Branch Cuts and Formal Methods?

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The (Bourbakist) Theory

In principle, (pure) mathematics is clear about "function".

> *On dit qu'un graphe F est un graphe fonctionnel si, pour tout x, il existe au plus un objet correspondant à x par F (I, p. 40). On dit qu'une correspondance $f = (F, A, B)$ est une fonction si son graphe F est un graphe fonctionnel, et si son ensemble de départ A est égal à son ensemble de définition $\mathrm{pr}_1 F$ [pr_1 is "projection on the first component"]. [Bourbaki, Ensembles]*

So for Bourbaki a function includes the definition of the domain and codomain, and is *total* and *single-valued*. We will write $(F, A, B)_{\mathcal{B}}$ for such a function definition.

Notation

$\mathbf{P}(A)$ denotes the power set of the set A.
For a function f, we write $\mathrm{graph}(f)$ for $\{(x, f(x)) : x \in \mathrm{Domain}(f)\}$ and $\mathrm{graph}(f)^T$ for $\{(f(x), x) : x \in \mathrm{Domain}(f)\}$.

Convention (Generally undocumented)

Where an underspecified object, such as $\sqrt{x}$, occurs more than once in a formula, the same *value, or interpretation, is meant at each occurrence.*

For example, $\sqrt{x} \cdot \frac{1}{\sqrt{x}} = 1$ for non-zero x, even though one might think that one root might be positive and the other negative. More seriously, in the formula for the roots of a cubic $x^3 + bx + c$,

$$\frac{1}{6}\sqrt[3]{-108\,c + 12\,\sqrt{12\,b^3 + 81\,c^2}} - \frac{2b}{\sqrt[3]{-108\,c + 12\,\sqrt{12\,b^3 + 81\,c^2}}},$$

the two occurrences of $\sqrt{12\,b^3 + 81\,c^2}$ are meant to have the same value, similarly $\sqrt[3]{-108\,c + 12\,\sqrt{12\,b^3 + 81\,c^2}}$.

Examples of statements [Dav10]

As statements about equality[1] of functions, we consider these:

$$\sqrt{z-1}\sqrt{z+1} \stackrel{?}{=} \sqrt{z^2-1}. \tag{1}$$

$$\sqrt{1-z}\sqrt{1+z} \stackrel{?}{=} \sqrt{1-z^2}. \tag{2}$$

$$\log z_1 + \log z_2 \stackrel{?}{=} \log z_1 z_2. \tag{3}$$

$$\arctan x + \arctan y \stackrel{?}{=} \arctan\left(\frac{x+y}{1-xy}\right). \tag{4}$$

(1) is valid for $\Re(z) > 0$, also for $\Re(z) = 0$, $\Im(z) > 0$.
(2) is valid everywhere, despite the resemblance to (1).
(3) is valid with $-\pi < \arg(z_1) + \arg(z_2) \leq \pi$.
(4) is valid, even for *real* x, y, only when $xy < 1$.

[1] At least at the moment, this is to be considered as extensional, i.e. do the l.h.s. and r.h.s. give the same results for the same inputs?

(4) is curious: arctan is nice

(as a real-valued function, at least).

$$\arctan x + \arctan y \stackrel{?}{=} \arctan\left(\frac{x+y}{1-xy}\right). \qquad (4)$$

On $\mathbf{R}$, $\frac{-\pi}{2} < \arctan < \frac{\pi}{2}$, so the l.h.s. of (4) is in (all of) $(-\pi, \pi)$ whereas the r.h.s. is only in $(\frac{-\pi}{2}, \frac{\pi}{2})$, so (4) can't be an equality.

In fact there is a "branch cut at infinity", since $\lim_{x\to+\infty} \arctan x = \frac{\pi}{2}$, whereas $\lim_{x\to-\infty} \arctan x = -\frac{\pi}{2}$ and $xy = 1$ therefore falls on this cut of the right-hand side of (4).

This is also the branch cut that many symbolic integrators (used to) fall over.

Setting

Various basic facts

- A 1:1 function f has an inverse function f^{-1}

defined on $\mathrm{Codomain}(f) = \mathrm{Domain}(f^{-1})$.

- A 1:1 continuous function f has a continuous inverse function.
- A 1:1 differentiable function f has a differentiable inverse function.

except when $f' = 0$.

- Similarly a 1:1 analytic function f has an analytic inverse function (except when $f' = 0$).

But all this depends on 1:1, and in general the inverse of a continuous etc. function is multivalued.
One way to see lack of 1:1 is via winding numbers.

Multi-valued functions, e.g. [Car58]

Traditionally written with initial capitals.

- $\sin^{-1}(0) = 0$
- $\mathrm{Sin}^{-1}(0) = \{0 + k\pi : k \in \mathbf{Z}\}$
- $\cos^{-1}(1) = 0$
- $\mathrm{Cos}^{-1}(1) = \{0 + 2k\pi : k \in \mathbf{Z}\}$
- $\sin^{-1}(\frac{1}{2}) = \frac{\pi}{6}$
- $\mathrm{Sin}^{-1}(\frac{1}{2}) = \{\frac{\pi}{6} + 2k\pi : k \in \mathbf{Z}\} \cup \{\frac{5\pi}{6} + 2k\pi : k \in \mathbf{Z}\}$
- $2\,\mathrm{Sin}^{-1}(0) = \{0 + 2k\pi : k \in \mathbf{Z}\}$, but
  $\mathrm{Sin}^{-1}(0) + \mathrm{Sin}^{-1}(0) = \{0 + k\pi : k \in \mathbf{Z}\}$

And $\mathrm{Sin}^{-1}(0) - \mathrm{Sin}^{-1}(0) = \{0 + k\pi : k \in \mathbf{Z}\}$

$\mathrm{Sin}^{-1}(\frac{1}{2}) + \mathrm{Sin}^{-1}(\frac{1}{2}) = \{\frac{2\pi}{6}, \frac{6\pi}{6}, \frac{10\pi}{6}\} + \{2k\pi : k \in \mathbf{Z}\}$, so
$\frac{1}{2}\left(\mathrm{Sin}^{-1}(\frac{1}{2}) + \mathrm{Sin}^{-1}(\frac{1}{2})\right) \ni \frac{3\pi}{6}$, whose sin is not $\frac{1}{2}$.

Possible solutions

- Deal in multi-valued functions. This is difficult (as we have seen), but intellectually honest.
- Use the Riemann surface formalism to underpin the multvalued thinking
- Choose a suitable domain on which f is single-valued, so we can talk about f^{-1}
- But this f^{-1}, on this domain, might not be the same as someone else's f^{-1} on their domain, or on the intersection.
  - In particular, not necessarily the same as a software implementation/table.
- Use a standard definition, which defines a principal domain D, and admits that, as z leaves D, then $f^{-1}(f(z))$ will (probably) have a discontinuity, or "branch cut"
- "The nice thing about standards is that there are so many to choose from". Where applicable,we use [AS64, printing ≥ 9], with behaviour on the branch cut defined by [Kah87].

The branch view: [Cartan1973]

p. 32 “The mapping $y \mapsto e^{iy}$ induces an isomorphism ϕ of the quotient group $\mathbf{R}/2\pi\mathbf{Z}$ on the group $\mathbf{U}$. The inverse isomorphism ϕ^{-1} of $\mathbf{U}$ on $\mathbf{R}/\pi\mathbf{Z}$ associates with any complex number u such that $|u| = 1$, a real number which is defined up to the addition of an integral multiple of 2π; this class of numbers is called the argument of u and is denoted by $\arg u$.” In our notation this is $\left(\mathrm{graph}(\phi)^T, U, \mathbf{R}/2\pi\mathbf{Z}\right)_{\mathcal{B}}$.

p. 33 “We define

$$\log t = \log |t| + i \arg t, \qquad (5)$$

which is a complex number defined only up to addition of an integral multiple of $2\pi i$.” In our notation this is $((5), \mathbf{C}, \mathbf{C}/2\pi i\mathbf{Z})_{\mathcal{B}}$.

p. 33 "For any complex numbers t and t' both $\neq 0$ and for any values of $\log t$, $\log t'$ and $\log tt'$, we have

$$\log tt' = \log t + \log t' \pmod{2\pi i}.\text{''} \qquad (6)$$

p. 33 "So far, we have not defined $\log t$ as a *function* in the proper sense of the word".

p. 61 "$\log z$ has a branch in any simply connected open set which does not contain 0."

So any given branch would be $(G, D, I)_{\mathcal{B}}$, where D is a simply connected open set which does not contain 0, G is a graph obtained from one element of the graph (i.e. a pair $(z, \log(z))$ for some $z \in D$) by analytic continuation, and I is the relevant image set.

Branch Cuts of Elementary Functions [Kah87]

exp / ln $\exp(z+2\pi i)=\exp(z)$. These days the principal domain is generally chosen as $\pi < \Im(z) \le \pi$, which translates to a branch cut for ln along the negative real axis, so that $\ln(-1+\epsilon i) \approx i\pi+\epsilon)$, but $\ln(-1-\epsilon i) \approx -i\pi-\epsilon)$.

tan / atan $\tan(z+\pi)=\tan(z)$. Principal domain is $-\frac{\pi}{2} < \Re(z) \le \frac{\pi}{2}$. This translates into a branch cut for atan on $\{0+iy : |y|>1\}$.

cot / acot $\cot(z+\pi)=\cot(z)$. Today the principal domain is $0 \le \Re(z) < \pi$. This translates into a branch cut for acot on $\{0+iy : |y|<1\}$.

cos / acos $\cos(z+\pi)=\cos(z)=-\cos(z)$. The principal domain is $0 \le \Re(z) < \pi$. This translates into a branch cut for acos on $\{x+0i : |x|>1\}$.

Similarly sec etc. and the hyperbolics sinh etc.

False sense of simplicity

Towards an algorithm (I)

$$\sqrt{z-1}\sqrt{z+1} \stackrel{?}{=} \sqrt{z^2-1}. \tag{1}$$

$$\sqrt{1-z}\sqrt{1+z} \stackrel{?}{=} \sqrt{1-z^2}. \tag{2}$$

(2) is correct but (1) is only partially correct. How can we distinguish? The branch cut of $\sqrt{\ }$ is the negative real axis. Regard $\mathbf{C}(z)$ as $\mathbf{R}(x,y)$. Then the branch cuts of (1) are

$\sqrt{z-1}$ $x < 1, y = 0$

$\sqrt{z+1}$ $x < -1, y = 0$

$\sqrt{z^2-1}$ $2xy = 0; x^2 - y^2 - 1 < 0.$

$[\{-1 < x < 1, y = 0\} \cup \{x = 0, y \text{ free}\}]$

These define semi-algebraic (polynomial equations and inequalities) sets in $\mathbf{R}^2$, so partition $\mathbf{R}^2$ into a finite number of cells (found by Cylindrical Algebraic Decomposition), and analyse each cell C_i (which comes with a sample point s_i) separately.

Towards an algorithm (II)

Q1,. . . ,Q4 are the four quadrants of the Argand diagram ($Q1 = \{x \geq 0, y \geq 0\}$ etc.): the branch cut for $\sqrt{}$ means that $\sqrt{Q2} \subset Q1$ and $\sqrt{Q3} \subset Q4$

$x > 0$ (and not $y - 0, x < 1$)Typical point $z = 2$, and (1) becomes $\sqrt{1}\sqrt{3} \stackrel{?}{=} \sqrt{3}$: correct.

$x < 0; y > 0$ Typical point $z = -1 + i$ and (1) becomes
$$\underbrace{\sqrt{\underbrace{-2+i}_{\text{Q2}}}}_{\text{Q1}} \underbrace{\sqrt{\underbrace{i}_{\text{Q2}}}}_{\text{Q1}} \stackrel{?}{=} \underbrace{\sqrt{\underbrace{(-1+i)^2-1}_{\text{Q3}}}}_{\text{Q4}}, \text{ false}$$

$x < 0; y < 0$ Typical point $z = -1 - i$ and (1) becomes $\sqrt{-2-i}\sqrt{-i} \stackrel{?}{=} \sqrt{(-1-i)^2 - 1}$, also false.

Cuts In principle we need to do similar analysis on these.

Towards an algorithm (III)

Not quite so simple: on each cell, the proposed identity is either *everywhere true* ot *generically false*.

Consider multiplying (1) by $z^2 + 2z + 2$, which vanishes at both $z = -1 + i$ and $z = -1 - i$.

Then this is "accidentally" true at the sample points $s_i = -1 \pm i$, even though false elsewhere in their regions. How do we deal with this?

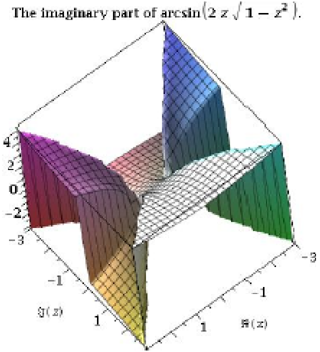
[BBD03] Regard our equation as power series, and use an explicit zero test for these [vdH02].

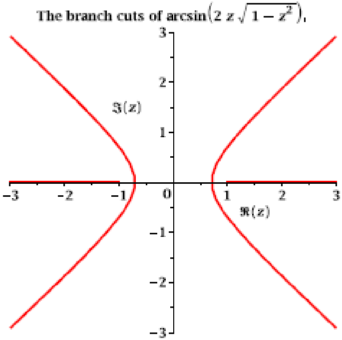
In practice a poly-algorithmic approach is useful [BBDP07], and for branch cuts, we can ask what full-dimensional cell they "adhere" to [BBDP05].

This is implemented in the package `BranchCuts` in Maple: see [EBDW13]. For example given $\operatorname{asin}(2z\sqrt{1-z^2})$, it can produce

$$\{\Im(z)=0, 1<\Re(z)\} \quad \{\Im(z)=\Im(z), \Re(z)=-\tfrac{1}{2}\sqrt{2+4\Im(z)^2}\}$$
$$\{\Im(z)=0, \Re(z)<-1\} \quad \{\Im(z)=\Im(z), \Re(z)=\tfrac{1}{2}\sqrt{2+4\Im(z)^2}\}$$

and the branch cuts on the right (left is a Maple plot).

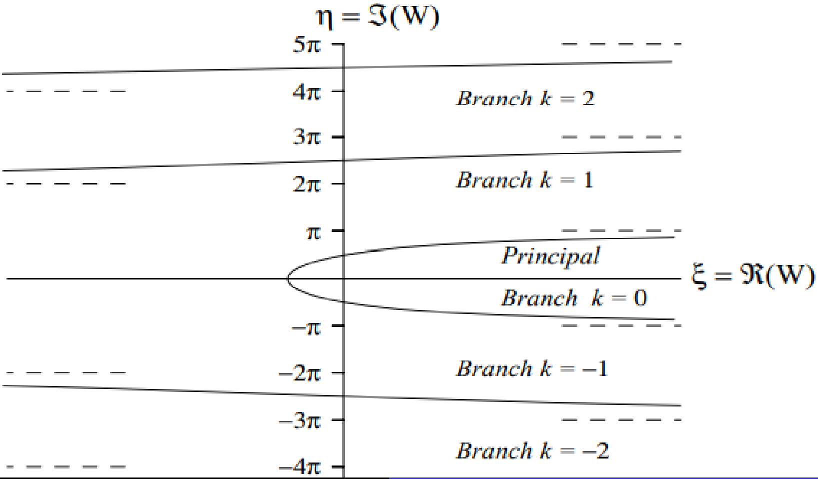




Branch cuts: Lambert W

W is the solution of $W(z)e^{W(z)} = z$, and is not Liouvillian [BCDJ08]. Its branches are more complicated [JHC96].

Figure: Branches of W [JHC96, Figure 2]



Interactions with Proving/Verification

- Can we be more formal than the "proof" I sketched via CAD?
- In an ideal world, that sketch would become a tactic, or possibly a generator of counter-examples.
- And how dependent is this on a "fully verified" CAD?
- Code can be generated from prover output (as in [FM24]), but is that code, with its choice of branch cuts, actually compatible with the prover?
- What if the branch cuts aren't semi-algebraic? As in W.

Interactions with Proving/Verification

- **Lean** I see nothing in [AM24]
- **Isabelle** There's a lot of underpinning stuff around winding numbers in [Gro24], but no branch cuts as such.
- **Rocq** See [Bru11], which treats winding numbers but not branch cuts, and is explicitly "non-constructive".
- **JHD** asked for other input.
- **PVS** NASA have a tool `precision` which, the responder thought, did some of this as well as simple precision checking.

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