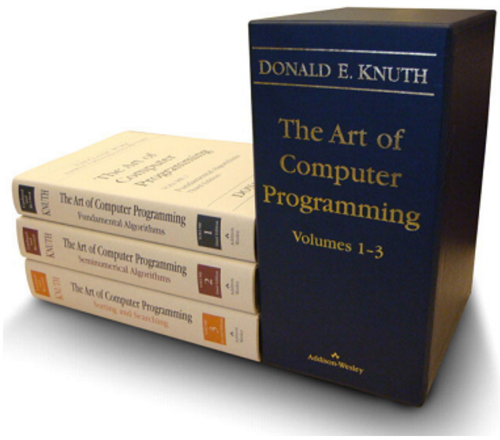
Symbolic Summation

Victor Adamchik

Carnegie Mellon University

Introduction to Summation



Exercise 1.2.6.63 in a book by D. Knuth "*The art of computer programming*" Vol. 1: Fundamental Algorithms, Addison-Wesley Publishing Co., Reading, Mass.-London-Don Mills, Ont, 1969 (1st or 2nd editions) says

develop computer programs for simplifying sums that

involve binomial coefficients

In 1997's 3rd edition, that exercise is replaced by a pure technical problem.

The summation problem

$$S = \sum_k f(n, k)$$

consists in finding a *closed form* for S. By a closed form we mean a finite combination of elementary functions and constants.

Consider a finite sum, where the summand $f(k)$ is free of n

$$S(n) = f(1) + f(2) + \ldots + f(n) = \sum_{k=1}^{n} f(k)$$

Shifting n by 1, we observe that

$$S(n+1) = f(1) + \ldots + f(n) + f(n+1) = \sum_{k=1}^{n} f(k) + f(n+1)$$

Thus

$$S(n+1) = S(n) + f(n+1)$$
$$S(1) = f(1)$$

and the problem of summation is reduced to solving a recurrence equation of the first order. The success of this approach mainly depends on ability to solve recurrence equations of different types and orders. As an example, the following sum

$$S(n) = \sum_{k=1}^{n} k$$

is reduced to solving this recurrence equation

$$S(n+1) - S(n) = n+1$$
$$S(1) = 1$$

If the summand is a function of n

$$S(n) = \sum_{k=0}^{n} f(n, k)$$

the above procedure does not lead so easily to a difference equation.

Before we proceed with summation algorithms, we need to review elementary techniques of solving difference equations.

Recurrence relations

Definition. If n-th term of a sequence can be expressed as a function of previous terms

$$x_n = F(x_{n-k}, x_{n-k+1}, \ldots, x_{n-1}) + g_n, \quad n > k$$

then this equation is called a k-th order recurrence relation. The values $x_1, x_2, \ldots, x_k$ must be explicitely given. They are called initial conditions. The function F in the definition above may depend upon all or some previous terms. If $g_n = 0$, the recurrence equation is called homogeneous. Otherwise, it's called non-homogeneous.

In this lecture we will outline some methods of solving recurrence relations (later on we will study the most general method of hypergeometric summation.) By solving we mean to find an explicit form of x_n as a function of n that is free of previous terms except ones given in initial conditions. For example, the Towers of Hanoi recurrence relation

$$x_n = 2\, x_{n-1} + 1$$
$$x_1 = 1$$

has the following solution

$$x_n = 2^n - 1$$

Recurrences are classified by the way in which terms are combined. Here is a list of some of the recurrences

■ First Order

Linear $a_n = 2 * a_{n-1} + 1$

Non-Linear $a_n = a_{n-1}^2 + z$

■ Second Order

Linear $a_n = a_{n-1} + a_{n-2}$

Non-Linear $a_n = a_{n-1} * a_{n-2}$

■ Higher Order

$$a_n = a_{n-1} + a_{n-2} + a_{n-3}$$

$$a_n = a_0\, a_{n-1} + a_1\, a_{n-2} + \ldots + a_{n-1}\, a_0$$

■ Divide and Conquer

Binary Search $a_n = a_{n/2} + 1$

Merge Sort $a_n = 2\, a_{n/2} + n - 1$

Solving First Order Recurrences

This class of recurrences can be solved by iteration: namely apply the recurrence to itself until only an initial value left.

Example 1

Consider the following recurrence

$$a_n = \lambda * a_{n-1}$$

$$a_1 = 1$$

It iterates to

$$a_n = \lambda * a_{n-1} = \lambda^2 * a_{n-2} = \lambda^3 * a_{n-3} = ... = \lambda^{n-1} * a_1 = \lambda^{n-1}$$

Towers of Hanoi

This is a non-homogeneous equation

$$a_n = 2 * a_{n-1} + 1$$
$$a_1 = 1$$

Shifting n, we obtain the following set of equations

$$a_n = 2 * a_{n-1} + 1$$
$$a_{n-1} = 2 * a_{n-2} + 1$$
$$a_{n-2} = 2 * a_{n-3} + 1$$
$$...$$
$$a_2 = 2 * a_1 + 1$$

that can be rewritten as

$$a_n = 2 * a_{n-1} + 1$$
$$2\, a_{n-1} = 4 * a_{n-2} + 2$$
$$4\, a_{n-2} = 8 * a_{n-3} + 4$$
$$...$$
$$2^{n-2} a_2 = 2^{n-1} * a_1 + 2^{n-2}$$

Next, we sum up the above equations to get

$$a_n = 2^{n-1} * a_1 + \left(1 + 2 + 4 + ... + 2^{n-2}\right)$$

or (since $a_1 = 1$)

$$a_n = 2^{n-1} + 2^{n-2} + 2^{n-1} + \ldots + 2 + 1 = 2^n - 1$$

In *Mathematica*

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RSolve[{a[n] == 2 a[n - 1] + 1, a[1] == 1}, a[n], n]
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```
{{a[n] → -1 + 2^n}}
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■ Example 2

$$a_n = \lambda\, a_{n-1} + n$$
$$a_1 = 1$$

We have

$$a_n = \lambda\, a_{n-1} + n$$
$$\lambda\, a_{n-1} = \lambda^2\, a_{n-2} + \lambda(n-1)$$
$$\lambda^2 a_{n-2} = \lambda^3\, a_{n-3} + \lambda^2(n-2)$$
$$\ldots$$
$$\lambda^{n-2} a_2 = \lambda^{n-1}\, a_1 + \lambda^{n-2}\, 2$$

Summing them up, yields

$$a_n = \lambda^{n-1}\, a_1 + n + \lambda(n-1) + \lambda^2(n-2) + \ldots + \lambda^{n-2}\, 2$$

Hence,

$$a_n = \lambda^{n-1} + \sum_{k=0}^{n-2} \lambda^k\, (n-k)$$

$$a_n = \lambda^{n-1} + \sum_{k=2}^{n} \lambda^{n-k}\, k$$

In *Mathematica*

```
RSolve[{a[n] == λ a[n - 1] + n, a[1] == 1}, a[n], n]
```

$$\left\{\left\{a[n] \to -\left(\left(\left(\frac{1}{\lambda}\right)^{-1+n} + n \left(\frac{1}{\lambda}\right)^{-1+n} - n \left(\frac{1}{\lambda}\right)^{n} - \lambda\right) \lambda^n\right) \Big/ (-1+\lambda)^2\right\}\right\}$$

Solving Second Order Recurrences

This class of recurrences can be solved using a characteristic equation - a method of solving linear recurrences with constant coefficients (coefficients by a_k are free of n).

Fibonacci numbers

The Fibonacci sequence is defined by

$$a_n = a_{n-1} + a_{n-2}$$
$$a_0 = 0, \quad a_1 = 1 \tag{1}$$

Our goal is to find a closed form representation for a_n. It's easy to see that we cannot find it by iteration, since unwinding recursive calls will lead to a binary tree. But what if we look at the ratio of two consecutive terms? The ratio could be any function, though the simplest one is a constant

$$\frac{a_n}{a_{n-1}} = \lambda$$

where λ is to be determined. To find λ, we divide (1) by a_{n-1}

$$\frac{a_n}{a_{n-2}} = \frac{a_{n-1}}{a_{n-2}} + 1$$

Since

$$\frac{a_n}{a_{n-2}} = \frac{a_n}{a_{n-1}} \frac{a_{n-1}}{a_{n-2}} = \lambda^2$$

we obtain apolynomial equation

$$\lambda^2 = \lambda + 1$$

which is called a characteristic equation. The equation has two roots

$$\lambda_1 = \frac{1-\sqrt{5}}{2} \text{ and } \lambda_2 = \frac{1+\sqrt{5}}{2}$$

Therefore,

$$\left(\frac{1-\sqrt{5}}{2}\right)^n \text{ and } \left(\frac{1+\sqrt{5}}{2}\right)^n$$

are two solutions to the Fibonacci recurrence. But we have more solutions! Since ${\lambda_1}^n$ and ${\lambda_2}^n$ are solutions, then so is their linear combination

$$a_n = c_1 * {\lambda_1}^n + c_2 * {\lambda_2}^n$$

where c_1 and c_2 are arbitrary constants. Such solution is called a *general* solution. How would you prove this result? By substitution this into the original equation

$$c_1 * {\lambda_1}^n + c_2 * {\lambda_2}^n - \left(c_1 * {\lambda_1}^{n-1} + c_2 * {\lambda_2}^{n-1}\right) - \left(c_1 * {\lambda_1}^{n-2} + c_2 * {\lambda_2}^{n-2}\right)$$

and collecting terms wrt c_1 and c_2

$$c_1 * \left(\lambda_1{}^n - \lambda_1{}^{n-1} - \lambda_1{}^{n-2}\right) + c_2 * \left(\lambda_2{}^n - \lambda_2{}^{n-1} - \lambda_2{}^{n-2}\right)$$

This is zero, since λ_1 and λ_2 are the roots of the charcateristic equation.

Back to the general solution

$$a_n = c_1 * \lambda_1{}^n + c_2 * \lambda_2{}^n$$

where coefficients c_1 and c_2 are unknown. How do we find c_1 and c_2? From initial conditions

$$a_0 = 0, \ \ a_1 = 1$$

This leads to a system of two equations

$$a_0 = c_1 * \lambda_1{}^0 + c_2 * \lambda_2{}^0 = 0$$
$$a_1 = c_1 * \lambda_1{}^1 + c_2 * \lambda_2{}^1 = 1$$

or

$$c_1 + c_2 = 0$$
$$c_1 * \frac{1-\sqrt{5}}{2} + c_2 * \frac{1+\sqrt{5}}{2} = 1$$

that can be easily solved by elimination. We obtain

$$c_1 = -\frac{1}{\sqrt{5}} \text{ and } c_2 = \frac{1}{\sqrt{5}}$$

Hence,

$$a_n = -\frac{1}{\sqrt{5}} * \left(\frac{1-\sqrt{5}}{2}\right)^n + \frac{1}{\sqrt{5}} * \left(\frac{1+\sqrt{5}}{2}\right)^n$$

is the solution to (1).

■ **Example 3**

Solve this recurrence

$$a_n = 3\, a_{n-1} + 4\, a_{n-2}$$
$$a_0 = 0, \ \ a_1 = 1$$

Assuming the solution in the form

$$a_n = \lambda^n$$

we get the following characteristic equation

$$\lambda^2 - 3\,\lambda - 4 = 0$$

that has two roots

$$\lambda_1 = -1 \text{ and } \lambda_2 = 4$$

Thus, the general solution is

$$a_n = c_1 * (-1)^n + c_2 * 4^n$$

We find c_1 and c_2 from initial conditions. This yields the following system

$$\begin{cases} c_1 + c_2 = 0 \\ -c_1 + 4\, c_2 = 1 \end{cases}$$

Its solution is

$$c_1 = -\frac{1}{5}, \; c_2 = \frac{1}{5}$$

Finally, the solution to the original recurrence is

$$a_n = -\tfrac{1}{5} * (-1)^n + \tfrac{1}{5} * 4^n$$

■ Multiple roots

What would be the solution of the recurrence if all (or few) roots of the characteristic equation are the same? Consider the following example.

$$a_n = 2\, a_{n-1} - a_{n-2}$$
$$a_0 = 1, \quad a_1 = 2$$

The characteristic equation

$$\lambda^2 - 2\,\lambda + 1 = 0$$

has two identical roots

$$\lambda_1 = \lambda_2 = 1$$

The first solution is

$$1^n$$

But what is the second solution? To get a notion of the second solution we consider a new equation

$$b_n = (2 + \epsilon)\, b_{n-1} - (1 + \epsilon)\, b_{n-2}$$
$$b_0 = 1, \quad b_1 = 2$$

It's easy to see that if $\epsilon \to 0$ then the sequence b_n approaches a_n. The characteristic equation for b_n sequence is

$$\lambda^2 - (2 + \epsilon)\, \lambda + (1 + \epsilon) = 0$$

It has two roots

$$\lambda_1 = 1, \;\; \lambda_2 = 1 + \epsilon$$

Therefore, a general solution is

$$b_n = c_1 * 1^n + c_2 * (1+\epsilon)^n$$

where c_1 and c_2 are arbitrary. Let us find them from the initial conditions

$$b_0 = c_1 + c_2 = 1$$

$$b_1 = c_1 + c_2 * (1+\epsilon) = 2$$

It follows,

$$c_1 = 1 - \frac{1}{\epsilon}, \;\; c_2 = \frac{1}{\epsilon}$$

Thus,

$$b_n = \left(1 - \frac{1}{\epsilon}\right) + \frac{1}{\epsilon} * (1+\epsilon)^n$$

Now, consider a general solution when $\epsilon \to 0$

$$a_n = \lim_{\epsilon \to 0} b_n = 1 + \lim_{\epsilon \to 0} \frac{(1+\epsilon)^n - 1}{\epsilon} = 1 + \lim_{\epsilon \to 0} \frac{\left(1^n + n * \epsilon * 1^{n-1} + \ldots + \epsilon^n\right) - 1}{\epsilon} = 1 + n$$

This is the second solution for a_n sequence. Then the general solution for a_n is

$$a_n = 1 + n$$

In *Mathematica*

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RSolve[{a[n] == 2 a[n - 1] - a[n - 2], a[0] == 1, a[1] == 2}, a[n], n]
```

```
{{a[n] → 1 + n}}
```

■ More on multiple roots

We have showed that if the characteristic equation has a multiple root λ then both

$$a_n = \lambda^n \text{ and } a_n = n\,\lambda^n$$

are solutions. We prove this for the second order recurrence equation

$$a_n = \alpha * a_{n-1} + \beta * a_{n-2}$$

The characteristic equation

$$\lambda^2 - \alpha\,\lambda - \beta = 0$$

has two identical roots

$$\lambda_1 = \frac{\alpha - \sqrt{\alpha^2 + 4\beta}}{2}, \ \lambda_2 = \frac{\alpha + \sqrt{\alpha^2 + 4\beta}}{2}$$

if and only if $\beta = -\frac{\alpha^2}{4}$. It follows $\lambda = \frac{\alpha}{2}$. To prove that

$$a_n = n\,\lambda^n$$

is the solution we substitute this into the original recurrence

$$n\,\lambda^n = \alpha\,(n-1)\,\lambda^{n-1} + \beta\,(n-2)\,\lambda^{n-2}$$

Divide this by λ^{n-2}

$$n\ \lambda^2 - \alpha\,(n-1)\,\lambda - \beta\,(n-2) = 0$$

and then collect terms with respect to n

$$n\,\left(\lambda^2 - \alpha\,\lambda - \beta\right) + \alpha\,\lambda + 2\,\beta = 0$$

The first term is zero because λ is the roots of the characteristic equation. The second term is zero because $\beta = -\frac{\alpha^2}{4}$ and $\lambda = \frac{\alpha}{2}$.

Theorem. *Let λ be a root of multiplicity p of the characteristic equation. Then*

$$\lambda^n,\ n\,\lambda^n,\ n^2\,\lambda^n,\ \ ...,\ n^{p-1}\,\lambda^n$$

are all solutions to the recurrence.

Example. Find a general solution

$$a_n = 3\,a_{n-1} - 3\,a_{n-2} + a_{n-3}$$

The characteristic equation has a root $\lambda = 1$ of multiplicity 3. Therefore,

$$a_n = c_1 + c_2\,n + c_3\,n^2$$

is a solution of this recurrence equation.

Exercise. Solve the recurrence

$$a_n - 5\,a_{n-1} + 7\,a_{n-2} - 3\,a_{n-3} = 0$$

$$a_0 = 1,\ a_1 = 2,\ a_2 = 3$$

■ Non-homogeneous equations

Theorem. *A recurrence of the form*

$$x_n + c_1\,x_{n-1} + ... + c_k\,x_{n-k} = b^n\,P(n)$$

where all c_k and b are constants and $P(n)$ is a polynomial of the order d can be transformed into the characteristic equation

$$\left(r^k + c_1\, r^{k-1} + \ldots + c_k\right) (r - b)^{d+1} = 0$$

Generating Functions

They provide an alternative (and more general) approach to solving recurrence equations.

Definition. *A generating function $f(x)$ is a formal power series*

$$f(x) = \sum_{k=0}^{\infty} a_k\, x^k$$

whose coefficients give the sequence $a_0,\ a_1,\ \ldots$

As an example, recall a geometric series

$$1 + x + x^2 + \ldots = \frac{1}{1 - x}$$

The infinite sequence $1,\ 1,\ 1,\ \ldots$ has a generating function $\frac{1}{1-x}$. Consider

$$1 + x^2 + x^4 + \ldots = \frac{1}{1 - x^2}$$

The infinite sequence $1,\ 0,\ 1,\ 0,\ \ldots$ has a generating function $\frac{1}{1-x^2}$.

Generating functions transform discrete math problems about sequences into problems about functions. The advantage of this approach that we can carry out manipulations on sequences by performing algebraic operations on their associated generating functions.

■ Example 4

We are going to derive a generating function for the following sequence

$$a_n - 3\, a_{n-1} + 2\, a_{n-2} = 0$$

$$a_0 = 0,\ \ a_1 = 1$$

First, we define

$$f(x) = a_0 + a_1\, x + a_2\, x^2 + a_3\, x^3 + a_4\, x^4 + \ldots = \sum_{k=0}^{\infty} a_k\, x^k$$

Next, we write series for $-3\,x\,f(x)$ and $2\,x^2\,f(x)$:

$$-3\,x\,f(x) = -3\,a_0\,x - 3\,a_1\,x^2 - 3\,a_2\,x^3 - 3\,a_3\,x^4 + \ldots = -\sum_{k=1}^{\infty} 3\,a_{k-1}\,x^k$$

$$2\,x^2\,f(x) = 2\,a_0\,x^2 + 2\,a_1\,x^3 + 2\,a_2\,x^4 + \ldots = \sum_{k=2}^{\infty} 2\,a_{k-2}\,x^k$$

Add them up

$$f(x) - 3\,x\,f(x) + 2\,x^2\,f(x) =$$

$$\sum_{k=0}^{\infty} a_k\,x^k - \sum_{k=1}^{\infty} 3\,a_{k-1}\,x^k + \sum_{k=2}^{\infty} 2\,a_{k-2}\,x^k =$$

$$a_0 + a_1\,x - 3\,a_0\,x + \sum_{k=2}^{\infty} (a_k - 3\,a_{k-1} + 2\,a_{k-2})\,x^k =$$

$$a_0 + a_1\,x - 3\,a_0\,x$$

Furthermore, in view of initial conditions,

$$f(x) - 3\,x\,f(x) + 2\,x^2\,f(x) = x$$

Thus,

$$f(x) = \frac{x}{1 - 3\,x + 2\,x^2} = \frac{1}{1 - 2\,x} - \frac{1}{1 - x}$$

How can this be used for solving recurrence equations? By means of a geometric series

$$1 + x + x^2 + \ldots = \frac{1}{1 - x}$$

$$1 + 2\,x + 2^2\,x^2 + \ldots = \frac{1}{1 - 2\,x}$$

How can this be used for solving recurrence equations? By means of a geometric series

$$\frac{1}{1 - 2\,x} - \frac{1}{1 - x} =$$

$$\left(1 + 2\,x + 2^2\,x^2 + \ldots\right) - \left(1 + x + x^2 + \ldots\right) =$$

$$(2 - 1)\,x + \left(2^2 - 1\right)x + \ldots$$

The coefficient of a_k is $2^k - 1$. In *Mathematica*