06-100: Air Quality Module – Lecture Notes

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These lecture notes complement the material in the slides, namely "Air Quality Module - Lecture 01.pptx" (denoted as Lecture 1) and "Air Quality Module - Lecture 02.ptx" (denoted as Lecture 2).

Radiative Balance

Many concepts in *radiation* will be covered in the Heat Transfer course. The key concepts for this module are summarized below. When I took the Heat Transfer course, I used the book by Bergman *et al.* (2011), which is written by mechanical engineers. Another good and commonly used book is by Welty *et al.* (2008), in which some of the authors are chemical engineers.

- **Irradiance:** Power of electromagnetic radiation per unit area incident on a surface. SI units: $\mathrm{W\ m^{-2}}$.
- **Black Body:** Idealized physical body that absorbs all incident electromagnetic radiation.
- **Stefan-Boltzmann Law:** Also known as Stefan's Law, describes the irradiance from a black body in terms of its temperature.

$$I = \sigma T^4$$

where I is the irradiance, $\sigma = 5.6704 \times 10^{-8}\ \mathrm{J\ s^{-1}\ m^{-2}\ K^{-4}}$ is the Stefan-Boltzmann constant or Stefan's constant, and T is temperature.

In Lecture 1, the colors of the arrows in figures on slides 5 – 7 have the following meaning: orange indicates sunlight and red means infrared.

On slide 5, the heat balance is simply:

$$E = \bar{S}$$

where E is the Earth's irradiance if it is considered a black body disk and $\bar{S} = 345\ \mathrm{W\ m^{-2}}$ is the effective solar irradiance. Therefore, $E = 345\ \mathrm{W\ m^{-2}}$. And the temperature at the surface of a perfectly absorbing Earth is $T_s = \left(\frac{\bar{S}}{\sigma}\right)^{1/4} = 279\ \mathrm{K}$.

On slide 6, the heat balance is modified as we consider the reflectivity of the Earth (mostly by clouds), which is called albedo. The global average reflectivity is $A = 0.3$. Hence:

$$\bar{S} = A\bar{S} + E$$
$$E = (1 - A)\bar{S}$$
$$E = 241\,\mathrm{W\ m^{-2}}$$

and

$$T_s = \left[\frac{(1 - A)\bar{S}}{\sigma}\right]^{1/4} = 255\,\mathrm{K}$$

The more sophisticated (and realistic) approach on slide 7 requires concepts (Beer-Lambert Law, optical depth, *etc.*) that are beyond the scope of these notes. The key point is that the location of the optical depth level 1 dictates the temperature we feel on Earth's surface and that is affected by the concentration of greenhouse gases.

Coefficient of Determination (R^2)

The coefficient of determination, usually written as R^2, is a *statistic* that indicates how well data points fit a line or curve. A statistic is a single measure of some attribute of a sample, for example its arithmetic mean value. The R^2 is not the only goodness-of-fit measure and there is some criticism and controversy in the statistics community on its overuse and interpretation.

In Lecture 2, we fit a straight line to CO_2 annual data and used the R^2 as a measure of how well the line fit the data. The R^2 can be calculated after performing a *regression analysis*. Regression is a statistical process for estimating the relationships among variables. Say we have N data points in the pair $(x_i,\ y_i)$ for $i = 1,\ \ldots,\ N$, where x is the independent variable (also called input, covariate or predictor) and y is the dependent variable (also called output or response). We would like to obtain a mathematical relationship between x and y in order to predict outputs given new inputs. The mathematical relationship is a function (model) and can be represented as $f(\mathbf{x};\ \boldsymbol{\beta})$, where $\mathbf{x}$ is a vector of input values and $\boldsymbol{\beta}$ is a vector of parameters of the model. A simple regression model is a linear function, *i.e.* $f(x_i;\ a,\ b) = ax_i + b$. Figure 1 shows a schematic of the regression analysis in 2D.

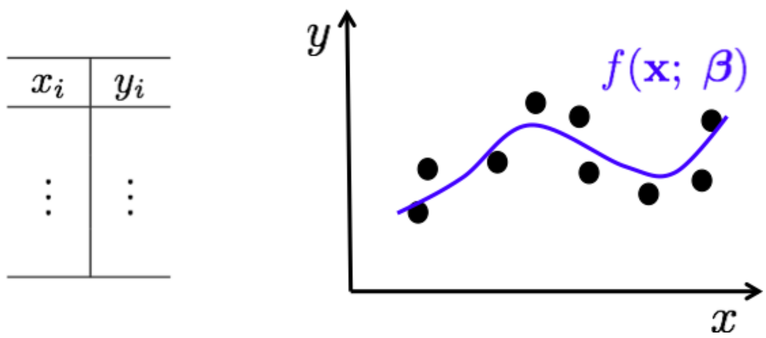

Figure 1: Regression analysis of data points $(x_i,\ y_i)$ and model $f(\mathbf{x};\ \boldsymbol{\beta})$.

The "variables" to be solved for in a regression problem are the model parameters, $\boldsymbol{\beta}$. In general, it requires solving a mathematical optimization problem. It is beyond the scope of these notes to explain the details of such process.

After regressing the model on the data, we obtain the values of the parameters and let us denote them by $\hat{\boldsymbol{\beta}}$. Thus, the output values obtained when evaluating the model at the input values are denoted by $\hat{\mathbf{y}} = f(\mathbf{x};\ \hat{\boldsymbol{\beta}})$. The R^2 is defined as follows:

$$\mathrm{R}^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

where

$$SS_{res} = \sum_{i=1}^{N} (\hat{y}_i - y_i)^2$$
$$SS_{tot} = \sum_{i=1}^{N} (y_i - \bar{y})^2$$

and $\bar{y}$ is the average of the output data values

$$\bar{y} = \frac{1}{N} \sum_{i=1}^{N} y_i$$

SS_{res} is the sum of squares of residuals, also called the residual sum of squares, and SS_{tot} is the total sum of squares (proportional to the sample variance). Clearly, the smaller the SS_{res} the closer to 1.0 (unity) R^2 is, which indicates a good fit or the closer the curve lies around the data points.

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References

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Welty, J.; Wicks, C. E.; Rorrer, G. L.; and Wilson, R. E. 2008. *Fundamentals of Momentum, Heat, and Mass Transfer*. John Wiley & Sons, Inc., 5^{th} edition.