Conditions on Minimization Criteria for Smoothing

By Boris Podolsky and Harry H. Denman

1. Introduction. Given a set of data points $\{Y_i(x_i)\}, i = 1, 2, \dots, n$, we wish to find the "smoothest" curve y(x) passing through or near the given set of points. Let us assume that the criterion for smoothness is that the integral of some function of y, y', and y'' (where y' = dy/dx, etc.) be a minimum, i.e.,

(1)
$$\delta \int_{x_1}^{x_n} f(y, y', y'') \, dx = 0.$$

As an example, we might minimize the integral (along the curve) of the square of the curvature, so that $f = (y'')^2/(1 + (y')^2)^{5/2}$.

However, the given data may come from physical measurements, where arbitrary units may be used for the physical quantities. If these points are plotted on a graph, the scales are usually chosen so that the set of points spans the available space on the sheet. If we are dealing numerically with the set of numbers representing these data, this method of selecting a scale is inappropriate. The problem here is to find f(y, y', y'') in (1) such that the smooth function y(x) remains unchanged with respect to the set of points $\{Y_i\}$ when these points are displaced or changed by a scale factor. That is, if y(x) is a smooth function associated with the data $\{Y_i\}$, and if these data undergo a linear transformation $\bar{Y}_i = aY_i + b$, the new solution \bar{y} of (1) should be $\bar{y} = ay + b$.

2. The Euler-Lagrange Equation. If we take the case where y and y' are known at x_1 and x_n , then the Euler-Lagrange equation resulting from (1) is

(2)
$$\frac{d^2}{dx^2} \left(\frac{\partial f}{\partial y''}\right) - \frac{d}{dx} \left(\frac{\partial f}{\partial y'}\right) + \frac{\partial f}{\partial y} = 0$$

Equation (2) is a fourth-order ordinary differential equation, which we may write as

(3)
$$L(y, y', y'', y''', y'''') = 0.$$

We shall denote $d^k y/dx^k$ by $y^{(k)}$, so that (3) may be written

(4a)
$$L(y^{(k)}) = 0$$
, where $k = 0, 1, 2, 3, \text{ and } 4$.

If the original data $\{Y_i\}$ have a different scale and origin, so that $\overline{Y}_i = aY_i + b$, the new solution of (4) should be $\overline{y} = ay + b$, and since f is the same function of \overline{y} that it was of y, (1) becomes

$$\delta \int_{x_1}^{x_n} f(\bar{y}, \bar{y}', \bar{y}'') \ dx = 0,$$

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with corresponding end conditions, and (4a) becomes

(4b)
$$L(\bar{y}^{(k)}) = 0.$$

The function L in (4b) is the same function of $\bar{y}^{(k)}$ as it is of the $y^{(k)}$ in (4a). Thus the differential equations represented by (4a) and (4b) have the same structure, and therefore the same family of solutions, but the boundary conditions will be different in the two cases. Therefore, we seek a differential equation (4a) which has solutions y(x) and $\bar{y}(x) = ay + b$, where a and b are arbitrary and independent parameters (except that $a \neq 0$).

Taking a = 1 and $b \neq 0$ in (4b), and subtracting (4a), we have

(5a)
$$L(y+b, y^{(k)}) - L(y, y^{(k)}) = 0, \qquad (k = 1, 2, 3, 4),$$

when L = 0. Dividing (5a) by b, and taking the limit as b approaches 0, we obtain^{*}

(6a)
$$\partial L(y^{(k)})/\partial y = 0$$
, when $L = 0$ $(k = 0, 1, 2, 3, 4)$

Taking b = 0 and $a = 1 + \epsilon$ in (4b), and subtracting (4a), we have

(5b)
$$L(y^{(k)} + \epsilon y^{(k)}) - L(y^{(k)}) = 0$$
, when $L = 0$.

Dividing (5b) by ϵ , and taking the limit as ϵ approaches 0, we obtain

(6b)
$$\sum_{0}^{4} y^{(k)} \frac{\partial L}{\partial y^{(k)}} = 0 \quad \text{if} \quad L = 0$$

Equation (4a) may be written

(7)
$$L(y^{(k)}) = L'(y, y^{(1)}, y^{(2)}, y^{(3)}) + f_{22} y^{(4)} = 0,$$

where we have introduced the notation $\partial^2 f / \partial y^{(i)} \partial y^{(j)} = f_{ij}$, etc., so that $f_{22} = \partial^2 f / (\partial y'')^2$. From (7), letting $L_0 = \partial L / \partial y$, etc.,

(8)
$$L_0 = L_0' + f_{022} y^{(4)}.$$

From (7) and (8), we obtain

$$f_{22}L_0 - f_{022}L = f_{22}L_0' - f_{022}L' = G(y, y^{(1)}, y^{(2)}, y^{(3)}).$$

Now, when L = 0, $\partial L/\partial y = L_0 = 0$ also, so that G = 0 whenever y is a solution of (4a). However, G = 0 is a differential equation of lower order than L = 0, so that not all the solutions of L = 0 are solutions of G = 0, unless G is *identically* zero, or

(9)
$$f_{22}L_0 - f_{022}L \equiv 0.$$

3. Case I. $f_{22} \neq 0$ at any point. (We consider the case $f_{22} \equiv 0$ in Case II.) Then (9) may be written

(10)
$$\partial L/\partial y \equiv gL,$$

where $g(y, y^{(1)}, y^{(2)}) = f_{022}/f_{22}$. We also have in this case

^{*} We assume here and in what follows that all the indicated partial derivatives of f and L exist, and moreover, that their mixed partial derivatives are equal.

(11)
$$\partial (L/f_{22})/\partial y \equiv 0$$
, so that L/f_{22} is independent of y.

Writing out the Euler-Lagrange equation (4a) in our notation,

(12)
$$L = f_0 - y^{(1)}f_{01} - y^{(2)}f_{11} + y^{(1)}(y^{(1)}f_{002} + 2y^{(2)}f_{012} + 2y^{(3)}f_{022}) + y^{(2)}(f_{02} + y^{(2)}f_{112} + 2y^{(3)}f_{122}) + (y^{(3)})^2f_{222} + y^{(4)}f_{22} = 0.$$

Substituting this expression into the identity (9), and equating terms in $y^{(4)}$, $(y^{(3)})^2$, and $y^{(3)}$, we obtain

(13a)
$$f_{022} \equiv g f_{22}$$
,

(13b)
$$f_{0222} \equiv g f_{222}$$
,

(13c)
$$y^{(1)}f_{0022} + y^{(2)}f_{0122} \equiv g(y^{(1)}f_{022} + y^{(2)}f_{122}).$$

Operating on (13a) with $\partial/\partial y^{(2)}$ and comparing with (13b), since f_{22} is never 0, we obtain $\partial g/\partial y^{(2)} \equiv 0$, so that g is at most a function of y and $y^{(1)}$. Operating on (13a) with $y^{(1)}\partial/\partial y$, and also with $y^{(2)}\partial/\partial y^{(1)}$, and adding,

$$y^{(1)}f_{0022} + y^{(2)}f_{0122} \equiv \left(y^{(1)}\frac{\partial g}{\partial y} + y^{(2)}\frac{\partial g}{\partial y^{(1)}}\right)f_{22} + g(y^{(1)}f_{022} + y^{(2)}f_{122}).$$

Thus, $y^{(1)}\partial g/\partial y + y^{(2)}\partial g/\partial y^{(1)} \equiv 0$, by subtraction of (13c). But since g is not a function of $y^{(2)}$, $\partial g/\partial y^{(1)}$ must be *identically* zero, and therefore also $\partial g/\partial y$; thus g is a constant.

Let E be defined by the expression

(14)
$$E = f_{22} \sum_{k=0}^{4} y^{(k)} \frac{\partial L}{\partial y^{(k)}} - \left(f_{22} + \sum_{j=0}^{2} y^{(j)} f_{j22} \right) L$$

which, from (6b), is zero when L = 0. Using (7) and (9), equation (14) can be rewritten, since all the terms in $y^{(4)}$ cancel, as

(15)
$$E = f_{22} \sum_{k=1}^{3} y^{(k)} \frac{\partial L'}{\partial y^{(k)}} - \left(f_{22} + \sum_{j=1}^{2} y^{(j)} f_{j22} \right) L' = 0.$$

Regarded as a differential equation in y, (15) is of lower order (third) than

$$L(y^{(k)}) = 0$$

but must be 0 when L = 0. Hence, $E \equiv 0$, and we may rewrite (14), using (10), as

(16)
$$\sum_{k=1}^{4} y^{(k)} \frac{\partial L}{\partial y^{(k)}} \equiv (h - gy)L,$$

where $h(y, y^{(1)}, y^{(2)}) = (y f_{022} + y^{(1)} f_{122} + y^{(2)} f_{222} + f_{22})/f_{22}$. Substituting (12) into (16), and equating terms in $y^{(4)}, (y^{(3)})^2$, and $y^{(3)}$,

(17a)
$$y^{(1)}f_{122} + y^{(2)}f_{222} \equiv (h - gy - 1)f_{22},$$

(17b)
$$y^{(1)}f_{1222} + y^{(2)}f_{2222} \equiv (h - gy - 2)f_{222},$$

(17c)
$$(y^{(1)})^2 f_{0122} + y^{(1)} y^{(2)} (f_{1122} + f_{0222}) + (y^{(2)})^2 f_{1222} \\ \equiv (h - gy - 2) (y^{(1)} f_{022} + y^{(2)} f_{122})$$

Operating on (17a) with $\partial/\partial y^{(2)}$ and combining with (17b), we obtain $\partial h/\partial y^{(2)} \equiv 0$,

and in a manner analogous to that used with equations (13), we find that h is also a *constant*.

From (13a), f_{22} may be written

(18)
$$f_{22} = e^{gy}w(y^{(1)}, y^{(2)}),$$

where w is some function of $y^{(1)}$ and $y^{(2)}$, and is never 0 in this case. Substituting in (17a), we get

(19)
$$h - gy - 1 \equiv \frac{1}{w} \left(y^{(1)} \partial w / \partial y^{(1)} + y^{(2)} \partial w / \partial y^{(2)} \right).$$

Since the right side of (19) is a function of $y^{(1)}$ and $y^{(2)}$ only, this implies that g = 0. Thus, $\partial L/\partial y \equiv 0$, or L is not a function of y. Then (16) becomes

(20)
$$\sum_{k=1}^{4} y^{(k)} \partial L / \partial y^{(k)} \equiv hL$$

so that L is a homogeneous function of degree h in dy/dx, d^2y/dx^2 , d^3y/dx^3 , and d^4y/dx^4 , and does not contain y explicitly.

Using (18), we may write f in the form

(21)
$$f = W(y^{(1)}, y^{(2)}) + y^{(2)}u + v,$$

where $W_{22} = w(y^{(1)}, y^{(2)})$, $u = u(y, y^{(1)})$, and $v = v(y, y^{(1)})$, and u and v are arbitrary. Equation (17a) becomes

$$y^{(1)} \frac{\partial f_{22}}{\partial y^{(1)}} + y^{(2)} \frac{\partial f_{22}}{\partial y^{(2)}} = y^{(1)} \frac{\partial w}{\partial y^{(1)}} + y^{(2)} \frac{\partial w}{\partial y^{(2)}} \equiv (h - 1)w,$$

so that w is homogeneous of degree h - 1 in $y^{(1)}$ and $y^{(2)}$. We next show that u and v can be chosen so that $W(y^{(1)}, y^{(2)})$ is a homogeneous function of degree h + 1.

 $W(y^{(1)}, y^{(2)})$ can be written, by a power series expansion in $y^{(2)}$ with a remainder term,

(22)
$$W(y^{(1)}, y^{(2)}) = W(y^{(1)}, 0) + W_2(y^{(1)}, 0)y^{(2)} + W_{22}(y^{(1)}, \theta y^{(2)})(y^{(2)})^2/2!,$$

where $W_2 = \partial W/\partial y^{(2)}$, etc., and $0 \leq \theta \leq 1$. Since $W_{22}(y^{(1)}, \theta y^{(2)}) = w(y^{(1)}, \theta y^{(2)})$ is homogeneous of degree h - 1 in its variables, the last term in (22) is homogeneous of degree h + 1 in $y^{(1)}$ and $y^{(2)}$. Since u and v are arbitrary, they may be chosen so that the first two terms of W are also homogeneous of degree h + 1, and we have the desired result.

Since $f_{022} = 0$, the Euler-Lagrange equation (12) becomes

(23)
$$L = f_0 - y^{(1)} f_{01} - y^{(2)} f_{11} + y^{(1)} (y^{(1)} f_{002} + 2y^{(2)} f_{012}) + y^{(2)} (f_{02} + y^{(2)} f_{112} + 2y^{(3)} f_{122}) + (y^{(3)})^2 f_{222} + y^{(4)} f_{22} = 0.$$

Since $f_{22} = w$ is homogeneous of degree h - 1 in $y^{(1)}$ and $y^{(2)}$, the terms $y^{(2)}y^{(3)}f_{122}$, $(y^{(3)})^2 f_{222}$, and $y^{(4)}f_{22}$ are homogeneous of degree h in $y^{(1)}$, $y^{(2)}$, $y^{(3)}$, and $y^{(4)}$. L is also homogeneous of degree h, and therefore, if L'' is defined by

$$L'' = L - 2y^{(2)}y^{(3)}f_{122} - (y^{(3)})^2f_{222} - y^{(4)}f_{22},$$

L'' must also be homogeneous of degree h in $y^{(1)}$, $y^{(2)}$. Also, L and f_{22} do not contain

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y explicitly; thus $\partial L''/\partial y \equiv 0$. Using (21), L'' becomes

$$L'' = 2y^{(2)}u_0 + v_0 - y^{(1)}v_{01} - y^{(2)}(W_{11} + v_{11}) + y^{(1)}(y^{(1)}u_{00} + y^{(2)}u_{01}) + (y^{(2)})^2W_{112}$$

Since W is homogeneous of degree h + 1 in $y^{(1)}$ and $y^{(2)}$, $-y^{(2)}W_{11} + (y^{(2)})^2W_{112}$ is homogeneous of degree h in $y^{(1)}$ and $y^{(2)}$ and does not contain y; therefore

$$y^{(2)}(2u_0 + y^{(1)}u_{01} - v_{11}) + v_0 - y^{(1)}v_{01} + (y^{(1)})^2 u_{00}$$

must be homogeneous of degree h in $y^{(1)}$ and $y^{(2)}$, and does not contain y.

The terms $v_0 - y^{(1)}v_{01} + (y^{(1)})^2 u_{00}$ do not contain $y^{(2)}$, so that they must be independent of y, and homogeneous of degree h in $y^{(1)}$. The terms $2u_0 + y^{(1)}u_{01} - v_{11}$ must be independent of y and homogeneous of degree h - 1 in $y^{(1)}$. These conditions result in the following equations

(24a)
$$2u_{00} + y^{(1)}u_{001} - v_{011} \equiv 0$$

(24b)
$$v_{00} - y^{(1)}v_{001} + (y^{(1)})^2 u_{000} \equiv 0,$$

(24c)
$$3y^{(1)}u_{01} + (y^{(1)})^2u_{011} - y^{(1)}v_{111} \equiv (h-1)(2u_0 + y^{(1)}u_{01} - v_{11}),$$

$$(24d) \quad (y^{(1)})^3 u_{001} + 2(y^{(1)})^2 u_{00} - (y^{(1)})^2 v_{011} \equiv h(v_0 - y^{(1)}v_{01} + (y^{(1)})^2 u_{00}).$$

It can be shown that a general solution of these equations is given by the relation

(25)
$$v = y^{(1)} \int u_0 \, dy^{(1)} + c_1 (y^{(1)})^{h+1} + y^{(1)} r(y) + c_2$$

where r(y) is an arbitrary function, c_1 and c_2 are arbitrary constants, and y is fixed in $\int u_0 dy^{(1)}$.

Now f can be written

(26)
$$f = W(y^{(1)}, y^{(2)}) + y^{(2)}u + y^{(1)} \int u_0 \, dy^{(1)} + y^{(1)}r(y) + c_2 \, dy^{(1)}$$

where the term $c_1(y^{(1)})^{h+1}$ has been incorporated into W.

Let $\phi(y, y^{(1)}, x) = \int u \, dy^{(1)} + R(y) + c_2 x$, where dR/dy = r(y). Then, $d\phi/dx = y^{(1)} \int u_0 \, dy^{(1)} + y^{(1)} r(y) + y^{(2)} u + c_2$, and f can be written

(27)
$$f = W(y^{(1)}, y^{(2)}) + d\phi/dx,$$

where W is homogeneous of degree h + 1 in $y^{(1)}$ and $y^{(2)}$. The term $d\phi/dx$ will not contribute to the Euler-Lagrange differential equation. Thus if we substitute the result (27) into (1), it is simple to verify that the resulting Euler-Lagrange equation will not contain y, and will be homogeneous of degree h in $y^{(1)}$, $y^{(2)}$, $y^{(3)}$, $y^{(4)}$, so that both y and $\bar{y} = ay + b$ will be solutions.

Thus we have established the theorem: A necessary and sufficient condition that the function f used in the smoothing criterion $\delta \int_{x_1}^{x_n} f(y, y', y'') dx = 0$, with y and dy/dx known at x_1 and x_n , result in a smooth function y(x) which is independent of origin and scale changes in the given data is that

$$f = W(y', y'') + \frac{d\phi(x, y, y')}{dx},$$

where $\partial^2 f / (\partial y'')^2 \neq 0$, and W is a homogeneous function of y' and y''.

4. Case II. $\partial^2 f/(\partial y'')^2 \equiv 0$.

In this degenerate case, f may be written, in our previous notation,

$$f(y, y^{(1)}, y^{(2)}) = p(y, y^{(1)}) + q(y, y^{(1)})y^{(2)},$$

and the Euler-Lagrange expression is

(28)
$$L = y^{(2)}(2q_0 - p_{11} + y^{(1)}q_{01}) + p_0 - p_{01}y^{(1)} + (y^{(1)})^2 q_{00}$$

If the expression (28) is set equal to 0, a second-order ordinary differential equation results, and its solution y(x) cannot in general satisfy four conditions at x_1 and x_n . The variational equation (2) becomes here

(29)
$$\int_{x_1}^{x_n} L\delta y \, dx + (p_1 - q_0 \, y^{(1)}) \delta y |_{x_1}^{x_n} + q \, \delta y^{(1)} |_{x_1}^{x_n} = 0.$$

If we know the values of y at x_1 and x_n , which is the case if the smooth function y is to have the values Y_1 and Y_n at the end points, then (29) becomes

(30)
$$\int_{x_1}^{x_n} L\delta y \ dx + q \ \delta y^{(1)}|_{x_1}^{x_n} = 0.$$

Since δy is arbitrary in the interval (x_1, x_n) , (30) requires L = 0 and $q \delta y^{(1)} |_{x_1}^{x_n} = 0$. But if $\delta y^{(1)}$ is arbitrary at the end points, q must be 0 there. Then either $q \equiv 0$, or q = 0 at the end points. But if q is 0 only at the end points, f must be a function of the particular end points of the problem and if a different set of data points $\{Y_i\}$ were used, f would have to be changed. Therefore, we shall consider here only the case $q \equiv 0$, and $\delta y = 0$ at x_1 , x_n .^{*} Thus, $f = p(y, y^{(1)})$, and the Euler-Lagrange equation becomes

(31)
$$L = p_0 - y^{(1)} p_{01} - y^{(2)} p_{11} = 0.$$

The analysis leading to conditions (6a) and (6b) gives, in this case,

(32a)
$$\partial L/\partial y = 0$$
, when $L = 0$,

(32b)
$$\sum_{k=0}^{2} y^{(k)} \partial L / \partial y^{(k)} = 0, \text{ when } L = 0.$$

Writing (31) as

(33)
$$L = L' + s y^{(2)},$$

then, by procedures similar to those used in obtaining (11), we find, if $s \neq 0$,

(34)
$$\frac{\partial}{\partial y}\left(\frac{L}{s}\right) \equiv 0, \qquad \frac{\partial}{\partial y}\left(\frac{L'}{s}\right) \equiv 0.$$

Note. If $s \equiv 0$, $p = y^{(1)}A(y) + B(y)$. But $A(y)y^{(1)}$ is an exact derivative, and does not contribute to the Euler-Lagrange equation, which in this case would be

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^{*} Also, if f = p + y''q, minimization of $\int f dx$ can occur with large oscillations in y'', since positive and negative contributions to the integral may cancel. In certain tests which were performed, this resulted in large oscillations in the smoothing curve, which we wish to avoid.

 $\partial B/\partial y = 0$. This result is of no interest in smoothing, and therefore the case $s \equiv 0$ will be ignored here.

Since L'/s is independent of y,

(35)
$$L'/s = -z(y^{(1)}), \text{ or} \\ L' = -sz(y^{(1)}),$$

where z is an arbitrary function of $y^{(1)}$. Then

(36)
$$L = s(y^{(2)} - z(y^{(1)})).$$

Since $s \neq 0$, the resultant differential equation in y is

(37a)
$$y'' - z(y') = 0.$$

Substituting the result (36) into condition (32b), we obtain also

(37b)
$$(y s_0 + y^{(1)} s_1)(y^{(2)} - z) + s(y^{(2)} - y^{(1)} z_1) = 0$$
, when $L = 0$.

But when L = 0, $y^{(2)} = z$, and therefore $y^{(2)} - y^{(1)}z_1$ must be 0 also. This requires either:

A. dz/dy' = z/y'.

This equation yields z = Cy'. The Euler-Lagrange equation (37) then becomes

(38)
$$y'' - Cy' = 0,$$

which has as its solution

(39)
$$y = \alpha e^{Cx} + \beta.$$

The constant C is fixed by the particular form of f, and therefore cannot vary between different pairs of data points. If the smoothing curve y(x) must pass through the given data $\{Y_i\}$, then α and β are fixed by these conditions for each interval, and therefore y' will in general not be continuous. Since discontinuities in y' are not compatible with the concept of smoothness, the solution (39) is not satisfactory.

B. z = 0.

This condition satisfies (37a) and (37b) if y'' = 0, which requires that y(x) be a straight line between each pair of data points. Since this also results in discontinuities in y', the case $\partial^2 f/(\partial y'')^2 = 0$ seems of no interest in the smoothing problem.

Note. This same conclusion may be drawn from equation (37a) without application of condition (32b), since this equation may be integrated twice to give yas a two-parameter function of x. Use of (32b) gives us the exact form of that function, but the same drawback exists in either case.

5. Conclusions. Given a set of data $\{Y_i\}$ for which a "smooth" function y(x) is desired. This function y is to be obtained by a minimization criterion of the form $\delta \int_{x_1}^{x_n} f(y, y', y'') dx = 0$, where y and y' are known at the end points, and

$$\partial^2 f/(\partial y'')^2 \neq 0.$$

Then a necessary and sufficient condition that the solution y(x) of the resultant

Euler-Lagrange ordinary differential equation become ay + b when Y_i is replaced by $aY_i + b$ is that f be of the form,

$$f = W(y', y'') + d\phi(y, y', x)/dx,$$

where W is a homogeneous function in y' and y''. Since $d\phi/dx$ does not contribute to the Euler-Lagrange equation for y(x), it may be ignored. Also, f (or W) should not be chosen linear in y''.

6. Applications. The simplest Lagrangian function f(y', y'') satisfying the requirements set forth above would seem to be $f = (y'')^2$. This choice appears to have been studied first by Holladay [1], and used first in smoothing by Podolsky [2]. It has also been used by Phillips [3] in the numerical solution of linear integral equations of a certain kind. Cook [4] has used $f = (y')^2$ and $f = (y'')^2$, both of which satisfy the criterion given here, in the numerical solution of a linear integral equation arising in the analysis of the photonuclear yields from bremstrahlen. Except in [4], where the author was aware of the present work, the choice $f = (y'')^2$ seems to have been made for simplicity, or because, if $y' \ll 1$, $(y'')^2$ is approximately the square of the curvature, which is a natural quantity to minimize if one is seeking a "smooth" curve. However, if f is the square of the curvature, it will not satisfy our criterion.

The result of the choice $f = (y'')^2$ leads, of course, to the Euler-Lagrange equation

(40)
$$y^{(4)} = 0,$$

so that the smooth curve is a set of cubic functions, which may be adjusted to give continuity of y and certain derivatives at or near the data points.

The simplicity, approximation to curvature, and fact that it satisfies the invariance properties studied here (which are to be expected for any "smooth" curve associated with our data) make the choice $f = (y'')^2$ a natural one; the results thus obtained show this choice is also a good one.

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