

LAFF-On Programming for Correctness

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Preface

Acknowledgments



Getting Started

0.1 Opening Remarks

0.1.1 Welcome to LAFF-On Programming for Correctness

Opening video.

Learn in Section 0.2.1 how and where to download videos onto your computer.

0.1.2 Outline

Following the "opener" we give the outline for the week:

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0.1.3 What You Will Learn

The third unit of the week informs you of what you will learn. This describes the knowledge and skills that you can expect to acquire. In addition, this provides an opportunity for you to self-assess upon completion of the week.

Upon completion of this week, you should be able to

- Navigate the different components of LAFF-On.
- Download and start MATLAB.
- Recognize the structure of a typical week.

You may want to print out Appendix ?? to track your progress throughout the course.

0.2 How to LAFF-On

0.2.1 Setting Up to LAFF

It helps if we all set up our environment in a consistent fashion. If you obtained this file from the github repository, it is already in a directory, LAFF-On, with a hierarchy similar to that illustrated in Figure 1. You should us Acrobat Reader or similar PDF viewer when reading this document so that hyperlinks work properly.

0.3 Software to LAFF-On

0.3.1 Why MATLAB

We use MATLAB as a tool because it was invented to support learning about matrix computations. You will find that the syntax of the language used by MATLAB, called M-script, very closely resembles the mathematical expressions in linear algebra.

Those not willing to invest in MATLAB will want to consider **GNU** Octave instead.

0.3.2 Installing MATLAB

Instructions can be found at **►** http://www.mathworks.org.

0.3.3 MATLAB Basics

Below you find a few short videos that introduce you to MATLAB. For a more comprehensive tutorial, you may want to visit — MATLAB Tutorials at MathWorks and clicking "Launch Tutorial".

HOWEVER, you need very little familiarity with MATLAB in order to learn what we want you to learn about how abstraction in mathematics is linked to abstraction in algorithms. So, you could just skip these tutorials altogether, and come back to them if you find you want to know more about MATLAB and its programming language (M-script).

What is MATLAB?



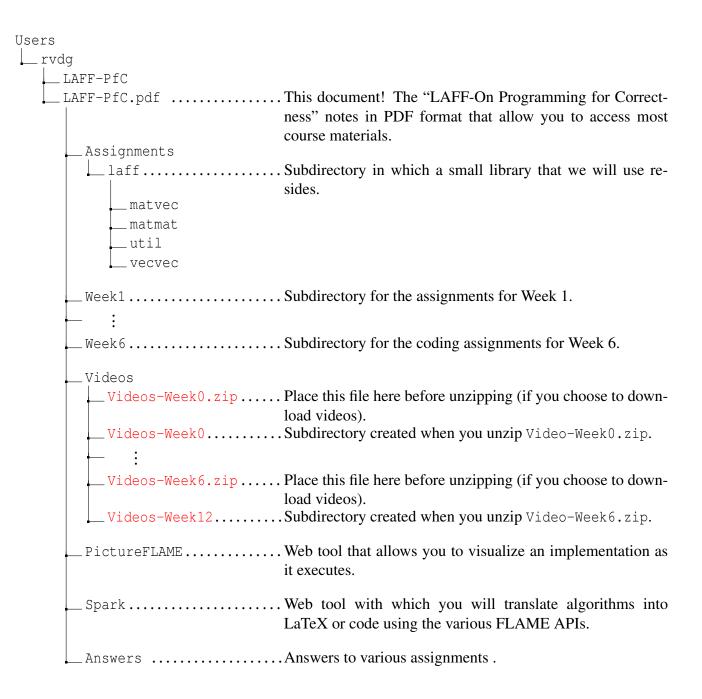


Figure 1: Directory structure for your LAFF-PfC materials. Items in red will be placed into the materials by you. In this example, we placed LAFF-PfC.zip in the home directory Users/rvdg before unzipping. You may want to place it on your account's "Desktop" instead.

The MATLAB Environment



MATLAB Variables



MATLAB as a Calculator



0.4 Typesetting LAFF-On

0.4.1 Typesetting mathematics

The tool of choice for typesetting mathematics is a document typesetting system called LATEX. We will use it to typeset many of our exercises in a way that captures how we want you to think about discovering algorithms hand-in-hand with their proofs of correctness.

We recommend that you use TeXstudio:

"TeXstudio an integrated writing environment for creating LaTeX documents."

It is the environment I typically use in the videos for this course and that I used to create the notes and many of the activities. You are, of course, free to use whatever such environment you prefer.

0.4.2 Downloading TeXstudio

You can download TeXstudio from www.texstudio.org.

0.4.3 Testing TeXstudio

- Open the file Assignments/Week0/LaTeX/HelloWorld.tex.
 - I would recommend opening it with your "Finder" (or whatever it is called in Windows or Linux) so that you can make the default application for ".tex" files the TeXstudio application.
 - Alternatively, you can open the TeXstudio application and then click on

choosing the file.

- At this point, it is a good idea to click on

```
Options -> Root Document -> Set Current Document as Explicit Root
```

which will make the "HelloWorld.tex" file the root file for the "compilation" of the document. This is important when the root file itself includes other files in some hierarchical fashion.

• Once you have opened "Hello@World.tex" Click on on the top bar. Eventually you will see a "Process exited normally" in the message box in the lower left-hand orner as well as the formatted text to the right.

0.4.4 LATEX and TeXstudio Primer

Insert video on LATEX and TeXstudio.

The source for the LATEX example in that video:

Assignments/Week0/LaTeX/LaTeXPrimer.tex

We will use LATEX in a very limited way. But you may want to become more familiar with this tool by following some tutorials that you can find on the internet. (Search "LaTeX tutorial").

The following is probably a pretty good place to start:

☞ LATEX Tutorials - a Primer.

Whenever it talks about latex myfile and xdvi myfile instead just click on



0.5 Enrichments

0.5.1 The Origins of MATLAB



0.5.2 The Origins of LATEX

You may enjoy this interview with Dr. Leslie Lamport, who created LATEX.

https://www.infoq.com/interviews/lamport-latex-paxos-tla

0.6 Wrap Up

0.6.1 Additional Homework

For a typical week, additional assignments may be given in this unit.

0.6.2 Summary

You will see that we develop a lot of the theory behind the various topics in linear algebra via a sequence of homework exercises. At the end of each week, we summarize theorems and insights for easy reference.

Part

Introduction

1.1 Opening Remarks

1.1.1 Launch

Homework 1.1.1.1 Compute

$$\begin{pmatrix} 1 & -1 & 2 \\ -2 & 2 & 0 \\ -1 & 1 & -2 \end{pmatrix} \begin{pmatrix} 2 \\ -1 \\ 1 \end{pmatrix} + \begin{pmatrix} 3 \\ 1 \\ 0 \end{pmatrix} =$$

SEE ANSWER

Given $m \times n$ matrix A, vector x of size n, and vector y of size m, we expose their elements as

$$A = \begin{pmatrix} \alpha_{0,0} & \alpha_{0,1} & \cdots & \alpha_{0,n-1} \\ \alpha_{1,0} & \alpha_{1,1} & \cdots & \alpha_{1,n-1} \\ \vdots & \vdots & & \vdots \\ \alpha_{m-1,0} & \alpha_{m-1,0} & \cdots & \alpha_{m-1,n-1} \end{pmatrix}, x = \begin{pmatrix} \chi_0 \\ \chi_1 \\ \vdots \\ \chi_{n-1} \end{pmatrix}, \text{ and } y = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{m-1} \end{pmatrix}$$

then the matrix-vector multiplication operation y := Ax + y (y is overwritten with Ax + y or "y becomes A times x plus y") is computed as

$$egin{array}{lll} \psi_0 &:= lpha_{0,0} & \chi_0 + lpha_{0,1} & \chi_1 + \cdots + lpha_{0,n-1} & \chi_{n-1} \ \psi_1 &:= lpha_{1,0} & \chi_0 + lpha_{1,1} & \chi_1 + \cdots + lpha_{1,n-1} & \chi_{n-1} \ dots & dots & dots & dots \ \psi_{m-1} &:= lpha_{m-1,0} \, \chi_0 + lpha_{m-1,1} \, \chi_1 + \cdots + lpha_{m-1,n-1} \, \chi_{n-1} \end{array}$$

This computation translates into the MATLAB function MatVec1 given in Figure 1.1.

```
function [ y_out ] = MatVecl( A, x, y )
% Compute y := A x + y

% Extract the row and column size of A
[ m, n ] = size( A );

% (Strictly speaking you should check that x is a vector size n and y is a
% vector of size m...)

% Copy y into y_out
y_out = y;

% Compute y_out = A * x + y_out
for i = 1:m
    for j=1:n
        y_out( i ) = A( i,j ) * x( j ) + y_out( i );
    end
end
end
```

Assignments/Week1/matlab/MatVec1.m

Figure 1.1: Function that computes y := Ax + y, returning the result in vector y_out.

.

```
Homework 1.1.1.2 Open the Live Script
```

Assignments/Week1/matlab/MatVec1LS.mlx

and follow the directions in it.

SEE ANSWER

Notice that we tend to start indexing of elements in arrays at zero:

while MATLAB start at one: our $\alpha_{0,0}$ is stored in A (1, 1). Better get used to this!

With few exceptions, we will use upper case Roman letters to denote matrices, lower case Roman letters to denote vectors, and lower case Greek letters to denote scalars.

Consider an $m \times n$ matrix A. We will often partition such a matrix into its columns

$$A = \left(a_0 \mid a_1 \mid \cdots \mid a_{n-1} \right).$$

Since each column is a vector, we use a lower case Roman letter to denote it. To further link the columns to the original matrix A, we use the lower case letter a.

Sometimes, we partition a matrix, A, into rows

$$A = \begin{pmatrix} a_0^T \\ \hline a_1^T \\ \hline \vdots \\ \hline a_{m-1}^T \end{pmatrix}.$$

Each row is a row vector, which we denote with the lower case Roman letter a. But we view vectors as column vectors, which is why we add the T to indicate it is a vector that has been transposed to become the row.

When we expose individual entries of a matrix, for its scalar entries we typically use the lower case Greek letter that is similar to the letter used to denote the matrix.

Now, if m = n then matrix A is square and if $\alpha_{i,j} = \alpha_{j,i}$ then it is said to be a symmetric matrix. In this case

where the *s are meant to indicate that the upper triangular part of the matrix needs not be stored.

Homework 1.1.1.3 Knowing that the matrix is symmetric, compute

$$\begin{pmatrix} 1 & \star & \star \\ -2 & 2 & \star \\ -1 & 1 & -2 \end{pmatrix} \begin{pmatrix} 2 \\ -1 \\ 1 \end{pmatrix} + \begin{pmatrix} 3 \\ 1 \\ 0 \end{pmatrix} =$$

SEE ANSWER

Homework 1.1.1.4 Copy the file MatVec1.m to file SymMatVec1.m, change the name of the function to SymMatVec1 and change the implementation so that it only accesses entries of array A that are on or below the diagonal. Test your implementation with the Live Script in

Assignments/Week1/matlab/SymMatVec1LS.mlx

SEE ANSWER

```
function [y_out] = SymMatVec1(A, x, y)
% Compute y := A x + y, assuming A is symmetric and stored in lower
% triangular part of array A.
% Extract the row and column size of A
[m, n] = size(A);
% (Strictly speaking you should check that m = n, x is a vector size n and y is a
% vector of size n...)
% Copy y into y_out
y_out = y;
% Compute y_out = A * x + y_out
for i = 1:n
    for j=1:i
        y_out(i) = A(i,j) * x(j) + y_out(i);
    end
    for j=i+1:n
        y_out(i) = A(j,i) * x(j) + y_out(i);
    end
end
end
```

Assignments/Week1/matlab/SymMatVec1.m

Figure 1.2: Function that computes y = Ax + y, returning the result in vector y_{out} . Matrix A is assumed to be symmetric and only stored in the lower triangular part of array A.

.

Now, MATLAB stores matrices in column-major order, which means that a matrix

$$\left(\begin{array}{cccc}
1 & -1 & 2 \\
-2 & 2 & 0 \\
-1 & 1 & -2
\end{array}\right)$$

```
function [ y_out ] = MatVec2( A, x, y )
% Compute y := A x + y
% Extract the row and column size of A
[ m, n ] = size( A );
% (Strictly speaking you should check that x is a vector size n and y is a
% vector of size m...)
% Copy y into y_out
y_out = y;
% Compute y_out = A * x + y_out
for j = 1:n
    for i = 1:m
        y_out( i ) = A( i, j ) * x( j ) + y_out( i );
    end
end
```

Assignments/Week1/matlab/MatVec2.m

Figure 1.3: Function that computes y = Ax + y, returning the result in vector y_out.

.

is stored in memory by stacking columns:

 $\begin{array}{c|c}
1 \\
-2 \\
-1 \\
2 \\
1 \\
2 \\
0 \\
-2 \\
\end{array}$

Computation tends to be more efficient if one accesses memory contiguously. This means that an algorithm that accesses *A* by columns often computes the answer faster than one that accesses *A* by columns.

In a linear algebra course you should have learned that,

$$\begin{pmatrix} 1 & -1 & 2 \\ -2 & 2 & 0 \\ -1 & 1 & -2 \end{pmatrix} \begin{pmatrix} 2 \\ -1 \\ 1 \end{pmatrix} + \begin{pmatrix} 3 \\ 1 \\ 0 \end{pmatrix} = (2) \begin{pmatrix} 1 \\ -2 \\ -1 \end{pmatrix} + (-1) \begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix} + (1) \begin{pmatrix} 2 \\ 0 \\ -2 \end{pmatrix} + \begin{pmatrix} 3 \\ 1 \\ 0 \end{pmatrix}$$

$$= \left((1) \begin{pmatrix} 2 \\ 0 \\ -2 \end{pmatrix} + \left((-1) \begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix} + \left((2) \begin{pmatrix} 1 \\ -2 \\ -1 \end{pmatrix} + \begin{pmatrix} 3 \\ 1 \\ 0 \end{pmatrix} \right) \right) \right),$$

which means that the implementation in Figure 1.1 can be rewritten as the one in Figure 1.3, which accesses the matrix by columns. Notice that the two implementations differ only in the order of the loops indexed by i and j.

Homework 1.1.1.5 Copy the file MatVec2.m to file SymMatVec2.m, change the name of the function to SymMatVec2 and change the implementation so that it only accesses entries of array A that are on or below the diagonal. Test your implementation with the Live Script in

Assignments/Week1/matlab/SymMatVec2LS.mlx

SEE ANSWER

Now we get to two exercises that help motivate the course. They are surprisingly hard, even for an expert:

Homework 1.1.1.6 Modify the code in Figure 1.2 so that it only accesses the lower triangular part of array A by columns, resulting in routine SymMatVec3. Test your implementation with the Live Script in

Assignments/Week1/matlab/SymMatVec3LS.mlx

SEE ANSWER

Homework 1.1.1.7 Find someone who knows a little (or a lot) about linear algebra and convince this person that the answer to the last exercise is correct. Alternatively, if you did not managed to come up with an answer for the last exercise, look at the answer to that exercise and convince yourself it is correct.

SEE ANSWER

The point of these last two exercises is:

- It is difficult to find algorithms with specific (performance) properties even for relatively simple operations.
- It is difficult to give a convincing argument that even a relatively simple algorithm is correct.

One could ask "But isn't having any algorithm to compute the result good enough?" The graph in Figure 1.4 illustrates the difference in performance of the different implementations (coded in C). The implementation that corresponds to SymMatVec3 is roughly five times faster than the other implementations. It demonstrates there is a definite performance gain that results from picking the right algorithm.

In this course, we hope to equip you with the tools to systematically develop whole families of algorithms that are correct by construction. From this family of algorithms the one that has a desirable property (e.g., that it accesses memory contiguously so that better performance can be achieved) can then be chosen.

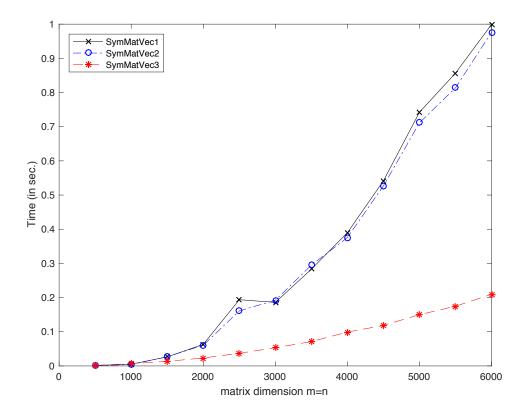


Figure 1.4: Execution time as a function of matrix size for the different implementations of symmetric matrix-vector multiplication.

1.1.2 Outline Week 1

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1.1.4 What you will learn

This week introduces the reader to the systematic derivation of algorithms for linear algebra operations. Through a very simple example we illustrate the core ideas: We describe the notation we will use to express algorithms; we show how assertions can be used to establish correctness; and we propose a goal-oriented methodology for the derivation of algorithms. We also discuss how to incorporate an analysis of the cost into the algorithm. Finally, we show how to translate algorithms to code so that the correctness of the algorithm implies the correctness of the implementation.

Upon completion of this week, you should be able to

•

Track your progress in Appendix ??.

1.2. A Farewell to Indices

1.2 A Farewell to Indices

1.2.1 A motivating example: dot product

In this section, we introduce a notation for expressing algorithms that avoids the pitfalls of intricate indexing and will allow us later to more easily derive, express, and implement algorithms. We present the notation through a simple example, the *inner product* of two vectors, an operation that will be used throughout this chapter for illustration.

Given two vectors, x and y, of length m, the inner product (or dot product) of these vectors is given by

$$\alpha := x^{\mathrm{T}} y = \sum_{i=0}^{m-1} \chi_i \psi_i$$

where χ_i and ψ_i equal the *i*th elements of x and y, respectively:

$$x = \begin{pmatrix} \chi_0 \\ \chi_1 \\ \vdots \\ \chi_{m-1} \end{pmatrix}$$
 and $y = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{m-1} \end{pmatrix}$.

We will use the symbol ":=" ("becomes") to denote assignment while the symbol "=" is reserved for equality.

Example 1.1 Let

$$x = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad and \quad y = \begin{pmatrix} 2 \\ 4 \\ 1 \end{pmatrix}.$$

Then $x^Ty = 1 \cdot 2 + 2 \cdot 4 + 3 \cdot 1 = 13$. Here we make use of the symbol "·" to denote the arithmetic product.

A traditional loop for implementing the updating of a scalar by adding an inner product to it, $\alpha := x^T y + \alpha$, is given by

$$k := 0$$

while $k < m$ do
 $\alpha := \chi_k \psi_k + \alpha$
 $k := k + 1$
endwhile

Some will find this loop a bit cumbersome, since the algorithm can be more easily expressed with "for" loop. Why we use a while loop will become clear later.

Algorithm:
$$\alpha := \text{SAPDOT_VAR1}(x, y, \alpha)$$

$$x \to \left(\frac{x_T}{x_B}\right), y \to \left(\frac{y_T}{y_B}\right)$$
where x_T and y_T have 0 elements
while $m(x_T) < m(x)$ do
$$\left(\frac{x_T}{x_B}\right) \to \left(\frac{x_0}{x_1}\right), \left(\frac{y_T}{y_B}\right) \to \left(\frac{y_0}{y_1}\right)$$
where χ_1 and ψ_1 are scalars
$$\alpha := \chi_1 \psi_1 + \alpha$$

$$\left(\frac{x_T}{x_B}\right) \leftarrow \left(\frac{x_0}{\chi_1}\right), \left(\frac{y_T}{y_B}\right) \leftarrow \left(\frac{y_0}{\psi_1}\right)$$
endwhile

Figure 1.5: Algorithm for computing $\alpha := x^T y + \alpha$.

1.2.2 A new notation for presenting algorithms

in Figure 1.5 we present a loop that updates with a dot product with an alternate notation, which we call the *FLAME notation*. The name of the algorithm in that figure reflects that it performs an <u>alpha plus dot</u> product (APDOT). To interpret the algorithm in Figure 1.5 note the following:

- We bid farewell to intricate indexing: In this example only indices from the sets $\{T,B\}$ (\underline{Top} and \underline{Bottom}) and $\{0,1,2\}$ are required.
- Each vector has been subdivided into two subvectors, separated by thick lines. This is how we will represent systematic movement through vectors (and later matrices).
- Subvectors x_T and y_T include the "top" elements of x and y that, in this algorithm, have already been used to compute a partial update to α . Similarly, subvectors x_B and y_B include the "bottom" elements of x and y that, in this algorithm, have not yet been used to update α . Referring back to the traditional loop, x_T and y_T consist of elements $0, \dots, k-1$ and x_B and y_B consist of elements

 $k, \ldots, m-1$:

$$\left(\frac{x_T}{x_B}\right) = \begin{pmatrix} \chi_0 \\ \vdots \\ \chi_{k-1} \\ \vdots \\ \chi_{m-1} \end{pmatrix} \quad \text{and} \quad \left(\frac{y_T}{y_B}\right) = \begin{pmatrix} \psi_0 \\ \vdots \\ \psi_{k-1} \\ \vdots \\ \psi_{m-1} \end{pmatrix}.$$

• The initialization before the loop starts

$$x \to \left(\frac{x_T}{x_B}\right), y \to \left(\frac{y_T}{y_B}\right)$$

takes the place of the assignment k := 0 in the traditional loop.

- The loop is executed as long as $m(x_T) < m(x)$ is *true*, which takes the place of k < m in the traditional loop. Here m(x) equals the length of vector x so that the loop terminates when x_T includes all elements of x.
- The statement

$$\left(\begin{array}{c} x_T \\ \hline x_B \end{array}\right) \to \left(\begin{array}{c} x_0 \\ \hline \chi_1 \\ \hline x_2 \end{array}\right), \left(\begin{array}{c} y_T \\ \hline y_B \end{array}\right) \to \left(\begin{array}{c} y_0 \\ \hline \psi_1 \\ \hline y_2 \end{array}\right)$$

exposes the top elements of x_B and y_B , χ_1 and ψ_1 respectively, which were χ_k and ψ_k in the traditional loop.

• The exposed elements χ_1 and ψ_1 are used to update α in

$$\alpha := \chi_1 \psi_1 + \alpha$$
,

which takes the place of the update $\alpha := \chi_k \psi_k + \alpha$ in the traditional loop.

It is important not to confuse the single elements exposed in our repartitionings, such as χ_1 or ψ_1 , with the second entries of corresponding vectors.

• The statement

$$\left(\frac{x_T}{x_B}\right) \leftarrow \left(\frac{x_0}{\chi_1}\right), \left(\frac{y_T}{y_B}\right) \leftarrow \left(\frac{y_0}{\psi_1}\right)$$

Algorithm:
$$\alpha := SAPDOT_VAR2(x, y, \alpha)$$

$$x \to \left(\frac{x_T}{x_B}\right), y \to \left(\frac{y_T}{y_B}\right)$$

where x_T and y_T have 0 elements

while $m(x_T) < m(x)$ do

$$\left(\begin{array}{c} x_T \\ \hline x_B \end{array}\right) \to \left(\begin{array}{c} x_0 \\ \chi_1 \\ x_2 \end{array}\right), \left(\begin{array}{c} y_T \\ \hline y_B \end{array}\right) \to \left(\begin{array}{c} y_0 \\ \psi_1 \\ y_2 \end{array}\right)$$

where χ_1 and ψ_1 are scalars

$$\left(\frac{x_T}{x_B}\right) \leftarrow \begin{pmatrix} x_0 \\ \chi_1 \\ x_2 \end{pmatrix}, \left(\frac{y_T}{y_B}\right) \leftarrow \begin{pmatrix} y_0 \\ \psi_1 \\ y_2 \end{pmatrix}$$

endwhile

Figure 1.6: Partial algorithm for computing $\alpha := x^T y + \alpha$.

moves the top elements of x_B and y_B to x_T and y_T , respectively. This means that these elements have now been used to update α and should therefore be added to x_T and y_T .

Homework 1.2.2.8 Consider the following loop, which computes $\alpha := x^Ty + \alpha$ by traversing the vectors backwards:

```
k := m - 1

while k \ge 0 do

\alpha := \chi_k \psi_k + \alpha

k := k - 1

endwhile
```

Complete the algorithm in Figure 1.6 so that it expresses this alternative algorithmic variant.

SEE ANSWER

1.2.3 Typesetting algorithms with FLAME notation and LATEX

One drawback of how we typeset our algorithms with the FLAME notation is that it takes considerably more room and time to write them down. To overcome this, we suggest using LATEX. In Week 0 you presumably installed a tool, TeXstudio, for writing LATEX documents.

Homework 1.2.3.9 Follow the instructions in the following video to duplicate Figure 1.5. Useful links:

• A partial LATEX document can be found in

Assigments/Week1/LaTeX/Sapdot_unb_var1.tex.

• The local install of the Spark webpage is in Spark/index.html. (If version does not update correctly, click here).

SEE ANSWER

Homework 1.2.3.10 Typeset the algorithm from Homework 1.2.2.8. Useful links:

• A partial LATEX document can be found in

Assignents/Week1/LaTeX/Sapdot_unb_var2.tex.

• The local install of the Spark webpage is in Spark/index.html. (If version does not update correctly, click here).

Make sure you "march" through the vectors in the correct direction.

SEE ANSWER

1.2.4 Representing (FLAME) algorithms in code

We now have a new notation for expressing algorithms. What we will find out later in the course is how to derive correct algorithms using this notation. The problem is that a correct algorithm still has to be translated into code. Programming bugs can be easily introduced as part of that translation. To overcome this, we will use an Application Programming Interface (API) that allows the code to closely resemble the algorithm.

Homework 1.2.4.11 Follow the instructions in the following video and the Live Script in

Assignments/Week1/matlab/Sapdot_unb_var1_LS.mlx

to translate the algorithm in Figure 1.5 into code using the FLAME@lab API. Useful links:

• The local install of the Spark webpage is in Spark/index.html. (If version does not update correctly, click here).

SEE ANSWER

Homework 1.2.4.12 Translate the algorithm from Homework 1.2.2.8 into code. Useful links:

- The local install of the Spark webpage is in Spark/index.html. (If version does not update correctly, click here).
- Live Script to test your implementation:

Assignments/Week1/matlab/Sapdot_unb_var2_LS.mlx

Make sure you "march" through the vectors in the correct order.

SEE ANSWER

1.3 Correctness of a Loop

1.3.1 Predicates as assertions about the state

To reason about the correctness of algorithms, predicates will be used to express assertions about the state (contents) of the variables. Recall that a *predicate*, *P*, is simply a ()*Boolean*) *expression* that evaluates to *true* or *false* depending on the state of the variables that appear in the predicate. The placement of a predicate at a specific point in an algorithm means that it must evaluate to *true* so that it asserts the state of the variables that appear in the predicate. An *assertion* is a predicate that is used in this manner.

For example, after the command

$$\alpha := 1$$

which assigns the value 1 to the scalar variable α , we can assert that the predicate "P: $\alpha = 1$ " holds (is true). An assertion can then be used to indicate the state of variable α after the assignment as in

$$\alpha := 1$$
$$\{P : \alpha = 1\}$$

(Here *P* : is just a label so we can refer to the predicate.)

Assertions will be enclosed by curly brackets in the algorithms.

If P_{pre} and P_{post} are predicates and S is a sequence of commands, then $\{P_{pre}\}S\{P_{post}\}$ is a predicate that evaluates to true if and only if the execution of S, when begun in a state satisfying P_{pre} , terminates in a finite amount of time in a state satisfying P_{post} . Here $\{P_{pre}\}S\{P_{post}\}$ is called the *Hoare triple*, and P_{pre} and P_{post} are referred to as the *precondition* and *postcondition* for the triple, respectively.

Example 1.2 $\{\alpha = \beta\} \alpha := \alpha + 1 \{\alpha = \beta + 1\}$ evaluates to true. Here " $\alpha = \beta$ " is the precondition while " $\alpha = (\beta + 1)$ " is the postcondition.

1.3.2 Reasoning about the correctness of a loop (example)

Let us again consider the computation $\alpha := x^T y + \alpha$. Let us use $\widehat{\alpha}$ to denote the *original contents* (or state) of α . Then we define the precondition for the algorithm as

$$P_{pre}: (\alpha = \widehat{\alpha}) \wedge (0 \leq m(x)) \wedge (m(x) = m(y)),$$

Step	Algorithm: $\alpha := SAPDOT(x, y, \alpha)$
1a	$(\alpha = \widehat{\alpha}) \wedge (0 \le m(x)) \wedge (m(x) = m(y))$
4	$x \to \left(\frac{x_T}{x_B}\right), y \to \left(\frac{y_T}{y_B}\right)$ where x_T and y_T have 0 elements
2	$(\alpha = x_T^T y_T + \widehat{\alpha}) \wedge (0 \le m(x_T)) \wedge (m(x_T) = m(y_T)) \wedge (m(x_T) \le m(x))$
3	while $m(x_T) < m(x)$ do
2,3	$(\alpha = x_T^{T} y_T + \widehat{\alpha}) \wedge (0 \leq m(x_T)) \wedge (m(x_T) = m(y_T)) \wedge (m(x_T) \leq m(x)) \wedge m(x_T) < m(x)$
5a	$\left(\frac{x_T}{x_B}\right) \to \left(\frac{x_0}{\chi_1}\right), \left(\frac{y_T}{y_B}\right) \to \left(\frac{y_0}{\psi_1}\right)$
	where χ_1 and ψ_1 are scalars
6	$(\alpha = x_0^{\mathrm{T}} y_0 + \widehat{\alpha}) \wedge (0 \leq m(x_0)) \wedge (m(x_0) = m(y_0)) \wedge (m(x_0) \leq m(x))$
8	$\alpha := \chi_1 \psi_1 + \alpha$
5b	$\left(\frac{x_T}{x_B}\right) \leftarrow \left(\frac{x_0}{\chi_1}\right), \left(\frac{y_T}{y_B}\right) \leftarrow \left(\frac{y_0}{\psi_1}\right)$
7	$(\alpha = x_0^{T} y_0 + \chi_1 \psi_1 + \widehat{\alpha}) \wedge (0 \le m(x_0)) \wedge (m(x_0) = m(y_0)) \wedge (m(x_0) \le m(x))$
2	$(\alpha = x_T^T y_T + \widehat{\alpha}) \wedge (0 \le m(x_T)) \wedge (m(x_T) = m(y_T)) \wedge (m(x_T) \le m(x))$
	endwhile
2,3	$(\alpha = x_T^T y_T + \widehat{\alpha}) \wedge (0 \leq m(x_T)) \wedge (m(x_T) = m(y_T)) \wedge (m(x_T) \leq m(x)) \wedge \neg (m(x_T) < m(x))$
1b	$\alpha = x^{\mathrm{T}}y + \widehat{\alpha}$

Figure 1.7: Annotated algorithm for computing $\alpha := x^T y + \alpha$.

and the postcondition as

$$P_{post}: \alpha = x^{\mathrm{T}}y + \widehat{\alpha};$$

that is, the result the operation to be computed.

In order to prove correctness, we next annotate the algorithm in Figure 1.5 with assertions that describe the state of the variables, as shown in Figure 1.7. Each command in the algorithm has the property that, when entered in a state described by the assertion that precedes it, it will complete in a state where the assertion immediately after it holds.

1.3.3 Equivalent reasoning without the FLAME notation

Let us instead look at how the loop

$$k := 0$$

while $k < m$ do
 $\alpha := \chi_k \psi_k + \alpha$
 $k := k + 1$
endwhile

can be annotated to reason about correctness.

$$\alpha = \widehat{\alpha}$$

$$i := 0$$

$$\alpha = \sum_{k=0}^{i-1} \chi_k \psi_k + \widehat{\alpha}$$

$$\mathbf{while} \ i < m \ \mathbf{do}$$

$$\alpha = \sum_{k=0}^{i-1} \chi_k \psi_k + \widehat{\alpha}$$

$$\alpha := \chi_i \psi_i + \alpha$$

$$\alpha := \chi_i \psi_i + \sum_{k=0}^{i-1} \chi_k \psi_k + \widehat{\alpha}$$

$$i := i + 1$$

$$\alpha = \sum_{k=0}^{i-1} \chi_k \psi_k + \widehat{\alpha}$$

$$\mathbf{endwhile}$$

$$\alpha = \sum_{k=0}^{i-1} \chi_k \psi_k + \widehat{\alpha} \wedge i = m$$

$$\alpha = \sum_{k=0}^{m-1} \chi_k \psi_k + \widehat{\alpha}$$

1.4. Enrichment 27

$$\alpha = \widehat{\alpha}$$

$$i := m$$

$$\alpha = \sum_{k=i}^{m-1} \chi_k \psi_k + \widehat{\alpha}$$

$$\text{while } i > 0 \text{ do}$$

$$\alpha = \sum_{k=i}^{m-1} \chi_k \psi_k + \widehat{\alpha}$$

$$i := i - 1$$

$$\alpha = \sum_{k=i+1}^{m-1} \chi_k \psi_k + \widehat{\alpha}$$

$$\alpha := \chi_i \psi_i + \alpha$$

$$\alpha := \chi_i \psi_i + \alpha$$

$$\alpha = \chi_i \psi_i + \sum_{k=i+1}^{m-1} \chi_k \psi_k + \widehat{\alpha}$$

$$\alpha = \sum_{k=i}^{m-1} \chi_k \psi_k + \widehat{\alpha}$$
endwhile
$$\alpha = \sum_{k=i}^{m-1} \chi_k \psi_k + \widehat{\alpha} \wedge i = 0$$

$$\alpha = \sum_{k=0}^{m-1} \chi_k \psi_k + \widehat{\alpha}$$

1.3.4 Deriving a correct loop

What we have now argued is that we can annotate the algorithm for computing the APDOT operation to prove it correct. Dijkstra has this to say about this:

Today a usual technique is to make a program and then to test it. But: program testing can be a very effective way to show the presence of bugs, but is hopelessly inadequate for showing their absence. The only effective way to raise the confidence level of a program significantly is to give a convincing proof of its correctness. But one should not first make the program and then prove its correctness, because then the requirement of providing the proof would only increase the poor programmers burden. On the contrary: the programmer should let correctness proof and program grow hand in hand.— Edsger W. Dijkstra, *The Humble Programmer*.

What you will learn later in the course is how to grow correctness proof and program grow hand in hand.

1.4 Enrichment

1.5 Wrap Up

1.5.1 Additional Exercises

Most of these exercises need to be moved.

A number of other commonly encountered operations involving vectors is presented in Table 1.1. These operations will resurface in later chapters and are therefore natural choices for further exercises.

Homework 1.5.1.12 *Use the worksheet in Figure* ?? *to derive an algorithm for computing* $\alpha := \alpha + x^T y$ *by choosing the loop-invariant as* $P_{inv} : \alpha = \widehat{\alpha} + x_R^T y_B$.

Part 1. Introduction 28

Step	Algorithm:
1a	
4	
	where
2	
3	while do
2,3	^
5a	
Ja	
	where
6	
0	
8	
5b	
30	
7	
2	
	endwhile
2,3	$\wedge \neg (\hspace{1cm})$
1b	

 $Figure \ 1.8: \ Blank \ worksheet. \ You \ may \ want \ to \ print \ {\tt Resources/BlankWorksheet.pdf}.$

1.5. Wrap Up 29

Operation	Math.	Defined as	Cost
	Notation	$(0 \le i < m)$	(flops)
Scaling (SCAL)	$x := \alpha x$	$\chi_i := \alpha \chi_i$	m
Addition (ADD)	y := x + y	$\psi_i := \chi_i + \psi_i$	m
Inner product (DOT)	$\alpha := x^{\mathrm{T}}y$	$\alpha := \sum_{k=0}^{m-1} \chi_k \psi_k$	2m-1
APDOT	$\alpha := \alpha + x^{\mathrm{T}} y$	$\alpha := \alpha + \sum_{k=0}^{m-1} \chi_k \psi_k$	2 <i>m</i>
AXPY	$y := \alpha x + y$	$\psi_i := \alpha \chi_i + \psi_i$	2 <i>m</i>

Table 1.1: Basic operations involving vectors. In the table, α is a scalar and x, y are vectors of length m with their corresponding ith elements denoted as χ_i , ψ_i , respectively.

Homework 1.5.1.12 *Use the worksheet in Figure* **??** *to derive algorithms for the following two operations (see Table 1.1):*

(a) The scaling of a vector.

Hint: Since x is modified in this operation, we recommend using \hat{x} to denote its original contents. In reasoning about correctness, \hat{x}_T , \hat{x}_B , \hat{x}_0 , $\hat{\chi}_1$, and \hat{x}_2 will be encountered.

(b) The AXPY.

The name of this operation comes from \underline{s} calar \underline{a} lpha times \underline{x} plus y.

Homework 1.5.1.12 *Prove the costs for the scaling of a vector and the* AXPY *shown in Table* 1.1.

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 $_{\mathsf{Part}} 2$

Deriving Algorithms to be Correct

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2.1.3 What you should know

2.1.4 What you will learn

This week introduces the reader to the systematic derivation of algorithms for linear algebra operations. Through a very simple example we illustrate the core ideas: We describe the notation we will use to express algorithms; we show how assertions can be used to establish correctness; and we propose a goal-oriented methodology for the derivation of algorithms. We also discuss how to incorporate an analysis of the cost into the algorithm. Finally, we show how to translate algorithms to code so that the correctness of the algorithm implies the correctness of the implementation.

Upon completion of this week, you should be able to

•

Track your progress in Appendix ??.

2.2 Deriving Algorithms for APDOT

2.2.1 Goal-oriented programming

While so far we discussed how to add annotations to an existing algorithm in an effort to prove it correct, we now demonstrate how one can methodically and constructively *derive* correct algorithms. *Goaloriented* derivation of algorithms starts with the specification of the operation for which an algorithm is to be developed. From the specification, assertions are systematically determined and inserted into the algorithm before commands are added. By then inserting commands that make the assertions true at the indicated points, the algorithm is developed, hand-in-hand with its proof of correctness. We will illustrate this with the by now familiar APDOT operation.

Homework 2.2.1.1 Print a blank "worksheet" from file

Resources/BlankWorksheet.pdf

SEE ANSWER

2.2.2 Step 1: Specifying the operation

The APDOT operation is mathematically given by $[\alpha] := SAPDOT_UNB_VAR1(x, y, \alpha)$, This means that upon completion the variable α needs to satisfy the *postcondition* for this algorithm

$$\alpha = \widehat{\alpha} + x^T y$$
.

Here $\widehat{\alpha}$ is a "dummy variable" introduced to represent the *original* contents of α , as is indicated in Step 1a as

$$\alpha = \widehat{\alpha}$$
,

which is known as the *precondition* for this algorithm.

Now, strictly speaking we should also indicate that x and y are vectors of the same length. We will assume this is implicitly true, since otherwise x^Ty (the dot product of x and y) is not well-defined.

Homework 2.2.2.2 On the worksheet, enter the precondition and postcondition as Step 1a and Step 1b, respectively.

SEE ANSWER

2.2.3 Step 2: Deriving loop-invariants

As part of the computation of $[\alpha] := SAPDOT_UNB_VAR1(x, y, \alpha)$ we will sweep through vectors x and y in a way that creates two different subvectors of each of those vectors: the parts that have already been used to update α and the parts that remain yet to be used in this update. This suggests a partitioning of x and y as

$$x \to \left(\frac{x_T}{x_B}\right)$$
 and $y \to \left(\frac{y_T}{y_B}\right)$,

where $m(x_T) = m(y_T)$ (the size of x_T equals the size of y_T) since otherwise $x_T^T y_T$ is not well-defined.

We take these partitioned vectors and substitute them into the postcondition to find that

$$\alpha = \left(\frac{x_T}{x_B}\right)^{\mathrm{T}} \left(\frac{y_T}{y_B}\right) + \widehat{\alpha} = \left(x_T^{\mathrm{T}} \mid x_B^{\mathrm{T}}\right) \left(\frac{y_T}{y_B}\right) + \widehat{\alpha},$$

or.

$$\alpha = x_T^T y_T + x_B^T y_B + \widehat{\alpha}.$$

This partitioned matrix expression (PME) expresses the final value of α in terms of its original value and the partitioned vectors.

The partitioned matrix expression (PME) is obtained by substitution of the partitioned operands into the postcondition.

Now, at an intermediate iteration of the loop, α does not contain its final value. Rather, it contains some *partial* result towards that final result. This partial result should be reflected in the loop-invariant. One such intermediate state is given by

$$P_{inv}: \alpha = \widehat{\alpha} + x_T^T y_T,$$

which we note is exactly the loop-invariant that we used to prove the algorithm correct in Figure 1.7. But

Once it is decided how to partition vectors and matrices into regions that have been updated and/or used in a consistent fashion, loop-invariants can be systematically determined *a priori*.

Homework 2.2.3.3 Enter the loop-invariant on the worksheet in the four places where Step 2 appears.

SEE ANSWER

2.2.4 Step 3: Determining the loop-guard.

The condition

$$P_{inv} \wedge \neg G \equiv (\alpha = \widehat{\alpha} + x_T^T y_T) \wedge \neg G$$

must imply that " P_{post} : $\alpha = \widehat{\alpha} + x^T y$ " holds. If x_T and y_T equal all of x and y, respectively, then the loop-invariant implies the postcondition: The choice 'G: $m(x_T) < m(x)$ " satisfies the desired condition that $P_{inv} \wedge \neg G$ implies that $m(x_T) = m(x)$, as x_T must be a subvector of x, and

$$\underbrace{(\alpha = \widehat{\alpha} + x_T^T y_T)}_{P_{inv}} \land \underbrace{(m(x_T) \ge m(x))}_{\neg G}$$

$$\Rightarrow \alpha = \widehat{\alpha} + x^T y.$$

Homework 2.2.4.4 Enter the loop-guard on the worksheet in the three places where Step 3 appears.

SEE ANSWER

The chosen loop-invariant and the postcondition together *prescribe* a (non-unique) loop-guard G.

2.2.5 Step 4: Initialization.

If we partition

$$x \to \left(\frac{x_T}{x_B}\right)$$
 and $y \to \left(\frac{y_T}{y_B}\right)$,

where x_T and y_T have *no* elements, then we place variables α , x_T , x_B , y_T , and y_B in a state where the loop-invariant is satisfied.

Homework 2.2.5.5 Enter the initial partitioning in Step 4 of the worksheet.

SEE ANSWER

The chosen loop-invariant and the precondition together *prescribe* the initialization.

2.2.6 Step 5: Progressing through the vectors.

We now note that, as part of the computation, x_T and y_T start by containing no elements and must ultimately equal all of x and y, respectively. Thus, as part of the loop, elements must be taken from x_B and y_B and must be added to x_T and y_T , respectively. This is denoted in Figure 1.7 by the statements

Repartition

$$\left(\frac{x_T}{x_B}\right) \to \left(\frac{x_0}{\chi_1}\right), \left(\frac{y_T}{y_B}\right) \to \left(\frac{y_0}{\psi_1}\right)$$

where χ_1 has 1 row, ψ_1 has 1 row,

and

Continue with

$$\left(\frac{x_T}{x_B}\right) \leftarrow \left(\frac{x_0}{\chi_1}\right), \left(\frac{y_T}{y_B}\right) \leftarrow \left(\frac{y_0}{\psi_1}\right).$$

This notation simply captures the movement of χ_1 , the top element of x_B , from x_B to x_T . Similarly ψ_1 moves from y_B to y_T . The movement through the vectors guarantees that the loop eventually terminates, which is one condition required for the Fundamental Invariance Theorem to apply.

Homework 2.2.6.6 Enter how the algorithm progresses through the vectors as Steps 5a and 5b in the worksheet.

SEE ANSWER

The initialization and the loop-guard together prescribe the movement through the vectors.

2.2.7 Step 6: Determining the state after repartitioning.

The repartitionings in Step 5a do not change the contents of α : it is an "indexing" operation. We can thus ask ourselves the question of what the contents of α are in terms of the exposed parts of x and y. We can derive this state, P_{before} , via *textual substitution*: The repartitionings in Step 5a imply that

$$\frac{x_T = x_0}{x_B = \left(\frac{\chi_1}{x_2}\right)} \quad \text{and} \quad \frac{y_T = y_0}{y_B = \left(\frac{\psi_1}{y_2}\right)} .$$

If we substitute the expressions on the right of the equalities into the loop-invariant we find that

$$\alpha = x_T^{\mathrm{T}} y_T + \widehat{\alpha}$$

implies that

$$\alpha = \underbrace{x_0}_{x_T} \underbrace{x_0}_{y_T} + \widehat{\alpha}.$$

Homework 2.2.7.7 Enter the stae of the variable α , in terms of the subparts of vectors x and y that were exposed in Step 5a, in the worksheet as Step 6.

SEE ANSWER

The state in Step 6 is determined via textual substitution.

2.2.8 Step 7: Determining the state after moving the thick lines.

The movement of the thick lines in Step 5b means that now

$$x_T = \left(\frac{x_0}{\chi_1}\right) \qquad \text{and} \qquad y_T = \left(\frac{y_0}{\psi_1}\right)$$
$$x_B = x_2 \qquad y_B = y_2$$

so that

$$\alpha = x_T^{\mathrm{T}} y_T + \widehat{\alpha}$$

implies that

$$\alpha = \underbrace{\left(\frac{x_0}{\chi_1}\right)}_{x_T} T \underbrace{\left(\frac{y_0}{\psi_1}\right)}_{y_T} + \widehat{\alpha} = x_0^{\mathrm{T}} y_0 + \chi_1 \psi_1 + \widehat{\alpha}.$$

Homework 2.2.8.8 Enter the stae of the variable α , in terms of the subparts of vectors x and y that were exposed in Step 5b, in the worksheet as Step 7.

SEE ANSWER

The state in Step 7 is determined via textual substitution and the application of the rules of linear algebra.

2.2.9 Step 8: Determining the update.

Comparing the contents in Step 6 and Step 7 now tells us that the state of α must change from

$$P_{before}: \alpha = x_0^{\mathrm{T}} y_0 + \widehat{\alpha}$$

to

$$P_{after}: \alpha = \underbrace{x_0^{\mathrm{T}} y_0 + \widehat{\alpha}}_{\text{already in } \alpha} + \underbrace{\chi_1 \psi_1}_{\text{+} \chi_1 \psi_1},$$

which can be accomplished by updating α as

$$\alpha := \chi_1 \psi_1 + \alpha$$
.

Homework 2.2.9.9 Enter the update to variable α as Step 8.

SEE ANSWER

It is *not* the case that $\widehat{\alpha}$ (the original contents of α) must be saved, and that the update $\alpha = x_0^T y_0 + \chi_1 \psi_1 + \widehat{\alpha}$ must be performed. Since α already contains $x_0^T y_0 + \widehat{\alpha}$, only $\chi_1 \psi_1$ needs to be added. Thus, $\widehat{\alpha}$ is only needed to be able to reason about the correctness of the algorithm.

2.2.10 Final algorithm.

Finally, we note that all the annotations (in the yellow boxes) in the worksheet were only introduced to derive the statements of the algorithm. Deleting these produces the algorithm already stated in Figure 1.5.

FIATEX command	Result
\FlaTwoByOne{x_T} {x_B}	$\left(\begin{array}{c} x_T \\ \hline x_B \end{array}\right)$
\FlaThreeByOneB{x_0} {x_1} {x_2}	$\left(\begin{array}{c} x_0 \\ \hline x_1 \\ \hline x_2 \end{array}\right)$
\FlaThreeByOneT{x_0}	$\left(\frac{x_0}{x_1}\right)$
\FlaOneByTwo{x_L}{x_R}	$\begin{pmatrix} x_L & x_R \end{pmatrix}$
\FlaOneByThreeR{x_0}{x_1}{x_2}	$\left(\begin{array}{c c} x_0 & x_1 & x_2 \end{array}\right)$
lem:lem:lem:lem:lem:lem:lem:lem:lem:lem:	$\left(\begin{array}{c c} x_0 & x_1 & x_2 \end{array}\right)$
\FlaTwoByTwo{A_{TL}}}{A_{TR}} {A_{BL}}}{A_{BR}}	$\left(egin{array}{c c} A_{TL} & A_{TR} \ \hline A_{BL} & A_{BR} \end{array} ight)$
\FlaThreeByThreeBR{A_{00}}{A_{01}}{A_{02}} {A_{10}}{A_{11}}{A_{12}} {A_{20}}{A_{21}}{A_{22}}	$ \left(\begin{array}{c c c} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right) $
\FlaThreeByThreeBL{A_{00}}{A_{01}}{A_{02}} {A_{10}}{A_{11}}{A_{12}} {A_{20}}{A_{21}}{A_{22}}	$ \left(\begin{array}{c c c} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right) $
\FlaThreeByThreeTR{A_{00}}{A_{01}}{A_{02}} {A_{10}}{A_{11}}{A_{12}} {A_{20}}{A_{21}}{A_{22}}	$ \left(\begin{array}{c c c} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right) $
\FlaThreeByThreeTL{A_{00}}{A_{01}}{A_{02}} {A_{10}}{A_{11}}{A_{12}} {A_{20}}{A_{21}}{A_{22}}	$ \left(\begin{array}{c cccc} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right) $

Table 2.1: Various FLATEX commands for typesetting partitioned matrices.

2.2.11 Typesetting a derivation

Homework 2.2.11.10 With TeXstudio open file

Assignments/Week2/LaTeX/DeriveSapdotVar1.tex.

With the Spark webpage create a "worksheet" for deriving Variant 1 for the routine

Sapdot_unb_var1(x, y, alpha)

indicating that x and y are input parameters and alpha is both input and output. Move through both vectors from top to bottom and choose FLaTeX - Worksheet as output language. Next, cut and past the text generated on the right into DeriveSapdotVarl.tex at the location indicated by

Insert output from http://www.cs.utexas.edu/users/flame/Spark/ here

If you now "compile" this LATEX source, you will see a partially filled out worksheet. Now look carefully at what was inserted from Spark. The comments will guide you through where you need to enter the various steps. Every time you add a step, recompile so that you can see what you are typesetting and so you can catch errors. When you are all done, flip through all the pages that are created. You will see the various Steps fill the worksheet.

2.3 A More Advanced Example

In this section, we will revisit the problem of finding algorithms for computing y := Ax + y where A is a symmetric matrix and only the lower triangular matrix is stored.

Homework 2.3.0.11 Print a blank "worksheet" from file

Resources/BlankWorksheet.pdf

and/or open file Assignments/Week2/LaTeX/Symv_l_unb_var1.tex with TeXstudio.

SEE ANSWER

Required linear algebra knowledge

Consider the matrix vector operation Ax where A and x are of appropriate sizes so that this multiplication makes sense. Partition

$$A
ightharpoonup \left(egin{array}{c|c} A_{TL} & A_{TR} \ \hline A_{BL} & A_{BR} \end{array}
ight), \quad ext{and} x
ightharpoonup \left(egin{array}{c} x_T \ \hline x_B \end{array}
ight).$$

Then

$$Ax = \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right) \left(\begin{array}{c} x_T \\ \hline x_B \end{array}\right) = \left(\begin{array}{c|c} A_{TL}x_T + A_{TR}x_B \\ \hline A_{BL}x_T + A_{BR}x_B \end{array}\right)$$

provided x_T and x_B have the appropriate size for the subexpressions to be well-defined.

2.3.1 Step 1: Specifying the operation

The operation we wish to implement is mathematically given by y := Ax + y, where we are implicitly remembering that only the lower triangular part of matrix A can be accessed, since the strictly upper triangular part is not stored.

Homework 2.3.1.12 On the worksheet, enter the precondition and postcondition for this operation as Step 1a and Step 1b, respectively.

SEE ANSWER

2.3.2 Step 2: Deriving loop-invariants

Since matrix A is symmetric, we want to partition

$$A
ightarrow \left(egin{array}{c|c} A_{TL} & A_{TR} \ \hline A_{BL} & A_{BR} \end{array}
ight)$$

where A_{TL} is square because then, because of the symmetry of A, we know that

- A_{TL} and A_{BR} are symmetric,
- $A_{TR} = A_{RI}^T$, and

• if we partition

$$x \to \left(\frac{x_T}{x_B}\right)$$
 and $y \to \left(\frac{y_T}{y_B}\right)$

then entering the partitioned matrix and vectors into the postcondition $y = Ax + \hat{y}$ yields

$$\left(\begin{array}{c} \underline{y_T} \\ \underline{y_B} \end{array}\right) = \left(\begin{array}{c} A_{TL} & A_{TR} \\ A_{BL} & A_{BR} \end{array}\right) \left(\begin{array}{c} x_T \\ \underline{x_B} \end{array}\right) + \left(\begin{array}{c} \widehat{y_T} \\ \widehat{y_B} \end{array}\right) \\
= \left(\begin{array}{c} A_{TL}x_T + A_{TR}x_B + \widehat{y_T} \\ A_{BL}x_T + A_{BR}x_B + \widehat{y_B} \end{array}\right) \\
= \left(\begin{array}{c} A_{TL}x_T + A_{TL}^T +$$

This last observation gives us our PME for this operation:

$$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + A_{BL}^T x_B + \widehat{y}_T}{A_{BL}x_T + A_{BR}x_B + \widehat{y}_B}\right).$$

Now, how do we come up with possible loop-invariants? Before and after each iteration of the loop, only part of the computation has been performed. For the remainder of the section we will consider the loop-invariant yielding

$$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + \widehat{y}_T}{\widehat{y}_B}\right).$$

Homework 2.3.2.13 Enter the loop-invariant on the worksheet in the four places where Step 2 appears.

SEE ANSWER

2.3.3 Step 3: Determining the loop-guard.

The condition

$$P_{inv} \wedge \neg G \equiv \left(\left(\frac{y_T}{y_B} \right) = \left(\frac{A_{TL}x_T + \widehat{y}_T}{\widehat{y}_B} \right) \wedge \neg G$$

must imply that

$$P_{post}: y = Ax + \widehat{y}$$

holds.

Homework 2.3.3.14 Enter the loop-guard on the worksheet in the three places where Step 3 appears.

2.3.4 Step 4: Initialization.

When we derived the PME in Step 2, we decided to partition the matrices like

$$A o \left(egin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right), \quad x o \left(egin{array}{c} x_T \\ \hline x_B \end{array} \right), \quad ext{and} \quad y o \left(egin{array}{c} y_T \\ \hline y_B \end{array} \right).$$

The question now is how to choose the sizes of the submatrices and vectors so that the precondition

$$y = \hat{y}$$

implies that the loop-invariant

$$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + \widehat{y}_T}{\widehat{y}_B}\right)$$

holds after the initialization (and before the loop commenses).

Homework 2.3.4.15 Enter the initial partitioning in Step 4 of the worksheet.

SEE ANSWER

2.3.5 Step 5: Progressing through the vectors.

We now note that, as part of the computation, A_{TL} , x_T and y_T start by containing no elements and must ultimately equal all of A, x and y, respectively. Thus, as part of the loop, elements must be taken from x_B and y_B and must be added to x_T and y_T , respectively.

Homework 2.3.5.16 Enter how the algorithm progresses through the matrix and vectors as Steps 5a and 5b in the worksheet.

SEE ANSWER

2.3.6 Step 6: Determining the state after repartitioning.

This is where things become less than straight forward. The repartitionings in Step 5a do not change the contents of y: it is an "indexing" operation. We can thus ask ourselves the question of what the contents of y are in terms of the newly exposed parts of A, x, and y. We can derive this state, P_{before} , via textual substitution: The repartitionings in Step 5a imply that

If we substitute the expressions on the right of the equalities into the loop-invariant we find that

$$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + \widehat{y}_T}{\widehat{y}_B}\right)$$

becomes

$$\left(\begin{array}{c}
 y_0 \\
\hline
\left(\begin{array}{c}
 \psi_1 \\
\hline
y_2
\end{array}\right)
\right) = \left(\begin{array}{c}
 A_{00}x_0 + \widehat{y}_0 \\
\hline
\left(\begin{array}{c}
 \widehat{\psi}_1 \\
\hline
\widehat{y}_2
\end{array}\right)
\right)$$

and hence

$$\left(\begin{array}{c}
\underline{y_0} \\
\underline{\psi_1} \\
\underline{y_2}
\end{array}\right) = \left(\begin{array}{c}
\underline{A_{00}x_0 + \widehat{y_0}} \\
\underline{\widehat{\psi}_1} \\
\underline{\widehat{y}_2}
\end{array}\right)$$

Homework 2.3.6.17 Enter the stae of the variable y, in terms of the subparts of matix A, and vectors x and \hat{y} that were exposed in Step 5a, in the worksheet as Step 6.

SEE ANSWER

2.3.7 Step 7: Determining the state after moving the thick lines.

The movement of the thick lines in Step 5b means that now

$$A_{TL} = \begin{pmatrix} A_{00} & a_{01} \\ \hline a_{10}^T & \alpha_{11} \end{pmatrix} A_{TR} = \begin{pmatrix} A_{02} \\ \hline a_{12}^T \end{pmatrix}, \quad x_T = \begin{pmatrix} x_0 \\ \hline \chi_1 \end{pmatrix}, \quad \text{and} \quad y_T = \begin{pmatrix} y_0 \\ \hline \psi_1 \end{pmatrix}$$

$$A_{BL} = \begin{pmatrix} A_{20} & a_{21} \end{pmatrix} A_{BR} = A_{22} \qquad x_B = x_2 \qquad y_B = y_2$$

If we substitute the expressions on the right of the equalities into the loop-invariant we find that

$$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + \widehat{y}_T}{\widehat{y}_B}\right)$$

becomes

where we recognize that due to symmetry $a_{01} = (a_{10}^T)^T$ and hence

$$\left(\frac{y_0}{\psi_1}\right) = \left(\frac{A_{00}x_0 + (a_{10}^T)^T \chi_1 + \widehat{y}_0}{a_{10}^T x_0 + \alpha_{11} \chi_1 + \widehat{\psi}_1}\right)$$

$$\widehat{y}_2$$

Homework 2.3.7.18 Enter the state of the variable y, in terms of the subparts of matrix A, and vectors x and \hat{y} that were exposed in Step 5b, in the worksheet as Step 7.

2.3.8 Step 8: Determining the update.

Comparing the contents in Step 6 and Step 7 now tells us that the state of y must change from

$$P_{before}: \left(\frac{y_0}{\psi_1} \right) = \left(\frac{A_{00}x_0 + \widehat{y}_0}{\widehat{y}_2} \right)$$

to

$$P_{after}: \left(\frac{y_0}{\psi_1} \right) = \left(\frac{A_{00}x_0 + (a_{10}^T)^T \chi_1 + \widehat{y}_0}{a_{10}^T x_0 + \alpha_{11} \chi_1 + \widehat{\psi}_1} \right),$$

which can be accomplished by updating

$$y_0 := \chi_1(a_{10}^T)^T + y_0$$

 $\psi_1 := a_{10}^T x_0 + \alpha_{11} \chi_1 + \psi_1$

Homework 2.3.8.19 Enter this update as Step 8 in the worksheet.

SEE ANSWER

2.3.9 Final algorithm.

Finally, we note that all the annotations (in the yellow boxes) in the worksheet were only introduced to derive the statements of the algorithm.

2.3.10 Typesetting the derivation

Homework 2.3.10.20 With TeXstudio open file

Assignments/Week2/LaTeX/Symv_l_unb_var1.tex.

With the Spark webpage create a "worksheet" for deriving Variant 1 for the routine

$$Symv_l_unb_var1(A, x, y)$$

Next, cut and past the text generated on the right into Symv_l_unb_varl.tex at the location indicated by

Insert output from http://www.cs.utexas.edu/users/flame/Spark/ here

If you now "compile" this LATEX source, you will see a partially filled out worksheet. Now look carefully at what was inserted from Spark. The comments will guide you through where you need to enter the various steps. Every time you add a step, recompile so that you can see what you are typesetting and so you can catch errors. When you are all done, flip through all the pages that are created. You will see the various Steps fill the worksheet.

PME:
$$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + A_{BL}^T x_B + \widehat{y}_T}{A_{BL}x_T + A_{BR}x_B + \widehat{y}_B}\right).$$

Var#	Loop-invariant	Var#	Loop-invariant
1	$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + \widehat{y}_T}{\widehat{y}_B}\right)$	5	$\left(\frac{y_T}{y_B}\right) = \left(\frac{\widehat{y}_T}{A_{BR}x_B + \widehat{y}_B}\right)$
2	$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + A_{BL}^T x_B + \widehat{y}_T}{\widehat{y}_B}\right)$	6	$\left(\frac{y_T}{y_B}\right) = \left(\frac{\widehat{y}_T}{A_{BL}x_T + A_{BR}x_B + \widehat{y}_B}\right)$
3	$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + \widehat{y}_T}{A_{BL}x_T + \widehat{y}_B}\right)$	7	$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{BL}^T x_B + \widehat{y}_T}{A_{BR} x_B + \widehat{y}_B}\right)$
4	$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + A_{BL}^T x_B + \widehat{y}_T}{A_{BL}x_T + \widehat{y}_B}\right)$	8	$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{BL}^T x_B + \widehat{y}_T}{A_{BL} x_T + A_{BR} x_B + \widehat{y}_B}\right)$

Figure 2.1: Loop-invariants for y := Ax + y where A is symmetric and only its lower triangular part is stored.

The result can be viewed in

Assignments/Week2/LaTeX/Symv_l_unb_var1_answer.pdf.

2.3.11 Other loop invariants

Other loop invariants can be derived by examining the PME

$$\left(\frac{y_T}{y_B}\right) = \left(\frac{A_{TL}x_T + A_{BL}^T x_B + \widehat{y}_T}{A_{BL}x_T + A_{BR}x_B + \widehat{y}_B}\right)$$

and removing different terms. There are four terms each of which either does or does not appear in the loop-invariant. This gives 2^4 different possible loop-invariants. However, some of these do not lead to valid loop invariants for various reasons that we will discuss later. There are eight loop-invariants that do yield valid algorithms, tabulated in Figure 2.1. Algorithms corresponding to the invariants on the left (Variants 1-4) traverse A from the top-left to bottom right, and vectors x and y from top to bottom. The ones on the right (Variants 5-8) traverse A from bottom-right to top-left, and vectors x and y from bottom to top.

Homework 2.3.11.21 Derive algorithms for Variants 2-8, corresponding to the indicated loop-invariants in Figure 2.1. Typeset the resulting algorithms with TeXstudio, starting with

Assignments/Week2/LaTeX/Symv_l_unb_varX.tex

by first coping this file to

Assignments/Week2/LaTeX/Symv_l_unb_var<n>.tex

where <n> is replaced by the appropriate digit 2 through 8.

Bibliography