Fast Cubic Spline Interpolation

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List of Codes

0.1 Abstract

The *Numerical Recipes* series of books are a useful resource, but all the algorithms they contain cannot be used within open-source projects. In this paper we develop drop-in alternatives to the two algorithms they present for cubic spline interpolation, showing as much of our work as possible to allow for replication or criticism. The output of the new algorithms is compared to the old, and found to be no different within the limits imposed by floating-point precision. Benchmarks of all these algorithms, plus variations which may run faster in certain instances, are performed. In general, all these algorithms have approximately the same execution time when interpolating curves with few control points on feature-rich Intel processors; as the number of control points increases or processor features are removed, the new algorithms become consistently faster than the old. Exceptions to that generalization are explored to create implementation guidelines, such as when to expect division to be faster than multiplication.
1 Introduction

Since first being released in 1986, the Numerical Recipes series has sold over a quarter-million copies, according to its authors, and been cited tens of thousands of times, according to Google Scholar. Several editions have been published, the most recent in 2007, with the computer code in this series translated into C, Fortran, Pascal, BASIC, and C++. This level of popularity is unusual for a thousand-page technical publication that consists of hundreds of small algorithms intended for use in engineering and scientific computing. The series’ appeal can be explained by the breadth of algorithms it includes, a desire to describe “what is inside the black box,” as well as an informal writing style.

The two Numerical Recipes books are marvellous. The principal book, The Art of Scientific Computing, contains program listings for almost every conceivable requirement, and it also contains a well written discussion of the algorithms and the numerical methods involved. The Example Book provides a complete driving program, with helpful notes, for nearly all the routines in the principal book.3

The authors express their opinions on methods and their usage and offer valuable insights in a highly readable and personable prose. For the novice or less mathematically inclined user, this guidance makes it possible to arrive at solutions using the computer routines more or less as black boxes. The more seasoned user can easily tailor the routines to his specific needs, assisted by the clear and consistent code, the inclusion of utility routines, and the meticulous documentation throughout.4

The two central characteristics of this book that I find the most compelling are its informality and the readiness of the authors to go out on a limb and present their own opinions. … Formality and a “close” style offer a warm refuge from a more daring and perceptive use of the language. This should not be so, as has been repeatedly demonstrated in a few excellent books (e.g. Gilbert Strang’s Introduction to Applied Mathematics) - it is possible, without compromising mathematical precision, to write well and comprehensibly (and even with a sense of humour). This is also the impression with Numerical Recipes and, reading it, I repeatedly felt that the authors are simply enjoying the task of explaining their subject matter. This enjoyment will be shared by the readers.5

The Numerical Recipes series has not escaped criticism, however. The authors created a web page devoted to countering rumours that the code within their book was full of mistakes. Other reviewers have argued the text contains inefficient, outdated, or inaccurate algorithms. Pavel Holoborodko tested a number of algorithms and libraries for calculating modified Bessel functions, and according to Jutta Degener found that “tests reveal that Numerical Recipes algorithms delivers the lowest accuracy in many cases!” Even the format and style which makes the series appealing has been a source of critique.

In order to present a great many topics, the authors devote little space to any one method. The treatment of each method is adequate to appreciate the basic idea, and references are provided to the literature. Generally the treatment is too superficial for a textbook. Further, the lack of examples, illustrative computations, and exercises make the book unsuitable for the classroom. … The codes themselves are of better than average quality for a survey book. However, they are far from being mathematical software. Even in the cases of a high quality code taken from the literature, the documentation expected of mathematical software is absent. Although the authors repeatedly express their distaste for “black boxes,” they do refer the reader to such codes in a number of instances. With few exceptions, the reader would be well advised to turn to reputable sources of mathematical software rather than to the codes given in this book. The advice offered does not always correspond to the methods advocated by leading practitioners and implemented in leading libraries.6
The critique of *Numerical Recipes* we are most concerned with is the license the programming code is released under. One of two licenses may apply, depending on whether access was purchased as an individual or as an institution.

By purchasing this disk or code download, you acquire a *Numerical Recipes* Personal Single-User License. This license lets you personally use *Numerical Recipes* code (“the code”) on any number of computers, but only one computer at a time. You are not permitted to allow anyone else to access or use the code. You may, under this license, transfer precompiled, executable applications incorporating the code to other, unlicensed, persons, providing that (i) the application is noncommercial (e.g., does not involve the selling or licensing of the application for a fee or its use in developing commercial products or services), and (ii) the application was first developed, compiled, and successfully run by you, and (iii) the code is bound into the application in such a manner that it cannot be accessed as individual routines and cannot practically be unbound and used in other programs. That is, under this license, your application user must not be able to use *Numerical Recipes* code as part of a program library or “mix and match” workbench.\(^8\)

The institutional license allows computers with a range of IP addresses to share *Numerical Recipes* programming code among themselves, but not to any computer outside that range. The license explicitly forbids the use of Network Address Translation or proxies to circumvent this restriction. Executables may be shared and sold outside this range, provided they were compiled within this range and *Numerical Recipes*’ source code “cannot practically be unbound and used in other programs.” Both licenses are unusually restrictive and impractical.

Free sharing of data after publication is a requirement in science (read the *Astrophysical Journal* policy if you don’t believe me). Algorithms and code are not data, but the tradition of sharing them helps the sciences to develop. The net effect of the NR license on science is to discourage people from helping others by sharing their work. I personally have a body of useful code that I want to distribute, but haven’t devoted the time to extracting it from the death grip of the NR license, because in a publish-or-perish world, I can’t justify spending the time when I could be writing a paper instead.\(^9\)

Both licenses are also incompatible with open-source software, where the source code must be shared with whoever asks for it. These restrictions were a major obstacle for us, when we found ourselves in need of a cubic B-spline interpolation routine. The version published in *Numerical Recipes* was perfect for our needs, and yet because the code would be used in a scientific publication and redistributed under an open-source license we found ourselves unable to use it. The available alternatives were either part of an existing library or poorly documented.

Our goal for this paper is to create a functional equivalent of the cubic B-spline code in *Numerical Recipes*. By deriving this code from the relevant mathematics, without reference to the original code, we are free to release our code under the license of our choosing.

Dedicating works to the public domain is difficult if not impossible for those wanting to contribute their works for public use before applicable copyright or database protection terms expire. Few if any jurisdictions have a process for doing so easily and reliably. Laws vary from jurisdiction to jurisdiction as to what rights are automatically granted and how and when they expire or may be voluntarily relinquished. More challenging yet, many legal systems effectively prohibit any attempt by these owners to surrender rights automatically conferred by law, particularly moral rights, even when the author wishing to do so is well informed and resolute about doing so and contributing their work to the public domain.

CC0 helps solve this problem by giving creators a way to waive all their copyright and related rights in their works to the fullest extent allowed by law. CC0 is a universal instrument that is not adapted to the laws of any particular legal jurisdiction, similar to many open source software
licenses. And while no tool, not even CC0, can guarantee a complete relinquishment of all copyright and database rights in every jurisdiction, we believe it provides the best and most complete alternative for contributing a work to the public domain given the many complex and diverse copyright and database systems around the world.¹⁰

We thus release the two algorithms necessary for cubic B-spline interpolation under the Creative Commons Zero license.¹¹ Unless stated otherwise, the other source code relating to the derivation of those two routines is released under the Creative Commons Attribution-ShareAlike 4.0 International license.¹² To conserve space, that source code is not embedded within this document and can instead be obtained online.¹³

Since the author has purchased one edition of the book, we are allowed access to the original code under the Numerical Recipes Personal Single-User License. We will take advantage of this to also compare the accuracy and efficiency of our replacement routines to those of the originals. These comparisons should be helpful to others interested in a replacing the original Numerical Recipes code.
2 Fast Interpolation

We can think of B-spline interpolation as a recreation of an unknown function based on sparse inputs. Each knot, $x_j$, is fed into the function and generates an output value, $y_j = f(x_j)$. The usual approach to cubic B-spline interpolation requires four knots and values to be referenced, in order to guarantee the proper continuity. *Numerical Recipes* points out there is another method which relies on two knots and values, plus two second derivatives.

\[
y = Ay_j + By_{j+1} + Cy''_j + Dy''_{j+1}, \quad (2.1)
\]

\[
A = \frac{x_{j+1} - x}{x_{j+1} - x_j}, \quad (2.2)
\]

\[
B = \frac{x - x_j}{x_{j+1} - x_j}, \quad (2.3)
\]

\[
C = \frac{1}{6}(A^3 - A)(x_{j+1} - x_j)^2, \quad (2.4)
\]

\[
D = \frac{1}{6}(B^3 - B)(x_{j+1} - x_j)^2, \quad (2.5)
\]

where $x$ is the location we wish to interpolate at, $x_j$ is the $j$th knot, $y''_j$ is the second derivative at $x_j$, $x_{j+1} \geq x \geq x_j$, and $x_{j+1} > x_j$. *Numerical Recipes* do not go into detail on how they derived this equation, but Arne Morten Kvarving fills in some of the details in their lecture notes.\(^{14}\)

Some analysis reveals that a number of the $(x_{j+1} - x_j)$ terms in $C$ and $D$ will cancel out. Manually canceling these values out may reduce the number of operations necessary. *Sympy* can automate much of this work for us.\(^{15}\) We begin with the original equation.

```python
import sympy as sp

def peq(math):
    txt = str(math)
    latex = sp.latex(math)
    display({'
        text/latex': '$$' + latex + '$$','
        text/txt': txt }, raw=True)

knots = sp.symbols('x_{-3} x_{-2} x_{-1} x_j x_{j+1} x_{j+2} x_{j+3}', real=True)
values = sp.symbols('y_{-1} y_j y_{j+1} y_{j+2}', real=True)
second_values = sp.symbols('y''_{-1} y''_{j} y''_{j+1} y''_{j+2}', real=True)
x, y, ypp, A, B, C, D = sp.symbols('x y y'' A B C D', real=True)

def xj(n):
    return knots[n+3]

def yj(n):
    return values[n+1]

def yppj(n):
```
return second_values[n+1]

def compare_math( a, b ):
    temp = sp.simplify( a - b )
    if temp == 0:
        display( {'text/latex': "The two statements are equivalent.",
                 'text/txt': "The two statements are equivalent."},
                 raw=True)
    else:
        peq( temp )

nr_interpolate = sp.Eq( y, A*yj(0) + B*yj(1) + C*yppj(0) + D*yppj(1) )
peq( nr_interpolate )

y = A y_j + B y_{j+1} + C y''_j + D y''_{j+1} \hspace{1cm} (2.6)

Next, we perform the substitutions, being careful of the order of substitution.

complex_y = sp.Eq( y, nr_interpolate.rhs.subs( [(C, (A**3 - A)*( (xj(1) - xj(0))**2 )/6), (D, (B**3 - B)*( (xj(1) - xj(0))**2 )/6), 
                                               (A, (xj(1) - x)/(xj(1) - xj(0))), (B, (x - xj(0))/(xj(1) - xj(0)))] ) )

Finally, we ask Sympy to perform the cancellations.

simpler_y = sp.Eq( y, sp.simplify( complex_y.rhs ) )
peq( simpler_y )

\begin{align*}
y &= \frac{y''_{j+1}((-x+x_j)(x_{j+1}-x)^2+(x-x_j)^3)}{6} - \frac{y''_j((-x+x_{j+1})(x_{j+1}-x_j)^2+(x-x_{j+1})^3)}{6} + y'_{j+1}(x-x_j) - y_j(x-x_{j+1}) \\
&\frac{x_{j+1}-x_j}{x_{j+1}-x_j}
\end{align*}

While this has been improved, there is still more which can be manually done. For instance, the equivalent of the C term has a common factor of \((x_{j+1} - x)\) and the D has \((x - x_j)\). Sympy also tends to reorder variables, resulting in a change of signs. Some manual work results in the following variation.

\begin{align*}
y &= \frac{y_j(x_{j+1} - x) + y_{j+1}(x - x_j) + \frac{1}{6} V}{x_{j+1} - x_j}, \hspace{1cm} (2.7) \\
V &= y'_j(x_{j+1} - x) \left( (x_{j+1} - x)^2 - (x_{j+1} - x_j)^2 \right) + y''_{j+1}(x-x_j) \left( (x-x_j)^2 - (x_{j+1} - x_j)^2 \right) \hspace{1cm} (2.8)
\end{align*}

We can use Sympy to verify the original and variation are equivalent.

variant_y = ( yj(0)*(xj(1) - x) + yj(1)*(x - xj(0)) + \ 
(yppj(0)*(xj(1) - x)*((xj(1)-x)**2 - (xj(1)-xj(0))**2) + \ 
yppj(1)*(x-xj(0))*((x-xj(0))**2 - (xj(1) - xj(0))**2))/6 
\hspace{1cm} \rightarrow ) / ( xj(1) - xj(0) )
The two statements are equivalent.

It does not follow that this variation is an improvement, though. The only proper test is to convert it into computer code, and compare it against the listing in *Numerical Recipies*. For obvious reasons, the latter code cannot be included here.

```python
# Released under a CC0 license by Haysn Hornbeck
def newint(x, a, b, u, v, up, vp):
    assert b > a
    ba = (b - a)
    xa = (x - a)
    inv_ba = 1. / ba
    bx = (b - x)
    ba2 = ba * ba  # 3 adds, 1 mult, 1 div
    lower = xa*v + bx*u
    C = (xa*xa - ba2)*xa*vp
    D = (bx*bx - ba2)*bx*up  # 1 add, 2 subs, 8 mults
    # 2 adds, 2 mult = 19 ops + 1 div
    return (lower + (.16666666666666666666) *( C + D ) ) * inv_ba
```

In theory, we could check this algorithm by substituting SymPy symbols into it, subtracting the simplified version, and cancelling terms. In practice, SymPy was unable to even though a visual inspection supports equivalence. We can still verify the algorithm via substitution, but this requires being able to generate derivatives. We defer on this for now.

If we ignore the initial bisection, the *Numerical Recipies* code consisted of three additions, five subtractions, ten multiplications, and three divisions. One of those divisions was of a constant, though, so in theory a compiler could convert it to a multiply, in which case nineteen basic operations plus two divisions would be done.

The new code consists of six additions, two subtractions, eleven multiplications, and one division, improving on *Numerical Recipes* by a single division. It also attempts to interleave operations so that the result of the next calculation does not require the input of another. This is redundant on desktop CPUs and modern compilers, which reorder operations, but could be useful on GPUs or mobile CPUs with poor compilers.

In practice, users of `newint` will likely translate it into C or C++ to maximize performance. Compiler Explorer is an ideal way to explore how a compiled language would deal with this code. Here is the assembly output of `newint` converted to C++ and compiled with `clang` version 9.0.0, with the `-O2 -msse4.1` optimization flags.

```
.LCPI0_0:
.long 1065353216 # float 1
.LCPI0_1:
.long 1042983595 # float 0.166666672
```

1.-O3 gives identical output.
newint(float, float, float, float, float, float, float, float):
    movaps xmm7, xmm0
    insertps xmm7, xmm2, 16  # xmm7 = xmm7[0],xmm2[0],xmm7[2,3]
    subss  xmm2, xmm1
    movss xmm8, dword ptr [rip + .LCPI0_0]  # xmm8 = mem[0],zero,zero,zero
    divss xmm8, xmm2
    insertps xmm1, xmm0, 16  # xmm1 = xmm1[0],xmm0[0],xmm1[2,3]
    mulss xmm2, xmm2
    insertps xmm4, xmm3, 16  # xmm4 = xmm4[0],xmm3[0],xmm4[2,3]
    mulps xmm4, xmm7
    movshdup xmm1, xmm4  # xmm1 = xmm4[1,1,3,3]
    addss xmm1, xmm4
    movaps xmm0, xmm7
    movshdup xmm0, xmm2  # xmm2 = xmm2[0,0,2,2]
    mulps xmm0, xmm0
    mulps xmm0, xmm7
    insertps xmm6, xmm5, 16  # xmm6 = xmm6[0],xmm5[0],xmm6[2,3]
    mulps xmm6, xmm0
    movshdup xmm0, xmm6  # xmm0 = xmm6[1,1,3,3]
    addss xmm0, xmm6
    mulss xmm0, dword ptr [rip + .LCPI0_1]
    addss xmm0, xmm1
    mulss xmm0, xmm8
    ret

In total there is nine instructions which move data between registers or memory (movaps, insertps, movshdup), three additions (addss), three subtractions (subps, subss), seven multiplications (mulps, mulss), and one division (divss). It is possible to eliminate the need to load LCPI0_0 into a register by removing inv_ba and simply dividing the return by ba, which also eliminates a multiplication, though this moves the division to just before the return statement and may cause execution to stall.

Compiling with gcc version 9.2 gives similar results, this time with seven data moves (movaps, movss), three additions, five subtractions (subps, subss), eleven multiplies (mulss), and one division. gcc will order the division to occur just before ret with these compiler options. Some experimentation reveals that declaring inv_ba to be volatile pins the division in place, at the cost adding two extra memory moves. As the location is likely stored in L1, this could still lead to a net speed-up as is gives the processor maximal flexibility in scheduling the division.

The compiled results of splint_one, Numerical Recipes’ equivalent algorithm, result in one less instruction relative to the above, though gcc’s output contains three divisions. clang is capable of simultaneously dividing two separate numbers by a third, unlike gcc, so it only requires two divisions. As astute readers may have noticed, neither gcc nor clang automatically converted division by a constant into a multiplication. The authors of both compilers are aware of how floating-point precision can change depending on the operation, and because of that refuse to change floating-point operations unless the -ffast-math flag is present. Here we know the precision loss is trivial, so this division can easily be eliminated without needing that flag.
3 Generating Second Derivatives

Numerical Recipes’ interpolation algorithm assumes that each data point’s second derivative is known, something which is rarely true. Their solution is to include spline, a second algorithm that generates those second derivatives by satisfying the following equation for all values of \( j \):

\[
\text{initial_value_prob} = \text{Eq}((xj(0) - xj(-1)) \times yppj(-1) + 2 *(xj(1) - xj(-1)) \times yppj(0) + 6 *((yj(1) - yj(0)) / (xj(1) - xj(0)) - (yj(0) - yj(-1)) / (xj(0) - xj(-1))))
\]

\[\text{peq} (\text{initial_value_prob})\]

\[
y''_{j+1} \left( x_{j+1} - x_j \right) + y''_{j-1} \left( -x_{j-1} + x_j \right) + y''_{j} \left( 2x_{j+1} - 2x_{j-1} \right) = -6 \left( -y_{j-1} + y_j \right) \left( x_{j+1} - x_{j} \right) + 6 \left( y_{j+1} - y_j \right) \left( x_{j+1} - x_{j} \right)
\]

(3.1)

The above equation has three unknowns, \( y''_{j+k} \), \( k \in \{-1, 0, 1\} \). As they point out, those unknowns form a tri-diagonal system. In matrix notation, this is equivalent to

\[
\begin{bmatrix}
 b_1 & c_1 & 0 \\
 a_2 & b_2 & c_2 \\
 a_3 & b_3 & \ddots \\
 \vdots & \ddots & \ddots \\
 0 & a_n & b_n
\end{bmatrix}
\begin{bmatrix}
 y''_1 \\
y''_2 \\
y''_3 \\
 \vdots \\
y''_n
\end{bmatrix}
= \begin{bmatrix}
 d_1 \\
d_2 \\
d_3 \\
 \vdots \\
d_n
\end{bmatrix}
\]

(3.2)

From the above, it is obvious that

\[
a_j = x_j - x_{j-1}
\]

(3.3)

\[
b_j = 2(x_{j+1} - x_{j-1})
\]

(3.4)

\[
c_j = x_{j+1} - x_j
\]

(3.5)

\[
d_j = 6 \left( \frac{y_{j+1} - y_j}{x_{j+1} - x_j} - \frac{y_j - y_{j-1}}{x_j - x_{j-1}} \right)
\]

(3.6)

for \( 2 \leq j < n \). A common approach is to solve this via Thomas’ algorithm, which operates in \( O(n) \) time.\textsuperscript{17}

We must show that the above system is either diagonally dominant or positive definite, however, in order to invoke Thomas’ algorithm. The former is easiest, as it means proving that

\[
|b_j| \geq |a_j| + |c_j|
\]

(3.7)

\[
|2(x_{j+1} - x_{j-1})| \geq |x_j - x_{j-1}| + |x_{j+1} - x_j|
\]

(3.8)

Note that the knots are written in increasing order, such that \( x_{j+1} \geq x_j \). Thus \( |x_{j+1} - x_j| = x_{j+1} - x_j \), and we can simplify Equation 3.8 to
\[ 2(x_{j+1} - x_j) \geq x_j - x_{j-1} + x_{j+1} - x_j \]  
\[ 2(x_{j+1} - x_{j-1}) \geq x_{j+1} - x_{j-1} \]  
\[ 2 \geq 1 \]  

As this is true for \( 2 \leq j < n \), we have established diagonal dominance in that range.

We still need values for \( b_1, c_1, d_1, a_n, b_n, \) and \( d_n \), however. If we try to use Equation 3.1 to satisfy the first two, we find

\[
\begin{align*}
\frac{y''_0}{-x_0 + x_1} &+ \frac{y''_1}{-2x_0 + 2x_2} + \frac{y''_2}{-x_1 + x_2} = \frac{6(-y_1 + y_2)}{-x_1 + x_2} - \frac{6(-y_0 + y_1)}{-x_0 + x_1}
\end{align*}
\]  

which contains numerous undefined values. A common workaround is to state that \( x_j = x_1 \) and \( y_j = y_1 \) for \( j < 1 \), which reduces the continuity at one end point. Careful substitution spares us from both an undefined division and having to define \( y_0'' \).
This allows us to extract the following values.

\[
\begin{align*}
b_1 &= 2(x_2 - x_1) \\
c_1 &= x_2 - x_1 \\
d_1 &= 6\frac{y_2 - y_1}{x_2 - x_1}
\end{align*}
\]

(3.13)

Note that the matrix continues to be diagonally dominant, as \( b_1 > c_1 \).

\( a_n, b_n, \) and \( d_n \) are handled in a similar manner. This time we declare \( x_j = x_n \) and \( y_j = y_n \) for \( j > n \), and again exploit a cancellation.

```python
# set up the offset values we're substituting in
temp_x = ""
temp_y = ""
temp_ypp = ""
for v in range(-1,2):
    base = "n"
    if v > 0:
        base += "-{0}".format(v)
    else:
        base += "{+0}".format(-v)
    temp_x += 'x_{{{{}}}{{{}}}{{{}}}{{{}}}{{{}}}{{{}}}{{}}}'.format(base)
    temp_y += 'y_{{{{}}}{{{}}}{{{}}}{{{}}}{{{}}}{{{}}}{{}}}'.format(base)
    temp_ypp += 'y''_{{{{}}}{{{}}}{{{}}}{{{}}}{{{}}}{{{}}}{{}}}'.format(base)

knots_upper = sp.symbols(temp_x, real=True)
values_upper = sp.symbols(temp_y, real=True)
accels_upper = sp.symbols(temp_ypp, real=True)

def xn(index):
    return knots_upper[1-index]
def yn(index):
    return values_upper[1-index]
def yppn(index):
    return accels_upper[1-index]

# do the actual substitution
upper_prob = initial_value_prob.subs(\n    [(y[n-1], \n    [(x[n-1], x[n-1])] for j in range(0,3)] + \n    \n3 Generating Second Derivatives
```
\[(y_j(1-j), y_n(1-j)) \text{ for } j \in \text{range}(0,3) \] + \[(ypp_j(1-j), yppn(1-j)) \text{ for } j \in \text{range}(0,3) \] 

peq( upper_prob.subs( [(yn(1), yn(0)), (xn(1), xn(0))] ) )

\[y''_{n-1}(-x_{n-1} + x_n) + y''_n(-2x_{n-1} + 2x_n) = -6\frac{(-y_{n-1} + y_n)}{-x_{n-1} + x_n} \quad (3.17)\]

Converting to the variables within the matrix, we find

\[a_n = x_n - x_{n-1} \quad (3.18)\]
\[b_n = 2(x_n - x_{n-1}) \quad (3.19)\]
\[d_n = -6\frac{y_n - y_{n-1}}{x_n - x_{n-1}} \quad (3.20)\]

With all matrix variables filled in, we have confirmed diagonal dominance for the entire system. Thomas’ algorithm can be used to solve it.

### 3.1 Implementation

That algorithm can be summarized as follows.

\[c_1' = \frac{c_1}{b_1} \quad (3.21)\]
\[d_1' = \frac{d_1}{b_1} \quad (3.22)\]
\[c_i' = \frac{c_i}{b_i - a_i c_{i-1}} \quad (3.23)\]
\[d_i' = \frac{d_i - a_i d_{i-1}}{b_i - a_i c_{i-1}} \quad (3.24)\]
\[y''_n = d_n \quad (3.25)\]
\[y''_i = d'_i - c'_i y''_{i+1} \quad (3.26)\]

Note that \(a_{j+1} = c_j\), and \(d_j\) also reuses prior values in part. As we advance \(j\), the only new values we need to fetch from memory are \(x_{j+1}\) and \(y_{j+1}\). Everything else is either equivalent to existing values, or can be calculated from them. While the algorithm suggests two temporary lists, we can reduce that to one by temporarily storing \(d'_j\) in \(y''_j\).

Some of these values can be simplified, based on the above calculations.

\[c_1' = \frac{c_1}{b_1} = \frac{1}{2} \quad (3.27)\]
\[d_1' = \frac{d_1}{b_1} = 3\frac{y_2 - y_1}{(x_2 - x_1)^2} \quad (3.28)\]
We have enough information to begin writing an implementation in Python code.

```python
# Released under a CC0 license by Haysn Hornbeck
def new_second_derivative_simple( knots, values):

    assert len(knots) == len(values)
    assert len(knots) > 2

    n = len(knots)
    c_p = [0] * n
    ypp = [0] * n

    # recycle these values in later routines
    new_x = knots[1]
    new_y = values[1]
    cj = knots[1] - knots[0]
    new_dj = (values[1] - values[0]) / cj

    # initialize the forward substitution
    c_p[0] = 0.5
    ypp[0] = 3 * new_dj / cj

    # forward substitution portion
    j = 1
    while j < (n-1):

        # shuffle new values to old
        old_x = new_x
        old_y = new_y

        aj = cj
        old_dj = new_dj

        # generate new quantities
        new_x = knots[j+1]
        new_y = values[j+1]

        cj = new_x - old_x
        new_dj = (new_y - old_y) / cj
        bj = 2*(cj + aj)
        inv_denom = 1. / (bj - aj*c_p[j-1])
        dj = 6*(new_dj - old_dj)

        ypp[j] = (dj - aj*ypp[j-1]) * inv_denom
        c_p[j] = cj * inv_denom

        j += 1

    # manually do the last round, as it saves some comparisons
    old_x = new_x
    old_y = new_y
```

3 Generating Second Derivatives
aj = cj
old_dj = new_dj

cj = 0  # this has the same effect as skipping c_n and altering d_n
new_dj = 0
bj = 2*(cj + aj)
inv_denom = 1. / (bj - aj*c_p[j-1])
dj = 6*(new_dj - old_dj)
ypp[j] = (dj - aj*ypp[j-1]) * inv_denom
c_p[j] = cj * inv_denom

# as we're storing d_j in y''_j, y''_n = d_n is a no-op

# backward substitution portion
while j > 0:
    j -= 1
    ypp[j] = ypp[j] - c_p[j]*ypp[j+1]

return ypp

This is very memory-efficient, at the cost of requiring a non-trivial number of registers. For RISC or 64-bit architectures, this usually isn’t a problem. GPU architectures may benefit from a rewrite that uses fewer variables and more memory fetches, as registers are at a premium while their wide memory bandwidth encourages cache use. Alternatively, the literature on fast GPU tridiagonal solvers may yield a faster algorithm.\(^\text{18}\)

While not feature-complete yet, this code is sufficiently developed to benchmark. We have translated \texttt{spline} into Python for this purpose.

```python
import numpy as np
import timeit
test_knots = np.linspace(0, np.pi*2, 256)
test_values = np.random.rand(256)

bench = timeit.Timer(lambda: spline(test_knots, test_values, 1e31, 1e31))
count, time = bench.autorange()
count *= 20  # inflate the runtime from about 0.2s to about 4s

result_nr = bench.timeit(number=count)

print("Time to generate second derivatives via NR's code: \{:.3f\}s ({} trials)\).format(result_nr, count))

bench = timeit.Timer(lambda: new_second_derivative_simple(test_knots, test_values))
result_sk = bench.timeit(number=count)
```

3 Generating Second Derivatives
print("Time to generate second derivatives via the sketch:	 {:.3f}s ({} trials)").format( result_sk , count ))

print(" Speedup: approx {:.2f}x".format( result_nr / result_sk ) )

Time to generate second derivatives via NR's code: 4.899s (4000 trials)
Time to generate second derivatives via the sketch: 2.809s (4000 trials)
Speedup: approx 1.74x

The new algorithm is faster by a non-trivial amount. It's possible that switching to a compiled language could narrow the difference, by reducing memory fetches and optimizing the underlying code. Since generating second derivatives is unlikely to be a performance bottleneck in practice, this line of investigation is not worth pursuing.

### 3.2 Start and End Derivatives

`new_second_derivative` is not a drop-in replacement for `Numerical Recipes`' spline, unfortunately. The latter also provides a way to alter the slope at the start of the curve, the end, or both places.

Earlier we declared that $x_j = x_1$ and $y_j = y_1$ for $j < 1$, in order to cancel out a term in the matrix representation of this problem. Another approach is to declare $y''_j = 0$ for $j < 1$.

```
lower_prob_sub = lower_prob . subs( yppv(0) ,0 )
peq( lower_prob_sub )
```

\[
y''_1 (-2x_0 + 2x_2) + y''_2 (-x_1 + x_2) = \frac{6(-y_1 + y_2)}{-x_1 + x_2} - \frac{6(-y_0 + y_1)}{-x_0 + x_1}
\]

(3.29)

While this may not seem like progress, observe that $\frac{y_1 - y_0}{x_1 - x_0}$ is a good approximation of the slope between two knots on the curve. The code in `Numerical Recipes` in fact simply replaces that term with the desired starting derivative, which we will denote as $y'_1$, and asserts $x_0 = x_1$. It is worth re-deriving this result, if only to check it results in the correct derivative.

We begin with evaluating Equation 2.1 at $j = 0$, taking its derivative at $x = x_1$, and asserting $y''_j = 0$ for $j < 1$.

```
yp1 = sp.Symbol("y'_1", real=True )
variant_y_first = variant_y . subs( \n    [(xj(j), xv(j)) for j in range (0,2) ] + \n    [(yj(j), yv(j)) for j in range (0,2) ] + \n    [(yppj (j), yppv (j)) for j in range (0,2) ] \n    )

var_y_first_deriv = sp.Eq( yp1, sp.simplify( sp.diff( variant_y_first, \n    x )).subs( [(ypvv(0), 0),(x,xv(1))] ) ) )
```

### Generating Second Derivatives
Unfortunately, this is an equation with three unknowns. If we assume that \( x_2 > x_1 \), however, we can assert that \( x_0 = x_1 - (x_2 - x_1) = 2x_1 - x_2 \). This will allow us to solve for \( y_0 \).

\[
\text{var}_y\text{first}_\text{subs} = \text{var}_y\text{first}_\text{deriv}.\text{subs}(\text{xv}(0), 2*\text{xv}(1) - \text{xv}(2))
\]
\[
\text{var}_y\text{first}_\text{sol} = \text{sp.solve}(\text{var}_y\text{first}_\text{subs}, \text{yv}(0))[0].\text{collect}(\text{yp1})
\]
\[
\text{sp.Eq}(\text{yv}(0), \text{var}_y\text{first}_\text{sol})
\]

\[
y_0 = \frac{y''_2(x_1 - x_2)^2}{3} + y'_1(x_1 - x_2) + y_1
\] (3.31)

We can now substitute Equation 3.31 into Equation 3.29, along with our other assertions.

\[
\text{lower}_\text{prob}_\text{int} = \text{sp.simplify}(\text{lower}_\text{prob}_\text{sub}.\text{subs}([\text{(xv}(0), 2*\text{xv}(1) - \leftrightarrow \text{xv}(2)), (\text{yv}(0), \text{var}_y\text{first}_\text{sol}]])
\]
\[
\text{lower}_\text{prob}_\text{tidy} = \text{sp.Eq}(\text{yppv}(1), \text{sp.solve}(\text{lower}_\text{prob}_\text{int}, \text{yppv}(1))\rightarrow [0].\text{collect}(\text{yp1}))
\]
\[
\text{peq}(\text{lower}_\text{prob}_\text{tidy})
\]

\[
y'_1 = \frac{-y''_2(x_1 - x_2)^2 + y'_1(6x_1 - 6x_2) - 6y_1 + 6y_2}{2(x_1 - x_2)^2}
\] (3.32)

Sympy has difficulty rearranging this equation to match Equation 3.1, but the task is trivial for a human.

\[
\text{lower}_\text{prob}_\text{sol} = \text{sp.Eq}(2*\text{yppv}(1)*xv(2) - xv(1)) + \text{yppv}(2)*(xv(2) - xv(1)), \text{6*((yv}(2) - yv(1))/(xv(2) - xv(1)) - yp1))
\]
\[
\text{peq}(\text{lower}_\text{prob}_\text{sol})
\]
\[
\text{compare}\_\text{math}(\text{sp.solve}(\text{lower}_\text{prob}_\text{sol}, \text{yppv}(1))[0], \text{lower}_\text{prob}_\text{tidy}.)
\]
\[
2y''_1(-x_1 + x_2) + y''_2(-x_1 + x_2) = -6y'_1 + \frac{6(-y_1 + y_2)}{-x_1 + x_2}
\] (3.33)

The two statements are equivalent.

Converting this to matrix form, we find
\[ c'_1 = \frac{c_1}{b_1} = \frac{x_2 - x_1}{2(x_2 - x_1)} = \frac{1}{2} \]  
\[ d'_1 = \frac{d_1}{b_1} = \frac{6\left(\frac{y_2 - y_1}{x_2 - x_1} - y'_1\right)}{2(x_2 - x_1)} = \frac{3}{x_2 - x_1}\left(\frac{y_2 - y_1}{x_2 - x_1} - y'_1\right) \]  

which matches *Numerical Recipes* exactly. Similar logic applies to the solution at the other end, this time we assert \( y''_j = 0 \) for \( j > n \) and \( x_{n+1} = x_n + (x_n - x_{n-1}) = 2x_n - x_{n-1} \).

\[
y'_{n+1} = 6\left(y_2 - y_{n-1}\right) + 6\left(y_2 - y_{n-1}\right) - 6(y_{n+1} - y_{n-1}) \]  
\[ = 3x_2 - x_1 \left(y_2 - y_{n-1}\right) \]  

(3.36)
\[ y''_{n-1}(-x_{n-1} + x_n) + 2y''_{n}(-x_{n-1} + x_n) = 6y'_n - \frac{6(-y_{n-1} + y_n)}{-x_{n-1} + x_n} \] (3.37)

The two statements are equivalent.

When converted to matrix form, we again find agreement with *Numerical Recipes*, though it should be noted their code takes a different approach to the end of the matrix than ours.

\[
\begin{align*}
a_n &= 2(x_n - x_{n-1}) \\
b_n &= x_n - x_{n-1} \\
d_n &= 6\left(y'_n - \frac{y_n - y_{n-1}}{x_n - x_{n-1}}\right)
\end{align*}
\] (3.38)  
(3.39)  
(3.40)

We are now capable of providing a feature-complete drop-in replacement for *spline*.

```python
# Released under a CC0 license by Haysn Hornbeck
def new_second_derivative(knots, values, start_deriv, end_deriv):
    assert len(knots) == len(values)
    assert len(knots) > 2
    for i, _ in enumerate(knots):
        assert (i == 0) or (knots[i] > knots[i-1])

    n = len(knots)
c_p = [0] * n
ypp = [0] * n

    # recycle these values in later routines
    new_x = knots[1]
    new_y = values[1]
cj = knots[1] - knots[0]
new_dj = (values[1] - values[0]) / cj

    # initialize the forward substitution
    if start_deriv > .99e30:
        c_p[0] = 0
        ypp[0] = 0
    else:
        c_p[0] = 0.5
        ypp[0] = 3 * (new_dj - start_deriv) / cj

    # forward substitution portion
    j = 1
    while j < (n-1):
        # shuffle new values to old
```

3 Generating Second Derivatives
old_x = new_x
old_y = new_y

aj = cj
old_dj = new_dj

# generate new quantities
new_x = knots[j+1]
new_y = values[j+1]

cj = new_x - old_x
new_dj = (new_y - old_y) / cj
bj = 2*(cj + aj)
inv_denom = 1. / (bj - aj*c_p[j-1])
dj = 6*(new_dj - old_dj)

ypp[j] = (dj - aj*ypp[j-1]) * inv_denom

# as we're storing d_j in y''_j, y''_n = d_n is a no-op
# backward substitution portion
while j > 0:
    j -= 1
    ypp[j] = ypp[j] - c_p[j]*ypp[j+1]

return ypp
As the inner loop of this code is no different from `new_second_derivative_simple`, it will offer similar performance.
4 Quality Checks

Since our goal is to create a drop-in replacement, we must be assured the new code generates the same results as the old. One approach is to hand-generate a set of control points and observe what happens when both routines are applied to it. The curve we will use is designed to have a mix of close and distant knots, sharp edges and smooth transitions. Figure 4.1 plots its control points.

test_knots = [0, 0.5, 1, 1.01, 1.25, 1.5, 1.58, 1.79, 2.12, 2.30, 2.402, 2.451, 2.5]
test_values = [1, 1.2, 2, 0.25, 0.25, 0.25, 0.63, 0.96, 1.17, 1.23, 1.245, 1.249, 1.25]

%matplotlib inline
import matplotlib.pyplot as plt
plt.figure(num=None, figsize=(8, 4), dpi=600, facecolor='w', edgecolor='k')

plt.plot(test_knots, test_values, 'xk')
plt.xlabel("X")
plt.ylabel("Y")
plt.xticks([0, 1, 1.5, 2.5])
plt.yticks([0, 0.25, 1, 2])
plt.show()

Figure 4.1: The hand-generated control points.

The simplest quantitative comparison is to calculate the second derivatives with both `spline` and `new_second_derivative`, and create a table of the different values calculated by each routine. There are three important cases to test: “natural” cubic b-splines that have $y''_1 = y''_n = 0$, cubic b-splines with $y'_1 = y'_n = 0$, and cubic b-splines with non-trivial derivatives. For the latter case, we will use $y'_1 = -1$ to exaggerate the curvature at the beginning of the curve and $y'_n = 1$ to skew what would otherwise be a nearly flat portion of the curve.
We begin by comparing what each routine generates when asked for a “natural” cubic b-spline.

```python
import pandas as pd
test_secdir_old = spline(test_knots, test_values, 1e32, 1e32)
test_secdir_new = new_second_derivative(test_knots, test_values, 1e32)

table = pd.DataFrame({'$x$': test_knots, '$y$': test_values, 'NR': test_secdir_old, 'our': test_secdir_new, '$\Delta$': [a-b for a,b in zip(test_secdir_old, test_secdir_new)]})

Table 4.1: A comparison of the two routines for a “natural” cubic b-spline. The calculations were done with double-precision floating-point numbers. Deltas are calculated by subtracting the old implementation from the new.

|   |   |   |   |   |
|---|---|---|---|---|
| 0.000 | 1.000 | 0.000000 | 0.000000 | 0.000000e+00 |
| 0.500 | 1.200 | 306.924794 | 306.924794 | 5.684342e-14 |
| 1.000 | 2.000 | -1213.299177 | -1213.299177 | -2.273737e-13 |
| 1.010 | 0.250 | 2450.276370 | 2450.276370 | -4.547474e-13 |
| 1.250 | 0.250 | -679.188305 | -679.188305 | 3.410605e-13 |
| 1.500 | 0.250 | 310.152841 | 310.152841 | -1.136868e-13 |
| 1.580 | 0.630 | -80.047486 | -80.047486 | 1.421085e-14 |
| 1.790 | 0.960 | 12.113742 | 12.113742 | -3.552714e-15 |
| 2.120 | 1.170 | -5.706845 | -5.706845 | 0.000000e+00 |
| 2.300 | 1.230 | 0.029250 | 0.029250 | -2.220446e-16 |
| 2.402 | 1.245 | -1.048158 | -1.048158 | 2.220446e-16 |
| 2.451 | 1.249 | -1.612180 | -1.612180 | -2.220446e-16 |
| 2.500 | 1.250 | 0.000000 | 0.000000 | 0.000000e+00 |
```

Table 4.1 demonstrates close agreement between *Numerical Recipes* routine and ours, with the differences at the precision limit for double-precision floating-point numbers. Which routine is the closest to the true value, however, if we could calculate values with infinite precision? We can approximate an answer with the arbitrary precision math routine *mpmath*. The Python versions of both *Numerical Recipes*’ code and ours work transparently with this library, so the only code changes involve generating the input arrays and adding the proper comparisons.

```python
from mpmath import mp
test_knots_hp = [mp.mpf('0'), mp.mpf('0.5'), mp.mpf('1'), mp.mpf('1.01'), mp.mpf('1.25'), mp.mpf('1.5'), mp.mpf('1.58'), mp.mpf('1.79'), mp.mpf('2.12'), mp.mpf('2.30'), mp.mpf('2.402'), mp.mpf('2.451'), mp.mpf('2.5')]
test_values_hp = [mp.mpf('0'), mp.mpf('1'), mp.mpf('1.2'), mp.mpf('2'), mp.mpf('2.25'), mp.mpf('0.25'), mp.mpf('0.63'), mp.mpf('0.96'), mp.mpf('1.17')]
```

4 Quality Checks
precis = dict()
for precision in range(10, 150, 20):
    with mp.workdps(precision):
        precis[precision] = mp.nstr(mp.max([(a-b) for a,b in zip(
            np.max([[(a-b) for a,b in zip(
                spline(test_knots_hp, test_values_hp,
                new_second_derivative(test_knots_hp, test_values_hp,
                test_values_hp, 1e32, 1e32))],
            test_values_hp, 1e32, 1e32))]), 5))

table = pd.DataFrame(precis, index=['maximal disagreement:'])
table.columns.name = 'decimal precision:'
display({'text/latex': table.to_latex(index=True), 'text/html': table.to_html(index=True)}, raw=True)

Table 4.2: The maximal divergence between NR code and ours, for varying degrees of precision.

| decimal precision: | 10   | 30   | 50   | 70   | 90   | 110  | 130  |
|--------------------|------|------|------|------|------|------|------|
| maximal disagreement: | 7.4506e-9 | 2.0195e-28 | 1.3685e-48 | 9.273e-69 | 2.5135e-88 | 3.4064e-108 | 2.3082e-128 |

Table 4.2 suggests that the precision of both Numerical Recipes code and ours are dependent only on the precision of the underlying floating-point storage. This means that we can approximate the true output of either routine by using mpmath with a precision sufficiently smaller than IEEE binary64’s typical precision of 15-17 decimal places. We have arbitrarily chosen to use spline and a precision of 30 decimal places to calculate the “true” value.

mp.dps = 30

test_secdir_true = spline(test_knots_hp, test_values_hp, 1e32, 1e32)

table = pd.DataFrame({'$x$':test_knots, '$y$':test_values, 'NR $\Delta$, "true"':
    [mp.nstr(a-b,5) for a,b in zip(test_secdir_old, test_secdir_true)],
    'our $\Delta$, "true"':
    [mp.nstr(a-b,5) for a,b in zip(test_secdir_new, test_secdir_true)])

display({'text/latex':table.to_latex(index=False), 'text/html':table.to_html(index=False)}, raw=True)
Table 4.3: A comparison of the two routines for a “natural” cubic b-spline. The calculations were done with double-precision floating-point numbers, this time comparing each to the “true” value.

| $x$  | $y$  | NR $\Delta$ | "true" | our $\Delta$ | "true" |
|------|------|--------------|--------|--------------|--------|
| 0.000| 1.000| 0.0          | 0.0    |              |        |
| 0.500| 1.200| 4.5507e-14   | -1.1336e-14 | 1.3416e-13  |
| 1.000| 2.000| -9.3212e-14  | 1.3416e-13  | -2.6939e-13 |
| 1.010| 0.250| 2.2244e-13   | 6.7179e-13  |              |
| 1.250| 0.250| 7.1667e-14   | -2.6939e-13 | 9.8311e-14  |
| 1.500| 0.250| -1.4856e-14  | 9.8311e-14  |              |
| 1.580| 0.630| -5.6305e-15  | -1.9841e-14 |              |
| 1.790| 0.960| 1.985e-15    | 5.5377e-15  |              |
| 2.120| 1.170| -8.3121e-16  | -8.3121e-16 |              |
| 2.300| 1.230| 5.7138e-16   | 7.9343e-16  |              |
| 2.402| 1.245| -3.2598e-16  | -5.4802e-16 |              |
| 2.451| 1.249| -8.7028e-17  | 1.3502e-16  |              |
| 2.500| 1.250| 0.0          | 0.0      |              |        |

Table 4.3 shows both the old and new routines are remarkably close to the true value. We can quantify their overall difference by calculating the mean square error.

```python
import numpy as np

test_secdir_old = spline( test_knots , test_values , 0 , 0 )
test_secdir_new = new_second_derivative( test_knots , test_values , 0 , 0 )
test_secdir_true = spline( test_knots_hp , test_values_hp , 0 , 0 )

table = pd.DataFrame( {'$x$':test_knots , '$y$':test_values , 'NR $\Delta$': test_secdir_old - test_secdir_true , 'our $\Delta$': test_secdir_new - test_secdir_true })

display( { "text/latex":table.to_latex(index=False), "text/html":table.to_html(index=False)}, raw=True )
```

Table 4.4: The mean square error of each set of routines from the “true” value, for a “natural” cubic B-spline.

| MSE, NR   | MSE, our   |
|-----------|------------|
| 5.04867e-27 | 4.30368e-26 |

According to Table 4.4, Numerical Recipes’ routine is closer to the “true” value than ours. It is worth noting that this difference appears chaotic. This paper was created using an interactive Jupyter notebook, and the minor differences between the interactive environment and the non-interactive one used to execute the final paper were enough to cause our routine to appear more accurate in the latter. This is consistent with both routines being unbiased in the limit, while for finite precision both have a bounded yet chaotic imprecision.

Next, we will compare the two routines when the initial and final slope is a horizontal line.

```python

test_secdir_old = spline( test_knots , test_values , 0 , 0 )
test_secdir_new = new_second_derivative( test_knots , test_values , 0 , 0 )
test_secdir_true = spline( test_knots_hp , test_values_hp , 0 , 0 )

table = pd.DataFrame( {'$x$':test_knots , '$y$':test_values , 'NR $\Delta$': test_secdir_old - test_secdir_true , 'our $\Delta$': test_secdir_new - test_secdir_true })

display( { "text/latex":table.to_latex(index=False), "text/html":table.to_html(index=False)}, raw=True )
```
Table 4.5: A comparison of the two routines for a cubic b-spline with $y'_1 = y'_n = 0$.

| $x$  | $y$  | NR $\Delta$, "true" | our $\Delta$, "true" |
|------|------|----------------------|----------------------|
| 0.000| 1.000| 1.7473e-14           | 1.7473e-14           |
| 0.500| 1.200| -2.2512e-14          | -2.2512e-14          |
| 1.000| 2.000| 4.7705e-14           | 4.7705e-14           |
| 1.010| 0.250| 6.9425e-15           | 6.9425e-15           |
| 1.250| 0.250| -8.3012e-14          | 3.0675e-14           |
| 1.500| 0.250| 7.3029e-14           | 1.6186e-14           |
| 1.580| 0.630| -5.6357e-15          | 5.6357e-15           |
| 1.790| 0.960| 2.5403e-15           | 2.5403e-15           |
| 2.120| 1.170| -9.4845e-16          | 6.027e-17            |
| 2.300| 1.230| 3.9991e-16           | 1.2336e-16           |
| 2.402| 1.245| -1.8866e-16          | 1.8866e-16           |
| 2.451| 1.249| -1.9206e-16          | 2.9989e-17           |
| 2.500| 1.250| 6.0745e-17           | -1.613e-16           |

Table 4.6: The mean square error of each set of routines from the “true” value.

| MSE, NR | MSE, our |
|---------|----------|
| 1.18459e-27 | 3.36714e-28 |

As Table 4.5 demonstrates, these routines again agree to floating-point precision. Table 4.6 shows that our routine is closer the “true” value than Numerical Recipes. The Jupyter notebook version again says the opposite.

Finally, we change the start and end derivatives to be non-trivial, $y'_1 = -1$ and $y'_n = 1$.

test_secdir_old = spline( test_knots, test_values, -1, 1 )
test_secdir_new = new_second_derivative( test_knots, test_values, -1, 1 )
test_secdir_true = spline( test_knots_hp, test_values_hp, -1, 1 )
Table 4.7: A comparison of the two routines for a cubic b-spline with 
\( y'_1 = -1 \) and \( y'_n = 1 \). The calculations were done with double-precision floating-point numbers. Deltas are calculated by subtracting the old implementation from the new.

| \( x \)  | \( y \)  | NR \( \Delta \), "true" | our \( \Delta \), "true" |
|---------|---------|-------------------------|-----------------------|
| 0.000   | 1.000   | 1.4693e-14              | 4.3115e-14            |
| 0.500   | 1.200   | -1.6952e-14             | -7.3795e-14           |
| 1.000   | 2.000   | -2.8599e-14             | 1.9877e-13            |
| 1.010   | 0.250   | -4.4446e-13             | -4.4446e-13           |
| 1.250   | 0.250   | 1.3114e-13              | 2.4483e-13            |
| 1.500   | 0.250   | -5.115e-14              | -5.115e-14            |
| 1.580   | 0.630   | -5.6418e-15             | -5.6418e-15           |
| 1.790   | 0.960   | -1.7248e-15             | 1.8279e-15            |
| 2.120   | 1.170   | 1.6451e-15              | -1.0194e-15           |
| 2.300   | 1.230   | -2.9414e-15             | 3.7199e-16            |
| 2.402   | 1.245   | -2.4384e-16             | -6.8792e-16           |
| 2.451   | 1.249   | 1.8995e-15              | 1.8995e-15            |
| 2.500   | 1.250   | 1.7419e-15              | 1.7419e-15            |

Table 4.8: The mean square error of each set of routines from the “true” value.

| MSE, NR | MSE, our |
|---------|----------|
| 1.68251e-26 | 2.36125e-26 |

As expected, Table 4.7 shows no significant differences between the two routines. Table 4.8 shows that the Numerical Recipes code is closer to the true value, and the interactive version agrees with this.

We will use this last set of second derivatives to perform a qualitative check on an interpolated curve, relying on both Numerical Recipes’ splint_one and our newint.

4 Quality Checks
```python
x_values = np.linspace(min(test_knots), max(test_knots), 2048)
y_values_old = list()
y_values_new = list()
y_values_true = list()

i = 0
for x in x_values:
    # find the proper lower index
    while (i+1 < len(test_knots)) and (test_knots[i+1] < x):
        i += 1
    y_values_old.append( splint_one( x, test_knots[i], test_knots[i+1],
    test_values[i], test_values[i+1],
    test_secdir_old[i], test_secdir_old[i+1] ) )

    y_values_new.append( newint( x, test_knots[i], test_knots[i+1],
    test_values[i], test_values[i+1],
    test_secdir_new[i], test_secdir_new[i+1] ) )

    y_values_true.append( splint_one( x, test_knots_hp[i],
    test_knots_hp[i+1],
    test_values_hp[i], test_values_hp[i+1],
    test_secdir_true[i], test_secdir_true[i+1] ) )
```

As Figure 4.2 shows, both sets of algorithms are in broad agreement. The resolution is very coarse, however, and does not answer which is closer to the “true” value.

```python
plt.figure(num=None, figsize=(8, 4), dpi=600, facecolor='w', edgecolor='k')
plt.plot( test_knots, test_values, 'xk' )
plt.plot( x_values, y_values_old, '-', color='#0000FF7F' )
plt.plot( x_values, y_values_new, '-', color='#FF00007F' )
plt.legend( ["control points","old algorithms","new algorithms"] )
plt.xlabel("X")
plt.ylabel("Y")
plt.ylim([-10,20])
plt.show()
```
Figure 4.2: A qualitative check of the old and new B-spline routines.

Table 4.9: The mean square error of each set of routines from the “true” value.

| MSE, NR        | MSE, our     |
|----------------|--------------|
| 9.03518e-31    | 1.5724e-30   |

Overall, both Figure 4.3 and Table 4.9 show that our code has less precision than the code of Numerical Recipes. The interactive Jupyter notebook agrees with this, though its Figure 4.3 looks quite different.
Figure 4.3: Comparing the divergence between the routines and the “true” value. Here we subtract the “true” value from the double-precision one.

It should be stressed that this imprecision is very small, on the order of the precision expected for IEEE binary64 floating point numbers. This level of imprecision can usually be safely ignored. It is also notable that the mean square error has dropped as more points have been introduced. This is further evidence neither algorithm has a systematic bias from the true value.
Figure 4.4: Figure 4.3, as seen in the Jupyter notebook used to construct this paper.
5 Benchmarks

nanoBench benchmarks a short fragment of programming code by repeatedly executing it multiple times in batches, while monitoring a number of internal CPU counters. The default measure used to summarize all batches is a trimmed mean that excludes the top and bottom 20% of samples, though users can select a median and minimum instead. Both the trimmed mean and median assume execution times are described by a Gaussian distribution. In theory, this cannot be the case, as the Gaussian distribution has range $[-\infty, \infty]$ and thus allows for negative times.

A more realistic model states that execution can be delayed via rare events which occur with a fixed probability on any given clock tick. This implies execution should follow a Poisson distribution, rather than a Gaussian. For short code fragments where delays are unlikely this Poisson distribution could resemble an Exponential distribution, while for very long code fragments the Poisson may resemble a Gaussian distribution more. The Poisson distribution can take a wide variety of shapes, and no one metric of central tendency can hope to represent all of them. This would be be less of a concern if nanoBench displayed all three of the trimmed mean, median, and minimum, however users can only select one of the three. Multiple measures require multiple executions, or manual calculation based on the raw times displayed in “verbose” mode.

nanoBench also lacks a good measure of variance, which can provide vital information. Even $O(1)$ code can have variable execution time when given certain inputs. For instance, the authors have observed one branchless series of floating-point operations that took four times longer to execute when it was fed not-a-number or infinite values. We have also seen that a code fragment which incorporated division had more variance in execution times than one which did not. It is entirely plausible for one code fragment to be 25% faster on average than a second that accomplishes the same task, yet the execution times of the former exhibit so much variance that it only has a 51% chance of finishing before the latter. Knowledge of execution variance is especially critical in real-time execution where code must finish before a specific deadline.

Finally, nanoBench only tests a fixed number of repeats. Testing a code fragment with $O(n)$ behaviour requires manually running it multiple times for various $n$. This makes it difficult to check that an algorithm does indeed have $O(n)$ behaviour. Caches in particular are notorious for exhibiting non-linear behaviour that could bias performance measurements. By accident or design, a researcher could select values of $n$ which avoid non-linear cache behaviour for their algorithm while triggering it in others’ algorithms, distorting their performance metrics.

We do not single out nanoBench because it is unusually flawed. On the contrary, it has a better methodology than nearly all benchmarking programs we have encountered. It shares a critical flaw of nearly all benchmark methodologies within Computer Science: none of them present enough information to assess their own fitness. This is especially problematic for algorithms with run-times in the nanosecond range, where even subtle sources of noise have a strong influence.

The ideal benchmarking methodology would instead attempt to execute the algorithm over as much of the parameter space as possible, using a process that minimizes systematic bias. Rather than assume a model, it would either infer or assess a model against the raw data.

5.1 Curve Interpolation

The curve interpolation routines, splint_one and newint, are typically used on lists of control points. The most common use is interpolation at fixed, regular distances along the curve for display. As both algorithms are $O(1)$, the typical approach to benchmarking would generate a list of control points of a fixed size and evaluate both routines. The runtime per evaluation is gathered by clocking the time taken to process the entire list, then dividing by the length of that list.
There is a hidden variable, however, the length of that list. If it is fairly short, it may fit entirely within the L1 cache. If it is large, it may spill into the L2 or L3 caches, if present, or main memory. All of those memory pools have different access times, which in the case of a fast algorithm may be enough to modify its expected runtime. Thus we should treat both algorithms as if they were $O(n)$ and use the resulting dataset to either verify $O(1)$ behaviour despite the caches or extract their effect on performance.

While Python is an excellent prototyping language, users of newint are likely to translate it into C or C++. We have thus written our benchmarking program in C++. For the Intel i7-7700k, gcc 9.2.1 was used to compile the program. The optimization flags -O3 -march=native were used to maximize performance, as it consistently generated faster code than -O2.

Each algorithm also comes in at least two variants. The original splint_one relied on division by a constant, which as mentioned earlier was not converted to a multiplication by the compiler. Thus we tested both a splint_one__div, which retained the original division, as well as a splint_one__mul which converted the division to multiplication by a constant. As for our algorithms, newint__orig corresponds exactly to newint. We also tested a newint__noinv variant that eliminated the inv_ba variable in favour of division by ba. Finally, the volatile trick was tested via a newint__vol variant.

For all variations of splint_one and newint, we applied the following methodology.

1. We executed all algorithms on curves with everywhere between four and 1,048,576 control points.
2. The number of control points to use for any given run was contained in a list, which was generated by interpolation of $0 \leq r \leq 1$ according to \( r(\sqrt{1,048,576} - \sqrt{4}) + \sqrt{4} \)\(^2\).
3. That list was generated by linearly interpolating \( r \) at a fixed number of points with constant spacing, totaling 524,288 points in most cases. Duplicates were not removed.
4. This list was shuffled into a random order.
5. Entries were drawn from that list to generate random control points of the form \( y_i = \epsilon \) and \( x_i = x_{i-1} + \epsilon \), where \( \epsilon \leftarrow U(0, 1) \). If \( \epsilon = 0 \), however, then \( x_i = x_{i-1} + 0.0001 \). This ensures \( x_i > x_{i-1} \).
6. Second-order derivatives were generated for the control points using new_second_derivative.
7. A second list was generated with each draw, consisting of the order to execute the variants. This list was shuffled into a random order as well.
8. For each algorithm, a for loop generated uniformly-spaced points between \( x_1 \) and \( x_n \) and interpolated the curve, taking advantage of the strictly increasing knots to simplify bracketing. One loop will not execute any of the algorithms but still calculate uniformly-spaced points and proper bracketing.
9. Execution was timed via C++’s high_resolution_clock.
10. These benchmarks were executed in a single thread.

IEEE binary64 floating-point numbers were used. Large values of \( n \) cause catastrophic precision loss for binary32 floating-point numbers.

The given formula was used instead of linear interpolation to create a bias towards shorter list lengths, where those aforementioned secondary factors would inject the most noise. As an intended side-effect, our benchmarking code sampled some curve counts multiple times. For instance, curves with four control points could be tested 1,376 times. This over-sampling helps establish the statistical distribution of the noisest execution regime.

The list of control point counts was randomized to ensure the computer was not allowed to “warm up” to any given choice of control points. As an intended side effect, should another process become active on the same core it will show up as random noise in the data, provided the task is only active for a short amount of time. If it is active for a substantial time, a “shadow” of the true execution will show up in the data. To ensure no algorithm had an advantage via cache warming, the second list was introduced to randomly choose which algorithm to execute first. The loop that does not run any algorithms will help estimate the overhead of scanning over the control points and generating uniformly-spaced points.
glibc aliases high_resolution_clock to system_clock, which on Linux provides approximately nanosecond precision. While that clock does change as the system time is updated, such updates occur with negligible chance and would be drowned out by the amount of data collected. The use of a single thread is to minimize the effects of hyperthreading and other processes executing on the computer. Unless stated otherwise, these tests were executed on an idle Intel i7-7700K processor, and the four cores it possesses should minimize the effects of another process becoming active on the same core.

As the benchmark is a C++ program that executes for hours, only the output will be included here. The code is available online, though Numerical Recipes’ code has been stripped out to remain in compliance with its license.

```python
interp_bench = pd.read_csv("data/interp_range.i7-7700k.tsv", sep="\t")

temp = interp_bench.copy()
temp.columns = [c.replace('_', '\_') for c in interp_bench.columns]
temp.tail()
```

Table 5.1: The last few entries in the benchmark results. See the text for a full explanation.

| n  | noop | splint_one__div | splint_one__mul | newint__orig | newint__noinv | newint__vol | order |
|----|------|----------------|----------------|--------------|--------------|------------|-------|
| 524283 | 474729 | 2629686 | 2918642 | 2938789 | 2940122 | 2884746 | 2860716 | 80480 |
| 524284 | 474729 | 2629686 | 2918642 | 2938789 | 2940122 | 2884746 | 2860716 | 80480 |
| 524285 | 105076 | 557215 | 630008 | 636847 | 632320 | 608602 | 619475 | 9003  |
| 524286 | 30750  | 174446 | 185269 | 186036 | 185787 | 178701 | 181247 | 115221 |
| 524287 | 687429 | 3840017 | 4227429 | 4305190 | 4267566 | 4138725 | 4158264 | 132329 |

All timing entries are in nanoseconds. n is the number of control points in the curve, and order encodes the order of execution of each algorithm. For the latter, the least three significant bits specify the first algorithm run, the next three the second, and so on. noop is the loop through the control points that calls none of the above algorithms.

We can begin the benchmark analysis by graphing the timings for one of the algorithms. One concern is whether or not the order of execution matters.

```python
# free up some memory
del temp

# the full dataset is too much clutter, instead pick a random subset
subset = interp_bench.sample( 64*1024 )

colors = ['#377eb8', '#4daf4a', '#984ea3', '#e41a1c', '#ff7f00']
plt.figure(num=None, figsize=(8, 4), dpi=600, facecolor='w', edgecolor='k')

for r in range(0,5):
    mask = (subset['order'] & (0x7 << 3*r)) == (3 << 3*r)
    plt.scatter( subset['n'][mask], (subset['newint__orig'] / subset['n']) [mask], marker='.', s=.03, color=colors[r], label="newint (original), round {}").format(r+1) )

plt.xlabel( "n" )
```

5 Benchmarks
Figure 5.1 shows the execution times of `newint__orig`. In general it shows no sign of achieving better times if its execution comes after other algorithms. One notable exception is the $200,000 < n < 600,000$ range, where being executed last provides a small but noticeable advantage. The dataset also shows a distinctive “goose neck” starting at approximately $n = 160,000$. A possible explanation for both phenomenon relies on the L3 cache, which for the Intel i7-7700k is 2MiB per core but shared across the four cores. As there are three lists needed for the control points, and each IEEE binary64 point within each list occupies eight bytes of memory, 2MiB can completely hold $n \leq 87,381$ control points. Performance begins to degrade when $n$ is half the size of L3 and levels off when $n$ is twice the size of L3. The order-dependency between $200,000 < n < 600,000$ can be explained by the cache’s pre-fetch logic “warming up” to the data access patterns of the interpolation task, and thus giving a minor performance boost to algorithms executed later. Intelligent pre-fetching cannot help when the control point list is entirely contained within L3, nor when the list is significantly larger, so neither case shows order dependence.

Similar effects might be visible as the algorithm shifts from being dominated by L1 fetches to L2 fetches, and from L2 to L3 fetch dominance. The latter transition should begin at $5,461 \leq n \leq 10,922$, however there is a significant amount of noise that could mask it and the former transition period between $682 \leq n \leq 1,365$ is even more obscured. The change in memory-access latency may also be trivial next to the algorithm’s execution time, limiting the impact any performance increase could have. Out-of-order execution could even eliminate the performance penalty, as the processor could shuffle opcodes based on whether or not their memory fetches have completed.
A secondary, slower performance profile is visible, following a Patero distribution but merging with the primary execution profile at approximately \( n = 300,000 \). A third is faintly visible, with a similar shape but slightly faster execution times. All execution orders seem equally likely to appear, so the most likely explanation for these profiles is contention with another process during execution.

The noise profile appears to follow a Poisson distribution. It is dependent on \( n \) and scales with it. There is an increase in noise for \( n < 50,000 \) that is inversely proportional to \( n \), which implies a second noise profile that does not scale with \( n \).

The “goose neck” can be explained by a Weibull distribution. This is commonly found when describing a process with a failure rate \( \lambda \) that changes according to a power of the current time, \( k \). Rather than describing one process, though, consider a very large number of them simultaneously. The odds of these processes failing is no longer described by a probability density function, but instead the cumulative distribution function of the Weibull distribution,

\[
\text{CDF}_{\text{Weibull}}(x|k, \lambda) = 1 - e^{-\left(\frac{x}{\lambda}\right)^k},
\]

as the finite execution time limits how much of the PDF’s domain could be reached by any given process. If the Weibull distribution provides a probabilistic model of cache misses within L3, this implies that the replacement policy involves random replacement in some fashion. This is in line with other research on Intel’s cache policies.\(^{21}\)

```python
plt.figure(num=None, figsize=(8, 4), dpi=600, facecolor='w', edgecolor='k')
for r in range(0, 5):
    mask = (subset['order'] & (0x7 << 3*r)) == (3 << 3*r)
    plt.scatter(subset['n'][mask], (subset['noop'] / subset['n'])[mask] / any algorithm, round {}".format(r+1) )
plt.xlabel( "n" )
plt.ylabel( "nanoseconds / n" )

legend = plt.legend( loc='best' )
for i in range(0, 5):
    legend.legendHandles[i]._sizes = [100]

plt.ylim([4.8, 6.6])
plt.show()
```

Figure 5.2 shows the execution times when the benchmarked code is run but no interpolation algorithm is executed. Two execution paths are evident, with the slower of the two fading out roughly when \( n \) is large enough to become main-memory dependent. No order dependence is evident, surprisingly. Perhaps algorithm execution is interfering with the cache policy logic.

The `noop` numbers make it clear that out-of-order execution plays a major role in algorithm performance, at least on the i7-7700k. If we estimate the mode of `noop`’s fastest execution path to be 5.3 ns/point, and the mode of `newint_orig`’s slowest execution point to be 6.2 ns/point, that leaves about one nanosecond per point to execute the algorithm. Either the i7-7700k is executing two dozen machine operations in about

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Figure 5.2: Execution times per list length for ‘noop’.

five clock cycles, or it is reordering instructions so it can continue calculation while waiting for memory-dependent operations to finish. It is also likely that register renaming is allowing it to calculate multiple interpolants simultaneously, further increasing performance.

```python
# the algorithms tested, in order of their ID
algorithms = [
    'splint_one__div',
    'splint_one__mul',
    'newint__orig',
    'newint__noinv',
    'newint__vol'
]

plt.figure(num=None, figsize=(8, 4), dpi=600, facecolor='w', edgecolor='k')

for i, alg in enumerate(algorithms):
    # only include the middle execution
    mask = (subset['order'] & (0x7 << 3*2)) == ((i+1) << 3*2)
    plt.scatter(subset['n'][mask], (subset[alg]/subset['n'])[mask],
                alpha=0.3,
                marker='.', s=.1, color=colors[i], label=f'{}, round 3'.
                format(alg)

plt.ylabel("nanoseconds / n")

legend = plt.legend( loc='best' )
for i in range(0,5):
```

5 Benchmarks
Figure 5.3: Normalized execution times for all five algorithms.

Figure 5.3 shows the execution times of all algorithms. All of them exhibit the same pattern of behaviour as \texttt{newint\_orig}. This strongly implies the performance of all of them can be captured by one model.

### 5.2 Execution Model

For this model, we can merge the two noise processes into one distribution. The first key insight is that we do not need to rely on the Poisson distribution.

\[
\text{Pois}(x|\lambda) = \frac{1}{x!} \lambda^x e^{-\lambda}, x \in \mathbb{Z} \quad (5.2)
\]

\[
\Gamma(x|\kappa, \theta) = \frac{\theta^{-\kappa}}{\Gamma(\kappa)} x^{\kappa-1} e^{-\theta x}, x \in \mathbb{R} \quad (5.3)
\]

Equation 5.3 is the Gamma distribution, expressed in terms of a shape parameter \(\kappa\) and a scale parameter \(\theta\). This is not to be confused with the single-parameter \(\Gamma(x)\), which is the Gamma function applied to \(x\). Note that \(\text{Pois}(x|\lambda) = \Gamma(\lambda|x + 1, 1)\), thus the Gamma distribution is an analytic continuity of Equation 5.2, which describes the Poisson distribution. By using the Gamma distribution, we do not have to concern ourselves with the quantized nature of the Poisson distribution. The scale parameter exists only as a convenience, as
The second key insight is that both the mode and standard deviation of any given Gamma distribution have a simple closed form, provided $\kappa \geq 1$.

We can rearrange Equations 5.5 and 5.6 to reparameterize the Gamma distribution, so it instead takes a mode and standard deviation as input.
Equations 5.8 and 5.7 allow us to combine both noise distributions into one. We hold the mode to be constant, and vary the standard deviation according to

\[ \sigma = n \cdot \sigma_\infty + \sigma_0 \]  (5.9)

That mode constitutes the offset above a baseline execution time, the fastest the algorithm could be executed on the given processor in theory. As Figure 5.1 demonstrates, there are two primary execution profiles, one where access to the L3 cache dominates performance, and one where access to main memory dominates. These both are \( O(n) \), which means both can be represented as a linear relation on \( n \). After some transition point \( t \), the execution time transitions between the L3-dominated profile to the main-memory dominated profile according to the cumulative Weibull distribution. We can express this baseline as

\[
\text{baseline} = w(n \cdot m_{L3} + b_{L3}) + (1 - w)(n \cdot m_{MM}), \quad (5.10)
\]

\[
w = \begin{cases} e^{-(n-t)s}p, & n > t \\ 1, & \text{otherwise.} \end{cases} \quad (5.11)
\]

where \( m_{L3} \) and \( m_{MM} \) are the slope of the L3-dependent and main-memory-dependent execution profiles, plus \( s \) and \( p \) are scaling and power factors for the Weibull distribution. The intercept for the main-memory-dependent profile was dropped as the execution times are sufficiently large that it would have negligible influence.

Those large execution times pose a practical problem, as floating-point numbers only offer a finite precision. To remove that problem, we divide both the execution times and Equations 5.9 and 5.10 by \( n \). This also makes the model easier to fit.

\[
p(y|n, m_{L3}, b_{L3}, m_{MM}, t, s, p, M_0, \sigma_0, \sigma_\infty) = \Gamma \left( \frac{y}{n} - \text{baseline} | M_0, \sigma \right) \]

\[
\sigma = \sigma_\infty + \frac{\sigma_0}{n} \quad (5.13)
\]

\[
\text{baseline} = w(m_{L3} + \frac{b_{L3}}{n}) + (1 - w)m_{MM} \quad (5.14)
\]

\[
w = \begin{cases} e^{-(n-t)s}p, & n > t \\ 1, & \text{otherwise.} \end{cases} \quad (5.15)
\]

We used \texttt{emcee} to fit this model to the data, \texttt{PyMC3} would have been a more natural choice, but it ran into difficulties generating a derivative. While the former is likely slower to converge on the posterior than the latter, it relies on pure Python functions which are easier to include in this paper.

As a full round of MCMC can take hours, we will not include the programming code here. Those wishing to check our work are encouraged to view the source code repository, where the notebooks used to test various models are stored alongside the datasets. These also include model checks, to ensure a goodness of fit. For now, we will simply load an archived copy of the resulting posteriors and chart the fitted values.
```python
postiors = list()
for alg in algorithms:
    posteriors.append( np.loadtxt("posterior{}.interp_range.i7-7700k.variable_gamma.tsv".format(alg),
                                 delimiter='\t'))
np.random.shuffle(posteriors[-1])  # shuffle to destroy any
print("There are {} samples within each posterior.".format(len(posteriors[0])))

There are 4096 samples within each posterior.

table = pd.DataFrame( {'variable': ['$m_{L3}$', '$m_{MM}$', '$b_{L3}$', '$t$', '$L$'],
                      'sigma': ['0', '0', '0', '0', '0']},
                      index = [16, 50, 84],
                      order = [1, 2, 3, 4, 5])

table = table.to_latex(index=False)

display( {"text/latex":table.to_latex(index=False), "text/html":table.to_html(index=False), raw=True})
```

| variable | splint_one_div | splint_one_mul | newint_orig | newint_noinv | newint_vol |
|----------|----------------|----------------|-------------|--------------|------------|
| $m_{L3}$ | 5.32e + 07 | 5.25e + 07 | 5.28e + 07 | 4.90e + 07 | 5.16e + 07 |
| $m_{MM}$ | 5.53e + 07 | 5.46e + 07 | 5.49e + 07 | 5.14e + 07 | 5.38e + 07 |
| $b_{L3}$ | 2.39e - 03 | 2.04e - 03 | 3.05e - 03 | 8.27e - 03 | 1.63e - 03 |
| $t$      | 2.18e + 05 | 2.19e + 05 | 2.37e + 05 | 2.17e + 05 | 2.20e + 05 |
| $s$      | 5.63e - 06 | 5.33e - 06 | 5.53e - 06 | 5.47e - 06 | 5.68e - 06 |
| $p$      | 8.03e - 01 | 7.91e - 01 | 6.85e - 01 | 8.09e - 01 | 7.96e - 01 |
| $Mo$     | 6.67e - 01 | 8.03e - 01 | 7.53e - 01 | 8.93e - 01 | 7.29e - 01 |
| $c_{0}$  | 4.81e + 02 | 6.46e + 02 | 5.90e + 02 | 6.01e + 02 | 7.87e + 02 |
| $c_{\infty}$ | 7.95e - 02 | 7.59e - 02 | 7.68e - 02 | 7.42e - 02 | 7.23e - 02 |

**Table 5.2:** The posterior distribution for each variable of the model, including 16/84 credible intervals.

One surprise is that the fitted Weibull power is below one for every algorithm, leading to a sharp transition point instead of the smooth “goose neck” transition observed in the data. One possible explanation is that the Weibull distribution assumes the failure rate changes according to a constant power of the time. The failure rate may instead change according to a variable power of the time. Another is that there are multiple execution profiles with different parameters for each, rather than just one, and the fitted power was the best compromise among all of them. Whatever the explanation, the cumulative Weibull portion of the model is the least certain portion of the model.
columns = ['n', 'count'] + [s.replace('_', '\_') for s in algorithms]
data = [list() for i in columns]

for n in [4, 8, 16, 32, 64, 128]:
    aggregated = interp_bench[interp_bench['n'] == n].drop(columns=['order', 'noop']).agg(
        [lambda x: np.percentile(x/n, 16),
         lambda x: np.median(x/n),
         lambda x: np.percentile(x/n, 84),
         'len']).reset_index()
    data[0].append(n)
data[1].append(aggregated[('newint_vol', 'len')].iloc[0])

    for i, alg in enumerate(algorithms):
        data[i+2].append(f"\{\{:.2f\}^{{+ {:.2f}}} _{{- {:.2f}}} \}"
            .format(aggregated[(alg, '<lambda_1>')].iloc[0],
                     aggregated[(alg, '<lambda_2>')].iloc[0] - aggregated[(alg, '<lambda_0>')].iloc[0]))

del aggregated
table = pd.DataFrame({columns[i]:data[i] for i, _ in enumerate(data)})

display({"text/latex":table.to_latex(index=False), "text/html":table.to_html(index=False)}, raw=True)

Table 5.3: Calculated medians and 16/84 percentiles for select small values of \( n \).

| \( n \) | count | splint_one__div | splint_one__mul | newint__orig | newint__noinv | newint__vol |
|--------|-------|----------------|---------------|-------------|--------------|------------|
| 4      | 122   | 13.00+0.53     | 14.50+2.25    | 12.50+6.81  | 12.00+3.73   | 13.50+13.25|
| 8      | 89    | 9.88+1.62      | 10.50+1.85    | 9.38+1.49   | 9.88+2.73    | 9.88+5.74  |
| 16     | 63    | 8.19+1.06      | 8.38+1.00     | 8.06+1.20   | 7.62+1.52    | 7.88+2.57  |
| 32     | 45    | 7.31+0.53      | 7.44+1.29     | 7.16+0.90   | 7.03+1.09    | 7.56+1.39  |
| 64     | 31    | 6.84+0.53      | 6.88+0.82     | 6.80+0.36   | 6.80+0.47    | 6.80+0.83  |
| 128    | 23    | 6.46+0.41      | 6.47+0.62     | 6.53+0.36   | 6.29+0.28    | 6.48+0.57  |

Of all the variables, \( b_{L3} \) shows the most uncertainty within the model and is on the order of a few picoseconds. Combined with a consistently large \( \sigma_0 \) that exhibits little uncertainty, this would suggest \( b_{L3} \) contributes little to the overall fit. As Table 5.3 demonstrates, however, there is an increase in the median execution time per \( n \) as \( n \) approaches zero, which argues an offset variable like \( b_{L3} \) should play a significant role in any model. The output of this model for small \( n \) should not be trusted.

import scipy.stats as sps

def gamma_param( mode, sigma ):
Convert the given mode and standard deviation into a Gamma shape and scale parameter.

```python
root = np.sqrt(mode*mode + 2*sigma*sigma)  # simplify calculation
rootmode = root - mode
theta = 0.5*rootmode
kappa = (mode + root) / rootmode
return (kappa, theta)
```

```python
def model_bilinear(theta, n):
    """Calculate the model's baseline.""

    m_l3, m_mm, b_l3, t_l3_mm, w_s, w_p, mode, sigma_0, sigma_infty = theta

    model = m_l3 + b_l3/n

    # early exit, if possible
    if ((type(n) is np.int64) or (type(n) is int)) and (n < t_l3_mm):
        return model

    # use clipping to ensure sane values
    frac = np.clip(np.nan_to_num(np.exp(-(n - t_l3_mm)*w_s)**w_p), nan=1.), 0., 1.)

    model = model*frac + m_mm*(1 - frac)
    return model
```

```python
def model_noise_stdev(theta, n):
    """Calculate the noise standard deviation, given n."

    m_l3, m_mm, b_l3, t_l3_mm, w_s, w_p, mode, sigma_0, sigma_infty = theta

    return sigma_infty + sigma_0/n
```

```python
def model_range_vargamma(theta, n, fraction=(2./3.)):
    """Determine the credible interval for the given parameter set.""

    m_l3, m_mm, b_l3, t_l3_mm, w_s, w_p, mode, sigma_0, sigma_infty = theta

    baseline = model_bilinear(theta, n)

    model_stdev = model_noise_stdev(theta, n)
    model_kappa, model_theta = gamma_param(mode, model_stdev)

    low, high = sps.gamma.interval(fraction, model_kappa, 0, model_theta)
    return (baseline + low, baseline + high)
```
In comparison, Figure 5.4 suggests the model is a good fit overall. We can resolve this contradiction by randomly drawing sampling from the posterior, and evaluating the likelihood of a subset of datapoints.

def lnprior_vargamma(theta):
    """Calculate the prior probability of the given parameters."""

5 Benchmarks
Figure 5.4: Execution times per list length for ‘newint’, original version, for when it is run third among the algorithms. A sample of the model’s posterior is displayed for comparison. The solid line is the modal execution time, while the 16/84 confidence interval is the filled region.

```python
m_l3, m_mm, b_l3, t_l3_mm, w_s, w_p, mode, sigma_0, sigma_infty = theta

if (m_l3 <= 0) or (m_mm <= 0):
    return -np.inf
if m_l3 > m_mm:  # L3 MUST be faster
    return -np.inf
if b_l3 < 0:
    return -np.inf
if (t_l3_mm < 32000) or (t_l3_mm > 350000):  # i7-7700k
    return -np.inf
if (w_s > 1e-2) or (w_s <= 0):
    return -np.inf
if (w_p <= 0) or (w_p > 1000):  # i7-7700k
    return -np.inf
if (mode <= 0) or (sigma_0 <= 0) or (sigma_infty <= 0):
    return -np.inf
if (sigma_infty > sigma_0):  # we know the noise decreases
    return -np.inf

return -1.5 * (np.log1p(m_l3 * m_l3) + np.log1p(m_mm * m_mm))
```

def lnlike_vargamma(theta, x, y):

5 Benchmarks
Calculate the likelihood of the observed y, given the dependent x and a set of parameters.

\[ m_{l3}, m_{mm}, b_{l3}, t_{l3-mm}, w_s, w_p, \text{mode}, \sigma_0, \sigma_{\infty} = \theta \]

\[ \text{normed} = y / x \]
\[ \text{model_floor} = \text{model_bilinear}(\theta, x) \]
\[ \text{model_stdev} = \text{model_noise_stdev}(\theta, x) \]
\[ \text{model_kappa}, \text{model_theta} = \gamma_{\text{param}}(\text{mode}, \text{model_stdev}) \]
\[ \text{return} \ \text{np.sum}(\ \text{sps.gamma.logpdf}(\ \text{normed}, \text{model_kappa}, \text{model_floor}, \ \text{model_theta})) \]

```python
plt.figure(num=None, figsize=(8, 4), dpi=600, facecolor='w', edgecolor='k')
total_points = 64*1024
total_posteriors = 128
points_per_posterior = total_points // total_posteriors

# only take the middle execution, as well as values of n below a threshold
mask = ((interp_bench['order'] & (0x7 << 3*2)) == (3 << 3*2)) & (interp_bench['n'] < 300000)

for theta in posteriors[2][0:total_posteriors]:
    subsubset = interp_bench[mask].sample(points_per_posterior)
    x_subset = subsubset['n']
    y_subset = subsubset['newint__orig']
    llike = [lnlike_vargamma(theta, x_subset.iloc[i], y_subset.iloc[i]) for i in range(len(x_subset))]
    plt.scatter(x_subset, llike, alpha=0.3, marker='.', s=.1, color=colors[2])
plt.xlabel("n")
plt.ylabel("log(likelihood)")
plt.ylim([-5,2.2])
plt.show()
```

Figure 5.5 charts the log-likelihoods of this model. The data is fit well, even for \( n > 220,000 \) where the model uses a sharp transition point instead of a smooth "goose neck," and yet the model systematically misrepresents the data for \( n < 100,000 \). Even so, it takes until approximately \( n < 1,100 \) for the maximal likelihood to drop below 1.

Note that the median times of Table 5.3 are all within the 16/84th percentile of one another, and that the ordering does not remain consistent. While this model does not give accurate predictions for small \( n \), its
The likelihood of a sample of datapoints, drawn from a sample of the poseterior.

assertion that execution times show much more variance as n decreases is born out. If the spline interpolation routine is not used on large lists, the performance differences between all the variants are negligible.

The slope portions of the model show very confident fits. Surprisingly, newint__noinv has the fastest baseline of all the algorithms while newint__vol comes in second. A modified Numerical Recipes’ algorithm, splint_one__mul, manages to have a slightly better baseline than the original newint variant, and the original Numerical Recipes variant has the slowest baseline. The baseline only represents the lowest possible execution time in theory, however, and the Gamma distribution assigns it zero probability of occurring. A fairer evaluation of execution times incorporates the Gamma distribution, which not only adds an offset above the baseline but also introduces variation in execution times.
The upper half of Figure 5.6 is based on the model’s prediction for $n \to \infty$, while the lower half is based on $n = 100,000$. Both show that incorporating the noise component led to the two *Numerical Recipes* algorithms switching orders.

This provides consistent evidence for an unexpected conclusion, that floating-point division does not carry the same penalty for the Intel i7-7700k that it once did for older processors. Of the newer algorithms, the fastest is the one which calculates the division last, without loading it from memory, and converting a division into a multiplication in *Numerical Recipes*’ algorithm resulted in a loss in performance. More surprisingly, `newint_vol`’s two additional memory access result in a performance improvement over `newint_orig`. While this could be explained by the prior observation that `gcc` will shift the division to occur near the end of the algorithm, that code was compiled on *Compiler Explorer* with generic optimization flags. For the i7-7700k with `-march=native`, `gcc` does not move the division, so the only significant difference...
Figure 5.6: Predicted execution times according to each algorithm’s model, for large $n$. See text for details.

between `newint__orig` and `newint__vol` is that the latter adds two `vmovsd` instructions. The order of operations is slightly different, for instance `newint__orig` executes the division one instruction earlier and interleaves some operations differently, but out-of-order execution should eliminate any advantage that would provide.

```python
arch_text = [ "AMD FX-4100",
    "Intel Xeon Gold 6148",
    "Intel Atom X5-Z8350",
    "Raspberry Pi 3 b+"
]

interp_range_bench = [ pd.read_csv("data/interp_range.fx-4100.clean.tsv", sep="\t" ),
    pd.read_csv("data/interp_range.x6148.tsv", sep="\t" ),
    pd.read_csv("data/interp_range.x5-z8350.tsv", sep="\t" ),
    pd.read_csv("data/interp_range.pi-3b+.tsv", sep="\t" )
]

# control the y-axis range manually
y_limits = [ [12, 30],
    [12, 30],
    [35,100],
    [50,130],
]
Running the same benchmark code on different processors provides further evidence. Figure 5.7 shows the timing results from the same code on an AMD FX-4100 (compiled with gcc 9.2.1), an Intel Xeon Gold 6148 (Intel compiler 19.0.3.199), an Intel Atom x5-z8350 (gcc 9.2.1), and a Raspberry Pi 3 b+ (gcc 6.3.0). All of them are either older, simpler, or more specialized than an i7-7700k, and all of them provide evidence for division being a costly operation. In all cases Numerical Recipes’ algorithm runs faster with one division converted to a multiplication. On the Xeon Gold 6148 newint__orig has the same performance as newint__noinv, while for all other microarchitectures the former is consistently faster. The Atom x5-z8350 chart may suggest that extra memory writes lead to a significant speed increase, but an examination of the assembly code reveals that gcc has deferred the division in newint__orig to just before it’s needed. Unlike the other cases, the volatile hack is working as intended.

None of these processors have the same cache layout as the i7-7700k, so we’d expect their “goose neck” to be different or nonexistent. The FX-4100 also has 8MiB of L3, so we’d expect performance to degrade at roughly the same location as the i7-7700k, and we do observe that. But while the latter’s 256KiB L2 cache has been rendered useless long before that point, leading to a flat line, the FX-4100’s 2MiB L2 cache shared between two cores is still gradually degrading and so it looks more like a smooth curve than a “goose neck.” The x5-Z8350 lacks any L3 cache, so the start of its “goose neck” instead marks when \( n \) occupies half its 1MiB of L2 cache shared across two cores.

The Raspberry Pi 3 B+ also lacks an L3 cache, so its “goose neck” begins when half its shared 512KiB of L2 is occupied and ends when \( n \) corresponds to roughly twice the size of L2. The Xeon Gold 6148 is very similar,
as its performance drop coincides with half its 1MiB-per-core L2 cache. We expect to see a performance degradation when the dataset exhausts half the 27.5 MiB L3 cache, but that occurs for $n > 6,040,234$.

Figure 5.7 also demonstrates there's less overlap between the algorithms' performance for small $n$. Switching from Numerical Recipes' code is much more likely to lead to a performance increase for these microarchitectures.

More benchmarks on Intel processors help further demonstrate the decreasing cost of division. On the i5-3230m\(^2\) and i7-4790\(^3\) processors, Numerical Recipes' splint\_one algorithm runs faster when the division is converted to a multiplication. On an i3-6100\(^4\), the conversion does not have a strong effect on performance. On the i7-7700k\(^5\) and i7-8700\(^6\), the conversion causes a decrease in performance. Interestingly, newint\_noinv has better performance than newint\_orig on all the microarchitectures listed in this paragraph. This is unlikely to be explained by the extra memory fetch and multiplication in the latter algorithm, as newint\_vol outperforms newint\_orig for all but the i5-3230m despite adding two extra memory fetches.

\(^2\)Part of the Ivy Bridge microarchitecture, released in 2013
\(^3\)Haswell, 2014
\(^4\)Skylake, 2015
\(^5\)Kaby Lake, early 2017
\(^6\)Coffee Lake, late 2017

Figure 5.7: Execution times for a variety of processor architectures. The colour coding is the same as Figure 4.7(fig:model_times).
6 Conclusion

Based on the results of these benchmarks, we can make a number of suggestions for programmers hoping to implement this code.

The critical factor in deciding which algorithm to implement appears to be the speed of the division instruction and the processor’s ability to organize out-of-order execution. On Intel processors with the Ivy Bridge microarchitecture or better, out-of-order execution appears to favour newint__noinv, a variant of newint which eliminates the inv_ba variable in favour of division by ba. If the architecture is Skylake or later, however, and the goal is to interpolate evenly-spaced points across a curve with less than tens of thousands of points, execution noise greatly reduces the performance advantage for any one algorithm, including those from *Numerical Recipes*.

For processors with slow division, or those with weak or no ability to reorder instruction execution, a straightforward implementation of newint is likely to give the best performance, and to maintain that performance for curves containing fewer than tens of thousands of control points. CPUs designed for high-performance computation typically fall into this category. One exception to look out for is if the compiler shuffles the declaration of inv_ba to occur immediately before the return statement, which could impair performance. Examine the assembly output to determine if this is happening. If it is, either manually adjust the assembly code or declare inv_ba to be volatile to prevent the division from migrating.

Surprisingly, on some processors the volatile hack leads to a performance increase even though it introduces an extra memory store and an extra fetch. This is unlikely to be faster than both a straightforward implementation of newint and newint__noinv, but if performance is absolutely critical it may be worth running some benchmarks to verify this.

As generating second derivatives is unlikely to be a performance bottleneck, we did only a minimal comparison between *Numerical Recipes*’ spline and our new_second_derivative. Still, there is reason to expect that there will be little performance difference between the two for small n.

Our replacements for spline and splint_one show only minor divergences in accuracy, all of which can be explained by the imprecision of floating-point operations. Other than the performance differences outlined above, there should be no intrinsic obstacle to replacing those *Numerical Recipes* routines with ours.

In future, we would like to benchmark our code on more recent AMD processors, as well as GPUs. The former are likely to run the newint__noinv variant faster than the original newint, and the latter are likely to show the opposite behaviour, but without running the experiment we cannot be sure. We are uncomfortable with insisting that CPU benchmarks be single-threaded while allowing GPU benchmarks unconstrained access to all hardware execution units, so we would also like to perform some multithreaded CPU benchmarks.
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