

CDM

Iteration

KLAUS SUTNER

CARNEGIE MELLON UNIVERSITY

SPRING 2024



1 Iteration, Trajectories and Orbits

2 Finding Cycles

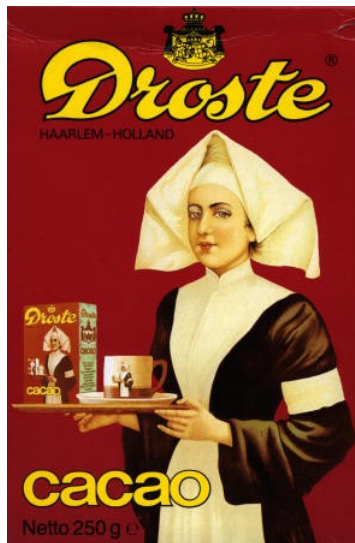
3 Goodstein Sequences

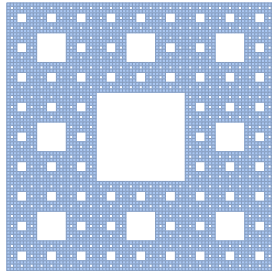
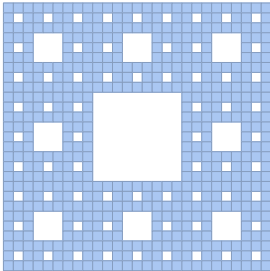
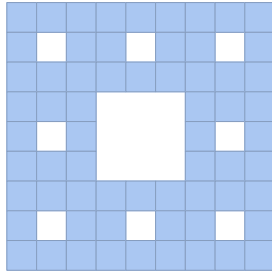
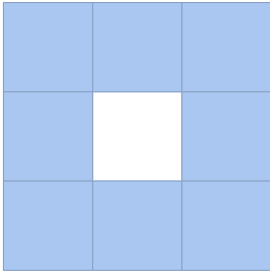
There are several general ideas that are useful to organize computation, perhaps the two most important ones being

- Recursion (self-similarity)
- Iteration (repetition)

Recursion is quite popular and directly supported in many programming languages.

Iteration usually requires some amount of extra work (and, to really make sense, support for functions as first class citizens).





Definition

Let $f : A \rightarrow A$ be an endofunction. The k th power of f (or k th iterate of f) is defined by induction as follows:

$$\begin{aligned}f^0 &= I_A \\f^k &= f \circ f^{k-1}\end{aligned}$$

Here I_A denotes the identity function on A and $f \circ g$ denotes composition of functions.

Informally, this just means: compose function f with itself, $(k-1)$ -times.

$$f^k = \underbrace{f \circ f \circ f \circ \dots \circ f}_{k \text{ terms}}$$

Without any further knowledge about f there is not much one can say about the iterates f^k . But the following always holds.

Lemma (Laws of Iteration)

- $f^n \circ f = f^{n+1}$
- $f^n \circ f^m = f^{n+m}$
- $(f^n)^m = f^{n \cdot m}$

Exercise

Prove these laws by induction using associativity of composition.

Prof. Dr. Alois Wurzelbrunft* stares at these equations and immediately recognizes a deep analogy to exponentiation.

He also remembers that there is a method for fast exponentiation based on squaring:

$$\begin{aligned}a^{2e} &= (a^e)^2 \\ a^{2e+1} &= (a^e)^2 \cdot a\end{aligned}$$

which allows us to compute a^e in $O(\log e)$ multiplications.

Wurzelbrunft's Conclusion:

There is an analogous “fast iteration” method.

*A famous if fictitious professor in the Bavarian hinterland.

A mathematician is a person who can find analogies between theorems; a better mathematician is one who can see analogies between proofs and the best mathematician can notice analogies between theories. One can imagine that the ultimate mathematician is one who can see analogies between analogies.

S. Banach

So is Wurzelbrunft brilliant?

Suppose we want to compute f^{1000} . The obvious way requires 999 compositions of f with itself.

By copying the standard divide-and-conquer approach for fast exponentiation we could try

$$\begin{aligned}f^{2n} &= (f^n)^2 \\ f^{2n+1} &= f \circ (f^n)^2\end{aligned}$$

This seems to suggest that we can compute $f^n(x)$ in $O(\log n)$ applications of the basic function f .

After all, it's just like exponentiation, right?

There is an interesting idea here: we would like to take a plain computation

$$C = C_0, C_1, C_2, \dots, C_{42}, \dots, C_n$$

and somehow translate it into another computation

$$C' = C'_0, C'_1, \dots, C'_m$$

such that

- the result is the same, but
- $m \ll n$

Of course, this won't always be possible, but sometimes we might be able to "compress" a computation (by using a smarter algorithm).

Consider the orbit of a under the rational function (this is a clear case of abuse of a Möbius transformation)

$$f(x) = \frac{2 + 2x}{3 + x}$$

A little fumbling shows that

$$f^t(x) = \frac{2(a-1) + (a+2)x}{2a+1 + (a-1)x} \quad a = 4^t$$

So there is no need to iterate f , we can simply do the coefficient arithmetic.

$$f^5(x) = \frac{2 + \frac{2 \left(2 + \frac{2 \left(2 + \frac{2(2+2x)}{3+x} \right)}{3 + \frac{2+2x}{3+x}} \right)}{2 + \frac{2(2+2x)}{3 + \frac{2+2x}{3+x}}}}{2 + \frac{2 \left(2 + \frac{2(2+2x)}{3+x} \right)}{2 + \frac{2+2x}{3 + \frac{2(2+2x)}{3 + \frac{2+2x}{3+x}}}}} = \frac{2 + \frac{2 \left(2 + \frac{2(2+2x)}{3+x} \right)}{2 + \frac{2+2x}{3 + \frac{2(2+2x)}{3 + \frac{2+2x}{3+x}}}}}{3 + \frac{2 \left(2 + \frac{2(2+2x)}{3+x} \right)}{2 + \frac{2+2x}{3 + \frac{2(2+2x)}{3 + \frac{2+2x}{3+x}}}}}$$

The obvious bottom-up method to compute F_n requires essentially n additions (we will ignore the growing size of the numbers).

We can exploit matrix multiplication to get an alternative description:

$$M = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{implies} \quad M^n = \begin{pmatrix} F_{n-1} & F_n \\ F_n & F_{n+1} \end{pmatrix}$$

But the computation of M^n involves only $\log n$ matrix multiplications (8 integer multiplications plus 4 integer additions).

Asymptotically this is much faster, even though multiplication is substantially more expensive than addition.

If the function f in question is linear it can be written as

$$f(x) = M \cdot x$$

where M is a square matrix over some suitable algebraic structure. Then

$$f^t(x) = M^t \cdot x$$

and M^t can be computed in $O(\log t)$ matrix multiplications.

So this is an exponential speed-up over the standard method.

Another important case is when f is a polynomial map

$$f(x) = \sum a_i x^i$$

given by a coefficient vector $\mathbf{a} = (a_d, \dots, a_1, a_0)$.

In this case the coefficient vector for $f \circ f$ can be computed explicitly by substitution. This is useful in particular when computation takes place in a quotient ring such as $R[x]/(x^n - 1)$ so that the expressions cannot blow up.

Again, an exponential speed-up over the standard method.

But we cannot conclude that $f^t(x)$ can always be computed in $O(\log t)$ operations.

The reason fast exponentiation and the examples above work is that we can explicitly compute a representation of $f \circ f$, given the representation of f .

But, in general, there is no fast representation for $f \circ f$, we just have to evaluate f twice.

Just think of f as being given by an executable, a compiled piece of C code. We can wrap a loop around the executable to compute f^t , but that just evaluates f t -times, in the obvious brute-force way. No speed-up whatsoever.

Exercise

Ponder deeply. Assume the speed-up trick always works and figure out what that would mean for complexity theory.

Speaking about hasty conclusions, here is a simple inductively defined sequence of integers.

$$\begin{aligned}a_1 &= 1 \\a_n &= a_{n-1} + (a_{n-1} \bmod 2n)\end{aligned}$$

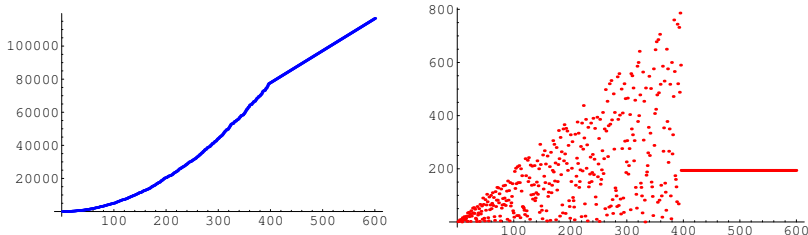
Thus, the sequence starts like so:

1, 2, 4, 8, 16, 20, 26, 36, 36, 52, 60, 72, 92, 100, 110, 124, 146, 148, 182, 204

This seems rather complicated. The function appears to be increasing in a somewhat complicated manner.

Alas, there is a rude surprise.

The sequence is ultimately linear: $a_{396+k} = a_{396} + k \cdot 194$ for $k \geq 0$.



The plot on the left is the sequence, on the right (in red) are the forward differences.

Exercise

Figure out why the sequence is ultimately linear.

Here is another strange integer sequence:

$$a_n = \lceil 2/(2^{1/n} - 1) \rceil - \lfloor 2n/\ln 2 \rfloor$$

This time, the sequence starts like so:

0, ...

and continues like this for a long, long time, for trillions of terms.

Note that it is a minor pain to compute the terms; it's not even clear that $n \mapsto a_n$ is primitive recursive[†]. At any rate, it sure looks like the sequence is constant 0. Alas

$$a_{777\,451\,915\,729\,368} = 1$$

[†]The expression looks like real arithmetic, but it can be handled with just integer arithmetic.

Innocent Question:

Are $n^{19} + 6$ and $(n + 1)^{19} + 6$ relatively prime for all n ?

Sure looks like it, for a long, long time. But there is a counterexample at

$$n = 1578270389554680057141787800241971645032008710129107338825798 \\ \approx 1.5783 \times 10^{60}$$

where the gcd jumps to

$$5299875888670549565548724808121659894902032916925752559262837$$

Intuitively, there are two basic ways to evaluate a recursive function:

bottom-up Use a loop to calculate result for large arguments, starting at small arguments.

top-down Unfold the recursion starting from large arguments and tracing things downward till termination occurs at small arguments.

The unfolding part requires a bit of bureaucracy, one needs to keep track of pending calls. On the other hand, the number of calls may be smaller than in the bottom-up approach.

Iteration can be construed as a special case of primitive recursion.

$$\begin{aligned}F(0, y) &= y \\ F(x + 1, y) &= f(F(x, y))\end{aligned}$$

Then $F(x, y) = f^x(y)$.

Again, this is just the standard bottom-up approach to computing an primitive recursive function, expressed in an elegant and concise way.

Conversely, iteration can be used to express recursion. Suppose

$$\begin{aligned}f(0, \mathbf{y}) &= g(\mathbf{y}) \\ f(x+1, \mathbf{y}) &= h(x, f(x, \mathbf{y}), \mathbf{y})\end{aligned}$$

Define a new function H by

$$\begin{aligned}H : \mathbb{N} \times \mathbb{N} \times \mathbb{N}^k &\longrightarrow \mathbb{N} \times \mathbb{N} \times \mathbb{N}^k \\ H(x, z, \mathbf{y}) &= (x+1, h(x, z, \mathbf{y}), \mathbf{y})\end{aligned}$$

Then

$$f(x, \mathbf{y}) = \text{snd}(H^x(0, g(\mathbf{y}), \mathbf{y}))$$

This is perhaps the most natural definition, but if we wanted to we could make H unary by coding everything up as a sequence number.

More surprisingly, suppose we have some simple basic functions such as

$$x + y \quad x * y \quad x \dot{-} y \quad \text{rt}(x)$$

Here $\text{rt}(x)$ is the integer part of $\sqrt{x}$. These functions suffice to set up the usual coding machinery. If we add an additional operation of iteration

$$f(x) = g^x(0)$$

we can replace primitive recursion by unary iteration.

Exercise

Come up with a precise version of this statement (define a clone) and give a detailed proof.

Definition

The **trajectory** or **orbit** of $a \in A$ under f is the infinite sequence

$$\text{orb}_f(a) = a, f(a), f^2(a), \dots, f^n(a), \dots$$

The set of all infinite sequences with elements from A is often written A^ω . Hence we can think of the trajectory as an operation of type

$$(A \rightarrow A) \times A \rightarrow A^\omega$$

that associates a function on A and element in A with an infinite sequence over A .

Sometimes one is not interested in the actual sequence of points but rather in the set of these points:

$$\{ f^i(a) \mid i \geq 0 \}$$

While the sequence is always infinite, the underlying set may well be finite, even when the carrier set is infinite.

In a sane world one would refer to the sequences as **trajectories**, and use the term **orbit** for the underlying sets. Alas, in the literature the two notions are hopelessly mixed up.

So, when we refer to a “trajectory” we will always mean the sequence, but, bending to custom, we will use “orbit” for both.

Here is a clever definition due to Dedekind: given an endofunction f and a point a , the corresponding **chain** is defined to be

$$\bigcap \{ X \subseteq A \mid a \in X, f(X) \subseteq X \}$$

Thus, the chain is the least set that contains a and is closed under f . That is exactly the orbit of a under f , considered as a set.

Who cares?

Dedekind's definition does not require the natural numbers. In fact, it can be used to define them. In Dedekind's view, this means that arithmetic can be reduced to logic.

Here is how. Suppose we have a function $f : A \rightarrow A$ and a point $a \in A$ such that

- f is an injection,
- a is not in the range of f ,
- A is the chain of f and a .

Dedekind calls these sets **simply infinite**.

We can think of a as 0 and, more generally, we can think of $f^n(a)$ as n .

So this is a way of describing the natural numbers, the smallest infinite set, without any hidden references to the naturals.

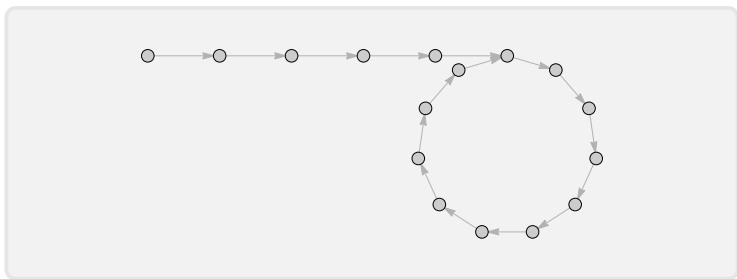
According to Dedekind, the chain C defined by f and a has the form

$$C = \bigcap \{ X \subseteq A \mid a \in X, f(X) \subseteq X \}$$

But note that C is one of the X 's on the right hand side. So there is some (non-vicious) circularity in this approach. Most mathematicians would not bat an eye when confronted with definitions like this one, they are totally standard.

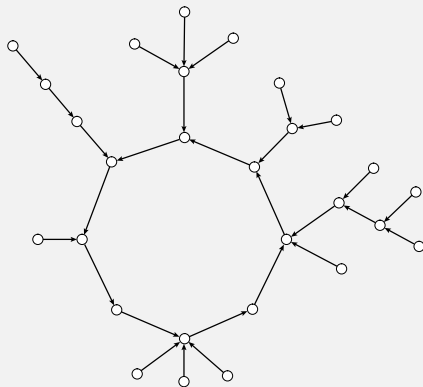
And the payoff is huge. For example, when Bernstein told Dedekind about his correct proof of the “Cantor-Schröder-Bernstein” theorem, he was shocked to hear that Dedekind had a much better proof, based on his chains.

At any rate, if the carrier set is finite, all trajectories must ultimately wrap around and all orbits must be finite:



What changes is only the length of the transient part and the length of the cycle (in the picture 5 and 11).

The lasso shows the general shape of any single orbit, but in general orbits overlap. All orbits with the same limit cycle are called a **basin of attraction** in dynamics.



The geometric perspective afforded by the diagram also suggests to study path-existence problems.

Definition

Let f be a function on A and $a, b \in A$ two points in A . Then point b is **reachable** from a if for some $i \geq 0$:

$$f^i(a) = b$$

In other words, point y belongs to the orbit of x .

Proposition

Reachability is reflexive and transitive but in general not symmetric.

Reachability is symmetric when A is finite and f injective (and therefore a permutation): each orbit then is a cycle and forms an equivalence class.

Definition

Let f be a function on A and $a, b \in A$ two points in A . Points a and b are **confluent** if for some $i, j \geq 0$:

$$f^i(a) = f^j(b)$$

In other words, the orbits of a and b merge, they share the same limit cycle (which may be infinite and not really a cycle).

Reachability implies confluence but not conversely. For finite carrier sets reachability is the same as confluence iff the map is a bijection.

Proposition

Confluence is an equivalence relation.

Reflexivity and symmetry are easy to see, but transitivity requires a little argument.

Let $f^i(x) = f^j(y)$ and $f^k(y) = f^l(z)$, assume $j \leq k$. Then with $d = k - j \geq 0$ we have

$$f^{i+d}(x) = f^{j+d}(y) = f^k(y) = f^l(z).$$

Each equivalence class contains exactly one cycle of f , and all the points whose orbits lead to this cycle – just as in the last picture.

1 Iteration, Trajectories and Orbits

2 **Finding Cycles**

3 Goodstein Sequences

How do we compute the transient t and period p of the orbit of $a \in A$ under $f : A \rightarrow A$ for finite carrier sets A ?

The obvious brute force approach is to use a container to keep track of everything we have already seen:

$$a, f(a), f^2(a), \dots, f^i(a)$$

and then to compare $f^{i+1}(a)$ to all these previous values.

In most cases, the data structure of choice is a hash table or tree: we can check whether $f^{i+1}(a)$ is already present in expected constant time or logarithmic time, respectively. Memory requirement is linear in the size of the orbit assuming the elements in A require constant space (a fairly safe assumption, if the elements are big use pointers).

A (simplified version of a) classical problem from the early days of Lisp: Suppose we have a pointer-based linked list structure in memory and we want to check if there are any cycles in the structure (as opposed to having all lists end in `nil`).

We can think of this as an orbit problem:

- A is the set of all nodes of the structure,
- $f(x) = y$ means there is a pointer from x to y .

The Problem:

Suppose further the structure consumes 90% of memory, so we cannot afford to build a large hash table or tree.

Can we compute transients and periods in $O(1)$ space?

At first glance, this may seem quite impossible: if we forget already discovered elements we *obviously* cannot detect cycles. Right?

Not at all: we have an element $b = f^t(a)$, and we want to check if it is new.

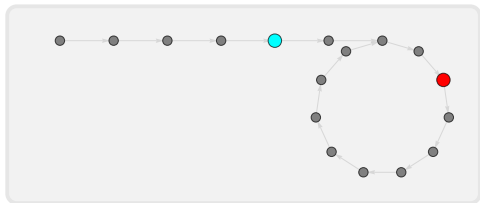
We can simply compare b to all $f^s(a)$ for $s < t$.

This requires an absurd amount of recomputation and is thus highly inefficient, but it trivially works and it uses only constant memory.

The method is actually quite simple: instead of storing an object, we recompute whenever necessary.

Here is a better way to handle the time/space tradeoff: race two pebbles down the orbit.

```
u = f(a);  
v = f(u);  
while( u != v ) {  
    u = f(u);  
    v = f(f(v));  
}
```



Claim

Upon termination, $u = v$ is a position on the cycle.

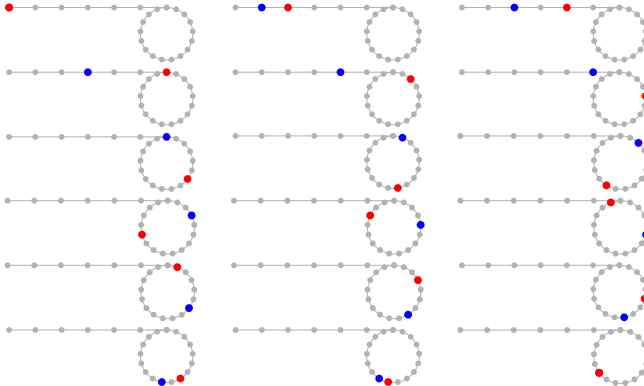
Think of two pebbles u and v , moving at speed 1 and 2, respectively.

The slow pebble u enters the limit cycle at time t , the transient, when the fast pebble v is already there. From now on, v gains one place on u at each step. So pebble v must catch up at time s where $s \leq t + p$, where p is the period. The meeting time is called the **Floyd-time**.

Once we have a foothold on the cycle it is not hard to compute transient and period, see below.

One can make a nice movie out of this. OK, it is pretty boring after all, but what do you expect.

Here the transient is 6, and the period 17.



The Floyd-time here is 17.

One can also write out a simple table of the process. Here we think of the points on the orbit as $-\tau, \dots, -1, 0, 1, \dots, \pi - 1$. To avoid visual clutter, we write $-k$ as $\underline{k}$.

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
<u>6</u>	<u>5</u>	<u>4</u>	<u>3</u>	<u>2</u>	<u>1</u>	0	1	2	3	4	5	6	7	8	9	10	11
<u>6</u>	<u>4</u>	<u>2</u>	0	2	4	6	8	10	12	14	16	1	3	5	7	9	11

Not as pretty, but potentially more useful. Note that when the slow pebbles enters the cycle at time 6, the fast one is in position 6. $6 + 11 = 17$.

Suppose we already have a point b on the cycle.

```
t = 1;  
u = f(b);  
  
while( u != b ) {  
    u = f(u);  
    t++;  
}  
return t;
```

We walk around the cycle, and count steps.

Suppose we already know p , the period.

```
t = 0;
u = a;
v = iterate( f, a, p );    // v = f^p(a)
while( u != v ) {
    u = f(u);
    v = f(v);
    t++;
}
return t;
```

v has a headstart of p . So, when u first enters the cycle, v has just gone around once, and they meet at the contact point.

Let us assume f to be computable in time $O(1)$ and elements of the carrier set A to take space $O(1)$.

Theorem

One can determine the transient t and period p of a point in A under f in time $O(t + p)$, and space $O(1)$.

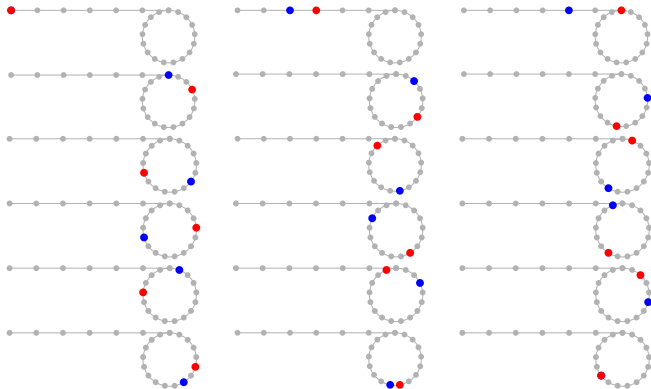
Linear time cannot be avoided in general (why?), so this is optimal.

Floyd's cycle finding algorithm is an excellent general purpose tool in particular when the evaluation of the function in question is cheap.

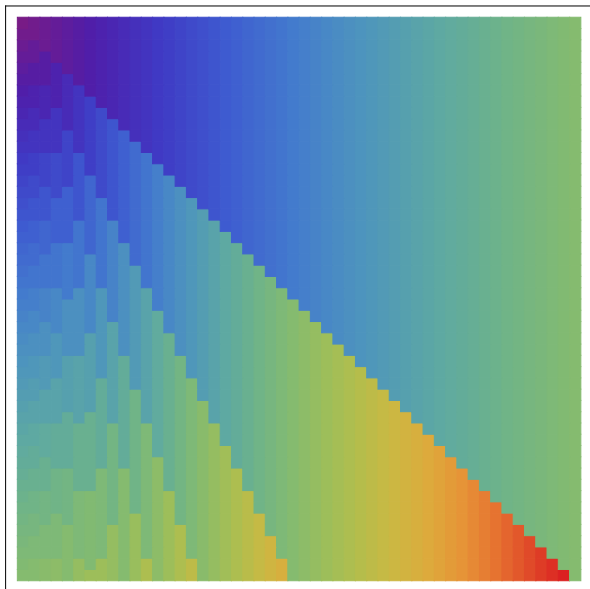
But note that in the special case where the function is known to be a permutation on a finite domain there is, of course, no need to use Floyd's or similar cycle finding algorithms: since the components of the diagram are all cycles we can simply trace a cycle once to determine its length. So the natural method to compute cycle length is automatically memoryless (if we assume the objects in question can be stored in constant space).

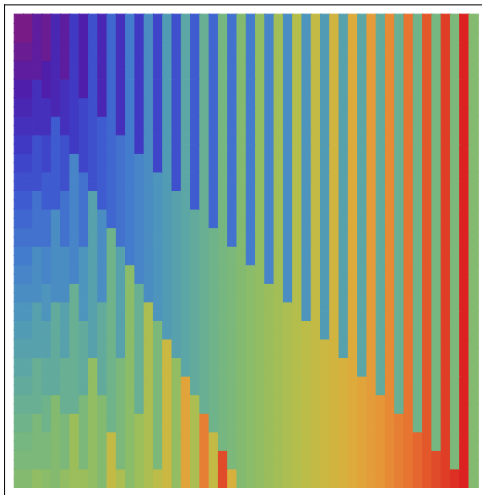
Incidentally, determining cycle lengths of permutations is very important for some advanced counting methods, more later.

It is tempting to try different pebble speeds. Here is transient 6, period 17, pebbles at speeds 2 and 3, respectively.



Surprisingly, the pebbles meet at time 17, just like the ordinary algorithm. Ponder deeply.





This uses speeds 2 and 4. Seems fairly complicated.

Exercise

What would happen to the Floyd-time if we changed the pebble speeds to u and v , where $1 \leq u < v$?

Would the algorithm even work for all transients and period?

Exercise

Try to find an algebraic way to compute the Floyd-time directly from the parameters τ and π . Do this for the $(1, 2)$ version first, then generalize to speeds $u < v$.

Exercise

*Call the place where the pebbles meet the **Floyd-point**. Study it.*

Here is a method to compute the period using “teleportation.”

```
slow = a;
fast = f(a);
cnt = pow2 = 1;
while( fast != slow )
    if( cnt == pow2 )
        { slow = fast; cnt = 0; pow2 *= 2; }
    fast = f(fast);
    cnt++;

return cnt;
```

Exercise

Figure out how this works. Compare its performance to Floyd's method.

There is another algorithm due to Nivasch that uses a bit of extra memory (a small stack) to speed up the search.

Applications:

- discrete dynamical systems (such as cellular automata)
- Pollard's factorization method
- analysis of hash functions

1 Iteration, Trajectories and Orbits

2 Finding Cycles

3 **Goodstein Sequences**

We have already seen that iteration can produce very rapidly growing functions (much like recursion). Here is another example where iteration produces a rather perplexing result: every orbit ends in fixed point 0, though it looks like it should diverge towards infinity.

Suppose we write a number in base 2, say

$$266 = 2^8 + 2^3 + 2$$

We can turn this into the **hereditary binary expansion** by writing the exponents also in base 2, and so on.

$$266 = 2^{2^{2+1}} + 2^{2+1} + 2$$

where we really should write 2^0 instead of 1, but c'mon.

Now suppose we replace 2 in the representation everywhere by 3:

$$3^{3^{3+1}} + 3^{3+1} + 3$$

Unsurprisingly, this new number is much larger:

$$443426488243037769948249630619149892887 \approx 4 \times 10^{38}$$

Next, we write this number in hereditary base 3, and bump the base to 4. We get something like 3×10^{616} .

Then we write this number in hereditary base 4 and bump to 5 ... Obviously, this process leads to a very rapidly increasing sequence of numbers.

More precisely, define the base bump function $G_b(x)$ to be the operation that bumps x from hereditary base b to $b + 1$. Given a natural number n , define

$$\begin{aligned} n_1 &= n \\ n_{b+1} &= \begin{cases} G_{b+1}(n_b) - 1 & \text{if } n_b \neq 0 \\ 0 & \text{otherwise.} \end{cases} \end{aligned}$$

The sequence (n_k) is the **Goodstein sequence** for n . Note that there is a primitive recursive function g such that $g(n, k) = n_k$.

We follow the base bump by subtracting 1, so the result will be a tiny little bit smaller than with a pure base bump. It seems fairly clear that a Goodstein sequence will diverge. Alas . . .

Theorem (Goodstein 1944)

All Goodstein sequences converge to 0.

Goodstein's proof of his theorem uses set theory and in particular a class of countable ordinals.

The argument is extremely elegant, but feels very “non-elementary,” one might try to come up with a more pedestrian proof that only uses the standard tools of arithmetic.

Sadly, it is very hard to come up with good examples.

Starting at 2 and 3 we get the short sequences

$$n = 2 \quad 2, 2, 1, 0$$

$$n = 3 \quad 3, 3, 3, 2, 1, 0$$

But starting at $n = 4$, things already spin out of control:

$$4, 26, 41, 60, 83, 109, 139, 173, 211, 253, 299, \dots, 402653183^2, \dots$$

It takes some $10^{121,210,695}$ steps to get to 0.

Why does this really work? Because once the base is sufficiently large, we keep chipping away at the constant term until we ultimately have to borrow from one of the previous terms.

Consider the sequence for $n = 4$. When we get to base $b = 402653183$, the sequence locally looks like

$$n_{b-1} = b^2$$

$$n_b = b(b+1) + b$$

$$n_{b+1} = b(b+2) + b - 1$$

$$n_{b+2} = b(b+3) + b - 2$$

...

$$n_{2b} = b(2b+1)$$

Ponder deeply.

We can define the **stopping time** $G : \mathbb{N} \rightarrow \mathbb{N}$ that counts the number of steps it takes to reach 0 in a Goodstein sequence:

$$G(n) = \min(k \geq 1 \mid n_k = 0)$$

Note that G is computable; in fact, the algorithm is not at all complicated. The theorem says that G is a total computable function.

Alas, the proof requires induction up to

$$\epsilon_0 = \omega^{\omega^{\omega^{\dots}}}$$

Which is enough to prove that (DPA) is consistent.

Theorem (Kirby, Paris 1982)

Goodstein's theorem is not provable in Dedekind-Peano arithmetic.

It is not terribly difficult to build a register machine M that, on input x , computes the stopping time $G(x)$. In fact, this just requires one while-loop wrapped around a primitive recursive function.

We know that G is total, i.e., M halts on all inputs, but this assertion cannot be proven in (DPA).

The totality statement for M is slightly more complicated than previous examples we have seen, it is Π_2 :

$$\forall x \exists t R(x, t)$$

where R is primitive recursive (and means: the Goodstein sequence for x converges after t steps).