Linear Least Squares: Versatile Curve and Surface Fitting (CDT-17)

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Abstract

The minimization method known as linear least squares – LLS – provides a straightforward, intuitive and effective means for fitting curves and surfaces (as well as hypersurfaces) to given sets of points. This text aims at presentng the LLS methodology in an intuitive manner, starting by defining the problem, introducing the concept of least squares error, and then describing the LLS method in an intuitive way based on systems of linear equations. Several examples of curve and surface fitting are provided in order to illustrate the flexibility and potential of the LLS approach.

'*Conoscere non è abbastanza, dobbiamo applicare.*'

Leonardo da Vinci.

1 Introduction

Often in science and technology, one faces the problem of fitting a curve or surface to a set of points. In case interest is focused on the interval where the points are contained, we have an *interpolation* problem. Otherwise, if we are aiming at extending the function outside that interval, an *extrapolation* problem arises. Given the frequency and importance of the above problems, several respective methods have been developed and reported in the literature (e.g. [1]). Typically, these methods involve the *optimization* of some merit or error function related to the adherence of the aimed curve/surface and the original points.

One of the simplest methods for fitting a curve/surface to a set of points is the *linear least squares* – LLS. Despite its simplicity, LLS is surprisingly powerful and versatile in its applications, allowing not only several types of candidate curves to be considered, as well as being extensible to higher dimensional problems involving several types of surfaces. These properties are not always fully realized, in the sense that LLS is sometimes understood mainly with respect to the more restricted situation of fitting straight lines to points.

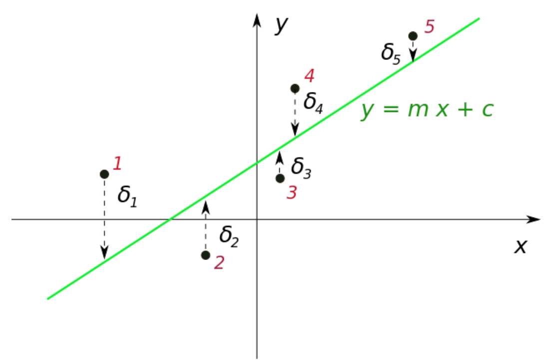

Figure 1: A set of $N = 5$ points (x_i, y_i), $i = 1, 2, \ldots, N$, and a possible straight line $y = mx + c$ fitting these points in the sense of passing near them. The adjustment parameters (coefficients) m and c allow the straight line to be rotate and translated, respectively, yielding varying levels of adherence. It is possible to define the distances δ_i from the $y-$value of each point i, namely y_i to the respectively fitted value $mx_i + c$. LLS involves minimizing the sum of $\sum_{i=1}^{N} \delta_i^2$.

As several other fitting methodologies, LLS is based on the optimization of an error function corresponding to the sum of squares differences between the given values and those produced by the sought curve/surface. By using matrix notation, LLS can be summarized in a very simple equation that can be easily applied to a wide range of interesting and important fitting problems. The computational cost mostly refers to matrix inversion ($\approx O(n^3)$,where n is the number of involved adjustment parameters, or coefficients). The matrix product $(A^T A)$

also requires $O(Nn)$ real products and sums.

The present didactic text has as its main objective to present an intuitive and relatively accessible introduction to the LLS method, covering not only straight line fitting, but also illustrating the potential of LLS with respect to other curves and surfaces.

2 Specifying the Problem

Let's first consider the situation where a set of points (x_i, y_i), $i = 1, 2, \ldots N$, are to be fitted by a straight line $y = mx + c$, as illustrated in Figure 1. Observe that the N points do not need to be equally spaced along the x domain. Also, keep in mind that several other curves could be equally considered.

The parameters, or coefficients, m and c in the sought line $y = mx + c$ can be understood as controlling two important aspects of the respective straight line, namely its inclination (m) and intercection with the $y-$axis (c). So, as we change these two parameters, we scan among an infinitude of possible solutions, each specified by the respective parameter values m and c. It can be soon realized that some of these solutions will provide better or worse fittings of the original points, and some configuration can lead to an optimal result. However, it is first necessary to objectively define some merit figure that can be used to gauge the quality of the possible fittings. A possible approach is described in the following section.

3 Mean Squares Error

As we desire that the fitted curve results as near as possible to the original points, we can define the differences δ_i from the values of y at each point i, namely y_i, to the respectively fitted values $mx_i + c$. As we want to minimize these differences, a first approach could be to define an error corresponding to the sum of all differences, i.e.

$$\lambda = \sum_{i=1}^{N} \delta_i \tag{1}$$

where $\delta_i = (mx_i + c) - y_i$.

However, this approach does not work properly because δ_i's with negative values tend to cancel those with positive values, eventually implying a small overall value of λ even when the straight line is far from the original points.

A possible alternative approach that circumvents this shortcoming would be to use the sum of the absolute values of the differences, namely $\sum_{i=1}^{N} |\delta_i|$. Though this criterion would avoid the aforementioned sign cancelations, the absolute value function incorporates a discontinuity of derivative at zero, which complicates analytical handling of the respective equations. This difficulty is avoided by taking the square instead of the absolute function, which yields the mean squared error often expressed as

$$MSE = \frac{1}{N} \sum_{i=1}^{N} \delta_i^2 \tag{2}$$

This measurement is called, for immediate reasons, *mean squares error*, MSE.

Now, the fitting problem illustrated in Figure 1 can be effectively formulated as finding the coefficient configuration (m, c) that minimizes the mean square error MSE. Because N is a constant, it can be removed during the minimization, which yields the simplified error function

$$\varepsilon = \sum_{i=1}^{N} \delta_i^2 \tag{3}$$

Interestingly, the problem illustrated in Figure 1 is more general and can consider several other types of functions. The problem of finding a curve that best adheres to the original points can, therefore, be approached by minimizing ε, which will be discussed in the following.

4 Linear Least Squares Fitting

An interesting insight about the workings of LLS minimization can be derived by considering a sequence of successive fitting situations expressed as the solution of systems of simultaneous linear equations. Let's start by considering the elementary situation in which we have only one point (x_1, y_1) to be fitted by a straight line $y = mx+c$. We can immediately plug the point coordinates into the straight line equation to obtain

$$y_1 = mx_1 + c. \tag{4}$$

Now, this equation has two unknowns, implying that it is soluble but undetermined or, in other words, that there is an infinite number of straight lines specified by $c = y_1 - mx_1$, each of which perfectly adhering to the original point by passing over it.

Let's proceed to another situation in which there is not one, but two distinct points (x_1, y_1) and (x_2, y_2). The imposition that the straight line passes through these two points can be mathematically expressed in terms of following system of linear equations

$$\begin{cases} y_1 = mx_1 + c \\ y_2 = mx_2 + c \end{cases} \tag{5}$$

Since the two points are distinct, the two equations composing the above system are linearly independent, so that the system is soluble and determined, presenting just one solution given as:

$$\begin{cases} \tilde{c} = \frac{x_1 y_2 - x_2 y_1}{x_1 - x_2} \\ \tilde{m} = \frac{y_1 - y_2}{x_1 - x_2} \end{cases} \tag{6}$$

and the straight line defined by $(\tilde{m}, \tilde{c})$ can be verified to pass precisely through the two original points (x_1, y_1) and (x_2, y_2).

The system of linear equations in Eq. 5 can be conveniently expressed in matrix form. In order to do so, we define a vector containing the $y-$values as

$$\vec{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \tag{7}$$

as well as a vector containing the adjustment coefficients

$$\vec{p} = \begin{bmatrix} c \\ m \end{bmatrix} \tag{8}$$

and the matrix

$$A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \end{bmatrix} \tag{9}$$

Now the system of linear equations in Eq. 5 can be compactly expressed as

$$\vec{y} = A\vec{p} \tag{10}$$

Observe that A is a 2×2 square matrix, which has A^{-1} as inverse. By left-multiplying both sides of the above equation by A^{-1}, we have

$$A^{-1}\vec{y} = A^{-1}A\vec{p} \implies \vec{p} = A^{-1}\vec{y} \tag{11}$$

which can be verified to provide the same solution as in Equation 6.

Now, we proceed to a fitting problem involving three distinct original points (x_1, y_1), (x_2, y_2) and (x_3, y_3). Let's impose that the straight line $y = mx + c$ passes through these three points, which leads to the respective system of linear equations

$$\begin{cases} y_1 = mx_1 + c \\ y_2 = mx_2 + c \\ y_3 = mx_3 + c \end{cases} \tag{12}$$

We have a system with two unknowns and three equations. The type of respective solution depends on the three involved equations being or not linearly independent. In the case of the three points being collinear, we have that two of these equations will be linearly dependent, so that a unique, determined solution will be obtained.

Otherwise, in case the three points are not aligned, the system is *overdetermined* and can only be solved in an optimization sense, for instance by imposing that the least square error between the original points and the fitted curve is minimum.

Let's start by expressing the above system in terms of a matrix equation, in an analogous way as that applied to the previous system involving two equations. We make

$$\vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}, \tag{13}$$

$$\vec{p} = \begin{bmatrix} c \\ m \end{bmatrix}, \tag{14}$$

and

$$A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{bmatrix} \tag{15}$$

and the system of linear equations in Eq. 12 can be summarized by the same equation as before, i.e.

$$\vec{y} = A\vec{p} \tag{16}$$

The problem in solving this system stems from the fact that A is no longer square, having instead dimension 3×2. Let's left-multiply both sides of the previous equation by A^T

$$A^T\vec{y} = A^T A\vec{p} \tag{17}$$

and define a new matrix S as

$$S = A^T A \tag{18}$$

Since S is now square, we can possibly derive its inverse $S^{-1} = (A^T A)^{-1}$ and left-multiply it to both sides of Equation 19, yielding

$$\begin{aligned} (A^T A)^{-1}\, A^T\vec{y} = (A^T A)^{-1}\, (A^T A)\, \vec{p} \implies \\ \implies \vec{p} = (A^T A)^{-1}\, A^T\vec{y} \end{aligned} \tag{19}$$

Let's make

$$U = (A^T A)^{-1}\, A^T \tag{20}$$

So that

$$\vec{p} = U\vec{y} \tag{21}$$

By comparing the previous equation with Equation 6, we see that the matrix U plays a role similar to that of the inverse of the square matrix A, i.e. A^{-1} in the case of determined systems. For this reason, matrix U is often called the *pseudo-inverse* of the non-square matrix A.

A good news is that Equation 21 can be verified to provide the least mean square *solution* to the fitting problem

Table 1: Coordinates (x_i, y_i) of five points to be fitted by a straight line function.

point i	x_i	y_i
1	-0.47	1.14
2	-0.26	1.21
3	0.15	1.28
4	0.82	1.47
5	-0.60	0.93

(e.g. [2, 1]). What is more, as we will illustrate in this text, this formulation holds for several other curves and surfaces. This approach will henceforth be called *LLS fitting*.

However, it should be kept in mind that the above development does *not* constitutes a proof that Equation 21 gives the least mean squares solution to the fitting problem. The manner in which we obtained that equation provides only an intuitive 'mnemonic' way to reach the pseudo-inverse equation that is motivated by the linear system of equations formulation of the considered fitting problem.

5 Curve Fitting

Let's apply the LLS method presented in the previous section to a problem involving real values. More specifically, consider the 5 original points given in Table 1.

We immediately have that

$$\vec{y} = \begin{bmatrix} 1.14 \\ 1.21 \\ 1.28 \\ 1.47 \\ 0.93 \end{bmatrix}, \tag{22}$$

$$\vec{p} = \begin{bmatrix} c \\ m \end{bmatrix} \tag{23}$$

and

$$A = \begin{bmatrix} 1 & -0.47 \\ 1 & -0.26 \\ 1 & 0.15 \\ 1 & 0.82 \\ 1 & -0.60 \end{bmatrix} \tag{24}$$

from which we obtain (up to 2 decimals)

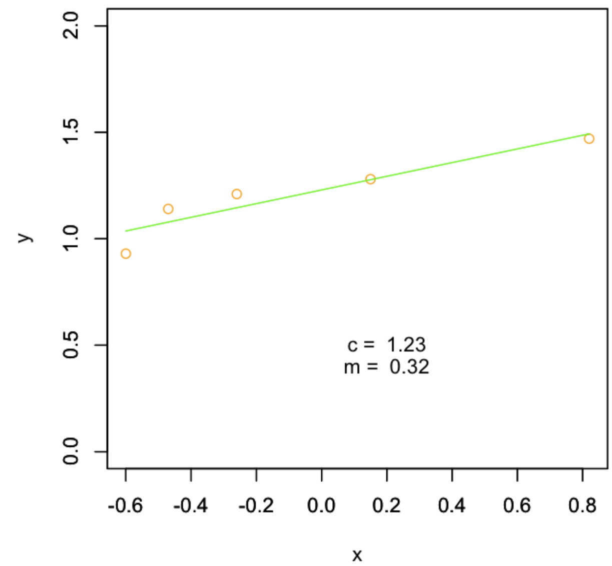

Figure 2: Five points (in orange) and respective LLS fitting by a straight line function. The parameters (m, c) corresponding to the best fitting are given in the legend up to two decimals.

$$(A^T A)^{-1} A^T = \begin{bmatrix} 0.18 & 0.19 & 0.21 & 0.25 & 0.17 \\ -0.30 & -0.14 & 0.17 & 0.68 & -0.40 \end{bmatrix}$$

so that the best adjustment parameters, in the least mean error sense, are easily determined as

$$\vec{p} = (A^T A)^{-1} A^T \vec{y} = \begin{bmatrix} 1.23 \\ 0.32 \end{bmatrix} = \begin{bmatrix} c \\ m \end{bmatrix}$$

The thus obtained LLS straight line fitting is shown in green in Figure 2. Observe that the LLS method does not warrant that the fitted curve passes through the original points. Also, it should be kept in mind that such good agreement as obtained in this example is by no means guaranteed. It will all depends on wether the chosen curve is indeed compatible to the points, in the sense of providing a good adherence to them. The mean squares error can be used to quantify the effectivity of the respective fitting, in the sense that better adherence will yield smaller mean squares errors.

Figure 2 illustrates another application of LLS for fitting 5 points, now by a cubic polynomial of the type:

$$y = a_0 + a_1 x + a_2 x^2 + a_3 x^3 \tag{25}$$

where a_0, a_1, a_2, and a_3 are the adjustment parameters to be determined. The coordinates of the 5 original points are given in Table 2.

Now, matrix A is constructed as follows:

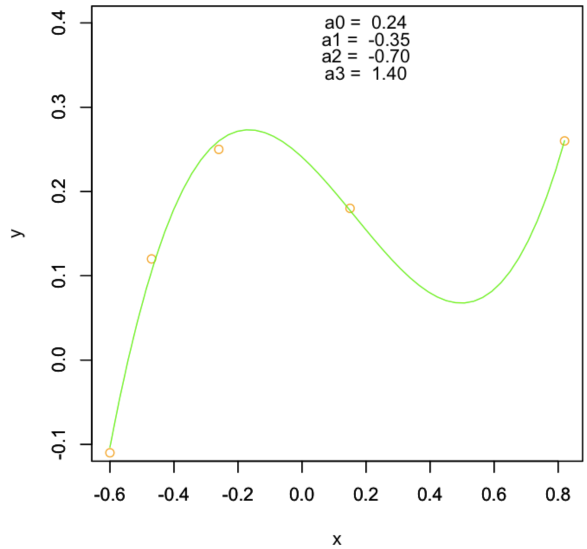

Figure 3: Five points (in orange) and respective LLS fitting by a cubic polynomial function. The parameters (a_0, a_1, a_2, a_3) corresponding to the best fitting are given in the legend up to two decimals.

Table 2: Coordinates (x_i, y_i) of five points to be fitted by a cubic polynomial function.

point i	x_i	y_i
1	-0.47	0.12
2	-0.26	0.25
3	0.15	0.18
4	0.82	0.26
5	-0.60	-0.11

$$A = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3 \\ 1 & x_5 & x_5^2 & x_5^3 \end{bmatrix}$$

and the coeffivients vector is given as

$$\vec{p} = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} \tag{26}$$

Again, a good adherence has been obtained. However, notice that this type of LLS-based curve fitting requires us to have a good guess or knowledge of the type of curve to be considered. In case the candidate curve is not proper, the adherence will not be good.

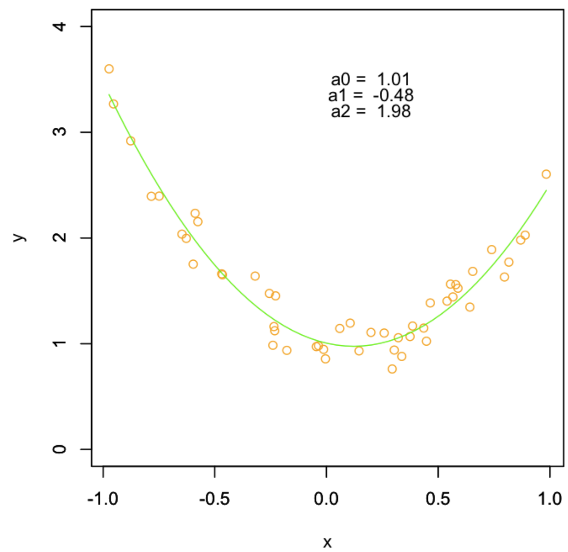

Figure 4: In some cases, LLS can be used as a 'filter' to remove added noise. In this example, the points originally followed a square function with $a_0 = 1$, $a_1 = -0.5$, and $a_2 = 2$, and noise values uniformly distributed in the interval $[-0.3, 0.3]$ were added to the original $y-$coordinates. In this specific case, as the original function was known, it was possible to recover the original curve (in green) and parameters with relatively good accuracy.

Interestingly, LLS fitting can be also used to remove noise added to a curve of a type that is known or that can be suitably inferred. This is illustrated in Figure 4.

The 50 points were generated from a square function

$$y = a_0 + a_1 x + a_2 x^2 \tag{27}$$

with $a_0 = 1$, $a_1 = -0.5$, and $a_2 = 2$. Uniformly distributed noise within the interval $[-0.3, 0.3]$ has been added to the $y-$coordinates of the original points. The green curve indicates the result of LLS fitting on the original points, and the original parameters were recovered with relatively good accuracy. This 'filtering' action of LLS filter is not so often realized, but can be an interesting option in some circumstances, such as when the nature of the original curve is known, in presence of low/moderate additive noise.

6 Non-Linear Fitting

The curves considered for fitting in the previous examples are linear with respective to all involved coefficients. This requirement is implied by the presented method, which is called *linear* least squares. In principle, LLS can be applied only to these situations, but is sometimes possible to transform a curve with nonlinear relationship between the coefficients so as to obtain a respective linear form. This extends the applicability of LLS.

Let's illustrate the above possibility with respect to

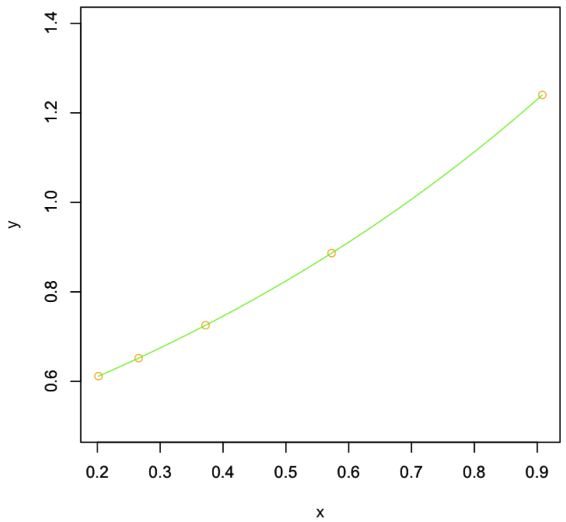

Figure 5: Fitting 5 points by an exponential function. The original points had their $x-$coordinates generated with uniform probability between $(0, 1]$ and respective $y-$coordinates were obtained by plugging the $x-$values into Equation 28 with $a = 0.5$ and $b = 0.1$. LLS was performed over the linearized version of the original curve, yielding coefficients (observe that a is obtained from the estimated coefficient c as $a = e^c$) that are substantially close to the original values.

the specific example involving an exponential fitting curve such as

$$y = a\, e^{bx} \tag{28}$$

involving non-linearity among the two involved coefficients a and b. If we take logarithm at both sides, and this requires that the values at both these sides are positive, we obtain

$$z = ln(y) = ln(a) + bx = c + bx \tag{29}$$

which can be understood as a new, transformed equation with linear coefficients b and c.

Figure 5 illustrates the application of LLS for fitting a set of 5 points by a curve as in Equation 29. The points were generated by using this same equation with $a = 0.5$ and $b = 0.1$.

7 Surface Fitting

The LLS method can be immediately applied to fitting of surfaces in multidimensional data. Let's consider $N = 15$ points with coordinates (x, y, z) as shown in orange in Figure 6.

A quadratic surface with $2-$dimensional domain can be expressed as

$$y = a_0 + a_1 x + a_2 y + a_3 xy + a_4 x^2 + a_5 y^2 \tag{30}$$

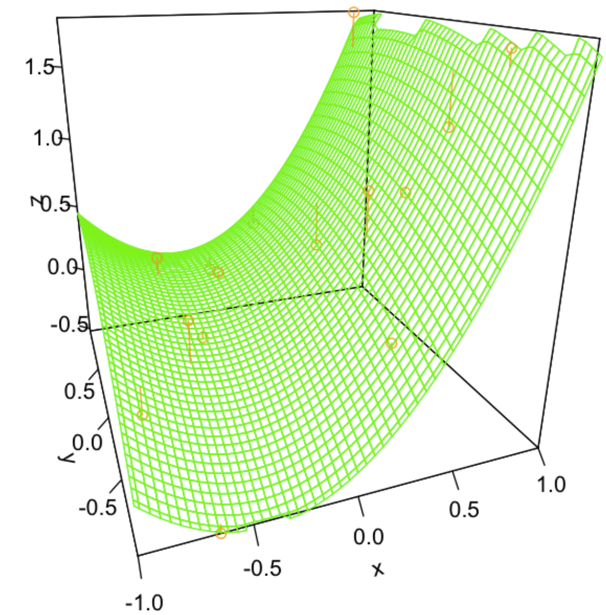

Figure 6: A quadratic surface fitted to 15 original points by using the LLS method.

The A matrix for this case can be constructed as

$$A = \begin{bmatrix} 1 & x_1 & y_1 & x_1\, y_1 & x_1^2 & y_1^2 \\ 1 & x_2 & y_2 & x_2\, y_2 & x_2^2 & y_2^2 \\ 1 & x_3 & y_3 & x_3\, y_3 & x_3^2 & y_3^2 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 1 & x_{15} & y_{15} & x_{15}\, y_{15} & x_{15}^2 & y_{15}^2 \end{bmatrix}$$

with respective coefficient vector

$$\vec{p} = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix} \tag{31}$$

The sought coefficients are estimated by using the Equation 21.

Figure 6 depicts the estimated quadratic surface (in green) fitted to the 15 original points.

8 Concluding Remarks

Linear least squares fitting is a well-established, flexible and efficient method for adjusting curves and surfaces to sets of points. In this text, we aimed at providing an intuitive and hopefully simple introduction to the LLS fitting methodology. We started by outlining the fitting problem, and proceeded by discussing curve and surface fitting as an optimization of the mean squares error between the original data and the candidate curve/surface.

By addressing curve fitting in terms of linear systems of equations, and respective compact matrix equations, we then developed an intuitive (though not a proof) approach to LLS fitting. The potential of this methodology was illustrated with respect to several situations including different types of curves, the possibility of linearizing some types of curves, as well as surface fitting. The flexibility and efficiency of the LLS approach contributed to applications of its application to a wide range of areas and problems, from signal processing (e.g. [3]) to statistics(e.g. [4]). LLS fitting is also related to the problem of scientific modeling (e.g. [5], in the sense that the obtained curves/surfaces can be understood as a simple, direct mathematical model underlying the original points, which often corresponds to measurements obtained from experiments.

Acknowledgments.
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Costa's Didactic Texts – CDTs

CDTs intend to be a halfway point between a formal scientific article and a dissemination text in the sense that they: (i) explain and illustrate concepts in a more informal, graphical and accessible way than the typical scientific article; and (ii) provide more in-depth mathematical developments than a more traditional dissemination work.

It is hoped that CDTs can also integrate new insights and analogies concerning the reported concepts and methods. We hope these characteristics will contribute to making CDTs interesting both to beginners as well as to more senior researchers.

Though CDTs are intended primarily for those who have some experience in the covered concepts, they can also be useful as summary of main topics and concepts to be learnt by other readers interested in the respective CDT theme.

Each CDT focuses on a few interrelated concepts. Though attempting to be relatively self-contained, CDTs also aim at being relatively short. Links to related material are provided in order to complement the covered subjects.

The complete set of CDTs can be found at: `https://www.researchgate.net/project/Costas-Didactic-Texts-CDTs`.