

The Euler–MacLaurin summation formula

Manuel Eberl

February 23, 2021

Abstract

The Euler–MacLaurin formula relates the value of a discrete sum $\sum_{i=a}^b f(i)$ to that of the integral $\int_a^b f(x) dx$ in terms of the derivatives of f at a and b and a remainder term. Since the remainder term is often very small as b grows, this can be used to compute asymptotic expansions for sums.

This entry contains a proof of this formula for functions from the reals to an arbitrary Banach space. Two variants of the formula are given: the standard textbook version and a variant outlined in *Concrete Mathematics* [3] that is more useful for deriving asymptotic estimates.

As example applications, we use that formula to derive the full asymptotic expansion of the harmonic numbers and the sum of inverse squares.

Contents

1	The Euler–MacLaurin summation formula	2
1.1	Auxiliary facts	2
1.2	The remainder terms	3
1.3	The conventional version of the Euler–MacLaurin formula	8
1.4	The “Concrete Mathematics” version of the Euler–MacLaurin formula	9
1.5	Bounds on the remainder term	12
1.6	Application to harmonic numbers	13
1.7	Application to sums of inverse squares	14
2	Connection of Euler–MacLaurin summation to Landau symbols	14
2.1	O -bound for the remainder term	15
2.2	Asymptotic expansion of the harmonic numbers	15
2.3	Asymptotic expansion of the sum of inverse squares	16

1 The Euler–MacLaurin summation formula

theory *Euler-MacLaurin*

imports

HOL-Complex-Analysis.Complex-Analysis

Bernoulli.Periodic-Bernpoly

Bernoulli.Bernoulli-FPS

begin

1.1 Auxiliary facts

lemma *pbernpoly-of-int [simp]*: $pbernpoly\ n\ (of-int\ a) = bernoulli\ n$
<proof>

lemma *continuous-on-bernpoly' [continuous-intros]*:

assumes *continuous-on A f*

shows *continuous-on A* $(\lambda x. bernpoly\ n\ (f\ x)) :: 'a :: real-normed-algebra-1$

<proof>

lemma *sum-atLeastAtMost-int-last*:

assumes $a < (b :: int)$

shows $sum\ f\ \{a..b\} = sum\ f\ \{a..<b\} + f\ b$

<proof>

lemma *sum-atLeastAtMost-int-head*:

assumes $a < (b :: int)$

shows $sum\ f\ \{a..b\} = f\ a + sum\ f\ \{a<..b\}$

<proof>

lemma *not-in-nonpos-Reals-imp-add-nonzero*:

assumes $z \notin \mathbb{R}_{\leq 0}\ x \geq 0$

shows $z + of-real\ x \neq 0$

<proof>

lemma *negligible-atLeastAtMostI*: $b \leq a \implies negligible\ \{a..(b::real)\}$

<proof>

lemma *integrable-on-negligible*:

$negligible\ A \implies (f :: 'n :: euclidean-space \Rightarrow 'a :: banach)\ integrable-on\ A$

<proof>

lemma *Union-atLeastAtMost-real-of-int*:

assumes $a < b$

shows $(\bigcup n \in \{a..<b\}. \{real-of-int\ n..real-of-int\ (n + 1)\}) = \{real-of-int\ a..real-of-int\ b\}$

<proof>

1.2 The remainder terms

The following describes the remainder term in the classical version of the Euler–MacLaurin formula.

definition *EM-remainder'* :: $\text{nat} \Rightarrow (\text{real} \Rightarrow 'a :: \text{banach}) \Rightarrow \text{real} \Rightarrow \text{real} \Rightarrow 'a$
where

$\text{EM-remainder}' n f a b = ((-1) \wedge \text{Suc } n / \text{fact } n) *_R \text{integral } \{a..b\} (\lambda t. \text{pbernpoly } n t *_R f t)$

Next, we define the remainder term that occurs when one lets the right bound of summation in the Euler–MacLaurin formula tend to infinity.

definition *EM-remainder-converges* :: $\text{nat} \Rightarrow (\text{real} \Rightarrow 'a :: \text{banach}) \Rightarrow \text{int} \Rightarrow \text{bool}$
where

$\text{EM-remainder-converges } n f a \longleftrightarrow (\exists L. ((\lambda x. \text{EM-remainder}' n f a (\text{of-int } x)) \longrightarrow L) \text{ at-top})$

definition *EM-remainder* :: $\text{nat} \Rightarrow (\text{real} \Rightarrow 'a :: \text{banach}) \Rightarrow \text{int} \Rightarrow 'a$ **where**

$\text{EM-remainder } n f a =$
(if EM-remainder-converges n f a then
Lim at-top (λx. EM-remainder' n f a (of-int x)) else 0)

The following lemmas are fairly obvious – but tedious to prove – properties of the remainder terms.

lemma *EM-remainder-eqI*:

fixes L
assumes $((\lambda x. \text{EM-remainder}' n f b (\text{of-int } x)) \longrightarrow L) \text{ at-top}$
shows $\text{EM-remainder } n f b = L$
<proof>

lemma *integrable-EM-remainder'-int*:

fixes $a b :: \text{int}$ **and** $f :: \text{real} \Rightarrow 'a :: \text{banach}$
assumes $\text{continuous-on } \{\text{of-int } a.. \text{of-int } b\} f$
shows $(\lambda t. \text{pbernpoly } n t *_R f t) \text{ integrable-on } \{a..b\}$
<proof>

lemma *integrable-EM-remainder'*:

fixes $a b :: \text{real}$ **and** $f :: \text{real} \Rightarrow 'a :: \text{banach}$
assumes $\text{continuous-on } \{a..b\} f$
shows $(\lambda t. \text{pbernpoly } n t *_R f t) \text{ integrable-on } \{a..b\}$
<proof>

lemma *EM-remainder'-bounded-linear*:

assumes $\text{bounded-linear } h$
assumes $\text{continuous-on } \{a..b\} f$
shows $\text{EM-remainder}' n (\lambda x. h (f x)) a b = h (\text{EM-remainder}' n f a b)$
<proof>

lemma *EM-remainder-converges-of-real*:

assumes *EM-remainder-converges* n f a *continuous-on* $\{of-int\ a..\}$ f
shows *EM-remainder-converges* n $(\lambda x. of-real (f\ x))$ a
 $\langle proof \rangle$

lemma *EM-remainder-converges-of-real-iff*:
fixes $f :: real \Rightarrow real$
assumes *continuous-on* $\{of-int\ a..\}$ f
shows *EM-remainder-converges* n $(\lambda x. of-real (f\ x)) ::$
 $'a :: \{banach, real-normed-algebra-1, real-inner\}$ $a \longleftrightarrow EM-remainder-converges$
 $n\ f\ a$
 $\langle proof \rangle$

lemma *EM-remainder-of-real*:
assumes *continuous-on* $\{a..\}$ f
shows *EM-remainder* n $(\lambda x. of-real (f\ x)) ::$
 $'a :: \{banach, real-normed-algebra-1, real-inner\}$ $a =$
 $of-real (EM-remainder\ n\ f\ a)$
 $\langle proof \rangle$

lemma *EM-remainder'-cong*:
assumes $\bigwedge x. x \in \{a..b\} \implies f\ x = g\ x\ n = n'\ a = a'\ b = b'$
shows *EM-remainder'* $n\ f\ a\ b = EM-remainder'\ n'\ g\ a'\ b'$
 $\langle proof \rangle$

lemma *EM-remainder-converges-cong*:
assumes $\bigwedge x. x \geq of-int\ a \implies f\ x = g\ x\ n = n'\ a = a'$
shows *EM-remainder-converges* $n\ f\ a = EM-remainder-converges\ n'\ g\ a'$
 $\langle proof \rangle$

lemma *EM-remainder-cong*:
assumes $\bigwedge x. x \geq of-int\ a \implies f\ x = g\ x\ n = n'\ a = a'$
shows *EM-remainder* $n\ f\ a = EM-remainder\ n'\ g\ a'$
 $\langle proof \rangle$

lemma *EM-remainder-converges-cnj*:
assumes *continuous-on* $\{a..\}$ f **and** *EM-remainder-converges* $n\ f\ a$
shows *EM-remainder-converges* n $(\lambda x. cnj (f\ x))\ a$
 $\langle proof \rangle$

lemma *EM-remainder-converges-cnj-iff*:
assumes *continuous-on* $\{of-int\ a..\}$ f
shows *EM-remainder-converges* n $(\lambda x. cnj (f\ x))\ a \longleftrightarrow EM-remainder-converges$
 $n\ f\ a$
 $\langle proof \rangle$

lemma *EM-remainder-cnj*:
assumes *continuous-on* $\{a..\}$ f
shows *EM-remainder* n $(\lambda x. cnj (f\ x))\ a = cnj (EM-remainder\ n\ f\ a)$
 $\langle proof \rangle$

lemma *EM-remainder'-combine*:

fixes $f :: \text{real} \Rightarrow 'a :: \text{banach}$
assumes [*continuous-intros*]: *continuous-on* $\{a..c\} f$
assumes $a \leq b \leq c$
shows $EM\text{-remainder}' n f a b + EM\text{-remainder}' n f b c = EM\text{-remainder}' n f a c$
<proof>

lemma *uniformly-convergent-EM-remainder'*:

fixes $f :: 'a \Rightarrow \text{real} \Rightarrow 'b :: \{\text{banach}, \text{real-normed-algebra}\}$
assumes *deriv*: $\bigwedge y. a \leq y \implies (G \text{ has-real-derivative } g y) \text{ (at } y \text{ within } \{a..\})$
assumes *integrable*: $\bigwedge a' b y. y \in A \implies a \leq a' \implies a' \leq b \implies$
 $(\lambda t. \text{pbernpoly } n t *_R f y t) \text{ integrable-on } \{a'..b\}$
assumes *conv*: *convergent* $(\lambda y. G (\text{real } y))$
assumes *bound*: *eventually* $(\lambda x. \forall y \in A. \text{norm } (f y x) \leq g x) \text{ at-top}$
shows *uniformly-convergent-on* $A (\lambda b s. EM\text{-remainder}' n (f s) a b)$
<proof>

lemma *uniform-limit-EM-remainder*:

fixes $f :: 'a \Rightarrow \text{real} \Rightarrow 'b :: \{\text{banach}, \text{real-normed-algebra}\}$
assumes *deriv*: $\bigwedge y. a \leq y \implies (G \text{ has-real-derivative } g y) \text{ (at } y \text{ within } \{a..\})$
assumes *integrable*: $\bigwedge a' b y. y \in A \implies a \leq a' \implies a' \leq b \implies$
 $(\lambda t. \text{pbernpoly } n t *_R f y t) \text{ integrable-on } \{a'..b\}$
assumes *conv*: *convergent* $(\lambda y. G (\text{real } y))$
assumes *bound*: *eventually* $(\lambda x. \forall y \in A. \text{norm } (f y x) \leq g x) \text{ at-top}$
shows *uniform-limit* $A (\lambda b s. EM\text{-remainder}' n (f s) a b)$
 $(\lambda s. EM\text{-remainder } n (f s) a) \text{ sequentially}$
<proof>

lemma *tendsto-EM-remainder*:

fixes $f :: \text{real} \Rightarrow 'b :: \{\text{banach}, \text{real-normed-algebra}\}$
assumes *deriv*: $\bigwedge y. a \leq y \implies (G \text{ has-real-derivative } g y) \text{ (at } y \text{ within } \{a..\})$
assumes *integrable*: $\bigwedge a' b . a \leq a' \implies a' \leq b \implies$
 $(\lambda t. \text{pbernpoly } n t *_R f t) \text{ integrable-on } \{a'..b\}$
assumes *conv*: *convergent* $(\lambda y. G (\text{real } y))$
assumes *bound*: *eventually* $(\lambda x. \text{norm } (f x) \leq g x) \text{ at-top}$
shows *filterlim* $(\lambda b. EM\text{-remainder}' n f a b)$
 $(\text{nhds } (EM\text{-remainder } n f a)) \text{ sequentially}$
<proof>

lemma *EM-remainder-0* [*simp*]: $EM\text{-remainder } n (\lambda x. 0) a = 0$

<proof>

lemma *holomorphic-EM-remainder'*:

assumes *deriv*:
 $\bigwedge z t. z \in U \implies t \in \{a..x\} \implies$
 $((\lambda z. f z t) \text{ has-field-derivative } f' z t) \text{ (at } z \text{ within } U)$
assumes *int*: $\bigwedge b c z e. a \leq b \implies c \leq x \implies z \in U \implies$

$(\lambda t. \text{of-real } (\text{bernpoly } n \ (t - e)) * f \ z \ t) \text{ integrable-on } \{b..c\}$
assumes *cont*: *continuous-on* $(U \times \{a..x\}) \ (\lambda(z, t). f' \ z \ t)$
assumes *convex* U
shows $(\lambda s. \text{EM-remainder}' \ n \ (f \ s) \ a \ x) \text{ holomorphic-on } U$
 $\langle \text{proof} \rangle$

lemma

assumes *deriv*: $\bigwedge y. a \leq y \implies (G \text{ has-real-derivative } g \ y) \ (\text{at } y \ \text{within } \{a..x\})$
assumes *deriv'*:
 $\bigwedge z \ t \ x. z \in U \implies x \geq a \implies t \in \{a..x\} \implies$
 $((\lambda z. f \ z \ t) \text{ has-field-derivative } f' \ z \ t) \ (\text{at } z \ \text{within } U)$
assumes *cont*: *continuous-on* $(U \times \{\text{of-int } a..\}) \ (\lambda(z, t). f' \ z \ t)$
assumes *int*: $\bigwedge b \ c \ z \ e. a \leq b \implies z \in U \implies$
 $(\lambda t. \text{of-real } (\text{bernpoly } n \ (t - e)) * f \ z \ t) \text{ integrable-on } \{b..c\}$
assumes *int'*: $\bigwedge a' \ b \ y. y \in U \implies a \leq a' \implies a' \leq b \implies$
 $(\lambda t. \text{pbernpoly } n \ t *_{\mathbb{R}} f \ y \ t) \text{ integrable-on } \{a'..b\}$
assumes *conv*: *convergent* $(\lambda y. G \ (\text{real } y))$
assumes *bound*: *eventually* $(\lambda x. \forall y \in U. \text{norm } (f \ y \ x) \leq g \ x) \ \text{at-top}$
assumes *open* U
shows *analytic-EM-remainder*: $(\lambda s :: \text{complex}. \text{EM-remainder } n \ (f \ s) \ a) \ \text{analytic-on } U$
and *holomorphic-EM-remainder*: $(\lambda s :: \text{complex}. \text{EM-remainder } n \ (f \ s) \ a) \ \text{holomorphic-on } U$
 $\langle \text{proof} \rangle$

The following lemma is the first step in the proof of the Euler–MacLaurin formula: We show the relationship between the first-order remainder term and the difference of the integral and the sum.

context

fixes $f \ f' :: \text{real} \Rightarrow 'a :: \text{banach}$
fixes $a \ b :: \text{int}$ **and** $I \ S :: 'a$
fixes $Y :: \text{real set}$
assumes $a \leq b$
assumes *fin*: *finite* Y
assumes *cont*: *continuous-on* $\{\text{real-of-int } a..\text{real-of-int } b\} \ f$
assumes *deriv* [*derivative-intros*]:
 $\bigwedge x :: \text{real}. x \in \{a..b\} - Y \implies (f \ \text{has-vector-derivative } f' \ x) \ (\text{at } x)$
defines *S-def*: $S \equiv (\sum_{i \in \{a <..b\}}. f \ i)$ **and** *I-def*: $I \equiv \text{integral } \{a..b\} \ f$
begin

lemma

diff-sum-integral-has-integral-int:
 $((\lambda t. (\text{frac } t - 1/2) *_{\mathbb{R}} f' \ t) \text{ has-integral } (S - I - (f \ b - f \ a) /_{\mathbb{R}} 2)) \ \{a..b\}$
 $\langle \text{proof} \rangle$

lemma *diff-sum-integral-has-integral-int'*:

$((\lambda t. \text{pbernpoly } 1 \ t *_{\mathbb{R}} f' \ t) \text{ has-integral } (S - I - (f \ b - f \ a) /_{\mathbb{R}} 2)) \ \{a..b\}$
 $\langle \text{proof} \rangle$

lemma *EM-remainder'-Suc-0*: $EM\text{-remainder}' (Suc\ 0) f' a\ b = S - I - (f\ b - f\ a) /_R\ 2$
 ⟨proof⟩

end

Next, we show that the n -th-order remainder can be expressed in terms of the $n + 1$ -th-order remainder term. Iterating this essentially yields the Euler–MacLaurin formula.

context

fixes $f\ f' :: real \Rightarrow 'a :: banach$ **and** $a\ b :: int$ **and** $n :: nat$ **and** $A :: real\ set$
assumes $ab: a \leq b$ **and** $n: n > 0$
assumes $fin: finite\ A$
assumes $cont: continuous\text{-on}\ \{of\text{-int}\ a..of\text{-int}\ b\}\ f$
assumes $cont': continuous\text{-on}\ \{of\text{-int}\ a..of\text{-int}\ b\}\ f'$
assumes $deriv: \bigwedge x. x \in \{of\text{-int}\ a<..<>of\text{-int}\ b\} - A \implies (f\ \text{has}\text{-vector}\text{-derivative}\ f'\ x)\ (at\ x)$
begin

lemma *EM-remainder'-integral-conv-Suc*:

shows $integral\ \{a..b\}\ (\lambda t. pbernpoly\ n\ t\ *_R\ f\ t) =$
 $(bernoulli\ (Suc\ n) / real\ (Suc\ n)) *_R\ (f\ b - f\ a) -$
 $integral\ \{a..b\}\ (\lambda t. pbernpoly\ (Suc\ n)\ t\ *_R\ f'\ t) /_R\ real\ (Suc\ n)$
 ⟨proof⟩

lemma *EM-remainder'-conv-Suc*:

$EM\text{-remainder}'\ n\ f\ a\ b =$
 $((-1) \wedge Suc\ n * bernoulli\ (Suc\ n) / fact\ (Suc\ n)) *_R\ (f\ b - f\ a) +$
 $EM\text{-remainder}'\ (Suc\ n)\ f'\ a\ b$
 ⟨proof⟩

end

context

fixes $f\ f' :: real \Rightarrow 'a :: banach$ **and** $a :: int$ **and** $n :: nat$ **and** $A :: real\ set$ **and** C
assumes $n: n > 0$
assumes $fin: finite\ A$
assumes $cont: continuous\text{-on}\ \{of\text{-int}\ a..\}\ f$
assumes $cont': continuous\text{-on}\ \{of\text{-int}\ a..\}\ f'$
assumes $lim: (f \longrightarrow C)\ at\text{-top}$
assumes $deriv: \bigwedge x. x \in \{of\text{-int}\ a<..\}\ - A \implies (f\ \text{has}\text{-vector}\text{-derivative}\ f'\ x)\ (at\ x)$
begin

lemma

shows *EM-remainder-converges-iff-Suc-converges*:
 $EM\text{-remainder-converges}\ n\ f\ a \longleftrightarrow EM\text{-remainder-converges}\ (Suc\ n)\ f'\ a$
and *EM-remainder-conv-Suc*:
 $EM\text{-remainder-converges}\ n\ f\ a \implies$

$EM\text{-remainder } n f a =$
 $((-1) \wedge Suc n * bernoulli (Suc n) / fact (Suc n)) *_R (C - f a) +$
 $EM\text{-remainder } (Suc n) f' a$

<proof>

end

1.3 The conventional version of the Euler–MacLaurin formula

The following theorems are the classic Euler–MacLaurin formula that can be found, with slight variations, in many sources (e. g. [1, 2, 3]).

context

fixes $f :: real \Rightarrow 'a :: banach$

fixes $fs :: nat \Rightarrow real \Rightarrow 'a$

fixes $a b :: int$ **assumes** $ab: a \leq b$

fixes $N :: nat$ **assumes** $N: N > 0$

fixes $Y :: real\ set$ **assumes** $fin: finite\ Y$

assumes $fs\text{-}0$ [*simp*]: $fs\ 0 = f$

assumes $fs\text{-}cont$ [*continuous-intros*]:

$\bigwedge k. k \leq N \implies continuous\text{-}on\ \{real\text{-}of\text{-}int\ a..real\text{-}of\text{-}int\ b\}\ (fs\ k)$

assumes $fs\text{-}deriv$ [*derivative-intros*]:

$\bigwedge k\ x. k < N \implies x \in \{a..b\} - Y \implies (fs\ k\ has\text{-}vector\text{-}derivative\ fs\ (Suc\ k)\ x)$

(*at x*)

begin

theorem *euler-maclaurin-raw-strong-int*:

defines $S \equiv (\sum i \in \{a <..b\}. f\ (of\text{-}int\ i))$

defines $I \equiv integral\ \{of\text{-}int\ a..of\text{-}int\ b\}\ f$

defines $c' \equiv \lambda k. (bernoulli' (Suc\ k) / fact (Suc\ k)) *_R (fs\ k\ b - fs\ k\ a)$

shows $S - I = (\sum k < N. c' k) + EM\text{-remainder}'\ N\ (fs\ N)\ a\ b$

<proof>

end

theorem *euler-maclaurin-strong-raw-nat*:

assumes $a \leq b\ 0 < N\ finite\ Y\ fs\ 0 = f$

$(\bigwedge k. k \leq N \implies continuous\text{-}on\ \{real\ a..real\ b\}\ (fs\ k))$

$(\bigwedge k\ x. k < N \implies x \in \{real\ a..real\ b\} - Y \implies$

$(fs\ k\ has\text{-}vector\text{-}derivative\ fs\ (Suc\ k)\ x)\ (at\ x))$

shows $(\sum i \in \{a <..b\}. f\ (real\ i)) - integral\ \{real\ a..real\ b\}\ f =$

$(\sum k < N. (bernoulli' (Suc\ k) / fact (Suc\ k)) *_R (fs\ k\ (real\ b) - fs\ k\ (real$

$a))) +$

$EM\text{-remainder}'\ N\ (fs\ N)\ (real\ a)\ (real\ b)$

<proof>

1.4 The “Concrete Mathematics” version of the Euler–MacLaurin formula

As explained in *Concrete Mathematics* [3], the above form of the formula has some drawbacks: When applying it to determine the asymptotics of some concrete function, one is usually left with several different unwieldy constant terms that are difficult to get rid of.

There is no general way to determine what these constant terms are, but in concrete applications, they can often be determined or estimated by other means. We can therefore simply group all the constant terms into a single constant and have the user provide a proof of what it is.

```

locale euler-maclaurin-int =
  fixes F f :: real  $\Rightarrow$  'a :: banach
  fixes fs :: nat  $\Rightarrow$  real  $\Rightarrow$  'a
  fixes a :: int
  fixes N :: nat assumes N: N > 0
  fixes C :: 'a
  fixes Y :: real set assumes fin: finite Y
  assumes fs-0 [simp]: fs 0 = f
  assumes fs-cont [continuous-intros]:
     $\bigwedge k. k \leq N \implies \text{continuous-on } \{\text{real-of-int } a..\} (fs\ k)$ 
  assumes fs-deriv [derivative-intros]:
     $\bigwedge k\ x. k < N \implies x \in \{\text{of-int } a..\} - Y \implies (fs\ k\ \text{has-vector-derivative } fs\ (Suc\ k)\ x)\ (at\ x)$ 
  assumes F-cont [continuous-intros]: continuous-on  $\{\text{of-int } a..\} F$ 
  assumes F-deriv [derivative-intros]:
     $\bigwedge x. x \in \{\text{of-int } a..\} - Y \implies (F\ \text{has-vector-derivative } f\ x)\ (at\ x)$ 
  assumes limit:
     $((\lambda b. (\sum_{k=a..b} f\ k) - F\ (\text{of-int } b) -$ 
       $(\sum_{i < N} (\text{bernoulli}'\ (Suc\ i) / \text{fact}\ (Suc\ i)) *_R fs\ i\ (\text{of-int } b))) \longrightarrow C)$ 
  at-top
begin

context
  fixes C' T
  defines C'  $\equiv -f\ a + F\ a + C + (\sum_{k < N} (\text{bernoulli}'\ (Suc\ k) / \text{fact}\ (Suc\ k))$ 
   $*_R (fs\ k\ (\text{of-int } a)))$ 
  and T  $\equiv (\lambda x. \sum_{i < N} (\text{bernoulli}'\ (Suc\ i) / \text{fact}\ (Suc\ i)) *_R fs\ i\ x)$ 
begin

lemma euler-maclaurin-strong-int-aux:
  assumes ab: a  $\leq$  b
  defines S  $\equiv (\sum_{k=a..b} f\ (\text{of-int } k))$ 
  shows S - F (of-int b) - T (of-int b) = EM-remainder' N (fs N) (of-int a)
  (of-int b) + (C - C')
  <proof>

lemma EM-remainder-limit:

```

assumes $ab: a \leq b$
defines $D \equiv EM\text{-remainder}' N (fs N) (of\text{-int } a) (of\text{-int } b)$
shows $EM\text{-remainder } N (fs N) b = C' - D$
and $EM\text{-remainder-converges: } EM\text{-remainder-converges } N (fs N) b$
 $\langle proof \rangle$

theorem *euler-maclaurin-strong-int*:
assumes $ab: a \leq b$
defines $S \equiv (\sum_{k=a..b} f (of\text{-int } k))$
shows $S = F (of\text{-int } b) + C + T (of\text{-int } b) - EM\text{-remainder } N (fs N) b$
 $\langle proof \rangle$

end
end

The following version of the formula removes all the terms where the associated Bernoulli numbers vanish.

locale *euler-maclaurin-int'* =
fixes $F f :: real \Rightarrow 'a :: banach$
fixes $fs :: nat \Rightarrow real \Rightarrow 'a$
fixes $a :: int$
fixes $N :: nat$
fixes $C :: 'a$
fixes $Y :: real \text{ set}$ **assumes** $fin: finite Y$
assumes $fs\text{-}0 [simp]: fs 0 = f$
assumes $fs\text{-}cont [continuous\text{-}intros]:$
 $\bigwedge k. k \leq 2*N+1 \implies continuous\text{-}on \{real\text{-}of\text{-}int a..\} (fs k)$
assumes $fs\text{-}deriv [derivative\text{-}intros]:$
 $\bigwedge k x. k \leq 2*N \implies x \in \{of\text{-}int a..\} - Y \implies (fs k \text{ has-vector-derivative } fs (Suc k) x) (at x)$
assumes $F\text{-}cont [continuous\text{-}intros]: continuous\text{-}on \{of\text{-}int a..\} F$
assumes $F\text{-}deriv [derivative\text{-}intros]:$
 $\bigwedge x. x \in \{of\text{-}int a..\} - Y \implies (F \text{ has-vector-derivative } f x) (at x)$
assumes $limit:$
 $((\lambda b. (\sum_{k=a..b} f k) - F (of\text{-int } b) -$
 $(\sum_{i < 2*N+1} (bernoulli' (Suc i) / fact (Suc i)) *_R fs i (of\text{-int } b))) \longrightarrow$
 $C) \text{ at-top}$

begin

sublocale *euler-maclaurin-int* $F f fs a 2*N+1 C Y$
 $\langle proof \rangle$

theorem *euler-maclaurin-strong-int'*:
assumes $a \leq b$
shows $(\sum_{k=a..b} f (of\text{-int } k)) =$
 $F (of\text{-int } b) + C + (1 / 2) *_R f (of\text{-int } b) +$
 $(\sum_{i=1..N} (bernoulli (2*i) / fact (2*i)) *_R fs (2*i-1) (of\text{-int } b)) -$
 $EM\text{-remainder } (2*N+1) (fs (2*N+1)) b$
 $\langle proof \rangle$

end

For convenience, we also offer a version where the sum ranges over natural numbers instead of integers.

lemma *sum-atLeastAtMost-of-int-nat-transfer*:

$$(\sum k=int\ a..int\ b.\ f\ (of-int\ k)) = (\sum k=a..b.\ f\ (of-nat\ k))$$

<proof>

lemma *euler-maclaurin-nat-int-transfer*:

fixes F **and** $f :: real \Rightarrow 'a :: real-normed-vector$
assumes $((\lambda b. (\sum k=a..b.\ f\ (real\ k)) - F\ (real\ b) - T\ (real\ b)) \longrightarrow C)$ *at-top*
shows $((\lambda b. (\sum k=int\ a..b.\ f\ (of-int\ k)) - F\ (of-int\ b) - T\ (of-int\ b)) \longrightarrow C)$ *at-top*
<proof>

locale *euler-maclaurin-nat* =

fixes $F\ f :: real \Rightarrow 'a :: banach$
fixes $fs :: nat \Rightarrow real \Rightarrow 'a$
fixes $a :: nat$
fixes $N :: nat$ **assumes** $N: N > 0$
fixes $C :: 'a$
fixes $Y :: real\ set$ **assumes** $fin: finite\ Y$
assumes $fs-0$ [*simp*]: $fs\ 0 = f$
assumes $fs-cont$ [*continuous-intros*]:
 $\bigwedge k. k \leq N \implies continuous-on\ \{real\ a..\}\ (fs\ k)$
assumes $fs-deriv$ [*derivative-intros*]:
 $\bigwedge k\ x. k < N \implies x \in \{real\ a..\} - Y \implies (fs\ k\ has-vector-derivative\ fs\ (Suc\ k)\ x)$ (*at\ x*)
assumes $F-cont$ [*continuous-intros*]: $continuous-on\ \{real\ a..\}\ F$
assumes $F-deriv$ [*derivative-intros*]:
 $\bigwedge x. x \in \{real\ a..\} - Y \implies (F\ has-vector-derivative\ f\ x)$ (*at\ x*)
assumes *limit*:
 $((\lambda b. (\sum k=a..b.\ f\ k) - F\ (real\ b) - (\sum i < N. (bernoulli'\ (Suc\ i) / fact\ (Suc\ i)) *_R\ fs\ i\ (real\ b)))) \longrightarrow C)$ *at-top*

begin

sublocale *euler-maclaurin-int* $F\ f\ fs\ int\ a\ N\ C\ Y$

<proof>

theorem *euler-maclaurin-strong-nat*:

assumes $ab: a \leq b$
defines $S \equiv (\sum k=a..b.\ f\ (real\ k))$
shows $S = F\ (real\ b) + C + (\sum i < N. (bernoulli'\ (Suc\ i) / fact\ (Suc\ i)) *_R\ fs\ i\ (real\ b)) - EM-remainder\ N\ (fs\ N)\ (int\ b)$
<proof>

end

```

locale euler-maclaurin-nat' =
  fixes F f :: real ⇒ 'a :: banach
  fixes fs :: nat ⇒ real ⇒ 'a
  fixes a :: nat
  fixes N :: nat
  fixes C :: 'a
  fixes Y :: real set assumes fin: finite Y
  assumes fs-0 [simp]: fs 0 = f
  assumes fs-cont [continuous-intros]:
    ∧k. k ≤ 2*N+1 ⇒ continuous-on {real a..} (fs k)
  assumes fs-deriv [derivative-intros]:
    ∧k x. k ≤ 2*N ⇒ x ∈ {real a..} - Y ⇒ (fs k has-vector-derivative fs (Suc
k) x) (at x)
  assumes F-cont [continuous-intros]: continuous-on {real a..} F
  assumes F-deriv [derivative-intros]:
    ∧x. x ∈ {real a..} - Y ⇒ (F has-vector-derivative f x) (at x)
  assumes limit:
    ((λb. (∑ k=a..b. f k) - F (real b) -
      (∑ i<2*N+1. (bernoulli' (Suc i) / fact (Suc i)) *R fs i (real b))) → C)
at-top
begin

```

```

sublocale euler-maclaurin-int' F f fs int a N C Y
  ⟨proof⟩

```

```

theorem euler-maclaurin-strong-nat':
  assumes a ≤ b
  shows (∑ k=a..b. f (real k)) =
    F (real b) + C + (1 / 2) *R f (real b) +
    (∑ i=1..N. (bernoulli (2*i) / fact (2*i)) *R fs (2*i-1) (real b)) -
    EM-remainder (2*N+1) (fs (2*N+1)) b
  ⟨proof⟩

```

```

end

```

1.5 Bounds on the remainder term

The following theorems provide some simple means to bound the remainder terms. In practice, better bounds can often be obtained e.g. for the n -th remainder term by expanding it to the sum of the first discarded term in the expansion and the $n + 1$ -th remainder term.

```

lemma
  fixes f :: real ⇒ 'a :: {real-normed-field, banach}
  and g g' :: real ⇒ real
  assumes fin: finite Y
  assumes pbernpoly-bound: ∀ x. |pbernpoly n x| ≤ D
  assumes cont-f: continuous-on {a..} f

```

assumes *cont-g*: *continuous-on* {*a..*} *g*
assumes *cont-g'*: *continuous-on* {*a..*} *g'*
assumes *limit-g*: (*g* \longrightarrow *C*) *at-top*
assumes *f-bound*: $\bigwedge x. x \geq a \implies \text{norm } (f x) \leq g' x$
assumes *deriv*: $\bigwedge x. x \in \{a..\} - Y \implies (g \text{ has-field-derivative } g' x) (at x)$
shows *norm-EM-remainder-le-strong-int*:
 $\forall x. \text{of-int } x \geq a \longrightarrow \text{norm } (EM\text{-remainder } n f x) \leq D / \text{fact } n * (C - g$
x)
and *norm-EM-remainder-le-strong-nat*:
 $\forall x. \text{real } x \geq a \longrightarrow \text{norm } (EM\text{-remainder } n f (\text{int } x)) \leq D / \text{fact } n * (C$
 $- g x)$
<proof>

lemma

fixes *f* :: *real* \Rightarrow '*a* :: {*real-normed-field, banach*}
and *g g'* :: *real* \Rightarrow *real*
assumes *fin*: *finite* *Y*
assumes *pbernpoly-bound*: $\forall x. |pbernpoly n x| \leq D$
assumes *cont-f*: *continuous-on* {*a..*} *f*
assumes *cont-g*: *continuous-on* {*a..*} *g*
assumes *cont-g'*: *continuous-on* {*a..*} *g'*
assumes *limit-g*: (*g* \longrightarrow 0) *at-top*
assumes *f-bound*: $\bigwedge x. x \geq a \implies \text{norm } (f x) \leq g' x$
assumes *deriv*: $\bigwedge x. x \in \{a..\} - Y \implies (g \text{ has-field-derivative } -g' x) (at x)$
shows *norm-EM-remainder-le-strong-int'*:
 $\forall x. \text{of-int } x \geq a \longrightarrow \text{norm } (EM\text{-remainder } n f x) \leq D / \text{fact } n * g x$
and *norm-EM-remainder-le-strong-nat'*:
 $\forall x. \text{real } x \geq a \longrightarrow \text{norm } (EM\text{-remainder } n f (\text{int } x)) \leq D / \text{fact } n * g x$
<proof>

lemma *norm-EM-remainder'-le*:

fixes *f* :: *real* \Rightarrow '*a* :: {*real-normed-field, banach*}
and *g g'* :: *real* \Rightarrow *real*
assumes *cont-f*: *continuous-on* {*a..*} *f*
assumes *cont-g'*: *continuous-on* {*a..*} *g'*
assumes *f-bigo*: *eventually* ($\lambda x. \text{norm } (f x) \leq g' x$) *at-top*
assumes *deriv*: *eventually* ($\lambda x. (g \text{ has-field-derivative } g' x) (at x)$) *at-top*
obtains *C D* **where**
 $\text{eventually } (\lambda x. \text{norm } (EM\text{-remainder}' n f a x) \leq C + D * g x)$ *at-top*
<proof>

1.6 Application to harmonic numbers

As a first application, we can apply the machinery we have developed to the harmonic numbers.

definition *harm-remainder* :: *nat* \Rightarrow *nat* \Rightarrow *real* **where**

$\text{harm-remainder } N n = EM\text{-remainder } (2*N+1) (\lambda x. -\text{fact } (2*N+1) / x \wedge$
 $(2*N+2)) (\text{int } n)$

lemma *harm-expansion*:
assumes $n: n > 0$ **and** $N: N > 0$
shows $\text{harm } n = \ln n + \text{euler-mascheroni} + 1 / (2*n) -$
 $(\sum_{i=1..N}. \text{bernoulli } (2*i) / ((2*i) * n ^ (2*i))) - \text{harm-remainder}$
 $N n$
 $\langle \text{proof} \rangle$

lemma *of-nat-ge-1-iff*: *of-nat* $x \geq (1 :: 'a :: \text{linordered-semidom}) \iff x \geq 1$
 $\langle \text{proof} \rangle$

lemma *harm-remainder-bound*:
fixes $N :: \text{nat}$
assumes $N: N > 0$
shows $\exists C. \forall n \geq 1. \text{norm } (\text{harm-remainder } N n) \leq C / \text{real } n ^ (2*N+1)$
 $\langle \text{proof} \rangle$

1.7 Application to sums of inverse squares

In the same vein, we can derive the asymptotics of the partial sum of inverse squares.

lemma *sum-inverse-squares-expansion*:
assumes $n: n > 0$ **and** $N: N > 0$
shows $(\sum_{k=1..n}. 1 / \text{real } k ^ 2) =$
 $\pi ^ 2 / 6 - 1 / \text{real } n + 1 / (2 * \text{real } n ^ 2) -$
 $(\sum_{i=1..N}. \text{bernoulli } (2*i) / n ^ (2*i+1)) -$
 $\text{EM-remainder } (2*N+1) (\lambda x. -\text{fact } (2*N+2) / x ^ (2*N+3)) (\text{int}$
 $n)$
 $\langle \text{proof} \rangle$

lemma *sum-inverse-squares-remainder-bound*:
fixes $N :: \text{nat}$
assumes $N: N > 0$
defines $R \equiv (\lambda n. \text{EM-remainder } (2*N+1) (\lambda x. -\text{fact } (2*N+2) / x ^ (2*N+3))$
 $(\text{int } n))$
shows $\exists C. \forall n \geq 1. \text{norm } (R n) \leq C / \text{real } n ^ (2*N+2)$
 $\langle \text{proof} \rangle$

end

2 Connection of Euler–MacLaurin summation to Landau symbols

theory *Euler-MacLaurin-Landau*
imports
 Euler-MacLaurin
 $\text{Landau-Symbols.Landau-More}$
begin

2.1 O-bound for the remainder term

Landau symbols allow us to state the bounds on the remainder terms from the Euler–MacLaurin formula a bit more nicely.

lemma

fixes $f :: \text{real} \Rightarrow 'a :: \{\text{real-normed-field, banach}\}$
and $g\ g' :: \text{real} \Rightarrow \text{real}$
assumes $\text{fin}: \text{finite } Y$
assumes $\text{cont-f}: \text{continuous-on } \{a..\} f$
assumes $\text{cont-g}: \text{continuous-on } \{a..\} g$
assumes $\text{cont-g}': \text{continuous-on } \{a..\} g'$
assumes $\text{limit-g}: (g \longrightarrow 0) \text{ at-top}$
assumes $\text{f-bound}: \bigwedge x. x \geq a \implies \text{norm } (f\ x) \leq g'\ x$
assumes $\text{deriv}: \bigwedge x. x \in \{a..\} - Y \implies (g \text{ has-field-derivative } -g'\ x) \text{ (at } x)$
shows $\text{EM-remainder-strong-bigo-int}: (\lambda x::\text{int}. \text{norm } (\text{EM-remainder } n\ f\ x)) \in O(g)$
and $\text{EM-remainder-strong-bigo-nat}: (\lambda x::\text{nat}. \text{norm } (\text{EM-remainder } n\ f\ x)) \in O(g)$
 $\langle \text{proof} \rangle$

2.2 Asymptotic expansion of the harmonic numbers

We can now show the asymptotic expansion

$$H_n = \ln n + \gamma + \frac{1}{2n} - \sum_{i=1}^m \frac{B_{2i}}{2i} n^{-2i} + O(n^{-2m-2})$$

lemma *harm-remainder-bigo*:

assumes $N > 0$
shows $\text{harm-remainder } N \in O(\lambda n. 1 / \text{real } n \wedge (2 * N + 1))$
 $\langle \text{proof} \rangle$

lemma *harm-expansion-bigo*:

fixes $N :: \text{nat}$
defines $T \equiv \lambda n. \ln n + \text{euler-mascheroni} + 1 / (2 * n) -$
 $(\sum_{i=1..N}. \text{bernoulli } (2 * i) / ((2 * i) * n \wedge (2 * i)))$
defines $S \equiv (\lambda n. \text{bernoulli } (2 * (\text{Suc } N)) / ((2 * \text{Suc } N) * \text{real } n \wedge (2 * \text{Suc } N)))$
shows $(\lambda n. \text{harm } n - T\ n) \in O(\lambda n. 1 / \text{real } n \wedge (2 * N + 2))$
 $\langle \text{proof} \rangle$

lemma *harm-expansion-bigo-simple1*:

$(\lambda n. \text{harm } n - (\ln n + \text{euler-mascheroni} + 1 / (2 * n))) \in O(\lambda n. 1 / n \wedge 2)$
 $\langle \text{proof} \rangle$

lemma *harm-expansion-bigo-simple2*:

$(\lambda n. \text{harm } n - (\ln n + \text{euler-mascheroni})) \in O(\lambda n. 1 / n)$
 $\langle \text{proof} \rangle$

lemma *harm-expansion-bigo-simple'*:

harm = *o* ($\lambda n. \ln n + \text{euler-mascheroni} + 1 / (2 * n)$) + *o* ($O(\lambda n. 1 / n ^ 2)$)

<proof>

2.3 Asymptotic expansion of the sum of inverse squares

Similarly to before, we show

$$\sum_{i=1}^n \frac{1}{i^2} = \frac{\pi^2}{6} - \frac{1}{n} + \frac{1}{2n^2} - \sum_{i=1}^m B_{2i} n^{-2i-1} + O(n^{-2m-3})$$

context

fixes $R :: \text{nat} \Rightarrow \text{nat} \Rightarrow \text{real}$

defines $R \equiv (\lambda N n. \text{EM-remainder } (2*N+1) (\lambda x. -\text{fact } (2*N+2) / x ^ (2*N+3)))$
(int n)

begin

lemma *sum-inverse-squares-remainder-bigo*:

assumes $N > 0$

shows $R N \in O(\lambda n. 1 / \text{real } n ^ (2 * N + 2))$

<proof>

lemma *sum-inverse-squares-expansion-bigo*:

fixes $N :: \text{nat}$

defines $T \equiv \lambda n. \pi ^ 2 / 6 - 1 / n + 1 / (2*n ^ 2) -$
 $(\sum i=1..N. \text{bernoulli } (2*i) / (n ^ (2*i+1)))$

defines $S \equiv (\lambda n. \text{bernoulli } (2*(\text{Suc } N)) / (\text{real } n ^ (2*N+3)))$

shows $(\lambda n. (\sum i=1..n. 1 / \text{real } i ^ 2) - T n) \in O(\lambda n. 1 / \text{real } n ^ (2 * N + 3))$

<proof>

lemma *sum-inverse-squares-expansion-bigo-simple*:

$(\lambda n. (\sum i=1..n. 1 / \text{real } i ^ 2) - (\pi ^ 2 / 6 - 1 / n + 1 / (2*n ^ 2))) \in O(\lambda n. 1 / n ^ 3)$

<proof>

lemma *sum-inverse-squares-expansion-bigo-simple'*:

$(\lambda n. (\sum i=1..n. 1 / \text{real } i ^ 2)) =_o (\lambda n. \pi ^ 2 / 6 - 1 / n + 1 / (2*n ^ 2)) +_o O(\lambda n. 1 / n ^ 3)$

<proof>

end

end

References

- [1] M. Abramowitz and I. A. Stegun. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*. Dover, New York,

tenth printing edition, 1964.

- [2] T. M. Apostol. *An Elementary View of Euler's Summation Formula*. *The American Mathematical Monthly*, 106(5):409–418, 1999.
- [3] R. L. Graham, D. E. Knuth, and O. Patashnik. *Concrete Mathematics: A Foundation for Computer Science*. Addison–Wesley, Boston, MA, USA, 2nd edition, 1994.