R: Numerical Algorithms

Signal Data Science

things to cover:

profvis

Now that you're acquainted with the basics of R's functional programming toolkit and have a strong grasp of the most important aspects of R's internals, we'll wrap up our R curriculum with some materials on a variety of useful and interesting numerical algorithms.

Numerical optimization

Gradient descent

Backpropagation

Stochastic gradient descent

The Newton-Raphson method

The Nelder-Mead method

Fast modular exponentiation

Before we can implement more complex algorithms, we'll need a fast implementation of modular exponentiation, consisting of the task of calculating $a^b \mod c$, *i.e.*, the remainder of dividing a^b by c. In addition to being intrinsically useful, modular exponentiation through repeated squaring (which is the end goal of this section) is a common programming question in interviews.

• Write a function pow(a, b, c) that calculates $a^b \mod c$. Begin with a naive implementation that simply evaluates the calculation directly. Verify that $6^{17} \mod 7 = 6$ and that $50^{67} \mod 39 = 2$.

- To improve the runtime of pow(), start at 1 and repeatedly multiply an intermediate result by *a*, calculating the answer mod *c* each time, until the *b*th power of *a* is reached. Implement this as pow2().
- Using the tictoc package, quantify the resulting improvement in runtime. How does runtime improve as *a* or *c* increase in size? Is the runtime improvement merely a constant-factor scaling change (is the new runtime a constant multiple of the previous runtimes)?

In order to make our algorithm even faster, we'll want to write a short utility function:

Write a function decompose(n) which takes as input an integer n and returns a vector of integers such that when you calculate 2 to the power of each element of the result and take the sum of those powers of 2, you obtain n. (Hint: First, calculate all powers of 2 less than or equal to n. After that, iteratively subtract off the highest power from n, keeping track of which power of 2 it was, until you get to 0.)

Now, we can implement a quite rapid algorithm for modular exponentiation with the trick of repeated squaring:

• You can improve the runtime of pow() further by decomposing b into a sum of powers of 2, starting with a and repeatedly squaring modulo c (to calculate $a^1, a^2, a^4, a^8, \ldots \mod c$), and then forming the final answer as a *product* of those intermediate calculations. (For example, for $6^{17} \mod 7$, you are essentially calculating $17 = 2^0 + 2^4 \mod 6^{17} \mod 7 = 6^{2^0} \cdot 6^{2^4} \mod 7$.) Using decompose(n), implement this improvement as pow3(), making sure to calculate every intermediate result modulo c. Verify that pow3() is faster than pow2().

Random number generation

Random number generators are not truly random (unless you use quantum techniques!) and are in fact pseudorandom, meaning that their output only approximates true randomness. A pseudorandom number generator (pRNG) can take a starting point, known as a seed, as input; a pRNG, given the same seed twice, will produce the exact same output in the exact same order both times. R uses inversion transform sampling by default to generate random numbers.

We will consider the implementation of a xorshift pRNG, one of the simplest and fastest classes of pRNGs which work by repeatedly taking the bitwise XOR of a number with bit-shifted versions of itself. The speed of xorshift pRNGs results from the fact that the numerical operations involved are directly implemented by the CPU. (Regrettably, they do fail certain statistical tests for randomness because they are fundamentally based on linear recurrences.)

Implementing bitwise operations in R

First, we need to implement bitwise operations in R.

In order to do so, we need functions which allow us to convert between decimal and binary representations of integers. The binary representation of a number encodes it as sums of powers of 2; for example, the binary number "100101" is equal to $2^5 + 2^2 + 2^0$, because (counting from the right and starting at 0) the 0th, 2nd, and 5th positions in "100101" are 1s. Representations of integers as sums of powers of 2 are *unique*, meaning that no two numbers have the same binary representation.

- Write a function to_binary(n) which takes an integer n and returns its binary representation in a string with no leading zeroes (e.g., "10100" instead of "0010100").
- Write a function to_decimal(b) which takes a binary representation b and returns the corresponding decimal integer.

The bitwise XOR operation takes two binary numbers of equal length and outputs another number of the same length, where the ith position in the output is 1 if the ith positions in the two input numbers are different and 0 if they are the same. For example, $0101 \oplus 0011 = 0110$ and $0010 \oplus 1010 = 1000$.

Implement bitwise XOR as bitwise_xor(a, b). If the inputs are of different lengths, remember to pad the shorter binary number with zeroes on the left.

A logical left shift of k bits can be thought of as discarding the leftmost k digits of a binary number and appending k zeroes to the right end. Similarly, a logical right shift of k bits discards the k rightmost digits and appends k zeroes to the left end. (If k is equal to or greater than the length of the binary number, then the entire number is placed with zeroes.)

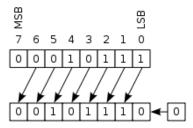


Figure 1: Illustration of a logical left shift by 1 bit.

These operations are called *shifts* because of how they are carried out in the CPU register.

 Implement left and right logical shifts of k bits as left_shift(b, k) and right_shift(b, k).

Implementing a xorshift pRNG

We can implement an algorithm to generate a random positive 32-bit integer. In order for logical left shifting to work properly, our binary numbers must be long enough to encode 32 bits of information:

 Write a function to_binary_len(n, k) which converts an integer n to a binary representation and then pads it with 0s on the left until the length of the string is equal to k.

Finally, we are ready to implement a simple xorshift algorithm. It will take as input 4 *seed* values x, y, z, and w which determine its initial state. In the following, let $x \ll n$ represent x left logical shifted by n bits, let $x \gg n$ represent x right logical shifted by x bits, and let x represent the bitwise XOR operation. The algorithm is as follows:

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1. Set t = x.

2. Set t = t \oplus (t \ll 11).

3. Set t = t \oplus (t \gg 8).

4. Set x = y, y = z, and z = w.

5. Set w = w \oplus (w \gg 19).

6. Set w = w \oplus t.

7. Return w.
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Now you have everything you need to write a custom implementation of a xorshift pRNG!

• Fill in the following code template for a xorshift() function:

xorshift() will return a xorshift pRNG seeded with the specified values which can then be repeatedly called to generate random values, e.g., r = xorshift(0, 3, 93, 59); r();. Verify that with (x, y, z, w) = (1, 2, 3, 4) as the seed, the first three generated numbers are 2061, 6175, and 4. Visualize 10,000 randomly generated numbers with a histogram of their values.

Saving and loading pRNG state in R

It is occasionally important to be able to save and load the pRNG state in R. For example, you may want to be able to reproduce the output of two "interwoven" random sequences beginning from different seeds.

The state of R's built-in pRNG is simply saved in the .Random.seed variable in the global environment. It can be written to a different variable and restored via simple assignment. There is one caveat: attempting to set .Random.seed within a function call will *create a local variable* called .Random.seed instead of changing the value of the *global* .Random.seed variable. Thankfully, the seed variable corresponding to R's pRNG can always be accessed with .GlobalEnv\$.Random.seed.

Fast primality testing

Checking whether a number is prime or composite is a classic algorithmic task, stretching all the way back to 200 BC with the Sieve of Erastosthenes developed by Erastosthenes of Cyrene. We will first implement the Sieve and then work toward writing an implementation of the Miller–Rabin primality test, a modern test for primality known to be very fast in practice for reasonably small numbers.

The Sieve of Erastosthenes

The Miller–Rabin primality test

In the Miller–Rabin primailty test, we test the primality of a number n > 2 as follows: Since n is odd, n-1 must be even, so we can write $n-1=2^s \cdot d$, where d is odd. (For example, if n=13, then $n-1=12=2^2 \cdot 3$ with s=2 and d=3.) The Miller–Rabin primality test is based on the observation that if we can find a number a such that $a^d \not\equiv 1 \pmod{n}$ and $a^{2^r d} \not\equiv -1 \pmod{n}$ for all integers r in the range $0 \le r \le s-1$, then n is not prime. Otherwise, n is likely to be prime.

Note that the Miller–Rabin primality test, as formulated here for a specific value of a, is *probabilistic* rather than *deterministic* – it cannot definitively establish that n is prime. It can be made deteterministic by checking all $a \le 2(\ln n)^2$. Better yet, when n is sufficiently small, it has been found that we only need to consider a couple different values of a; for example, for n < 4,759,123,141, we only have to check $a \in \{2,7,61\}$.

We have one more utility function to write:

Write a function decompose_even(n) which takes as input an even integer
n and returns a vector of two integers c(s, d) such that n is equal to 2^s
* d and d is odd.

With decompose(), decompose_even(), and pow3(), we are now ready to implement the entire primality test.

- Following the above description, implement the deterministic Miller–Rabin test as miller_rabin(n) for n < 4,759,123,141, returning TRUE for a prime number and FALSE otherwise. (Note that checking if $x \equiv -1 \pmod{n}$ is equivalent to checking if $x \equiv n 1 \pmod{n-1}$.)
- Write a function simple_check(n) that checks if n is a prime by checking
 if n is divisible by any integers from 2 up to floor(sqrt(b)). Verify that
 miller_rabin() and simple_check() produce the same output for the
 first 100 integers. Use timeit to compare the performance of the two
 functions as n grows.

A small primality problem

We can apply the Miller–Rabin primality test to solve a simple problem in computational number theory.

• Find a counterexample to the following statement: By changing at most a single digit of any positive integer, we can obtain a prime number. Use the memoise package to easily perform memoization for the output of miller_rabin(). How much faster is your code with memoization compared to without memoization?