

Tricks of the Trade

Edited by Paul Abbott

This is a column of programming tricks and techniques, most of which, we hope, will be contributed by our readers, either directly as submissions to *The Mathematica Journal* or as an edited answer to a question posted in the *Mathematica* newsgroup, comp.soft-sys.math.mathematica.

■ Sum-Free Set

The *sumset* of two or more subsets of an additive group is the set of all sums formed by taking one element from each set (see planetmath.org/encyclopedia/Sumset.html). The sumset can be computed using **Tuples**.

```
In[1]:= SumSet[s_List] := Union[Plus @@@ Tuples[{s}]]
```

Define \oplus to be **SumSet**.

```
In[2]:= CirclePlus := SumSet
```

Here is the sumset $\{1, 2\} \oplus \{1, 3, 5\} \oplus \{2\}$.

```
In[3]:= {1, 2} \oplus {1, 3, 5} \oplus {2}
```

```
Out[3]= {4, 5, 6, 7, 8, 9}
```

A sum-free set S is a set for which the intersection of S and the sumset $S \oplus S$ is empty (see mathworld.wolfram.com/Sum-FreeSet.html).

```
In[4]:= SumFreeQ[s_List] := s \cap (s \oplus s) == {}
```

For example, the sum-free subsets of $\{1, 2, 3\}$ are $\emptyset \equiv \{\}, \{1\}, \{2\}, \{3\}, \{1, 3\}$, and $\{2, 3\}$.

```
In[5]:= SumFreeQ /@ {{}, {1}, {2}, {3}, {1, 3}, {2, 3}}
```

```
Out[5]= {True, True, True, True, True, True}
```

Note that $\{1, 2\}$ is not sum-free.

```
In[6]:= SumFreeQ[{1, 2}]
```

```
Out[6]= False
```

Here are the sum-free subsets of $\{1, 3, 5, 7, 8\}$.

```
In[7]:= Select[Subsets[{1, 3, 5, 7, 8}], SumFreeQ]
```

```
Out[7]= {{}, {1}, {3}, {5}, {7}, {8}, {1, 3}, {1, 5}, {1, 7}, {1, 8}, {3, 5},  
         {3, 7}, {3, 8}, {5, 7}, {5, 8}, {7, 8}, {1, 3, 5}, {1, 3, 7}, {1, 3, 8},  
         {1, 5, 7}, {1, 5, 8}, {3, 5, 7}, {3, 7, 8}, {5, 7, 8}, {1, 3, 5, 7}}
```

Sum-free subsets of $\{1, 2, \dots, n\}$ can be computed recursively as follows.

```
In[8]:= SumFreeSet[0] = {};
```

```
In[9]:= SumFreeSet[n_] := SumFreeSet[n] = SumFreeSet[n - 1] ∪
      (# ∪ {n} &)/@ Select[SumFreeSet[n - 1], # ∩ (n - #) = {} &]
```

The key to this computation is the use of the test $\# \cap (n - \#) = \{\}$ & on **SumFreeSet[n - 1]** to construct elements of **SumFreeSet[n]**.

Here are the sum-free subsets for $n = 0, 1, \dots, 4$.

```
In[10]:= Table[SumFreeSet[n], {n, 0, 4}] // ColumnForm
```

```
Out[10]= {}
      {}, {1}
      {}, {1}, {2}
      {}, {1}, {2}, {3}, {1, 3}, {2, 3}
      {}, {1}, {2}, {3}, {4}, {1, 3}, {1, 4}, {2, 3}, {3, 4}
```

Alternatively, sum-free subsets can be computed using **NestList**, starting from the empty set.

```
In[11]:= Module[{n = 0},
      NestList[(++n; # ∪ (# ∪ {n} &)/@ Select[# , # ∩ (n - #) = {} &]) &, {}, 5] //
      ColumnForm]
```

```
Out[11]= {}
      {}, {1}
      {}, {1}, {2}
      {}, {1}, {2}, {3}, {1, 3}, {2, 3}
      {}, {1}, {2}, {3}, {4}, {1, 3}, {1, 4}, {2, 3}, {3, 4}
      {}, {1}, {2}, {3}, {4}, {5}, {1, 3}, {1, 4}, {1, 5}, {2, 3}, {2, 5}, {3, 4}, {3, 5}, {4, 5},
      {1, 3, 5}, {3, 4, 5}
```

The number of sum-free subsets for each n are 1, 2, 3, 6, 9, 16, Searching for this sequence at www.research.att.com/~njas/sequences, we find that it is A007865.

```
In[12]:= Length /@ First[%]
```

```
Out[12]= {1, 2, 3, 6, 9, 16}
```

Using **Sow** and **Reap**, here is the number of sum-free subsets for $0 \leq n \leq 25$.

```
In[13]:= Module[{n = 0},
      First@Last@Reap@Nest[(++n; Sow[Length[#]]; # ∪ (# ∪ {n} &)/@
      Select[# , # ∩ (n - #) = {} &]) &, {}, 25]
```

```
Out[13]= {1, 2, 3, 6, 9, 16, 24, 42, 61, 108, 151, 253, 369, 607, 847,
      1400, 1954, 3139, 4398, 6976, 9583, 15456, 20982, 32816, 45417}
```

■ Google™ Search for *Mathematica*

Chris Chiasson

chris.chiasson@gmail.com

A Google search for “keyword site:documents.wolfram.com inurl:mathematica” searches for *keyword* in *The Mathematica Book* and in the current version of the online documentation. For example, a search for `NVariationalBound` returns a link to `documents.wolfram.com/mathematica/Add-onsLinks/StandardPackages/Calculus/VariationalMethods.html`.

Firefox users can make a bookmark with the URL

`www.google.com/search?q=%s+site%3Adocuments.wolfram.com+inurl%3Amathematica&sourceid=mozilla-search` and then fill in the keyword field for that bookmark as `mhelp`. Typing “`mhelp NVariationalBound`” into the Firefox address bar searches the documentation for `NVariationalBound`.

■ Asymptotic Expansion and π

Gregory’s series (`mathworld.wolfram.com/GregorySeries.html`) is a slowly convergent formula for π .

$$\text{In}[1]:= 4 \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{2k-1}$$

`Out[1]= π`

Truncating the series after 50,000 terms (half a power of 10, in this case 10^5) yields a result that is incorrect in the 6th digit.

$$\text{In}[2]:= \text{gregory} = 4 \cdot 50 \sum_{k=1}^{50000} \frac{(-1)^{k-1}}{2k-1}$$

`Out[2]= 3.1415726535897952384626423832795041041971666293751`

`In[3]:= pi = N[π , 50]`

`Out[3]= 3.1415926535897932384626433832795028841971693993751`

`In[4]:= 1 - [log10(pi - gregory)]`

`Out[4]= 6`

However, comparing these two numbers, it is surprising how many digits they have in common [1, 2].

`In[5]:= RealDigits[pi] - RealDigits[gregory]`

`Out[5]= {{0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -2, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, -2, 7, 8, 0, 0, 0, 0, 0, 0, 3, -3, 7, 0, 0, 0, 0, 0}, 0}`

Moreover, the index of the position of the least significant digit of each block of different digits is an odd multiple of 5.

`In[6]:= Partition[Rest@First[%, 5]`

$$\text{Out[6]} = \begin{pmatrix} 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 7 & 8 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & -3 & 7 & 0 \end{pmatrix}$$

The differences can be computed using **FromDigits**.

`In[7]:= FromDigits /@ %`

`Out[7]= {2, 0, -2, 0, 10, 0, -122, 0, 2770}`

We can represent the difference between π and Gregory's series truncated after 50,000 terms as

$$3.14159265358979\overset{2}{3}23846264\overset{122}{33832795028841971693993751},$$

$\frac{2}{2}$
 $\frac{122}{10}$
 $\frac{2770}{2770}$

where numbers above the center line are negative and those below the line are positive.

Searching for the sequence of differences at www.research.att.com/~njas/sequences, we find that they are twice the Euler numbers, E_{2k} .

`In[8]:= Table[{k, 2 E_{2k}}, {k, 0, 4}]`

$$\text{Out[8]} = \begin{pmatrix} 0 & 2 \\ 1 & -2 \\ 2 & 10 \\ 3 & -122 \\ 4 & 2770 \end{pmatrix}$$

Empirically, we have determined the asymptotic difference between π and the truncated Gregory's series.

$$\text{In[9]} := \text{diff}[n_, m_] = 2 \sum_{k=0}^m \frac{E_{2k}}{n^{2k+1}};$$

See [1] for a proof of this result.

Adding the asymptotic difference to the truncated Gregory's series and putting $n = 2 \times 50000 = 10^5$, we can recover π to (at least) 50 decimal places.

`In[10]:= π - gregory - diff[105, 4]`

`Out[10]= $0. \times 10^{-50}$`

The asymptotic difference can be computed directly using **Series**.

`In[11]:= FullSimplify[Series[$\pi - 4 \sum_{k=1}^{\frac{n}{2}} \frac{(-1)^{k-1}}{2k-1}$, {n, ∞ , 9}], n > 0 \wedge $\frac{n}{4} \in \mathbb{Z}$]`

`Out[11]= $\frac{2}{n} - 2\left(\frac{1}{n}\right)^3 + 10\left(\frac{1}{n}\right)^5 - 122\left(\frac{1}{n}\right)^7 + 2770\left(\frac{1}{n}\right)^9 + O\left(\left(\frac{1}{n}\right)^{10}\right)$`

See also [3].

■ Hadamard Regularization

Hadamard regularization is a technique for handling divergent integrals (essentially keeping only the finite part of the integral) and plays an important role in several branches of mathematical physics (see [4, 5] and mathworld.wolfram.com/HadamardIntegral.html). Consider evaluating

$$K^\alpha[f] \equiv \frac{1}{\Gamma(-\alpha)} \int_{-1}^1 \frac{f(y)}{(1-y)^{\alpha+1}} dy$$

in the Hadamard sense, where $0 \leq n < \alpha < n+1$ and $n \in \mathbb{Z}$, that is, $n = \lfloor \alpha \rfloor$ and $f \in C^{n+1}[-1, 1]$.

Using integration by parts via pattern matching, we can increase the exponent of $(1-y)^{-p}$ until it is integrable, that is, $-1 < p \leq 0$.

`In[1]:= byparts =`

$$\int (1-y)^p f[y] dy \rightarrow f(y) \int (1-y)^p dy - \int \left(\int (1-y)^p dy \right) \partial_y f(y) dy;$$

Here is the formal result of integrating by parts once.

`In[2]:= $\frac{1}{\Gamma(-\alpha)} \int \frac{f(y)}{(1-y)^{\alpha+1}} dy$ /. byparts // FullSimplify // Expand`

`Out[2]= $\frac{\int (1-y)^{-\alpha} f'(y) dy}{\Gamma(1-\alpha)} - \frac{(1-y)^{-\alpha} f(y)}{\Gamma(1-\alpha)}$`

The $(1-y)^{-\alpha} f(y)$ term is singular at $y = 1$ if $\alpha > 0$. Here is the result of three partial integrations.

`In[3]:= Collect[Nest[# /. byparts &, $\frac{1}{\Gamma(-\alpha)} \int \frac{f(y)}{(1-y)^{\alpha+1}} dy$, 3],
 $\{f(y), f^{(\cdot)}(y)\}$, FullSimplify]`

`Out[3]:= $-\frac{f'(y)(1-y)^{1-\alpha}}{\Gamma(2-\alpha)} - \frac{f''(y)(1-y)^{2-\alpha}}{\Gamma(3-\alpha)} - \frac{f(y)(1-y)^{-\alpha}}{\Gamma(1-\alpha)} + \frac{\int(1-y)^{2-\alpha} f^{(3)}(y) dy}{\Gamma(3-\alpha)}$`

Neglecting the singular terms at $y = 1$, we evaluate the partial integrals at $y = -1$.

`In[4]:= -% /. HoldPattern[Integrate[_]] := 0 /. y -> -1`

`Out[4]:= $\frac{2^{-\alpha} f(-1)}{\Gamma(1-\alpha)} + \frac{2^{1-\alpha} f'(-1)}{\Gamma(2-\alpha)} + \frac{2^{2-\alpha} f''(-1)}{\Gamma(3-\alpha)}$`

The pattern is clear. Dropping the singular terms at $y = 1$, we obtain

$$K^\alpha[f] \equiv \frac{1}{\Gamma(-\alpha)} \int_{-1}^1 \frac{f(y)}{(1-y)^{\alpha+1}} dy =$$

$$\sum_{k=0}^n \frac{2^{k-\alpha}}{\Gamma(k-\alpha+1)} f^{(k)}(-1) + \frac{1}{\Gamma(n-\alpha+1)} \int_{-1}^1 (1-y)^{n-\alpha} f^{(n+1)}(y) dy.$$

As a definite example, consider

$$\int_{-1}^1 \frac{\exp(y)}{(1-y)^{\alpha+1}} dy.$$

Direct integration followed by series expansion about $\epsilon = 0$ reveals the singular terms.

`In[5]:= Assuming[1 > ϵ > 0, $\frac{1}{\Gamma(-\alpha)} \int_{-1}^{1-\epsilon} \frac{\exp(y)}{(1-y)^{\alpha+1}} dy$]`

`Out[5]:= $\frac{e(\Gamma(-\alpha, \epsilon) - \Gamma(-\alpha, 2))}{\Gamma(-\alpha)}$`

`In[6]:= Series[%, { ϵ , 0, 1}]`

`Out[6]:= $\frac{e((\frac{1}{\alpha} + \frac{\epsilon}{1-\alpha} + O(\epsilon^2))\epsilon^{-\alpha} + \Gamma(-\alpha) - \Gamma(-\alpha, 2))}{\Gamma(-\alpha)}$`

Now $\epsilon^{-\alpha}$ is singular at $\epsilon = 0$ for $\alpha > 0$, and $\epsilon^{1-\alpha}$ is either singular if $\alpha > 1$ or vanishes if $0 < \alpha < 1$. So both terms are ignorable. Hence the nonsingular part can be extracted as follows.

`In[7]:= $K_{\alpha-}$ [Exp] = % /. $\epsilon^{-\alpha} \rightarrow 0$ // FullSimplify`

`Out[7]:= $e - \frac{e \Gamma(-\alpha, 2)}{\Gamma(-\alpha)}$`

For example, here is the exact result for $\alpha = 3/2$.

`In[8]:= K3/2[Exp] // FunctionExpand // Simplify`

$$\text{Out[8]} = \frac{3}{4 e \sqrt{2} \pi} + e \operatorname{erf}(\sqrt{2})$$

Alternatively, using the identity obtained using integration by parts, we obtain the same answer.

`In[9]:= Module[{α = 3/2, n, f = Exp}, n = Floor[α]; $\sum_{k=0}^n \frac{2^{k-\alpha}}{\Gamma(k-\alpha+1)} f^{(k)}(-1) +$`

$$\frac{1}{\Gamma(n-\alpha+1)} \int_{-1}^1 (1-y)^{n-\alpha} f^{(n+1)}(y) dy] // Simplify$$

$$\text{Out[9]} = \frac{3}{4 e \sqrt{2} \pi} + e \operatorname{erf}(\sqrt{2})$$

■ References

- [1] J. M. Borwein, P. B. Borwein, and K. Dilcher, "Pi, Euler Numbers, and Asymptotic Expansions," *American Mathematical Monthly*, **96**(8), 1989 pp. 681–687.
- [2] G. Almkvist, "Many Correct Digits of π , Revisited," *American Mathematical Monthly*, **104**(4), 1997 pp. 351–353. DOI-Link: [dx.doi.org/10.2307/2974583](https://doi.org/10.2307/2974583)
- [3] S. Matsumoto, "Convergence Improvement of Infinite Series by Linear Fractions," in *Applied Mathematica: Electronic Proceedings of the Eighth International Mathematica Symposium (IMS06)*, Avignon, France (Y. Papegay, ed.), Rocquencourt: INRIA, 2006 ISBN 2-7261-1289-7.
- [4] D. Elliott, "Three Algorithms for Hadamard Finite-Part Integrals and Fractional Derivatives," *Journal of Computational and Applied Mathematics*, **62**(3), 1995 pp. 267–283.
- [5] L. Blanchet and G. Faye, "Hadamard Regularization," *Journal of Mathematical Physics*, **41**, 2000 pp. 7675–7714.

Paul Abbott

School of Physics, M013
The University of Western Australia
35 Stirling Highway
Crawley WA 6009, Australia
tmj@physics.uwa.edu.au
physics.uwa.edu.au/~paul