Supplementary Material for
Random Data Interpolation (Dirac-Monte Carlo formulation)

(1) Methodology
(Monte-Carlo Method, Dirac Delta Function, Error analysis, Convergence)
(2) Estimate of Delta Width
(3) More Discussion of bias ε value and statistical errors
(4) References

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(1) METHODOLOGY

It is challenging to construct "interpolant" which can be deduced through mathematical analysis by use of given input function values at random locations. The well-known Lagrangian interpolation formula (ref. 1) in one-dimension is still in use today. Though the Lagrangian formula can be shown by using polynomials through mathematical derivation. However, it is not straightforward to extend the formula to 2-dimension and above. Popular interpolation methods (Shepard's distance-weighted, Hardy's multiquadrics, Kriging, etc.) have been developed and practiced successfully in the past few decades in different industries, as well as in scientific and engineering research (refs 2, 3). On the other hand, in statistics community the so-called nonparametric kernel regression (ref. 4) has been studied in the past 50 years, and many analytical results have been discovered, including interpolants (called estimators) and their associated errors and convergence rates. In fact, the original Shepard's interpolant looks somewhat similar to the well-known "Nadaraya-Watson estimator" practiced in kernel regression analysis. Starting from a different approach through our observation, we are able to derive analytically, and establish quickly the interpolant formula for 1-dimension, 2-dimension and any higher dimension. The interpolant found in Dirac-Monte Carlo method has been identified and it is closely related to Nadaraya-Watson estimator. However, one distinct feature of DMC interpolant, different from other interpolants/estimators, is that DMC interpolant is dependent upon individual "coordinate separation", not on the "distance". This difference makes DMC interpolant capable of handling non-convex domain (For example, in between two concentric spherical shells in 3-D or two concentric circles in 2-D, or L-shape corridor.). With the help of Dirac delta function, it is straightforward to generalize DMC interpolants in terms of non-Cartesian coordinates, such as polar coordinates, spherical coordinates, cylindrical coordinates, etc. (ref. 5). Furthermore, the error (uncertainty) analysis of DMC interpolant is derived directly through the use of Central Limit Theorem and different from the findings of kernel regression method. Due to the fact that DMC is a new interpolation formulation, we present the mathematical analysis below to describe DMC method. (Please also view web pages, including references, FAQs, and comparison with other intepolants provided at RDIC)

First, the two ingredients, *Dirac delta function* and *Monte-Carlo method*, used in the formulation are presented:

(1) Dirac delta function (Refs. 6, 7)

Dirac delta function is a special impulse, weighting function which has the following properties:

$$f(x) = \int_a^b f(x')\,\delta(x'-x)\,dx' \;;\; \text{where } a<x<b \qquad \text{(Eq. 1)}$$

$f(x)$ is continuous and bounded;
δ(x'-x) = 0 when x' not equal to x
δ(x'-x) = ∞ (infinity) when x' equal to x

$$\int_{-\infty}^{+\infty} \delta(x'-x)dx' = 1 \; ; \qquad \text{(Eq. 2)}$$

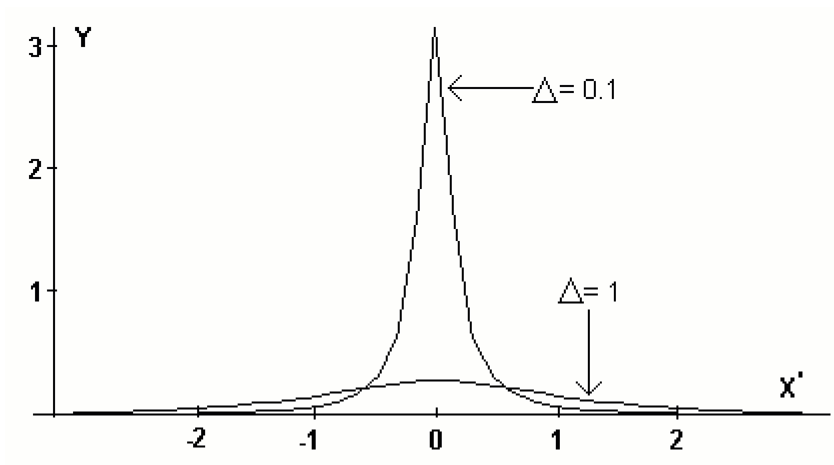
Note that the delta function was introduced by Paul Dirac in theoretical physics in the early 20th century. The function has been given a rigorous, mathematical treatment by L. Schwartz with theory of Distribution. A number of analytical expressions of delta function are commonly used in the literature. They exist in the forms of rational function, transcendental function and infinite series expansion. The rational function below will be used to approximately represent the original Dirac delta function in our work. [Please note the subscript Δ is added to δ(x'-x).]

$$\delta_\Delta(x'-x) = \frac{1}{\pi}\left[\frac{\Delta}{(x'-x)^2+\Delta^2}\right] \qquad \text{(Eq. 3)}$$

$$\lim_{\Delta\to 0}\delta_\Delta(x'-x) = \delta(x'-x)$$

It should be said that the rational function $\delta_\Delta(x'-x)$ in (Eq. 3) is known as "Lorentzian" or "Breit-Wigner distribution" in physics and widely used for "resonance" phenomena in classical mechanics and quantum mechanics. It is also known as "Cauchy density" in statistics. A graphical display of delta function (Eq. 3) is shown in Figure A, where Δ =0.1 and Δ =1.0 with x=0. The abscissa is x' axis and the ordinate Y is $\delta_\Delta(x'-x)$.

Figure A. Approximated Dirac Delta Function



Note that the smaller Δ is, the higher the peak will be and the more narrow the peak will become. The approximated Dirac delta function is peaked symmetrically and drops quickly towards zero value. The function has half peak value when x'-x = $\pm\Delta$. The area under the curve is always equal to 1 according to Eq. 2. Note that in theory Dirac delta function demands that the width approaches zero. However, in numerical computation, it can be set to a small (relative to the domain interval) and finite number. The delta width is an important parameter and will be discussed further later in the section.

(2) Monte-Carlo Integration (ref. 8 and ref. 9)

In the late 1940's, a novel technique was developed by E. Fermi, J. von Neumann, and S. Ulam in the area of evaluating integrals numerically. The method has been proven a powerful tool to handle computations of multi-variable problems in diverse subjects, physics, chemistry, biology, economics etc. In particular, Monte-Carlo method has been a great help to numerically evaluate multiple integrals in applications. There are two fundamental theorems behind Monte-Carlo method: (a) Strong law of large numbers; (b) Central limit theorem. They are briefly stated below to facilitate the presentation of Dirac-Monte Carlo method.

(a) Strong law of large numbers

If a sequence of N random variables x_1 to x_N are picked from a population with the probability density function $g(x)$ and a new random variable A defined by the equation,

$$A= \frac{1}{N}\sum_{i=1}^{N} Z(x_i)\,, \qquad \text{(Eq. 4)}$$

where Z(x) is a given integrable function, and if the integral

$$\overline{Z}=\int_{-\infty}^{+\infty} Z(x)g(x)dx \qquad \text{(Eq. 5)}$$

exists, then A, with probability 1, approaches $\overline{Z}$ as a limit as N approaches infinity.

(b) Central limit theorem

For large N, the probability density distribution of A, G(A), is Gaussian, centered at $\overline{Z}$ with a standard deviation ($\frac{1}{\sqrt{N}}$) times that of the distribution of Z,

$$G(A)\xrightarrow[N\to\infty]{} \frac{1}{\sqrt{2\pi}\,(\frac{\sigma}{\sqrt{N}})}\exp[-\frac{(A-\overline{Z})^2}{2(\frac{\sigma}{\sqrt{N}})^2}] \qquad \text{(Eq. 6)}$$

where σ is the standard deviation of Z.(That is, $\sigma^2 = \overline{(Z-\overline{Z})^2}$). The above result is independent of the nature of Z(x) or $g(x)$. In essence, the probability that the deviation of A from $\overline{Z}$ will exceed $\pm\frac{\sigma}{\sqrt{N}}$ is 31.7%, $\pm\frac{2\sigma}{\sqrt{N}}$ 4.5%, $\pm\frac{3\sigma}{\sqrt{N}}$ 0.3%.

Now, the Dirac-Monte Carlo (DMC) formulation of interpolation is described below. We observe that the following equation exists,

$$\int_{a_1}^{b_1} [f(x') - f(x)]\ \delta(x' - x)dx'=0 \qquad \text{(Eq.7)}$$

and with the substitution of $\delta(x'-x)$ by $\delta_\Delta(x'-x)$ of (Eq. 3) , (Eq. 7) becomes

$$\int_{a_1}^{b_1} [f(x') - f(x)]\ \delta_\Delta(x' - x)dx'=\varepsilon \qquad \text{(Eq. 7A)}$$

where x is the arbitrary value of x' variable and $a_1<x<b_1$, $f(x')$ is continuous and ε is a finite number and is a function of x and the delta width Δ. As Δ approaches zero, so does ε regardless of the value of x. Next, using the density function defined as,

$g(x') = 1/(b_1-a_1)$, for $a_1\le x'\le b_1$, and $g(x') = 0$, otherwise; (Eq. 8)

(Eq. 7A) is recast by use of (Eq. 4) and $Z(x) = (b_1-a_1)\ [f(x')-f(x)]\delta_\Delta(x'-x)$, $M'=N$, and it gives,

$$\frac{(b_1-a_1)}{M'}\sum_{i=1}^{M'}[f(x_i)-f(x)]\delta_\Delta(x_i-x)\approx\varepsilon \qquad \text{(Eq. 9)}$$

and changing the “approximate” sign to “equal” sign”, we obtain

$$\frac{(b_1 - a_1)}{M'}\sum_{i=1}^{M'}[f(x_i) - f(x)]\delta_\Delta(x_i - x) = \varepsilon \pm E$$

$$f(x)\sum_{i=1}^{M'}\delta_\Delta(x_i - x) = -\frac{\varepsilon M'}{(b_1 - a_1)} - \frac{\pm EM'}{(b_1 - a_1)} + \sum_{i=1}^{M'}[f(x_i)]\delta_\Delta(x_i - x) \quad \text{(Eq.9A)}$$

where E is the statistical error occurred by using Monte-Carlo integration. By suppressing the first two terms on the right hand side of the above equation (Eq.9A), we define $f_A(x)$ as,

$$f_A(x) = \frac{\sum_{i=1}^{M'}[f(x_i)]\delta_\Delta(x_i - x)}{\sum_{i=1}^{M'}\delta_\Delta(x_i - x)} = \frac{\sum_{i=1}^{M'}\frac{[f(x_i)]}{[(x_i - x)^2 + \Delta^2]}}{\sum_{i=1}^{M'}\frac{1}{[(x_i - x)^2 + \Delta^2]}} \quad \text{(Eq.10)}$$

where x_i are randomly chosen in the interval (a_1, b_1). It can be seen that by providing x_i, and $f(x_i)$, (Eq. 10) can be used to interpolate the function $f(x)$ at location x where $a_1<x<b_1$. Note that $f_A(x)$ is the searched interpolant. The accuracy and the convergence of $f_A(x)$ are governed by two factors, ε *and* E .They will be discussed later in detail in the error analysis below. In essence, ε factor controls the "systematic bias" error and E factor controls the statistical random error. The ε factor depends on the value of Δ and x , and is assumed small (See an example in Section 3) across the entire supported domain, except near the boundary. It should be said that (Eq. 10) has the same form as the famous nonparametric "Nadaraya-Watson" kernel regression estimator, $f_{NW}(x)$ which is defined as, (ref.10 and ref. 11)

$$f_{NW}(x) = \frac{\sum_{i=1}^{M'}[f(x_i)]K_H(x - x_i)}{\sum_{i=1}^{M'}K_H(x - x_i)} \quad \text{where} \quad K_H(x - x_i) = (\frac{1}{H})K(\frac{x - x_i}{H})$$

Compare the above equation with Eqs. 10 and 3, one obtains that $\delta_\Delta(x_i - x) = \delta_\Delta(x - x_i) =$ $K_H(x - x_i)$ and Δ = H. Furthermore,

$$K(\frac{x - x_i}{H}) = \delta_\Delta(\frac{x - x_i}{\Delta}) = (\frac{1}{\pi})[\frac{1}{(\frac{x - x_i}{\Delta})^2 + 1}]$$

H factor is also called "width" or "band width" in nonparametric kernel regression and controls the kernel smoothing property. The connection between our derivation of the interpolant (Eq. 10) and nonparametric kernel regression can be understood because the original Dirac delta function is defined as a special "local, weighting function".

For 2-dimension Cartesian space, (Eq. 7), (Eq. 7A) and (Eq. 9) are generalized respectively to,

$$\int_{a_2}^{b_2}\int_{a_1}^{b_1}[f(x_1', x_2') - f(x_1, x_2)]\delta(x_1' - x_1)\,\delta(x_2' - x_2)\,dx_1'dx_2' = 0 \quad \text{(Eq. 11)}$$

$$\int_{a_2}^{b_2}\int_{a_1}^{b_1}[f(x_1', x_2') - f(x_1, x_2)]\delta_{\Delta_1}(x_1' - x_1)\delta_{\Delta_2}(x_2' - x_2)dx_1'dx_2' = \varepsilon_2 \quad \text{(Eq. 11A)}$$

where ε_2 is a function of X_1, X_2, Δ_1 and Δ_2.

$$f_{\mathrm{A}}(x_1, x_2) = \frac{\sum_{i=1}^{M'} f(x_{1i}, x_{2i}) \delta_\Delta(x_{1i} - x_1) \delta_\Delta(x_{2i} - x_2)}{\sum_{i=1}^{M'} \delta_\Delta(x_{1i} - x_1) \delta_\Delta(x_{2i} - x_2)} \qquad \text{(Eq.12)}$$

With the use of (Eq. 3), we rewrite (Eq. 12) as,

$$f_{\mathrm{A}}(x_1, x_2) = \frac{\sum_{i=1}^{M'} \frac{[f(x_{1i}, x_{2i})]}{[(x_{1i} - x_1)^2 + \Delta_1^{\ 2}][(x_{2i} - x_2)^2 + \Delta_2^{\ 2}]}}{\sum_{i=1}^{M'} \frac{1}{[(x_{1i} - x)^2 + \Delta_1^{\ 2}][(x_{2i} - x_2)^2 + \Delta_2^{\ 2}]}} \qquad \text{(Eq. 13)}$$

The above equation (Eq. 13) is the 2-dimensional interpolant where x_1 is the x-coordinate and x_2 is the y-coordinate. Thus, (x_{1i}, x_{2i}) is the i[th] input random location and $f(x_{1i}, x_{2i})$ is the associated function value. (x_1, x_2) is the requested location where interpolation is to be calculated. M' is the total number of input locations. With Δ_1 and Δ_2 values given (preset), (Eq. 13) can be used to calculate the interpolated function value, $f_{\mathrm{A}}(x_1,x_2)$. It can be seen that the interpolant, (Eq. 13), depends on the "product"of two coordinate-separation terms,

$$[(x_{1i}-x_1)^2+\Delta_1^{\ 2}]\,[(x_{2i}-x_2)^2+\Delta_2^{\ 2}]$$

and not on the distance which is defined as the square root of $(x_{1i}-x_1)^2 + (x_{2i}-x_2)^2$.

At this point, it should be said that Δ_1 and Δ_2 values can be estimated within the framework of DMC. The following formula can be found (See detailed presentation below in Section 2),

$$\frac{(b_1 - a_1)(b_2 - a_2)}{M'\pi^2 \Delta_1 \Delta_2} \approx 1 \qquad \text{(Eq. 14)}$$

If $(b_1 - a_1) = (b_2 - a_2)$, then $\Delta_1 = \Delta_2$ (See Section 2) and (Eq. 14) becomes

$$\frac{(b_1 - a_1)^2}{M'\pi^2 \Delta_1^{\ 2}} \approx 1 \qquad \text{(Eq. 15)}$$

One can easily calculate the value of Δ_1 when the interval length $(b_1 - a_1)$ is provided .

We now begin the analysis of ***accuracy*** of (Eq. 13) and present the error analysis in terms of the Central Limit Theorem. Recalling (Eq. 9A),

$$f(x)\sum_{i=1}^{M'} \delta_\Delta(x_i - x) = -\frac{\varepsilon M'}{(b_1 - a_1)} - \frac{\pm EM'}{(b_1 - a_1)} + \sum_{i=1}^{M'} [f(x_i)] \delta_\Delta(x_i - x)$$

where E is the statistical error, and both ε and E are dependent on x and Δ. The interpolant f_{A} is defined by (Eq. 10). So, the difference between f(x) and f_{A}(x) is the deviation incurred in the interpolation process,

$$f(x)-f_A(x)=\frac{\sum_{i=1}^{M'}[f(x_i)]\delta_\Delta(x_i-x)-\frac{M'\varepsilon}{(b_1-a_1)}-\frac{\pm M'E}{(b_1-a_1)}}{\sum_{i=1}^{M'}\delta_\Delta(x_i-x)} - \frac{\sum_{i=1}^{M'}[f(x_i)]\delta_\Delta(x_i-x)}{\sum_{i=1}^{M'}\delta_\Delta(x_i-x)}$$

$$=\frac{-\varepsilon\mp E}{\frac{(b_1-a_1)}{M'}\sum_{i=1}^{M'}\delta_\Delta(x_i-x)}=\frac{-\varepsilon}{\frac{(b_1-a_1)}{M'}\sum_{i=1}^{M'}\delta_\Delta(x_i-x)}+\frac{\mp E}{\frac{(b_1-a_1)}{M'}\sum_{i=1}^{M'}\delta_\Delta(x_i-x)} \qquad \text{(Eq. 15A)}$$

Note that the denominator is always "positive" and "not equal to zero" and in fact it is in the form when the integral

$$\int_{a_1}^{b_1}\delta_\Delta(x'-x)dx'$$ (Note that this integral approaches 1 when Δ approaches zero.)

is calculated by use of Monte-Carlo integration and is also governed by the Central Limit Theorem .(See more of this connection in Section 2).

For 2-dimension case, the deviation is generalized to,

$$f(x_1, x_2)-f_A(x_1, x_2)=\frac{-\varepsilon_2\mp E}{\frac{(b_1-a_1)(b_2-a_2)}{M'}\sum_{i=1}^{M'}\delta_{\Delta_1}(x_{1i}-x_1)\delta_{\Delta_2}(x_{2i}-x_2)}$$

(Eq. 16)

where $\delta_{\Delta_1}(x_{1i}-x_1)$ and $\delta_{\Delta_2}(x_{2i}-x_2)$ are defined by (Eq. 3). Note that on the right hand side of (Eq. 16), the denominator can be computed for the requested location (x_1, x_2) and E in the numerator is governed by the Central Limit Theorem. As said earlier about (Eq. 6), the deviation error E will exceed $\pm\frac{\sigma}{\sqrt{N}}$ with probability 31.7%, $\pm\frac{2\sigma}{\sqrt{N}}$ with probability 4.5%, and $\pm\frac{3\sigma}{\sqrt{N}}$ with probability 0.3%. Again, N is equal to the input location number M '. All needs to be done is to find the value of ε and σ. We shall do so as follows.

Let us recall Eq. 7A,

$$\int_{a_1}^{b_1}[f(x')-f(x)]\,\delta_\Delta(x'-x)dx'=\varepsilon$$

and Eq. 5,

$$\int_{-\infty}^{+\infty}Z(x')g(x')dx'=\overline{Z}$$

Comparing the above two integrals, we obtain,

$$\overline{Z}=\varepsilon$$

$$(b_1-a_1)\,[f(x')-f(x)]\delta_\Delta(x'-x)=Z(x')$$

and the density function,

$$g(x') = \begin{cases} 1/(b_1-a_1), & \text{for } a_1 \le x' \le b_1 \\ 0, & \text{otherwise} \end{cases}$$

By definition $\sigma^2 = \overline{(Z-\overline{Z})^2}$ and $\overline{Z} = \varepsilon$, it gives $\sigma^2 = \overline{(Z-\varepsilon)^2}$.

$$\sigma^2 = \overline{(Z-\varepsilon)^2} = \int_{-\infty}^{+\infty} (Z(x')-\varepsilon)^2 g(x')dx'$$

$$= \int_{-\infty}^{+\infty} (Z^2(x') - 2Z(x')\varepsilon + \varepsilon^2) g(x')dx' = \int_{-\infty}^{+\infty} Z^2(x') g(x') dx' - \varepsilon^2 \qquad \text{(Eq. 17)}$$

As can be seen, both ε and σ^2 can not be calculated because they involve the unknown function $f(x')$. However, the sample estimates of ε and σ^2 can be computed by use of,

$$\varepsilon = \overline{Z} = \frac{1}{M'} \sum_{i=1}^{M'} Z_i = \frac{1}{M'} \sum_{i=1}^{M'} (b_1 - a_1)[f(x_i) - f(x)]\delta_\Delta(x_i - x) \qquad \text{(Eq. 18)}$$

$$\sigma^2 = \overline{(Z-\varepsilon)^2} = \frac{1}{M'} \sum_{i=1}^{M'} (Z_i - \varepsilon)^2 = \frac{1}{M'} \sum_{i=1}^{M'} \{(b_1 - a_1)[f(x_i) - f(x)]\delta_\Delta(x_i - x) - \varepsilon\}^2 \qquad \text{(Eq. 18A)}$$

The 2-dimensional case of (Eq. 18) and (Eq. 18A) have the following forms,

$$\varepsilon_2 = \overline{Z} = \frac{1}{M'} \sum_{i=1}^{M'} Z_i = \frac{1}{M'} \sum_{i=1}^{M'} (b_1 - a_1)(b_2 - a_2)[f(x_{1i}, x_{2i}) - f(x_1, x_2)]\delta_{\Delta_1}(x_{1i} - x_1)\delta_{\Delta_2}(x_{2i} - x_2) \qquad \text{(Eq. 19)}$$

$$\sigma^2 = \overline{(Z-\varepsilon_2)^2} = \frac{1}{M'} \sum_{i=1}^{M'} (Z_i - \varepsilon_2)^2 =$$

$$\frac{1}{M'} \times \sum_{i=1}^{M'} \{(b_1 - a_1)(b_2 - a_2)[f(x_{1i}, x_{2i}) - f(x_1, x_2)]\delta_{\Delta_1}(x_{1i} - x_1)\delta_{\Delta_2}(x_{2i} - x_2) - \varepsilon_2\}^2 \qquad \text{(Eq. 19A)}$$

The above two equations and (Eq. 16) can be used to calculate the uncertainty for the interpolation result. The function value $f(x_1, x_2)$ is set to the true value if known. In the event when no true value is given, then $f(x_1, x_2)$ can be set to the interpolated value, $f_A(x_1, x_2)$. When doing so, the sample ε_2 value (or ε value for one-dimension case) will always be zero, because

$$\sum_{i=1}^{M'} [f(x_i) - f_A(x)]\delta_\Delta(x_i - x) = \sum_{i=1}^{M'} [f(x_i) - \frac{\sum_{j=1}^{M'} f(x_j)\delta_\Delta(x_j - x)}{\sum_{j=1}^{M'} \delta_\Delta(x_j - x)}]\delta_\Delta(x_i - x)$$

$$= \sum_{i=1}^{M'} f(x_i)\delta_\Delta(x_i - x) - \frac{\sum_{j=1}^{M'} f(x_j)\delta_\Delta(x_j - x)}{\sum_{j=1}^{M'} \delta_\Delta(x_j - x)} \sum_{i=1}^{M'} \delta_\Delta(x_i - x)$$

$$= \sum_{i=1}^{M'} f(x_i)\delta_\Delta(x_i - x) - \sum_{j=1}^{M'} f(x_j)\delta_\Delta(x_j - x) = 0$$

and the deviation is given only in terms of the statistical factor ***E*** which can be computed.

We note in passing that, by reducing the delta width Δ_1 and Δ_2 used in (Eq. 13) towards zero, the interpolation semi-norm, $\sum_{i=1}^{M'} \left| f(x_{1i}, x_{2i}) - f_A(x_{1i}, x_{2i}) \right|$ approaches zero as well (See the simple proof in Section 2). This property of semi-norm approaching zero will remain true in our formulation for any higher dimensional space.

Finally, we shall address the ***convergence rate*** for 2-dimension and the same procedure can be applied to any other dimension.. As Δ_1 and Δ_2 approach zero, and M' approaches infinity, ε_2 approaches zero according to the following analysis. We recall (Eq. 11A),

$$\int_{a_2}^{b_2}\int_{a_1}^{b_1} [f(x_1', x_2') - f(x_1, x_2)](\frac{\Delta_1}{\pi})[\frac{1}{(x_1'-x_1)^2 + \Delta_1^2}](\frac{\Delta_2}{\pi})[\frac{1}{(x_2'-x_2)^2 + \Delta_2^2}]dx_1'dx_2' = \varepsilon_2$$

Due to the fact that $\delta_{\Delta_1}(x_1'-x_1)$ and $\delta_{\Delta_2}(x_2'-x_2)$ are now sharply peaked near the point (x_1, x_2) as Δ_1 and Δ_2 approach zero and drop their values quickly toward zero when $|x_1'-x_1| > \Delta_1$ and $|x_2'-x_2| > \Delta_2$, we only need to be concerned with x_1' and x_1' values when $|x_1'-x_1| \le \Delta_1$ and $|x_2'-x_2| \le \Delta_2$. Thus, $f(x_1', x_2')$ can be expanded by Taylor's series,

$$f(x_1', x_2') \approx f(x_1, x_2) + (x_1'-x_1)\frac{\partial f}{\partial x_1'} + (x_2'-x_2)\frac{\partial f}{\partial x_2'} + (ignoring - higher - order - terms)$$

Substituting the expansion to the above integral, we obtain,

$$\varepsilon_2 \approx \int_{a_2}^{b_2}\int_{a_1}^{b_1} [(x_1'-x_1)\frac{\partial f}{\partial x_1'}(\frac{\Delta_1}{\pi})[\frac{1}{(x_1'-x_1)^2 + \Delta_1^2}](\frac{\Delta_2}{\pi})[\frac{1}{(x_2'-x_2)^2 + \Delta_2^2}]dx_1'dx_2' \; +$$
$$\int_{a_2}^{b_2}\int_{a_1}^{b_1} [(x_2'-x_2)\frac{\partial f}{\partial x_2'}(\frac{\Delta_1}{\pi})[\frac{1}{(x_1'-x_1)^2 + \Delta_1^2}](\frac{\Delta_2}{\pi})[\frac{1}{(x_2'-x_2)^2 + \Delta_2^2}]dx_1'dx_2'$$

$$= (\frac{\partial f}{\partial x_1'})\int_{a_1}^{b_1} (x_1'-x_1)(\frac{\Delta_1}{\pi})[\frac{1}{(x_1'-x_1)^2 + \Delta_1^2}]dx_1' \int_{a_2}^{b_2} (\frac{\Delta_2}{\pi})[\frac{1}{(x_2'-x_2)^2 + \Delta_2^2}]dx_2' \; +$$

$$(\frac{\partial f}{\partial x_2'})\int_{a_2}^{b_2}(x_2'-x_2)(\frac{\Delta_2}{\pi})[\frac{1}{(x_2'-x_2)^2+\Delta_2^{\,2}}]dx_2'\int_{a_1}^{b_1}(\frac{\Delta_1}{\pi})[\frac{1}{(x_1'-x_1)^2+\Delta_1^{\,2}}]dx_1'$$

$$=(\frac{\partial f}{\partial x_1'})(\frac{\Delta_1}{2\pi})[\log\frac{(b_1-x_1)^2+\Delta_1^{\,2}}{(a_1-x_1)^2+\Delta_1^{\,2}}](\frac{1}{\pi})[\tan^{-1}(\frac{b_2-x_2}{\Delta_2})-\tan^{-1}(\frac{a_2-x_2}{\Delta_2})]\ +$$

$$(\frac{\partial f}{\partial x_2'})(\frac{\Delta_2}{2\pi})[\log\frac{(b_2-x_2)^2+\Delta_2^{\,2}}{(a_2-x_2)^2+\Delta_2^{\,2}}](\frac{1}{\pi})[\tan^{-1}(\frac{b_1-x_1}{\Delta_1})-\tan^{-1}(\frac{a_1-x_1}{\Delta_1})]$$

As Δ_1 and Δ_2 approach zero, the above equation gives,

$$\varepsilon_2 \rightarrow (\text{constant 1})\ \Delta_1 + (\text{constant 2})\ \Delta_2 \qquad \text{(Eq. 20)}$$

From the analysis in Section 2, we know that Δ_1 and Δ_2 are proportional to $\frac{1}{\sqrt{M'}}$. Thus ε_2 is proportional to $\frac{1}{\sqrt{M'}}$.

In contrast, in 1-D, Δ is proportional to $\frac{1}{M'}$, ε is proportional to Δ or equivalently $\frac{1}{M'}$.

Now let us turn the attention to the *E* factor in (Eq. 16). Due to the complexity of 2-D *E* factor, we perform the analysis in 1-D below and the whole presentation can be extended to 2-D in a straightforward manner. Recalling (Eq. 7A) and (Eq. 17), they give

$$\int_{a_1}^{b_1}[f(x')-f(x)]\ \delta_\Delta(x'-x)dx'=\varepsilon \qquad \text{(Eq. 7A)}$$

$$\sigma^2=\overline{(Z-\varepsilon)^2}=\int_{-\infty}^{+\infty}(Z(x')-\varepsilon)^2 g(x')dx' = \int_{-\infty}^{+\infty}Z^2(x')g(x')dx'-\varepsilon^2 \qquad \text{(Eq. 17)}$$

where for bounded domain support $[a_1, b_1]$, $g(x')$ equals to $1/(b_1-a_1)$ for $a_1 \le x' \le b_1$ and

$$(b_1-a_1)\ [f(x')-f(x)]\delta_\Delta(x'-x)=Z(x')$$

Let us calculate the integral in (Eq. 17) under the condition that Δ approaches zero. We obtain,

$$\int_{-\infty}^{+\infty}Z^2(x')g(x')dx'=\int_{a_1}^{b_1}Z^2(x')g(x')dx'=(\frac{\Delta}{\pi})^2(b_1-a_1)\int_{a_1}^{b_1}[f(x')-f(x)]^2(\frac{1}{(x'-x)^2+\Delta^2})^2dx'$$

$$\approx(\frac{\Delta}{\pi})^2(b_1-a_1)\int_{a_1}^{b_1}[f'(x)(x'-x)]^2[\frac{1}{(x'-x)^2+\Delta^2}]^2dx'$$

$$= (\frac{\Delta}{\pi})^2 (b_1 - a_1)[f'(x)]^2 \int_{a_1}^{b_1} (x'-x)^2 [\frac{1}{(x'-x)^2 + \Delta^2}]^2 dx'$$

$$= (\frac{\Delta}{\pi})^2 (b_1 - a_1)[f'(x)]^2 \int_{a_1-x}^{b_1-x} \frac{y^2}{[y^2 + \Delta^2]^2} dy = (\frac{\Delta}{\pi})^2 (b_1 - a_1)[f'(x)]^2 \int_{\frac{a_1-x}{\Delta}}^{\frac{b_1-x}{\Delta}} \frac{z^2}{(\Delta)[z^2+1]^2} dz$$

$$= (\frac{\Delta}{\pi^2})(b_1 - a_1)[f'(x)]^2 \int_{\frac{a_1-x}{\Delta}}^{\frac{b_1-x}{\Delta}} \frac{z^2}{[z^2+1]^2} dz$$

$$= (\frac{\Delta}{\pi^2})(b_1 - a_1)[f'(x)]^2 \{(\frac{1}{2})[\tan^{-1} z]_{\frac{a_1-x}{\Delta}}^{\frac{b_1-x}{\Delta}} - (\frac{1}{2})[\frac{z}{z^2+1}]_{\frac{a_1-x}{\Delta}}^{\frac{b_1-x}{\Delta}}\}$$

$$= (\frac{\Delta}{\pi^2})(b_1 - a_1)[f'(x)]^2 \bullet$$

$$\{(\frac{1}{2})[\tan^{-1}(\frac{b_1-x}{\Delta}) - \tan^{-1}(\frac{a_1-x}{\Delta})] - (\frac{1}{2})[\frac{\frac{b_1-x}{\Delta}}{(\frac{b_1-x}{\Delta})^2+1} - \frac{\frac{a_1-x}{\Delta}}{(\frac{a_1-x}{\Delta})^2+1}]\}$$

$$\approx \text{(constant) } \Delta \qquad \text{(Eq. 21)}$$

Thus, (Eq. 17) becomes for 1-D, (Note that ε is proportional to Δ in 1-D.)

$$\sigma^2 = \overline{(Z-\varepsilon)^2} \approx \text{(constant) } \Delta - \varepsilon^2 \approx \text{(constant) } \Delta \qquad \text{(Eq. 22)}$$

Hence, in 1-D we can see that the *E* factor, which is proportional to $\frac{\sigma}{\sqrt{M'}}$, converges according to $\sim \frac{1}{M'}$.

Now, let us generalize the above σ^2 analysis for 2-D.

In 2-D,

$$\sigma^2 = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} Z^2(x_1', x_2') g(x_1', x_2') dx_1' dx_2' - \varepsilon_2^{\,2}$$

$$= (\frac{\Delta_1}{\pi})^2 (\frac{\Delta_2}{\pi})^2 (b_1 - a_1)(b_2 - a_2) \bullet$$

$$\int_{a_2}^{b_2} \int_{a_1}^{b_1} [f(x_1', x_2') - f(x_1, x_2)]^2 [\frac{1}{(x_1'-x_1)^2 + \Delta_1^2}]^2 [\frac{1}{(x_2'-x_2)^2 + \Delta_2^2}]^2 dx_1' dx_2' - \varepsilon_2^2$$

$$\approx (\frac{\Delta_1}{\pi})^2 (\frac{\Delta_2}{\pi})^2 (b_1 - a_1)(b_2 - a_2) \bullet$$

$$\int_{a_2}^{b_2} \int_{a_1}^{b_1} [\frac{\partial f}{\partial x_1'}(x_1'-x_1) + \frac{\partial f}{\partial x_2'}(x_2'-x_2)]^2 [\frac{1}{(x_1'-x_1)^2 + \Delta_1^2}]^2 [\frac{1}{(x_2'-x_2)^2 + \Delta_2^2}]^2 dx_1' dx_2' - \varepsilon_2^2$$

$$= (\frac{\Delta_1}{\pi})^2 (\frac{\Delta_2}{\pi})^2 (b_1 - a_1)(b_2 - a_2) \bullet [(\frac{\partial f}{\partial x_1'})^2 \int_{a_1}^{b_1} [\frac{x_1'-x_1}{(x_1'-x_1)^2 + \Delta_1^2}]^2 dx_1' \int_{a_2}^{b_2} [\frac{1}{(x_2'-x_2)^2 + \Delta_2^2}]^2 dx_2'$$

$$+ 2(\frac{\partial f}{\partial x_1'})(\frac{\partial f}{\partial x_2'}) \int_{a_1}^{b_1} \frac{x_1'-x_1}{[(x_1'-x_1)^2 + \Delta_1^2]^2} dx_1' \int_{a_2}^{b_2} \frac{x_2'-x_2}{[(x_2'-x_2)^2 + \Delta_2^2]^2} dx_2'$$

$$+ (\frac{\partial f}{\partial x_2'})^2 \int_{a_1}^{b_1} [\frac{1}{(x_1'-x_1)^2 + \Delta_1^2}]^2 dx_1' \int_{a_2}^{b_2} [\frac{x_2'-x_2}{(x_2'-x_2) + \Delta_2^2}]^2 dx_2'] - \varepsilon_2^2$$

$$= (\frac{\Delta_1}{\pi})^2 (\frac{\Delta_2}{\pi})^2 (b_1 - a_1)(b_2 - a_2) \bullet [(\frac{\partial f}{\partial x_1'})^2 \int_{a_1}^{b_1} [\frac{x_1'-x_1}{(x_1'-x_1)^2 + \Delta_1^2}]^2 dx_1' \int_{a_2}^{b_2} [\frac{1}{(x_2'-x_2)^2 + \Delta_2^2}]^2 dx_2'$$

$$+ 2(\frac{\partial f}{\partial x_1'})(\frac{\partial f}{\partial x_2'}) \int_{a_1}^{b_1} \frac{x_1'-x_1}{[(x_1'-x_1)^2 + \Delta_1^2]^2} dx_1' \int_{a_2}^{b_2} \frac{x_2'-x_2}{[(x_2'-x_2)^2 + \Delta_2^2]^2} dx_2'$$

$$+ (\frac{\partial f}{\partial x_2'})^2 \int_{a_1}^{b_1} [\frac{1}{(x_1'-x_1)^2 + \Delta_1^2}]^2 dx_1' \int_{a_2}^{b_2} [\frac{x_2'-x_2}{(x_2'-x_2) + \Delta_2^2}]^2 dx_2'] - \varepsilon_2^2$$

(Eq. 23)

Note that the integral

$$\int_a^b [\frac{1}{(x'-x)^2 + \Delta^2}]^2 dx' = (\frac{1}{\Delta^3}) \int_{\frac{a-x}{\Delta}}^{\frac{b-x}{\Delta}} [\frac{1}{z^2+1}]^2 dz = (\frac{1}{2\Delta^3})[\tan^{-1} z]_{\frac{a-x}{\Delta}}^{\frac{b-x}{\Delta}} + (\frac{1}{2\Delta^3})[\frac{z}{z^2+1}]_{\frac{a-x}{\Delta}}^{\frac{b-x}{\Delta}}$$

$$= (\frac{1}{2\Delta^3})[\tan^{-1}(\frac{b-x}{\Delta}) - \tan^{-1}(\frac{a-x}{\Delta})] + (\frac{1}{2\Delta^3})[\frac{\frac{b-x}{\Delta}}{(\frac{b-x}{\Delta})^2+1} - \frac{\frac{a-x}{\Delta}}{(\frac{a-x}{\Delta})^2+1}] \quad \text{(Eq. 24)}$$

and the integral

$$\int_a^b (x'-x)[\frac{1}{(x'-x)^2+\Delta^2}]^2 dx' = (\frac{1}{2})\int_{(a-x)^2+\Delta^2}^{(b-x)^2+\Delta^2} \frac{dz}{z^2} = (\frac{1}{2})[\frac{1}{(a-x)^2+\Delta^2} - \frac{1}{(b-x)^2+\Delta^2}]$$

(Eq. 25)

We can now approximate (Eq. 23) as,

$$\sigma^2 \text{ (for 2-D)} \approx \text{(constant 1)} (\frac{\Delta_1^{\ 2}}{\Delta_2}) + \text{(constant2)} (\frac{\Delta_2^{\ 2}}{\Delta_1}) \qquad \text{(Eq. 26)}$$

Recalling in 2-D, Δ_1 and Δ_2 are proportional to $\sim \frac{1}{\sqrt{M'}}$. Therefore, the *E* factor converges as $\sim \frac{1}{M'}$ same as in 1-D.

There is one more factor which needs to be studied before we can find out the convergence rate of (Eq. 15A) for 1-D. It is the denominator of (Eq. 15A). As explained before, the denominator of (Eq. 15A) is the Monte-Carlo integration of the integral, $\int_{a_1}^{b_1} \delta_\Delta (x'-x) dx'$. The analytic result of this integral is,

$$I = \int_{a_1}^{b_1} \frac{1}{\pi}[\frac{\Delta}{(x'-x)^2+\Delta^2}]dx' = \frac{1}{\pi} [\tan^{-1}(\frac{b_1-x}{\Delta}) - \tan^{-1}(\frac{a_1-x}{\Delta})]$$

and the Monte-Carlo integration of the integral gives, by use of Central Limit Theorem,

$$\frac{(b_1-a_1)}{M'}\sum_{i=1}^{M'}\frac{1}{\pi}[\frac{\Delta}{(x'-x)+\Delta^2}] = I \pm G \ , \qquad \text{(Eq. 26)}$$

G is proportional to $\frac{\sigma_\Delta}{\sqrt{M'}}$ where σ_Δ is defined as,

$$\sigma_\Delta^{\ 2} = \int_{a_1}^{b_1} \{(b_1-a_1)\frac{1}{\pi}[\frac{\Delta}{(x'-x)^2+\Delta^2}] - I\}^2 g(x')dx'$$

$$= \frac{(b_1-a_1)\Delta^2}{\pi^2}\int_{a_1}^{b_1} [\frac{1}{(x'-x)^2+\Delta^2}]^2 dx' - I^2$$

We can find that when Δ is small, ignoring I^2,

$$\sigma_\Delta^{\ 2} \approx \frac{(b_1-a_1)}{2\pi\Delta}$$

Using the result found in the next section, that is,

$$\frac{(b_1-a_1)}{M'\pi\Delta} \approx 1$$

we found,

$$\sigma_{\Delta} \approx \sqrt{\frac{(b_1 - a_1)}{2\pi\Delta}} \approx \sqrt{\frac{M'}{2}}$$

Therefore, the G factor is proportional to $\frac{\sigma_{\Delta}}{\sqrt{M'}} \approx \sqrt{\frac{1}{2}} \approx 0.7$.

Similarly, in 2-D, the denominator of (Eq. 16) is the Monte-Carlo integration of the integral,

$$I_2 = \int_{a_2}^{b_2}\int_{a_1}^{b_1} \delta_{\Delta_1}(x_1' - x_1)\delta_{\Delta_2}(x_2' - x_2)dx_1'dx_2'$$

$$= \int_{a_1}^{b_1} \frac{1}{\pi}[\frac{\Delta_1}{(x_1' - x_1)^2 + \Delta_1^{\ 2}}]dx' \int_{a_1}^{b_1} \frac{1}{\pi}[\frac{\Delta_2}{(x_2' - x_2)^2 + \Delta_2^{\ 2}}]dx'$$

and we obtain,

$$\frac{(b_1 - a_1)(b_2 - a_2)}{M'}\sum_{i=1}^{M'}\frac{1}{\pi}[\frac{\Delta_1}{(x_{1i}' - x_1)^2 + \Delta_1^{\ 2}}]\frac{1}{\pi}[\frac{\Delta_2}{(x_{2i}' - x_2)^2 + \Delta_2^{\ 2}}] = I_2 \pm G_2 \qquad \text{(Eq. 27)}$$

where G_2 factor is proportional to $\frac{\sigma_{\Delta_1,\Delta_2}}{\sqrt{M'}}$ where $\sigma_{\Delta_1,\Delta_2}$ is defined as,

$$[\sigma_{\Delta_1,\Delta_2}]^2 = \int_{a_2}^{b_2}\int_{a_1}^{b_1}\{(b_1 - a_1)(b_2 - a_2)(\frac{1}{\pi^2})[\frac{\Delta_1}{(x_1' - x_1)^2 + \Delta_1^{\ 2}}][\frac{\Delta_2}{(x_2' - x_2) + \Delta_2^{\ 2}}] - I_2\}^2 g(x_1', x_2')dx_1'dx_2'$$

$$= (b_1 - a_1)(b_2 - a_2)(\frac{\Delta_1^{\ 2}\Delta_2^{\ 2}}{\pi^4})\int_{a_2}^{b_2}\int_{a_1}^{b_1}[\frac{1}{(x_1' - x_1)^2 + \Delta_1^{\ 2}}]^2[\frac{1}{(x_2' - x_2) + \Delta_2^{\ 2}}]^2 dx_1'dx_2' - I_2^{\ 2}$$

$$\approx (b_1 - a_1)(b_2 - a_2)(\frac{\Delta_1^{\ 2}\Delta_2^{\ 2}}{\pi^4}) \bullet (\frac{\pi}{2\Delta_1^{\ 3}})(\frac{\pi}{2\Delta_2^{\ 3}}) = (b_1 - a_1)(b_2 - a_2)(\frac{1}{4\pi^2\Delta_1\Delta_2}) \qquad \text{(Eq. 28)}$$

In Section 2, we also found, a general form of (Eq. D-9),

$$\frac{(b_1 - a_1)(b_2 - a_2)}{M'\pi^2} = \Delta_1\Delta_2$$

Therefore, we obtain

$$[\sigma_{\Delta_1,\Delta_2}]^2 \approx \frac{M'}{4} \quad \text{and} \quad \sigma_{\Delta_1,\Delta_2} \approx \frac{\sqrt{M'}}{2}$$

Thus, G_2 factor is proportional to $\frac{\sigma_{\Delta_1,\Delta_2}}{\sqrt{M'}} \approx \frac{1}{2}$.

At last, we can conclude that the convergence rate of (Eq. 15A) for 1-D. It converges according to,

$$| f(\mathrm{x}) - f_A(\mathrm{x}) | \rightarrow \frac{1}{M'}$$

and (eq. 16) for 2-D,

$$| f(\mathrm{x}_1, \mathrm{x}_2) - f_A(\mathrm{x}_1, \mathrm{x}_2) | \rightarrow \frac{1}{\sqrt{M'}}$$

In more than 2-dimension, each individual delta width is proportional to $\frac{1}{\sqrt[n]{M'}}$ where n is the dimensionality.

Therefore, the convergence rate is proportional to $\frac{1}{\sqrt[n]{M'}}$ which is much slower. Indeed the Curse of Dimensionality (COD) inevitably shows up in the analysis. In summary, in one dimension, the convergence is controlled by ε and *E*. In two dimension, the convergence is dominated by ε_2. For n-dimension (n > 2), the convergence is again dominated and controlled by the ε_n bias factor.

CONVERGENCE SUMMARY

Dimension	ε_n Bias term	*E* Random error term
1-D	$\frac{1}{M'}$	$\frac{1}{M'}$
2-D	$\frac{1}{\sqrt{M'}}$	$\frac{1}{M'}$
n-D	$\frac{1}{\sqrt[n]{M'}}$	$\frac{1}{M'}$

Appendix A. More about Monte-Carlo Method

It should be said that Strong law of large numbers and Central Limit Theorem do not give prescriptions for deciding how large N should be. However, in real life calculations when Z(x) is well-behaved, N generally can be a finite number in the neighborhood of 10 to 20 for one dimension problems. Of course, with higher N the interpolant will yield better accuracy results. In addition, these two theorems do not depend on the dimensionality of the integral. It can be anticipated that the number of points required to evaluate a multi-dimensional integral could still be manageable.

In using Monte-Carlo method, one needs to generate a set of random numbers x_i distributed uniformly over the interval $a \leq x \leq b$ (one dimension problem). The following procedure is generally used to find the set. The density function,

1/(b-a), for $a \leq x \leq b$

g(x) =

0, otherwise

and the two boundary conditions, namely, when R_i=0, x_i=a and R_i=1, x_i=b. One can easily obtain the following relation,

$$x_i = a + R_i*(b-a) \qquad \text{(Eq. A)}$$

where R_i is the random number between 0 and 1, and it is generally produced by using the random number generator available on the computer. This whole process can easily be extended to multi-dimensional space when all variables are constrained in the specified intervals. The user generates sets of random numbers (R_1, R_2,....,R_n) and each set will be used to calculate the coordinate locations of the sample point in design space. There are n equations similar to Eq. A and one for each coordinates.

Appendix B. More about Delta width

Our earlier experience indicated that the delta width Δ can be set as a few percent of the variable interval length. See more detailed analysis about estimating delta width value in Section 2. This is an important parameter and its proper setting is closely related to the number of random sample points N. Analytically, one can estimate the value of Δ for the interpolation as shown in the next section.

Note that there is a scaling property of the delta width Δ with respect to the interval length. Let us illustrate this property by using the following equation, (For simplicity, choose x=0.)

$$1 = \int_{-\infty}^{+\infty} \delta(x'-x)\,dx' = \int_{-\infty}^{+\infty} \frac{1}{\pi}\left[\frac{\Delta}{(x'-x)^2+\Delta^2}\right]dx' = \int_{-\infty}^{+\infty} \frac{1}{\pi}\left[\frac{\Delta}{(x')^2+\Delta^2}\right]dx'$$

$$\approx \int_{-l}^{+l} \frac{1}{\pi}\left[\frac{\Delta}{(x')^2+\Delta^2}\right]dx' = \frac{1}{\pi}\left[\tan^{-1}\left(\frac{l}{\Delta}\right) - \tan^{-1}\left(\frac{-l}{\Delta}\right)\right]; \qquad \text{(Eq. B)}$$

In real computation, l and Δ are both finite numbers. Thus, for example, if the interval length $2l$ equals 20 (That is l=10.), one can choose Δ close to 1 and it gives,

$$\frac{1}{\pi}\left[\tan^{-1}\left(\frac{l}{\Delta}\right) - \tan^{-1}\left(\frac{-l}{\Delta}\right)\right] = \frac{1}{\pi}\left[\tan^{-1}(10) - \tan^{-1}(-10)\right] \approx 0.936$$

which is close to 1. Henceforth, if the interval length is 200, then Δ can be chosen close to 10. Conversely, if the interval length is 2, then Δ can be chosen close to 0.1. The important thing to keep in mind is that Δ is "small" with respect to the interval length. Furthermore, in two-dimension case, if x-interval length l_x and y-interval length l_y do not have the same length. Then one needs to make sure that Δ_x and Δ_y are chosen such that they satisfy,

$$\frac{l_x}{\Delta_x} = \frac{l_y}{\Delta_y} \qquad \text{(Eq. C)}$$

The same argument should be applied to multi-dimension situation.

(2) Estimate of Delta width

Use the definition of Dirac delta function for the interval (a,b),

$$\int_a^b \delta(x'-x)dx' = 1 \quad \text{(where x is between a and b)}$$

We use the rational function $\delta_\Delta(x'-x)$ to approximate Dirac delta function. It gives

$$\int_a^b \delta_\Delta(x'-x)dx' = \int_a^b (\frac{\Delta}{\pi})[\frac{1}{(x'-x)^2+\Delta^2}]dx' = \frac{1}{\pi}[\tan^{-1}(\frac{b-x}{\Delta}) - \tan^{-1}(\frac{a-x}{\Delta})] \qquad \text{(Eq. D)}$$

and recast the integral using Monte-Carlo method,

$$\int_a^b \delta_\Delta(x'-x)dx' \overset{(approximated)}{\approx} \frac{(b-a)}{M'}\sum_{i=1}^{M'}(\frac{\Delta}{\pi})[\frac{1}{(x_i-x)^2+\Delta^2}] \overset{(approximat\ ed)}{\approx}$$
$$\frac{1}{\pi}[\tan^{-1}(\frac{b-x}{\Delta}) - \tan^{-1}(\frac{a-x}{\Delta})] \qquad \text{(Eq. D-1)}$$

The two-dimensional extension of (Eq. D-1) is,

$$\frac{(b_1-a_1)(b_2-a_2)}{M'}\sum_{i=1}^{M'}(\frac{\Delta_1\Delta_2}{\pi^2})[\frac{1}{(x_{1i}-x_1)^2+\Delta_1{}^2}][\frac{1}{(x_{2i}-x_2)^2+\Delta_2{}^2}] \approx$$
$$\frac{1}{\pi}[\tan^{-1}(\frac{b_1-x_1}{\Delta_1}) - \tan^{-1}(\frac{a_1-x_1}{\Delta_1})]\ \frac{1}{\pi}[\tan^{-1}(\frac{b_2-x_2}{\Delta_2}) - \tan^{-1}(\frac{a_2-x_2}{\Delta_2})] \qquad \text{(Eq. D-2)}$$

To be more exact, let us change the "approximate" sign to equal sign in (Eq. D-1) as,

$$\frac{(b-a)}{M'}\sum_{i=1}^{M'}(\frac{\Delta}{\pi})[\frac{1}{(x_i-x)^2+\Delta^2}] = \frac{1}{\pi}[\tan^{-1}(\frac{b-x}{\Delta}) - \tan^{-1}(\frac{a-x}{\Delta})] \pm \frac{3\sigma_D}{\sqrt{M'}}$$

(Eq. D-3)

where σ_D, originated from the Monte-Carlo integration error, is a function of (Δ ,x,a,b) and it is expressed in the analytical form,

$$\sigma_D = \int_a^b \frac{1}{(b-a)}\{(b-a)(\frac{\Delta}{\pi})[\frac{1}{(x'-x)^2+\Delta^2}] - \frac{1}{\pi}[\tan^{-1}(\frac{b-x}{\Delta}) - \tan^{-1}(\frac{a-x}{\Delta})]\}^2 dx'$$

(Eq. D-4)

Note that (Eq. D-3) can be recast into

$$\frac{-3\sigma_D}{\sqrt{M'}} \le \frac{(b-a)}{M'}\sum_{i=1}^{M'}(\frac{\Delta}{\pi})[\frac{1}{(x_i-x)^2+\Delta^2}] - \frac{1}{\pi}[\tan^{-1}(\frac{b-x}{\Delta}) - \tan^{-1}(\frac{a-x}{\Delta})] \le \frac{3\sigma_D}{\sqrt{M'}}$$

(Eq. D-5)

The above inequality equation holds true with probability 99.7% in accordance with Central Limit Theorem. As can be seen, Δ can take a range of values to satisfy (Eq. D-5). Given M',b, a, x_i, and x, one can solve Δ analytically from (Eq. D-5) in principle. However, this is not an easy task and the closed form solution is unlikely to be found. However, one can try to solve Δ in (Eq. D-5) by use of numerical methods. But, it will also be tedious because for each x-value, one needs to calculate the corresponding Δ values. Instead, we propose to use the following approach to find a "first-cut value" of Δ. First, let us define the symbol "**S**" in the following equation, (Eq. D-6),

$$\mathbf{S} = \frac{(b-a)}{M'}\sum_{i=1}^{M'}(\frac{\Delta}{\pi})[\frac{1}{(x_i-x)^2+\Delta^2}] \qquad \text{(Eq. D-6)}$$

Empirically, we have found that **S** is generally greater than one when x is near or at x_i and less than one when otherwise, if Δ value is about 5 to 10% of the interval length. Thus, we use the following equation to find an approximate, "first-cut value" of Δ, namely,

$$\frac{(b-a)}{M'}\sum_{i=1}^{M'}(\frac{\Delta}{\pi})[\frac{1}{(x_i-x)^2+\Delta^2}] = 1 \qquad \text{(Eq. D-7)}$$

Note that both M' and Δ are finite. In principle one can solve the Δ value in (Eq. D-7) and Δ value found depends on the value of x. However, it is easier to use the following argument to find the answer. We note that when Δ is a small percentage of the interval length, (Eq. 10) in Section 1 becomes, when $x=x_i$, by keeping the dominant term,

$$f_A(x_i) = \frac{\sum_{i=1}^{M'}\frac{[f(x_i)]}{[(x_i-x)^2+\Delta^2]}}{\sum_{i=1}^{M'}\frac{1}{[(x_i-x)^2+\Delta^2]}} \approx \frac{\frac{f(x_i)}{\Delta^2}}{\frac{1}{\Delta^2}} = f(x_i)$$

This demonstrates that the interpolated value $f_A(x_i)$ reproduces the input function value $f(x_i)$ when Δ is small and this property is independent of dimensionality. In the same token, let $x=x_i$, one obtains, keeping the dominant term of **S** of (Eq. D-7) and ignoring contribution from any other sample points,

$$\frac{(b-a)}{M'\pi\Delta} \approx 1$$

By doing so, we find the first-cut value of Δ. For example, Giving (b-a)=20 and M'=10, the above equation gives $\Delta = 0.63$, and $\Delta = 0.31$ if M'=20. The Δ found can be used for the entire domain supported.

For two dimension case, the above formulas (Eqs. D-6, 7) are generalized to,

$$S = \frac{(b_1-a_1)(b_2-a_2)}{M'}\sum_{i=1}^{M'}(\frac{\Delta_1\Delta_2}{\pi^2})[\frac{1}{(x_{1i}-x_1)^2+\Delta_1^{\ 2}}][\frac{1}{(x_{2i}-x_2)^2+\Delta_2^{\ 2}}]$$

(Eq. D-8)

and,

$$\frac{(b_1-a_1)(b_2-a_2)}{M'}\sum_{i=1}^{M'}(\frac{\Delta_1\Delta_2}{\pi^2})[\frac{1}{(x_{1i}-x_1)^2+\Delta_1^{\ 2}}][\frac{1}{(x_{2i}-x_2)^2+\Delta_2^{\ 2}}] = 1$$

For a square region $a=a_1=a_2$, and $b=b_1=b_2$ (choosing $\Delta_1 = \Delta_2 = \Delta$), one obtains

$$\frac{(b-a)^2}{M'\pi^2\Delta^2} \approx 1 \qquad \text{(Eq. D-9)}$$

Again, choosing (b-a)=20 and M'=40, one gets $\Delta = 1.006$, and $\Delta = 1.83$ if M'=12. Again, these are "first-cut" values for Δ_1 and Δ_2. For n-dimension, use the following formula to calculate Δ (assuming all Δ s have the same value),

$$\frac{(b-a)^n}{M'\pi^n\Delta^n} \approx 1$$

If the supported domain is not a square (in 2-D) but a rectangle, then one needs to find the relationship between Δ_x (or defined as Δ_1) and Δ_y (or defined as Δ_2) first. By use of the equation found earlier,

$$\frac{l_x}{\Delta_x} = \frac{l_y}{\Delta_y}$$

the ratio is $\frac{l_x}{l_y} = \frac{\Delta_x}{\Delta_y}$ and (Eq. D-9) is written as,

$$\frac{l_x l_y}{M'\pi^2 \Delta_x \Delta_y} \approx 1$$

Thus,

$$\Delta_x = \frac{l_x}{\sqrt{M'\pi^2}}$$

$$\Delta_y = \frac{l_y}{\sqrt{M'\pi^2}}$$

The whole analysis can be easily extended to n-dimension.

Once the first-cut value of Δ is found, one can fine tune the value according to the application at hand. For example, if one wants the interpolant to reproduce more correctly at input locations for the global peak and global valley value of the input function, one generally needs to reduce the first-cut value and check if the newly interpolated value is closer to the global peak or global valley value. By doing so, we can check the sensitivity and self-consistency of the interpolant. This fine tuning is an iterative process and typically, one can stop the iteration when the reproduced value is about 95% of the peak and valley value. On the other hand, if one wants to generate more smoothly interpolated values (say for Response Surface applications), then one can increase the first-cut value to achieve the smoothness. The general rule of thumb is, "a larger width value will erode the peak and fill in the valley" and "a smaller width value will raise the peak and deepen the valley". In addition, a large width may over-smooth the interpolated function and a small width may produce "spikes" artifacts which are unwanted. For SIC 2004 exercise (http://www.fanginc.com/sic1.pdf), it involves the interpolation of "natural ambient radioactivity" in the atmosphere. Due to the stochastic nature (many peaks and valleys) of the radioactivity distribution, we reduced the first-cut value so that the interpolant can generate the interpolated values more sensibly in compliance with (global maximum) input peak and (global minimum) valley values. Furthermore, even though the supported domain has a rectangular shape for the exercise, we found $\Delta_x = \Delta_y$ works well to achieve better the fine-tuning. (See Example 2 below at the end of this Section) Finally, quite often, the first-cut value can be used for interpolation right away without any change. This statement is more correct in high-dimension (3D and above) than in low-dimension (1D, 2D) because in higher dimensional space, the input locations are more sparsely distributed and hard to find one another in close-by neighborhood.

In this section, we have established, for any dimension, a relationship between the first-cut delta width and the sample number M' with the use of (Eq. D-6) . It can be seen clearly that as M' goes to infinity, the first-cut delta width will approach zero (and vice versa), even though at a slower rate, and the product ($M'\Delta$) will approach infinity, except in one-dimension. This limit result of ($M'\Delta$) is compatible to the finding (That is, the optimized kernel width calculated through Mean-Squared-Error.) obtained by the standard nonparametric kernel regression analysis, except in one-dimension.

Before closing, let us present two examples to illustrate the steps to find delta width values. Both examples are for 2-D.

Example 1: There are 12 input locations together with the associated function values. They are listed in the following table. Both x_1 and x_2 are defined between -10 and +10.

Location Number	Input Location (X_1, X_2)	Input Function $f(x_1, x_2)$
1	(1.6, 9.0)	226.06
2	(5.6, -4.2)	79.54
3	(-1.0, -10.)	8.93
4	(-4.6, -4.0)	9.87
5	(3.6, -2.4)	60.36
6	(-7.4, 6.6)	119.93
7	(1.6, -8.2)	12.23
8	(-4.6, 2.4)	52.36
9	(-8.4, 9.8)	183.89
10	(9.4, 3.8)	302.61
11	(8.6, -5.8)	134.51
12	(-7.4, 7.2)	129.86

Solution: From (Eq. D-9), we obtain $\Delta_1 = \Delta_2 = 1.83$. We substitute the delta width value into (Eq. D-8) and compute **S** values. We can see that the calculated S-value is in line with the assumption in our analysis, namely, **S =1**. The reproduced function values at input locations are also given below. It can be seen that the first-cut delta width value gives fairly good reproduced function values at 12 input locations. If one wants to reproduce the function value at location #3 more close to the original input value, then one reduces the width to 1.40 to improve the results.

Location Number	S value found ($\Delta_1 = \Delta_2 = 1.83$) (average of S =1.41)	Reproduced function value ($\Delta_1 = \Delta_2 = 1.83$)	Reproduced function value ($\Delta_1 = \Delta_2 = 1.40$)	Input Function $f(x_1, x_2)$
1	1.09978634732106	216.063	221.18	226.06
2	1.46188852514591	80.88	80.047	79.54
3	1.20993373995982	11.733	10.153	8.93
4	1.18970951468216	19.048	14.885	9.87
5	1.35469744099448	65.12	62.931	60.36
6	2.16053954169866	128.622	127.123	119.93
7	1.28607451881441	19.435	15.924	12.23
8	1.19872814418426	58.945	54.846	52.36
9	1.48191667295652	165.82	172.105	183.89
10	1.06703321688486	289.698	296.599	302.61
11	1.24509553961353	126.336	130.604	134.51
12	2.21934025360859	131.241	129.369	129.86

Example 2: This example is copied from the problem used in SIC 2004 exercise. The supported domain has a rectangular shape with interval length 360,000 meters along x-axis and 700,000 meters along y-axis.

There are 200 input locations given together with function values. Also, there are 800 output locations where function values are to be interpolated. (The reader can download the input locations and output locations at: "http://www.ai-geostats.org/events/sic2004/index.htm" and click on "training data".).

Solution: We begin the analysis, by using the equation,

$$\Delta_x = \frac{l_x}{\sqrt{M'\pi^2}}$$ where l_x=360000, M'=200. Thus $\Delta_x = \Delta_1$ =8102. (in meters)

$$\Delta_y = \frac{l_y}{\sqrt{M'\pi^2}}$$ where l_y=700000, M'=200. Thus $\Delta_y = \Delta_2$ =15755. (in meters)

Substituting the delta width values into (Eq. D-8), we obtain the following average values of **S** for both 200 input and 800 output locations. Again, they are near the value of one. Following the same procedure as in the previous example by reducing delta width values to match the global maximum and minimum, we found that when Δ_x=4000 and Δ_y= 4000, the interpolant can reproduce the global maximum and minimum input function values within a few percent. For SIC 2004 exercise, we have chosen and preset $\Delta_x = \Delta_y$ = 4000 in the actual contest. All the measures of merit for the exercise have been calculated and they all indicate good results. (Please read the document at "http://www.fanginc.com/sic1.pdf")

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Δ_1	Δ_2	**S values found** (for all 200 input locations)	**S values found** (for all 800 output locations)
8102	15755	**average=1.86** **$1.11 \le S \le 3.44$**	**average=0.84** **$0.13 \le S \le 2.66$**
4000	4000	**average=8.57** **$7.9 \le S \le 12.6$**	**average=0.61** **$0.04 \le S \le 7.2$**

(3) More Discussion of ε value and statistical errors

Let us recall (Eq. 7A),

$$\int_{a_1}^{b_1} [f(x') - f(x)]\, \delta_\Delta(x' - x)dx' = \varepsilon \qquad \text{(Eq. 7A)}$$

Note that the above integral is with respect to *x*', and Δ and *x* values are fixed. ε is a function of Δ and *x*. We define C(Δ, *x*) in the following equation,

$$\int_{a_1}^{b_1} c(\Delta, x)\delta_\Delta(x' - x)dx' = c(\Delta, x)\int_{a_1}^{b_1} \delta_\Delta(x' - x)dx' = \varepsilon \qquad \text{(Eq. D-10)}$$

where $\int_{a_1}^{b_1} \delta_\Delta(x' - x)dx' = \frac{1}{\pi}[\tan^{-1}(\frac{b_1 - x}{\Delta}) - \tan^{-1}(\frac{a_1 - x}{\Delta})]$ from (Eq. D).

Now we rearrange (Eq. 7A) as,

$$\int_{a_1}^{b_1} [f(x') - f(x)]\ \delta_\Delta(x' - x)dx' - \varepsilon = \int_{a_1}^{b_1} [f(x') - f(x) - c(\Delta, x)\ ]\ \delta_\Delta(x' - x)dx' = 0 \qquad \text{(Eq. D-11)}$$

Recast the above integral by use of Monte-Carlo integration and we obtain,

$$\frac{(b_1 - a_1)}{M'} \sum_{i=1}^{M'} [f(x_i) - f(x) - c(\Delta, x)] \delta_\Delta(x_i - x) = 0 \pm F$$

$$[f(x) + c(\Delta, x)] \sum_{i=1}^{M'} \delta_\Delta(x_i - x) = -\frac{\pm M'F}{(b_1 - a_1)} + \sum_{i=1}^{M'} [f(x_i)] \delta_\Delta(x_i - x)$$

$$[f(x) + c(\Delta, x)] = \frac{\sum_{i=1}^{M'} [f(x_i)] \delta_\Delta(x_i - x) - \frac{\pm M'F}{(b_1 - a_1)}}{\sum_{i=1}^{M'} \delta_\Delta(x_i - x)}$$

$$f_A(x) = \frac{\sum_{i=1}^{M'} [f(x_i)] \delta_\Delta(x_i - x)}{\sum_{i=1}^{M'} \delta_\Delta(x_i - x)}$$

$$[f(x) + c(\Delta, x)] = f_A(x) \mp \frac{F}{\frac{(b_1 - a_1)}{M'} \sum_{i=1}^{M'} \delta_\Delta(x_i - x)} \qquad \text{(Eq. D-12)}$$

$$[f(x) - f_A(x)] = -c(\Delta, x) \mp \frac{F}{\frac{(b_1 - a_1)}{M'} \sum_{i=1}^{M'} \delta_\Delta(x_i - x)} \qquad \text{(Eq. D-13)}$$

From (Eq. D-10), we also obtain through Monte-Carlo integration,

$$c(\Delta, x) \frac{(b_1 - a_1)}{M'} \sum_{i=1}^{M'} \delta_\Delta(x_i - x) = \varepsilon \pm H \qquad \text{(Eq. D-14)}$$

Substituting this equation into (Eq. D-12), we get

$$[f(x)-f_A(x)]=\frac{-\varepsilon}{\frac{(b_1-a_1)}{M'}\sum_{i=1}^{M'}\delta_\Delta(x_i-x)}\mp\frac{F+H}{\frac{(b_1-a_1)}{M'}\sum_{i=1}^{M'}\delta_\Delta(x_i-x)} \qquad \text{(Eq. D-15)}$$

Comparing (Eq. D-15) and (Eq. 15A), one obtains that $F+H = E$. The reason for us to show the above derivation is to understand better the values of ε and the statistical error incurred. As commented in the last section, if one does not have the true function value and uses the f_A value to calculate the ε value, then it always gives the value zero for ε. It is not possible to find the correct sample estimate of ε. From (Eq. D-12), it can be seen that the interpolant $f_A(x)$ defined indeed is the "unbiased" estimator for the function which is a combination of,

$$[f(x)+c(\Delta,x)]$$

Therefore, one needs to keep in mind that to use $f_A(x)$ as the interpolant for $f(x)$ will be a good approximation as long as $C(\Delta, x)$ is small in magnitude as compared with $f(x)$. This condition is generally satisfied, as shown in the last section, when Δ is very small. Also, if Δ is finite and when x is not near, say 3Δ away from, the boundary of the domain, $C(\Delta, x)$ will remain small. Note again that $C(\Delta, x)$ is related analytically to ε through (Eq. D-10) and (Eq. D).

One explicit calculation of ε value is given below by use of the specified function $f(x)$.

Example: Find ε value when function $f(x) = x^2$ and the supported domain is (-10, 10).

Solution: Follow the definition of ε, (Eq. 7A).

$$\int_{a_1}^{b_1}[f(x')-f(x)]\,\delta_\Delta(x'-x)dx'=\varepsilon \qquad \text{(Eq. 7A)}$$

Choose x=2 as an example. We obtain,

$$\int_{-10}^{10}[x'^2-4]\,\delta_\Delta(x'-2)dx'=\int_{-10}^{10}[x'^2-4]\,\frac{\Delta}{\pi}[\frac{1}{(x'-2)^2+\Delta^2}]dx'=\varepsilon$$

Let x'-2= y, and we obtain

$$\int_{-12}^{8}[y^2+4y]\,\frac{\Delta}{\pi}[\frac{1}{y^2+\Delta^2}]dy=\varepsilon$$

$$\int_{-12}^{8} [y^2+4y]\frac{\Delta}{\pi}[\frac{1}{y^2+\Delta^2}]dy = \int_{-12}^{8}\frac{\Delta}{\pi}[\frac{y^2}{y^2+\Delta^2}]dy + \int_{-12}^{8}\frac{\Delta}{\pi}[\frac{4y}{y^2+\Delta^2}]dy$$

$$= \frac{\Delta}{\pi}\{[y]_{-12}^{8} - \Delta^2\int_{-12}^{8}\frac{dy}{y^2+\Delta^2}\} + \frac{2\Delta}{\pi}\int_{-12}^{8}\frac{dy^2}{y^2+\Delta^2}$$

$$= \frac{\Delta}{\pi}(20) - \frac{\Delta^2}{\pi}[\tan^{-1} z]_{\frac{-12}{\Delta}}^{\frac{8}{\Delta}} + \frac{2\Delta}{\pi}[\log w]_{144+\Delta^2}^{64+\Delta^2} =$$

$$= \frac{20\Delta}{\pi} - \frac{\Delta^2}{\pi}[\tan^{-1}(\frac{8}{\Delta}) - \tan^{-1}(\frac{-12}{\Delta})] + \frac{2\Delta}{\pi}[\log(64+\Delta^2) - \log(144+\Delta^2)] = \varepsilon$$

(Eq. D-17)

Using (Eq. D-17) and with 3 different Δ values, we obtain

Δ	ε
2	8.27
1	4.9
0.5	2.5

One more example, if x=9. Then

$$\int_{-19}^{1} [y^2+18y]\frac{\Delta}{\pi}[\frac{1}{y^2+\Delta^2}]dy = \varepsilon$$

$$\int_{-19}^{1} [y^2+18y]\frac{\Delta}{\pi}[\frac{1}{y^2+\Delta^2}]dy = \int_{-19}^{1}\frac{\Delta}{\pi}[\frac{y^2}{y^2+\Delta^2}]dy + \int_{-19}^{1}\frac{\Delta}{\pi}[\frac{18y}{y^2+\Delta^2}]dy$$

$$= \frac{\Delta}{\pi}\{[y]_{-19}^{1} - \Delta^2\int_{-19}^{1}\frac{dy}{y^2+\Delta^2}\} + \frac{2\Delta}{\pi}\int_{-19}^{1}\frac{dy^2}{y^2+\Delta^2}$$

$$= \frac{\Delta}{\pi}(20) - \frac{\Delta^2}{\pi}[\tan^{-1} z]_{\frac{-19}{\Delta}}^{\frac{1}{\Delta}} + \frac{9\Delta}{\pi}[\log w]_{361+\Delta^2}^{1+\Delta^2} =$$

$$= \frac{20\Delta}{\pi} - \frac{\Delta^2}{\pi}[\tan^{-1}(\frac{1}{\Delta}) - \tan^{-1}(\frac{-19}{\Delta})] + \frac{9\Delta}{\pi}[\log(1+\Delta^2) - \log(361+\Delta^2)] = \varepsilon$$

(Eq. D-18)

Again with 3 different Δ values, we obtain

Δ	ε
2	-14.28
1	-9.25
0.5	-5.45

Indeed, near the edge of the boundary, we can see that the magnitude (absolute value) of ε gets larger as expected. This, in fact, gives a theoretical proof to what is generally known as "edge effect" in nonparametric kernel regression.

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