Numerical Investigation of the *3n+1* Problem and its Continuous Extension

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ABSTRACT

We numerically investigate commonalities between the iterative behavior of a variant $T : \mathbb{N} \to \mathbb{N}$ of the discrete Collatz function and a continuous function $f : \mathbb{R}^+ \to \mathbb{R}^+$ that is equivalent to T on $\mathbb{N}$. The function f is a restriction to $\mathbb{R}^+$ of Letherman, Schleicher, and Wood's extension (1999) of T to $\mathbb{C}$. We then then generalize T and f to functions $\mathcal{T}_{a,b}$ and $F_{a,b}$, where the $3n+1$ rule becomes $an+b$, and we numerically investigate how a shared property appears to affect the iterative behavior of both functions. Finally, we relate this property to random walks whose proportionality of step size to displacement causes them to converge. It is important to note that the investigations in this paper consist primarily of numerical experiments, rather than proofs, regarding the $3n+1$ and $an+b$ maps.

INTRODUCTION

The $3n+1$ problem, also known as the Collatz problem, the Syracuse problem, Kakutani's problem, and Ulam's problem, is German mathematician Lothar Collatz's 1937 conjecture about the iterative behavior of the Collatz function C.

Definition The *Collatz function* $C : \mathbb{N} \to \mathbb{N}$ is defined by

$$C(n) = \begin{cases} 3n+1 & \text{if } n \equiv 1 \mod 2 \\ n/2 & \text{if } n \equiv 0 \mod 2 \end{cases}$$

Remark The acronym *HOTPO (Half Or Triple Plus One)* is frequently used to describe C.

Definition C^j is the jth *iteration* of C. That is, C^j is the composition of C with itself j times.

Example

$$\begin{aligned} C^0(n) &= n \\ C^1(n) &= C(n) \\ C^2(n) &= (C \circ C)(n) \\ C^3(n) &= (C \circ C \circ C)(n) \\ &\vdots \end{aligned}$$

Definition The *3n+1 problem* is to prove the *Collatz conjecture*: for each $n \in \mathbb{N}$, there is a $k \in \mathbb{N}$ such that $C^k(n) = 1$.

Because the $3n+1$ step for an odd n always yields an even number, investigations of the $3n+1$ problem often utilize the function $T : \mathbb{N} \to \mathbb{N}$ defined by

$$T(n) = \begin{cases} \frac{3n+1}{2} & \text{if } n \equiv 1 \mod 2 \\ \frac{n}{2} & \text{if } n \equiv 0 \mod 2 \end{cases}$$

which combines the $3n+1$ step with the inevitable $n/2$ step afterwards.

The Collatz conjecture is largely supported by computation: Oliveira e Silva (2010) has verified the conjecture for each natural number up to $5 \times 2^{60} \approx 5.8 \times 10^{18}$. Furthermore, Lagarias (1985) offered an intuitive argument for the Collatz conjecture by considering iteration sequences of natural numbers under T.

Definition Let $n \in \mathbb{N}$. The *iteration sequence* of n under T is the sequence $(n, T(n), T^2(n), ...)$, or, more compactly, $(T^j(n))_{j=0}^{\infty}$.

Lagarias showed that if each term of each iteration sequence of T is equally likely to be even or odd, then each odd number in the sequence is expected to be $3/4$ the previous odd number. Although Lagarias's argument provides intuitive support for convergence, it does not guard against periodic cycles and is not a proof because its hypothesis has not been proven.

Despite the $3n+1$ problem's apparent simplicity, every proposed proof has been shown incomplete, and the Collatz conjecture remains unproven over 70 years since its proposal. Although the $3n+1$ problem is not of immediate practical importance in itself, a solution technique could offer new insights to analysis of complex systems. The $3n+1$ problem lies in the intersection of number theory and dynamical systems, and the mathematics that produces a solution may unite aspects of the two fields.

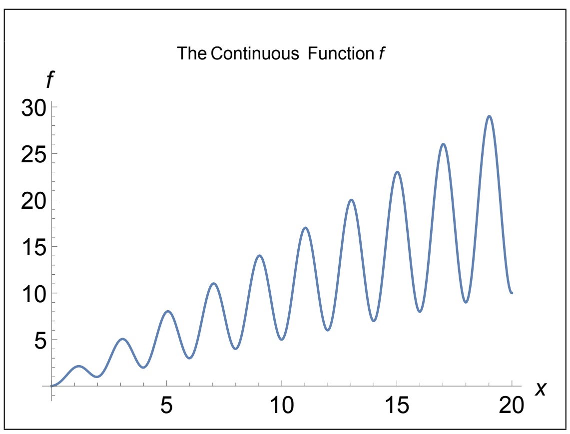
In this paper, we extend T to a continuous function $f : \mathbb{R}^+ \to \mathbb{R}^+$, and we discover commonalities between numerically-observed iterative behavior of T over $\mathbb{N}$ and f over $\mathbb{R}^+$. Then, we extend the $3n+1$ rule to $an+b$ and generalize T and f to $\mathcal{T}_{a,b}$ and $F_{a,b}$. We numerically investigate a shared property that appears to be related to the iterative behavior of the functions. Finally, we see how this property relates to random walks whose step size is proportional to displacement.

CONSTRUCTION OF f

Notice that T is bounded by the lines $u(x) = \frac{3x+1}{2}$ and $\ell(x) = \frac{x}{2}$. Thus, a sinusoid which runs along the equilibrium $e(x) = \frac{u(x)+\ell(x)}{2} = \frac{4x+1}{4}$ with amplitude $\alpha(x) = \frac{u(x)-\ell(x)}{2} = \frac{2x+1}{4}$ and period 2 will intersect $u(x)$ when x is odd and $\ell(x)$ when x is even. We define $f(x) = e(x) - \alpha(x)\cos(x\pi)$, which yields

$$f(x) = \frac{4x+1}{4} - \frac{2x+1}{4}\cos(\pi x).$$

A plot of $f(x)$ is shown below for $1 \leq x \leq 50$.



Proposition 1. *The functions f and T are equivalent on $\mathbb{N}$.*

Proof. If $n \in \mathbb{N}$ is even, then $\cos(n\pi) = 1$, so

$$f(n) = \frac{4n+1}{4} - \frac{2n+1}{4} = \frac{n}{2}.$$

If $n \in \mathbb{N}$ is odd, then $\cos(n\pi) = -1$, so

$$f(n) = \frac{4n+1}{4} + \frac{2n+1}{4} = \frac{3n+1}{2}.$$

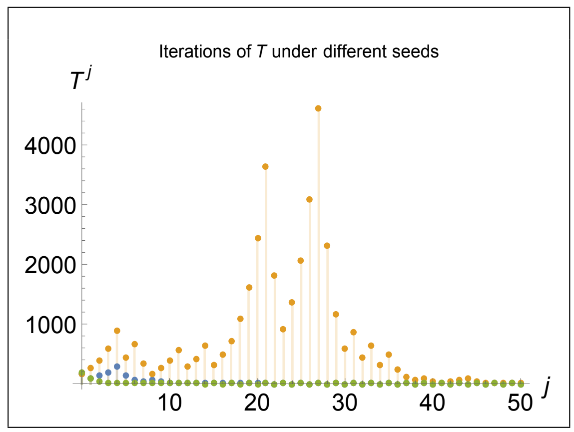
Thus, $f(\mathbb{N}) = T(\mathbb{N})$. □

Note that f can also be realized as a restriction to $\mathbb{R}^+$ of Letherman, Schleicher, and Wood's extension (1999) of T to $\mathbb{C}$.

ITERATIVE BEHAVIOR OF T & f

The Collatz conjecture says that for any $n \in \mathbb{N}$, $T^j(n)$ settles down and eventually reaches 1 for some choice of j.

Below are graphs of $T^j(174)$, $T^j(175)$, and $T^j(176)$ for $0 \leq j \leq 50$. Indeed, all three inputs, or seeds, are eventually mapped to 1, consistent with the Collatz conjecture. However, although these inputs, or seeds, are as close to each other as possible, their iterative behavior prior to reaching 1 differs significantly.



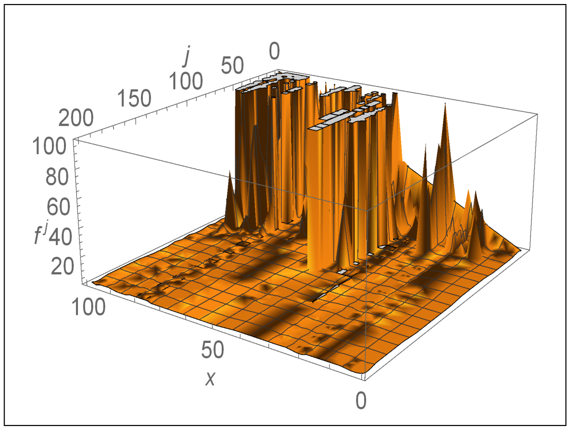
We see that small variations in $n \in \mathbb{N}$ can lead to unexpected changes in the iteration sequence of n under T.

Proposition 2. *If the Collatz conjecture holds for a number n, then there is a $k \in \mathbb{N}$ such that $T^j(n) \in \{1, 2\}$ for all natural numbers $j \geq k$.*

Proof. If n satisfies the Collatz conjecture, then there is a $k \in \mathbb{N}$ such that $T^k(n) = 1$. But if $T(1) = 2$ and $T(2) = 1$, so $1 \to 2 \to 1 \to 2 \to \cdots$ under T. □

Remark If the Collatz conjecture is true, then values of iterates of $\mathbb{N}$ under T are eventually confined to $\{1, 2\}$. This raises the question: how do iterates of $\mathbb{R}^+$ behave under f?

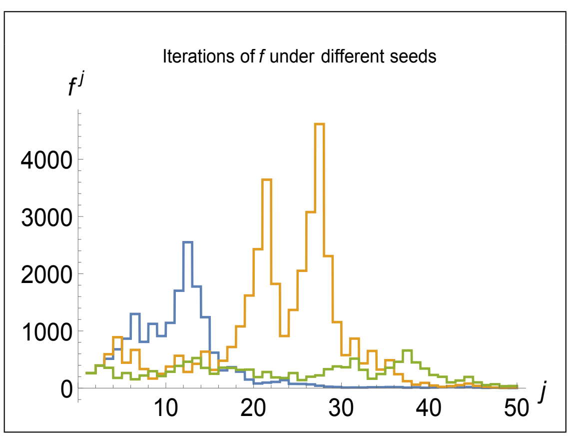
To visualize many iteration sequences at once, we create a 3D plot of $f^j(x)$ for $0 \leq j \leq 200$ on $1 \leq x \leq 100$:



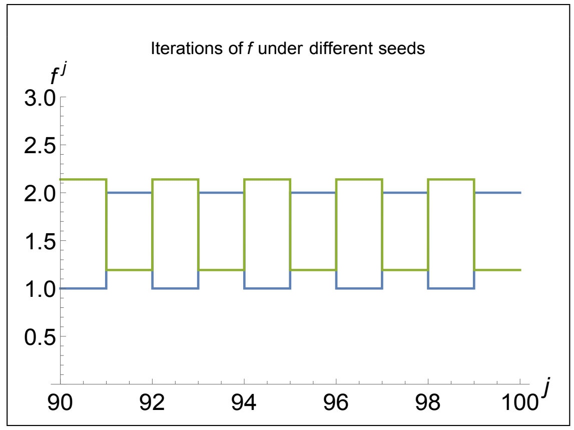
Although all computer programs are susceptible to roundoff error and cannot generate plots over the entirety of $\mathbb{R}^+$, it is interesting that every value plotted follows the same trend: the plot suggests that for most points x of f, as j increases, $f^j(x)$ settles down and eventually becomes trapped in approximately the interval $[1, 2]$ for $1 \leq x \leq 100$. Similar plots for larger values of x suggest that $f^j(x)$ displays the same settling behavior as j increases.

We also see in f the property that even when seeds (input values) are very close together, their iteration sequences can take quite different paths before they settle.

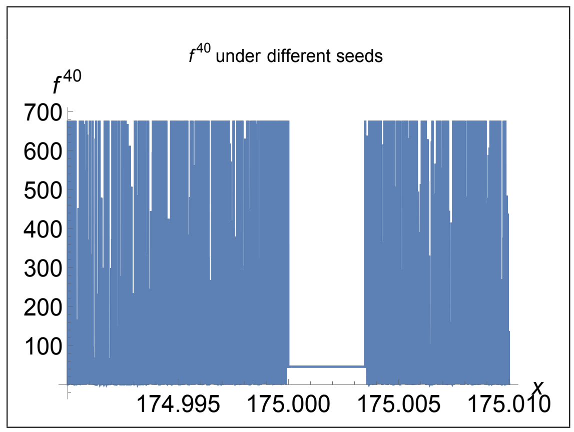
Below is a plot of $f^j(174.99)$, $f^j(175)$, and $f^j(175.01)$ for $0 \leq j \leq 50$. Although these three seeds are spaced at merely 0.01, their iteration sequences differ significantly. Small variations in $x \in \mathbb{R}^+$ can lead to unexpected changes in the iteration sequence of x under f.



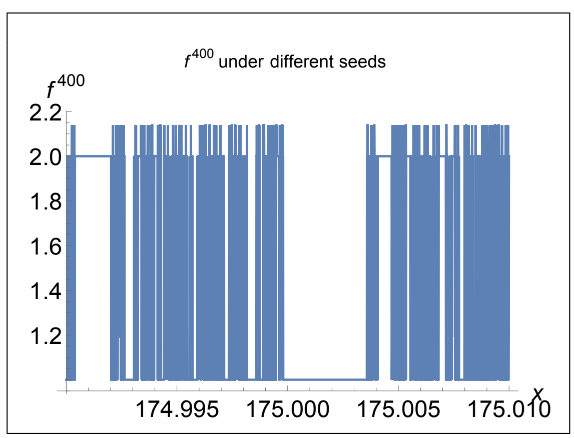
As j increases, $f^j(174.99)$ oscillates between 1 and 2 with period 1, and $f^j(175.01)$ oscillates between ~ 1.193 and ~ 2.139 with period 2.



Other points appear to demonstrate the same behavior: they first take different paths, reaching drastically different values after the same number of iterations.



However, after sufficiently many iterations, these points appear to converge into one of the cycles $(1, 2)$ or $(1.193.., 2.139...)$. This behavior occurs for all points that were tested, although we show only a small interval $[174.99, 175.01]$ for clarity because the graph oscillates so often.



Upon consideration of $\frac{df^2}{dx}$, the $(1, 2)$ and

$(1.193..., 2.105...)$, the cycles makes sense. By the chain rule, we know

$$\frac{df^2(x_0)}{dx} = \frac{df}{dx}(f(x_0))\frac{df}{dx}(x_0),$$

and we also have that

$$\frac{df(x)}{dx} = 1 + \frac{1}{2}\cos\pi x - \frac{2x+1}{4}\pi\sin\pi x.$$

We see that $\begin{cases} \frac{df}{dx}(1) = \frac{3}{2} \\ \frac{df}{dx}(2) = \frac{1}{2} \end{cases}$ and $\begin{cases} f(1) = 2 \\ f(2) = 1 \end{cases}$, so

$$\frac{df^2(1)}{dx} = \frac{df^2(2)}{dx} = \frac{3}{4}.$$

Also, because $\begin{cases} \frac{df}{dx}(1.193) = 2.105 \\ \frac{df}{dx}(2.139) = -0.300 \end{cases}$ and $\begin{cases} f(1.193) \approx 2.139 \\ f(2.139) \approx 1.193 \end{cases}$, we have that

$$\frac{df^2(1.193)}{dx} \approx \frac{df^2(2.139)}{dx} \approx -0.632.$$

Since we have $\left|\frac{df^2(p)}{dx}\right| < 1$ for $p = 1, 2, 1.193..., 2.139...,$ we know that the cycles $(1,2)$ and $(1.193..., 2.139...)$ are attracting.

GENERALIZATION TO $\mathcal{T}_{a,b}$ and $F_{a,b}$

Now, we will extend T and f to larger, more general classes of functions.

Define the function $\mathcal{T}_{a,b} : \mathbb{N} \to \mathbb{N}$ by

$$\mathcal{T}_{a,b} = \begin{cases} \frac{an+b}{2} & \text{if } n \equiv 1 \mod 2 \\ \frac{n}{2} & \text{if } n \equiv 0 \mod 2 \end{cases}$$

where $a, b \in \mathbb{N} \cup \{0\}$ with $a + b$ even and nonzero.

Proposition 3. *Provided that $a, b \in \mathbb{N} \cup \{0\}$ are chosen that $a + b$ is even and nonzero, $\mathcal{T}_{a,b}$ indeed maps $\mathbb{N}$ to $\mathbb{N}$*

Proof. If n is even, then $\mathcal{T}_{a,b}(n) = \frac{n}{2} \in \mathbb{N}$. Thus, we need only consider the case when n is odd.

If $a+b$ is even, then a, b are either both even or both odd. Suppose that n is odd. If a, b are both even, then an is even, so $an + b$ is even. Moreover, because a, b are not both zero, we have that $\mathcal{T}_{a,b}(n) = \frac{an+b}{2} \in \mathbb{N}$. Alternatively, if a, b are both odd, then an is odd, so $an + b$ is even. Hence $\mathcal{T}_{a,b}(n) = \frac{an+b}{2} \in \mathbb{N}$. □

Remark Notice that $\mathcal{T}_{2,1}$ is equivalent to T.

Using the method that we used to create the continuous extension f of T, we create the continuous extension $F_{a,b}$ of $\mathcal{T}_{a,b}$. It is given by:

$$F_{a,b}(x) = \frac{(a+1)x+b}{4} - \frac{(a-1)x+b}{4}\cos(\pi x)$$

Remark Notice that $F_{2,1}$ is equivalent to f.

Proposition 4. *The functions $F_{a,b}$ and $\mathcal{T}_{a,b}$ are equivalent on $\mathbb{N}$.*

Proof. If $n \in \mathbb{N}$ is even, then $\cos(n\pi) = 1$, so

$$F_{a,b}(n) = \frac{(a+1)n+1}{4} - \frac{(a-1)n+1}{4} = \frac{n}{2}.$$

If $n \in \mathbb{N}$ is odd, then $\cos(n\pi) = -1$, so

$$F_{a.b}(n) = \frac{(a+1)n+b}{4} + \frac{(a-1)n+b}{4} = \frac{an+b}{2}.$$

Thus, $F_{a,b}(\mathbb{N}) = \mathcal{T}_{a,b}(\mathbb{N})$ □

AREA INVESTIGATION OF $\mathcal{T}_{a,b}$

The overall iterative behavior of $\mathcal{T}_{a,b}$ is related to

- how frequently $\mathcal{T}_{a,b}(n) > n$ and $\mathcal{T}_{a,b}(n) < n$ occur relative to each other, and
- how much greater or lesser $\mathcal{T}_{a,b}(n)$ is than n.

Both of these aspects are encompassed in sum of a function's values function above the line $y = x$ versus below the line $y = x$.

Accordingly, define the function $H_{a,b} : \mathbb{N} \to \mathbb{N}$ by

$$H_{a,b}(t) = \sum_{n=1}^{t} \mathcal{T}_{a,b}(n) - n.$$

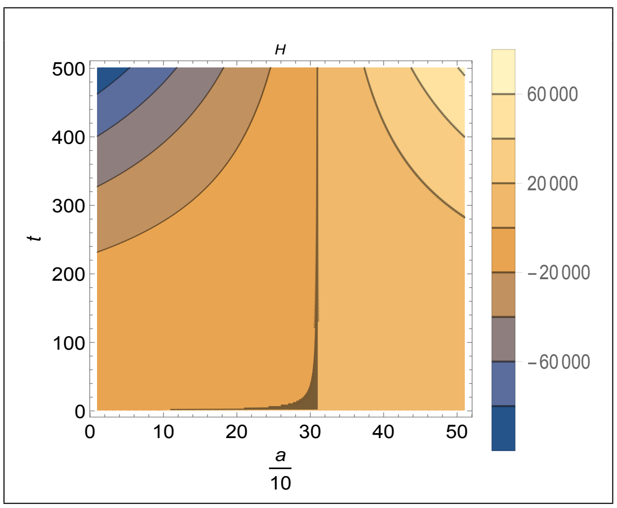
where t is odd (for simplicity).

Then

$$
\begin{aligned}
H_{a,b}(t) &= \sum_{n=0}^{\frac{t-1}{2}} \frac{a(2n+1)+b}{2} - (2n+1) + \sum_{n=0}^{\frac{t-1}{2}} \frac{2n}{2} - 2n \\
&= \sum_{n=0}^{\frac{t-1}{2}} \left[(a-3)n + \frac{a+b-2}{2} \right] \\
&= (a-3)\left(\frac{t^2-1}{8}\right) + \left(\frac{a+b-2}{2}\right)\left(\frac{t-1}{2}\right) \\
&= \frac{a-3}{4}t^2 + \frac{a+b-2}{4}t + \frac{7-3a-2b}{4}
\end{aligned}
$$

We see that b does not offer unique contribution to any of the above terms: b is not included in the t^2 term, and both a and b contribute in similar ways to the t term and the constant term. Thus, in our upcoming investigation, we will vary a and constrain $b = 1$.

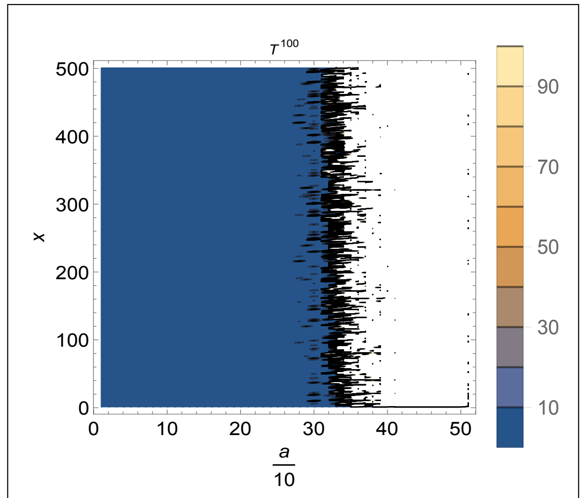
A contour plot of $H_{a,1}(t)$ is shown below for $0 \leq a \leq 5$ and $0 \leq t \leq 500$.



We see that the $H_{a,1} = 0$ isocline is given approximately by the line $a = 3$. This makes sense, because the t^2 term of $H_{a,1}(t)$ dominates the other terms: for very large t, we see that

$$H_{a,1}(t >> 0) \approx \frac{a-3}{8}t^2.$$

Interestingly, $a = 3$ also appears to be the crossover point from decreasing to increasing iterative behavior, as suggested by the following contour plot of $\mathcal{T}_{a,1}^{100}(x)$ for $0 \leq a \leq 5$ and $0 \leq x \leq 500$.



Note: white color denotes values that were were outside the range of the plot.

AREA INVESTIGATION OF $\mathcal{F}_{a,b}$

When we make the extension from discrete to continuous, the sum of values above versus below the line $y = x$ turns into an integral, or area, of the values above versus below the line $y = x$.

Define $G_{a,b} : \mathbb{R}^+ \to \mathbb{R}$ by

$$G_{a,b}(t) = \int_0^t [F_{a,b}(x) - x]dx.$$

Then

$$
\begin{aligned}
G_{a,b}(t) = &\int_0^t \left[\frac{(a+1)x+b}{4} \right. \\
&\left. - \frac{(a-1)x+b}{4}\cos(\pi x) - x \right] dx \\
= &\int_0^t \left[\frac{(a-3)x+b}{4} \right. \\
&\left. - \frac{(a-1)x+b}{4}\cos(\pi x) \right] dx \\
= &\frac{a-3}{8}t^2 + \frac{b}{4}t \\
&- \frac{b}{4\pi}\sin(\pi x) - \frac{a-1}{4}\int_0^t x\cos(\pi x)dx.
\end{aligned}
$$

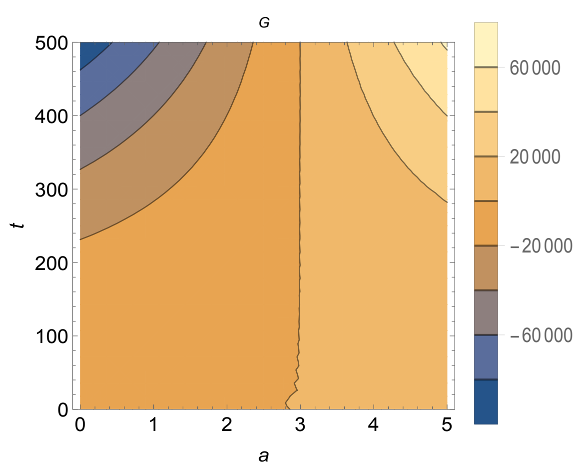
Using integration by parts, we know that

$$\int_0^t x\cos(\pi x)dx = \frac{1}{\pi}t\sin(\pi t) + \frac{1}{2\pi^2}\cos(\pi t) - \frac{1}{2\pi^2}.$$

Thus, we reach

$$G_{a,b}(t) = \frac{a-3}{8}t^2 + \left(\frac{b}{4} - \frac{a-1}{4\pi}\sin(\pi t)\right)t - \frac{b}{4\pi}\sin(\pi x) - \frac{a-1}{8\pi^2}\cos(\pi t) + \frac{a-1}{8\pi^2}.$$

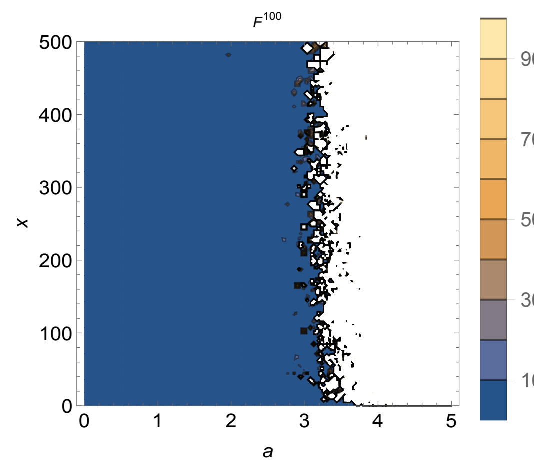
A contour plot of $G_{a,1}(t)$ is shown below for $0 \leq a \leq 5$ and $0 \leq t \leq 500$.



We see that, just as for $H_{a,b}$, the $G_{a,1} = 0$ isocline is given approximately by the line $a = 3$, and for very large t we have

$$G_{a,b}(t >> 0) \approx \frac{a-3}{8}t^2.$$

Again, $a = 3$ appears to be the crossover point from decreasing to increasing iterative behavior, as suggested by the following contour plot of $F_{a,1}^{100}(x)$ for $0 \leq a \leq 5$ and $0 \leq x \leq 500$.



Note: Again, white color denotes values that were outside the range of the plot. For example, $F_{4,1}^{100}(250) \approx 1.0836 * 10^9$.

COMPARISON TO RANDOM WALKS

In the previous two sections, we saw that the $\frac{a-3}{8}t^2$ term appears to tell us a lot about the behavior of $\mathcal{T}_{a,b}$ and $F_{a,b}$. In the case of $b = 1$, when one of the functions is positive in the t^2 term, it increases over time, but when one of the functions is zero or negative in the t^2 term, it appears to settle down regardless of the t or constant terms. Thus, the $\frac{a-3}{8}t^2$ term is the focal point of this last investigation.

Let $g_a : \mathbb{R}^+ \to \mathbb{R}$ be a function that satisfies

$$\int_0^t [g_a(x) - x]\, dx = \frac{a-3}{8}t^2.$$

Then we have

$$\int_0^t g_a(x)dx = \frac{a-3}{8}t^2 + \frac{1}{2}t^2 = \frac{a+1}{8}t^2$$

and we see that

$$g_a(x) = \frac{a+1}{4}x$$

When $-5 < a < 3$, we have that $|\frac{a+1}{4}| < 1$, and so the iterate $g_a^k(x)$ approaches 0 as k increases. However, when $a > 3$, we have that $|\frac{a+1}{4}| > 1$ and so the iterate $g_a^k(x)$ increases without bound as k increases. Thus, it is not surprising that $a = 3$ appears to form a boundary for the cross-over from decreasing to increasing iterative behavior (at least, when $b = 1$).

It may seem surprising that we saw eventually decreasing behavior for F and $\mathcal{T}$ when $a = 3$. When $a = 3$, we have that $g_3(x) = x$, and so $g_3^k(x) = x$ for all k. However, $F_{3,b}(x)$ and $\mathcal{T}_{3,b}(x)$ include fluctuations from the line $y = x$ on the order of x. These fluctuations may have a role in the convergent behavior for $a = 3$.

Indeed, fluctuations play a role in the dynamics of random walks. Consider a random walk of the form

$$r(x) = x + \delta x$$

where δ takes on values $+\lambda$ and $-\lambda$, where $\lambda > 0$, with equal probability. We see that $r(x)$ moves x right or left by λ units for each iteration. However, writing

$$r(x) = (1 + \delta)x,$$

we see that the expected value $E[r^k(x)]$ of $r^k(x)$ is

$$\begin{aligned} E[r^k(x)] &= x\,(1+\lambda)^{\frac{k}{2}}\,(1-\lambda)^{\frac{k}{2}} \\ &= x\left(1-\lambda^2\right)^{\frac{k}{2}}. \end{aligned}$$

As long as $0 < \lambda < \sqrt{2}$, we have that $0 < |1-\lambda^2| < 1$. Thus, even if λ is nonzero but arbitrarily small, we have that for each x, $E[r^k(x)] \to 0$ as $k \to \infty$.

CONCLUSIONS

We extended the discrete function T on $\mathbb{N}$ to the continuous function f on $\mathbb{R}^+$. Using plots we saw that although iteration sequences T and f change unexpectedly even with small changes in initial input, both functions appear to settle down after many iterations. T appears to cycle between the values 1 and 2, while f appears to become trapped in (or quite close to) the cycles $(1, 2)$ and $(1.193..., 2.139...)$.

We generalized T and f to larger classes of functions $\mathcal{T}_{a,b}$ and $F_{a,b}$, and we saw that their sums and integrals above the line $y = x$ on the interval $[0, t]$ depends heavily on the $\frac{a-3}{8}t^2$ term. For $b = 1$, when $a < 3$, the term is negative, and both $\mathcal{T}_{a,1}$ and $F_{a,1}$ appear to settle; when $a > 3$, the term is positive, and both $\mathcal{T}_{a,1}$ and $F_{a,1}$ appear to increase without bound. When $a = 3$, as in the Collatz conjecture, the term vanishes. However, when $a = 3$, the simplest function whose integral above the line $y = x$ on $[0, t]$ is $\frac{a-3}{8}t^2$ becomes the identity function, whose iterates do not settle. Analogy to random walks offers an intuitive explanation for why small fluctuations from $y = x$ that are proportional to x, as found in $\mathcal{T}_{a,b}$ and $F_{a,b}$, can give rise to settling behavior.

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