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Note

Numerical Differentiation by Spline Functions Applied to a Lake Temperature Observation

Observed data often need to be numerically differentiated. A classical interpolation formula, however, does not always yield a consistent result. For instance, numerical differentiation by use of a parabola passing through three consecutive points yields different values of the derivatives at a fixed point according to the location of the point relative to the parabola. Snyder [6, 7] proposed a method for overcoming the ambiguity of the numerical differentiation. A better method than Snyder's is the use of spline functions.

The superiority of the use of cubic splines for numerical differentiation over other methods was "measured," as reported in [8], by comparing the rates of convergence as the increase of subdivision and by computing "goodness" and "smoothness" of numerical interpolation defined as extensions of the best interpolation property (Ahlberg *et al.* [1]) and the smooth interpolation property (Greville [3]), respectively, of cubic splines. If minor details could be omitted, the result may be described simply as follows: Values of the first derivatives, the second derivatives, and the function itself, computed by cubic spline interpolation, are slightly better than the corresponding values obtained by the classical quartic polynomial interpolation and worse than those obtained by the classical quintic polynomial interpolation.

As an application, the temperature distribution in Post Pond, located 18 km north of Hannover, New Hampshire, measured by Parrott and Fleming [5] was analyzed to detect how the actual heat transfer differed from the vertical heat conduction.

To analyze the data, daily averages θ were evaluated from observed hourly temperatures as functions of depth and time. The cubic splines fitted as functions of time were used to compute $\partial\theta/\partial t$ and those fitted as functions of depth were used to compute $\partial^2\theta/\partial x^2$. The residual

$$D = \frac{\partial\theta}{\partial t} - a\,\frac{\partial^2\theta}{\partial x^2} \tag{1}$$

where α is the coefficient of thermal diffusivity of water, was thus computed, squared, and integrated over the depth to define the integral residual R

$$R = \int D^2\,dx. \tag{2}$$

The integral residual is a measure of the deviation of the actual heat transfer mechanism from the ideal vertical heat condutcion.

The integral residuals R, computed from December 1, 1968 to April 17, 1969 are plotted in Fig. 1. The curve is drawn to pass through the middle of the scattered points, and is intended to show the tendency of the change of R.

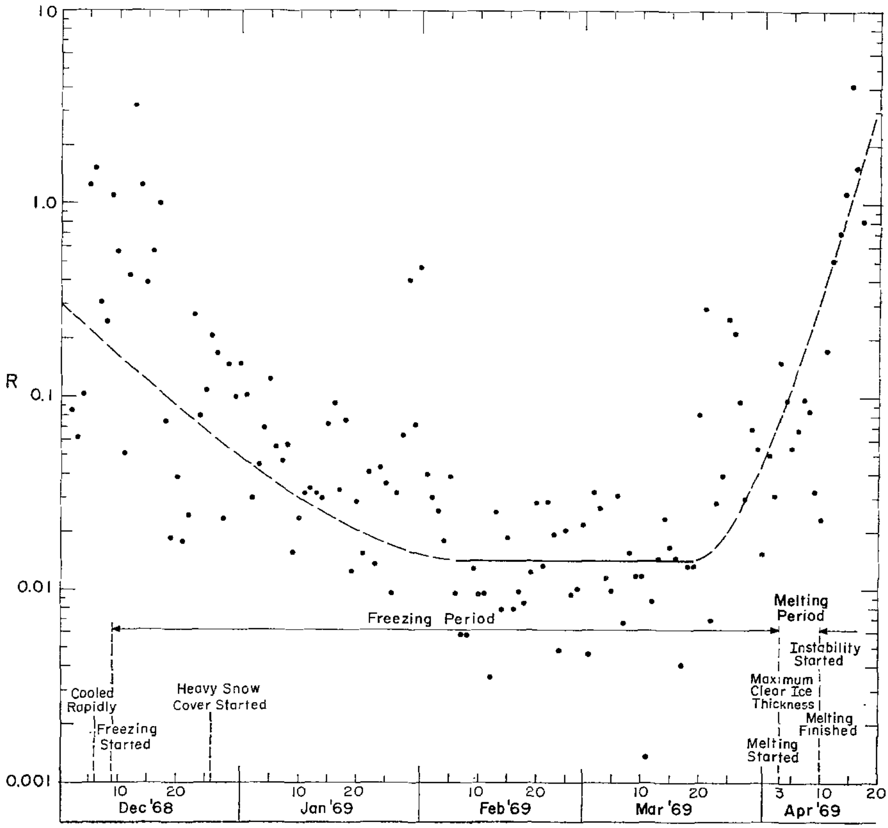

FIG. 1. Integral residuals of the temperatures between December 1, 1968 and April 17, 1969.

The curve reaches a minimum where it remains between February 6 and March 18. In this period, as shown later, we may assume that only vertical heat condution was the mechanism of heat transfer. The solid straight line in this period represents the means of the values of R. The curves extending to the left and to the right of the straight line were not calculated but were drawn from observation.

Four mechanisms of heat transfer other than the vertical heat conduction can be assumed: (1) radiation absorption, (2) convection, (3) current of water, and (4) horizontal heat flow. When the lake is covered with thick ice, radiation absorption in the water ceases. Horizontal heat flow may be disregarded for most of the period because, since the lake bottom at the observation site is uniform, we cannot find any cause for the horizontal heat flow, except the horizontal water flow which we believe occurred only immediately before and during the period of ice melt.

The following interpretations, therefore, may be made from Fig. 1: (1) Although radiation absorption and convection stopped after the freeze-up on December 9, their effects remained until February 6, when the flat portion in Fig. 1 began. (2) Melting of ice began on April 3, when the clear ice (frozen lake water, not the ice formed from snow) was thickest, and ended on April 10. According to Parrott and Fleming [5], the quick melting that took only seven days was a result of the inflow of snowmelt. Accepting their interpretation, we can say from Fig. 1 that the horizontal flow started on March 19, 15 days before the ice began to melt.

The factors contributing to the magnitude of R are: (1) deviation of the actual heat transfer mechanism from the vertical heat conduction, (2) observational errors, and (3) errors caused by spline function fitting. The third error is negligibly small as compared with the other two errors, as explained below.

To evaluate the errors in spline function fitting, two theoretical temperature distributions were assumed. One of these was the solution of a Neumann's problem (Carslaw and Jaegar [2]) defined as follows: water at 4°C extends in the region $0 \leqslant x < \infty$. At time $t = 0$, the temperature at $x = 0$ is changed to -2°C and maintained at this value throughout $0 \leqslant t < \infty$. The ice thickness in this problem reaches 40.13 cm on $t = 77$ days and 43.62 cm on $t = 91$ days. The numerical computation on $t = 84$ days showed a close approximation to the observation on April 3, 1969, when the ice thickness was 42 cm, the maximum in this observation.

It was found that the numerical values of $\partial\theta/\partial t$ agreed surprisingly well with the exact values (see Table I), but the numerical values of $\partial^2\theta/\partial x^2$ did not agree so well. The number of consecutive days used for the time differentiation was apparently too large, but no attempt was made to decrease the number of consecutive days. The integral residual thus obtained (see Table I) was negligibly small as compared with the residuals caused by observation errors (shown around the flat portion in Fig. 1).

The second theoretical temperature distribution was determined as follows: The temperature observation on March 26, 1969, was extended to the infinite region, $-\infty < x < \infty$, by defining the temperature in the region $-\infty < x \leqslant 0.5$ m by the tangent at $x = 0.5$ m and the temperature in the region 11.1 m $\leqslant x < \infty$ by the tangent at 11.1 m, where 0.5 m and 11.1 m are the depths of the top and bottom thermocouples used in this computation. The temperature distribution

TABLE I

Comparison of Numerical Computations and Exact Values in the Neumann Solution on $t = 84$ Day

Depths of thermocouples	°C	$\partial\theta/\partial t$ Numerical	$\partial\theta/\partial t$ Exact	$\partial^2\theta/\partial x^2$ Numerical	$\partial^2\theta/\partial x^2$ Exact	D (Eq. (1))
0.5	0.21981	-8.01745×10^{-3}	-8.01758×10^{-3}	$+0.624707$	-0.644417	-1.57898×10^{-2}
0.84	1.09163	-1.27087×10^{-3}	-1.27087×10^{-3}	-1.24941	-0.970833	3.46598×10^{-3}
1.47	2.39737	-1.49234×10^{-2}	-1.49235×10^{-2}	-1.17063	-1.19948	-3.58856×10^{-4}
2.06	3.20094	-1.27072×10^{-2}	-1.27072×10^{-2}	-1.05132	-1.02135	3.72864×10^{-4}
2.67	3.66432	-8.25931×10^{-3}	-8.25931×10^{-3}	-0.656064	-0.663846	-9.6822×10^{-5}
3.24	3.87033	-4.47719×10^{-3}	-4.7721×10^{-3}	-0.35029	-0.359858	-1.19019×10^{-4}
3.86	3.96068	-1.86092×10^{-3}	-1.86093×10^{-3}	-0.139583	-0.149574	-1.2428×10^{-4}
4.47	3.98969	-6.39109×10^{-4}	-6.39089×10^{-4}	-0.046652	-5.13671×10^{-2}	-5.86829×10^{-5}
5.07	3.99765	-1.84335×10^{-4}	-1.84332×10^{-4}	-1.28488×10^{-2}	-1.48158×10^{-2}	-2.44751×10^{-5}
5.68	3.99956	-4.30443×10^{-5}	-4.30221×10^{-5}	-2.85461×10^{-3}	-3.45792×10^{-3}	-7.52836×10^{-6}
6.27	3.99993	-8.79604×10^{-6}	-8.79311×10^{-6}	-5.70244×10^{-4}	-7.06751×10^{-4}	-1.7013×10^{-6}
6.88	3.99999	-1.40818×10^{-6}	-1.41618×10^{-6}	-7.97703×10^{-5}	-1.13826×10^{-4}	-4.15707×10^{-7}
7.48	4.	-2.13844×10^{-6}	-1.96032×10^{-7}	-1.26129×10^{-5}	-1.57561×10^{-5}	-5.69201×10^{-8}
8.08	4.	-9.09674×10^{-9}	-2.2695×10^{-8}	-9.08451×10^{-7}	-1.82412×10^{-6}	2.20584×10^{-9}
8.71	4.	2.65987×10^{-11}	-1.9482×10^{-9}	-1.18782×10^{-7}	-1.56587×10^{-7}	1.50444×10^{-9}
9.3	4.	0	-1.63751×10^{-10}	1.80622×10^{-8}	-1.31616×10^{-8}	-2.24723×10^{-10}
11.1	4.	0	-2.99384×10^{-14}	-9.30311×10^{-9}	-2.40631×10^{-12}	1.12361×10^{-10}

$R = 2.98081 \times 10^{-5}$

thus defined is fitted by a spline function and called $\psi(x)$. Using $\psi(x)$ as the initial condition, the rigorous solution for the infinite region

$$\theta(x, t) = \frac{1}{2\sqrt{\pi a t}} \int_{-\infty}^{\infty} \exp\left(-\frac{(x-\xi)^2}{4at}\right) \psi(\xi)\, d\xi \tag{3}$$

was computed. The integral residual for this case was $R = 1.65916 \times 10^{-4}$, which is negligibly small as compared with the residuals in Fig. 1 caused by observational errors.

The effect of observational error on R was estimated by substituting error obeying a normal distribution

$$\frac{1}{\sqrt{2\pi}\sigma} e^{-\epsilon^2/(2\sigma^2)} \tag{4}$$

in place of θ in (1). This substitution yields practically the same value as the substitution of ϵ plus a spline function interpolation fitted to a rigorous solution into θ of (1), because, as stated above, R obtained from a rigorous solution can be neglected.

Given a random number x_i of a uniform distribution ϵ of the distribution (4) can be computed by Hamming's [4] formula

$$\epsilon = \sigma\left(\sum_{i=1}^{12} x_i - 6.0\right). \tag{5}$$

The integral residual R computed from ϵ by assuming $\sigma = 0.03°C$ yielded the distribution of almost the same mean and scattering as those obtained from the

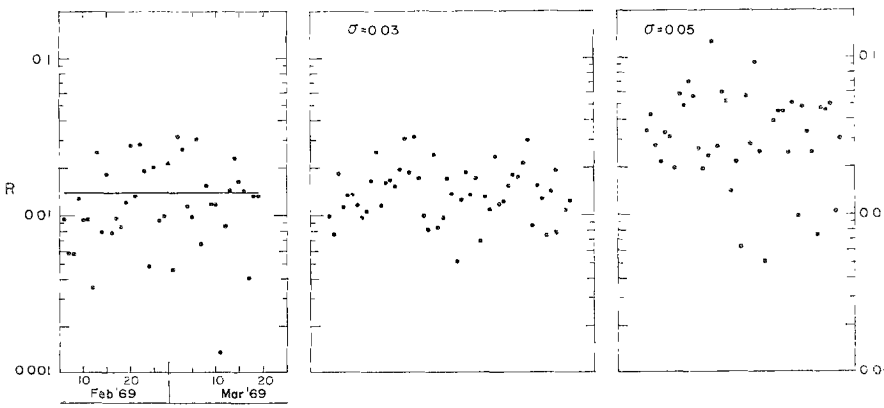

FIG. 2. Comparison of the scattering of R on various assumptions.

temperatures observed between February 6 and March 18, 1969, as shown in Fig. 2. For comparison, the value of R obtained by assuming $\sigma = 0.05°C$ is shown in Fig. 2. The number of computations of R is almost the same in all three cases.

To test the hypothesis that the empirical R is a stochastic distribution sampled from the population of theoretical R computed by assuming $\sigma = 0.03$, the number of theoretical computations was increased almost 10 times. The cumulative curve thus obtained, which is shown in Fig. 3 as the thick line, was regarded as the

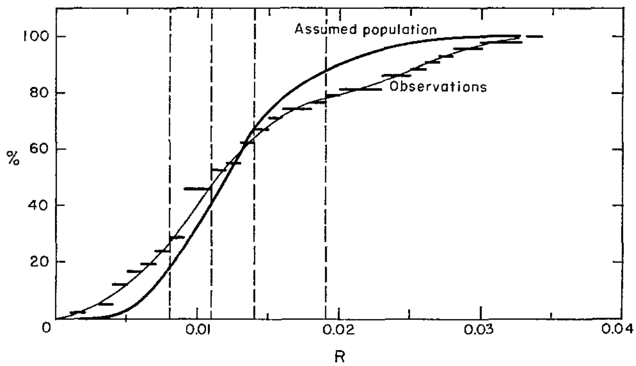

FIG. 3. Test of R (horizontal lines on the observation curve show the grouping).

population. The thin line in Fig. 3 shows the cumulative curve of the empirical R. The χ^2-test was performed, and it was concluded that the hypothesis cannot be rejected at the level of probability 0.05. (The χ^2-test was performed with five divisions as shown by the vertical lines in Fig. 3. The χ^2 thus obtained was 9.486, where the theoretical χ^2 with freedom 4 and at level 0.05 is 9.488.) Therefore, we may conclude that daily averages determined from the observations of Parrott and Fleming [5] obey the error distribution of $\sigma = 0.03°C$.

REFERENCES

1. J. H. AHLBERG, E. N. NILSON, AND J. L. WALSH, "The Theory of Splines and Their Applications," Academic Press, New York, 1967.
2. H. S. CARSLAW AND J. C. JAEGER, "Conduction of Heat in Solids," Oxford University Press, New York, 1959.
3. T. N. E. GREVILLE (Ed.), "Theory and Applications of Spline Functions," Academic Press, New York, 1969.
4. R. W. HAMMING, "Numerical Methods for Scientists and Engineers," pp. 34 and 389, McGraw-Hill, New York, 1962.

5. W. H. PARROTT AND W. M. FLEMING, "The Temperature Structure of a Mid-Latitude, Dimictic Lake During Freezing, Ice Cover, and Thawing," U. S. Army Cold Regions Research and Engineering Laboratory (USA CRREL) Research Report 291, Hanover, N.H., 1970.
6. W. R. SNYDER, Continuous parabolic interpolation, *J. Hydraulic Division*, Proc. ASCE, No. HY4, **87** (1961), 99–111.
7. W. R. SNYDER, Extended continuous interpolation, *J. Hydraulic Division*, Proc. ASCE, No. HY5, **93** (1967), 261–280.
8. S. TAKAGI, "Numerical Differentiation by Spline Functions and its Application to Analyzing a Lake Temperature Observation," USA CRREL Research Report, Hanover, N.H. (to be published); "Transactions of the Sixteenth Conference of Army Mathematicians," U.S. Army Research Office Durham, Box CM, Duke Station, Durham, North Carolina (to be published).

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