CHEBFUN GUIDE 2: INTEGRATION AND DIFFERENTIATION

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2.1 sum

We have seen that the `sum` command returns the definite integral of a chebfun over its range of definition. The integral is normally calculated by an FFT-based variant of Clenshaw-Curtis quadrature, as described first in [Gentleman 1972]. This formula is applied on each fun (i.e., each smooth piece of the chebfun), and then the results are added up.

Here is an example whose answer is known exactly:

```
f = chebfun(@(x) log(1+tan(x)),[0 pi/4]);
format long
I = sum(f)
Iexact = pi*log(2)/8
```

```
I =
   0.272198261287950
Iexact =
   0.272198261287950
```

Here is an example whose answer is not known exactly, given as the first example in the section "Numerical Mathematics in Mathematica" in The Mathematica Book [Wolfram 2003].

```
f = chebfun('sin(sin(x))',[0 1]);
sum(f)
```

```
ans =
   0.430606103120691
```

All these digits match the result 0.4306061031206906049... reported by Mathematica.

Here is another example:

```
F = @(t) 2*exp(-t.^2)/sqrt(pi);
f = chebfun(F,[0,1]);
I = sum(f)
```

```
I =
   0.842700792949715
```

The reader may recognize this as the integral that defines the error function evaluated at t=1:

```
Iexact = erf(1)
```

```
Iexact =
   0.842700792949715
```

It is interesting to compare the times involved in evaluating this number in various ways. Matlab's specialized erf code is the fastest:

```
tic, erf(1), toc
```

```
ans =
   0.842700792949715
Elapsed time is 0.000077 seconds.
```

Using Matlab's various quadrature commands is understandably slower:

```
tol = 3e-14;
tic, I = quad(F,0,1,tol); t = toc;
  fprintf('  QUAD:  I = %17.15f  time = %6.4f secs\n',I,t)
tic, I = quadl(F,0,1,tol); t = toc;
  fprintf(' QUADL:  I = %17.15f  time = %6.4f secs\n',I,t)
tic, I = quadgk(F,0,1,'abstol',tol,'reltol',tol); t = toc;
  fprintf('QUADGK:  I = %17.15f  time = %6.4f secs\n',I,t)
```

```
  QUAD:  I = 0.842700792949715  time = 0.0465 secs
 QUADL:  I = 0.842700792949715  time = 0.0312 secs
QUADGK:  I = 0.842700792949715  time = 0.0477 secs
```

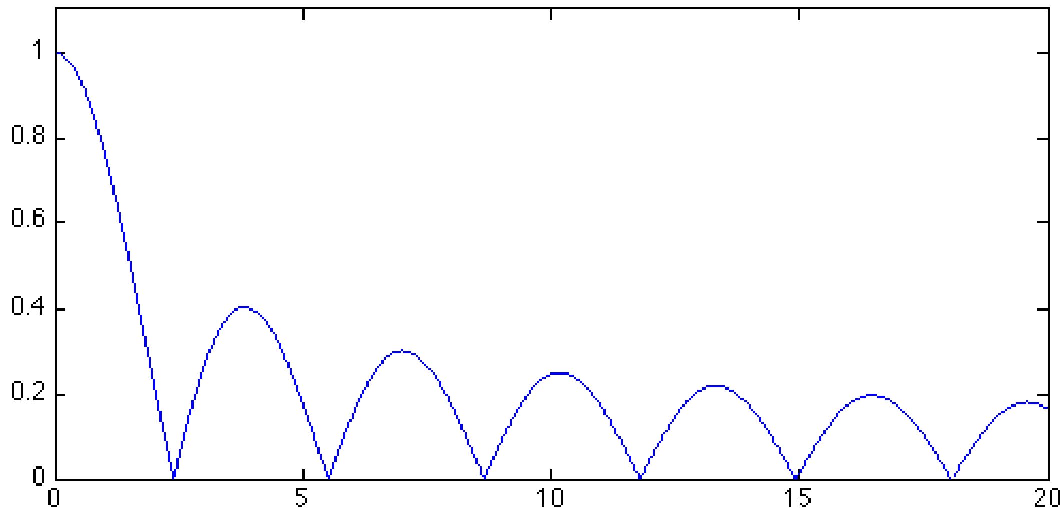
The timing for Chebfun comes out competitive:

```
tic, I = sum(chebfun(F,[0,1])); t = toc;
  fprintf('CHEBFUN:  I = %17.15f  time = %6.4f secs\n',I,t)
```

```
CHEBFUN:  I = 0.842700792949715  time = 0.0114 secs
```

Here is a similar comparison for a function that is more difficult, because of the absolute value, which leads with "splitting on" to a chebfun consisting of a number of funs.

```
F = @(x) abs(besselj(0,x));
f = chebfun(@(x) abs(besselj(0,x)),[0 20],'splitting','on');
plot(f), ylim([0 1.1])
```

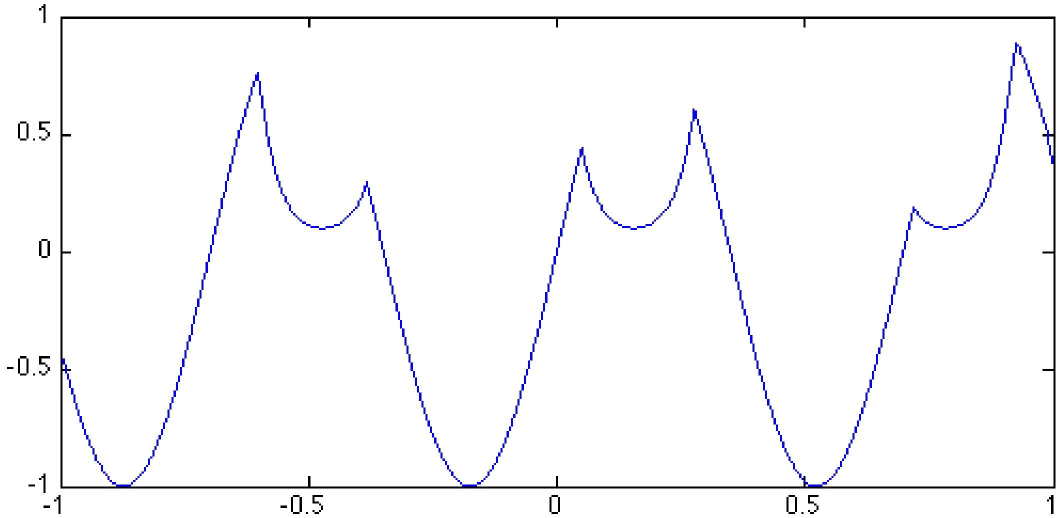



```
tol = 3e-14;
tic, I = quad(F,0,20,tol); t = toc;
  fprintf('   QUAD:  I = %17.15f  time = %5.3f secs\n',I,t)
tic, I = quadl(F,0,20,tol); t = toc;
  fprintf('  QUADL:  I = %17.15f  time = %5.3f secs\n',I,t)
tic, I = quadgk(F,0,20,'abstol',tol,'reltol',tol); t = toc;
  fprintf(' QUADGK:  I = %17.15f  time = %5.3f secs\n',I,t)
tic, I = sum(chebfun(@(x) abs(besselj(0,x)),[0,20],'splitting','on')); t = toc;
  fprintf('CHEBFUN:  I = %17.15f  time = %5.3f secs\n',I,t)
```

```
   QUAD:  I = 4.445031603001505  time = 0.131 secs
  QUADL:  I = 4.445031603001576  time = 0.079 secs
 QUADGK:  I = 4.445031603001578  time = 0.016 secs
CHEBFUN:  I = 4.445031603001566  time = 0.267 secs
```

This last example highlights the piecewise-smooth aspect of Chebfun integration. Here is another example of a piecewise smooth problem.

```
x = chebfun('x');
f = sech(3*sin(10*x));
g = sin(9*x);
h = min(f,g);
plot(h)
```



Here is the integral:

```
tic, sum(h), toc
```

```
ans =
  -0.381556448850250
Elapsed time is 0.001579 seconds.
```

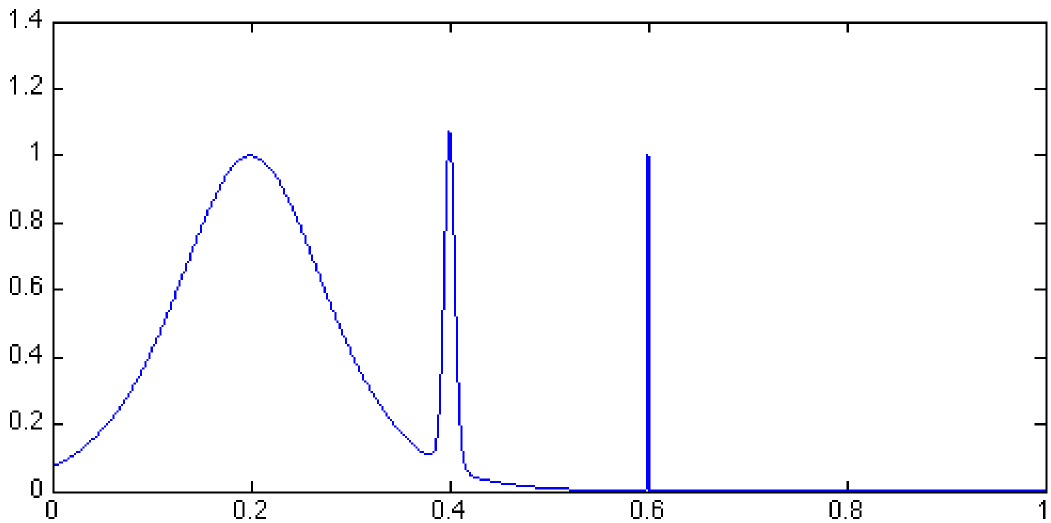
For another example of a definite integral we turn to an integrand given as example `F21F` in [Kahaner 1971]. We treat it first in the default mode of splitting off:

```
ff = @(x) sech(10*(x-0.2)).^2 + sech(100*(x-0.4)).^4 + sech(1000*(x-0.6)).^6;
f = chebfun(ff,[0,1])
```

```
f =
   chebfun column (1 smooth piece)
       interval       length    endpoint values
[       0,       1]     12724      0.071   4.5e-07
Epslevel = 1.473049e-13.  Vscale = 1.070655e+00.
```

The function has three spikes, each ten times narrower than the last:

```
plot(f)
```



The length of the global polynomial representation is accordingly quite large, but the integral comes out correct to full precision:

```
length(f)
sum(f)
```

```
ans =
       12724
ans =
   0.210802735500549
```

With splitting on, Chebfun misses the narrowest spike, and the integral comes out too small:

```
f = chebfun(ff,[0,1],'splitting','on');
length(f)
sum(f)
```

```
ans =
   234
ans =
   0.209736068833883
```

We can fix the problem by forcing finer initial sampling in the Chebfun constructor with the `minsamples' flag:

```
f = chebfun(ff,[0,1],'splitting','on','minsamples',100);
length(f)
sum(f)
```

```
ans =
   391
ans =
   0.210802735500549
```

Now the integral is correct again, and note that the length of the chebfun is much smaller than with the original global representation. For more about `minsamples` see Section 8.6.

As mentioned in Chapter 1 and described in more detail in Chapter 9, Chebfun has some capability of dealing with functions that blow up to infinity. Here for example is a familiar integral:

```
f = chebfun(@(x) 1./sqrt(x),[0 1],'blowup',2);
sum(f)
```

```
ans =
   2.000000000000000
```

Certain integrals over infinite domains can also be computed, though the error is often large:

```
f = chebfun(@(x) 1./x.^2.5,[1 inf]);
sum(f)
```

```
Warning: Result may not be accurate as the function decays slowly at infinity.
ans =
   1.229596649932262
```

Chebfun is not a specialized item of quadrature software; it is a general system for manipulating functions in which quadrature is just one of many capabilities. Nevertheless Chebfun compares reasonably well as a quadrature engine against specialized software. This was the conclusion of an Oxford MSc thesis by Phil Assheton [Assheton 2008], which compared Chebfun experimentally to quadrature codes including Matlab's `quad` and `quadl`, Gander and Gautschi's `adaptsim` and `adaptlob`, Espelid's `modsim`, `modlob`, `coteda`, and `coteglob`, QUADPACK's `QAG` and `QAGS`, and the NAG Library's `d01ah`. In both reliability and speed, Chebfun was found to be competitive with these alternatives. The overall winner was `coteda` [Espelid 2003], which was typically about twice as fast as Chebfun. For further comparisons of quadrature codes, together with the development of some improved codes based on a philosophy that has something in common with Chebfun, see [Gonnet 2009]. See also "Battery test of Chebfun as an integrator" in the Quadrature section of the Chebfun Examples collection.

2.2 norm, mean, std, var

A special case of an integral is the `norm` command, which for a chebfun returns by default the 2-norm, i.e., the square root of the integral of the square of the absolute value over the region of definition. Here is a well-known example:

```
norm(chebfun('sin(pi*theta)'))
```

```
ans =
     1
```

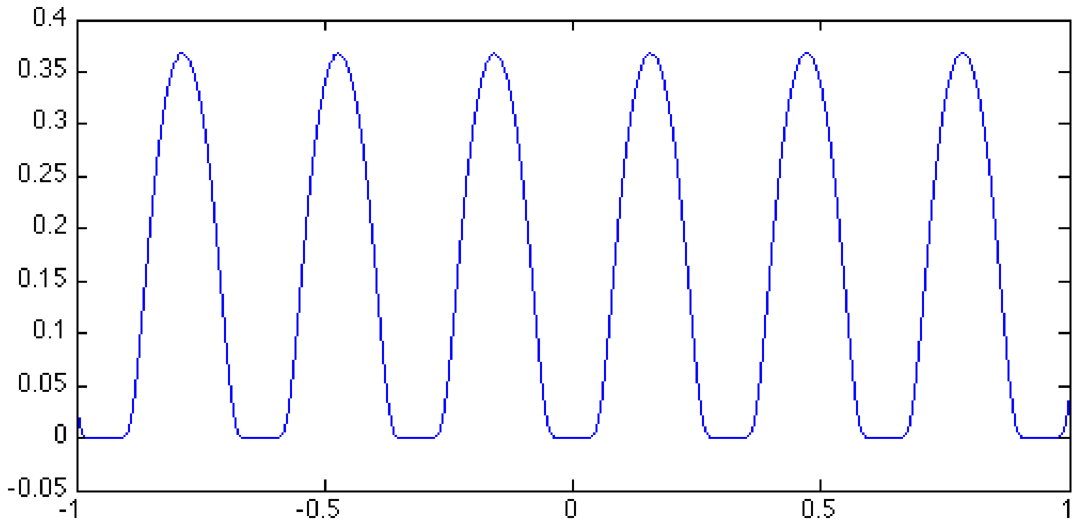
If we take the sign of the sine, the norm increases to $\sqrt{2}$:

```
norm(chebfun('sign(sin(pi*theta))','splitting','on'))
```

```
ans =
   1.414213562373095
```

Here is a function that is infinitely differentiable but not analytic.

```
f = chebfun('exp(-1./sin(10*x).^2)');
plot(f)
```



Here are the norms of `f` and its tenth power:

```
norm(f), norm(f.^10)
```

```
ans =
   0.292873834331035
ans =
     2.187941295308668e-05
```

2.3 cumsum

In Matlab, "cumsum" gives the cumulative sum of a vector,

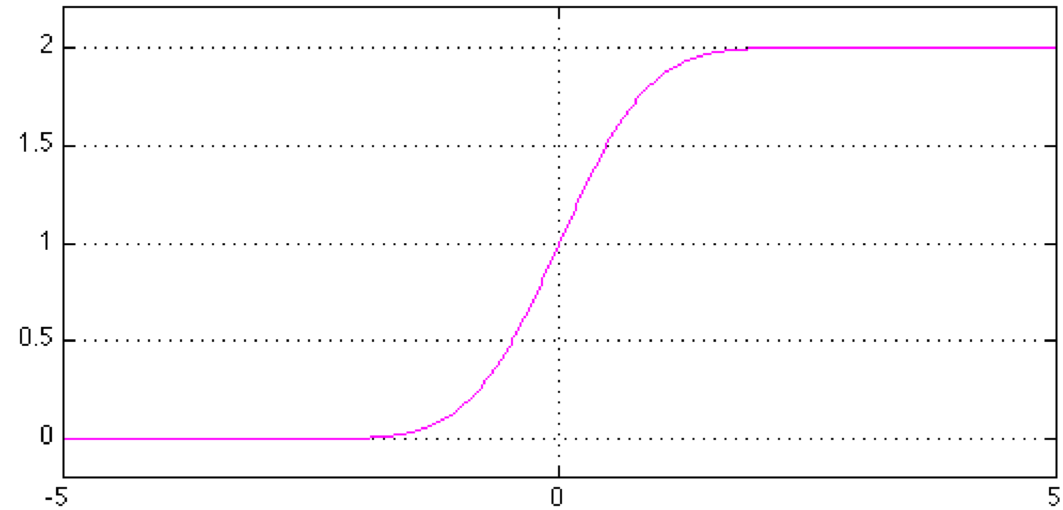
```
v = [1 2 3 5]
cumsum(v)
```

```
v =
     1     2     3     5
ans =
     1     3     6    11
```

The continuous analogue of this operation is indefinite integration. If `f` is a fun of length n, then `cumsum(f)` is a fun of length $n+1$. For a chebfun consisting of several funs, the integration is performed on each piece.

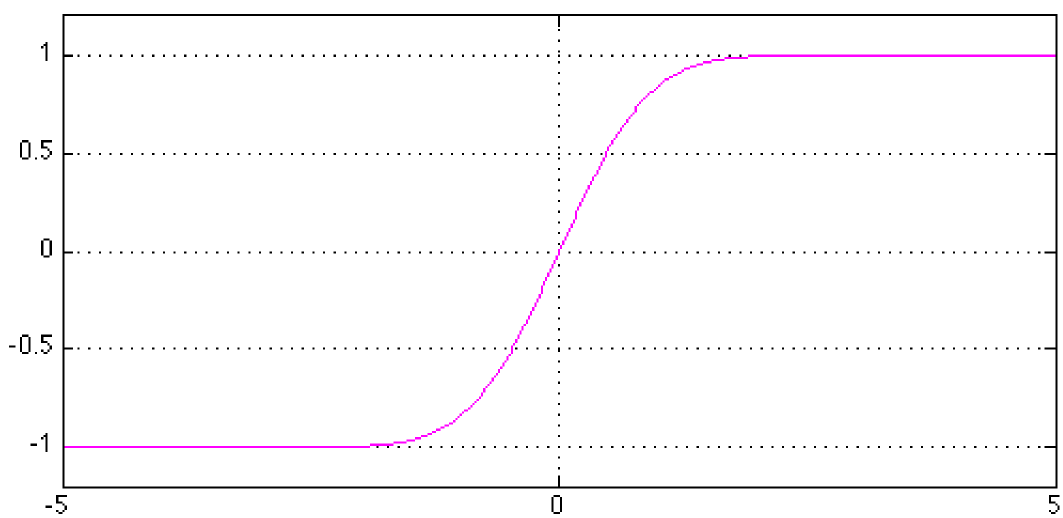
For example, returning to an integral computed above, we can make our own error function like this:

```
t = chebfun('t',[-5 5]);
f = 2*exp(-t.^2)/sqrt(pi);
fint = cumsum(f);
plot(fint,'m')
ylim([-0.2 2.2]), grid on
```



The default indefinite integral takes the value 0 at the left endpoint, but in this case we would like 0 to appear at $t=0$:

```
fint = fint - fint(0);
plot(fint,'m')
ylim([-1.2 1.2]), grid on
```



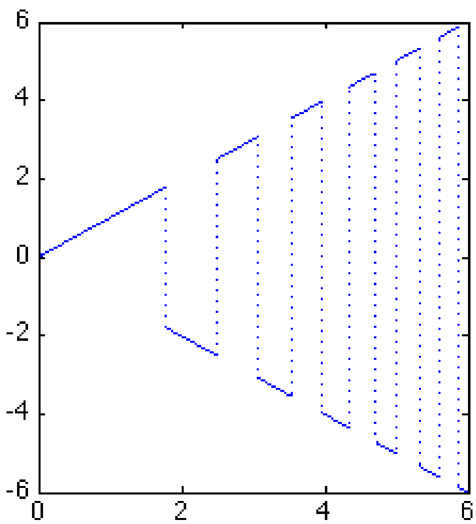
The agreement with the built-in error function is convincing:

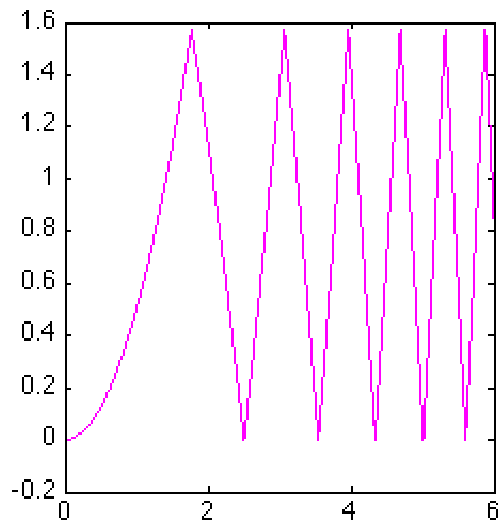
```
[fint((1:5)') erf((1:5)')]
```

```
ans =
   0.842700792949715   0.842700792949715
   0.995322265018952   0.995322265018953
   0.999977909503001   0.999977909503001
   0.999999984582742   0.999999984582742
   0.999999999998463   0.999999999998463
```

Here is the integral of an oscillatory step function:

```
x = chebfun('x',[0 6]);
f = x.*sign(sin(x.^2)); subplot(1,2,1), plot(f)
g = cumsum(f); subplot(1,2,2), plot(g,'m')
```





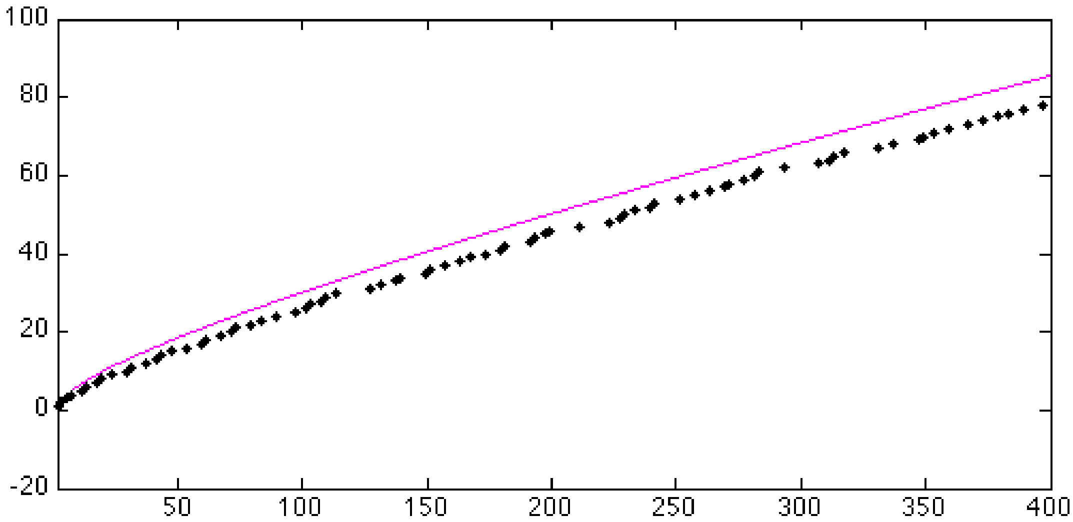
And here is an example from number theory. The logarithmic integral, $Li(x)$, is the indefinite integral from 0 to x of $1/\log(s)$. It is an approximation to $\pi(x)$, the number of primes less than or equal to x. To avoid the singularity at $x = 0$ we begin our integral at the point $\mu = 1.451...$ where $Li(x)$ is zero, known as Soldner's constant. The test value $Li(2)$ is correct except in the last digit:

```
mu = 1.45136923488338105;   % Soldner's constant
xmax = 400;
Li = cumsum(chebfun(@(x) 1./log(x),[mu xmax]));
lengthLi = length(Li)
Li2 = Li(2)
```

```
lengthLi =
   308
Li2 =
   1.045163780027057
```

(Chebfun has no trouble if `xmax` is increased to 10^5 or 10^{10}.) Here is a plot comparing $Li(x)$ with $\pi(x)$:

```
clf, plot(Li,'m')
p = primes(xmax);
hold on, plot(p,1:length(p),'.k')
```



The Prime Number Theorem implies that $\pi(x) \sim Li(x)$ as $x \to \infty$. Littlewood proved in 1914 that although $Li(x)$ is greater than $\pi(x)$ at first, the two curves eventually cross each other infinitely often. It is known that the first crossing occurs somewhere between $x = 10^{14}$ and $x = 2 \times 10^{316}$ [Kotnik 2008].

The `mean`, `std`, and `var` commands have also been overloaded for chebfuns and are based on integrals. For example

```
mean(chebfun('cos(x).^2',[0,10*pi]))
```

```
ans =
   0.500000000000000
```

2.4 diff

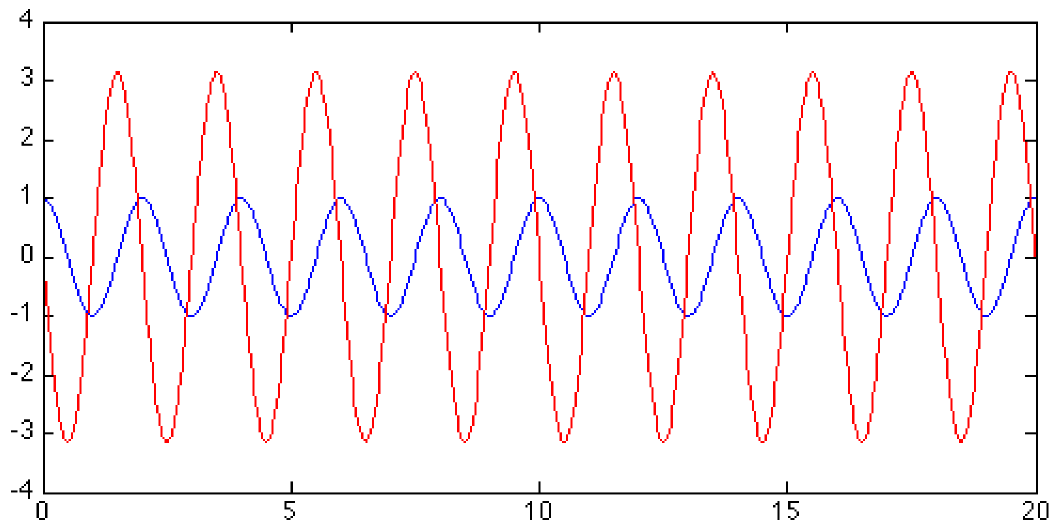
In Matlab, `diff` gives finite differences of a vector:

```
v = [1 2 3 5]
diff(v)
```

```
v =
     1     2     3     5
ans =
     1     1     2
```

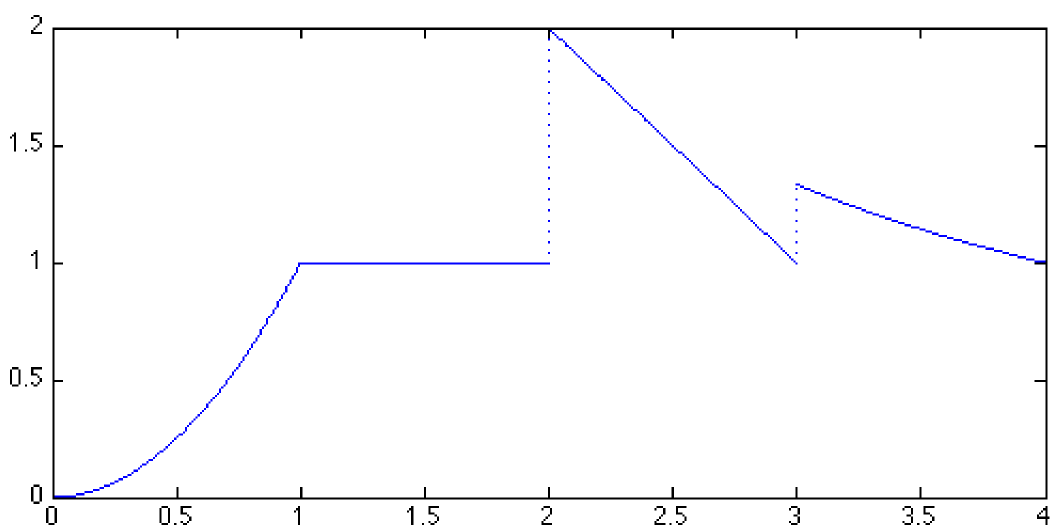
The continuous analogue of this operation is differentiation. For example:

```
f = chebfun('cos(pi*x)',[0 20]);
fprime = diff(f);
hold off, plot(f)
hold on, plot(fprime,'r')
```



If the derivative of a function with a jump is computed, then a delta function is introduced. Consider for example this function defined piecewise:

```
f = chebfun({@(x) x.^2, @(x) 1+0*x, @(x) 4-x, @(x) 4./x},0:4);
hold off, plot(f)
```



Here is the derivative:

```
  fprime = diff(f);
% plot(fprime,'r'), ylim([-2,3])
```

The first segment of f' is linear, since f is quadratic here. Then comes a segment with $f' = 0$, since f is constant. And the end of this second segment appears a delta function of amplitude 1, corresponding to the jump of f by 1. The third segment has constant value $f' = -1$. Finally another delta function, this time with amplitude $1/3$, takes us to the final segment.

Thanks to the delta functions, `cumsum` and `diff` are essentially inverse operations. It is no surprise that differentiating an indefinite integral returns us to the original function:

```
norm(f-diff(cumsum(f)))
```

```
ans =
     3.257618164241706e-14
```

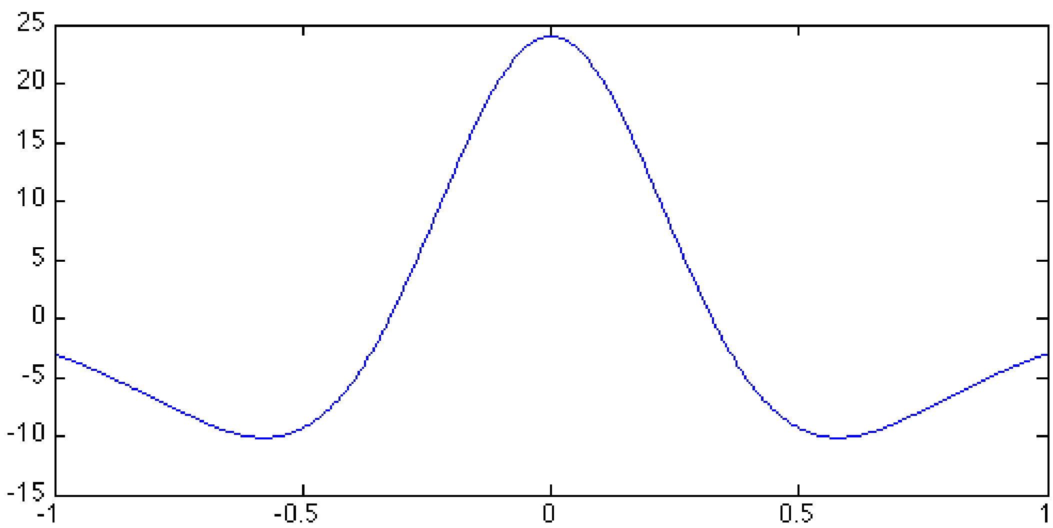
More surprising is that integrating a derivative does the same, so long as we add in the value at the left endpoint:

```
d = domain(f);
f2 = f(d(1)) + cumsum(diff(f));
norm(f-f2)
```

```
ans =
   1.000000000000004
```

Multiple derivatives can be obtained by adding a second argument to `diff`. Thus for example,

```
f = chebfun('1./(1+x.^2)');
g = diff(f,4); plot(g)
```



However, one should be cautious about the potential loss of information in repeated differentiation. For example, if we evaluate this fourth derivative at $x = 0$ we get an answer that matches the correct value 24 only to 11 places:

```
g(0)
```

```
ans =
  24.000000000057252
```

For a more extreme example, suppose we define a chebfun for $\exp(x)$ on $[-1, 1]$:

```
f = chebfun('exp(x)');
length(f)
```

```
ans =
    15
```

Since f is a polynomial of low degree, it cannot help but lose information rather fast as we differentiate, and 15 differentiations eliminate the function entirely.

```
for j = 0:length(f)
  fprintf('%6d %19.12f\n', j,f(1))
  f = diff(f);
end
```

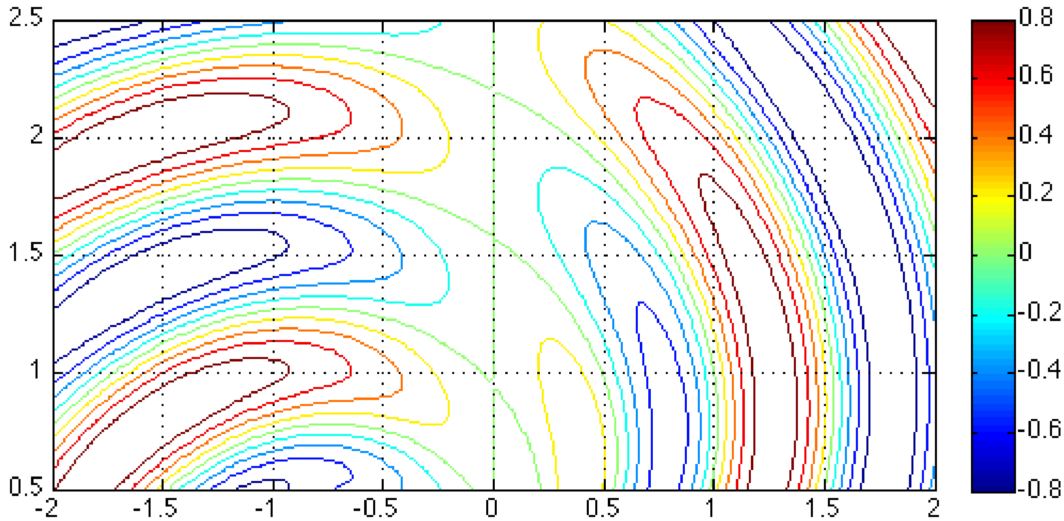
```
     0      2.718281828459
     1      2.718281828459
     2      2.718281828457
     3      2.718281828387
     4      2.718281826584
     5      2.718281790190
     6      2.718281193863
     7      2.718273153877
     8      2.718183811140
     9      2.717370444998
    10      2.711382775996
    11      2.676512700946
    12      2.521466381039
    13      2.025715330339
    14      1.008396873546
    15      0.000000000000
```

Is such behavior "wrong"? Well, that is an interesting question. Chebfun is behaving correctly in the sense mentioned in the second paragraph of Section 1.1: the operations are individually stable in that each differentiation returns the exact derivative of a function very close to the right one. The trouble is that because of the intrinsically ill-posed nature of differentiation, the errors in these stable operations accumulate exponentially as successive derivatives are taken.

2.5 Integrals in two dimensions

Chebfun can often do a pretty good job with integrals over rectangles. Here for example is a colorful function:

```
r = @(x,y) sqrt(x.^2+y.^2); theta = @(x,y) atan2(y,x);
f = @(x,y) sin(5*(theta(x,y)-r(x,y))).*sin(x);
x = -2:.02:2; y = 0.5:.02:2.5; [xx,yy] = meshgrid(x,y);
clf, contour(x,y,f(xx,yy),-1:.2:1)
axis([-2 2 0.5 2.5]), colorbar, grid on
```



Using 1D Chebfun technology, we can compute the integral over the box like this. Notice the use of the flag `vectorize` to construct a chebfun from a function only defined for scalar arguments.

```
Iy = @(y) sum(chebfun(@(x) f(x,y),[-2 2]));
tic, I = sum(chebfun(@(y) Iy(y),[0.5 2.5],'vectorize')); t = toc;
fprintf('CHEBFUN:  I = %16.14f  time = %5.3f secs\n',I,t)
```

```
CHEBFUN:  I = 0.02041246545700  time = 0.503 secs
```

Here for comparison is Matlab's `dblquad/quadl` with a tolerance of 10^{-11}:

```
tic, I = dblquad(f,-2,2,0.5,2.5,1e-11,@quadl); t = toc;
fprintf('DBLQUAD/QUADL:  I = %16.14f  time = %5.3f secs\n',I,t)
```

```
DBLQUAD/QUADL:  I = 0.02041246545700  time = 4.503 secs
```

This example of a 2D integrand is smooth, so both Chebfun and `dblquad` can handle it to high accuracy.

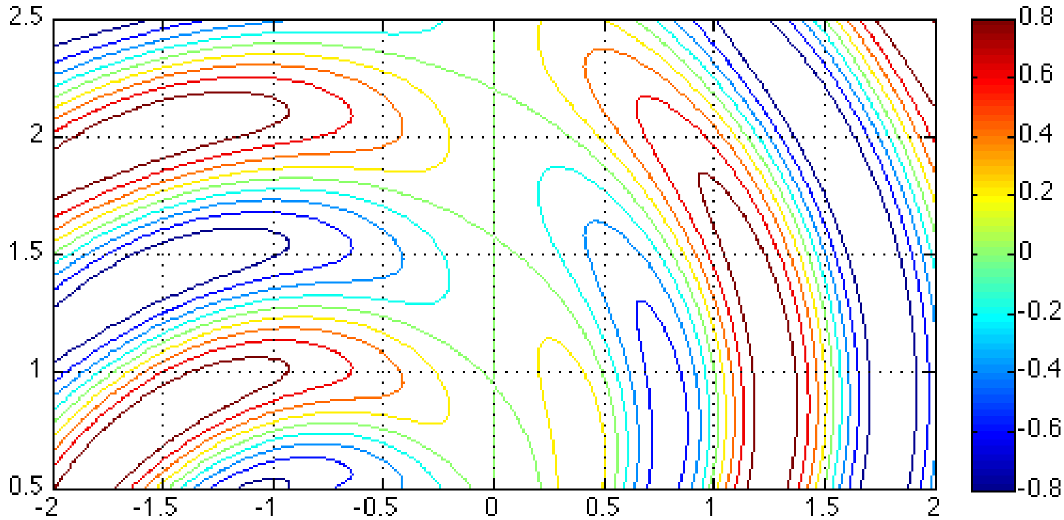
A much better approach for this problem, however, is to use Chebfun2, which is described in the Chebfun2 chapters of this guide. With this method we can compute the integral quickly,

```
tic
f2 = chebfun2(f,[-2 2 0.5 2.5]);
sum2(f2)
toc
```

```
ans =
   0.020412465456998
Elapsed time is 0.267550 seconds.
```

and we can plot the function without the need for `meshgrid` :

```
contour(f2,-1:.2:1), colorbar, grid on
```



2.6 Gauss and Gauss-Jacobi quadrature

For quadrature experts, Chebfun contains some powerful capabilities due to Nick Hale and Alex Townsend [Hale & Townsend 2013]. To start with, suppose we wish to carry out 4-point Gauss quadrature over $[-1, 1]$. The quadrature nodes are the zeros of the degree 4 Legendre polynomial `legpoly(4)` , which can be obtained from the Chebfun command `legpts` , and if two output arguments are requested, `legpts` provides weights also:

```
  [s,w] = legpts(4)
```

```
s =
  -0.861136311594053
  -0.339981043584856
   0.339981043584856
   0.861136311594053
w =
  Columns 1 through 3
   0.347854845137454   0.652145154862546   0.652145154862546
  Column 4
   0.347854845137454
```

To compute the 4-point Gauss quadrature approximation to the integral of $\exp(x)$ from -1 to 1, for example, we could now do this:

```
x = chebfun('x');
f = exp(x);
Igauss = w*f(s)
Iexact = exp(1) - exp(-1)
```

```
Igauss =
   2.350402092156377
Iexact =
   2.350402387287603
```

There is no need to stop at 4 points, however. Here we use 1000 Gauss quadrature points:

```
tic
[s,w] = legpts(1000); Igauss = w*f(s)
toc
```

```
Igauss =
   2.350402387287603
Elapsed time is 0.178298 seconds.
```

Even 100,000 points doesn't take very long:

```
tic
[s,w] = legpts(100000); Igauss = w*f(s)
toc
```

```
Igauss =
   2.350402387287603
Elapsed time is 0.243763 seconds.
```

Traditionally, numerical analysts computed Gauss quadrature nodes and weights by the eigenvalue algorithm of Golub and Welsch [Golub & Welsch 1969]. However, the Hale-Townsend algorithms are both more accurate and much faster [Hale & Townsend 2013].

For Legendre polynomials, Legendre points, and Gauss quadrature, use `legpoly` and `legpts` . For Chebyshev polynomials, Chebyshev points, and Clenshaw-Curtis quadrature, use `chebpoly` and `chebpts` and the built-in Chebfun commands such as `sum` . A third variant is also available: for Jacobi polynomials, Gauss-Jacobi points, and Gauss-Jacobi quadrature, see `jacpoly` and `jacpts` . These arise in integration of functions with singularities at one or both endpoints, and are used internally by Chebfun for integration of chebfuns with singularities (Chapter 9).

As explained in the help texts, all of these operators work on general intervals $[a, b]$, not just on $[-1, 1]$.

2.7 References

[Assheton 2008] P. Assheton, *Comparing Chebfun to Adaptive Quadrature Software*, dissertation, MSc in Mathematical Modelling and Scientific Computing, Oxford University, 2008.

[Espelid 2003] T. O. Espelid, "Doubly adaptive quadrature routines based on Newton-Cotes rules," *BIT Numerical Mathematics* 43 (2003), 319-337.

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