

## Some Plane Curvature Approximations\*

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**Abstract.** Second-order accurate approximations to the curvature function along a sufficiently smooth plane curve are presented, the curve being given in finite form (and thus, approximately) by  $N + 2$  points taken along its full length. The curvature estimates are continuous and invariant under translation and rotation, and they are based on local information—so are easy to implement computationally. In particular, second-order accurate estimates of surface tension forces halfway between immediate neighbors in the curve's mesh can thereby be made for hydrodynamic simulations.

The construction makes use of any of the common techniques one might contemplate for using the information present in three adjacent points (of the  $N + 2$  points) in order to estimate the curve's curvature near those three points. It may do this because each of these techniques yields a number which is, to within second order in the distances between the three points, the value of the true curvature function at the same place, namely, at the arithmetic mean of the location of the three points as measured along the curve. The asymptotic form, displaying all terms through the second order, of error estimates for these techniques is provided, along with comparison of gross properties and numerical examples. Finally, continuous, locally second-order accurate, global approximation to the curvature function is obtained by interpolation of successive local estimates between the locations of successive means.

A related result is given for the simpler but analogous situation concerning the  $n$ th-order difference quotient of a function of one variable. The broken line interpolant of successive  $n$ th difference quotients, between the successive mean values of their stencil points, provides a continuous, locally second-order accurate, global approximation to the  $n$ th derivative. It also coincides, between two successive stencil means, with the  $n$ th derivative of the polynomial interpolant of the  $n + 2$  data points associated with the two successive stencils.

**1. Introduction and summary.** Parametric interpolation provides a basis for one approach to curvature approximation; a comprehensive survey of the literature concerning such interpolation is contained in Ferguson's thesis [2], for example. But the form and implementation of such approximations is often nonlocal and thus rather complex computationally; moreover, analysis of the accuracy of the resulting curvature estimates is rarely detailed.

Less familiar is the use of intrinsic curvature estimation as explored by people involved in computer-aided design. We are indebted to J. C. Ferguson for such references as Nutbourne, McLellan, and Kensit [5], Pal [6], Schechter [7], and

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McLeod and Todd [4], among others. A relatively early work considering  $C^2$  piecewise Cornu spirals is Burns [1].

Our approach here is the appropriate local interpolation of sufficiently accurate local estimates of the curvature. We are motivated by approximation of the second derivative of a scalar function  $y(t)$ . First, a locally determined estimate is the function's second difference quotient. Next, this number is known to be a second-order accurate approximation to the value that  $y''$  assumes at the mean value of the three points in the stencil of the difference quotient (see, e.g., Kreiss, Manteuffel, Swartz, Wendroff, and White [3]). Finally, second-order accurate global approximation to  $y''$  can be associated with the broken line interpolant of the second difference quotient between successive stencil means. Proofs invoke both the accuracy and stability of local linear interpolation.

So, given three neighboring points  $X_-$ ,  $X_0$  and  $X_+$  (in that order) on a sufficiently smooth curve, we begin with four estimates of the size of the curvature nearby. The first is the number  $|\kappa_c|$ , the reciprocal of the radius of the (unique) circle passing through the points; cf. (2.2) below. The second number is  $|\kappa_d|$ , the length of a second difference quotient of the radius vectors (i.e., of the vector of the difference quotient of the coordinates); this difference quotient is taken with respect to distance along the broken line joining the three points; cf. (2.3)–(2.4). A third number, equipped with a sign as well, is  $\kappa_\times$ , the ratio of the sine of the angle between the two successive secant vectors to their average length; cf. (2.10). A fourth number—really, collection of numbers—consists of difference approximations to the classic expression for the curvature in terms of the derivatives of the curve's coordinates—approximations in which the increments in the independent variable are replaced with the Euclidean distances  $\Delta t_\pm$  between successive pairs of points; cf. (2.15).

We summarize our

RESULTS. (1)  $|\kappa_c|$ ,  $|\kappa_d|$ , and  $\kappa_\times$  are invariant under rigid motions of the plane, as are any of the difference approximations to the classic expression for the curvature, as long as the same difference operators are applied to each coordinate (for the last, cf. (2.15) below).

(2)  $|\kappa_d|$  and  $|\kappa_c|$  are equal to within second order; cf. (2.2).

(3)  $|\kappa_d|$  is also to within second order of the magnitude of the second difference quotient, with respect to *arclength*, on any sufficiently smooth (say,  $C^4$ ) curve which passes through the three points. This is so because, although the (vector) difference between the two difference quotients has length *first* order in size in general, it is sufficiently orthogonal to either of the difference quotients themselves; cf. (2.7).

(4) Consequently,  $|\kappa_d|$  and  $|\kappa_c|$  are, to within second order, the magnitude of the curve's curvature at the arithmetic mean of the locations of the three points  $X_-$ ,  $X_0$ , and  $X_+$  as measured along the curve; cf. (2.8).

(5)  $\kappa_\times$  is, to within second order, the (signed) curvature at the same location. It is suitable for providing a sign for  $|\kappa_d|$  and for  $|\kappa_c|$  as necessary; cf. (2.12).

(6) The second-order differentiations in the classic expression for the curvature in terms of its coordinates are most easily and consistently approximated by  $\Delta^2/\Delta t^2$ . But the numerator's first derivatives may be approximated by a one-parameter average (say,  $\lambda$ ) of the forward and backward difference quotients, and the denominator's by another (say,  $\mu$ ). The value of the numerator is then, in fact,  $\kappa_\times$ ,

independent of  $\lambda$ . And, the resulting number  $\kappa_{\lambda\mu}$  is also (to within second order) the (signed) curvature at the same average of  $X_-$ ,  $X_0$ , and  $X_+$  (if  $\mu$  is presumed appropriately bounded). The geometry of smooth curves asymptotically avoids the situation which can make the denominator zero; cf. (2.13)–(2.15).

(7) The gross properties of  $|\kappa_c|$ ,  $|\kappa_d|$ , and  $|\kappa_x|$  are compared; cf. (3.3). The asymptotic form of localized error estimates is provided through second-order terms; cf. (3.5). Their efficacy is explored in two numerical examples; the second example summarizes comparison of some twenty-seven hundred specific instances using a notion we call “the accuracy of the predicted error”; cf. Section 3.

(8) Using these results, one now may associate with a sequence of  $N + 2$  points along a plane curve another sequence of  $N$  points at which second-order accurate curvatures are known; these values are interpolated—in two ways—to obtain continuous, second-order accurate global approximations to the curve’s curvature function. We reject a third locally defined approximating function related to  $\kappa_x$  because we do not know how to join successive pieces continuously. The definition of these functions and proof of their local second-order accuracy must (and does) get around the fact that, unlike the approximation of a scalar function  $y(t)$ , one does not have in hand a smooth parametrization of one of the curve’s coordinates; cf. Section 4. *Second-order* accurate interpolation of the magnitude of a smooth function is not easy over an interval containing a zero of first order; this is where the utilization of the sign of  $\kappa_x$  becomes important.

(9) The continuous, second-order accurate global approximations to the curvature provide, in particular, second-order accurate curvatures half-way between pairs of mesh points on the curve. As used in hydrodynamic simulations, this allows second-order accurate estimation, at those locations, of the force due to surface tension—and thus of pressure jumps; cf. the paper’s penultimate paragraph.

**2. Three-Point Curvature Approximations.** Suppose we are given three noncollinear points in the plane, defined by the vectors  $X_-$ ,  $X_0$ , and  $X_+$ . We shall obtain and discuss certain approximations of the curvature of smooth (say,  $C^4$ ) curves  $X(w)$  passing through these points in the order presented.

We recall first the radius  $r$  of the circle interpolating the three points. For this, consider the two secant vectors

$$(2.1a) \quad \Delta_+X := X_+ - X_0, \quad \Delta_-X := X_0 - X_-,$$

with their associated unit vectors

$$(2.1b) \quad U_{\pm} := \Delta_{\pm}X / \Delta_{\pm}t, \quad \text{where } \Delta_{\pm}t := |\Delta_{\pm}X|,$$

and  $|V|$  is the Euclidean length of a vector  $V$ . The center  $Y$  of the interpolating circle lies on each of the perpendicular bisectors of the secant segments emanating from  $X_0$ . Hence the component of  $Z := Y - X_0$  along each secant segment is

$$Z \cdot U_{\pm} = \pm \Delta_{\pm}t / 2,$$

by our choice of direction for the  $U_{\pm}$ . It is the length  $r$  of  $Z$  we seek. From  $U_{\pm}$  we form the orthonormal pair

$$\tilde{U}_{\pm} := (U_{\pm} \pm U_{\mp}) / |U_{\pm} \pm U_{\mp}|,$$

concluding, from the components of  $Z$  along  $\tilde{U}_{\pm}$ , that

$$(2.2a) \quad 4r^2 = (\Delta_+t + \Delta_-t)^2 / |U_+ - U_-|^2 + (\Delta_+t - \Delta_-t)^2 / |U_+ + U_-|^2.$$

This provides our first estimate of the curvature, namely the number

$$(2.2b) \quad |\kappa_c| := 1/r \quad (c \text{ for circle}).$$

However, for three *neighboring* vectors  $X_-, X_0,$  and  $X_+$ , sampled successively along a smooth curve  $X(w)$ , the two unit vectors  $U_{\pm}$  are nearly parallel and in the same direction, so the final term in (2.2a) then contributes only  $O(\max \Delta_{\pm} t^2)$  to the curvature approximation (2.2b). This prompts, in these circumstances, the alternative curvature estimate

$$(2.3) \quad |\kappa_d| := |U_+ - U_-| / [(\Delta_+ t + \Delta_- t) / 2],$$

an approximation which may also be derived using the following, more analytic, considerations.

With  $U(s) := \dot{X}(s)$  ( $:= dX/ds$ ) the unit tangent, as a function of arclength  $s$  on a smooth curve  $X(s)$ , the curvature  $\kappa(s)$  is given by

$$|\kappa| := |\dot{U}| = |\ddot{X}|,$$

with  $\kappa$  taking the sign of the  $90^\circ$  angle from  $U$  to  $\dot{U}$ . But, using (2.1), we see (2.3) is the magnitude of the second difference quotient of  $X$ , i.e., of

$$(2.4) \quad \Delta^2 X / \Delta t^2 := (\Delta_+ X / \Delta_+ t - \Delta_- X / \Delta_- t) / [(\Delta_+ t + \Delta_- t) / 2],$$

taken with respect to the Euclidean distance  $t$  along the secant lines between the data points. So, in (2.3),  $d$  is for difference.

The more relevant (vector) difference quotient is the second arclength difference quotient,

$$\Delta^2 X / \Delta s^2,$$

given by replacing  $\Delta_{\pm} t$  in (2.4) with the magnitudes  $\Delta_{\pm} s$  of the (unknown) arclength increments along the curve. Near (2.9) below we show that (for smooth curves, with no nearby double points, passing through  $X_-, X_0,$  and  $X_+$  in that order)

$$(2.5) \quad 1 / \Delta_{\pm} s = [1 - \kappa_0^2 \Delta_{\pm} t^2 / 24 + O(\Delta_{\pm} t^3)] / \Delta_{\pm} t,$$

where  $\kappa_0$  is the curvature at  $X_0$ . It follows that, for such curves,

$$(2.6) \quad \Delta^2 X / \Delta s^2 = \Delta^2 X / \Delta t^2 - \kappa_0^2 (\Delta_+ t - \Delta_- t) \dot{X}_0 / 12 + O(\max \Delta_{\pm} t^2).$$

That is to say, these two vectors are separated by a first-order quantity in general. Now we *could* use (2.6) to compute  $\Delta^2 X / \Delta s^2$  to within second order—say, by invoking  $|\kappa_d|$  from (2.3) and any first-order estimate of  $\dot{X}_0$ . But it is not necessary to do so for our purposes. For, since  $\Delta^2 X / \Delta s^2$ , and hence  $\Delta^2 X / \Delta t^2$ , in (2.6) are each first-order approximations to  $\ddot{X}$  at  $X_0$ , and since  $\ddot{X} = \dot{U}$  is orthogonal to  $U = \dot{X}$ , we are allowed the conclusion that  $\dot{X}_0 \cdot \Delta^2 X / \Delta t^2 = O(\max \Delta_{\pm} t)$ . Hence, taking the scalar product of each side of (2.6) with itself, we find that the *lengths* of the two second difference quotients are the same within second order:

$$(2.7) \quad |\Delta^2 X / \Delta s^2| = |\kappa_d| + O(\max \Delta_{\pm} t^2).$$

It is known that the second difference quotient of a smooth function—like either component of  $X(s)$ —is a *second-order* accurate approximation to the function's second derivative when the latter is evaluated at the average of the three arguments

involved in the difference quotient (see, e.g., Kreiss, Manteuffel, Swartz, Wendroff and White [3, p. 538]). Hence, if arclength  $s$  runs from  $X_-$  through  $X_0$  and then  $X_+$ , and if  $s = 0$  at  $X_0$ , it follows from (2.3), (2.4), (2.5), and (2.7) that

$$(2.8) \quad |\kappa_d| = |\kappa(\bar{t})| + O(\max \Delta_{\pm} t^2), \quad \text{with } \bar{t} := (\Delta_+ t - \Delta_- t)/3$$

(if  $X$  is, say, a  $C^4$  curve); the same relation holds for  $|\kappa_c|$ , by (2.2) and (2.3).

Next, as promised, we prove (2.5), an estimate independent of translation and rotation of the plane. So we may assume we are given a sufficiently smooth plane curve  $X(s) := (x(s), y(s))$  parametrized by its arclength  $s$ , passing through the origin at  $s = 0$ , its unit tangent there being along the positive  $x$ -axis. Differentiating thrice and twice, respectively, the identities

$$\dot{x}^2 + \dot{y}^2 \equiv 1, \quad \ddot{x}^2 + \ddot{y}^2 \equiv \kappa^2,$$

we establish (with the convention that  $g_0 := g(0)$  for any function  $g(s)$ ) that

$$(2.9) \quad \begin{aligned} x_0 = 0, \quad \dot{x}_0 = 1, \quad \ddot{x}_0 = 0, \quad \ddot{x}_0 = -\kappa_0^2, \quad \ddot{\ddot{x}}_0 = -3\kappa_0 \dot{\kappa}_0; \\ y_0 = 0, \quad \dot{y}_0 = 0, \quad \ddot{y}_0 = \kappa_0, \quad \ddot{\ddot{y}}_0 = \dot{\kappa}_0. \end{aligned}$$

Computing the Maclaurin expansion of  $t^2(s) := (x^2 + y^2)(s)$  through 5th-degree terms, and choosing  $\dot{t}_0 = +1$  (so that  $t$  increases with  $s$ ), we conclude that

$$t(s) = [1 - \kappa_0^2 s^2/24 - \kappa_0 \dot{\kappa}_0 s^3/24 + O(s^4)]s,$$

so the  $O(s^3)$  factor is present unless  $\kappa^2$  is stationary at  $s = 0$ . But the existence of merely four derivatives of  $X$  now implies (2.5).

Finally, we must define the *sign* of our approximate curvatures, as it too is important. We intend eventually to interpolate (Section 4), and there is not enough information in the magnitudes of two successive values of a smooth function for them to be interpolated with *second-order* accuracy—at least, over an interval in which the function itself has a zero of first order. Towards this end, given two vectors  $V = (v_1, v_2)$  and  $W = (w_1, w_2)$ , we first define the number

$$(2.10a) \quad V \times W := v_1 w_2 - v_2 w_1$$

(the only nontrivial component of the vector product of the two vectors appropriately embedded in a right-handed coordinate system). Then, using the notation (2.1), we set

$$(2.10b) \quad \kappa_{\times} := (\Delta_- X/\Delta_- t \times \Delta_+ X/\Delta_+ t)/\bar{\Delta}t \quad (= (U_- \times U_+)/\bar{\Delta}t),$$

where  $\bar{\Delta}t := (\Delta_- t + \Delta_+ t)/2$ . From (2.1) and the properties of the vector product, we see that

$$(2.11a) \quad \kappa_{\times} = \Delta_{\lambda} X/\Delta t \times \Delta^2 X/\Delta t^2 \quad (= \Delta_{\lambda} X/\Delta t \times (U_+ - U_-)/\bar{\Delta}t),$$

in which  $\Delta_{\lambda} X/\Delta t$  is *any* average of  $\Delta_+ X/\Delta_+ t$  and  $\Delta_- X/\Delta_- t$ , i.e., of  $U_+$  and  $U_-$ :

$$(2.11b) \quad \Delta_{\lambda} X/\Delta t := (U_+ + U_-)/2 + \lambda(U_+ - U_-).$$

So,  $\kappa_{\times}$  is the only obvious approximation around for  $\dot{X} \times \ddot{X} (= U \times \dot{U} = \kappa)$ , whose sign we seek. And, indeed, we now complete our definitions of  $\kappa_c$  and  $\kappa_d$  with

$$(2.12a) \quad \kappa_c := \text{sgn}(\kappa_{\times})|\kappa_c| \quad \text{and} \quad \kappa_d := \text{sgn}(\kappa_{\times})|\kappa_d|$$

(cf. (2.2) and (2.3), respectively). But it follows from (2.10), (2.9) and (2.5) that

$$(2.12b) \quad \kappa_{\times} = \kappa(\bar{t}) + O(\max \Delta_{\pm} t^2) \quad (\bar{t} \text{ as in (2.8)}).$$

Hence we conclude from (2.8) that, with (2.12a),

$$(2.12c) \quad \kappa_c = \kappa(\bar{t}) + O(\max \Delta_{\pm} t^2) \quad \text{and} \quad \kappa_d = \kappa(\bar{t}) + O(\max \Delta_{\pm} t^2).$$

And we now have in hand *three* second-order accurate estimates of  $\kappa(\bar{t})$  itself, not just two of its magnitude.

The general parametric form for the curvature, in terms of the curve's coordinates, is

$$(2.13) \quad \kappa = (x'y'' - y'x'') / [(x')^2 + (y')^2]^{3/2} \quad (' = d/dw, w \text{ the parameter}).$$

We shall now see that, because of (2.11),  $\kappa_{\times}$  is related to a host of difference approximations to this expression—at least to those in which the parameter differences are taken to be  $\Delta_{\pm} t$ . It is quite reasonable to do this, for two reasons. First, the data  $X_{-}$ ,  $X_0$ , and  $X_{+}$  contains no information whatsoever about the parameter  $w$ . Second, if one uses typical difference approximations in (2.13) and replaces  $\Delta_{\pm} w$  in them with  $c\Delta_{\pm} t$  ( $c > 0$ ), then the result is independent of  $c$ . For there will be no effect on the ratio—at least as long as the resulting difference approximations to the first derivatives there are homogeneous of order  $-1$  in  $c$ , and those to the second derivatives, of order  $-2$ .

More specifically, for the numerator of (2.13): (a) If one approximates  $d^2u/dw^2$  by its simplest available consistent linear difference approximation, namely,  $\Delta^2 u / \Delta t^2$ ; (b) if one also approximates  $du/dw$  by any average of  $u$ 's forward and backward difference quotients, i.e., by

$$(2.14) \quad D_{\lambda} u := (\Delta_{+} u / \Delta_{+} t + \Delta_{-} u / \Delta_{-} t) / 2 + \lambda (\Delta_{+} u / \Delta_{+} t - \Delta_{-} u / \Delta_{-} t),$$

then the numerator is the number  $\kappa_{\times}$  (independent of  $\lambda$ —use (2.11)) and is, in particular, invariant under translation and rotation. Moreover, if one approximates the two differentiations in denominator of (2.13) by  $D_{\mu}$  ( $\mu$  not necessarily equal to  $\lambda$ , but the same  $\mu$  for each derivative there), then (1) the denominator is similarly invariant; and (2) if one presumes also that  $\mu$  is uniformly bounded, the denominator is  $1 + O(\max \Delta_{\pm} t^2)$ . (For the second: The two terms in the expression  $(U_{+} + U_{-})/2 + \mu(U_{+} - U_{-})$  are orthogonal. Now use (2.5) to conclude that the first term is, to within  $O(\max \Delta_{\pm} t^2)$ , the unit tangent at  $(\Delta_{+} t - \Delta_{-} t)/4$ , and use the boundedness of both  $\mu$  and  $\Delta^2 X / \Delta t^2$  to show the second term contributes  $O(\max \Delta_{\pm} t^2)$ .)

The resulting difference approximation to (2.13), then, is given in terms of (2.11b) as

$$(2.15) \quad \kappa_{\lambda\mu} := \Delta_{\lambda} X / \Delta t \times \Delta^2 X / \Delta t^2 / |\Delta_{\mu} X / \Delta t|^3 \quad \left( = \kappa_{\times} / |\Delta_{\mu} X / \Delta t|^3 \right),$$

its value is independent of  $\lambda$ , and it is a second-order approximation to  $\kappa(\bar{t})$  if  $\mu$  is bounded. We note that the denominator in (2.15) is zero if and only if  $\mu = 0$  and  $U_{+} = -U_{-}$ , i.e., the two successive secant segments are in opposite directions. (For, the line (2.11b) through two points on the unit circle contains the origin if and only if the two points are opposite each other. The limiting value of (2.15) can be infinite in this case although the numerator, too, goes to zero; cf. the discussion below (3.3b).)

For example, an unsophisticated approximation (i.e., not centered at  $\bar{i}$  (2.8)) to the numerator of (2.13) utilizes first-order centered differences and is given by the expression

$$(2.16a) \quad D_{\text{cen}x} \Delta^2 y / \Delta t^2 - D_{\text{cen}y} \Delta^2 x / \Delta t^2 \quad \text{with } D_{\text{cen}u} := (u_+ - u_-) / (2\bar{\Delta}t);$$

but the value of this expression is precisely  $\kappa_{\times}$ : Take

$$(2.16b) \quad 2\lambda = 2\lambda_{\text{cen}} := (\Delta_- t - \Delta_+ t) / (\Delta_+ t + \Delta_- t)$$

in (2.14) and in (2.11b). An even less sophisticated approximation utilizes the forward difference quotient  $D_+ u := \Delta_+ u / \Delta_+ t$ , but this also has the form (2.14) (take  $\lambda = +\frac{1}{2}$ ). Equally elementary approximations to use in the denominator of (2.13) are the number 1 (presuming the parameter to be arclength or, alternatively, that  $\mu = \pm\frac{1}{2}$ ), or the expression

$$(2.16c) \quad (D_{\text{cen}x})^2 + (D_{\text{cen}y})^2 \quad \left( = \left| (X_+ - X_-) / (2\bar{\Delta}t) \right|^2 \right) = 1 + O(\max \Delta_{\pm} t^2).$$

We believe that we have considered in this section all of the common techniques one might contemplate for using the information present in three successive points on a curve in order to estimate its curvature near those points. And it has turned out that the location of the point where a given estimate is correct is, to within second order, independent of the technique; more specifically, it is the arithmetic mean of the location of the three points as measured along the curve.

**3. Examples, Practical Remarks, Error Estimates.**

*Example 1.*  $\kappa = 1/R = \text{constant}$ : a circle with its center at the origin. We assume that  $X_-$ ,  $X_0$ , and  $X_+$  are at  $(R, -\theta_-)$ ,  $(R, 0)$ , and  $(R, \theta_+)$  in the associated polar coordinates, respectively. There is no loss of generality—except for the sign of  $\kappa_{\times}$ —in also presuming that  $\theta_{\pm} > 0$  while  $0 < \theta_+ + \theta_- < 2\pi$ . The circle yields quite special results, and not just that  $|\kappa_c| = 1/R$  is exact, (2.2). For this circular example, the quantities (2.1b) are

$$(3.1) \quad \Delta_{\pm} t = 2R \sin(\theta_{\pm}/2) \quad \text{and} \quad U_{\pm} = (\mp \sin(\theta_{\pm}/2), \cos(\theta_{\pm}/2)).$$

With this, we find from (2.3) that

$$(3.2a) \quad |\kappa_d| / |\kappa_c| = 1 / \cos[(\theta_+ - \theta_-) / 4] = 1 + (\theta_+ - \theta_-)^2 / 32 + O[(\theta_+ - \theta_-)^4].$$

Surprisingly, this is independent of  $\theta_+ + \theta_-$ . It also increases monotonically with  $|\theta_+ - \theta_-|$ ; we compute (on our TI SR-50)

Error in $ \kappa_d $	.01%	.1%	1%	10%	100%
$ \theta_+ - \theta_- $	3.24°	10.2°	32.3°	98.5°	240°

which exhibits the second-order accuracy.  $|\kappa_d| / |\kappa_c|$ , (3.2a), can indeed be unbounded: Let  $\theta_+ \rightarrow 2\pi$ . But, the additional restrictions  $\theta_{\pm} < \pi$  (or even more:  $U_+ \cdot U_- \geq 0$ , i.e.,  $\theta_+ + \theta_- \leq \pi$ ) bound  $|\kappa_d| / |\kappa_c|$ , (3.2a), by  $\sqrt{2}$ .

We now consider  $\kappa_{\times}$ , (2.10). From (3.1) we determine that

$$(3.2b) \quad \begin{aligned} \kappa_{\times} / |\kappa_c| &= \cos[(\theta_+ + \theta_-) / 4] / \cos[(\theta_+ - \theta_-) / 4] \\ &= 1 - \theta_+ \theta_- / 8 + O(\max \theta_{\pm}^4); \end{aligned}$$

so that, e.g.,  $\kappa_{\times}/|\kappa_d| = \cos[(\theta_+ + \theta_-)/4]$  is independent of  $\theta_+ - \theta_-$ . As  $\kappa_{\times}/|\kappa_c|$  depends on both  $\theta_+ + \theta_-$  and on  $\theta_+ - \theta_-$ , we tabulate no specific errors for  $\kappa_{\times}$ . We do conclude from (3.2b) and (3.2a) that (asymptotically)  $|\kappa_d|$  is the more accurate estimate of  $1/R$  for this circular example, except when  $\theta_+$  and  $\theta_-$  are quite disparate—more particularly, when  $\theta_{\pm} \geq (3 + 2\sqrt{2})\theta_{\mp}$ .

As for the difference approximations  $\kappa_{\lambda\mu}$ , (2.15), to the classic parametric expression for the curvature, it suffices (since the numerator is  $\kappa_{\times}$ , independent of  $\lambda$ ) to note that the denominator in (2.15) is given in terms of

$$(3.2c) \quad d_{\mu}^2 := |(U_+ + U_-)/2 + \mu(U_+ - U_-)|^2 = 1 + (4\mu^2 - 1)\sin^2[(\theta_+ + \theta_-)/4] \\ = 1 + (4\mu^2 - 1)(\theta_+ + \theta_-)^2/16 + O(\max \theta_{\pm}^4)$$

(for this, use (3.1)). Thus  $d_{\mu} \geq 1$  (and hence  $|\kappa_{\lambda\mu}| \leq |\kappa_{\times}|$ ) only when  $|\mu| \geq 1/2$  (i.e., only when  $U_+$  and  $U_-$  are *extrapolated*). In particular, using a forward or backward difference quotient (but not both) in the denominator gives the value  $d_{\pm 1/2}^2 = 1$  (and hence, the value  $\kappa_{\times}$  for the associated curvature). On the other hand, the value  $\mu_{\text{cen}}$  of  $\mu$  associated with using the centered difference quotient  $D_{\text{cen}}$  in the denominator satisfies  $|\mu_{\text{cen}}| < \frac{1}{2}$ , so  $|\kappa_{\lambda\mu_{\text{cen}}}| > |\kappa_{\times}|$ ; cf. (2.16).

Example 1 provides, for *arbitrary* data, an interpretation for both  $|\kappa_d|$  and  $\kappa_{\times}$  in terms of the geometry of the associated interpolating circle: For this, replace the origin here with that circle’s center, and  $R$  with  $r$ , (2.2a). We next use Example 1 in this way to help compare gross properties of our approximate curvatures.

Some practical remarks may be in order about the numbers  $|\kappa_c| := 1/r$  in (2.2),  $|\kappa_d|$  in (2.3),  $\kappa_{\times}$  in (2.10), and  $\kappa_{\lambda\mu}$  in (2.15). All four are independent of translation and rotation of the plane. The magnitudes of all but  $|\kappa_c|$  are affected by which one of three points one selects for the “middle” point  $X_0$ , but no magnitude is affected by interchanging  $X_+$  with  $X_-$ . From (3.2b), and from (2.2) and (2.3), we see that (modulo collinearity)

$$(3.3a) \quad 0 < |\kappa_{\times}| < |\kappa_c| \leq |\kappa_d|,$$

with equality in the last if and only if  $\Delta_+t = \Delta_-t$ . As we have seen,  $|\kappa_{\lambda\mu}| \leq |\kappa_{\times}|$  only for  $|\mu| \geq \frac{1}{2}$ ; otherwise,  $|\kappa_{\lambda\mu}|$  can exceed even  $|\kappa_d|$ ; cf. (3.2c).

The following individual bounds are sharp (and are of the order of the square root of corresponding bounds on the second difference quotient of bounded *scalar* functions)

$$(3.3b) \quad 0 \leq |\kappa_c| \text{ (or } |\kappa_{\times}|) \leq 2/\max \Delta_{\pm}t \quad \text{while} \quad 0 \leq |\kappa_d| \leq 4/\max \Delta_{\pm}t;$$

the first—for  $\kappa_c$ —because  $2r \geq \max \Delta_{\pm}t$  on geometric grounds, the second using the triangle inequality on (2.3).  $|\kappa_c| = 0$  and  $\kappa_{\times} = 0$  exactly when the points are collinear; for  $|\kappa_d| = 0$  one also needs that  $X_0$  lie between the points  $X_{\pm}$ . The above bound on  $|\kappa_d|$  may be divided by  $\sqrt{2}$  by imposing a natural gross restriction on the data; namely, that  $U_+ \cdot U_- \geq 0$ . As will be seen, the asymptotics will have little meaning unless the dimensionless parameter  $\kappa_0 \max \Delta_{\pm}t$  is relatively small.

On the other hand,  $|\kappa_{\lambda\mu}|$  can become infinite: Take  $\mu = 0$ ,  $\Delta_+t = \Delta_-t$ , let  $\theta_+ + \theta_-$  approach  $2\pi$  in (3.2c), and use (3.2b) and (2.2). This indicates that  $|\kappa_{\lambda\mu}|$  can grow unboundedly in related circumstances. For example, when using centered differencing (2.16) in the denominator, it grows unboundedly in most cases of the



analogous situation, i.e., when  $|X_+ - X_-| = o(|X_+ - X_0|)$ . More specifically, consider the following geometrical situation:  $X_0 := (\Delta t, 0)$ ,  $X_- := (0, 0)$ , while  $X_+ := \Delta t(x, cx^3)$ . Then,  $\lim_{x \rightarrow 0} |\kappa_{\lambda\mu_{\text{cen}}}| = |c/4|$  independent of  $\Delta t$ . The limit is zero if  $X_+ = \Delta t(x, o(x^3))$ , and is infinite if  $X_+ = \Delta t(o(y^{1/3}), y)$ ,  $y \rightarrow 0$ . However, according to (3.2c) or to the geometric argument below (2.15), the pair of values  $\mu = 0$  and  $\theta_+ + \theta_- = 2\pi$  is the only pair for which  $d_\mu$  can vanish.

It would be easy to consider more and more complex examples. For, given its (signed) curvature  $\kappa(s)$  in terms of its arclength, a plane curve is determined by the natural (or intrinsic) equations (see, e.g., Struik [8, p. 26])

$$(3.4a) \quad \dot{\phi} = \kappa; \quad \dot{x} = \cos \phi, \quad \dot{y} = \sin \phi;$$

that is to say,

$$(3.4b) \quad \begin{aligned} \phi(s) - \phi_0 &= \int_{s_0}^s \kappa(\sigma) d\sigma; \quad \text{and, with } \rho := 1/\kappa, \\ x - x_0 &= \int_{s_0}^s \cos \phi d\sigma = \int_{\phi_0}^\phi \rho \cos \phi d\zeta \\ y - y_0 &= \int_{s_0}^s \sin \phi d\sigma = \int_{\phi_0}^\phi \rho \sin \phi d\phi. \end{aligned}$$

(The three integration constants  $\phi_0$ ,  $x_0$ , and  $y_0$  rotate and translate the curve;  $s_0$  translates the arclength parameter. Thus, all four of these vanished in the special coordinate system used to establish (2.5).)

So, it is natural to develop a sequence of local approximants to a plane curve, beginning with lines ( $\kappa \equiv 0$ ), circles ( $\kappa \equiv \text{constant} \neq 0$ ), followed by curves with  $\kappa(s) \equiv \dot{\kappa}_0 s$ , etc. (This last mentioned is J. Bernoulli's clothoid (Cornu's spiral) (see, e.g., Struik [8, p. 201]); interpolating spirals could succeed interpolating circles when using four neighboring points, instead of three, to approximate sufficiently smooth curves.) The sequence could provide the basis for more examples.

Nevertheless, we record instead certain asymptotic expansions of our curvature estimates. Thus, using (3.4) and/or extending (2.9) to obtain  $\ddot{y}_0 = \ddot{\kappa}_0 - \kappa_0^3$ , and defining

$$(3.5a) \quad \delta_1 := \Delta_+ s - \Delta_- s, \quad \delta_{2a} := \Delta_+ s^2 - \Delta_+ s \Delta_- s + \Delta_- s^2,$$

$$(3.5b) \quad \hat{s} := s_0 + \delta_1/3, \quad \delta_{2b} := \Delta_+ s^2 + \Delta_+ s \Delta_- s + \Delta_- s^2$$

(here one could equally well have used  $\Delta_\pm t$ , by (2.5)), one finds that

$$(3.5c) \quad |\Delta^2 X / \Delta s^2| = |\kappa_0| \left[ 1 + \frac{\dot{\kappa}_0 \delta_1}{3\kappa_0} + \frac{\kappa_0^2 \delta_1^2}{18} + \frac{(\ddot{\kappa}_0 - \kappa_0^3) \delta_{2a}}{12\kappa_0} \right] + O(\max \Delta_\pm s^3)$$

$$(3.5d) \quad = |\kappa(\hat{s})| \left[ 1 + \frac{(\ddot{\kappa}_0 - \kappa_0^3) \delta_{2b}}{36\kappa_0} \right] + O(\max \Delta_\pm s^3),$$

$$(3.5e) \quad \begin{aligned} |\Delta^2 X / \Delta t^2| (= |\kappa_d|) &= |\kappa_0| \left[ 1 + \frac{\dot{\kappa}_0 \delta_1}{3\kappa_0} + \frac{\kappa_0^2 \delta_1^2}{32} + \frac{\ddot{\kappa}_0 \delta_{2a}}{12\kappa_0} \right] \\ &+ O(\max \Delta_\pm s^3) \end{aligned}$$

$$(3.5f) \quad = |\kappa(\hat{s})| \left[ 1 + \frac{\kappa_0^2 \delta_1^2}{32} + \frac{\ddot{\kappa}_0 \delta_{2b}}{36\kappa_0} \right] + O(\max \Delta_\pm s^3),$$

$$(3.5g) \quad |\kappa_c| = |\kappa_d| \left[ 1 - \kappa_0^2 \delta_1^2 / 32 \right] + O(\max \Delta_{\pm} s^3), \quad \text{and}$$

$$(3.5h) \quad \kappa_{\times} = \kappa_0 \left[ 1 + \frac{\dot{\kappa}_0 \delta_1}{3\kappa_0} + \frac{\ddot{\kappa}_0 \delta_{2a}}{12\kappa_0} - \frac{\kappa_0^2 \Delta_{+s} \Delta_{-s}}{8} \right] + O(\max \Delta_{\pm} s^3)$$

$$(3.5i) \quad = \kappa(\hat{s}) \left[ 1 + \frac{\ddot{\kappa}_0 \delta_{2b}}{36\kappa_0} - \frac{\kappa_0^2 \Delta_{+s} \Delta_{-s}}{8} \right] + O(\max \Delta_{\pm} s^3)$$

(if  $X$  is, say, a  $C^5$  curve). Taking the special case  $\kappa(s) \equiv \kappa_0$ , each expansion here is easily seen to be compatible with that associated with Example 1. The only uniformly valid expressions for  $\kappa_c := \text{sgn}(\kappa_{\times})|\kappa_c|$  and  $\kappa_d := \text{sgn}(\kappa_{\times})|\kappa_d|$  are the obvious combinations using the discontinuous “sgn” function; no polynomial expression can suffice if  $\kappa(s)$  changes sign in the interval  $|s| \leq \max \Delta_{\pm} s$ . Of course, from (2.15) and (3.2c), we also have the expansion

$$(3.6) \quad \kappa_{\lambda\mu} = \kappa_{\times} \left[ 1 + \kappa_0^2 3(1 - 4\mu^2)(\Delta_{+s} + \Delta_{-s})^2 / 32 \right] + O(\max \Delta_{\pm} s^3).$$

As an additional check on the expansions (3.5), we have used them to predict relative errors for all the combinations present in

*Example 2.*  $s_0 = 0 = \phi_0 = x_0 = y_0$ ;  $\kappa(s)$  cubic with

$$(3.7a) \quad \kappa_0 = 3/2, \pm 13/7; \quad \dot{\kappa}_0 = 0, \pm \sqrt{2}, \pm \sqrt{5}; \\ \ddot{\kappa}_0 = 0, \pm \pi/2, \pm \pi; \quad \ddot{\kappa}_0 = 0, \pm 11;$$

$$(3.7b) \quad \Delta_{+s} = p\Delta_{-s}, \quad |\kappa_0|\Delta_{-s} = 2^{-q}, \quad p = 1, 3/2, 5/2, \quad q = 5, 8, 11$$

(Cray XMP;  $\sigma$ -integrals (3.4b) calculated using the SLATEC program library’s adaptive 7-point Newton-Cotes quadrature program QNC79 with relative error request set to  $10^{-12}$ ). We report the results in terms of how accurately the principal parts of (3.5c)–(3.5i) predict errors in these cases. That is to say, the nonconstant, explicitly given polynomial part  $P$  of (3.5x) (polynomial in  $\Delta_{\pm} s$ ) may be regarded as a prediction of the error in the left-hand side (as an estimate of the constant term in the right); the number we shall discuss is the error in this prediction as a percent of the error actually incurred. Specifically: (3.5x) has the form  $A = B(1 + P) + O(\max \Delta_{\pm} s^3)$ ; we compute  $100|BP/(A - B)|$  and call it the “accuracy of the predicted error.”

For all cases considered with  $|\kappa_0|\Delta_{-s} = 2^{-11}$ , the accuracy of the predicted error was better than 4.8%. It was better than 0.6% for all cases with  $\Delta_{+s} = \Delta_{-s}$ ; orders of magnitude better for the smaller  $|\kappa_0|\Delta_{-s}$ ’s. Otherwise, the accuracy of the predicted error was better than 6.7% ( $p = 1.5$ ) and 57% ( $p = 2.5$ ) for  $|\kappa_0|\Delta_{-s} = 2^{-8}$ ; and better than 98% for  $p = 1.5$  and  $|\kappa_0|\Delta_{-s} = 2^{-5}$ . These maximal values occurred for cases in which a sign change or a doubling of one of the derivatives results in the division of the accuracy of the predicted error (and multiplication of the actual error) by a factor of five or so. That is to say, we had a hard time predicting when it involved cancellation. This was most apparent for  $|\kappa_0|\Delta_{-s} = 2^{-5}$  and  $p = 2.5$ , when in twelve of the 300 cases we predicted errors (for either (3.5d) or (3.5f)) which were more than a factor of two larger than actually observed. The worst of the twelve were the two cases  $\kappa_0 = \mp 13/7, \dot{\kappa}_0 = \pm \sqrt{2}, \ddot{\kappa}_0 = \pm \pi/2, \ddot{\kappa}_0 = 0$ ; the magnitude

of the actual error in (3.5f) was about  $3 \times 10^{-5}\%$  while the magnitude of the predicted error was about  $4 \times 10^{-4}\%$ . On the other hand, with  $|\ddot{\kappa}_0| = \pi$  instead, the actual error was .0066% and the prediction, .0061%. We point out that the case  $|\kappa_0|\Delta_{-s} = 2^{-5}$ ,  $p = 5/2$ , and constant  $\kappa \equiv \kappa_0$  corresponds to  $\theta_- \approx 1.8^\circ$ ,  $\theta_+ \approx 4.5^\circ$  in Example 1 above.

We take these results as supporting expansions (3.5), emphasizing that we are not reporting here the accuracies of  $\kappa_d$ ,  $\kappa_c$ , and  $\kappa_x$  as curvatures, but our ability to predict that accuracy. (In fact, the left-hand sides of (3.5c), (3.5e), and (3.5h) estimated  $\kappa_0$  to within 1.6%, with figures of better than .06% being associated with the remaining, second-order accurate formulae).

In practice, it is unusual to use asymptotic error estimates to predict actual errors; they are more often used to provide a conservative guess of an appropriate mesh size. In this connection, we report the following results using the 300 parameter values (3.7a) of Example 2. We fix  $p$ , (3.7b). We tabulate below the largest nonnegative integer  $q$  for which, with  $|\kappa_0|\Delta_{-s} = 2^{-q}$ , the magnitude of the nonconstant polynomial part  $P$  of (3.5x) overestimated the magnitude of the actual error by more than a factor of two for at least one of the 300 cases. (In this exercise,  $|P|$  exceeded the size of the constant term for some case only for (3.5c) and (3.5h),  $p = 2.5$ ,  $|\kappa_0|\Delta_{-s} = 1$ .) For the second subcolumn we used, instead of  $P$  itself, the number obtained by replacing each term in  $P$ —as expressed in (3.5x)—with its absolute value.

Expansion	(3.5c)	(3.5d)	(3.5e)	(3.5f)	(3.5g)	(3.5h)	(3.5i)
$p = 1.0$	1 1	1 1	- -	- -	- -	- -	- -
$p = 1.5$	3 1	4 4	2 2	3 3	- -	1 -	0 -
$p = 2.5$	2 0	5 5	2 2	6 3	0 0	2 -	3 -

For example, the content of the (3, 7) entry 3 - is the following. For  $p = 2.5$  in (3.7b): The nonconstant polynomial part  $P$  of (3.5i) was no larger than twice the actual error for  $|\kappa_0|\Delta_{-s}$  smaller than  $2^{-3}$  (for all parameter values (3.7a)). But this failed to be so for  $2^{-3}$  (for at least one set of the parameters). The blank second column means that if one summed instead the magnitude of  $P$ 's terms, then the resulting number never overestimated the actual error by more than a factor of two (at least for  $|\kappa_0|\Delta_{-s}$  a nonpositive power of two).

According to (3.5), for small errors one asks that the dimensionless parameters  $\kappa_0\Delta_{\pm t}$  be small while the dimensionless parameters  $\ddot{\kappa}_0/\kappa_0^2$  and  $\ddot{\kappa}_0/\kappa_0^3$  are of reasonable size ( $\approx 1$  in the calculations above). In their range of asymptotic validity,  $\kappa_d$ , (3.5f), could be substituted into (3.5g), leading to:  $\kappa_c$  estimates  $\kappa(\hat{\delta})$  better than  $\kappa_d$  does when  $\ddot{\kappa}_0 > 0$  or  $\Delta_{+s} = \Delta_{-s}$ ; but if  $\ddot{\kappa}_0 < 0$ , then there is a range of  $\delta_1$ 's (3.5a), for which  $\kappa_d$  yields the more accurate approximation. In the same asymptotic fashion, but using (3.5i),  $\kappa_c$  estimates  $\kappa(\hat{\delta})$  better than  $\kappa_x$  does when  $\ddot{\kappa}_0 < 0$ ; but if  $\ddot{\kappa}_0 > 0$ , then there is a range of values  $\kappa_0\Delta_{\pm s}$  for which  $\kappa_x$  yields the more accurate approximation. The asymptotics (3.5) should prove useful in other ways until overwhelmed by some of the unspecified cubic terms. Although our calculations above indicate that this phenomenon can begin before one might have anticipated it based on Example 1, it is our view that the variety of these unspecified terms precludes presentation of any additional, generally useful, sample calculations.

**4. A Broken Line Extension.** Suppose, now, we are given a sequence  $(X_i := X(s_i))_{i=0}^{N+1}$  of points along a sufficiently smooth ( $C^4$ ) but otherwise unknown plane curve  $X(s)$ ,  $s$  being arclength on  $X$ ,  $s_{i-1} < s_i$ , all relevant  $i$ . Using successive triples of neighbors in this sequence for the triple  $X_-, X_0, X_+$  of Section 2, we compute a sequence of curvature estimates  $(\bar{\kappa}_i)_{i=1}^N$ . Using (2.12) or (2.15), there is a corresponding sequence  $\bar{t}_i$  for which each associated  $\bar{\kappa}_i$  is a second-order accurate approximation of  $X$ 's curvature  $\kappa$  at  $\bar{t}_i$ . In this section we compose two (continuous) broken line interpolants in order to construct a broken line  $\hat{\kappa}(s)$  which approximates  $\kappa(s)$  with second-order accuracy. We describe below the use of  $\hat{\kappa}$  to estimate  $\kappa$  at any given fraction  $\alpha$  of the distance between  $s_{i-1}$  and  $s_i$ . Each such use will amount to applying a complicated difference approximation involving four adjacent  $X_j$ 's surrounding the desired point. Next, we show that another continuous approximation, based on the magnitude of a local cubic interpolant's second derivative, has second-order accuracy, too. Finally, we reject a third possibility, the vector product of a local cubic interpolant's first and second derivatives, because we do not know how to easily extend it globally as a continuous function.

The first broken line used in this construction is easy. Set

$$\Delta t_{i-1/2} := |X_i - X_{i-1}| > 0; \quad t_0 := 0, \quad t_i := \sum_{j=1}^i \Delta t_{j-1/2};$$

$$\bar{t}_i := (t_{i-1} + t_i + t_{i+1})/3, \quad \Delta \bar{t}_{i-1/2} := \bar{t}_i - \bar{t}_{i-1}.$$

Moreover, let  $\bar{\kappa}_i$  be  $\kappa_c$  (or  $\kappa_d$  or  $\kappa_\times$ ) based on the triple  $X_{i-1}, X_i$  and  $X_{i+1}$  (cf. Section 2). Then define  $\bar{\kappa}(t)$  to be the broken line interpolant of  $(\bar{t}_i, \bar{\kappa}_i)_{i=1}^N$ , so that  $\bar{\kappa}$  is linear on each  $[\bar{t}_{j-1}, \bar{t}_j]$  with  $\bar{\kappa}(\bar{t}_i) = \bar{\kappa}_i$ , each  $i$ . (The  $t$ -axis, here, is simply the broken line interpolant of the  $X_i$ , straightened out; each  $t_i$  corresponds to  $X_i$ , and each  $\bar{t}_i$  to the point where the number  $\bar{\kappa}_i$  is a second-order accurate curvature estimate.)

To convert  $\bar{\kappa}$  to curvature as a function of  $s$  along the unknown curve  $X$  we need a map  $\hat{T}: s \rightarrow t$ ; one would like  $\hat{T}$  to be continuous, strictly monotone, and to map each  $s_i$  onto  $t_i$ . A natural map having these properties is the broken line interpolating  $(s_i, t_i)_{i=0}^{N+1}$ . With this choice, define

$$\hat{\kappa}(s) := \bar{\kappa}(\hat{T}(s)).$$

Then  $\hat{\kappa}$ , too, is continuous and piecewise linear; it is defined on  $[\bar{s}_1, \bar{s}_N]$ , where

$$\bar{s}_i := \hat{T}^{-1}(\bar{t}_i) \quad (\text{so we set } \Delta \bar{s}_{i-1/2} := \bar{s}_i - \bar{s}_{i-1});$$

and  $\hat{\kappa}$  breaks slope not only at each  $s_j$  in that interval but also at each  $\bar{s}_j$ . (We observe below that  $\hat{\kappa}$  may be extrapolated to be defined on all of  $[s_0, s_{N+1}]$ .) Note that, because  $\hat{T}$  is strictly monotone, the points  $(\bar{s}_i)$  interlace the  $(s_i)$  in exactly the same way that the  $(\bar{t}_i)$  interlace the  $(t_i)$ —a characteristic not necessarily shared by the collection of averages  $(s_{i-1} + s_i + s_{i+1})/3$ .

The approximation  $\hat{\kappa}$  is easier to use than to describe. Thus, suppose one wants to estimate the curvature at a fraction  $\alpha$  ( $0 \leq \alpha \leq 1$ ) of the distance along the curve from  $X_{i-1}$  to  $X_i$ , i.e., from  $s_{i-1}$  to  $s_i$ . One first computes  $t_\alpha := t_{i-1} + \alpha \Delta t_{i-1/2}$  ( $t_\alpha$  being  $\hat{T}$  of the appropriate  $s$ ). Next, one picks an interval  $[\bar{t}_{j-1}, \bar{t}_j]$  which contains  $t_\alpha$ . (If  $\alpha = 1/2$ , then  $j = i$ ; but if  $\alpha < 1/2$ ,  $j$  may be  $i$  or  $i - 1$ ; and  $j$  may be  $i$  or

$i + 1$  otherwise.) Next, one finds the relative position  $\beta$  of  $t_\alpha$  in  $[\bar{t}_{j-1}, \bar{t}_j]$ :  $\beta := (t_\alpha - \bar{t}_{j-1})/\Delta\bar{t}_{j-1/2}$ . Then the curvature estimate is

$$(4.1) \quad \kappa_\alpha := (1 - \beta)\bar{\kappa}_{j-1} + \beta\bar{\kappa}_j.$$

To analyze the second-order accuracy of  $\hat{\kappa}$  we begin with the following remark:

$$(4.2) \quad \hat{T}(s) - t_{i-1} = s - s_{i-1} + O(\Delta s_{i-1/2}^3) \quad \text{for } s \text{ in } [s_{i-1}, s_i].$$

For

$$\hat{T}(s) = t_{i-1} + (s - s_{i-1})\Delta t_{i-1/2}/\Delta s_{i-1/2} = t_{i-1} + (s - s_{i-1})[1 + O(\Delta s_{i-1/2}^2)],$$

the last by (2.5). We conclude that  $\bar{\kappa}_i$ , a second-order estimate of  $\kappa(\bar{t}_i)$  by (2.12) or (2.15), also satisfies

$$|\bar{\kappa}_i - \kappa(\bar{s}_i)| = O(\max \Delta s_{i\pm 1/2}^2).$$

Let  $\tilde{\kappa}(s)$  be the linear interpolant of  $(\bar{s}_{i-1}, \bar{\kappa}_{i-1})$  and  $(\bar{s}_i, \bar{\kappa}_i)$ . Then, on  $[\bar{s}_{i-1}, \bar{s}_i]$ ,  $\tilde{\kappa}$  differs from the linear interpolant of  $(\bar{s}_{i-1}, \kappa(\bar{s}_{i-1}))$  and  $(\bar{s}_i, \kappa(\bar{s}_i))$  by  $O(\max_{j=0,\pm 1} \Delta s_{i-1/2+j}^2)$ , since the difference is linear and satisfies this inequality at the two endpoints. The latter interpolant is within  $O(\Delta \bar{s}_{i-1/2}^2)$  of  $\kappa$  on  $[\bar{s}_{i-1}, \bar{s}_i]$  in the usual fashion; hence,

$$|\tilde{\kappa} - \kappa|(s) = O(\Delta \bar{s}_{i-1/2}^2) = O(\Delta \bar{t}_{i-1/2}^2), \quad s \text{ in } [\bar{s}_{i-1}, \bar{s}_i];$$

the last since

$$(4.3) \quad \begin{aligned} \Delta s_{i-1/2}/\Delta t_{i-1/2} &= 1 + O(\Delta t_{i-1/2}^2), \quad \text{and} \\ \Delta \bar{s}_{i-1/2}/\Delta \bar{t}_{i-1/2} &= 1 + O(\Delta \bar{t}_{i-1/2}^2) \end{aligned}$$

by (2.5) and (4.2).

If  $|\hat{\kappa} - \tilde{\kappa}|$  satisfies this same inequality, then we shall have proved the error estimate we seek, namely that

$$(4.4) \quad |\hat{\kappa} - \kappa|(s) = O(\Delta \bar{t}_{i-1/2}^2), \quad s \text{ in } [\bar{s}_{i-1}, \bar{s}_i].$$

But, if  $\tilde{T}$  is the broken line interpolant of  $(\bar{s}_i, \bar{t}_i)_{i=1}^N$ , then  $\tilde{\kappa}$ , like  $\hat{\kappa}$ , is a composition:  $\tilde{\kappa}(s) = \bar{\kappa}(\tilde{T}(s))$ . Thus, on  $[\bar{s}_{i-1}, \bar{s}_i]$  (which is mapped by both  $\hat{T}$  and  $\tilde{T}$  onto  $[\bar{t}_{i-1}, \bar{t}_i]$ ),

$$\tilde{\kappa}(s) - \hat{\kappa}(s) = \bar{\kappa}'_{i-1/2}[\tilde{T}(s) - \hat{T}(s)],$$

where  $\bar{\kappa}'_{i-1/2}$  is the (constant) slope of  $\bar{\kappa}$  on  $(\bar{t}_{i-1}, \bar{t}_i)$  (and is hence bounded, being a first-order approximation to, say,  $\dot{\kappa}(s_i)$ ). And, it is not difficult, using (4.3), to verify that, in fact,

$$\tilde{T}(s) - \hat{T}(s) = O(\Delta \bar{t}_{i-1/2}^3) \quad \text{for } s \text{ in } [\bar{s}_{i-1}, \bar{s}_i].$$

Finally,  $\hat{\kappa}$  may be extrapolated from  $[\bar{s}_1, \bar{s}_N]$  to  $[s_0, s_{N+1}]$ : For points  $s$  in  $[s_0, \bar{s}_1]$  the corresponding  $\beta$  in (4.1) satisfies

$$0 < -\beta \leq \bar{t}_1/(\bar{t}_2 - \bar{t}_1) = (t_1 + t_2)/t_3 < 2,$$

so  $\beta$  is uniformly bounded. Consequently  $O(\Delta \bar{t}_{3/2}^2)$  accuracy here is not destroyed in the process—but recall that the endpoint error in extrapolating the linear interpolant of a quadratic, over an adjacent interval twice as long, is  $5^2 - 1^2 = 24$  times the maximum error incurred on the original interval.

As an aside for readers interested in piecewise polynomial approximation of the second derivative  $y''$  of a scalar function: The broken line interpolant, corresponding to what we did above, of  $(\bar{t}_i, (\Delta^2 y / \Delta t^2)_i)_{i=1}^N$  is locally second-order accurate. Moreover, it is exact, for cubic functions  $y(t)$ , at each  $\bar{t}_j$ . Consequently, it coincides, on  $[\bar{t}_{j-1}, \bar{t}_j]$ , with the second derivative of the cubic interpolant of the  $(t_i, y_i)_{i=j-2}^{j+1}$ . That is to say, the (linear) second derivatives of the cubic interpolants of two successive quadruples  $(t_i, y_i)_{i=j-2}^{j+1}$  and  $(t_i, y_i)_{i=j-1}^{j+2}$  cross at  $\bar{t}_j$  (whether  $y$  is cubic or not), since their common value at that point is  $(\Delta^2 y / \Delta t^2)_j$ . The congruent dual role of the broken line interpolant of translations of the  $n$ th difference quotient, at the corresponding averages of the  $n + 1$  points in its stencil (where it exactly yields the  $n$ th derivative of  $(n + 1)$ th degree polynomial functions according to Kreiss et al. [3, p. 538]), is now equally clear.

This suggests another continuous (but not piecewise linear) approximation to the curvature: namely, the magnitude of the second derivative of the local vector cubic interpolant (in secant length), evaluated at  $t_\alpha$  above, (4.1). Specifically, in the context of (4.1), we mean

$$(4.5) \quad \tilde{\kappa}_\alpha := |(1 - \beta)(\Delta^2 X / \Delta t^2)_{j-1} + \beta(\Delta^2 X / \Delta t^2)_j|.$$

It, too, is independent of translation and rotation. And, according to the previous paragraph, it is continuous at its breakpoints  $(\bar{s}_i)$ . We show now that it is also second-order accurate, because

$$(4.6) \quad \tilde{\kappa}_\alpha / |\kappa| = |\kappa_\alpha / \kappa| - (1/2)\beta(1 - \beta)\kappa^2 \Delta \bar{t}_j^2 [1 + o(1)];$$

here  $\kappa$  is any value of  $\kappa(t)$  on  $[\bar{t}_{j-1}, \bar{t}_j]$ , and  $\kappa_\alpha$ , (4.1), is that based on  $\kappa_d$ , (2.12). For this we use the identity

$$(bc - ad)^2 \equiv (a^2 + b^2)(c^2 + d^2) - (ac + bd)^2$$

to verify the identity

$$\begin{aligned} & 2\beta(1 - \beta)(bc - ad)^2 \\ & \equiv (\sqrt{a^2 + b^2}\sqrt{c^2 + d^2} + ac + bd) \left\{ [(1 - \beta)\sqrt{a^2 + b^2} + \beta\sqrt{c^2 + d^2}]^2 \right. \\ & \quad \left. - [((1 - \beta)a + \beta c)^2 + ((1 - \beta)b + \beta d)^2] \right\}. \end{aligned}$$

Then, using  $X_i = (x_i, y_i)$ ,  $i = j - 2, j - 1, j, j + 1$ , set

$$a := (\Delta^2 x / \Delta t^2)_{j-1}, \quad b := (\Delta^2 y / \Delta t^2)_{j-1}, \quad c := (\Delta^2 x / \Delta t^2)_j, \quad d := (\Delta^2 y / \Delta t^2)_j,$$

so that

$$\begin{aligned} \sqrt{a^2 + b^2} &= (\kappa_d)_{j-1}, & \sqrt{c^2 + d^2} &= (\kappa_d)_j, \\ (\kappa_d)_{j-1}(\kappa_d)_j + ac + bd &= 2\kappa^2 [1 + o(1)], \\ |bc - ad| &= |(\bar{x}\bar{y} - \bar{x}\bar{y})((\bar{t}_{j-1} + \bar{t}_j)/2)| \Delta \bar{t}_{j-1/2} [1 + o(1)] \\ &= |\kappa|^3 \Delta \bar{t}_{j-1/2} [1 + o(1)], \end{aligned}$$

the last using (3.4). And (4.6) follows.

A third local approximation to the curvature function would be given by the vector product of the first derivative of the local (vector) cubic interpolant (in secant distance) with its second derivative. Second-order accuracy seems certain here; but the way to switch *continuously* from one such local approximation to the next is not clear. As we have seen, given five stencil points, the *second* derivative of the cubic interpolant associated with the left four agrees with that of the right four when both are evaluated at the average of the middle three points. So, that location is the natural point to consider for switching from one vector product to the other. We now show that if  $X(t)$  is the (vector) cubic interpolant of four vectors  $X_1, \dots, X_4$  at the secant distances  $t_1, \dots, t_4$  along their broken line interpolant, then  $X' \times X''$ , at the mean  $\bar{t}$  of  $t_1, t_2$ , and  $t_3$ , depends upon  $X_4 - X_3$  in general (thereby showing that the middle mean will *not* do, in general, as a point to switch vector products). For this it suffices to demonstrate that  $(\partial L/\partial t)(X_4 \times X'')$  at  $\bar{t}$  depends nontrivially upon  $X_4 - X_3$ ; here  $L(t; t_1, t_2, t_3, t_4)$  is the Lagrange interpolation basis function, associated with the data at  $t_4$ , for cubic interpolation at  $t_1, \dots, t_4$ :

$$L(t; t_1, t_2, t_3, t_4) := p(t; t_1, t_2, t_3)/p(t_4; t_1, t_2, t_3),$$

$$p(t; t_1, t_2, t_3) := (t - t_1)(t - t_2)(t - t_3), \quad \bar{t} := (t_1 + t_2 + t_3)/3.$$

But

$$\begin{aligned} \partial L/\partial t|_{\bar{t}} &= [(t_1 t_2 + t_1 t_3 + t_2 t_3) - (t_1^2 + t_2^2 + t_3^2)]/[3p(t_4; t_1, t_2, t_3)]. \\ &=: f_1(|X_4 - X_3|, X_1, X_2, X_3) \neq f_2(X_1, X_2, X_3) \end{aligned}$$

(this to be contrasted with the now unsurprising fact that  $\partial^2 L/\partial t^2|_{\bar{t}} \equiv 0$ ); while

$$\begin{aligned} X_4 \times X''|_{\bar{t}} &= X_3 \times \Delta^2 X/\Delta t^2 + (X_4 - X_3) \times \Delta^2 X/\Delta t^2 \\ &=: f_3(X_4 - X_3, X_1, X_2, X_3) \neq f_4(|X_4 - X_3|, X_1, X_2, X_3) \end{aligned}$$

(the second difference quotient here being that based on  $t_1, t_2$ , and  $t_3$ ).

Since the difference between the two successive vector products is a cubic polynomial in the distance  $t$  along the broken line interpolant/extrapolant of the associated five points in the plane, it has at least one zero. Each such zero is a point at which one could switch continuously from one local curvature estimate to the next. But, we have not investigated the conditions under which (a) this zero (or zeros) lies between the five points, and (b) as one moves along the data from one quintuple to the next overlapping quintuple, the next zero comes after the previous one on the broken line joining the six points.

We discuss briefly the hydrodynamic context. The force due to surface tension acts continuously along a smooth boundary between two fluids. But this boundary is typically specified computationally only by its mesh points, and an apt approximate boundary is their broken line interpolant. For this it is natural to apply the force to the midpoint of each segment, so we require a curvature estimate at each midpoint and hence invoke the estimate (4.1) with  $\alpha = \frac{1}{2}$ . This particular value of  $\alpha$  means the estimate will amount to the use of a complex difference formula involving those four neighbors of this midpoint which are its four natural nodal neighbors in the curve. As we have seen, the estimate is independent of rigid motion of the plane and is locally second-order accurate (in terms of the three mesh sizes associated with the

four neighbors used). We hasten to point out, though, that the story is far from complete for this application of our curvature estimates. For: (1) although our work can contribute to hydrodynamic schemes having second-order truncation error, it does so using a stencil which is not as compact as that of more elementary schemes, and this could lead to different stability problems. Moreover, (2) although second-order truncation suffices for second-order convergence (assuming stability and a linear problem), it is not necessary in some contexts; see, e.g., Kreiss et al. [3] for the context of ordinary differential equations (with some references to partial differential equations), or the finite element literature concerning “lumped mass” schemes.

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