CSE 331 Winter 2023 – Reasoning About Code II

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Reasoning about loops

When you hear “loop,” you might think immediately of a `for` loop, but we’re going to focus on the more fundamental `while` loop:

```
while (B)
      S;
```

`for` loops can, of course, can be rewritten using `while`. The loop `for (`*init*`;` *test*`;` *step*`) S` is equivalent to

```
init;
while (test) {
      S;
      step
}
```

So we lose no generality by restricting our attention to `while`. (There is one difference we won’t emphasize here: The meaning of `continue` is different for the two kinds of loops: For the for-loop, `continue` will execute *step* before the next iteration. Another difference is that *init* can contain declarations of variables local to the loop, but the same effect can be achieved by surrounding the entire loop in braces `{` and `}` .)

When reasoning about a chunk of code involving a loop, there’s often an initialization step between the precondition and the start of the loop. The complete code looks more like:

```
{P}
[initialization steps]
while (B)
      S;
{Q}
```

Loops are trickier to reason about than assignment and if/else statements because you don’t know how many times the loop body will execute. We have to show that our code is correct if the loop iterates 0 times, 1 times, 2 times, 3 times, 4 times, … . More generally, we need to prove that when the loop terminates, {Q} is satisfied regardless of how many times the loop ran. (We also need to prove that the loop will terminate, but we won’t worry too much about that for now.) To do this, we introduce the notion of a **loop invariant**.

A loop invariant, usually written `{I}`, is an assertion that is both a precondition and postcondition for the loop body. `{I}` must be true at the beginning and end of each iteration of the loop body, though it does not need to hold at every point in the middle of the loop. To show that a given loop invariant is valid, we show (1) that it holds immediately before entering the loop and (2) that if it holds at the beginning of the loop, it also holds at the end. (1) implies that `{I}` holds at the beginning of the first iteration. (We assume that evaluating B does not change any variables). By induction, we can then conclude that `{I}` holds at the beginning and end of every iteration. (Why?) We can also use the fact that `{B}` is true at the beginning of every iteration or the loop would have terminated.

Since `{I}` holds true at the end of any iteration, including the final iteration, it must also hold true immediately after the loop exits. We also know `{B}` is false when the loop terminates or the loop wouldn't have stopped. So to prove that `{Q}` holds after the loop, we just need to show that `{I∧!B}=>{Q}`. (You may have noticed an edge case: what if the loop terminates immediately so the loop body is never executed? Since `{I}` held before the non-executed loop, it will still hold afterward.)

In summary, to prove that the postcondition is satisfied and our code is correct, we need to show:

1. That `{I}` holds immediately before the loop, i.e., immediately after the initialization steps.
2. That `{I}` holds at the end of the loop body, given that `{I ∧ B}` hold at the beginning of the loop body.
3. That `{I∧ !B}=>{Q}`

Let's add these assertions to our generalized loop:

```
{P}
[initialization steps]
{I}
while (B)
      {I ∧ B}
      S;
      {I}
{I ∧ !B} => {Q}
```

Sound easy? The clever part is finding the loop invariant that makes these three conditions true. We often can get inspiration by looking at the postcondition `{Q}`. Very often a suitable invariant `{I}` is a weaker version of `{Q}` that captures how the loop has achieved part of the desired result, but not all.

As we will see in the examples below, this reasoning process should be performed *as you are writing the code*, shaping what you write. It guides your thought process to help you write clean and correct code on the first try.

When writing loops, you may be tempted to write your code sequentially, starting with {P} and working your way to {Q} one line at a time. It is usually more effective to work from the inside out in roughly the following order:

- Choose a loop invariant and write the loop body (in either order – this is the inventive step).
- Choose B so that `{I ∧ !B} => {Q}`.
- Add initialization steps to get from {P} to {I}.

This order isn't a hard-and-fast rule, but it's a good place to start.

One detail that we've glossed over is that sometimes a few statements need to be executed after the loop body to establish the postcondition `{Q}`. In that case, when the loop terminates, it might not be the case that `{I ∧ !B} => {Q}`. The additional statements `S′` that are inserted at the end need to allow us to prove that `{I && !B} S′ {Q}` is a valid Hoare triple, i.e., `S′` establishes `{Q}`. In most of our examples we won't need these extra termination steps, and it is often possible to design loops to minimize the need for extra steps at the end.

Example 1
Write a loop to set sum = 1 + 2 + … + n and prove that it is correct.

From the instructions, we have our postcondition: {sum = 1 + 2 + … n}.

Let's start with the loop body. We'll need a counter k. At each iteration, we'll add k to sum and increment k. So far, our code looks something like this:

```
{pre: ____________}
[Initialization]
{inv: ____________}
while (B:__________) {
      {inv: ____________}
      sum = sum + k;
      k = k+1;
      {inv: ____________}
}
{post: sum = 1 + 2 + … + n}
```

An aside: notation

Earlier, our preconditions and postconditions looked the same as any other assertions. Now, it will be helpful to be more precise:

`{pre: assertion}` denotes a precondition

`{post: assertion}` denotes a postcondition

`{inv: assertion}` denotes a loop invariant

What should our loop invariant be? In the loop body, we add `k` to `sum` and increment `k`. This suggests that `sum` should be `1+2+…+k-1` at the beginning of the loop body. Let's call this assertion `{I}`. If `{I}` holds at the beginning of the loop, is it guaranteed to hold at the end of the loop? We can find out by writing it as the postcondition for the loop body and reasoning backwards to find the weakest precondition:

```
{sum = 1+2+…+k-1}
sum = sum + k;
{sum = 1+2+…+k}
k = k+1;
{sum = 1+2+…+k-1}
```

Yes, if `{I}` holds at the beginning of the loop, the fact that we add `k` to `sum` and increment `k` will ensure that `{I}` also holds at the end of the loop. We will use `{I}` for our invariant, later adding the initialization steps needed to ensure that it holds on entering the loop for the first time. Notice that `{I}` is, in fact, a weaker version of the postcondition, i.e., when the postcondition is true, then so is the invariant. That was the inspiration for picking this particular invariant and designing the loop this way.

Now we need B. Remember that we need to have that `{I ∧ !B} => {Q}`, or

```
{sum = 1+2+…+k-1 ∧ !B} => {sum = 1 + 2 + … + n}.
```

This logic falls neatly into place if we let !B be {k-1 = n}. So then B = !(!B) is simply

```
{!(k-1 = n)} => {k-1 != n} => {k != n+1}
```

Let's add the new details to our code outline:

```
{pre: ________}
[Initialization]
{inv: sum = 1+2+…+k-1}
while (k != n+1) {
      {sum = 1+2+…+k-1}
      sum = sum + k;
      {sum = 1+2+…+k}
      k = k+1;
      {inv: sum = 1+2+…+k-1}
}
{sum = 1+2+…+k-1 ∧ k = n+1} => {post: sum = 1 + 2 + … + n}
```

We're almost there! We just need to initialize `sum` and `k` to values that will make the loop invariant true initially. One possible initialization is to set k=1 and `sum` to a value that establishes that `sum` is the sum of the elements in the set {1…k-1}. By convention, the set {i…j} for j < i is defined as the empty set, and the sum of an empty set is 0. Because k-1 = 0 < 1, we set `sum` to 0 to satisfy the invariant.

Finally, we just need the weakest precondition for the entire sequence of code. We need k <= n+1 initially or the loop will never terminate. Reasoning backwards, we arrive at the precondition n >= 0.

The complete code, with assertions, looks like this:

```
{pre: n >= 0}
sum = 0;
{n >= 0}
k = 1;
{inv: sum = 1+2+…+k-1}
{n+1 > 0 ∧ sum = 1+2+…+k-1}
while (k != n+1) {
      {inv: sum = 1+2+…+k-1}
      sum = sum + k;
      {sum = 1+2+…+k}
      k = k+1;
      {inv: sum = 1+2+…+k-1}
}
{sum = 1+2+…+k-1 ∧ k = n+1} => {post: sum = 1 + 2 + … + n}
```

Example 2
Write a loop to set max = largest value in items[0…size-1]

We get our postcondition directly from the problem: {max = largest value in items[0…size-1]}

A simple approach is to look through `items` one element at a time, keeping track of the largest value seen so far. The loop terminates when we've examined all elements. Much like in a typical `for` loop, we'll keep a counter k, examining items[k] during each iteration of the loop and updating max if needed. From this description, the invariant `{I}` emerges naturally: {max = largest in items[0…k-1]}.

To choose {B}, recall that we want `{I ∧ !B} => {Q}`, or

```
{max = largest in items[0..k-1] ∧ !B} =>
                               {max = largest in items[0..size-1]}.
```

This works if we set {!B} to {k = size}, or {B} = {k != size}.

Finally, we make `{I}` true initially by setting k = 1 and max = items[0]. This assumes the list is non-empty, so our precondition is size > 0.

Let's put this all together:

```
{pre: size > 0}
k = 1;
max = items[0];
{inv: max = largest in items[0..k-1]}
while (k != size) {
      {inv: max = largest in items[0..k-1]}
      if (max < items[k]) {
            {max = largest in items[0..k-1] ∧ max < items[k]}
            max = items[k];
            {max = largest in items[0..k]}
      else {
            // nothing to do
            {max = largest in items[0..k]}
      }
      k = k+1;
      {inv: max = largest in items[0..k-1]}

}
{max = largest in items[0…k-1] ∧ k = size}
      => {max = largest in items[0..size-1]}
```

An aside: the code works, but only for non-empty lists (size > 0). What if the list is empty? We could treat that as an error, but we might like to accept the broadest set of inputs possible (i.e., make the precondition as weak as possible). One way we could do that is to return the result Integer.MIN_VALUE if `size == 0`. (Is this a good design decision? It depends on what properties we want to hold for this method.) We end up with something like:

```
// return largest value in list if not empty
// otherwise, return Integer.MIN_VALUE
public int max() {
      if (size == 0) {
            return Integer.MIN_VALUE;
      } else {
            // code from above
      }
}
```

An aside: notation for historical values

Sometimes an assertion needs to refer to the earlier value of a variable. To prove that

```
t = x; x = y; y = t;
```

swaps x and y, the postcondition must refer to their initial values. You can do so with subscripts or case distinctions, e.g.:

{pre: $x=x_{pre} \land y=y_{pre}$}

{post: $x=y_{pre} \land y=x_{pre}$}

Example 3

Given a[0…n-1], reverse the elements in a.

Choosing the invariant is a little subtler than for previous problems. We need to say something about the state of the whole array at each iteration. Let's start with our precondition and postcondition to establish the initial and final state of the array:

```
              0                       n
pre:    a  | A[0]  A[1]  …  A[n-2]  A[n-1] |

              0                       n
post:   a  | A[n-1]  A[n-2]  …  A[1]  A[0] |
```

In our invariant, we will divide the array into three regions by weakening the postcondition: we have two regions at the front and back that have already been swapped and a region in the middle that still needs to be swapped.

```
              0                  L              R                N
inv:    a  | A[n-1]  A[n-2]  …  | original order | … A[1] A[0] |
```

At each step of the loop, we will swap the items at the beginning and end of the unswapped section and adjust the endpoints. Let us define L and R as the first and last indices of the unswapped section, respectively. Alternatively, L could be the index just before the unswapped section and/or R could be the index just afterward. It doesn't really matter which convention you use (though one might result in cleaner code) – just pick one and *use it consistently!* Bugs happen when someone forgets what they chose and writes part of the code assuming a different convention.

When the unswapped section only contains 0 or 1 elements, the entire list has been reversed. This occurs when L >= R, so {B} = {L < R}. Initially the entire list is unswapped, and we initialize L and R accordingly.

Putting it all together:

```
    L = 0;
    R = n-1;
    while (L < R) {
          swap(a[L],a[R]);
          L = L+1;
          R = R-1;
    }
```

To avoid extra detail and focus on reasoning about the loop, we assume we can write swap(x,y) to correctly interchange the values of variables x and y. We actually can't write such a function in Java, but it could easily be replaced with three assignment statements wherever it occurs if needed. (Making this replacement and proving it correct is left as an exercise for the reader. ☺)

Example 4

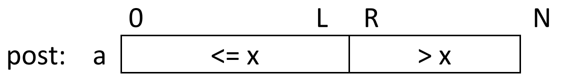
Binary search. Given a value x and sorted array a[0..n-1], find the index of x in a, if present. If x is not present, return an appropriate location in the array that can be used to insert x if desired.

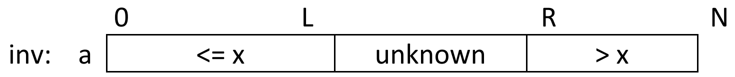
The basic idea of binary search is to keep track of three regions of the array: a region at the front where all values are known to be <= x, a region at the end where all values are known to be > x, and an "unknown" region in the middle. At each iteration of the loop, we compare x to the element at the center of the unknown region and adjust the endpoints of the unknown region accordingly. We repeat this process until the unknown region is empty. Then x will be located or can be inserted at the end of the first region.

We will use L and R to represent the indexes immediately before and after the unknown region. Notice that this is a different convention than we used in the previous example, where L and R were the first and last elements of the middle region. Again, it doesn't matter which convention we use as long as we are consistent, except that the one choice might make the code simpler or easier to follow than the other. When creating an algorithm it's sometimes useful to try different alternatives and see which one leads to simpler, cleaner code.

Our precondition is that the loop is already sorted. Our invariant shows what we know about the array at each step along the way, and our postcondition shows what we know at the end:

pre: a[0] <= a[1] <= … <= a[n-1]





We can also write our invariant as:

```
inv: a[0..L] <= x ∧ a[R..n-1] > x ∧ a[L+1..R-1] unknown
```

The loop terminates when the unknown region is empty, i.e. L+1=R. Initially the entire list is unknown, and we initialize L and R accordingly. (Notice that `a[L]` and `a[R]` are actually outside the array initially! But that is not a problem because we never reference those array elements.)

Putting it all together:

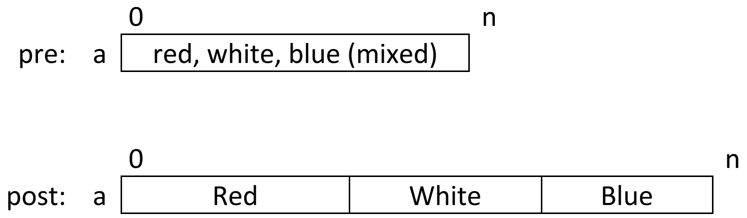
```
L = -1;
R = n;
while (L+1 != R) {
      mid = (L+R)/2;
      if (a[mid] <= x)
            L = mid;
      else  // a[mid] > x
            R = mid;
}

// x is found if L >= 0 && a[L] = x (note that the short-circuit
// property of && is essential here)
```

As in the previous example, we glossed over proving the body of the loop in detail.

Example 5

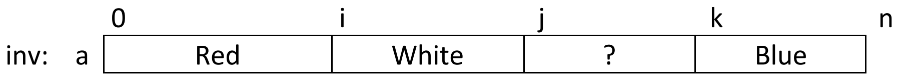
("Dutch National Flag" problem) Given an array of red, white, and blue pebbles, sort the array so the red pebbles are at the front, white are in the middle, and blue are at the end.

Once again, we describe the state of the array in the precondition, postcondition, and invariant. The precondition describes an array with red, white, and blue elements of unknown quantities in an unknown order. The postcondition is the correctly partitioned array.



We can see that the array naturally has three regions in the postcondition. For the invariant, we add an "unknown" region representing the values not yet sorted. We keep track of the endpoints of the four regions. At each step, we take a value from the unknown region, put it in the appropriate sorted region, and adjust the endpoints of all the regions accordingly.

Where should the unsorted region go? At the end? Somewhere in the middle? We choose to keep it between the white and blue regions, although it could just as easily have been between the red and white areas. Both of these choices have the advantage that pebbles that have been moved to the red and blue regions do not need to be moved further as the algorithm progresses. Our invariant is then:



a[0…i-1] red ∧ a[i…j-1] white ∧ a[j…k-1] unknown ∧ a[k…n-1] blue

The code is straightforward:

```
i = 0; j = 0; k = n;
while (j != k) {
      if (a[j] == white) {
            j = j+1;
      } else if (a[j] == blue) {
            swap(a[j], a[k-1]);
            k = k-1;
      } else {  // a[j] is red
            swap(a[i], a[j]);
            i = i+1;
            j = j+1;
      }
}
```

As before, we use the `swap` function to interchange array elements.

A note about termination

Some loops should run forever, for example a web server, but most of the loops we write should normally terminate. So a full proof that a loop is correct involves showing that it terminates as well as that it computes the right result. In fact, Hoare logic only says that *if* a loop terminates then the postcondition holds. We have ignored termination above to focus on the correctness issues.

There are various ways to prove termination, but a common strategy is the following:

- Map the state of the computation to a natural number somehow (only used "in the proof")
- Prove that the natural number decreases on every iteration
- Prove that the loop test is false by the time the natural number gets to 0, if not sooner

For many of our examples, the appropriate number is the size of the unprocessed input:

- The quantity *n-k* in when we sum the numbers from 1 to *n*
- The size of the part of the array that has not yet been examined in the "find the max" and binary search problems
- The size of the unprocessed part of the array in the Dutch National Flag problem

In all of these cases the number decreases by 1 or more (for binary search) on each iteration of the loop. Eventually the number reaches 0 and the loop must terminate at that point.