y_i)^2 \equiv Cost \ Function$$

$$\frac{\partial Cost Function}{\partial a} = 2\sum_{i=1}^{N} (a+b x_i - y_i) = 0$$

$$\frac{\partial Cost Function}{\partial b} = 2\sum_{i=1}^{N} (a+b x_i - y_i) x_i = 0$$

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$$\frac{\partial Cost Function}{\partial a} = 2\sum_{i=1}^{N} (a+b x_i - y_i) = 0$$

$$\frac{\partial Cost Function}{\partial b} = 2\sum_{i=1}^{N} (a+b x_i - y_i) x_i = 0$$

$$a N + b \Sigma x_i - \Sigma y_i = 0$$
$$a \Sigma x_i + b \Sigma x_i^2 - \Sigma x_i \cdot y_i = 0$$

Can show:

$$b = \frac{\sum x_i \cdot \sum y_i - N \cdot \sum x_i y_i}{(\sum x_i)^2 - N \cdot \sum x_i^2}$$

Slope of linear least squares fit

$$a = \frac{\Sigma y_i - b \cdot \Sigma x_i}{N}$$

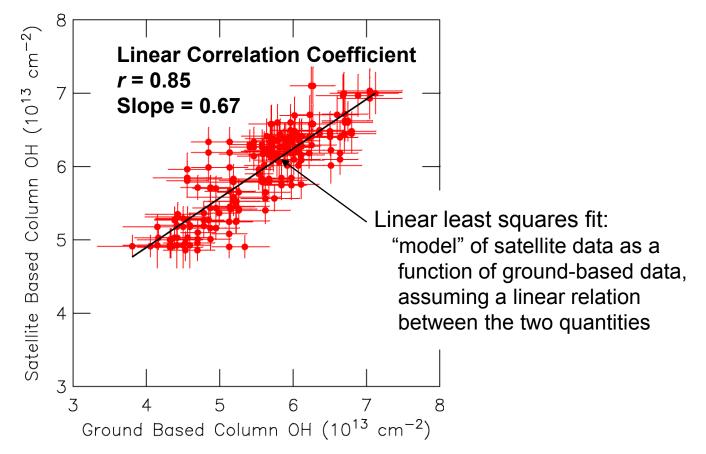
Intercept of linear least squares fit

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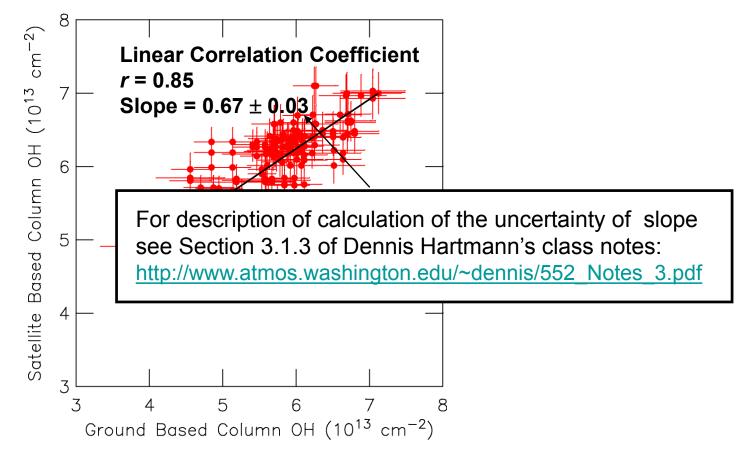
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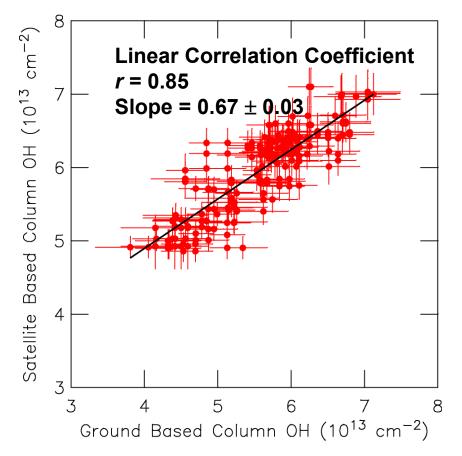
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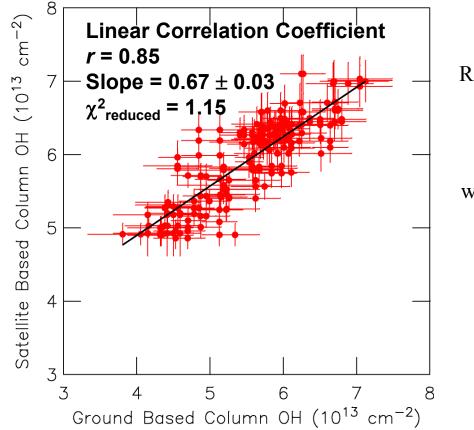
Suppose you have two sets of measurements (or data and model) that you'd like to relate.



#### How can we quantify the "goodness of the fit" ?

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Reduced  $\chi^2$  :

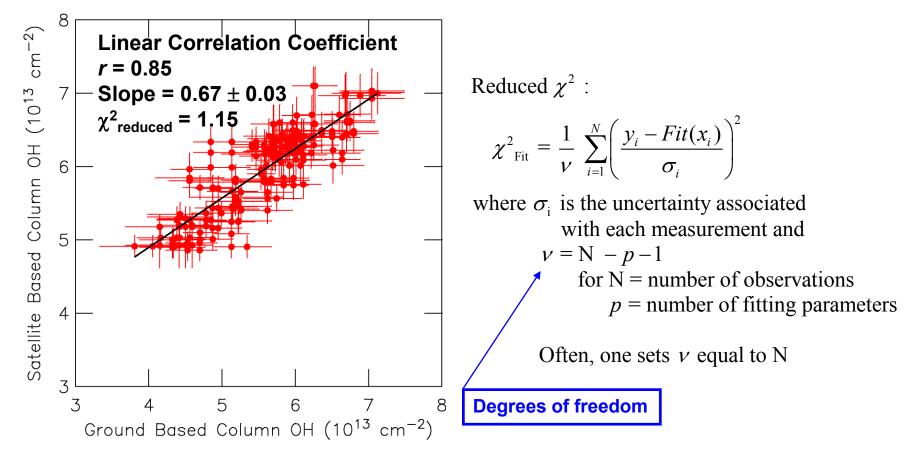
$$\chi^{2}_{\text{Fit}} = \frac{1}{\nu} \sum_{i=1}^{N} \left( \frac{y_{i} - Fit(x_{i})}{\sigma_{i}} \right)^{2}$$

where  $\sigma_i$  is the uncertainty associated with each measurement and v = N - p - 1for N = number of observations p = number of fitting parameters

Often, one sets v equal to N

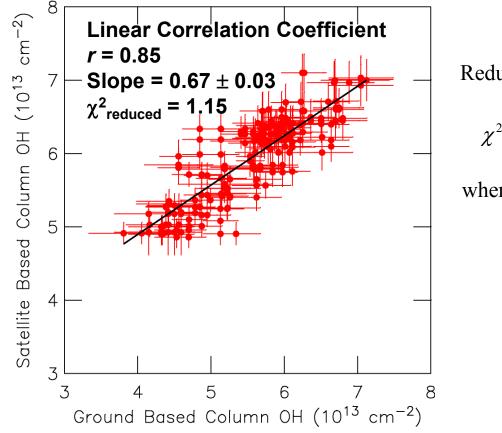
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# Reduced $\chi^2$ is an under-used, often unappreciated, quantitative measure of the degree of relation between a model and data, or two types of measurements (or, two types of models, if we can define uncertainties for each)

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Reduced  $\chi^2$  is very commonly used in the physics community

Indeed, in physics lab courses, students are sometimes cautioned to be critical of an experiment where reduced  $\chi^2$  lies close to zero. Why is this?

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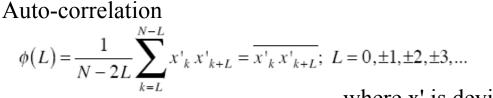
See <u>http://www.physics.csbsju.edu/stats/chi\_fit.html</u> for more for reduced  $\chi^2$ 

# A method for evaluating bias in global measurements of CO<sub>2</sub> total columns from space

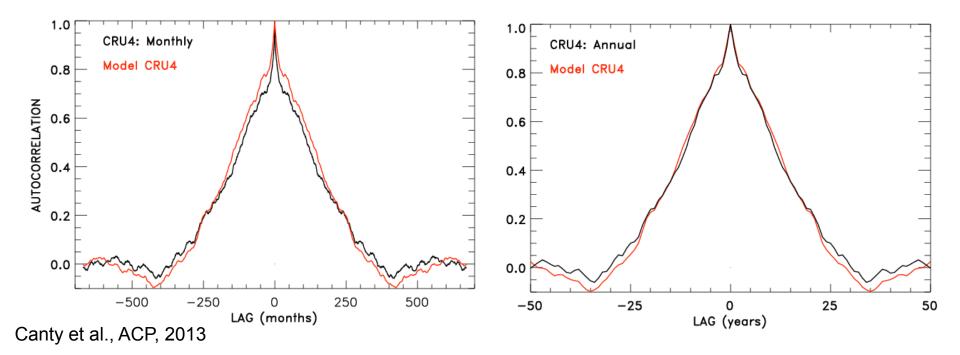
D. Wunch<sup>1</sup>, P. O. Wennberg<sup>1</sup>, G. C. Toon<sup>1,2</sup>, B. J. Connor<sup>3</sup>, B. Fisher<sup>2</sup>, G. B. Osterman<sup>2</sup>, C. Frankenberg<sup>2</sup>, L. Mandrake<sup>2</sup>, C. O'Dell<sup>4</sup>, P. Ahonen<sup>5</sup>, S. C. Biraud<sup>14</sup>, R. Castano<sup>2</sup>, N. Cressie<sup>6</sup>, D. Crisp<sup>2</sup>, N. M. Deutscher<sup>7,8</sup>, A. Eldering<sup>2</sup>, M. L. Fisher<sup>14</sup>, D. W. T. Griffith<sup>8</sup>, M. Gunson<sup>2</sup>, P. Heikkinen<sup>5</sup>, G. Keppel-Aleks<sup>1</sup>, E. Kyrö<sup>5</sup>, R. Lindenmaier<sup>15</sup>, R. Macatangay<sup>8</sup>, J. Mendonca<sup>15</sup>, J. Messerschmidt<sup>7</sup>, C. E. Miller<sup>2</sup>, I. Morino<sup>9</sup>, J. Notholt<sup>7</sup>, F. A. Oyafuso<sup>2</sup>, M. Rettinger<sup>10</sup>, J. Robinson<sup>12</sup>, C. M. Roehl<sup>1</sup>, R. J. Salawitch<sup>11</sup>, V. Sherlock<sup>12</sup>, K. Strong<sup>15</sup>, R. Sussmann<sup>10</sup>, T. Tanaka<sup>9,\*</sup>, D. R. Thompson<sup>2</sup>, O. Uchino<sup>9</sup>, T. Warneke<sup>7</sup>, and S. C. Wofsy<sup>13</sup>

> Retrievals are defined as successful by the master quality flag when they satisfy  $\chi^2 < 1.2$ . However, the  $\chi^2$  values have increased linearly over time, because the time-dependent radiometric calibration caused by a sensitivity degradation of the O<sub>2</sub> A-band channel was not applied to the noise model. To compensate for this, we adjust the cutoff value so that it starts at 1.2 and evolves with a linear increase in time, matching the increase in minimum  $\chi^2$ . As a result, a similar number of scenes are retained over time.

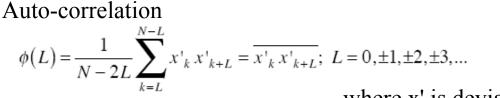
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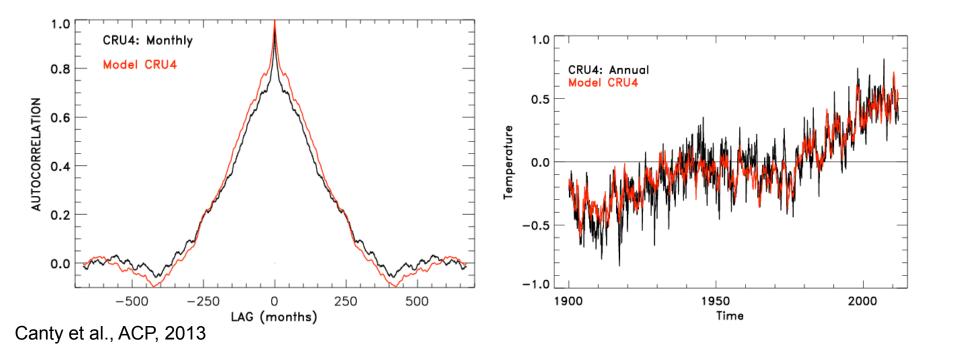
where x' is deviation from mean



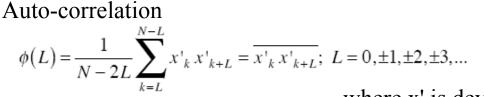
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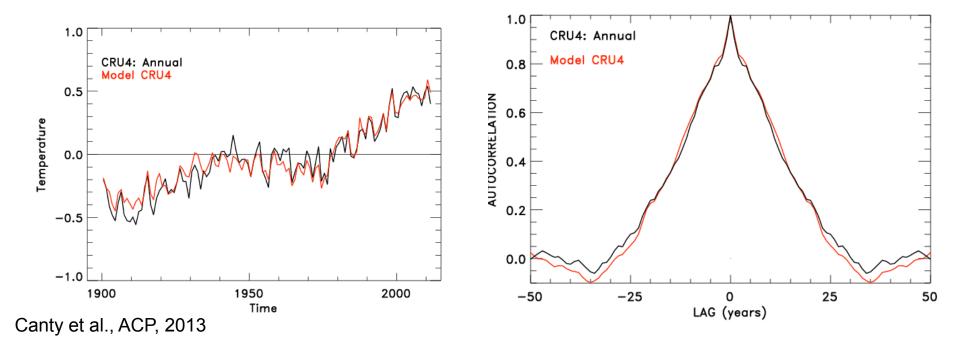
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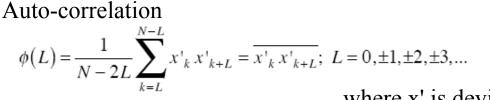
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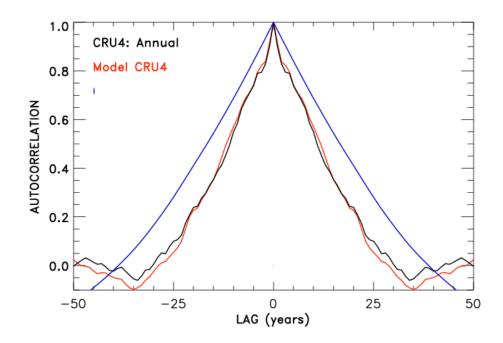
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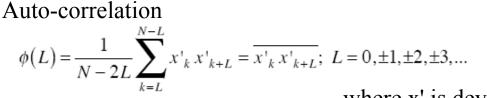


Canty et al., ACP, 2013

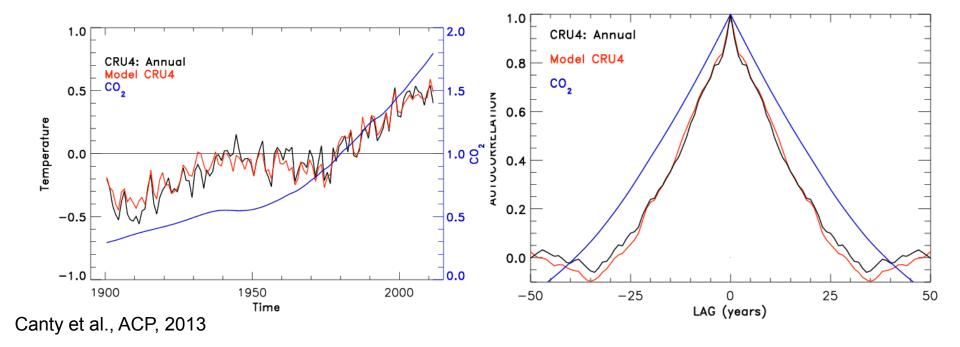
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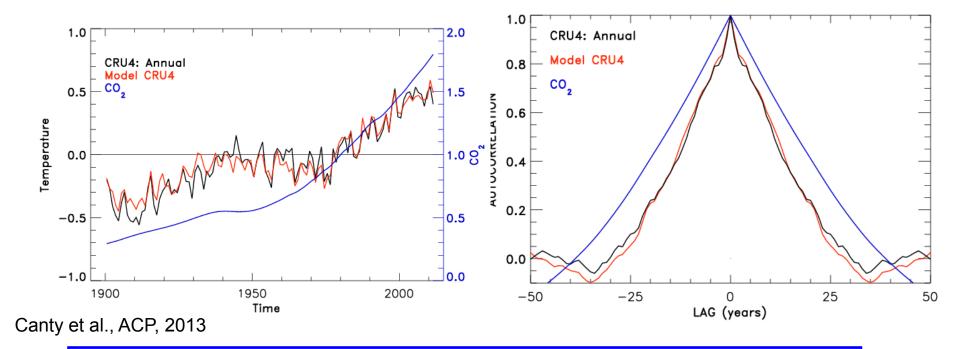
where x' is deviation from mean



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Auto-correlation  $\phi(L) = \frac{1}{N - 2L} \sum_{k=L}^{N-L} x'_{k} x'_{k+L} = \overline{x'_{k} x'_{k+L}}; \ L = 0, \pm 1, \pm 2, \pm 3, \dots$ where x' is devi

where x' is deviation from mean



The behavior of the auto-correlation of a signal is often used to infer degrees of freedom: see for example Dennis Hartmann's class notes: <a href="http://www.atmos.washington.edu/~dennis/552\_Notes\_6a.pdf">http://www.atmos.washington.edu/~dennis/552\_Notes\_6a.pdf</a>

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