

# UNIVERSITY OF VESZPRÉM DEPARTMENT OF MATHEMATICS AND COMPUTING

### SCATTERED DATA INTERPOLATION VIA IMPROVED SHEPARD-'S METHOD

by

### ISTVÁN SZALKAI

Department of Mathematics and Computing, University of Veszprém P.O. Box. 158, 8201 Veszprém, Hungary

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## SCATTERED DATA INTERPOLATION VIA IMPROVED SHEPARD'S METHOD I. CONTINUITY, DIFFERENTIABILITY AND LIMITS

István SZALKAI, Veszprém, Hungary

#### Abstract

We present here a complete investigation of Shepard's one-formula method for scattered interpolation for general weight functions (see (2) below) which might help to choose the optimal one for anyone's interpolation purposes.

We investigate, in any dimension, continuity, differentiability, limit and monotonicity of the approximating function, and at the end of the paper, the question of multiple measure data. We investigate pro and contra, that is we highlight also the bad properties of the approximating function given by Shepard's method!

We do not repeate the wellknown results of the large literature on Shepard's method, however the present paper can be read alone, no previous knowledge of the topic is required. Our general results are not easy generalizations of the ones in the literature.

The method we investigated is, in fact, a single formula, easy to build in into any computer program, works for any layout of data, and moreover can have many good properties, depending on the weight function  $\sigma$ , that is why we deal with it in a two-part paper.

#### TABLE OF CONTENTS

0	INTRODUCTION	p. 1
1	GENERAL RESULTS	p. 6
2	CONTINUITY and DIFFERENTIABILITY	p. 8
3	LIMITS	p. 12
4	MONOTONICITY	p. 18
	a) Negative results	
	4.0 The "Hill and Valley" Property	p. 19
	b) Positive results	
	4.1 The Case M=2	p.21
	4.2 The Case M>2	p.22
5	DUPLICATE DATAPOINTS	p. 25
6	GLOSSARY of Notations	p. 28
	References	p. 29

#### O INTRODUCTION and HISTORY

Inspite of the large number of interpolation methods only a few of them help us in the case of scattered dataset: the dataset do not have any regularity for its distribution. (The usual methods for approximation require some kind of regularity of the dataset. On the contrary, scattered data interpolation tasks arise almost everywhere both in practice and also in theoretical investigation, see eg. [Sz0] through [Sz2].) The problem of scattered data interpolation is the following: Let the dataset  $\{P_1, \ldots, P_n\}$   $\subseteq \mathbb{R}^N$  and the real numbers  $F_1, \ldots, F_n \in \mathbb{R}$  be given, and we seek for an interpolation function  $U: \mathbb{R}^N \to \mathbb{R}$  with best possible approximation. (This latter means that either  $U(P_1) = F_1$  for each  $1 \le M$  is required, or that the quadratic sum  $\sum_{i=1}^N (F_i - U(P_i))^2$  is to be minimized and U(P) would have some other good properties, too.)

We investigate here Shepard's method in all of these aspects.

The easiest method for scattered data interpolation is Shepard's one which is a single formula. Shepard's original formula reads

$$U(P) := \frac{\sum_{i=1}^{M} F_{i} \cdot \prod_{j \neq i} d(P, P_{j})}{\sum_{i=1}^{M} \prod_{j \neq i} d(P, P_{i})}$$

$$(0)$$

which has the simpler version

$$U(P) := \frac{\sum_{i=1}^{M} \frac{F_{i}}{d(P, P_{i})}}{\sum_{i=1}^{M} \frac{1}{d(P, P_{i})}}$$
(1)

where d(P,Q) denotes any Eucledian distance of the points  $P,Q\in\mathbb{R}^N$ . It is important to note that (0) is suitable for theoretical investigations only, as demonstrated in [GW], but numerical computations of (0) always do overand underflow! In the meantime (1) is always comfortable for computing. It is plausible that (1) is the weighted arithmetic mean of the values  $F_i$  with the weights  $\frac{1}{d(P,P_i)}$ , the inverse distance of the point P from the poits  $P_i$ . That is, the closer is P to the point  $P_i$  the greater weight corresponds to  $F_i$ . (See [HL] also for some other more or less complicated scattered data interpolation methods.)

The above method has a large number of good properties, among others: U(P) is defined on the whole space  $\mathbb{R}^N$ , it is exact ( $\forall i \ U(F_i) = P_i$ ) and continuous, it is invariant to many co-ordinate transformations and to changing measure units, has limit  $\lim_{P \to \infty} U(P) = \overline{F} = \frac{F1 + \ldots + FM}{M}$  and many more, we give a complete list in Section 1. Moreover, beeing this a small formula only, this simple and quick subroutine can be built in any program (also short ones, not only packages) and works for any dataset! Its theoretical and practical behaviour can also easily been investigated!

However, despite of the above numerous excellent properties, Shepard's above original method has a great disadvantage, which is not mentioned in the literature, and must be the reason why Shepard's method is *not* widely used: U(P) tends to the average  $\overline{F}$  not only when P goes to infinity but even also when P is in the convex hull of the dataset  $\{P_1, \ldots, P_M\}$ ! This is illustrated in the 1-dimensional Figure 1 below.

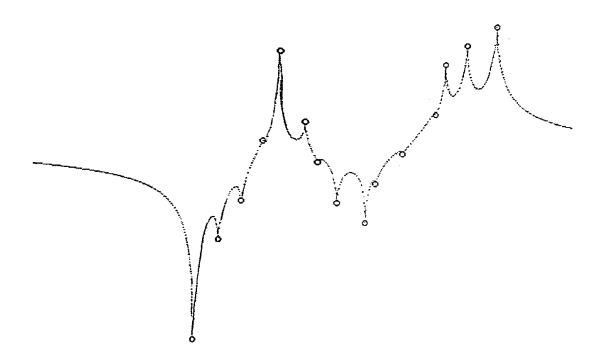


Figure 1

Sample for some 1-dimensional U(P),  $\sigma(d) = 1/d$ 

In Example 4.0 we show that these "bumps" are neccessary and further, in Theorems 4.1 and 4.2 we even calculate *the rate* of them. Roughly speaking the reason of this phenomena is that the weight function  $\frac{1}{d}$  (where  $d=d(P,P_i)$  is the distance) goes *slowly* to 0 when  $d\to\infty$  (when P moves off some of the points  $P_i$ ).

This problem could be avoided by choosing another weight function  $\sigma(d)$  instead of  $\frac{1}{d}$ . To be more precise, in this paper we investigate the below generalization of Shepard's formula (1):

Let for P∈RN

$$U(P) = \frac{\sum_{i=1}^{M} F_{i} \cdot \sigma(P, P_{i})}{\sum_{i=1}^{M} \sigma(P, P_{i})}$$
(2)

where  $\sigma: \mathbb{R}_+ \to \mathbb{R}_+$  is any positive, continuous and decreasing function, and for simplicity we write  $\sigma(PQ)$  instead of  $\sigma(d(PQ))$  for  $P, Q \in \mathbb{R}^N$ .

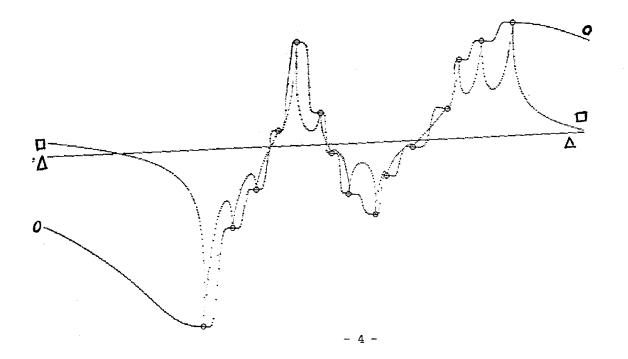
The main goal of our present paper is to investigate the behaviour of this modified interpolation method (2) for different weight functions  $\sigma$ .

Section 1 deals with general properties of U(P) for any weight function  $\sigma(d)$  while Section 2 is devoted to the exactness, continuity and differentiability properties of this method. Let us highlight here Theorem 2.1. The monotonicity and "bump" - problems pro and contra are investigated in Section 3, the limit of U in the infinity is dealt in Section 4.

In Section 5 we investigate the problem of multiple data - raised by specialists in practice. Shortly speaking, in practical applications we may measure multiple data at the same point, by chance. In Section 5 we reveal to what extend remain our previous results valid.

In the appendix we collected the notations we use and might be not common.

Also we allow arbitrary weight function  $\sigma$  in (2) unless we say otherwise. For example, we tried out the following ones by computer (d>0 unless stated otherwise):  $1/d^{\alpha}$ ,  $\frac{1}{1+d}\alpha$ ,  $\exp(-\lambda d^{\beta})$  for  $\alpha,\beta,\lambda>0$ ,  $\frac{1}{\ln(d+1)}$ ;  $-\ln(d)$  for 0<d<1 and 0 for d≥1; arccotan(d), and various multiplications and compositions of them. In Figure 2 we show some of our collection.



#### Figure 2

U(P) for various σ

 $\Box : \sigma(d) = \exp(-d^2)$ 

 $\Delta : \sigma(d) = \frac{1}{\ln(1+d)}$   $\circ : \sigma(d) = 1/d^{5}$ 

These diagrams demonstrate well the huge difference behaviour of the weight functions  $1/d^{\alpha}$  and  $\exp(-\lambda d^{\beta})$ . Theorem 2.1 and other results of Sections 2 and 3 explore many more differences between these two types of weight functions. Some type of "crossing" (eg.multiplication) of these functions might have better properties, at least from our computer experiments. However, also the theroretical methods with which these functions can be dealt, are also very different, so at this moment we do not have any hope for examining  $\exp(-d^{\beta})/d^{\alpha}$  for  $\alpha, \beta>0$ , for example.

In Sections 2 and 3 we will see that the behaviour of  $\sigma$  near to 0 and around  $\infty$  have prior importance for the behaviour of U. (See eg.our # operator in Section 3.) Another possibility would be to investigate weight functions which are equal to 0 for d>d for some fixed number d. We also do not deal with this interesting problem, but U certainly would have many breaks when d(P,P,) leaves d for any i≤M.

We work in the general n-dimensional space  $\mathbb{R}^{N}$ , and we talk about the distance of points P and Q, which we denote by d(P,Q) or simply by (P,Q), but we do not restrict ourselves to any specific metric! Though we do not deal with the question which metric d(P,Q) remain our results valid, but certainly for all the wellknown norms L for any  $n \in \mathbb{R}_+$  will do.

Though monotonicity properties are more important than limit ones, we have very few results on monotonicity because of the complex and not trivial problem. In the meantime, results on limits are much more easier to obtain, we even have a complete characterization in Section 3.

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#### 1 GENERAL RESULTS

Let us list first here the good properties of  $U:\mathbb{R}^N\to\mathbb{R}$  for  $\sigma(d)=1/d^{\alpha}$  for  $\alpha>0$  in (2). (Most of these properties are easy or proved in [GW],[HL].) U is defined on the whole space<sup>(1)</sup>  $\mathbb{R}^N$ , it is exact ( $\forall i \ U(P_i)=F_i$ ), it is continuous on the whole  $\mathbb{R}^N$ , it is even differentiable also at the points  $P_i$  for  $\alpha>1$ . In any case we have

$$\min_{i \le M} F_i \le U(P) \le \max_{i \le M} F_i$$
 (3)

for all PeR<sup>N</sup>. This especially implies that U(P) is positive if all  $F_i$  are positive, and that U is constant on the whole  $\mathbb{R}^N$  if  $F = \ldots = F_N$  are the same. Further, U has the finite limit  $\lim_{P \to \infty} U(P) = \overline{F} : \frac{F_1 + \ldots + F_N}{M}$ . Moreover, U is also invariant to any linear co-ordinate transformations  $P' := a \cdot P + \underline{b}$  and  $F'_i := c \cdot F_i + e$  for any  $a, c, e \in \mathbb{R}$ ,  $\underline{b} \in \mathbb{R}^N$  (i.e. translations and scalaring [changing measure units/zooming] in "both" directions).

Let us now deal with the general case when  $\sigma: \mathbb{R}_+ \to \mathbb{R}_+$  is any positive continuous and decreasing function.

Obviously the domain of U is again the whole  $\mathbb{R}^N$  but possibly excluding the data points  $\{P_1,\ldots,P_M\}$  and U is again continuous on its whole domain, the problem  $\lim_{P\to P_1} U(P)=F_1$  is completely handled in Theorem 2.1. Section 3 is devoted to the question of the limit  $\lim_{N\to\infty} U(P)$ .

The relation (3) can be easily proved for any positive  $\sigma: \mathbb{R}_+ \to \mathbb{R}$ : the below statement gives an easy proof for Theorem 2.2 of [GW].

STATEMENT 1.1 For any positive  $\sigma: \mathbb{R}_{+} \to \mathbb{R}_{+}$  we have  $\min_{i \leq M} F_{i} \leq U(P) \leq \max_{i \leq M} F_{i}$ 

for all P∈RN.

**PROOF** Using (2) and the fact that  $\sigma$  is always positive we have by (2) that the numerator of U is

$$(\min_{i \leq M} F_i) \cdot \sum_{i=1}^{M} \sigma(PP_i) \leq U_{num}(P) \leq (\max_{i \leq M} F_i) \cdot \sum_{i=1}^{M} \sigma(PP_i)$$

which clearly implies our statement.

To be more precise U(P) is not defined for P=P but using  $\lim_{P\to P_1} U(P)=F$  we can extend U to the whole  $\mathbb{R}^N$ .

The present Statement implies that U is positive if all the data  $F_i$  are all positive, or that U is constant on the whole  $\mathbb{R}^N$  for any  $\sigma$  if  $F_1 = \ldots = F_M$  are the same.

Clearly U is also invariant to the linear co-ordinate transformations  $F'_i := c \cdot F_i + e$  and translations P' := P + b for any  $c, e \in \mathbb{R}$  and  $b \in \mathbb{R}^N$  with no restriction on  $\sigma$ . However, the scaling  $P' := a \cdot P$  ( $a \in \mathbb{R}$ ) does not effect U only in the case when  $\sigma$  is multiplicative, that is if and only if

$$\sigma(\lambda d) = f(\lambda) \cdot \sigma(d) \tag{4}$$

holds for some positive continuous (but any) function  $f: \mathbb{R}_{+} \to \mathbb{R}_{+}$  and for all  $\lambda, d \in \mathbb{R}_{+}$ . The equality (4) is fulfilled for example when  $\sigma(d) = 1/d^{\alpha}$  ( $\alpha \in \mathbb{R}$ ) but unfortunately not in the case  $\sigma(d) = \exp(-d^{\beta})$  ( $\beta > 0$ ). This latter is a serious withdrawn for the weight function  $\sigma(d) = \exp(-d^{\beta})$  for any  $\beta \in \mathbb{R}$  — choosing too large or too small unit in the domain of U, we get surprisingly different shapes of U, as shown in Figure 3 below:

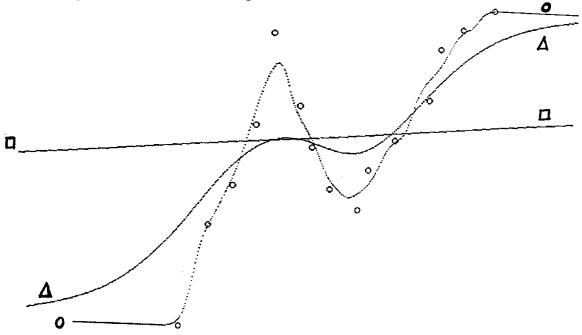


Figure 3

The case  $\sigma(d)=\exp(-d^2)$  with different units

 $\Box$  : e = 10

**Δ: e=** 2

o: e = 0.5

The wellknown diagrams of the weight functions  $\exp(-d^{\beta})$  itself for  $\beta>0$  explain this phenomena: the larger the units in Dom(U) are, the more equal weights are used in (2) to compute U(P), that is the more closer to the average value -- a straight line -- the diagram of U is.

STATEMENT 1.2 U is invariant to vertical translations for any distance function  $\sigma$ , i.e. if  $F_i^* = F_i + r$  for all i $\leq M$  and any fixed number  $r \in \mathbb{R}$ , then  $U^*(P) = U(P) + r$  for any  $P \in \mathbb{R}$ .

PROOF Using (2) we get

$$U^{*}(P) = \frac{\sum_{i=1}^{M} (F_{i}+r) \cdot \sigma(P, P_{i})}{\sum_{i=1}^{M} \sigma(P, P_{i})} = \frac{\sum_{i=1}^{M} F_{i} \cdot \sigma(P, P_{i}) + \sum_{i=1}^{M} r \cdot \sigma(P, P_{i})}{\sum_{i=1}^{M} \sigma(P, P_{i})} = U(P)+r. \blacksquare$$

#### 2 CONTINUITY and DIFFERENTIABILITY

U(P) is clearly continuously differentiable for  $P \neq P_i$  (i $\leq M$ ) for any continuously differentiable weight function  $\sigma: \mathbb{R}_+ \rightarrow \mathbb{R}$ . In this section we investigate the behaviour of U(P) at the points  $P = P_i$  for several weight functions  $\sigma$ .

But first consider the following Theorem, which solves completely the question of continuity of U.

THEOREM 2.1 Assume that  $\sigma: \mathbb{R}_{\rightarrow} \mathbb{R}$  is positive, continuous and  $\lim_{o \to} \sigma$  does exists, either finite or infinite. Then U is exact at least on one point  $P_i$  (ie.  $\lim_{p \to p_1} U(p) = F_i$ ) for any dataset  $F_1, \dots, F_n$  if and only if  $\lim_{o \to} \sigma = +\infty$ . Moreover, we may require the above exactness of U either for one or for all points  $P_i$  (i  $\leq M$ ).

PROOF For the sake of simplicity, let investigate the case i=1. Simplifying (2) with  $\sigma(P,P_1)$  we get

$$U(P) = \frac{F_1 + \sum_{i=2}^{M} F_i \cdot \frac{\sigma(P, P_i)}{\sigma(P, P_1)}}{1 + \sum_{i=2}^{M} \frac{\sigma(P, P_i)}{\sigma(P, P_1)}} \rightarrow \frac{F_1 + \sum_{i=2}^{M} F_i \cdot \frac{\sigma_i}{\sigma_o}}{1 + \sum_{i=2}^{M} \frac{\sigma_i}{\sigma_o}}$$
(5)

as P→P<sub>1</sub> where

$$\sigma_{i} = \sigma(P_{i}P_{i}) = \lim_{P \to P_{i}} \sigma(PP_{i}) \qquad (2 \le i \le M)$$

and

$$\sigma = \lim_{\alpha \to 0} \sigma$$
.

Now, the limit of (5) does exist and equals to  $F_1$  iff

$$\sum_{i=2}^{M} (F_i - F_i) \cdot \frac{\sigma_i}{\sigma_0} = 0 .$$
 (6)

Since  $\sigma$  is continuous and positive on the whole  $\mathbb{R}_{+}$ , (6) holds for any dataset  $F_{1}, \ldots, F_{M}$  if and only if  $\sigma = \infty$ .

Now we turn to the question: for which weight functions  $\sigma: \mathbb{R} \to \mathbb{R}$  is U differentiable at the points  $P=P_i$  for some/all points  $P_i$ ? Our results below give an almost complete characterization of the question, but before we need a Lemma.

In what follows we use the Euclidean distance (the L\_-norm)

$$d(P,Q) = \sqrt{\sum_{i=1}^{N} (x_i - x_i^Q)^2}$$

for any points  $P, Q \in \mathbb{R}^N$ ,  $P = (x_1, \dots, x_N)$ ,  $Q = (x_1^Q, \dots, x_N^Q)$ . Of course generalizations of the below results for other distance – functions are also possible.

**LEMMA 2.2** The partial derivative of the above distance function, for fixed  $Q \in \mathbb{R}^N$ , is

$$\frac{\partial}{\partial x_{t}} d(P,Q) = \frac{x_{t}^{-} x_{t}^{Q}}{d(P,Q)}$$

To prove our results we are adviced to rewrite the formula (2) for  $\,\,$  U(P) as

$$U(P) := \frac{\sum_{i=1}^{M} F_{i} \cdot \prod_{j \neq i} \frac{1}{\sigma(P, P_{j})}}{\sum_{i=1}^{M} \prod_{j \neq i} \frac{1}{\sigma(P, P_{j})}}$$
(7)

that is we introduce the function

$$\rho(d) := \frac{1}{\sigma(d)}$$

for d∈R<sub>1</sub>:

Now, Theorem 2.3 below generalizes the result 3.1 in [GW] while Theorem 2.4 almost completes the remainder cases.

THEOREM 2.3 If  $\sigma:\mathbb{R}_+\to\mathbb{R}$  is differentiable on  $\mathbb{R}_+$  and  $\lim_{o+}\rho=\lim_{o+}\rho'=0$  then  $U:\mathbb{R}^N\to\mathbb{R}$  is differentiable on all  $\mathbb{R}^N$ , moreover  $\frac{\partial}{\partial \times t}U(P_i)=0$  for  $i\leq M$  and  $t\leq N$ .

This statement clearly generalizes the result 3.1 from [GW].

PROOF We have written U(P) as

$$U(P) = \frac{\sum_{i=1}^{M} F_{i} \cdot \left( \prod_{j \neq i} \rho(d(P, P_{j})) \right)}{\sum_{i=1}^{M} \left( \prod_{j \neq i} \rho(d(P, P_{j})) \right)} = \frac{\sum_{i=1}^{M} F_{i} \cdot B_{i}}{\sum_{i=1}^{M} B_{i}}$$

$$\left(\frac{\partial}{\partial x_{t}} U_{NUM}(P)\right) = \sum_{i=1}^{M} F_{i} \cdot B_{i}' = \sum_{i=1}^{M} F_{i} \cdot \left(\sum_{j \neq i} \rho'(d_{j}) \cdot \frac{\partial}{\partial x_{t}} d(d_{j}) \cdot \prod_{m \neq j, j} \rho(d_{m})\right)$$

which has limit, after  $d_1 \rightarrow 0$  and separating the term i=1:

$$\lim_{P \to P_1} \left[ \frac{\partial}{\partial x_t} U_{NUM}(P) \right] = F_1 \cdot \sum_{j \neq 1} \left[ \rho'(d_j^1) \cdot \frac{\partial}{\partial x_t} d(d_j^1) \cdot \prod_{m \neq 1, j} \rho(d_m^1) \right] +$$

$$+ \sum_{i \neq 1}^M F_i \cdot \rho'(d_1^1) \cdot \frac{\partial}{\partial x_t} d(d_1^1) \cdot \prod_{m \neq i, j} \rho(d_m^1)$$

by our assumptions, where  $d_j^1 := d(P_1P_j)$  (j≤M), since  $\rho(d_1^1+0)=0$ . The denumerator's partial derivatives are almost the same, so the numerator

of the limit of the partial derivative  $\frac{\partial}{\partial x_{+}}U(P)$  reads

$$\begin{split} &\left[\frac{1}{P} \frac{1}{\partial P} \frac{\partial}{\partial x_{t}} U(P)\right]_{\text{NUM}} = \\ &= \left[F_{1} \cdot \sum_{j \neq 1} \left[\rho' \cdot (d_{j}^{1}) \cdot \frac{\partial}{\partial x_{t}} d(d_{j}^{1}) \cdot \prod_{m \neq 1, j} \rho \cdot (d_{m}^{1})\right] + \sum_{i \neq 1}^{M} \left[F_{i} \cdot \rho' \cdot (d_{1}^{1}) \cdot \frac{\partial}{\partial x_{t}} d(d_{1}^{1}) \cdot \prod_{m \neq 1, 1} \rho \cdot (d_{m}^{1})\right]\right] \cdot \\ & \cdot \left[\prod_{m \neq 1} \rho \cdot (d_{m}^{1})\right] - \\ & - \left[\sum_{j \neq 1} \left[\rho' \cdot (d_{j}^{1}) \cdot \frac{\partial}{\partial x_{t}} d(d_{j}^{1}) \cdot \prod_{m \neq 1, j} \rho \cdot (d_{m}^{1})\right] + \sum_{i \neq 1}^{M} \left[\rho' \cdot (d_{1}^{1}) \cdot \frac{\partial}{\partial x_{t}} d(d_{1}^{1}) \cdot \prod_{m \neq 1, 1} \rho \cdot (d_{m}^{1})\right]\right] \cdot \\ & \cdot \left[F_{1} \cdot \prod_{m \neq 1} \rho \cdot (d_{m}^{1})\right] \end{split}$$

which can be transformed into

$$= \left[ \sum_{i \neq 1}^{M} \left[ F_{i} \cdot \rho' \left( d_{1}^{1} \right) \cdot \frac{\partial}{\partial x_{t}} d(d_{1}^{1}) \cdot \prod_{m \neq i, 1} \rho(d_{m}^{1}) \right] - F_{1} \cdot \sum_{i \neq 1}^{M} \left[ \rho' \left( d_{1}^{1} \right) \cdot \frac{\partial}{\partial x_{t}} d(d_{1}^{1}) \cdot \prod_{m \neq i, 1} \rho(d_{m}^{1}) \right] \right] \cdot \left[ \prod_{m \neq 1} \rho(d_{m}^{1}) \right]$$

$$= \left[ \sum_{i \neq 1}^{M} \left( F_{i} - F_{1} \right) \cdot \prod_{m \neq i, 1} \rho(d_{m}^{1}) \right] \cdot \rho' \left( d_{1}^{1} \right) \cdot \frac{\partial}{\partial x_{t}} d(d_{1}^{1}) \cdot \left[ \prod_{m \neq 1} \rho(d_{m}^{1}) \right] = 0$$

since  $\rho'(d_1^1)=0$  and  $\left|\frac{\partial}{\partial x_t}d(d_1^1)\right|=1$ , and using the assumptions of the Theorem.

THEOREM 2.4 If  $\sigma: \mathbb{R} \to \mathbb{R}$  is differentiable on  $\mathbb{R}_+$ ,  $\lim_{\sigma \to 0} \sigma$  exists and is finite and  $\lim_{\sigma \to 0} \sigma' = 0$ , then  $U: \mathbb{R}^N \to \mathbb{R}$  is differentiable on all  $\mathbb{R}^N$ .

PROOF Clearly we must check the differentiability of U at the datapoints  $P_i$  (i $\leq$ M) only. Let us investigate the case i=1 for short. Now, for any fixed t $\leq$ N and P $\neq$ P, we have

$$\frac{\partial}{\partial x_{t}} U(P) = \frac{\partial}{\partial x_{t}} \frac{\sum_{i=1}^{M} F_{i} \cdot \sigma(d(P, P_{i}))}{\sum_{i=1}^{M} \sigma(d(P, P_{i}))} =$$

$$= \frac{\sum_{i=1}^{M} F_{i} \cdot \frac{\partial}{\partial xt} \sigma(d(P, P_{i})) \cdot \sum_{i=1}^{M} \sigma(d(P, P_{i})) - \sum_{i=1}^{M} \frac{\partial}{\partial xt} \sigma(d(P, P_{i})) \cdot \sum_{i=1}^{M} F_{i} \cdot \sigma(d(P, P_{i}))}{\left(\sum_{i=1}^{M} \sigma(d(P, P_{i}))\right)^{2}}$$

$$= \frac{(F_1 \cdot \frac{\partial}{\partial xt} \sigma(d(P, P_1)) + A) \cdot (\sigma(d(P, P_1)) + B) - (\frac{\partial}{\partial xt} \sigma(d(P, P_1)) + C) \cdot (F_1 \cdot \sigma(d(P, P_1)) + D)}{K^2}$$

where A,B,C,D,K are appropriate parts of the previous expression. Since the denumerator is continuous and  $\lim_{o} K \neq 0$ , we may deal with the numerator only, which can be transformed into

$$\begin{split} \left(\frac{\partial}{\partial x_{t}}U(P)\right)_{NUM} &= \frac{\partial}{\partial xt}\sigma(d(P,P_{1}))\cdot(F_{1}B-D) + \sigma(d(P,P_{1}))\cdot(A-F_{1}C) - (A\cdot B-C\cdot D) \\ &= \sigma'(d(P,P_{1}))\cdot\frac{x_{t}-x_{t}^{P1}}{d(P,P_{1})}\cdot(F_{1}B-D) + \sigma(d(P,P_{1}))\cdot(A-F_{1}C) - (A\cdot B-C\cdot D) \end{split}$$

Now using the assumptions  $\lim_{d\to o+} \sigma'(d)=0$ ,  $\lim_{d\to o+} \sigma(d)\in \mathbb{R}$  and that A,B,C,D,K are all finite since  $\sigma: \mathbb{R} \to \mathbb{R}_+$  is differentiable on  $\mathbb{R}_+$  we may conclude that  $\frac{\partial}{\partial xt} U(P)$  must exist since the part

$$\frac{x_t - x_t^{P1}}{d(P, P_t)}$$

of the last expression is bounded.

We plan to investigate the convexity properties of (U) in a forthcoming paper.

#### 3 LIMITS

Let us mention again that our investigations are made in any dimension, that is  $U:\mathbb{R}^N \to \mathbb{R}$  where  $N\geq 1$  is any number. After clearing the concept "P goes to infinity" we use, the arguments will show that the main points of the results are decided in certain 3-dimensional hyperspaces of  $\mathbb{R}^N$ . Our results generalize the ones in [GW], but ours are made for any weight function  $\sigma$ .

DEFINITION 3.0 We say (in  $\mathbb{R}^N$ ) that a point P goes to infinity along a straight line if  $P=P+\lambda v$  where P,  $v\in\mathbb{R}^N$  are fixed and  $\lambda\to\infty$  ( $\lambda\in\mathbb{R}$ ).

**LEMMA 3.1** If P goes to infinity along a straight line in  $\mathbb{R}^N$  then we may suppose (assuming a suitable, fixed renumbering of the points  $P_1, \dots, P_N$ ) that

$$d(P,P_1) \le d(P,P_2) \le \ldots \le d(P,P_N)$$

if  $d(P, P_1)$  are all large enough.

The Lemma says that we have to renumber the points  $P_1, \dots, P_M$  only once, before we start to move P, and the order of the distances  $d(P,P_1)$  do not change after a while when the point P tends to infinity along the straight line. The order of the points, of course, depends on the line P moves along.

PROOF So  $P=P_0+\lambda v$  where  $P_0,v\in\mathbb{R}^N$  are fixed and  $\lambda\to\infty$  ( $\lambda\in\mathbb{R}$ ). Denote e the straight line  $\{P_1+\lambda v:\lambda\in\mathbb{R}\}$  P moves along. For any index  $i\le M$  the distance of P and  $P_i$  can be measured in the two-dimensional hyperplane  $S_i$  spanned by  $P_i$  and e, no matter wherever  $S_i\subseteq\mathbb{R}^N$  lies. That is, to compare  $d(P,P_i)$  with  $d(P,P_j)$  we may assume that both  $P_i$  and  $P_j$  together with e lie in the same 2-dimensional hyperplane (in other words  $S_i=S_j$ , say, after rotating  $S_i$  around e in order to match  $S_j$ ). Now, a wellknown geometrical theorem from secondary school (about the perpendicular straight line halving the section  $P_iP_j$ ) says that one of  $d(P,P_i)$  and  $d(P,P_j)$  is always the larger than the other if  $\lambda$  is large enough. Examining all the pairs (i,j) we may find a threshold  $\lambda\in\mathbb{R}_+$  such that the order of the distances  $d(P,P_1)$ ,  $d(P,P_2)$ , ...,  $d(P,P_R)$  is the same for all  $\lambda>\lambda$ .

While computing  $\lim_{P\to\infty} U(P)$  in [GW] in one dimension  $\mathbb{R}^1$  (i.e.when  $U:\mathbb{R}^1\to\mathbb{R}$ ), and assuming

$$d(P, P_1) < d(P, P_1)$$
(8)

we could use the property  $d(P,P_i)=d(P,P_i)+d(P_i,P_i)$ , which is true for any three points in the one-dimensional line  $\mathbb{R}^1$ , but not in higher dimensions.

However, in higher dimensions (i.e.when  $U: \mathbb{R}^N \to \mathbb{R}$ ) we have the triangle-inequality

$$d(P, P_1) \le d(P, P_1) + d(P_1, P_1)$$
 (9)

only, which implies the upper bound

$$d(P, P, ) - d(P, P, ) \le d(P, P, )$$

For computing  $\lim_{P\to\infty} U(P)$  in  $\mathbb{R}^N$  in Theorem 3.4 we need also a *lower bound* for  $d(P,P_1)-d(P,P_1)$  which can be derived from (10) below in the next Lemma. Let us emphasize that (10) below is valid in any dimension  $\mathbb{R}^N$ !

**LEMMA 3.2** If  $P=P_0+\lambda \underline{v}$  goes to infinity along a straight line in  $\mathbb{R}^N$  ( $\lambda\to\infty$  but  $\underline{v}\in\mathbb{R}^N$  is fixed), and  $d(P,P_1)< d(P,P_1)$  for  $\lambda$  large enough,  $i\le M$  is any fixed, then

$$d(P, P_i) \ge d(P, P_1) + \varepsilon \cdot d(P_1, P_i)$$
(10)

holds for any  $\epsilon$ ,  $0 < \epsilon < m_i$  and for  $\lambda$  large enough  $(m_i$  is some fixed number,  $0 \le m_i \le 1$ , depending on  $P_1$ ,  $P_i \in \mathbb{R}^N$  and  $\underline{v} \in \mathbb{R}^N$ ).

PROOF So  $d(P,P_1) < d(P,P_1)$  and  $P = P_0 + \lambda v$  where  $P_0, v \in \mathbb{R}^N$  are fixed and  $\lambda \to \infty$  ( $\lambda \in \mathbb{R}$ ). As in the previous proof we may assume that  $P_1$ ,  $P_1$  and the line  $e = \{P_0 + \lambda v : \lambda \in \mathbb{R}\}$  lie in the same 2-dimensional hyperplane of  $\mathbb{R}^N$ . Now, working in this 2-dimensional hyperplane we may use a rectangular Cartesian co-ordinate system, and we may put  $P_1 := (0,a)$ ,  $P_1 := (0,-a)$  and e : y = mx + b where either m>0 or m=0 and b>0 since  $d(P,P_1) < d(P,P_1)$  must hold for  $\lambda$  large enough. Now, if  $P = \{x_p,y_p\}$  moves on e (i.e.  $y = mx_1 + b$  and  $x_1 \to \infty$ ), then we have

$$d(P, P_{i}) - d(P, P_{i}) = \sqrt{x_{p}^{2} + (y_{p} + a)^{2}} - \sqrt{x_{p}^{2} + (y_{p} - a)^{2}} = \frac{4ay_{p}}{\sqrt{x_{p}^{2} + (y_{p} + a)^{2}} + \sqrt{x_{p}^{2} + (y_{p} - a)^{2}}} = \frac{4a}{\sqrt{\left(\frac{x_{p}}{y_{p}}\right)^{2} + \left(\frac{y_{p} + a}{y_{p}}\right)^{2}} + \sqrt{\left(\frac{x_{p}}{y_{p}}\right)^{2} + \left(\frac{y_{p} - a}{y_{p}}\right)^{2}}}$$

which has the limit (if y = mx + b and  $x \to \infty$ )

$$\frac{4a}{2 \cdot \sqrt{\frac{1}{m^2} + 1}} = \frac{2am}{\sqrt{m^2 + 1}} = d(P_1, P_1) \cdot \frac{m}{\sqrt{m^2 + 1}} \qquad if m > 0$$

and equals to

$$= \frac{4a}{\sqrt{\left(\frac{x_p}{b}\right)^2 + \left(\frac{b+a}{b}\right)^2} + \sqrt{\left(\frac{x_p}{b}\right)^2 + \left(\frac{b-a}{b}\right)^2}} \rightarrow 0 \qquad \text{if } m=0.$$

So, in both cases we have

$$d(P, P_i) - d(P, P_1) \longrightarrow d(P_1, P_i) \cdot \frac{m}{\sqrt{m^2 + 1}}$$
(11)

This means that  $m_i := \frac{m}{\sqrt{m^2 + 1}}$  justifies the statement of the Lemma.

One can observe that  $\,m_{_{1}} \! = \! \sin(\alpha)\,$  where  $\alpha$  is the angle between the lines  $P_{_{1}}P_{_{1}}\,$  and e .

Let us further highlight that the limit of the distance- difference:

$$d(P,P_i)-d(P,P_i) \rightarrow d(P_i,P_i) \cdot m_i$$
 (12)

where  $0 \le m \le 1$ , and  $m_i$  depends on  $P_i, P_i \in \mathbb{R}^N$  and  $v \in \mathbb{R}^N$  only. Especially,  $m_i = 1$  for each  $i \le M$  in one dimension.

For stating our main Theorem on the limit of U(P) (when P goes to infinity along a straight line:  $P=P_0+\lambda \underline{v}$  and  $\lambda\to\infty$ ) we need also a notation:

**DEFINITION 3.3** For any function 
$$\sigma: \mathbb{R}^+ \to \mathbb{R}^+$$
 and real number  $m \in \mathbb{R}$  we let 
$$\sigma^\#(m) := \lim_{d \to \infty} \frac{\sigma(d+m)}{\sigma(d)}$$

The Theorem below uses the fact that  $\sigma^{\sharp}$  measures the rate of the quickness of the convergence  $\lim_{d\to\infty}\sigma(d)=0$ . Some main properties of the  $\sharp$  - operator are shortly listed *after* the following theorem.

THEOREM 3.4 If  $P=P + \lambda \underline{v}$  goes to infinity along a straight line in  $\mathbb{R}^N$  and

$$d(P,P_1) = d(P,P_2) = \dots = d(P,P_j) \leq d(P,P_{j+1}) \leq \dots \leq d(P,P_M)$$
 (14)

holds for all  $\lambda$  large enough and for a suitable fixed index  $1 \le j \le M$ , then

$$\lim_{P \to \infty} U(P) = \frac{F_1 + \dots + F_j + \sum_{i=j+1}^{M} F_i \cdot \sigma^{\#}(m_i)}{j + \sum_{i=j+1}^{M} \sigma^{\#}(m_i)}$$
(15)

where the numbers  $m_i$  depend on the relative position of the points P,  $P_1$ ,  $P_1$  and of the direction vector  $\underline{\mathbf{v}}$  of the straight line where P moves to infinity, computed in Lemma 3.2.

PROOF So  $P=P_0+\lambda v$  where  $P_0,\underline{v}\in\mathbb{R}^N$  are fixed and  $\lambda\to\infty$  ( $\lambda\in\mathbb{R}$ ). By Lemma 3.1 we may assume that (14) holds for all  $\lambda\in\mathbb{R}$  large enough. Now, after simplifying the formula of U(P) with  $\sigma(P_1)$ , we get

$$U(P) = \frac{\sum_{i=1}^{M} F_{i} \cdot \sigma(P, P_{i})}{\sum_{i=1}^{M} \sigma(P, P_{i})} = \frac{F_{1} + \ldots + F_{j} + \sum_{i=j+1}^{M} F_{i} \cdot \frac{\sigma(P, P_{i})}{\sigma(P, P_{1})}}{j + \sum_{i=j+1}^{M} \frac{\sigma(P, P_{i})}{\sigma(P, P_{1})}} \rightarrow \frac{F_{1} + \ldots + F_{j} + \sum_{i=j+1}^{M} F_{i} \cdot \sigma^{\#}(m_{i})}{j + \sum_{i=j+1}^{M} \sigma^{\#}(m_{i})}$$

using (10) by Lemma 3.2.

Before some applications of the above result let us deal shortly with the # -operator itself, defined in (13). We deal mainly but not exclusively with decreasing positive functions (i.e. for  $\sigma: \mathbb{R} \to \mathbb{R}$  decreasing).

Clearly  $0 \le \sigma^*(m) \le 1$  for  $m \in \mathbb{R}_+$ ; # is multiplicative (i.e.  $(\sigma \cdot \rho)^{\#} = \sigma^{\#} \cdot \rho^{\#}$ );  $c^{\#} = 1$  for constant functions  $c \in \mathbb{R}_+$ ;  $(f/g)^{\#} = f^{\#}/g^{\#}$  for any functions  $f, g: \mathbb{R}_+ \to \mathbb{R}$ ;  $(\sigma^{+u})^{\#} = \sigma^{\#}$  if  $\sigma^{+u}$  is a translation of  $\sigma$  with any  $u \in \mathbb{R}$  (i.e.  $\sigma^{+u}(d) = (d+u)$  for  $d \in \mathbb{R}$ );  $(\sigma^{\vee})^{\#} = (\sigma^{\#})^{\vee}$  where  $\sigma^{\vee}$  denotes the v-fold zoom of  $\sigma$  for any  $u \in \mathbb{R}$  (i.e.  $\sigma^{\vee}(d) = (v \cdot d)$  for  $d \in \mathbb{R}$ ).

In general, the steeper is  $\sigma(x)$  for  $x\to\infty$ , the closer is  $\sigma^{\sharp}(m)$  to 0 for any  $m\in\mathbb{R}_+$ ; and conversely, the more gently sloping is  $\sigma(x)$  for  $x\to\infty$ , the closer is  $\sigma^{\sharp}(m)$  to 1 for any  $m\in\mathbb{R}_+$ .

Especially,  $(1/x^{\alpha})^{\#} = (\frac{1}{1+x^{\alpha}})^{\#} = 1$  for any  $\alpha \in \mathbb{R}$ ,  $(\operatorname{arccotan})^{\#} = 1$ ,  $(\frac{1}{1+\ln(d)})^{\#} = 1$ , and finally

$$\left[e^{-\lambda x^{\beta}}\right]^{\#}(m) = \begin{cases} 0 & \text{for } \beta > 1\\ e^{-\lambda m} & \text{for } \beta = 1\\ 1 & \text{for } 0 < \beta < 1 \end{cases}$$
 (16)

since

$$(e^{-h})^{\#}(m) = \lim_{d \to \infty} e^{h(d) - h(d+m)}$$

holds for any function  $h: \mathbb{R}_1 \to \mathbb{R}_1$  and  $m \in \mathbb{R}$ .

Now we turn to some applications of Theorem 3.4. A short list below of several special cases of the above Theorem throws some light on the meaning of the result (15). We mean special weight-functions  $\sigma$  and special positions of the datapoints  $P_1,\ldots,P_{\varkappa}$ .

COROLLARY 3.5 If  $\sigma(d)=e^{-d^{\beta}}$  for some positive  $\beta\in\mathbb{R}$  and all the assumption of Theorem 3.4 hold, then  $\lim_{P\to\infty}U(P)$  has the value

$$\lim_{P\to\infty} U(P) \ = \ \begin{cases} \frac{F_1+\ldots+F_M}{M} & (\textit{the arithmetic mean}) & \textit{if } 0<\beta<1\\ \\ \frac{F_1+\ldots+F_j+\sum_{j=j+1}^M F_j \cdot e^{-mi}}{j+\sum_{j=j+1}^M e^{-mi}} & \textit{if } \beta=1\\ \\ \frac{F_1+\ldots+F_j}{j} & (\textit{the arithmetic mean} \\ & \textit{of the dominating values}) & \textit{if } \beta>1 \end{cases}$$

PROOF Use (15) and (16). ■

Let us remark immediately that in one dimension  $U:\mathbb{R}^1\to\mathbb{R}^1$  in the  $\beta=1$  case the above result imply that  $\lim_{P\to\infty}U(P)=U(P_1)$  if  $P_1$  is the closest point to P. Moreover, an easy calculation shows that even  $U(P)=U(P_1)$  just after P leaves  $P_1$  for all P, that is P is constant outside of the dataset  $P_1,\ldots,P_{\mathbb{R}}$ . See Figure 2 again for illustration.

The next case, when  $\sigma(d)=1/d^{\alpha}$ , we get a new proof for the result (2.18) of [GW] using our Theorem 3.4 above.

COROLLARY 3.6 If  $\sigma(d)=d^{-\alpha}$  for some positive  $\alpha\in\mathbb{R}$  and all the assumption of Theorem 3.4 hold, then for all  $\alpha$  we have

$$\lim_{P\to\infty} U(P) = \frac{F_1 + \dots + F_M}{M}$$
 (17)

(the arithmetic mean)

PROOF We have  $\sigma^{\#}(m) = \lim_{d \to \infty} \frac{(d+m)^{-\alpha}}{d^{-\alpha}} = \lim_{d \to \infty} (1+\frac{m}{d})^{-\alpha} = 1$  for all positive  $\alpha$  and  $m \in \mathbb{R}$ . Now use Theorem 3.4.

Certainly (17) also holds for all weight function  $\sigma$  whenever  $\sigma^{\sharp}=1$ , so we can put also, for example  $\frac{1}{1+d^{\alpha}}$ , arccotan(d),  $\frac{1}{\ln(d+1)}$  or any multiplication or power of these functions and  $1/d^{\alpha}$  into the role of  $\sigma$  to get (17).

It is interesting to mention also a two dimensional special case of Theorem 3.4. So let us focus on the positions of the points and lines on which P moves in the space  $\mathbb{R}^2$ :

COROLLARY 3.7 If  $P_1, P_2, P_3 \in \mathbb{R}^2$  and  $F_1, F_2, F_3 \in \mathbb{R}$  are arbitrary given datapoints/numbers respectively,  $\sigma^{\#}(d)=1$  and P moves along the line e, then for  $\lim_{P \to \infty} U(P)$  we have

$$\lim_{P\to\infty}\,U(P) \ = \ \begin{cases} \frac{F_1+F_j}{2} & \text{if } e \text{ halves and perpendicular to the segment } P_iP_j \\ F_k & \text{if } P_k \text{ is the closest point to } P \,. \end{cases}$$

Figure 4 below illustrates this case.

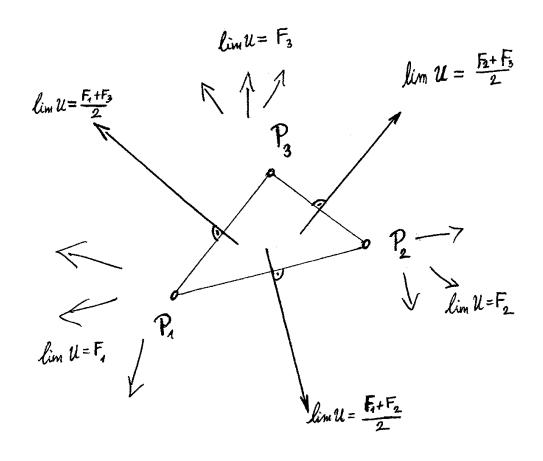


Figure 4

lim U(P) in  $\mathbb{R}^2$  for  $\sigma^{\#}(d)=1$  and M=3

#### 4 MONOTONICITY

In higher dimensions the question of monotonicity means that we must proceed along straight lines. Since the general case could easily be transformed into one dimension, we restrict ourselves to the case N=1, that is when  $P_1, \ldots, P_M \in \mathbb{R}$  and so  $U: \mathbb{R} \rightarrow \mathbb{R}$ .

One might think at once that the monotonicity of U between  $P_i$  and  $P_{i+1}$  — that is  $F_i < F_i$  implies  $U(P_i) < U(P_{i+1})$  — requires and also is ensured by that either the distances of the other points  $P_j$  for  $j \ne i, i+1$  are large enough, or the other values  $F_j$  for  $j \ne i, i+1$  are not so large. This feeling is justified in Theorem 4.3 in Subsection 4.2. But before we show that the bumps shown in Figure 1 are neccessary bad properties of U for certain weight functions  $\sigma$ .

#### a) NEGATIVE RESULTS

#### 4.0 The "Hill and Valley" Property

In this subsection we give a short but demonstrative computation for the rate of the non-monotonicity of Shepard's original formula  $\sigma(d)=1/d^{\alpha}$  for any  $\alpha \ge 1$ : we estimate the place (frequency) and the size of the bumps shown in Figure 1.

EXAMPLE 4.0 A special case of U:R $\rightarrow$ R when  $\sigma(d)=1/d^{\alpha}$ . Let the dataset  $P_0,\ldots,P_M\in$ R and  $F_0,\ldots,F_M\in$ R be equidistant, i.e. let  $P_i=P_0+i\cdot v$  and  $F_i=F_0+i\cdot u$  for  $i=1,\ldots,M$ , where  $P_0,F_0,u,v\in$ R are arbitrary fixed numbers. Now, using the definition (2) of U with  $\sigma(d)=1/d^{\alpha}$ , let us investigate U at the place  $x_0:=\frac{P_0+P_1}{2}=P_0+\frac{v}{2}$ . (Similar computations could be made for the point  $x_1:=P_M-\frac{v}{2}$ , or for any other pont  $x\in$ R.) The following Theorem shows that the size of the "bumps" must raise to the infinity when M goes to infinity.

THEOREM 4.1  $U(x_0)=u \cdot \ell(M,\alpha)$  where  $\ell(M,\alpha)\to\infty$  as  $M\to\infty$  for any fixed  $\alpha\ge 1$ . PROOF By (2) we have

$$U(x_{o}) = \frac{\sum_{i=1}^{M} F_{i} \cdot \frac{1}{(d(x_{o}, P_{i}))^{\alpha}}}{\sum_{i=1}^{M} \frac{1}{(d(x_{o}, P_{i}))^{\alpha}}} = \frac{F_{o} \cdot (\frac{2}{v})^{\alpha} + \sum_{i=2}^{M} iu \cdot \frac{1}{(iv - v/2)^{\alpha}}}{2 \cdot (\frac{2}{v})^{\alpha} + \sum_{i=2}^{M} \frac{1}{(iv - v/2)^{\alpha}}} = u \cdot \frac{2^{\alpha} + \sum_{i=2}^{M} \frac{i}{(i-1/2)^{\alpha}}}{2 \cdot 2^{\alpha} + \sum_{i=2}^{M} \frac{1}{(i-1/2)^{\alpha}}} = u \cdot \ell(M, \alpha) .$$

An easy computation shows that  $\ell(M,\alpha) \to \infty$  as  $M\to \infty$  for any fixed  $\alpha \ge 1$ .

The order of  $\ell(M,1)$  can also be determined easily.

STATEMENT 4.2 
$$\ell(M, 1) \approx \mathcal{O}\left(\frac{M}{\ln{(M)}}\right)$$
 as  $M \rightarrow \infty$ .

PROOF By the above computation we have

$$\ell(M,1) = \frac{2 + \sum_{i=2}^{M} \frac{i}{i-1/2}}{4 + \sum_{i=2}^{M} \frac{1}{i-1/2}} = \frac{2 + \sum_{i=2}^{M} (1 + \frac{1/2}{i-1/2})}{4 + \sum_{i=2}^{M} \frac{1}{i-1/2}} = \frac{M + \frac{1}{2} \cdot \sum_{i=2}^{M} \frac{1}{i-1/2}}{4 + \sum_{i=2}^{M} \frac{1}{i-1/2}}$$

and recall that

$$\lim_{M\to\infty} \left( \sum_{i=1}^{M} \frac{1}{i-1/2} - \ln(M) \right) = C + 2 \cdot \ln(2)$$

where  $C \approx 0.57722...$  is the Eulerian constant (see eg.[GR, 0.132]). So we can write

$$\ell(M,1) \approx \frac{M + \frac{1}{2} \cdot \ln(M) + C/2 + \ln(2) - 1}{4 + \ln(M) + C + 2 \cdot \ln(2) - 2} \approx O\left(\frac{M}{\ln(M)}\right)$$

as M goes to infinity.

The Reader could make similar easy but interesting computations in the case M=3 and varying either  $P_3$  or  $F_3$  or both of them.

#### b) POSITIVE RESULTS

In this subsection we justify the monotonicity of U in the sub-interval  $[P_iP_{i+1}]$  for the weight function  $\sigma(d) = \exp(-d^{\beta})$  if either the other points  $P_j$  (j≠i,i+1) are far enough from this interval or the data  $F_j$  are not extremaly large or small. Not only for curiosity but also for better understanding of the general case we have to deal with the case M=2 first.

#### 4.1 The Case M=2

THEOREM 4.3 U(P) is strictly increasing in the closed segment  $[P_1, P_2]$  for every positive strictly decreasing weight function  $\sigma$  if  $P_1 < P_2$  and  $F_1 < F_2$ .

**PROOF** Let  $P=P_1+r$  be a point in the segment  $[P_1,P_2]$ , i.e.  $0 \le r \le \delta$  where  $\delta=P_2-P_1$ . Now we have

$$U(d) = \frac{F_1 \cdot \sigma(r) + F_2 \cdot \sigma(\delta - r)}{\sigma(r) + \sigma(\delta - r)} = F_1 + \frac{F_2 - F_1}{1 + \frac{\sigma(r)}{\sigma(\delta - r)}}$$

which is clearly strictly increasing since  $F_2 - F_1 > 0$  and  $\sigma$  is strictly decreasing.

Let us mention here that the previous result can also be obtained by using the derivative of U, but that method wouldn't be easier at all.

Second, let us highlight the special case  $\sigma(d) = \frac{1}{d}$  when an easy computation shows for any  $P_1 \le P \le P_2$  that

$$U(P) = F_1 + \frac{F_2 - F_1}{P_2 - P_1} \cdot (P - P_1) ,$$

so the graph of U is the straight line segment connecting the points  $(P_1,F_1)$  and  $(P_2,F_2)$  .

#### 4.2 The Case M>2

Now we are ready to deal with the general case M>2. We focus here on the weight functions  $\sigma(d) = \exp(-\lambda d^{\beta})$  for fixed  $\lambda, \beta > 0$ . The case  $\beta = 1$  is handled in Theorem 4.4 while in Theorem 4.5 we settle many other exponents  $\beta > 0$ . More precisely, Theorem 4.5 deals with weight functions  $\sigma(d) = e^{F(d)}$  for certain functions  $F: \mathbb{R}_+ \mathbb{R}_+$ . These results compute precisely how large the distances of the other points  $P_j$  for  $j \neq i, i+1$  and how small the difference among the values  $F_j$  for  $j \neq i, i+1$  and  $F_i$ ,  $F_{i+1}$  must be (see eg. (14)) to ensure the monotonicity of U between  $P_i$  and  $P_{i+1}$  — that is  $P_i < P_i$  and  $P_i < P_{i+1}$  would imply  $U(P_i) < U(P_{i+1})$ .

THEOREM 4.4 Let  $P_1, \ldots, P_M \in \mathbb{R}$  and  $F_1, \ldots, F_M \in \mathbb{R}$  be any given numbers such that  $P_1 < P_2 < \ldots < P_M$ , and let  $\sigma(d) = e^{-\lambda d}$  (18)

for some fixed  $\lambda>0$  and for any  $d\in\mathbb{R}$ , d>0.

Let further  $L:=\min\{\big|F_i-F_j\big|:i,\,j{\le}M\}$  ,  $K:=\max\{\big|F_i-F_j\big|:i,\,j{\le}M\}$  and  $\epsilon:=\min\{\big|P_i-P_i\big|:i,\,j{\le}M\}.$  Suppose also that

$$\frac{4L}{KM^2} > e^{-2\varepsilon} \tag{19}$$

Then, for any i of index U is strictly monotone increasing/decreasing on the interval  $(P_{io}, P_{io+1})$  according whether  $F_{io} < F_{io+1}$  or  $F_{io} > F_{io+1}$ .

In the special case " $F_i < F_j$  for every  $1 \le i \le i_0 < j \le M$ " we can drop the assumption (18), this can easily seen from (24) at the end of the proof below.

In the proof we will use only the below properties of  $\boldsymbol{\sigma}$  :

$$\exists \lambda \ \forall d$$
  $\sigma'(d) = -\lambda \cdot \sigma(d)$  (20)

$$\forall \mathbf{u}, \mathbf{v} \qquad \qquad \sigma(\mathbf{u} \cdot \mathbf{v}) = \sigma(\mathbf{u}) \cdot \sigma(\mathbf{v}) . \tag{21}$$

PROOF Let us investigate the case  $F_{io} < F_{io+1}$ . By the definition (2) of U:R-R we have for  $P_{io} < x < P_{io+1}$ ,  $x \in \mathbb{R}$ :

$$U(x) = \frac{\sum_{i} F_{i} \cdot \sigma(x-P_{i}) + \sum_{j} F_{j} \cdot \sigma(P_{j}-x)}{\sum_{i} \sigma(x-P_{i}) + \sum_{i} \sigma(P_{i}-x)}$$
(22)

where  $\Sigma$  means  $\sum\limits_{i=1}^{i_0}$  while  $\Sigma$  stands for  $\sum\limits_{j=i_0+1}^{M}$  .

Now the numerator of the derivative U', using  $\sigma$ '(d)=- $\lambda \cdot \sigma$ (d), is :

$$U'_{\text{num}}(x) = (\sum_{i=1}^{n} \cdot (-\lambda) \cdot \sigma(x - P_i) - \sum_{j=1}^{n} \cdot (-\lambda) \cdot \sigma(P_j - x)) \cdot (\sum_{i=1}^{n} \sigma(x - P_i) + \sum_{j=1}^{n} \sigma(P_j - x)) - (\sum_{i=1}^{n} \cdot \sigma(x - P_i) + \sum_{j=1}^{n} \cdot \sigma(P_j - x)) \cdot (\sum_{i=1}^{n} (-\lambda) \cdot \sigma(x - P_i) - \sum_{j=1}^{n} (-\lambda) \cdot \sigma(P_j - x))$$

has form of  $(\mu A - \mu B)(C + D) - (A + B)(\mu C - \mu D)$ , so we can write

$$U'_{num}(x) = -2\lambda \cdot [ (\Sigma F_{i} \cdot \sigma(x - P_{i})) \cdot (\Sigma \sigma(P_{j} - x)) - (\Sigma F_{j} \cdot \sigma(P_{j} - x)) \cdot (\Sigma \sigma(x - P_{i})) ]$$

$$= -2\lambda \cdot \sum_{i,j} \sigma(x - P_{i}) \cdot \sigma(P_{j} - x) \cdot (F_{i} - F_{j})$$

$$= -2\lambda \cdot [ (F_{io} - F_{io+1}) \cdot \sigma(x - P_{io}) \cdot \sigma(P_{io+1} - x) +$$

$$+ \sum_{j>i_{o}+1} \sigma(x - P_{io}) \cdot \sigma(P_{j} - x) \cdot (F_{io} - F_{j}) ]$$

$$+ \sum_{i < i_{o}} \sigma(x - P_{i}) \cdot \sigma(P_{io+1} - x) \cdot (F_{i} - F_{io+1}) ]$$

$$+ \sum_{i < i_{o}} \sum_{j > i_{o}+1} \sigma(x - P_{i}) \cdot \sigma(P_{j} - x) \cdot (F_{i} - F_{j}) ]$$

$$+ \sum_{i < i_{o}} \sum_{j > i_{o}+1} \sigma(x - P_{i}) \cdot \sigma(P_{j} - x) \cdot (F_{i} - F_{j}) ]$$

$$= -2\lambda \cdot \sigma(x-P_{i_{0}}) \cdot \sigma(P_{i_{0}+1}-x) \cdot [ (F_{i_{0}}-F_{i_{0}+1}) + (24) + \sum_{1 \leq i_{0}} \sum_{j \geq i_{0}+1} \sigma(P_{i_{0}+1}-P_{i_{0}}) \cdot \sigma(P_{j}-P_{i_{0}+1}) \cdot (F_{i}-F_{j}) ]$$

The second term in the brackets has less than  $\frac{M^2}{4}$  term, so its absolute value is surely less than  $e^{-2\lambda\epsilon} \cdot K \cdot \frac{M^2}{4}$ , while the first one's absolute value is at least L. Using the assumption (18) we can derive that U'(x) is positive, which concludes the proof.

Let us observe, that the ratio  $\frac{L}{K}$  does not change during any vertical linear transformation of the data  $F_1, \ldots, F_M$  (translating, zooming, using another measure units or 0-point), so the requirement (18) of the above Theorem is independent from these transformations.

Now let us turn to the case  $\sigma(d)=\exp(-d^{\beta})$  where  $\beta>1$ . To be more precise, we need only a weaker assumption which, honestly, covers only the "half" of the cases  $\sigma(d)=\exp(-d^{\beta})$  for  $\beta>1$ .

THEOREM 4.5 Let  $P_1, \dots, P_M \in \mathbb{R}$  be any given numbers such that  $P_1 < P_2 < \dots < P_M$  . Let further

$$\sigma(d) = e^{F(d)}$$

be any even positive function with domain deR\{0} such that both  $\sigma$  and F' are decreasing for d>0 and for deR\{0} respectively. Now, assuming  $F_1 < F_2 < \ldots < F_M$  we get that U is strictly monotone increasing, too.

**PROOF** Since  $\sigma$  is even we can write U(x) for  $x \in \mathbb{R}$ ,  $P_{io} < x < P_{io+1}$  (i < M is any fixed index)

$$U(x) = \frac{\sum_{i} F_{i} \sigma(x-P_{i})}{\sum_{i} \sigma(x-P_{i})}$$

where  $\Sigma_{i}$  stands for  $\Sigma_{i=1}$ .

By the assumption we have that  $\sigma'(d)=f(d)\cdot\sigma(d)$  is an *odd* function where f(d)=F'(d) for  $d\in\mathbb{R}\setminus\{0\}$ . Now the numerator of U'(x) is

$$U'_{NUM}(x) =$$

$$= [\Sigma_i F_i f(x-P_i)\sigma(x-P_i)] \cdot [\Sigma_j \sigma(x-P_i)] - [\Sigma_i F_i \sigma(x-P_i)] \cdot [\Sigma_j f(P_j-x)\sigma(P_j-x)]$$

which turns, after elementary computation, to

$$= \sum_{i=1}^{M} \sum_{j=1}^{M} F_{i} \sigma(x-P_{i}) \sigma(P_{j}-x) \cdot [f(x-P_{i})-f(P_{j}-x)] =$$

$$= \sum_{i=1}^{M} \sum_{j=1}^{M} (F_{i}-F_{j}) \cdot \sigma(x-P_{i}) \sigma(P_{j}-x) \cdot [f(x-P_{i})-f(P_{j}-x)]$$

$$= \sum_{i=1}^{M} \sum_{j=1}^{M} (F_{i}-F_{j}) \cdot \sigma(x-P_{i}) \sigma(P_{j}-x) \cdot [f(x-P_{i})-f(P_{j}-x)]$$

which is positive for all x if  $P_i < x < P_j$  by our assumptions.

We think that sharper results (without assuming that  $F_1 < F_2 < \ldots < F_M$ ) could be proved with more sophisticated methods. Further, the differences between the functions  $d^{-\alpha}$  and  $\exp(-d^{\beta})$  presented in the Introduction and in this Section show that our present methods are not enough to investigate their product  $\exp(-d^{\beta})/d^{\alpha}$  ( $\alpha,\beta>0$ ). It may be better or worse than the original ones: computer graphic shows various pictures, see eg. Figure 2 in [Sz3]. Perhaps certain good pair of some  $\alpha$  and  $\beta$  would have good properties

We do not deal here with the cases x < P or x > P with respect of monotonicity of U.

Interesting (theoretical) computations can be made in the case M=3, the rate of the disturbing effect of  $F_2$  can be investigated when the distance  $|P_2-P_1|$  goes to  $\infty$ . However we have not found any close connection between the functions U constructed from M=2, M=3 or more datapoints.

#### 5 DUPLICATE DATAPOINTS

In the practice not only the values what we measure but the points where we measure them could not be determined precisely. One way to express this phenomena is that we suppose the fact of multiple measurements at the points  $P_i$  (1 $\leq$ i $\leq$ M). Denote these values by  $F_i^{(1)}$ ,  $F_i^{(2)}$ , ...,  $F_i^{(k)}$  where  $k_i \geq 1$  is

the number of all data we succeeded in measuring at the point  $P_i$  (i $\leq$ M). Using this assumption, (2) is replaced by the following formula:

$$U(P) = \frac{\sum_{i=1}^{M} F_{i}^{*} \cdot \sigma(P, P_{i})}{\sum_{i=1}^{M} k_{i} \cdot \sigma(P, P_{i})}$$
(25)

where

$$F_{i}^{*} := F_{i}^{(1)} + F_{i}^{(2)} + \dots + F_{i}^{(k_{i})}$$

is the  $sum^{(1)}$  of the values measured at the point  $P_i \in \mathbb{R}^N$  for  $i=1,\ldots,M$ . Let us highlight here that M is only the number of points  $P_i$  where we finally "managed" to measure, while the total number of measurements is

$$\mathfrak{M} := \sum_{i=1}^{M} k_{i}.$$

Let us mention again that the domain of U is the N-dimensional space  $\mathbb{R}^N$  .

Concerning basic-, limit and monotonicity properties of the function U(P) in (25) we mainly have to repeat almost all the theorems in the previous sections but with minor modifications.

Again we have  $Dom(U) \supseteq \mathbb{R}^{N} \setminus \{P_1, \dots, P_M\}$ , moreover U can be defined continuously also at the points  $P_i$  for each  $i \le M$  if  $\lim_{o} \sigma \in \mathbb{R}_+ \cup \{+\infty\}$  -- see Theorem 5.1 below.

Since o is always positive, we again have that

$$\min \{F_i^{(j)}: j \leq k_i, i \leq M\} \leq U(P) \leq \max \{F_i^{(j)}: j \leq k_i, i \leq M\}$$

and we again have its consequences, too (as seen in Section 1).

U is also invariant to linear transformations on  $\overline{F}_{i}^{*}$  and translations on  $P_{i}$  , etc.

Continuity properties of the modified U are similar to the ones in Section 2: Theorem 2.1 remains valid with the below modification:

THEOREM 5.1 Let  $\sigma: \mathbb{R} \to \mathbb{R}$  be any positive weight function, such that  $\sigma$  is bounded on a neighbourhood of each distance  $d(P_i P_j)$ . Then U is "exact", i.e.

$$\lim_{P \to P_{i}} U(P) = \frac{F_{i}^{(1)} + F_{i}^{(2)} + \dots + F_{i}^{(k_{i})}}{k_{i}} = \frac{F_{i}^{*}}{k_{i}}$$

<sup>(1)</sup> and NOT any arithmetic mean of the values  $F_i^{(1)}$ ,  $F_i^{(2)}$ , ...,  $F_i^{(k)}$ 

for any dataset  $F_1,\ldots,F_M$  and for any  $i\leq M$  if and only if  $\lim_{\sigma} \sigma = +\infty$ . Moreover, we may require the above "exactness" of U either for one or for all of the poits  $P_3$ .

Let us remark that the quotient  $F_i^*/k_i$  is the arithmetic mean of the dataset  $F_i^{(1)}$ ,  $F_i^{(2)}$ , ...,  $F_i^{(k_i)}$  measured at the point  $P_i$  for any  $i \le M$ .

PROOF Let i=1 for simplicity. Simplifying (25) with  $\sigma(PP_1)$  we get

$$U(P) = \frac{F_{1}^{*} + \sum_{i=2}^{M} F_{i}^{*} \cdot \frac{\sigma(PP_{1})}{\sigma(PP_{1})}}{k_{1} + \sum_{i=2}^{M} k_{i} \cdot \frac{\sigma(PP_{1})}{\sigma(PP_{1})}}$$

which clearly goes to  $\frac{F_1^*}{k_1}$  since  $\frac{\sigma(PP_1)}{\sigma(PP_1)} \to 0$  when  $d=d(PP_1)\to 0$ .

The other direction of the Theorem can be proved on a similar way.

The differentiability of U depends on  $\sigma$  exactly on the same way as we sew in Section 2, we do not repeat the big expressions here again.

Limit questions are similar to the ones in Section 3 of [Sz3], as follows below.

THEOREM 5.2 If P=P +  $\lambda \underline{v}$  goes to infinity along a straight line in in  $\mathbb{R}^N$  and

$$d(P, P_1) = \dots = d(P, P_j) \leq d(P, P_{j+1}) \leq \dots \leq d(P, P_k)$$

holds for all λ large enough and for a suitable fixed index 1≤j≤M, then

$$\lim_{P \to \infty} U(P) = \frac{F_1^* + \dots + F_j^* + \sum_{i=j+1}^M F_i^* \cdot \sigma^*(m_i)}{\sum_{i=1}^J k_i + \sum_{i=j+1}^M k_i \cdot \sigma^*(m_i)}$$
(26)

where the numbers  $\mathbf{m_i}$  depend on the common position of the points  $\mathbf{P_i}, \mathbf{P_i}$  and of the direction vector  $\mathbf{v}$  of the straight line where P moves to infinity.

PROOF The same as was in Theorem 3.4.

The below results are also obvious generalizations of Corollaries 3.5 and 3.6 from Section 3 of [Sz3].

COROLLARY 5.3 If  $\sigma(d)=e^{-d^{\beta}}$  for some positive  $\beta\in\mathbb{R}$  and all the assumptions of Theorem 5.2 hold, then  $\lim_{P\to\infty}$  U(P) has the value

$$\lim_{P \to \infty} U(P) = \begin{cases} \frac{F_1^* + \ldots + F_M^*}{\mathfrak{M}} & (\text{the arithmetic mean}) & \text{if } 0 < \beta < 1 \\ \frac{F_1^* + \ldots + F_j^* + \sum\limits_{i=j+1}^M F_i^* \cdot e^{-mi}}{\sum\limits_{i=1}^J k_i + \sum\limits_{i=j+1}^M e^{-mi}} & \text{if } \beta = 1 \\ \frac{F_1^* + \ldots + F_j^*}{\sum\limits_{i=1}^J k_i} & (\text{the arithmetic mean} \\ \frac{\sum\limits_{i=1}^J k_i}{\sum\limits_{i=1}^J k_i} & \text{of the dominating values}) & \text{if } \beta > 1 \end{cases}$$

Again, in one dimension  $U:\mathbb{R}^1\to\mathbb{R}^1$  in the  $\beta=1$  case the above result imply that  $U(P)=U(P_1)$  (U is constant) if P is outside of the dataset  $\{P_1,\ldots,P_n\}$ .

COROLLARY 5.4 If  $\sigma(d)=d^{-\alpha}$  for some positive  $\alpha\in\mathbb{R}$  and all the assumptions of Theorem 5.2 hold, then for all  $\alpha$  we have

$$\lim_{P\to\infty} U(P) = \frac{F_1^*+\ldots+F_M^*}{\mathfrak{M}}$$

(the arithmetic mean)

Concerning monotonicity, the result in Theorem 4.4 can not be transformed easily: though K and  $\epsilon$  would play the same role as in Theorem 4.2 but L would ultimately be small. This question is planned to be investigated in a forthcoming paper.

#### 6 GLOSSARY of NOTATIONS

R<sub>+</sub> = the set of positive real numbers

N = the dimension of R<sup>N</sup> where U is defined

M = the number of the datapoints P<sub>1</sub>, 1≤i≤M

P<sub>1</sub>,...,P<sub>M</sub> ∈ R<sup>N</sup> = the data/measuring points

F<sub>1</sub>,...,F<sub>M</sub>∈ R = the data/measured values

U: R<sup>N</sup> → R

d:  $\mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$  = distance d(P,Q), often shortened as PQ  $\mathbb{R}_+ = set$  of positive real numbers  $\sigma: \mathbb{R}_+ \to \mathbb{R}$   $\sigma(P,Q)$  instead of  $\sigma(d(P,Q))$  for  $P,Q \in \mathbb{R}^N$   $\sigma^{\#}(m) := \lim_{d \to \infty} \frac{\sigma(d+m)}{\sigma(d)}$ 

#### REFERENCES

- [GW] Gordon, W. J., Wixom, J. A.: Shepard's Method of "Metric Interpolation" to Bivariate and Multivariate Interpolation, Math. of Computation, 32 (1978), 253-264
- [HL] Hoschek, J., Lasser D.: Computer Aided Geometric Design, Ch. 9.:

  Scattered Data Interpolation und Approximation, A.K. Peters Ltd.,
  1993
- [GR] Gradstein, I.S., Rusik, I.M.: Tables of Integrals, Sums, Series and Products, Nauka, Moscow, 1971 (in Russian)
- [Sz0] Szalkai, I.: SALT3DIM.exe A Program for Handling 4 Component Mixtures, Preprint No. 047, Univ. of Veszprém, 1996
- [Sz1]  $\longrightarrow$ : Handling Multicomponent Systems in  $\mathbb{R}^n$ . I: Theoretical Results, J. of Math. Chemistry, in print
- [Sz2] ——— : Handling Multicomponent Systems in  $\mathbb{R}^n$ . II: Computational Results, to submit to J. Chem. Inf. Comput. Sci.

István Szalkai
University of Veszprém
Dept.of Math.and Comp.Sci.
H-8200 Veszprém, Hungary
szalkai@almos.vein.hu