Data Science in Ten Minutes*

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May 19, 2018

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Introduction

Data science is not machine learning. There is no machine learning in this guide, because machine learning is the wrong answer to most problems you're likely to run into. I've never deployed a machine learning system, although I've debugged several misbehaving ones (and will cover how to do that).

A lot of the code examples assume you're running Linux because Linux is the go-to platform for medium/big data processing. It's also ideal for small data due to optimizations in core utilities like sort. If you're running a non-Linux OS and want to try stuff, you have a few options:

• Install Docker and create a container from the ubuntu:18.04 image or similar (I'll assume you have this setup)

^{*}for extremely large values of ten

¹GNU sort will compress temporary files, unlike the sort that ships with OSX.

- Run a VM like VirtualBox and install Ubuntu Desktop inside it
- Rent a free tier Amazon EC2 instance (you can use the free-tier t2.nano or t2.micro for data science, and they're ideal for learning because they're resource-constrained)
- Buy a cheap rack server from eBay and drop Ubuntu Server on it

Realistically, you probably won't want to use OSX or Windows for distributed programming: your binaries won't be portable to cluster machines, and you'll be fighting with things like case-insensitive filesystems, slower core utilities, and general inconsistencies that will increase debugging time.²

Examples

This guide comes with example code in the original repository. Where necessary, I've included package installation commands required to install dependencies on Ubuntu 18.04.

²All of this is a non-issue for JVM processes, e.g. Hadoop and Spark, but a lot of data science is best done with native tools that use less memory and have lower iteration time.

1 Linux

Oh yes, we are totally going here. Here's why.

Backend programs and processing pipelines and stuff (basically, "big data" things) operate entirely by talking to the kernel, which, in big-data world, is usually Linux; and this is true regardless of the language, libraries, and framework(s) you're using. You can always throw more hardware at a problem³, but if you understand system-level programming you'll often have a better/cheaper option.

Some quick background reading if you need it for the homework/curiosity:

- How to write a UNIX shell
- How to write a JIT compiler
- ELF executable binary spec (more readable version on Wikipedia, and this StackOverflow answer may be useful)
- Intel machine code documentation

1.1 Virtual memory

This is one of the two things that comes up a lot in data science infrastructure. Basically, any memory address you can see is virtualized and may not be resident in the RAM chips in your machine. The kernel talks to the MMU hardware to maintain the mapping between software and hardware pages, and when the virtual page set overflows physical memory the kernel swaps them to disk, usually with an LRU strategy.

Here's where things get interesting. Linux (and any other server OS) gives you a mmap system call to request that the kernel map pages into your program's address space. mmap, however, has some interesting options:

- MAP_SHARED: map the region into multiple programs' address spaces (this
 reuses the same physical page across processes)
- MAP_FILE: map the region using data from a file; then the kernel will load file data when a page fault occurs

MAP_FILE is sort of like saying "swap this region to a specific file, rather than the shared swapfile you'd normally use." The implication is important, though: all memory mappings go through the same page allocation cache, and any page fault has the potential to block your program on disk IO. Clever data structures like Bloom filters, Count-min sketches, and so forth are all designed to give you a way to trade various degrees of accuracy for a much smaller memory footprint.

Sometimes you won't have any good options within the confines of physical RAM, so you'll end up using IO devices to supply data; then the challenge

³Until you can't

becomes optimizing for those IO devices (SSDs are different from HDDs, for instance). I'll get to some specifics later on when we talk about sorting, joins, and compression.

1.2 File descriptors

This is the other thing you need to know about.

Programs don't typically use mmap for general-purpose IO. It's more idiomatic, and sometimes faster, to use read and write on a file descriptor. Internally, these functions ask the kernel to copy memory from an underyling file/socket/pipe/etc into mapped pages in the address space. The advantage is cache locality: you can read a small amount of stuff into a buffer, process the buffer, and then reuse that buffer for the next read. Cache locality does matter; for example:

```
# small block size: great cache locality, too much system calling overhead
$ dd if=/dev/zero count=262144 bs=32768 of=/dev/null
262144+0 records in
262144+0 records out
8589934592 bytes (8.6 GB, 8.0 GiB) copied, 0.774034 s, 11.1 GB/s

# medium block size: great cache locality, insignificant syscall overhead
$ dd if=/dev/zero count=8192 bs=1048576 of=/dev/null
8192+0 records in
8192+0 records out
8589934592 bytes (8.6 GB, 8.0 GiB) copied, 0.574597 s, 14.9 GB/s

# large block size: cache overflow, insignificant syscall overhead
$ dd if=/dev/zero count=2048 bs=$((1048576 * 4)) of=/dev/null
2048+0 records in
2048+0 records out
8589934592 bytes (8.6 GB, 8.0 GiB) copied, 1.14022 s, 7.5 GB/s
```

This makes sense considering the processor hardware:

```
$ grep cache /proc/cpuinfo
cache size : 3072 KB
cache_alignment : 64
```

1.3 Pulling this together: let's write a program

...in machine language. For simplicity, let's write one that prints hello world and then exits successfully (with code 0).

This is also a good opportunity to talk about how we might generate and work with binary data with things like fixed offsets. Two simple functions for this are pack() and unpack(), variants of which ship with both Perl and Ruby.

The first part of any Linux executable is the ELF header, usually followed directly by a program header; here's what those look like as C structs for 64-bit executables (reformatted slightly, and with docs for readability):

```
typedef struct {
  unsigned char e_ident[16];
                               // 0x7f, 'E', 'L', 'F', ...
 uint16_t
                                // ET_EXEC = 2 for executable files
               e_type;
                               // EM_X86_64 = 62 for AMD64 architecture
 uint16_t
               e_machine;
 uint32_t
              e_version;
                               // EV_CURRENT = 1
                               // virtual address of first instruction
 uint64_t
               e_entry;
                               // file offset of first program header
  uint64 t
               e_phoff;
               e_shoff;
                               // file offset of first section header
 uint64_t
                               // always zero
 uint32_t
              e_flags;
                               // size of the ELF header struct (this one)
 uint16_t
               e_ehsize;
                               // size of a program header struct
 uint16_t
               e_phentsize;
               e_phnum;
                               // number of program header structs
  uint16_t
               e_shentsize;
                               // size of a section header struct
 uint16_t
                               // number of section header structs
  uint16_t
                e_shnum;
                e_shstrndx;
                               // string table linkage
  uint16_t
} Elf64_Ehdr;
typedef struct {
                                // the purpose of the mapping
  uint32_t p_type;
 uint32_t p_flags;
                               // permissions for the mapped pages (rwx)
 uint64_t p_offset;
                               // file offset of the first byte of data
                               // virtual memory offset of the data (NB below)
 uint64_t p_vaddr;
 uint64_t p_paddr;
                               // physical memory offset (usually zero)
                               // number of bytes from the file
 uint64_t p_filesz;
 uint64_t p_memsz;
                               // number of bytes to be mapped into memory
  uint64_t p_align;
                               // segment alignment
} Elf64_Phdr;
  If we want a very minimal executable, here's how we might write these
headers from Perl:
# elf-header.pl: emit an ELF binary and program header to stdout
use strict;
use warnings;
print pack('C16 SSL',
```

```
0x7f, ord 'E', ord 'L', ord 'F',
           2, 1, 1, 0,
           0, 0, 0, 0,
           0, 0, 0, 0,
                                          # e_type
                                                      = ET_EXEC
           2,
           62,
                                          # e_machine = EM_X86_64
                                          # e_version = EV_CURRENT
           1)
    . pack('QQQ',
           0x400078,
                                          \# e_{entry} = 0x400078
                                          # e_phoff
           64,
           0)
                                          # e_shoff
    . pack('LSS SSSS',
                                          # e_flags
           0,
                                          # e_ehsize
           64.
           56,
                                          # e_phentsize
                                          # e_phnum
           1,
           0,
                                          # e_shentsize
           0,
                                          # e_shnum
           0)
                                          # e_shstrndx
    . pack('LLQQQQQQ',
                                          # p_type = PT_LOAD (map a region)
           1,
           7,
                                          # p_flags = R|W|X
                                          # p_offset (must be page-aligned)
           0,
                                          # p_vaddr
           0x400000,
                                          # p_paddr
           0,
                                          # p_filesz: 4KB
           0x1000,
           0x1000,
                                          # p_memsz: 4KB
           0x1000);
                                          # p_align: 4KB
  Now we can generate the ELF header:
$ sudo apt install perl
                                          # if perl is missing
$ perl elf-header.pl > elf-header
   You can verify that the header is correct using file, which reads magic
```

numbers and tells you about the format of things:

```
$ sudo apt install file
$ file elf-header
elf-header: ELF 64-bit LSB executable, x86-64, version 1 (SYSV), statically
linked, corrupted section header size
```

Awesome, now let's get into the machine code.

1.4 hello world in machine code

The first thing to note is that we're talking directly to the kernel here. Our ELF header above is very minimalistic, with no linker instructions or anything else to complicate things. So we have none of the usual libc functions like printf or exit; it's up to us to define those in terms of Linux system calls.

There are two calls we'll use for this: write(2) and exit(2). You can view the documentation for these using man:

```
$ sudo apt install man manpages-dev
$ man 2 write
$ man 2 exit
```

We'll need to pass arguments in registers to match the kernel calling convention. I'll spare you the gory details and cut straight to the machine code:

```
# elf-hello.pl: emit machine code for hello world, then exit successfully
use strict;
use warnings;
print pack('H*', join '',
  '4831c0',
                                         # xorq %rax, %rax
  'b001',
                                         # movb $01, %al (1 = write syscall)
  'e80c000000',
                                         # call %rip+12 (jump over the message)
  unpack('H*', "hello world\n"),
                                         # the message
  '5e',
                                         # pop message into %rsi (buf arg)
  'ba0c000000'.
                                         # movl $12, %rdx (len arg)
  '48c7c701000000',
                                         # movl $1, %rdi (fd arg)
  '0f05',
                                         # syscall instruction
  '4831c0',
                                         # xorq %rax, %rax
  'b03c',
                                         # movb $3c, %rax (3c = exit syscall)
                                         # xorq %rdi, %rdi (exit code arg)
  '4831ff'.
  '0f05');
                                         # syscall instruction
```

Now we can build the full executable, verify it, and run:

```
$ sudo apt install nasm
$ perl elf-hello.pl | cat elf-header - > elf-hello
$ chmod 755 elf-hello
$ tail -c+121 elf-hello | ndisasm -b 64 -
00000000 4831C0
                           xor rax, rax
00000003 B001
                           mov al.0x1
00000005 E80C000000
                           call 0x16
0000000A 68656C6C6F
                           push qword 0x6f6c6c65
                                                    # corruption from message
000000F 20776F
                                                    # (which we jumped over)
                           and [rdi+0x6f],dh
00000012 726C
                           jc 0x80
00000014 640A5EBA
                           or bl,[fs:rsi-0x46]
```

```
or al,0x0
00000018 0C00
0000001A 0000
                            add [rax],al
                                                    # now we're back on track
0000001C 48C7C701000000
                            mov rdi,0x1
00000023 0F05
                            syscall
00000025 4831C0
                            xor rax, rax
00000028 B03C
                            mov al,0x3c
0000002A 4831FF
                            xor rdi, rdi
0000002D 0F05
                            syscall
```

The moment we've been waiting for:

```
$ ./elf-hello
hello world
$ echo $? # check exit status
0
```

Whether through libraries, JIT, or anything else, this is the exact mechanism being used by any program that performs IO of any sort: the program lives in a completely virtual world and interacts with the kernel using the 0f05 syscall instruction, referring to virtual addresses in the process.

1.5 Homework, if that's your thing

- 1. Write an ELF Linux executable that consumes data from stdin and writes that data to stdout, then exits successfully. In other words, cat without file support.
- 2. Use pack() to produce a RIFF WAV file containing a 440Hz sine wave for ten seconds. It may be helpful to use unpack() to inspect the headers of existing WAV files because it's challenging to find detailed documentation of the format.
- 3. Problem (2), but have no more than 256 bytes of string data resident at any given moment.

2 Wikipedia

You can download the full English language Wikipedia as a giant bzip2-compressed XML file. For reference, here's the exact torrent file I downloaded. It's about 14GB compressed, which is not big data by any means; you could process this on a Raspberry Pi with a 64GB SD card if you wanted to.⁴

While that's downloading, let's take a moment to talk about compression formats.

2.1 Compression

There are a few standard, general-purpose data compressors you're likely to encounter regularly:⁵

Compressor	Compression speed	Decompression speed	Efficiency
XZ	4MB/s	200MB/s TODO	High
bzip2	8MB/s	24MB/s	High-ish
gzip	23MB/s	120MB/s	Medium
lzo	200MB/s	300MB/s TODO	Low
1z4	240MB/s	800MB/s TODO	Low

If you take one thing away from this table, it's *don't use bzip2*. bzip2 is horrible, even though the algorithm is pretty cool. If you are ever cursed with a bzip2 file, you can accelerate decompression by parallelizing it across multiple cores using pbzip2, which is installable under Ubuntu using sudo apt install pbzip2.

Roughly speaking, here's how these compressors operate:⁶

Compressor	Structure
XZ	Large-dictionary LZ77 + LZMA + statistical prediction
bzip2	RLE + BWT + MTF + RLE + Huffman + bit-sparse
gzip	LZ77 + Huffman
lzo	Dictionary
1z4	Dictionary

It's worth knowing the broad strokes because the nature of the data will impact compression performance, both in space and time. For example, the Reddit comments dataset contains a bunch of identical-schema JSON objects that look roughly like this (reformatted for readability):

$\{$ "author": "CreativeTechGuyGames",

⁴Be careful with SD cards and Flash storage in general; if you write the memory too many times you'll destroy the drive. I'll mention this hazard anytime I have an IO-intensive process.

⁵I ran these tests by compressing an infinite stream of copies of the ni repository, which is large enough to overflow any buffers used by these algorithms. The exact script template was ni ::self[//ni] npself zx9 zn.

⁶And here's some background on the theory, if that's of interest

```
"author_flair_css_class":null,
"author_flair_text":null,
"body":"You are looking to create a reddit bot? You will want to check out
        the [reddit API](https://www.reddit.com/dev/api). Many people do
        this in Python and there are many tutorials on the internet showing
        how to do so.",
"can_gild":true,
"controversiality":0,
"created_utc":1506816001,
"distinguished":null,
"edited":false,
"gilded":0,
"id":"dnqik29",
"is_submitter":false,
"link_id":"t3_73if9c",
"parent_id":"t1_dnqihqz",
"permalink":"/r/learnprogramming/comments/73if9c/how_i_would_i_go_around_making_something_
"retrieved_on":1509189607,
"score":1,
"stickied":false,
"subreddit": "learnprogramming",
"subreddit_id":"t5_2r7yd" }
```

A nontrivial amount of the bulk in this file is stored in the JSON field names, so dictionary encoding alone is likely to save us a nontrivial amount of space. LZ4 is worthwhile here just for that, and would almost certainly be faster than reading directly from the underlying IO device.

Sometimes you need Huffman encoding, though; for example, random ASCII floats don't have enough repetition to behave well with dictionary compressors. On my test case gzip gets about 4x better compression than 1z4, and that might justify preferring it to LZ4 over slow IO devices even if it creates a CPU bottleneck.

I generally start with gzip at its default level and change algorithms later if I need to.

2.2 OK, back to Wikipedia

So we have 14GB of bzip2 data:

```
$ ls -lh enwiki-20170820-pages-articles.xml.bz2
-rw-rw-r- 1 114 122 14G May 20 00:38 enwiki-20170820-pages-articles.xml.bz2
```

What do we do with this? I'll present the next section two ways, one with standard UNIX tools and one with ni, a tool I wrote for data science.

In both cases we're solving the same problem: let's build a list of articles sorted by the fraction of web citations, as opposed to other types like books or journals.

2.3 Wikipedia with standard UNIX tools

First we need a way to preview the data without decompressing the whole thing. The simplest strategy is to decompress into less:

```
$ bzip2 -dc enwiki* | less
<mediawiki xmlns="http://www.mediawiki.org/xml/export-0.10/"</pre>
           xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
           xsi:schemaLocation="http://www.mediawiki.org/xml/export-0.10/
                                http://www.mediawiki.org/xml/export-0.10.xsd"
           version="0.10" xml:lang="en">
  <siteinfo>
    <sitename>Wikipedia</sitename>
    <dbname>enwiki</dbname>
    <base>https://en.wikipedia.org/wiki/Main_Page</base>
    <generator>MediaWiki 1.30.0-wmf.14
    <case>first-letter</case>
  Paging around a bit, the basic structure looks roughly like this:
<page>
  <title>AccessibleComputing</title>
  <ns>0</ns>
  <id>10</id>
  <redirect title="Computer accessibility" />
  <revision>
    <id>767284433</id>
    <parentid>631144794</parentid>
    <timestamp>2017-02-25T00:30:28Z</timestamp>
    <contributor>
      <username>Godsy</username>
      <id>23257138</id>
    </contributor>
    <comment>[[Template:This is a redirect]] has been deprecated, change to [[Template:Redinerated]
    <model>wikitext</model>
    <format>text/x-wiki</format>
    <text xml:space="preserve">#REDIRECT [[Computer accessibility]]
{{Redirect category shell|
{{R from move}}
{{R from CamelCase}}
{{R unprintworthy}}
}}</text>
    <sha1>ds1crfrjsn7xv73djcs4e4aq9niwanx</sha1>
  </revision>
</page>
```

Inline citations are in the text and look like this (normally one line; I've reformatted here):

Overall we have two stages to this process. The first should convert the XML stream to a series of rows, let's say TSV of webcount othercount title, one per article. So the AccessibleComputing not-really-article above would look like 0 0 AccessibleComputing.

This runs one line at a time and streams its output, so we can quickly preview/debug/iterate. Here's what that looks like:

```
0 0 AfghanistanMilitary
0 0 AfghanistanTransnationalIssues
0 0 AssistiveTechnology
0 0 AmoeboidTaxa
18 207 Autism
0 0 AlbaniaHistory
```

OK, we want a ratio, so let's remove citation-free articles and calculate web/total as a fraction:

```
$ bzcat enwiki* \
    | perl wikipedia-cite-extract.pl \
    | perl -ane 'print join("\t", F[0] / (F[0] + F[1]), @F[2..$#F]), "\n"
                   if $F[0] + $F[1]' \
    | less
0.435114503816794
                        Anarchism
80 0
        Autism
0.566666666666667
                        Albedo
0.272727272727273
                        Α
0.826086956521739
                        Alabama
                        Achilles
0.181818181818182
0.123529411764706
                        Abraham Lincoln
0.147540983606557
                        Aristotle
```

...and finally, before we write anything, let's sort the list by the fraction using sort. Before I do that, though, I want to talk a little about how sort works.

If you're sorting a stream of things, you have to store the whole stream first. Then, once you have everything, you shuffle stuff $\log n$ times and emit the sorted values.

This requires O(n) space, of course, which is inconvenient: you now have at least one temporary copy of the data you're sorting. If you were running this in a language like Python, Perl, or Ruby this would all happen in memory, which limits the size of data you can sort using standard APIs. UNIX sort is different, though.

Internally, sort keeps only a very small amount of data in memory, by default something like 4MB at a time. Once it hits that limit, it writes the sorted buffer to a temporary file and sorts the next one, later merging them back from disk. GNU sort in particular supports some extra options that are useful for data like this: --compress-program and --parallel. --compress-program instructs sort to compress its temporary files, effectively reducing the *disk* space-complexity of the sort to O(k), where k is the compressed size of your data. This, obviously, can make a huge difference.

So, with that said, here's the final pipeline:

pv is cat, but with a progress meter that looks like this:

```
164MiB 0:00:31 [5.39MiB/s] [> ] 1% ETA 0:42:08
```

Having progress meters is crucial for long-running data jobs, if for no other reason than to make sure it looks reasonable.

While that's running and before I get to the ni version, let's talk about some tools useful for performance monitoring.

2.4 Monitoring tools

I have a standard set of things I install on Linux boxes:

- htop: top, but better
- atop: top for CPU, memory, disk, network, etc
- units: a unit-aware calculator (e.g. 50GB/5Mbps in hours)

TODO: expand the above list

2.5 Wikipedia with ni

```
$ sudo apt install git pbzip2 perl perl-modules
$ git clone git://github.com/spencertipping/ni
$ sudo ln -s $PWD/ni/ni /usr/bin/
```

ni will preview compressed data automatically, so you can use it like a compression-aware less by default. It also knows to use pbzip2 if you have it installed.

```
$ ni enwiki*  # preview data
$ ni enwiki* r/cite/ # select rows matching the regex /cite/, preview those
```

There's extensive documentation on how ni works, which may be helpful to understand what these commands do.

wikipedia-cite-extract.pl and the following perl command can be folded into a four-liner, and sort -rn | gzip becomes oz:

```
$ ni enwiki* p'return () unless /<title>(.*)<\/title>/;
    my $t = $1;
    my @cs = map /\{\{cite (\w+)/, ru {/<\/text>/} or return ();
    r grep(/^web$/, @cs) / @cs, $t' oz > wiki-sorted.gz
```

ni monitors the data progress for you, so you can see a preview of the data moving out of each pipeline stage as well as speed and bottleneck pressure.

Whether you use ni, perl, or something else, command-line data processing is crucial to fast iteration on datasets. It's far less typing, instant startup, and no data movement.

2.6 Homework

TODO