J Math Chem (2011) 49:619–624
DOI 10.1007/s10910-010-9781-4

BRIEF COMMUNICATION

Logical Kronecker delta deconstruction of the absolute value function and the treatment of absolute deviations

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Received: 3 November 2010 / Accepted: 18 November 2010 / Published online: 4 December 2010

Abstract A logical Kronecker delta reformulation of the absolute value function and the related discrete problem of the optimal absolute deviation are studied as the basic step towards applications of first order norms in theoretical chemistry. Absolute value function derivatives appear in the present context related to unit step function, Dirac delta function and its derivatives. The absolute value of the difference of two Minkowski normalized Gaussian functions is analyzed as an example. The proposed logical Kronecker delta deconstruction manner to express the absolute value function is also applied to the absolute deviation from the median of a set of numerical values, which looks to be just the optimal first order norm.

Keywords Logical Kronecker delta · First order norm · Absolute value function · Step function · Dirac delta function · Gaussian functions absolute difference · Absolute value deviation · Median

1 Introduction

The absolute value function and first order norms can be undoubtedly associated to some important problems in theoretical and mathematical chemistry, which still are waiting to be fully developed. This communication wants to clarify some points which still are not well understood about the absolute value function, see for example [1]. This effort can be taken as a preliminary step to be later used as the basic mathematical structure in defining fundamental aspects of Minkowski norms and distances, which in turn could be subsequently employed into new quantum similarity definitions as well as quantum mechanical wave and density functions analysis, classification and

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comparison. The role of Minkowski norms in several aspects of quantum similarity has been already analyzed in previous papers [2–5], thus the development of this earlier introduction can be supposed started by the present study. Here, will be just considered, as it seems of some fundamental importance, the differentiation of the absolute value function and a statistical application in the search of optimal absolute value deviation. They constitute the two related sides of the problem, providing a continuous and a discrete example, associated to the Minkowski norm applications.

2 Redefinition of the absolute value function in terms of logical Kronecker deltas

The deconstruction of the absolute value function in terms of logical Kronecker deltas[1] [6–8] becomes an easy task, if one accepts that the following expression holds:

$$f(x) = |x| \rightarrow |x| = \delta(x \geq 0)\, x - \delta(x \leq 0)\, x \tag{1}$$

3 First absolute value function derivative and step functions

Then, the formal above possibility of writing the absolute value function as in Eq. 1, allows expressing the derivative as a difference of logical Kronecker deltas:

$$\frac{d|x|}{dx} = \delta(x \geq 0) - \delta(x \leq 0)$$

obviating in this way the problem of the usual definition of the absolute value derivative

$$\frac{d|x|}{dx} = \frac{|x|}{x} \tag{2}$$

which becomes indefinite at $x = 0$.

However, in the present deconstruction of $|x|$, the right and left derivatives of the absolute function as shown in Eq. 1 are not coincident, but at $x = 0$ are going from -1 on the left derivative to $+1$ on the right derivative. Such a problem could be arranged using a cumbersome description of Eq. 1, where the two logical Kronecker deltas could be used without the equal sign and a third term added: $\delta(x = 0)\, x$.

To obviate this problem now one can use the Heaviside or unit step function [9]:$H(x)$, which in turn can be also defined in terms of a logical Kronecker delta as:

$$H(x) = \delta(x \geq 0) \tag{3}$$

[1] A logical Kronecker delta is a generalization of the well-known mathematical symbol: $\mathbf{I} = \{\delta_{IJ}\}$, used to represent the elements of the unit matrix. A logical Kronecker delta can be written in general as: $\delta(L)$, where L is a logical expression. Therefore one assumes that: $\delta(.T.) = 1$ and $\delta(.F.) = 0$. In fact, logical Kronecker deltas are mathematical symbols, which can be translated into the high level computer language conditional instruction: *if* ([*logical expression*])...

Having in mind the present description of the $|x|$ first derivative at $x = 0$ in one hand and the Heaviside definition (3) on the other, the anomalous first derivative of the absolute value function deconstruction can be easily related to the step function. That is, one can also write:

$$\frac{d\,|x|}{dx} = 2H\,(x) - 1 \tag{4}$$

4 Higher derivatives of the absolute value function

It is well known that the derivative of the step function as above defined is the Dirac's delta function [9]. Then, in this way one can associate the second derivative of the absolute value function to a Dirac function. First and higher derivatives of the Dirac functions also exists [9], thus the absolute value function can be considered smooth in the sense of Dirac's function smoothness.

Absolute value function derivatives can be in this way thought as a member of the distributions family.

5 First derivative of the absolute value of the difference of two Gaussian functions

In order to visualize the underlying idea and the algebraic power contained into the above redefinition of the absolute value function, suppose two normalized Gaussian functions:

$$g\,(a\,|x\,) = N\,(a)\exp(-ax^2) \wedge g\,(b\,|x\,) = N\,(b)\exp(-bx^2)$$

with:

$$N\,(a) = \left(\frac{a}{\pi}\right)^{\frac{1}{2}} \wedge N\,(b) = \left(\frac{b}{\pi}\right)^{\frac{1}{2}}$$

thus, the Minkowski norms become:

$$\int_{-\infty}^{+\infty} g\,(a\,|x\,)\,dx = \langle g\,(a\,|x\,)\rangle = 1 \wedge \int_{-\infty}^{+\infty} g\,(b\,|x\,)\,dx = \langle g\,(b\,|x\,)\rangle = 1$$

so the difference of both Gaussians and their absolute value is easily defined as:

$$\Delta_g\,(x) = g\,(a\,|x\,) - g\,(b\,|x\,) \to A_g\,(x) = \left|\Delta_g\,(x)\right|;$$

therefore as it has been earlier described, the absolute value of the difference can be also deconstructed in the following way:

$$A_g\,(x) = \left|\Delta_g\,(x)\right| = [\delta\,(g\,(a\,|x\,) > g\,(b\,|x\,)) - \delta\,(g\,(a\,|x\,) < g\,(b\,|x\,))]\,\Delta_g\,(x)$$

and calling:

$$\Gamma = [\delta\,(g\,(a\,|x\,) > g\,(b\,|x\,)) - \delta\,(g\,(a\,|x\,) < g\,(b\,|x\,))]$$

for simplicity sake, then it can be written:

$$A_g\,(x) = \left|\Delta_g\,(x)\right| = \Gamma\Delta_g\,(x).$$

The first derivative of the absolute value of the Gaussian difference can be readily set as:

$$\begin{aligned}\frac{dA_g\,(x)}{dx} &= \frac{d\Gamma}{dx}\Delta_g\,(x) + \Gamma\frac{d\Delta_g\,(x)}{dx}\\ &= \frac{d\Gamma}{dx}\Delta_g\,(x) + 2\Gamma x\left(b\left(\frac{b}{\pi}\right)^{\frac{1}{2}}\exp(-bx^2) - a\left(\frac{a}{\pi}\right)^{\frac{1}{2}}\exp(-ax^2)\right)\end{aligned}$$

which is a well-defined function, but depending of the first derivative of the step function, similar to the one encountered in Eq. 4 and the sign of the previously defined difference of Gaussian functions playing a role in the second derivative term. Higher order derivatives can be obtained in the same way.

6 Absolute deviation and the median

A related problem to the above discussion, but in the discrete side of the absolute value point of view, corresponds to the optimal absolute deviation of a set of ordered numerical values: $X = \{x_I\,|I = 1, N\}$ from a given parameter. The problem still is transcribed into modern books, see for example [1], as related to the absolute value function first derivative indetermination as defined in Eq. 2. As the problem possible solution has been previously discussed, the same technique will be employed now in this discrete context.

In order to obtain a possible definition of the absolute deviation of a numerical set like X from an optimal parameter λ, such deviation can be described as:

$$D\,(\lambda) = \sum_I |x_I - \lambda|, \tag{5}$$

producing an extremum for the sum of the absolute differences in a way parallel to the one which can be employed in obtaining the optimal variance, yielding in this case the arithmetic mean as the optimal parameter.

Such an extremum can be obtained in the absolute deviation case, by preliminarily using the alternative logical Kronecker delta definition (1) on Eq. 5:

$$D\,(\lambda) = \sum_I [\delta\,((x_I - \lambda) \geq 0)\,(x_I - \lambda) + \delta\,((x_I - \lambda) \leq 0)\,(\lambda - x_I)]$$

yielding a derivative, which can be easily written as:

$$\frac{dD(\lambda)}{d\lambda} = \sum_I \left[-\delta\left((x_I - \lambda) \geq 0\right) + \delta\left((x_I - \lambda) \leq 0\right)\right]$$
$$= N_Q - N_P \wedge N = N_P + N_Q$$

where N_P and N_Q are the cardinalities of the positive and negative differences between the elements of the set X and the parameter, respectively. To become an extremum the above derivative shall be null and then the obvious result is obtained:

$$N_Q = N_P.$$

Consequently, it can be trivially deduced that the optimal parameter λ must be a central value of the numerical set X, dividing the whole into two subsets of equal cardinality.

That means that if the cardinality of X is even, then:

$$N = 2K \to \lambda = \frac{1}{2}\left(x_K + x_{K+1}\right)$$

and in case of X possessing an odd cardinality:

$$N = 2K + 1 \to \lambda = x_{K+1}.$$

Therefore, the sought optimal parameter becomes the median of the numerical set X in both cases.

7 Conclusion

The reformulation of the absolute value symbol in terms of logical Kronecker deltas permits to study the analytical structure of the absolute value function, opening the way of systematically utilize first order Minkowski norms in quantum mechanical problems.

Acknowledgments The author wants to acknowledge professor I. Gutman sharp comments on a previous study, where the absolute value function was classified as smooth. Most surely this paper could never have been written or, at least, delayed *sine die*, without Gutman's kind intervention. Also, the discussion on the nature of the first derivative of the present absolute value formulation with Professor P. G. Mezey has deeply clarified some aspects of a first draft of this work. This contribution has been partially sponsored by the Spanish Ministerio de Educación y Ciencia, under the fellowship: CTQ2006-04410/BQU.

References

1. D. Koks, *Explorations in Mathematical Physics* (Springer, New York, 2006)
2. R. Carbó-Dorca, J. Math. Chem. **32**, 201–223 (2002)
3. R. Carbó-Dorca, J. Math. Chem. **33**, 227–244 (2003)

4. P. Bultinck, R. Carbó-Dorca, J. Math. Chem. **36**, 191–200 (2004)
5. R. Carbó-Dorca, J. Math. Chem. **44**, 628–636 (2008)
6. R. Carbó-Dorca, E. Besalú, J. Math. Chem. **13**, 331–342 (1993)
7. R. Carbó-Dorca, E. Besalú, Comput. Chem. **18**, 117–125 (1994)
8. E. Besalú, R. Carbó, J. Math. Chem. **18**, 37–72 (1995)
9. V. Ya Arsenin, *Basic Equations and Special Functions of Mathematical Physics* (Iliffe Books Ltd, London, 1968)