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TAYLOR MODELS AND COMPUTATIONS IN THE COMPLEX PLANE

ABSTRACT In this note we show how Taylor model methods can successfully alleviate the problems of conventional interval arithmetic in the complex plane being susceptible to significant overestimations caused by the dependency problems in the elementary operations. The use of Taylor models on the other hand results in self-validated methods that fully utilize the rich structure of the complex numbers.

To show how high order methods can be used for self-validated computations in the complex plane, we extend real-valued Taylor model methods to complex ones. The extension provides the tools to compute enclosures of the results of elementary operations and standard functions. We show how the new methods provide sharp and validated descriptions of image sets of analytic functions even after extended computations.

Keywords: Taylor models, complex interval arithmetic, dependency problem, wrapping effect.

Introduction Interval arithmetic on the field R of real numbers provides sharp and rigorous enclosures for the images of compact intervals under the elementary operations and intrinsic functions. However, while complex interval arithmetic can be seen as a straightforward extension of real-valued interval methods, it generally fails to provide sharp enclosures of the mathematically correct results since the necessary wrapping of results in new interval boxes often leads to significant overestimations [1, 2, 3].

Realistic problems often require the evaluation of complicated functions composed of multiple elementary operations and intrinsics. Evaluating such functions with conventional interval methods suffers from the dependency problem: if the computation involves several occurrences of the same variable, the result will be an overly pessimistic enclosure of the mathematically correct result. For the case of real-valued interval arithmetic, this has long been recognized as one of the main limitations of interval methods[4], and it has been shown [5] that high order Taylor model methods can avoid the dependency problem for practical purposes. In the case of interval arithmetic on the field C of complex numbers, the situation is further complicated by the fact that even the elementary operations and intrinsic functions are subject to the dependency problem. Thus, complex interval arithmetic is prone to significant overestimations and often fails to provide rigorous bounds with a sufficient sharpness even for polynomial expressions [6].

Complex numbers are commonly represented by pairs of two numbers: split into real and imaginary part or characterized by argument and absolute value

$$z = x + i \cdot y = r \exp(i\varphi) \tag{1}$$

Both representations are equivalent but lead to significantly different results when used in the context of complex interval arithmetic. Writing complex numbers in terms of real and imaginary part is equivalent to identifying C with the real linear space R^2. In this representation, we write complex interval numbers as $X + i \cdot Y$ with the real intervals X and Y. As such, complex intervals represent rectangles in the complex plane and the interval methods provide optimal enclosures for the addition and the multiplication with reals. However, enclosing the product of two such complex intervals in another interval generally leads to significant overestimations.

As an alternative to representing complex interval numbers by rectangles, the characterization by arguments and absolute values can be used to enclose sets of complex numbers. In that case we describe sets as $r \exp(i\Phi)$ with real intervals $r \subset R_0^+$ and $\Phi \subset [0, 2\pi]$. This description provides optimal validated enclosures for the product of sets of complex numbers. However, such a description generally overestimates the sum of these objects.

By not providing optimal enclosures for the elementary operations, neither of the two presented approaches utilizes the full power and rich structure of the complex field C. Other approaches of bringing self-validated computations to the complex plane while avoiding the excessive overestimation have been based on complex disks, represented by center and radius [7, 3]. However, in all cases the problem of overestimating the results of elementary operations is further aggravated in the case of the standard mathematical functions, where the actual overestimation may be arbitrary large. Thus, it has been recognized that conventional interval techniques are insufficient to properly deal with computations in the complex plane. In this paper we will show how the use of high order Taylor model methods can successfully overcome the limitations of conventional interval methods when it comes to rigorously enclosing the image sets of analytic functions defined on the complex plane.

Complex Taylor Models Let us introduce Complex Taylor Models (CTM). The definition and set of its operations are very similar to Taylor Models (TM) in the real case. And one of the two variants presented of CTM constructing will be based on real TMs completely. Real TM were suggested and their properties were investigated in details in [8, 9]. TM are presented as a data type in the Cosy Infinity code [10]. All examples of section 3 were calculated with using of this code.

For convenience we start with definition of Taylor Models for real functions of two real variables.

Definition 1 *Let u be a real function of two real variables $x, y \in R$. Suppose the function is defined and has continuous partial derivatives up to order $n+1$ (at least) at each point of two-dimensional box*

$$M = \{(x, y) : a_1 \leq x \leq b_1, a_2 \leq y \leq b_2\} \subseteq R^2. \tag{2}$$

Assume that $(x_0, y_0) \in M$ and we have a pair of objects: a polynomial

$$P_{\alpha,u}(x - x_0, y - y_0) = \sum_{\substack{0 \leq j,k \leq n \\ j+k \leq n}} K_{j,k} (x - x_0)^j (y - y_0)^k \tag{3}$$

and a real interval $I_{\alpha,u}$ (the interval remainder bound), such that for any $(x, y) \in M$ the following inclusion is true

$$u(x, y) \in P_{\alpha,u}(x - x_0, y - y_0) + I_{\alpha,u}. \tag{4}$$

Then we say the pair $T_{\alpha,u} = (P_{\alpha,u}, I_{\alpha,u})$ is a Taylor Model of function $u(x, y)$. Here the parameter $\alpha = (n, (x_0, y_0), M)$ contains information about the order of the Taylor polynomial, reference point (x_0, y_0) and domain M.

It is natural to consider the Taylor polynomial as corresponding truncated Taylor series, and interval remainder bounds as interval estimation of remainder term. But it is practically useless to consider this interpretation as a path of finding of Taylor Models. Instead of it we should introduce rules of Taylor Model arithmetic with elementary operations (sum, product), intrinsic functions etc. In the following we assume that these rules have been implemented. For details see [9]. For example, evidently we can define a Taylor Model for the sum of functions $u(x,y)$ and $w(x,y)$ as

$$T_{\alpha,u} + T_{\alpha,w} = T_{\alpha,u+w} = \left(P_{\alpha,u} + P_{\alpha,w}, I_{\alpha,u} + I_{\alpha,w}\right). \tag{5}$$

Here the additions of two polynomials and two real interval numbers should be done in the usual ways.

Consider a complex function f of one complex variable $z \in C$:

$$f(z) = u(x,y) + i \cdot w(x,y). \tag{6}$$

Here $x = \operatorname{Re} z$, $y = \operatorname{Im} z$. Suppose that assumptions of the definition 1 for $u = \operatorname{Re} f(z)$ and $w = \operatorname{Im} f(z)$ are fulfilled and we have separate real Taylor Models $T_{\alpha,u}$ and $T_{\alpha,w}$ of the real and imaginary parts of as real functions of two variables.

Definition 2 *We say an ordered pair of Taylor Models $T^{cc}_{\alpha,f} = (T_{\alpha,u}, T_{\alpha,w})$ is a Coordinate Complex Taylor Model (CCTM) of the complex function $f(z)$. Thus we have the following statement for any $z = x + i \cdot y$ (where $(x,y) \in M$):*

$$f(z) \in T^{cc}_{\alpha,f} = T_{\alpha,u} + i \cdot T_{\alpha,w} \tag{7}$$

The next step is the introduction elementary operations and standard functions for Coordinate Complex Taylor Models. Let us start with addition and multiplication. Consider two complex functions $f(z) = u(x,y) + i \cdot w(x,y)$, $g(z) = q(x,y) + i \cdot r(x,y)$, and their Coordinate Complex Taylor Models. We can define the elementary operations like for complex numbers. For example:

$$\begin{aligned}
T^{cc}_{\alpha,f} + T^{cc}_{\alpha,g} &= T^{cc}_{\alpha,f+g} = \left(T_{\alpha,u} + T_{\alpha,q}, T_{\alpha,w} + T_{\alpha,r}\right) && (8)\\
T^{cc}_{\alpha,f} \cdot T^{cc}_{\alpha,g} &= T^{cc}_{\alpha,f\cdot g} \\
&= \left(T_{\alpha,u} \cdot T_{\alpha,q} - T_{\alpha,w} \cdot T_{\alpha,r}, T_{\alpha,u} \cdot T_{\alpha,r} + T_{\alpha,w} \cdot T_{\alpha,q}\right) && (9)
\end{aligned}$$

Now consider the exponential function

$$\exp f(z) = \exp u \cos w + i \cdot \exp u \sin w. \tag{10}$$

Obviously we have

$$T^{cc}_{\alpha,\exp f} = \left(T_{\alpha,\exp u} \cdot T_{\alpha,\cos u}, T_{\alpha,\exp u} \cdot T_{\alpha,\sin u}\right). \tag{11}$$

We should remind that the rules of obtaining real Taylor Models $T_{\alpha,\exp u}$, $T_{\alpha,\cos u}$, $T_{\alpha,\sin u}$ were described in [9].

So the key idea of the coordinate approach is to split the complex function into the real and imaginary parts and manipulate with well-known real Taylor Models for them. It is clear that in this approach, it is possible to develop a complete formalism for complex TM arithmetic like in its real counterpart, the resulting method helps in the suppression of the dependency problem [5] and the remainder bounds have the high-order scaling property.

But sometimes it is reasonable to have "pure" Complex Taylor Models. Let us consider the analytic complex function f of one variable z in a circle $S(r_0, z_0)$:

$$f(z) : S(r_0, z_0) \subset C \to C. \tag{12}$$

Here $z \in C$; $z_0 \in C$ is a reference point; $r_0 \in R_+$ is the radius of the circle:

$$S(r_0, z_0) = \{z : |z - z_0| < r_0, r_0 > 0\}. \tag{13}$$

Now let us introduce Complex Taylor Models. Further we assume that $z_0 \in D \subset S(r_0, z_0)$ where $D = \{z \in C : a_1 \leq \operatorname{Re} z \leq b_1, a_2 \leq \operatorname{Im} z \leq b_2\}$ is a complex box. Here $a_1, b_1, a_2, b_2 \in R$.

Definition 3 *Let us assume that for the analytic complex function $f(z) : D \subset C \to C$ we have a pair of objects: a complex polynomial*

$$P_{\delta,f}(z - z_0) = \sum_{j=0}^{n} K_j \cdot (z - z_0)^j \tag{14}$$

and complex interval $I_{\delta,f}$, such that for any $z \in D$

$$f(z) \in P_{\delta,f}(z - z_0) + I_{\delta,f}. \tag{15}$$

Here the parameter δ contains information about the order of the polynomial, reference point and domain interval: $\delta = (n, z_0, D)$. Then we say the pair $T^c_{\delta,f} = (P_{\delta,f}, I_{\delta,f})$ is a Complex Taylor Model of the function f. We call n the order of the Taylor Model, z_0 the reference point of the Taylor Model, D the domain interval of the Taylor Model, δ the parameter of the Taylor Model. Also we call $P_{\delta,f}$ the Taylor polynomial, $I_{\delta,f}$ the interval remainder bound.

Let us introduce rules of the Complex Taylor Model constructing for the sum and product of two functions. We note that this is just a reformulation of the real Taylor Models case. With this aim we will consider a pair of analytical complex functions $f(z)$ and $g(z)$, for which Taylor models are known, i.e. $T^c_{\delta,f} = (P_{\delta,f}, I_{\delta,f})$ and $T^c_{\delta,g} = (P_{\delta,g}, I_{\delta,g})$ accordingly. Thus, it is evident that

$$\begin{aligned} f(z) + g(z) &\in ((P_{\delta,f}(z - z_0) + I_{\delta,f}) + (P_{\delta,g}(z - z_0) + I_{\delta,g})) \\ &= (P_{\delta,f}(z - z_0) + P_{\delta,g}(z - z_0)) + (I_{\delta,f} + I_{\delta,g}) \end{aligned} \tag{16}$$

or it means that a Taylor model $T^c_{\delta,f+g}$ for $f + g$ can be obtained via

$$P_{\delta,f+g} = P_{\delta,f} + P_{\delta,g} \quad \text{and} \quad I_{\delta,f+g} = I_{\delta,f} + I_{\delta,g} \tag{17}$$

Thus we define

$$T^c_{\delta,f} + T^c_{\delta,g} = T^c_{\delta,f+g} = (P_{\delta,f} + P_{\delta,g}, I_{\delta,f} + I_{\delta,g}). \tag{18}$$

In a similar way we will consider a product of the Taylor models. Let us write down a true for any $z \in D$ relation as follows

$$\begin{aligned} f(z) \cdot g(z) &\in ((P_{\delta,f}(z - z_0) + I_{\delta,f}) \cdot (P_{\delta,g}(z - z_0) + I_{\delta,g})) \\ &= (P_{\delta,f}(z - z_0) \cdot P_{\delta,g}(z - z_0)) + P_{\delta,f}(z - z_0) \cdot I_{\delta,g} \\ &\quad + P_{\delta,g}(z - z_0) \cdot I_{\delta,f} + (I_{\delta,f} \cdot I_{\delta,g}). \end{aligned} \tag{19}$$

We need to note, that $P_{\delta,f}(z-z_0)\cdot P_{\delta,g}(z-z_0)$ is a polynomial of 2n-th order. Let us divide this polynomial into the sum of two: the first one of n-th order and agrees with the Taylor polynomial $P_{\delta,f\cdot g}$ of $f\cdot g$ and an additional polynomial P_e so that

$$P_{\delta,f}(z-z_0)\cdot P_{\delta,g}(z-z_0)=P_{\delta,f\cdot g}(z-z_0)+P_e(z-z_0). \tag{20}$$

We denote bounds of polynomials by $B(P)$ for polynomial $P:D\subset C\to C$:

$$\forall z\in D, P(z-z_0)\in B(P). \tag{21}$$

Remark 4 *We demand that $B(P)$ is at least as sharp as direct interval evaluation of $P(z-z_0)$ on D. More sophisticated methods exist, but are not important for our purposes.*

Here $B(P)$ is a complex interval. Then $I_{\delta,f\cdot g}$ can be found in following way:

$$I_{\delta,f\cdot g}=B(P_e)+B(P_{\delta,f})\cdot I_{\delta,g}+B(P_{\delta,g})\cdot I_{\delta,f}+I_{\delta,f}\cdot I_{\delta,g}. \tag{22}$$

Thus it is possible to define

$$T^c_{\delta,f}\cdot T^c_{\delta,g}=T^c_{\delta,f\cdot g}=(P_{\delta,f\cdot g},I_{\delta,f\cdot g}). \tag{23}$$

By using of definition of sum and product of the Taylor models it is possible to calculate models for functions of the type $Q(f)$: $T^c_{\delta,Q(f)}=\left(P_{\delta,Q(f)},I_{\delta,Q(f)}\right)$, where Q is a complex polynomial of function f, for which the Taylor model will be considered as known. With this numerical coefficients $t_k\in C$ of polynomial $Q(f)=t_0+t_1\cdot f+\ldots+t_m\cdot f^m$ are represented as the following Taylor models $T^c_{\delta,t_k}=(P_{\delta,t_k},I_{\delta,t_k})$, where $P_{\delta,t_k}=t_k$ and $I_{\delta,t_k}=[(0+i\cdot 0),(0+i\cdot 0)]$.

For practical use of the Taylor models we need to have an algorithm of calculations of intrinsic functions of the Taylor models. This algorithm is based on the theorem of expansion of analytical function into the Taylor series.

As it is known, a function f that is analytic on $S(r_0,z_0)$ can be represented as the following power series for any $z\in S(r_0,z_0)$:

$$f(z)=\sum_{k=0}^{\infty}\frac{1}{k!}\frac{\partial^k f(z_0)}{\partial z^k}(z-z_0)^k. \tag{24}$$

One can also consider the complex function as a sum of two real-valued functions of real arguments:

$$f(z)=u(x,y)+i\cdot w(x,y), \tag{25}$$

where $x=\operatorname{Re} z\in R$, $y=\operatorname{Im} z\in R$.

After splitting $f(z)$ into real and imaginary parts we can employ Taylor expansions of the functions (with Lagrangian remainder term) $u(x,y)$ and $w(x,y)$ to represent them as finite sums

$$\begin{aligned} u(x,y) &= \sum_{k=0}^{n}\frac{1}{k!}\left(\Delta x\cdot\frac{\partial}{\partial x}+\Delta y\cdot\frac{\partial}{\partial y}\right)^k u(x_0,y_0)\\ &\quad+\frac{1}{(n+1)!}\left(\Delta x\cdot\frac{\partial}{\partial x}+\Delta y\cdot\frac{\partial}{\partial y}\right)^{n+1} u(x_{\theta_1},y_{\theta_1}), && (26)\\ w(x,y) &= \sum_{k=0}^{n}\frac{1}{k!}\left(\Delta x\cdot\frac{\partial}{\partial x}+\Delta y\cdot\frac{\partial}{\partial y}\right)^k w(x_0,y_0)\\ &\quad+\frac{1}{(n+1)!}\left(\Delta x\cdot\frac{\partial}{\partial x}+\Delta y\cdot\frac{\partial}{\partial y}\right)^{n+1} w(x_{\theta_2},y_{\theta_2}), && (27)\end{aligned}$$

where $\Delta x = \operatorname{Re}\Delta z$, $\Delta y = \operatorname{Im}\Delta z$, $\Delta z = z - z_0$, $x_0 = \operatorname{Re} z_0$, $y_0 = \operatorname{Im} z_0$, $x_{\theta_j} = x_0 + \theta_j \cdot \Delta x$, $y_{\theta_j} = y_0 + \theta_j \cdot \Delta y$, $0 \le \theta_j \le 1$, $j = 1, 2$; and the partial differential operator $\left(\Delta x \cdot \frac{\partial}{\partial x} + \Delta y \cdot \frac{\partial}{\partial y}\right)^k$ works as

$$\left(\Delta x \cdot \frac{\partial}{\partial x} + \Delta y \cdot \frac{\partial}{\partial y}\right)^k = \sum_{j=0}^{k} \frac{k!}{j!\,(k-j)!} \Delta x^j \Delta y^{(k-j)} \frac{\partial^k}{\partial x^j \partial y^{(k-j)}}. \tag{28}$$

For the analytic function f the following formulae are correct

$$i \cdot \frac{\partial}{\partial x} f(\widetilde{z}) = \frac{\partial}{\partial y} f(\widetilde{z}), \tag{29}$$

$$\frac{\partial}{\partial z} f(\widetilde{z}) = \frac{\partial}{\partial x} u(\widetilde{x}, \widetilde{y}) + i \cdot \frac{\partial}{\partial x} w(\widetilde{x}, \widetilde{y}), \tag{30}$$

$$\begin{aligned} \left(\Delta z \cdot \frac{\partial}{\partial z}\right)^k f(\widetilde{z}) &= \left((\Delta x + i \cdot \Delta y) \frac{\partial}{\partial x}\right)^k f(\widetilde{z}) \\ &= \left(\Delta x \cdot \frac{\partial}{\partial x} + \Delta y \cdot \frac{\partial}{\partial y}\right)^k f(\widetilde{z}), \\ &= \left(\Delta x \cdot \frac{\partial}{\partial x} + \Delta y \cdot \frac{\partial}{\partial y}\right)^k (u(\widetilde{x}, \widetilde{y}) + i \cdot w(\widetilde{x}, \widetilde{y})), \end{aligned} \tag{31}$$

where k is integer number,$\forall \widetilde{z} \in S(r_0, z_0)$, $\widetilde{x} = \operatorname{Re}\widetilde{z}$, $\widetilde{y} = \operatorname{Im}\widetilde{z}$.

Thus after taking into account these formulae, the Taylor expansions of $u(x, y)$ and $w(x, y)$, and the representation of $f(z)$ as the power series we can obtain the following statements

$$f(z) = \sum_{k=0}^{n} \frac{1}{k!} \frac{\partial^k f(z_0)}{\partial z^k} (z - z_0)^k + \operatorname{Re} R_{n+1}(\theta_1) + i \cdot \operatorname{Im} R_{n+1}(\theta_2), \tag{32}$$

where $R_{n+1}(\theta) = \frac{1}{(n+1)!} \frac{\partial^{(n+1)} f(z_0 + \theta(z - z_0))}{\partial z^{(n+1)}} (z - z_0)^{(n+1)}$ and $\theta_1, \theta_2 \in [0, 1]$.

Or in the following form:

$$\begin{aligned} f(z) &= \sum_{k=0}^{n} \frac{1}{k!} \frac{\partial^k f(z_0)}{\partial z^k} (z - z_0)^k \\ &+ \frac{\partial^{(n+1)} f(z_{\theta_1}) / \partial z^{(n+1)} + \partial^{(n+1)} f(z_{\theta_2}) / \partial z^{(n+1)}}{2(n+1)!} (z - z_0)^{n+1} \\ &+ \frac{\overline{\partial^{(n+1)} f(z_{\theta_1}) / \partial z^{(n+1)} - \partial^{(n+1)} f(z_{\theta_2}) / \partial z^{(n+1)}}}{2(n+1)!} \overline{(z - z_0)}^{n+1}. \end{aligned} \tag{33}$$

Here $\bar{}$ means conjugate complex value, $z_{\theta_1} = z_0 + \theta_1 (z - z_0)$, $z_{\theta_2} = z_0 + \theta_2 (z - z_0)$.

Let us emphasize that R_{n+1} has the same form as the well-known Lagrangian remainder term in Taylor theorem for real functions. So we can formulate

Theorem 5 *(Complex Interval analogy of Taylor's theorem). For the analytic function f the following inclusion is true with any $z \in S(r_0, z_0)$,*

$$\begin{aligned} f(z) \;\; &\in \;\; \sum_{k=0}^{n} \frac{1}{k!} \frac{\partial^k f(z_0)}{\partial z^k} (z - z_0)^k \\ &+ \frac{1}{(n+1)!} \frac{\partial^{(n+1)} f(z_0 + \Theta(z - z_0))}{\partial z^{(n+1)}} (z - z_0)^{(n+1)}, \end{aligned} \tag{34}$$

where $\Theta = [0,1] \subset R$ is a real interval. The last term (interval remainder term) has been considered as complex interval (a box in complex plane), that contains the set of values (curve on complex plane) of complex function $R_{n+1}(\theta) = \frac{1}{(n+1)!} \frac{\partial^{(n+1)} f(z_0 + \theta(z - z_0))}{\partial z^{(n+1)}} (z - z_0)^{(n+1)}$ with $\theta \in [0,1]$, and it can apparently be obtained by interval evaluation of R_{n+1}.

Let us illustrate this result for the special case $n = 0$.

$$\begin{aligned} f(z) \;\; &= \;\; f(z_0) + \mathrm{Re}\left(\frac{\partial}{\partial z} f(z_0 + \theta_1 \cdot (z - z_0)) \cdot (z - z_0)\right) \\ &+ i \cdot \mathrm{Im}\left(\frac{\partial}{\partial z} f(z_0 + \theta_2 \cdot (z - z_0)) \cdot (z - z_0)\right), \end{aligned} \tag{35}$$

Or we can write it in the following form:

$$\begin{aligned} f(z) \;\; &= \;\; f(z_0) + \frac{\partial f(z_{\theta_1})/\partial z + \partial f(z_{\theta_2})/\partial z}{2} (z - z_0) \\ &+ \overline{\frac{\partial f(z_{\theta_1})/\partial z - \partial f(z_{\theta_2})/\partial z}{2}}\,\overline{(z - z_0)}. \end{aligned} \tag{36}$$

Here $^{-}$ means conjugate complex value, $z_{\theta_1} = z_0 + \theta_1 (z - z_0)$, $z_{\theta_2} = z_0 + \theta_2 (z - z_0)$. The statements give us a practical way to bound remainder term of intrinsic functions.

Remark 6 *The remainder of the Taylor series in the complex plane is usually expressed in the form:*

$$R_{n+1} = \frac{(z - z_0)^{n+1}}{2\pi i} \oint_{\Gamma} \frac{f(\zeta)}{(\zeta - z)(\zeta - z_0)^{n+1}}. \tag{37}$$

Here $z \in int\Gamma$, $\Gamma = \{\zeta : |\zeta - z_0| = r\}$. But this form is not convenient for simple realization. Since it involves integration. The representation of the remainder term in the form suggested in this paper is similar to the real functions case, allows using almost the same formulae like in realized real Taylor Models and easier treatment of remainders.

Let consider us several examples of intrinsic functions. We start with the examination of the exponential function. As it is known, $(\exp z)^{(k)} = \exp z$, where $()^{(k)}$ is the operation of taking of derivative of k-th order. Bearing in mind that $\exp 0 = 1$, we can find following

$$\begin{aligned} \exp f(z) \;\; &= \;\; \exp(c_{\delta,f}) \cdot \exp\left(0 + \widetilde{f}(z)\right) \\ &\in \;\; \exp(c_{\delta,f}) \cdot \begin{pmatrix} 1 + \widetilde{f}(z) + \frac{1}{2}\left(\widetilde{f}(z)\right)^2 + \ldots + \frac{1}{k!}\left(\widetilde{f}(z)\right)^k \\ + \frac{1}{(k+1)!}\left(\widetilde{f}(z)\right)^{k+1} \exp\left(\Theta \cdot \widetilde{f}(z)\right) \end{pmatrix}. \end{aligned} \tag{38}$$

Here and further $f(z) = c_{\delta,f} + \widetilde{f}(z)$, $\Theta = [0,1]$. The right part of taken expression can serve as the source for constructing the Taylor model for the function $\exp f(z)$. It consists of the polynomial part and the remainder. The possibility of the constructing of the Taylor model for a polynomial has been discussed above. The remainder must be bounded by the complex interval and added into the interval remainder bounds of the Taylor model of the polynomial part.

The same scheme is used for the construction of the Taylor model for the function $\left\{\sqrt{f(z)}\right\}_j$, where $\{\}_j$ denotes one-valued branch of the multi-valued function of square root $\sqrt{f(z)}$. Let $0 \notin P_{\delta,f(z)}(z - z_0) + I_{\delta,f(z)}$ for any $z \in D$. We will also introduce such notations as

$$\begin{array}{c} c_{\delta,f} = r\exp(i\varphi),\ r = |c_{\delta,f}|,\ \varphi = \arg c_{\delta,f}, \\ \varepsilon_j = \left\{\sqrt{c_{\delta,f}}\right\}_j = \sqrt{r}\cdot\exp\left(i\left(\varphi/2 + \pi(j-1)\right)\right),\ j = 1,2. \end{array}$$

Then with taking into account of $\left(\{\sqrt{z}\}_j\right)^{(k)} = (-1)^{k-1}\frac{(2k-3)!!}{2^k\left(\{\sqrt{z}\}_j\right)^{2k-1}}$, we get

$$\begin{aligned} \left\{\sqrt{f(z)}\right\}_j &= \left\{\sqrt{c_{\delta,f} + \widetilde{f}(z)}\right\}_j \\ &\in \left(\begin{array}{c} \varepsilon_j \cdot \left(\begin{array}{c} 1 + \frac{\widetilde{f}(z)}{2c_{\delta,f}} - \frac{\left(\widetilde{f}(z)\right)^2}{2^2 2!(c_{\delta,f})^2} + \dots \\ +(-1)^{k-1}\frac{(2k-3)!!\left(\widetilde{f}(z)\right)^k}{2^k k!(c_{\delta,f})^k} \end{array}\right) \\ +(-1)^k\frac{(2k-1)!!}{2^{k+1}(k+1)!}\frac{\left(\widetilde{f}(z)\right)^{k+1}}{\left(\left\{\sqrt{c_{\delta,f}+\Theta\cdot\widetilde{f}(z)}\right\}_j\right)^{2k+1}} \end{array}\right) \end{aligned} \tag{39}$$

Here $(2k-1)!! = \prod\limits_{m=1}^{k}(2m-1)$, $c_{\delta,f} \neq 0$,

$0 \notin c_{\delta,f} + \Theta\cdot\left(B\left(P_{\delta,\widetilde{f}(z)}(z - z_0)\right) + I_{\delta,\widetilde{f}(z)}\right)$ for any $z \in D$.

Let us consider one-valued branches of the function of natural logarithm $Lnf(z)$. Let again $0 \notin P_{\delta,f(z)}(z - z_0) + I_{\delta,f(z)}$ for any $z \in D$. With this we keep that $\frac{\partial}{\partial z}\{Ln\,z\}_j = \frac{1}{z}$ and $\left(\{Ln\,z\}_j\right)^{(k)} = (-1)^{k+1}\frac{(k-1)!}{z^k}$ at $k \geq 2$. Thus

$$\begin{aligned} \{Lnf(z)\}_j &= \left\{Ln\left(c_{\delta,f} + \widetilde{f}(z)\right)\right\}_j \\ &\in \left(\begin{array}{c} \{Ln(c_{\delta,f})\}_j + \frac{\widetilde{f}(z)}{c_{\delta,f}} - \frac{1}{2}\frac{\left(\widetilde{f}(z)\right)^2}{(c_{\delta,f})^2} + \dots \\ +(-1)^{k+1}\frac{1}{k}\frac{\left(\widetilde{f}(z)\right)^k}{(c_{\delta,f})^k} \\ +(-1)^{k+2}\frac{1}{k+1}\frac{\left(\widetilde{f}(z)\right)^{k+1}}{\left(c_{\delta,f}+\Theta\cdot\widetilde{f}(z)\right)^{k+1}} \end{array}\right). \end{aligned} \tag{40}$$

As above $c_{\delta,f} \neq 0$, $0 \notin c_{\delta,f} + \Theta\cdot\left(B\left(P_{\delta,\widetilde{f}(z)}(z - z_0)\right) + I_{\delta,\widetilde{f}(z)}\right)$ for any $z \in D$.

Definition 7 *Let us consider a Complex Taylor Model* $T^c_{\delta,f} = \left(P_{\delta,f}(z - z_0), I_{\delta,f}\right)$. *Let* $|I|$ *denotes diameter of a complex interval* $I = [a_1,a_2] + i\cdot[b_1,b_2]$: $|I| = \sqrt{(a_2 - a_1)^2 + (b_2 - b_1)^2}$. *Then we say* $|I_{\delta,f}|$ *is sharpness of the Taylor Model.*

Theorem 8 *(Taylor Model Scaling Theorem). Let* $f(z)$ *and* $g(z)$ *are analytic complex functions that have n-th order Complex Taylor Models* $T^c_{\delta,f} = (P_{\delta,f}(z - z_0), I_{\delta,f})$ *and* $T^c_{\delta,g} = (P_{\delta,g}(z - z_0), I_{\delta,g})$ *correspondingly. Let us consider circle of minimal possible radius h with center in point* z_0 *such that it includes domain D:* $D \subset S(h, z_0)$*. Let the remainder bounds* $I_{\delta,f}$ *and* $I_{\delta,g}$ *satisfy* $|I_{\delta,f}| = O(h^{n+1})$ *and* $|I_{\delta,g}| = O(h^{n+1})$*. Then the Taylor Models for the sum and products of* $f(z)$ *and* $g(z)$ *obtained via addition and multiplication of Complex Taylor Models satisfy*

$$|I_{\delta,f+g}| = O\left(h^{n+1}\right) \quad \text{and} \quad |I_{\delta,f\cdot g}| = O\left(h^{n+1}\right). \tag{41}$$

Furthermore, let F be any of the intrinsic functions defined above, then the Complex Taylor Model for $F(f)$ *obtained by the above instructions satisfies*

$$\left|I_{\delta,F(f)}\right| = O\left(h^{n+1}\right). \tag{42}$$

We say the Complex Taylor Models have the $(n+1)$*st order scaling property.*

Proof. The proof for the binary operations follows directly from the definition of the remainder bounds for the binaries. Similarly, the proof for the intrinsics follows because all intrinsics are composed of binary operations as well as an additional complex interval, the width (diameter) of which scales at least with the $(n+1)$st power of a bound of a function that scales at least linearly with h. ■

Examples In this section we illustrate how the use of high order complex Taylor models can indeed provide sharp and guaranteed bounds on the ranges of complicated complex functions. The main advantage of Taylor models methods over the use of conventional interval techniques lies in the propagation of high order functional dependencies from one computational step to the next; suppressing the *wrapping* of intermediate results between each and every elementary operation.

As a first example of how even simple elementary operations in the complex plane can result in overestimating the function's ranges, we consider a simple monomial function of order six.

$$f_1(z) = z^6 \tag{43}$$

While linear methods cannot properly model f_1, it is clear that any high order method of at least order six can model the functional behavior up to machine precision. Figure 1 shows the the mathematically correct range of f_1 over the domain $D_1 = [3,5] + i[1,4]$. While conventional interval arithmetic in either the x/y or the r/φ convention is bound to overestimate the exact range, modeling that function with a single Taylor model over the whole domain results in a sharpness that is in the order of the machine precision.

As a second example for how Taylor model methods can provide sharp enclosures even for complicated functions, consider the function f_2 that is analytic in the whole complex plane C:

$$f_2(z) = z^2 + \cos(z) + 4i\exp\left(\frac{z^3}{7} + \sin\left(z + \exp\left(0.5 + z^2\right)\right)\right) \tag{44}$$

The figure 2 shows the exact range of f_2 over the domain $D_2 = [-0.01, 0.11] + i[-0.01, 0.11]$. Additionally, a range enclosure obtained with conventional interval arithmetic is included. While the interval enclosure is rigorous, it does not provide a sharp enclosure of the mathematically exact range. Utilizing complex Taylor model methods on the other hand, allows the computation of rigorous enclosures that are extremely sharp as shown in the figure 3.

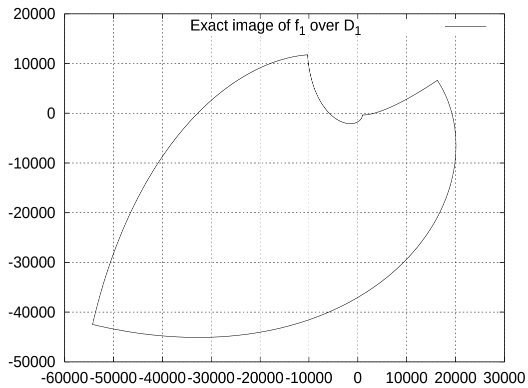

Figure 1: Exact range of z^6 over the complex interval domain $D_1 = [3,5] + i\,[1,4]$. The computed interval enclosure of the range exceeds the plotted range in all coordinate directions.

The graph also illustrates how for a given domain, the sharpness of Taylor model enclosures does indeed scale with the $(n+1)$-st order of that domain, where n is the order of the Taylor models.

As another example of how high order Taylor model methods can accurately enclose functional dependencies, Figure 4 shows the evaluation of f_2 over the domain $D_3 = [0, 0.02] + i[-0.1, 0.12]$. Like in the previous example, the plot shows the exact mathematical range and its interval enclosure and the strong non-linearity of f_2 leads to a significant overestimation in the interval enclosure of the mathematically exact range. As shown in the Figure 5 , complex Taylor models on the other hand succeed in finding sharp enclosures for the function f_2.

As an illustration of how the Taylor model approach can often significantly improve the sharpness of computed enclosures over sizable domains, consider the evaluation of the function f_2 over the domain box $D_4 = (0.01 + i0.01) + \lambda([-0.5, 0.5] + i[0.5, 0.5])$ Figure 6 shows the widths of the enclosures computed with interval and Taylor model methods for several different domain size parameters λ. Apparently, for each of the different methods, the size of the computed enclosure scales with a power of the domain size and is limited from below by the machine accuracy. However, while conventional intervals scales approximately linear with the domain width, the accuracy of Taylor model methods does indeed scale with the $(n + 1)$-st order of the domain size. Thus, once the domain size drops below a problem and order dependent threshold, Taylor model computations can often achieve a much higher sharpness over larger domains than conventional interval techniques.

This example also shows that “in the large”, the Taylor model approach can sometimes be worse than simple evaluation with conventional intervals. In fact, Taylor model methods will usually succeed if the contributions of all the highest order polynomial terms drop faster with order than the number of coefficients of a given order. Based on this rule of thumb, for polynomials with coefficients of magnitude 1, the Taylor model methods do not work well over domains with magnitudes larger than 1; on the other hand, if the domains have magnitudes of 0.1 or less, the Taylor model methods tend to work very well. Thus, if a given problem can be treated with conventional interval techniques, there is usually nothing to be gained by using Taylor models. However, if the problem requires domain splitting the use of Taylor models often becomes advantageous, especially if the interval

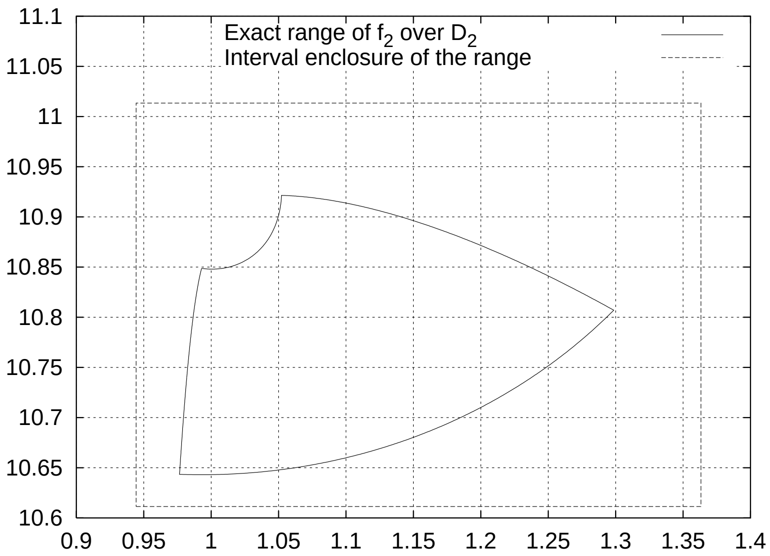

Figure 2: The plot shows the exact range and interval enclosure of the range of f_2 over the complex interval domain $D_2 = [-0.01, 0.11] + i\,[-0.01, 0.11]$.

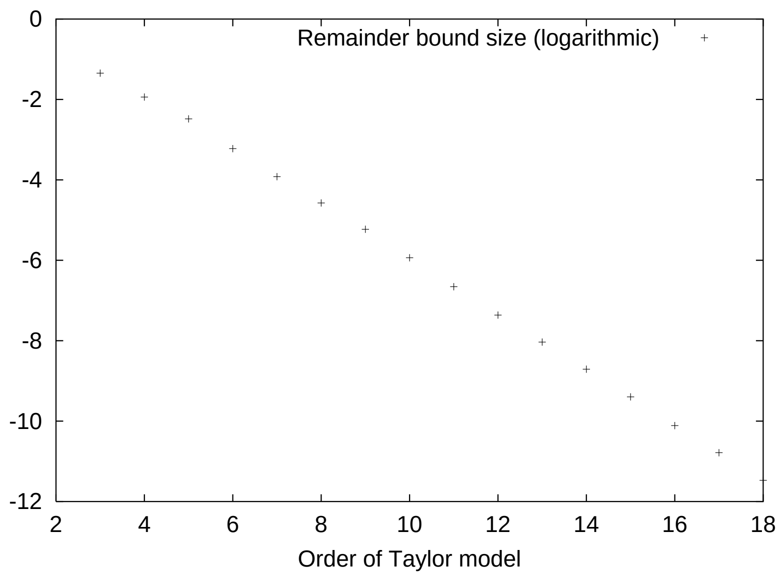

Figure 3: The graph shows the decadic logarithm of the size of the Taylor model remainder bounds for f_2 over the domain D_2 with the reference point $z_0 = 0.01 + i \cdot 0.01$ as a function of Taylor model orders.

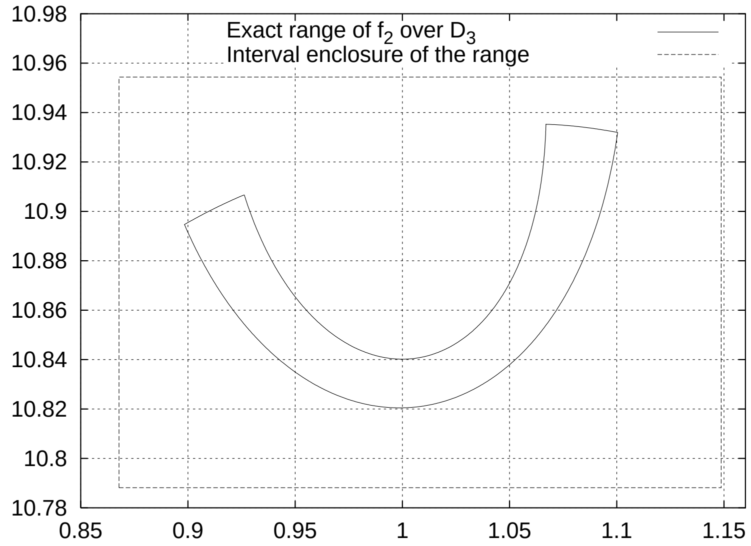

Figure 4: The plot shows the exact range and interval enclosure of the range of f_2 over the complex interval domain $D_3 = [0, 0.02] + i\,[-0.1, 0.12]$.

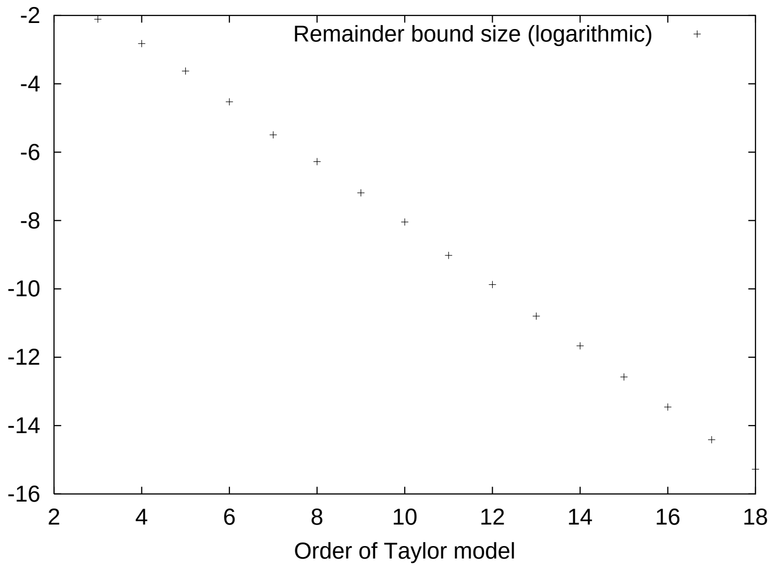

Figure 5: The graph shows the decadic logarithm of the size of the Taylor model remainder bounds for f_2 over the domain D_3 with the reference point $z_0 = 0.01 + i \cdot 0.01$ as a function of Taylor model orders.

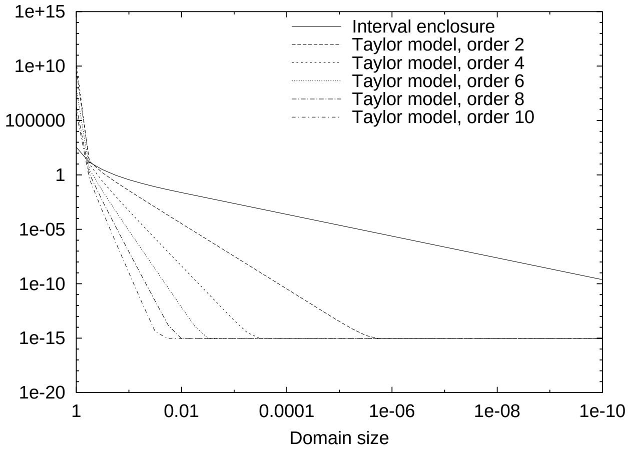

Figure 6: Dependence of the computed enclosure width on the size of the domain for conventional interval arithmetic and complex Taylor models of orders two, four, six, eight, and ten.

approach requires domain splitting beyond the threshold at which the Taylor approach shows significant improvements.

While Taylor model methods are computationally more expensive than conventional interval methods, the increased sharpness of the computed enclosures usually outweighs the computational expense. This is especially true if the desired sharpness requires domain splitting. To illustrate this, we measure the computational expense of evaluating f_2 over the domain D_4 by defining the information count as the number of floating point numbers that have to be stored and processed in order to obtain the desired sharpness in the enclosure. Thus, the information count equals the number of domain intervals multiplied with the actual storage requirements for a single instance of the underlying data type. For complex functions, the information counts for intervals N_I and n-th order Taylor models $N_{T,n}$ are given by

$$N_I = (\#boxes) \times 4 \tag{45}$$

$$N_{T,n} = (\#boxes) \times 2 \left(\frac{(n+2)!}{2 \cdot n!} + n + 2 \right). \tag{46}$$

Following table lists the maximum width of subdomains, and the corresponding information counts, necessary to enclose the range of f_2 over the domain D_4 with a uniform sharpness of 10^{-3} and 10^{-5}, respectively.

$Method$	$Required Domain Width$		$Information Count$	
$Sharpness$	10^{-3}	10^{-5}	10^{-3}	10^{-5}
$Interval$	0.418×10^{-3}	0.418×10^{-5}	$> 10^{200}$	$> 10^{200}$
$Taylor, n = 2$	0.304×10^{-1}	0.627×10^{-2}	1.3×10^{21}	2×10^{97}
$Taylor, n = 4$	0.104	0.040	26030646	4×10^{16}
$Taylor, n = 6$	0.180	0.100	158136	71217904
$Taylor, n = 8$	0.214	0.145	72659	1525956
$Taylor, n = 10$	0.317	0.181	12447	333208
$Taylor, n = 12$	0.318	0.209	16439	158038
$Taylor, n = 14$	0.321	0.316	20303	21791
$Taylor, n = 16$	0.332	0.316	22121	27351

Due to a prohibitively large number of domain splittings, straightforward interval methods and low order Taylor models fail to achieve the required sharpness. However, high order Taylor model methods can provide the requested accuracy with a moderate information count and without imposing excessive requirements on the computational overhead. Moreover, it is apparent that for each of the two problems there is an optimal computation order that finds the results at a minimal cost. At this point, any further increase of the computation order results in only negligible improvements in sharpness at the expense of increased information counts.

Conclusion We have developed an approach that allows the rigorous representation of analytic functions by complex Taylor models. Compared to conventional interval methods that model functions by range intervals, the new method propagates information on high order derivatives together with rigorous remainder bounds. As an important consequence, the sharpness of the computed enclosures scales with a high order of the size of the domain.

In computational mathematics, functions are frequently modeled by either one of the following methods: numerical tables, symbolic representations, range intervals, finite approximations. The Taylor model approach offers a novel approach to rigorous numerical analysis by combining many positive aspects of these seemingly different approaches. Taylor models use high order approximations with symbolic polynomial operations and interval methods to achieve sharp and guaranteed enclosures of functional dependencies.

Lastly, we point out that Taylor model methods are often transparent to the user of computational software. While conventional interval methods often require an adaptation of the underlying algorithms, Taylor model methods can usually be used as straightforward drop-in replacements for floating point number methods and provide rigorous answers to common questions.

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Summary

Ovsyannikov A., Berz M. Taylor Models and Computations in the Complex Plane.

This article is devoted to the extension of sphere of applications of Taylor models developed earlier. A definition of the complex Taylor model is introduced. A possibility of their use in the representation of complex analytical functions is considered. Rules for the construction of complex Taylor models are suggested for elementary functions. Arithmetic operations on models are introduced. A series of numerical patterns illustrating advantages of this approach are suggested. Calculations had been made with the help of the system Cosy infinite.

Овсянников А., Берц М. Модели Тейлора и вычисления на комплексной плоскости.

Данная статья посвящена расширению сферы применения моделей Тейлора, разработанных ранее. Вводится определение комплексной модели Тейлора. Рассматривается возможность представления с их помощью комплексных аналитических функций. Приводятся правила построения комплексных моделей Тейлора для элементарных функций. Вводятся арифметические операции над моделями. В работе рассматривается ряд численных примеров, иллюстрирующих возможности данного подхода. Вычисления проводились с помощью системы Cosy infinite.

РЕФЕРАТ

УДК 519.6

О v s y a n n i k o v A., B e r z M. **Taylor Models and Computations in the Complex Plane.** // Вестн. С.-Петерб. ун-та. Сер. 10. 2009. Вып. 2. С. 00-00.

The conduction of scientific and engineering computer calculations is non-trivial task. One of important components of this task is the assessment of received results and the assessment of preciseness (correctness) of calculated values. In practice it is common sense and professional experience of the calculator. More formal approach to the task means such organization of the calculation process that automatically makes correlation of calculation values with relation to possible errors, miscalculations on uncertainties of given data as well as approximation errors and errors which may occur due to computer representation of numerical values etc. The result of such calculations is certain interval or set that is certain to contain correct solution. Many publications deal with the construction of such mathematically approved methods of calculation. As a rule they are based on the interval mathematics and interval modifications of traditional (conventional) numerical methods. In this case it is not always possible to get as a result intervals, which are narrows enough. Thus in the process of calculations one can get catastrophic ballooning of intervals as the result, for example, of dependency effect which leads to certain overestimations. The usage of the method of representation of functions into the Taylor series with simultaneous control of remainders bounds effectively allows effective realization of the calculations with automatic control of the value of calculation errors. This approach developed in works by Martin Berz and Kyoko Makino for the case of real functions has, as it is shown, some advantages. With the turn to the complex plane all calculation problems are getting even more difficult. In this paper the development of the technique of calculations based on Taylor's model for complex analytical functions is considered. Calculation technique based on complex Taylor model appears to be free of many failures of interval calculations or at least it is able to reduce unwanted effects such as wrapping effect and dependency problem.

Keywords: Taylor models, complex interval arithmetic, dependency problem, wrapping effect.