Explicit double exponential numerical integration

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A mi familia
Rafaela, Sofía, Claudia y Rafael.

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Resumen

El método Doble Exponencial de integración numérica, descubierto por Masatake Mori y Hidetosi Takahasi hacia el año 1970, es sorprendentemente eficaz, pero no es utilizable en trabajos rigurosos al no haber constantes explícitas que acoten el error del método. En este trabajo obtenemos cotas sencillas y explícitas para este error.

Summary

The Double Exponential method of numerical integration, discovered by Masatake Mori and Hidetosi Takahasi around 1970, yields superb results. Unfortunately, the method could not be used in rigorous computations since no explicit bounds for the error were known. We give straight-forward and explicit bounds for this error.

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Introduction

The basic problem of numerical integration is to approximate $\int_a^b f(x)dx$. If f is sufficiently differentiable, and one does not require great accuracy, the usual techniques are sufficient. In number theory, however, one sometimes needs to compute such integrals with extraordinary accuracy. Even 1000 places or more may be needed to discover algebraic relations or various identities. Sometimes these are expected from standard conjectures such as Stark's [7], and sometimes they suggest new conjectures [1, p. 507]. Unfortunately, the traditional methods of numerical integration become totally useless when one needs huge accuracy.

The simplest quadrature formulas, such as the trapezoidal method, Simpson's rule or Gaussian formulas, fail to take advantage of the fact that in practice one nearly always integrates *analytic* functions. Towards the end of the 1960's and early 70's, several authors suggested taking advantage of analyticity and of changing variables [6], [2], [10], [11], [8]. Masao Iri, Sigeiti Moriguti and Yoshimitsu Takasawa [3] gave a new quadrature formula (called in 1973, by Hidetosi Takahasi and Masatake Mori, the IMT-Rule) for an integral of an analytic function f over a finite interval. They applied a change of variable $x = F(t)$ to the integral

$$\int_a^b f(x)\,dx = \int_0^\infty g(t)\,dt, \qquad (\text{where } g(t) = f\big(F(t)\big)F'(t))$$

and they approximated the latter integral simply as

$$\int_0^\infty g(t)\,dt \approx h\sum_{k=0}^{N} g(kh) \qquad (h = 1/N),$$

claiming an error bound of the form

$$\mathcal{O}\big(e^{-C_1\sqrt{N}}\big), \tag{0.0.1}$$

where C_1 is an unknown constant [5, p. 907], [11, p. 213].

Later in 1973 Takahasi and Mori described in [11] several quadratures formulas, using various changes of variable $x = F(t)$, claiming similar error bounds and specifying $C_1 = \pi$. Their functions F are much simpler than the IMT ones (they use, for example, $x = \tanh(t)$). They again do not give rigorous proofs, but point out that the common idea behind the various choices of change of variable F is to get exponential decrease of $g(t)$ as $t \to \pm\infty$. Stenger [8] around this same time makes similar claims.

A little later Takahasi and Mori [12] proposed the double exponential transformation

$$F(t) = \tanh\big(\pi \sinh(t)/2\big),$$

claiming a superb error bound of

$$\mathcal{O}\Big(\exp\big(-\frac{C_2 N}{\log(N)}\big)\Big), \tag{0.0.2}$$

again with no rigorous proofs or hypotheses, except that f be analytic. After more than twenty years, in 1997 Sugihara [9] gave a rigorous proof, specifying the constant C_2 in (0.0.2). However, he did not treat the implied $\mathcal{O}$ constant, so the method could not be used to provide rigorous numerical error bounds. His paper unfortunately couches all results in terms of the new function $g(t) = f\big(F(t)\big)F'(t)$, making the casual reader wonder what to do with his original knowledge of f, given that all he wanted was to compute $\int_a^b f(x)\,dx$.

The above story, very nicely told by Mori nearing retirement [5], went almost unnoticed outside a small circle in Japan. Many of the publications were in Japanese and few proofs were provided. The greatest recognition before around 2000 was the invitation of Mori to speak at the International Congress of Mathematicians in Kyoto in 1990 [4]. Even this was barely noticed, mainly because the numerical community has little need for computing integrals to very high accuracy.

The obscurity of the double exponential method began to change when number theorists heard of its miraculous accuracy early in the 2000's. In 2005 David Bailey and Jonathan Borwein [1, p. 507] made this rediscovery widely known and number theorist took notice. They recognized that the method worked experimentally (Henri Cohen incorporated it into the PARI software soon thereafter). Bailey and Borwein gave interesting examples in number theory by this method using 5000 decimal digits! The authors reaffirm that although the method works, it is not clear why. Only later did many people notice Sugihara's rigorous work.

In this thesis we complete Sugihara's work by giving explicit constants and simple hypotheses. We phrase our final results directly in terms of the function f. The aim is to allow the casual mathematician to easily get rigorous numerical bounds with the least work. The following is an illustration of the kind of results we will obtain, as explained after Corollary 3.3.2 below.

If the function $f(z)$ is analytic and bounded in the interior of the rectangle given by $|\mathrm{Re}(z)| < 1.51$, $|\mathrm{Im}(z)| < .49$, then for $n \geq 575$ we have the error bound

$$\Big|\int_{-1}^{1} f(x)dx - h\sum_{k=-n}^{n} g(hk)\Big| \leq 15.28\, M(f)\, \mathrm{e}^{-\pi n/\log(n)},$$

where $M(f)$ is the supremum of $|f(z)|$ for z in the rectangle, and

$$h = \frac{1}{n}\log\Big(\frac{2\pi n^2}{(n-\log(n))\log(n)}\Big), \qquad g(t) = \frac{f\big(\tanh(\sinh(t)/2)\big)\cosh(t)}{2\cosh^2\big(\sinh(t)/2\big)}.$$

The above result is stated for an integral over the interval $[-1,1]$. Of course, any integral over a *finite* interval can be brought to this form after an affine change of variable.

This thesis is divided into three chapters. In Chapter 1, we prove under appropriate hypothesis on $g(t) = f\big(F(t)\big)F'(t)$, a formula due to Mori and Takahasi for the error using the trapezoidal method over an infinite interval [12, p. 723]. Namely

$$\int_{-\infty}^{\infty} g(t)\,dt - h\sum_{k=-\infty}^{\infty} g(hk) = \frac{1}{2\pi i}\int_{\partial D_d} \phi_h(w)g(w)\,dw, \tag{0.0.3}$$

where the path ∂D_d consists of the horizontal line from $\infty + id$ to $-\infty + id$ together with the horizontal line from $-\infty - id$ to $\infty - id$, and $\phi_h(w)$ is an explicit function decaying exponentially as $h^+ \to 0$ or $|w| \to \infty$ in D_d.

In Chapters 2 and 3 this formula is applied to give explicit bounds for the simple exponential and double exponential methods.

In Chapter 2 we obtain bounds of the following kind.

Theorem 0.0.1. *Suppose that for some $0 < T \le 1$ the function $f(z)$ is analytic and bounded in the interior of the rectangle given by*

$$|\mathrm{Re}(z)| < 1, \qquad |\mathrm{Im}(z)| < T,$$

and let $d_T = 2\arctan(T)$. Then, for $n > 1/(4\pi d_T)$ we have the error bound

$$\left|\int_{-1}^{1} f(x)dx - h\sum_{k=-n}^{n} g(hk)\right| \le 16.6\, M_T(f)\, \mathrm{e}^{-\sqrt{2\pi d_T n}},$$

where $h = \sqrt{2\pi d_T/n}$, $M_T(f)$ is the supremum of $|f(z)|$ for z in the rectangle, and

$$g(t) = \frac{f\big(\tanh(t/2)\big)}{2\cosh^2(t/2)}.$$

Taking $d = \pi/2$ and being a little more careful with the domain we obtain a nice bound.

Corollary 0.0.1. *Suppose that the function $f(z)$ is analytic and bounded in the interior of the unit circle $|z| < 1$. Then, for $n \in \mathbb{N}$ we have the error bound*

$$\left|\int_{-1}^{1} f(x)dx - h\sum_{k=-n}^{n} g(hk)\right| \le 16.6\, S_{f,\pi/2}\, \mathrm{e}^{-\pi\sqrt{n}},$$

where $h = \pi/\sqrt{n}$, $g(t) = f\big(\tanh(t/2)\big)/2\cosh^2(t/2)$, and $S_{f,\pi/2}$ is the supremum of $|f(z)|$ on the unit circle.

If we have larger regions of analyticity of f, so they are not contained in rectangles with sides of length at most 2, we shall prove a slightly more complicated error bound. Namely,

Theorem 0.0.2. *Suppose that for some $T \geq 1$ the function $f(z)$ is analytic and bounded in the interior of the rectangle given by*

$$|\mathrm{Re}(z)| < (T+T^{-1})/2, \qquad |\mathrm{Im}(z)| < T,$$

and let $d_T = 2\arctan(T)$. Then, for $n \in \mathbb{N}$ we have the error bound

$$\left|\int_{-1}^{1} f(x)dx - h\sum_{k=-n}^{n} g(hk)\right| \leq 4M_T(f)\big(d_T(T+T^{-1})+1\big)\,\mathrm{e}^{-\sqrt{2\pi d_T n}},$$

where $h = \sqrt{2\pi d_T/n}$, $M_T(f)$ is the supremum of $|f(z)|$ for z in the rectangle, and

$$g(t) = \frac{f\big(\tanh(t/2)\big)}{2\cosh^2(t/2)}.$$

These bounds are much worse than those obtained with the double exponential method, but their simple proof will serve as guide and warm-up for chapter 3.

In chapter 3 we modify slightly Mori and Takahasi's choice of auxiliary function. They proposed

$$F(t) = \tanh\Big(\frac{\tau}{2}\sinh(t)\Big),$$

with τ fixed as π. We allow a variable τ in order to reduce the region in which f is required to be analytic. In the end we choose τ so as to have a small region and not too large a minimal number of steps.[1] The kind of result we will obtain at the end of this thesis is as follows.

Corollary 0.0.2. *Let $0 < d < \pi/2$ be one of the values in Table 1 and assume that f is analytic and bounded in the interior of the rectangle*

$$\big\{z \in \mathbb{C} : |\mathrm{Re}(z)| \leq a_d,\ |\mathrm{Im}(z)| \leq b_d\big\},$$

with a_d and b_d as given in Table 1. Then, we have for $n \geq N_d$ in Table 1, the error bound

$$\left|\int_{-1}^{1} f(x)dx - h\sum_{k=-n}^{n} g(hk)\right| < M_{a,b}(f)\cdot B(d)\cdot \mathrm{e}^{-2\pi d n/\log(n)},$$

where $M_{a,b}$ is the supremum of $|f(z)|$ on the rectangle, and $B(d)$ is given in Table 1.

[1] That is, not having N_d too large in Corollary 0.0.2 below.

d	a	b	N_d	$B(d)$
.1	1.42	.14	723	63.95
.2	1.43	.23	632	32.67
.3	1.44	.31	600	22.41
$\pi/8$	1.47	.39	585	17.89
.4	1.48	.4	585	17.68
.5	1.51	.49	575	15.28
$\pi/6$	1.53	.52	573	14.94
.6	1.58	.61	569	14.26
.7	1.68	.75	564	14.56
$\pi/4$	1.8	.9	561	15.69
.8	1.82	.93	560	15.98
.9	2.05	1.14	558	19.48
1	2.37	1.47	556	25.81
$\pi/3$	2.61	1.68	555	30.68
1.1	2.95	1.93	554	38.43
1.2	3.92	2.67	552	66.58
1.3	5.83	3.99	551	137.63
1.4	10.82	7.38	550	420.01
1.5	37.32	23.4	549	3587.33

Table 1: Table for Corollary 0.0.2

Chapter 1

The Mori-Takahasi Error Formula

In this section we prove that under appropriate hypotheses on g we have a nice formula for the error in the trapezoidal method [12, p. 723]. Namely

$$\int_{-\infty}^{\infty} g(t)\,dt - h\sum_{k=-\infty}^{\infty} g(hk) = \frac{1}{2\pi i}\int_{\partial D_d} \phi(w)g(w)\,dw, \tag{1.0.1}$$

where the path ∂D_d consists of the horizontal line from $\infty + id$ to $-\infty + id$ together with the horizontal line from $-\infty - id$ to $\infty - id$, and ϕ is given by

$$\phi(w) = \begin{cases} 2\pi i \exp(2\pi i w/h)/\big(1-\exp(2\pi i w/h)\big), & \mathrm{Im}(w) > 0 \\ 2\pi i \exp(-2\pi i w/h)/\big(\exp(-2\pi i w/h) - 1\big), & \mathrm{Im}(w) < 0. \end{cases} \tag{1.0.2}$$

The strength of this formula lies in the exponential decay as $h \to 0^+$ of $|\phi(w)|$ for $w \in \partial D_d$ (see (1.0.8) below).

Theorem 1.0.3. *(Mori-Takahasi) Let d, h and ε be positive real numbers, and assume that g is analytic in the strip $D_{d+\varepsilon} = \{w \in \mathbb{C} \mid |\mathrm{Im}(w)| < d+\varepsilon\}$. Assume also that*

$$\int_{-\infty}^{\infty} |g(t+ic)|\,dt < \infty \qquad \textit{for } c=-d,\ c=0 \textit{ and } c=d, \tag{1.0.3}$$

$$\int_{-d}^{d} |g(\pm M + it)|\,dt = o(1) \qquad \textit{as } M \to \infty, \tag{1.0.4}$$

$$\sum_{k=-\infty}^{\infty} |g(hk)| < \infty. \tag{1.0.5}$$

Then the Mori-Takahasi error formula (1.0.1) *holds.*

As usual, we have written $o(1)$ for a function that tends to 0 as $M \to +\infty$.

Proof. For $w \in \mathbb{C} - \mathbb{R}$, let

$$\phi_1(w) = \begin{cases} -i\pi, & \mathrm{Im}(w) > 0 \\ i\pi, & \mathrm{Im}(w) < 0 \end{cases},$$

and

$$\phi_2(w) = \pi \cot(\pi w/h).$$

One checks easily that

$$\phi(w) = \phi_1(w) - \phi_2(w).$$

The Mori-Takahasi formula will follow from

$$\frac{1}{2\pi i} \int_D \phi_1(w) g(w)\, dw = \int_{-\infty}^{\infty} g(t)\, dt, \tag{1.0.6}$$

and

$$\frac{1}{2\pi i} \int_D \phi_2(w) g(w)\, dw = h \sum_{k=-\infty}^{\infty} g(hk), \tag{1.0.7}$$

which we now prove. Note that $\cot(\pi w/h)$ is bounded on $D = \partial D_d$, so both sides of (1.0.6) and of (1.0.7) converge by assumptions (1.0.3) and (1.0.5). Take $M = M_n = h(n + \frac{1}{2})$, where $n \in \mathbb{N}$, and let C_M be the contour shown in Figure 1.1.

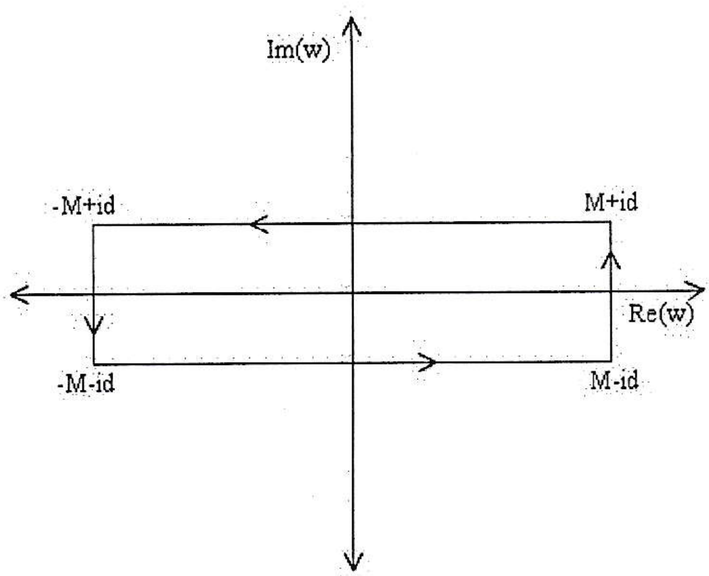

Figure 1.1: Path C_M

Since $\phi_2(w)$ has simple poles at integral multiples of h, with residue h, the residue theorem yields

$$\frac{1}{2\pi i} \int_{C_M} \phi_2(w) g(w)\, dw = h \sum_{k=-n}^{n} g(hk),$$

since g is assumed analytic in the strip $|\text{Im}(w)| < d + \varepsilon$. Claim (1.0.7) now follows on taking $n \to +\infty$, using assumption (1.0.4) and the boundedness of $\cot(\pi w/h)$ for $\text{Re}(w) = \pm M = \pm h(n + \frac{1}{2})$.

To prove (1.0.6), let C_M^+ be the part of C_M in the upper half-plane and C_M^- that in the lower half-plane. Then, since ϕ_1 is constant ($= \mp\pi i$) on each half-plane, the residue theorem again yields

$$\frac{1}{2\pi i}\int_{C_M^+}\phi_1(w)g(w)\,dw = \frac{1}{2}\int_{-M}^{M} g(t)\,dt,$$
$$\frac{1}{2\pi i}\int_{C_M^-}\phi_1(w)g(w)\,dw = \frac{1}{2}\int_{-M}^{M} g(t)\,dt.$$

Since

$$\int_{C_M}\phi_1(w)g(w)\,dw = \int_{C_M^+}\phi_1(w)g(w)\,dw + \int_{C_M^-}\phi_1(w)g(w)\,dw,$$

formula (1.0.6) again follows on taking $n \to +\infty$. □

From the definition (1.0.2) of ϕ, for $\mathrm{Im}(w) > 0$ we find

$$|\,\phi(w)| = \frac{2\pi|\,\mathrm{e}^{2\pi i w/h}|}{|\,\mathrm{e}^{2\pi i w/h} - 1|} \le \frac{2\pi \mathrm{e}^{-2\pi \mathrm{Im}(w)/h}}{1 - \mathrm{e}^{-2\pi \mathrm{Im}(w)/h}}.$$

Similarly, if $\mathrm{Im}(w) < 0$, we find

$$|\,\phi(w)| = \left|\frac{2\pi i\,\mathrm{e}^{-2\pi i w/h}}{\mathrm{e}^{-2\pi i w/h} - 1}\right| \le \frac{2\pi \mathrm{e}^{2\pi \mathrm{Im}(w)/h}}{1 - \mathrm{e}^{2\pi \mathrm{Im}(w)/h}}.$$

Combining these inequalities we find the exponential decay mentioned above, namely

$$|\,\phi(w)| \le \frac{2\pi \mathrm{e}^{-2\pi|\mathrm{Im}(w)|/h}}{1 - \mathrm{e}^{-2\pi|\mathrm{Im}(w)|/h}}, \tag{1.0.8}$$

for all $w \in \mathbb{C}$ with $\mathrm{Im}(w) \neq 0$.

Hence we find a more practical form of the Mori-Takahasi formula.

Theorem 1.0.4. *(Mori-Takahasi) Suppose $F : \mathbb{R} \to (-1, 1)$ is strictly increasing, satisfies*

$$\lim_{t\to-\infty} F(t) = -1, \qquad \lim_{t\to+\infty} F(t) = 1,$$

and that for some $d > 0$ and $\varepsilon > 0$, F is the restriction to $\mathbb{R}$ of an analytic function (also called F) on $D_{d+\varepsilon} = \{w \in \mathbb{C}|\ |\mathrm{Im}(w)| < d + \varepsilon\}$. Let $\Omega_{d+\varepsilon} = \Omega_{F,d+\varepsilon}$ be the image of $D_{d+\varepsilon}$ under F, so $\Omega_{d+\varepsilon}$ contains the interval $(-1, 1)$. Assume that

$$\int_{-d}^{d} |F'(\pm M + it)|dt = o(1) \qquad \text{as } M \to \infty. \tag{1.0.9}$$

Then, for any function f analytic on $\Omega_{d+\varepsilon}$, any real number $h > 0$ and any integer $n \ge 0$, we have the bound

$$\left|\int_{-1}^{1} f(x)\,dx - h\sum_{k=-n}^{n} g(hk)\right| \tag{1.0.10}$$
$$\le S_{f,d}\left(\frac{\mathrm{e}^{-2\pi d/h}\int_{-\infty}^{\infty}\left(|F'(t+id)| + |F'(t-id)|\right)dt}{1 - \mathrm{e}^{-2\pi d/h}} + h\sum_{|k|>n} F'(hk)\right),$$

where $g(w) = f(F(w))F'(w)$, *and* $S_{f,d}$ *is the supremum of* $|f(z)|$ *for* $z \in \Omega_d$.

Proof. Note that F is differentiable and $F'(t) \geq 0$ for $t \in \mathbb{R}$ since F is assumed increasing and to be the restriction of an analytic function. We may assume

$$\int_{-\infty}^{\infty} \left(|F'(t+id)| + |F'(t-id)|\right) dt < \infty, \quad \sum_{|k|>n} |F'(hk)| < \infty, \quad S_{f,d} < \infty, \tag{1.0.11}$$

for otherwise the bound (1.0.10) holds trivially. We now verify the hypotheses of Theorem 1.0.3. For $c = 0$ or $c = \pm d$ we have

$$\int_{-\infty}^{\infty} |g(t+ic)|\, dt \leq S_{f,d} \int_{-\infty}^{\infty} |F'(t+ic)|\, dt.$$

For $c = \pm d$ this integral is finite by (1.0.11). As for $c = 0$,

$$\int_{-\infty}^{\infty} |F'(t)|\, dt = \int_{-\infty}^{\infty} F'(t)\, dt = F(\infty) - F(-\infty) = 1 - (-1) < \infty.$$

Hence hypothesis (1.0.3) holds. Similarly, hypotheses (1.0.4) and (1.0.5) follow from (1.0.9) and (1.0.11), respectively.

Since f is bounded on $(-1, 1)$, Lebesgue's dominated convergence theorem shows that $\int_{-1}^{1} f(x)\, dx$ exists. On making the change of variables $x = F(t)$, we have

$$\int_{-1}^{1} f(x)\, dx = \int_{-\infty}^{\infty} g(t)\, dt.$$

Hence, from Theorem 1.0.3 and (1.0.8),

$$\begin{aligned}
\left| \int_{-1}^{1} f(x)\, dx - h \sum_{k=-n}^{n} g(hk) \right| &\leq \left| \int_{-\infty}^{\infty} g(t)\, dt - h \sum_{k=-\infty}^{\infty} g(hk) + h \sum_{|k|>n} g(hk) \right| \\
&= \left| \frac{1}{2\pi i} \int_{\partial D_d} \phi(w) g(w)\, dw + h \sum_{|k|>n} g(hk) \right| \\
&\leq \frac{S_{f,d}}{2\pi} \int_{-\infty}^{\infty} \left(\left|\phi(id+t)F'(id+t)\right| + \left|\phi(-id+t)F'(-id+t)\right| \right) dt + S_{f,d} h \sum_{|k|>n} F'(hk) \\
&\leq \frac{S_{f,d}\, \mathrm{e}^{-2\pi d/h}}{1 - \mathrm{e}^{-2\pi d/h}} \int_{-\infty}^{\infty} \left(\left|F'(id+t)\right| + \left|F'(-id+t)\right| \right) dt + S_{f,d} h \sum_{|k|>n} F'(hk),
\end{aligned}$$

as claimed in (1.0.10). □

In the following chapters we will apply the bound in Theorem 1.0.4 to different choices of F. In each case the procedure will be the same: We compute Ω_d (or, when this is too difficult, a region containing Ω_d), estimate the integral and sum on the right-hand side of (1.0.10), and then choose h (nearly) optimal for a given n.

Chapter 2

The simple exponential transformation

In this chapter we will show that the change of variables

$$x = F(t) = \tanh(t/2)$$

leads to a numerical integration method where $\mathcal{O}(n)$ function evaluations lead to an error of $\mathcal{O}\big(\exp(-\sqrt{2\pi d n})\big)$ in the evaluation of $\int_{-1}^{1} f(x)\,dx$. Here d depends on the region of analyticity of f around the interval of integration. This result converges far more slowly than the one obtained in the next chapter, but is far simpler to use since there is a simple relationship between d and the region of analyticity. For many purposes it gives sufficient accuracy.

2.1 The arcs bounding the region Ω_d

Since we are using the transformation $F(t) = \tanh(t/2)$, to obtain analyticity of F inside the horizontal strip $D_d = \big\{w \in \mathbb{C} \big| \, |\mathrm{Im}(w)| < d\big\}$ we require throughout this chapter

$$0 < d < \pi.$$

Proposition 2.1.1. *The region Ω_d, defined as image by F of the strip D_d is the region bounded by C_d^+ and C_d^-, each an arc of a circle. The arc C_d^+ is the piece above the x-axis of the circle of radius $1/\sin(d)$, centered at $\big(0, -\cot(d)\big)$. The arc C_d^- is the piece below the x-axis of the circle of radius $1/\sin(d)$, centered at $\big(0, \cot(d)\big)$.*

Of course, in the above Proposition we mean the interior region, *i. e.* the bounded connected component of $\mathbb{C} - (C_d^+ \cup C_d^-)$. In Figure 2.1 we have shaded Ω_d for $d = \pi/3$, $\pi/2$ and $2\pi/3$.

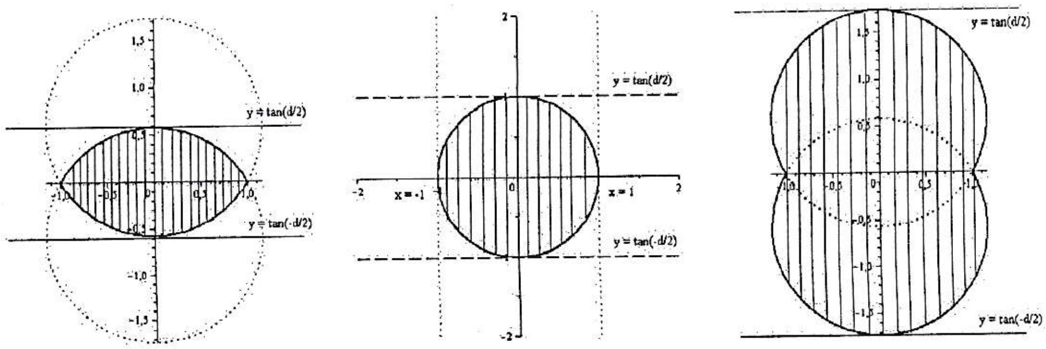

Figure 2.1:
Figure 2. The region Ω_d for $d = \pi/3$ (left) $d = \pi/2$ (center) and $d = 2\pi/3$ (right).

Proof. This is an exercise (admittedly, slightly painful) in high-school algebra using the identities

$$\mathrm{Re}\left(\tanh\left(\frac{t \pm id}{2}\right)\right) = \frac{b}{a + 2\cos(d)}, \qquad \mathrm{Im}\left(\tanh\left(\frac{t \pm id}{2}\right)\right) = \frac{\pm 2\sin(d)}{a + 2\cos(d)},$$

where t is real and

$$a = a(t) = \mathrm{e}^t + \mathrm{e}^{-t}, \qquad b = b(t) = \mathrm{e}^t - \mathrm{e}^{-t}, \qquad (\text{so } a^2 - b^2 = 4).$$

□

For $d = \pi/2$, the region Ω_d is simply the open unit disc $\{z \in \mathbb{C} : |z| < 1\}$. For $0 < d \leq \pi/2$ elementary geometry shows that Ω_d is contained in the rectangle

$$\{z \in \mathbb{C} : |\mathrm{Re}(z)| < 1, \ |\mathrm{Im}(z)| < \tan(d/2)\}.$$

For $\pi/2 \leq d < \pi$, the region Ω_d is contained in the rectangle

$$\{z \in \mathbb{C} : |\mathrm{Re}(z)| < 1/\sin(d), \ |\mathrm{Im}(z)| < \tan(d/2)\}.$$

2.2 Estimating the integral and sum

Proposition 2.2.1. *For $0 < d < \pi$ and $F(w) = \tanh(w/2)$, we have*

$$\int_{-\infty}^{\infty} \left(|F'(t + id)| + |F'(t - id)|\right) dt = 4d/\sin(d).$$

Proof. For $w = t + id$ we calculate,

$$\left|\frac{d}{dt}\tanh((t + id)/2)\right| = \frac{1}{2}\left|\frac{1}{\cosh^2(w/2)}\right| = \left|\frac{1}{\cosh(w) + 1}\right|,$$

and
$$\frac{1}{\cosh(w)+1} = \frac{1}{\big(\cos(d)\cosh(t)+1\big) + i\sin(d)\sinh(t)}.$$

Then
$$\begin{aligned}|\cosh(w)+1|^2 &= (\cos(d)\cosh(t)+1)^2 + \big(\sin(d)\sinh(t)\big)^2\\ &= \big(\cos(d)\cosh(t)\big)^2 + 1 + 2\cos(d)\cosh(t) + \sin^2(d)\sinh^2(t).\end{aligned}$$

But,
$$\big(\cos(d)\cosh(t)\big)^2 = \cos^2(d)\big(1+\sinh^2(t)\big) = \cos^2(d) + \cos^2(d)\sinh^2(t),$$

implies that
$$\begin{aligned}|\cosh(w)+1|^2 &= \cos^2(d) + \cos^2(d)\sinh^2(t) + 1 + 2\cos(d)\cosh(t) + \sin^2(d)\sinh^2(t)\\ &= \cos^2(d) + \sinh^2(t) + 1 + 2\cos(d)\cosh(t) = \big(\cos(d)+\cosh(t)\big)^2.\end{aligned}$$

Therefore,
$$\left|\frac{d}{dt}\tanh\big((t+id)/2\big)\right| = \frac{1}{\cos(d)+\cosh(t)} = \frac{2e^t}{2\cos(d)e^t + e^{2t} + 1}. \tag{2.2.1}$$

Thus far we have
$$\int_{-\infty}^{\infty}\left|\frac{d}{dt}\tanh\big((t+id)/2\big)\right|dt = \int_{-\infty}^{\infty}\frac{2e^t\,dt}{2\cos(d)e^t + e^{2t}+1}.$$

The substitution $u = e^t$ yields
$$\begin{aligned}\int_{-\infty}^{\infty}\left|\frac{d}{dt}\tanh\big((t+id)/2\big)\right|dt &= 2\int_0^{\infty}\frac{du}{2\cos(d)u + u^2 + 1}\\ &= 2\int_0^{\infty}\frac{du}{(u+\cos(d))^2 + \sin^2(d)}.\end{aligned}$$

The change of variable $v = u + \cos(d)$ yields
$$\int_{-\infty}^{\infty}\left|\frac{d}{dt}\tanh\big((t+id)/2\big)\right|dt = 2\int_{\cos(d)}^{\infty}\frac{dv}{v^2+\sin^2(d)} = \frac{2}{\sin(d)}\left(\frac{\pi}{2} - \arctan\big(\cot(d)\big)\right).$$

But $\arctan\big(\cot(d)\big) = \frac{\pi}{2} - d$ if $0 < d < \pi$, and so
$$\frac{2}{\sin(d)}\left(\frac{\pi}{2} - \arctan\big(\cot(d)\big)\right) = \frac{2}{\sin(d)}\left(\frac{\pi}{2} - \left(\frac{\pi}{2} - d\right)\right) = \frac{2d}{\sin(d)}.$$

Thus
$$\int_{-\infty}^{\infty}|F'(t+id)|\,dt = 2d/\sin(d),$$

whence the Proposition. □

Proposition 2.2.2. *For $F(t) = \tanh(t/2)$, for any real number $h > 0$ and any integer $n \geq 0$, we have*

$$h \sum_{|k|>n} F'(hk) < 4\mathrm{e}^{-nh}.$$

Proof. As in the beginning of the proof of the previous Proposition, but with $d = 0$, we find

$$F'(t) = \frac{1}{\cosh(t)+1},$$

so that

$$h \sum_{|k|>n} F'(hk) = h \sum_{|k|>n} \frac{1}{\cosh(hk)+1}.$$

For $h > 0$, the function $1/\big(\cosh(hk)+1\big)$ is even, and

$$\frac{1}{\cosh(hk)+1} = \frac{2}{\mathrm{e}^{hk}+\mathrm{e}^{-hk}+2} = \frac{2\mathrm{e}^{hk}}{(\mathrm{e}^{hk}+1)^2},$$

so that,

$$\begin{aligned} h \sum_{|k|>n} \frac{1}{\cosh(hk)+1} &= 2h \sum_{k=n+1}^{\infty} \frac{1}{\cosh(hk)+1} = 4h \sum_{k=n+1}^{\infty} \frac{\mathrm{e}^{hk}}{(\mathrm{e}^{hk}+1)^2} \\ &\leq 4h \sum_{k=n+1}^{\infty} \frac{\mathrm{e}^{hk}+1}{(\mathrm{e}^{hk}+1)^2} = 4h \sum_{k=n+1}^{\infty} \frac{1}{\mathrm{e}^{hk}+1} \\ &\leq 4h \sum_{k=n+1}^{\infty} \mathrm{e}^{-hk} = \frac{4h\mathrm{e}^{-(n+1)h}}{1-\mathrm{e}^{-h}} = \frac{4h\mathrm{e}^{-nh}}{\mathrm{e}^{h}-1}. \end{aligned}$$

But

$$\frac{h}{\mathrm{e}^h - 1} = \frac{h}{h + h^2/2! + h^3/3! + \ldots} = \frac{1}{1 + h/2! + h^2/3! + \ldots} < 1,$$

and so

$$h \sum_{|k|>n} \frac{1}{\cosh(hk)} \leq \frac{4h\mathrm{e}^{-nh}}{\mathrm{e}^h - 1} < 4\mathrm{e}^{-nh}.$$

□

2.3 Error bound for the simple exponential case

Theorem 2.3.1. *For $0 < d < \pi$, let Ω_d be the open region between two circular arcs defined in Proposition 2.1.1. Assume that f is analytic and bounded in Ω_d. Then, for any integer $n > 1/(4\pi d)$ we have the error bound*

$$\left| \int_{-1}^{1} f(x)dx - h \sum_{k=-n}^{n} g(hk) \right| \leq 4S_{f,d} \cdot \left(\frac{2d}{\sin(d)} + 1 \right) \cdot \mathrm{e}^{-\sqrt{2\pi d n}}, \tag{2.3.2}$$

where

$$h = \sqrt{2\pi d/n}, \qquad g(t) = \frac{1}{2} f\big(\tanh(t/2)\big)/\cosh^2(t/2),$$

and $S_{f,d}$ *is the supremum of* $|f(z)|$ *on* Ω_d.

Proof. In proving (2.3.2), we may assume that f is analytic in $\Omega_{d+\varepsilon}$ for some small $\varepsilon > 0$. Indeed, if we replace d by $d' = d - \varepsilon$, then this holds for d'. Taking the limit as $d' \to d$ of (2.3.2) then yields the claim for d. Clearly $F(t) = \tanh(t/2)$ is strictly increasing on $\mathbb{R}$, maps $\mathbb{R}$ to $(-1, 1)$ and is analytic on the strip $|\mathrm{Im}(z)| < \pi$. As we have assumed $0 < d < \pi$, to check that all the hypotheses of Theorem 1.0.4 are satisfied we must only prove

$$\int_{-d}^{d} |F'(\pm M + it)| dt = o(1) \qquad \text{as } M \to \infty.$$

From (2.2.1) we find

$$|F'(\pm M + it)| = \frac{2e^{\pm M}}{2\cos(t)e^{\pm M} + e^{\pm 2M} + 1},$$

from which the required bound readily follows. From Theorem 1.0.4 and Propositions 2.2.1 and 2.2.2 we obtain

$$\left| \int_{-1}^{1} f(x)\, dx - h \sum_{k=-n}^{n} g(hk) \right| \le S_{f,d} \cdot \left(\frac{4d\, e^{-2\pi d/h}}{\sin(d)(1 - e^{-2\pi d/h})} + 4e^{-nh} \right). \qquad (2.3.3)$$

The above is true for any $h > 0$ and any $n \in \mathbb{N}$. We choose h to balance the magnitude of the first term with the second term on the right-hand side. For this, disregarding $4d/\big(\sin(d)(1 - e^{2\pi d/h})\big)$, we equate

$$e^{-2\pi d/h} = e^{-nh},$$

or

$$h = \sqrt{2\pi d/n}.$$

Substituting h into (2.3.3), we get

$$\left| \int_{-1}^{1} f(x) dx - h \sum_{k=-n}^{n} g(hk) \right| \le S_{f,d} \cdot \left(\frac{4d\, e^{-\sqrt{2\pi dn}}}{\sin(d)(1 - e^{-\sqrt{2\pi dn}})} + 4e^{-\sqrt{2\pi dn}} \right).$$

Now, if $n \ge 1/(4\pi d)$, then $\sqrt{2\pi dn} > 1/\sqrt{2}$, and so

$$\frac{1}{1 - e^{-\sqrt{2\pi dn}}} < \frac{1}{1 - e^{-1/\sqrt{2}}} = 1.97265\cdots < 2.$$

Thus,

$$\left| \int_{-1}^{1} f(x) dx - h \sum_{k=-n}^{n} g(hk) \right| \le 4S_{f,d} \cdot \left(\frac{2d}{\sin(d)} + 1 \right) \cdot e^{-\sqrt{2\pi dn}}.$$

□

Corollary 0.0.1 in the Introduction follows from Theorem 2.3.1 on taking $d = \pi/2$ and noting that $\Omega_{\pi/2}$ coincides with the unit disk.

To deduce Theorems 0.0.1 and 0.0.2 in the Introduction, replace $\Omega_d = \Omega_{d_T}$ in Theorem 2.3.1 by the smallest rectangle R containing Ω_d. Notice (see Figure 2.1 and the remark at the end of §2.1) that the width of R is 2 for $0 < d \le \pi/2$ and $2/\sin(d)$ for $\pi/2 \le d < \pi$. In both cases the height of R is $2\tan(d/2)$. Theorem 0.0.1 follows from Theorem 2.3.1, noting that the function $d \to d/\sin(d)$ is increasing for $0 < d \le \pi/2$. Hence

$$4\Big(\frac{2d}{\sin(d)} + 1\Big) \le 4\Big(\frac{2d}{\sin(d)} + 1\Big)\Big|_{d=\pi/2} = 4(\pi + 1) < 16.6 \qquad (0 < d \le \pi/2).$$

Theorem 0.0.2 follows from Theorem 2.3.1, noting that $1/\sin(d_T) = \frac{1}{2}(T + T^{-1})$, since $\tan(d_T/2) = T$.

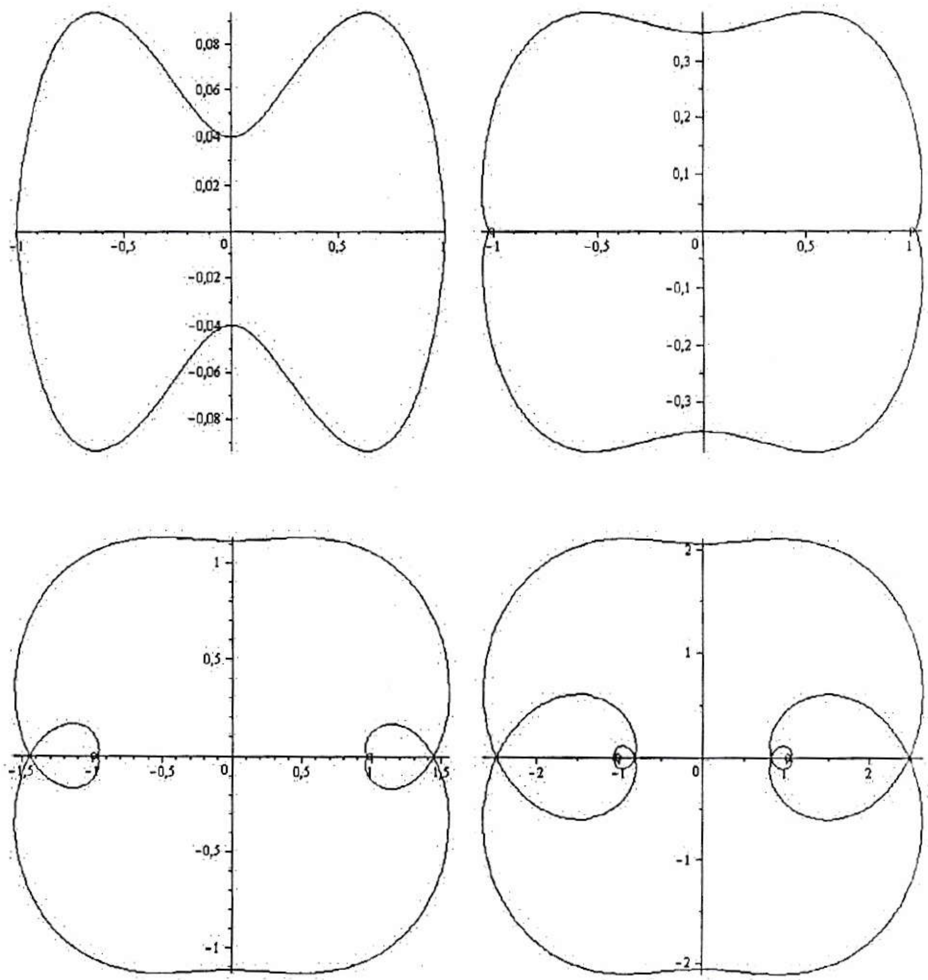

Figure 3.1 The region Ω_d, with $\tau = 2d$, for $d = .2$ (top left), $d = .6$ (top right), $d = 1$ (bottom left) and $d = 1.2$ (bottom right).

The complexity of these figures accounts for many complications in this section. Instead of capturing the exact region, we are forced to approximate it by rectangles, as shown in Figure 3.2.

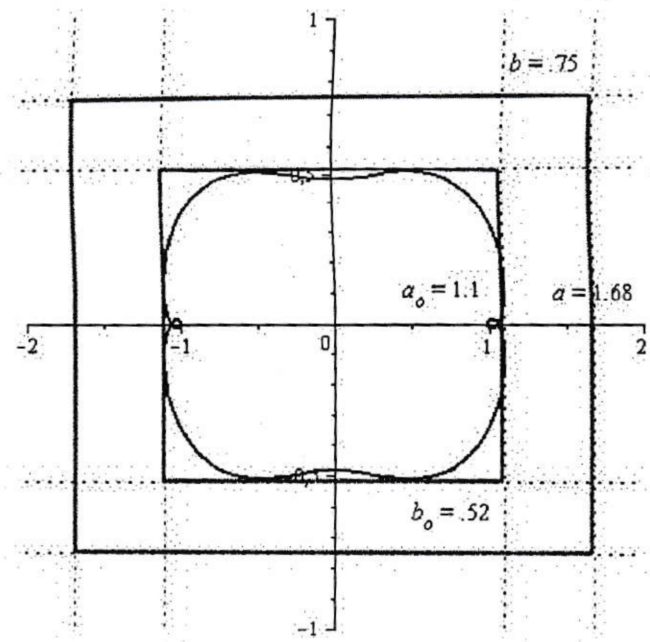

Figure 3.2 The region Ω_d for $d = .7,\ \tau = 1.4$, the real bounding rectangle and the bounding rectangle we will obtain.

Proposition 3.1.1. *Let $w = t + i\delta$, with t and δ real, not be a pole of F. Then*

$$\mathrm{Re}\big(F(t+i\delta)\big) = \frac{\sinh\big(\tau\cos(\delta)\sinh(t)\big)}{\cosh\big(\tau\cos(\delta)\sinh(t)\big) + \cos\big(\tau\sin(\delta)\cosh(t)\big)}, \tag{3.1.1}$$

$$\mathrm{Im}\big(F(t+i\delta)\big) = \frac{\sin\big(\tau\sin(\delta)\cosh(t)\big)}{\cosh\big(\tau\cos(\delta)\sinh(t)\big) + \cos\big(\tau\sin(\delta)\cosh(t)\big)}. \tag{3.1.2}$$

Proof. Since

$$\sinh(t+i\delta) = \cos(\delta)\sinh(t) + i\sin(\delta)\cosh(t),$$
$$\cosh(t+i\delta) = \cos(\delta)\cosh(t) + i\sin(\delta)\sinh(t).$$

if we define

$$a = \frac{\tau}{2}\cos(\delta)\sinh(t), \qquad b = \frac{\tau}{2}\sin(\delta)\cosh(t),$$

then

$$\tanh\left(\tfrac{\tau}{2}\sinh(t+i\delta)\right) = \frac{\sinh\big(\tau\sinh(t+i\delta)/2\big)}{\cosh\big(\tau\sinh(t+i\delta)/2\big)} = \frac{\sinh(a+ib)}{\cosh(a+ib)}.$$

Therefore, (replacing $\sinh(a)$ and $\cosh(a)$ by their definitions in terms of exponentials),

$$\tanh(a+ib) = \frac{\sinh(a+ib)}{\cosh(a+ib)} = \frac{\cos(b)(e^a - e^{-a}) + i\sin(b)(e^a + e^{-a})}{\cos(b)(e^a + e^{-a}) + i\sin(b)(e^a - e^{-a})} = \frac{N}{D},$$

with the obvious definitions of the numerator N and denominator D. But $N\overline{D} = e^{2a} - e^{-2a} + 2i\sin(2b)$ implies that

$$\tanh(a+ib) = \frac{N}{D} = \frac{N\overline{D}}{|D|^2} = \frac{e^{2a} - e^{-2a} + 2i\sin(2b)}{e^{2a} + e^{-2a} + 2\cos(2b)}.$$

□

We now show that the boundary of $\Omega_d = F(D_d)$ spirals around $x = \pm 1$ as $t \to \pm\infty$. Indeed, it is immediately obvious from (3.1.2) that $\operatorname{Im}(F(t+id))$ oscillates in sign infinitely as $|t| \to \infty$. To see that $\operatorname{Re}(F(t+id))$ oscillates around $x = 1$ as $t \to \infty$, we calculate from (3.1.1) (using the notation of its proof)

$$\operatorname{Re}(F(t+id)) - 1 = \frac{\sinh(2a) - \cosh(2a) - \cos(2b)}{\cosh(2a) + \cos(2b)} = \frac{\exp(-2a) - \cos(2b)}{\cosh(2a) + \cos(2b)},$$

where a and b tend to infinity with t, and exponentially fast at that. From this it is obvious that there is a fast oscillation of the sign of the (admittedly minute) quantity $\operatorname{Re}(F(t+id)) - 1$ as $t \to \infty$. Thus, the boundary of Ω_d spirals around $x = 1$. The behavior around $x = -1$ is the same, as F is an odd function. This complicated behavior probably explains why the region is hard to treat both rigorously and accurately, forcing us to approximate it by a considerably larger region below.

We now consider the region of analyticity of F. It follows from the previous Proposition that w is not a pole of F unless

$$\tau\cos(\delta)\sinh(t) = 0, \qquad \text{and} \qquad \tau\sin(\delta)\cosh(t) = \pi + 2k\pi \quad (k \in \mathbb{Z}).$$

It follows that $F(w)$ has no poles in the strip $|\delta| < \pi/2$ provided $0 < \tau < \pi/\sin(d)$, which we assume throughout this chapter. In fact, we will later take $\tau = 2d$, which is permissible since $0 < d < \pi/2$ implies $\tau = 2d < \pi < \pi/\sin(d)$.

In the next propositions we bound the real and imaginary parts of $F(w)$ for $w = t + id$, where $0 < d < \pi/2$. First we give a bound for the real part of $|F(t+id)|$ which is very accurate for large $|t|$.

Proposition 3.1.2. *Let* $f_R = f_{R,d} : (0,\infty) \to (0,\infty)$ *be*

$$f_R(t) = \coth\left(\tfrac{\tau}{2}\cos(d)\sinh(t)\right),$$

and assume $0 < d < \pi/2$ *and* $0 < \tau < \frac{\pi}{\sin(d)}$. *Then*

$$\left|\operatorname{Re}(F(t+id))\right| \le f_R(t)$$

for all $t > 0$. *Furthermore,* $t \to f_R(t)$ *is a decreasing function for* $t > 0$.

Proof. From Proposition 3.1.1,

$$\left|\operatorname{Re}(F(t+id))\right| = \left|\frac{\sinh\left(\tau\cos(d)\sinh(t)\right)}{\cosh\left(\tau\cos(d)\sinh(t)\right) + \cos\left(\tau\sin(d)\cosh(t)\right)}\right|.$$

Using

$$\cosh\big(\tau\cos(d)\sinh(t)\big) + \cos\big(\tau\sin(d)\cosh(t)\big) \geq \cosh(\tau\cos(d)\sinh(t)) - 1,$$

and

$$\sinh(2a) = 2\sinh(a)\cosh(a), \qquad 2\sinh^2(a) = \cosh(2a) - 1,$$

gives

$$\big|\mathrm{Re}\big(F(t+id)\big)\big| \leq \left|\frac{\sinh\big(\tau\cos(d)\sinh(t)\big)}{\cosh\big(\tau\cos(d)\sinh(t)\big) - 1}\right| = \left|\coth\big(\tfrac{\tau}{2}\cos(d)\sinh(t)\big)\right| = f_R(t).$$

Since f_R is the composition of the decreasing function coth with the increasing function $\tau\cos(d)\sinh(t)$, it is clearly decreasing. □

The next bound for the real part of $|F(t+id)|$ will be useful for small positive t.

Proposition 3.1.3. *Let*

$$\omega = \omega_d = \big\{t \geq 0 : \ \cosh(t) < \pi/\big(\tau\sin(d)\big)\big\},$$

and assume $0 < d < \pi/2$ *and* $0 < \tau < \frac{\pi}{\sin(d)}$. *Let* $g_R = g_{R,d} : \omega \to \mathbb{R}$ *be*

$$g_R(t) = \frac{\sinh\big(\tau\cos(d)\sinh(t)\big)}{1 + \cos\big(\tau\sin(d)\cosh(t)\big)}.$$

Then,

$$\big|\mathrm{Re}\big(F(t+id)\big)\big| \leq |g_R(t)|$$

for $t \in \omega$. *Furthermore,* $t \to g_R(t)$ *is an increasing function for* $t \in \omega$.

Proof. From (3.1.1),

$$\big|\mathrm{Re}\big(F(t+id)\big)\big| = \left|\frac{\sinh\big(\tau\cos(d)\sinh(t)\big)}{\cosh(\tau\cos(d)\sinh(t)) + \cos\big(\tau\sin(d)\cosh(t)\big)}\right|.$$

But

$$\cosh\big(\tau\cos(d)\sinh(t)\big) + \cos\big(\tau\sin(d)\cosh(t)\big) \geq 1 + \cos\big(\tau\sin(d)\cosh(t)\big),$$

and the hypothesis imply $\tau\cosh(t)\sin(d) < \pi$. So, $\cos\big(\tau\sin(d)\cosh(t)\big) \neq -1$ and

$$\big|\mathrm{Re}\big(F(t+id)\big)\big| \leq \left|\frac{\sinh\big(\tau\cos(d)\sinh(t)\big)}{1 + \cos\big(\tau\sin(d)\cosh(t)\big)}\right| = |g_R(t)|.$$

It is clear that g_R is increasing, since its numerator is increasing and its denominator is decreasing for $t \in \omega$. □

The next step gets the best of both of the bounds above. Figure 3.3 illustrates the following Proposition for $d = \pi/3$ and $\tau = 2d$.

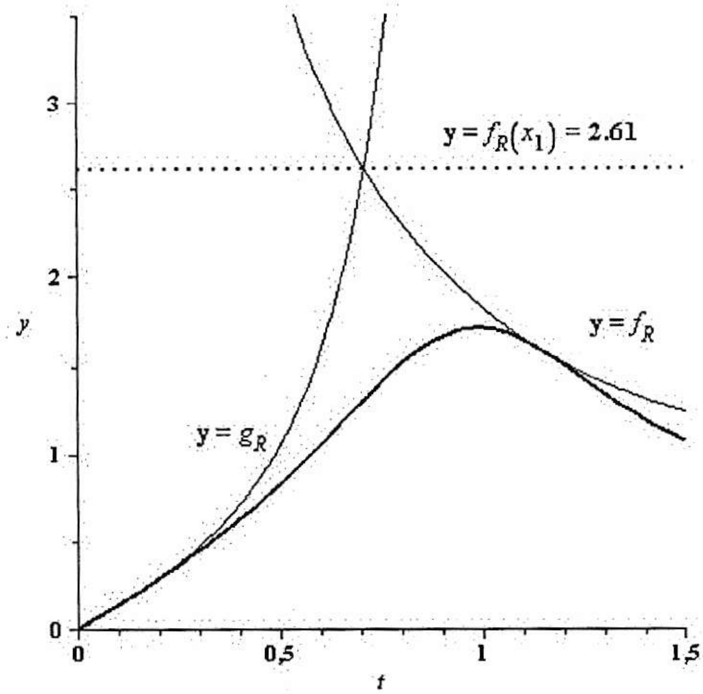

Figure 3.3 Why for $d = \pi/3$ and $\tau = 2d$ we have $\left|\mathrm{Re}\big(F(t+id)\big)\right| < 2.61$.

Proposition 3.1.4. *Let $f_R = f_{R,d}$ and $g_R = g_{R,d}$ be the functions defined in Propositions 3.1.2 and 3.1.3. Then for any $0 < d < \frac{\pi}{2}$ and $0 < \tau < \frac{\pi}{\sin(d)}$ there exists a unique x_1 such that $1 \leq \cosh(x_1) < \pi/\big(\tau\sin(d)\big)$ and $g_R(x_1) = f_R(x_1)$. Moreover, if $x_0 > 0$ and $g_R(x_0) \leq f_R(x_0)$, then for all w in the closure of the strip*

$$D_d = \{w \in \mathbb{C} | \; |\mathrm{Im}(w)| < d\}$$

we have $\left|\mathrm{Re}\big(F(w)\big)\right| \leq f_R(x_0)$.

Proof. We first consider $z = t + id$ with $t \geq 0$. The upper bound $g_R(t)$ for $\left|\mathrm{Re}\big(F(t+id)\big)\right|$ defined in Proposition 3.1.3 is continuous on its domain interval $[0, t_d)$, where $t_d > 0$ is defined by $\cosh(t_d) = \frac{\pi}{\tau\sin(d)}$, increasing on $[0, t_d)$, satisfies $g_R(0) = 0$ and has a vertical asymptote as $t \to t_d^-$. On the other hand, by Proposition 3.1.2, the other upper bound, *i. e.* the function f_R is positive, continuous and decreasing on $(0, \infty)$. Hence its graph crosses that of g_R exactly once. Therefore

$$\left|\mathrm{Re}\big(F(t+id)\big)\right| \leq f_R(x_0).$$

This has been proved for $t \geq 0$, but it holds for all $t \in \mathbb{R}$ since $t \to \text{Re}\big(F(t+id)\big)$ is an odd function of $t \in \mathbb{R}$, as is clear from (3.1.1). Also,

$$\text{Re}\big(F(t-id)\big) = \text{Re}\big(F(t+id)\big).$$

Thus for z on the boundary of the strip D_d we have the inequality

$$-f_R(x_0) \leq \text{Re}\big(F(z)\big) \leq f_R(x_0).$$

The maximum principle for the harmonic function $\text{Re}\big(F(z)\big)$ on the strip

$$D_d = \big\{w \in \mathbb{C}\big|\ |\text{Im}(w)| < d\big\}$$

readily implies that the above bound extends to all $z \in D_d$, as claimed in the Proposition. Indeed, as one easily checks that $\text{Re}\big(F(z)\big)$ is bounded on the whole strip D_d, it must assume its maximum and minimum value on the boundary. □

We now turn to bounding Ω_d in the vertical direction.

Proposition 3.1.5. *Let* $f_I = f_{I,d} : (0,\infty) \to (0,\infty)$ *be*

$$f_I(t) = \frac{1}{\sinh\big(\tau\cos(d)\sinh(t)\big)},$$

and assume $0 < d < \pi/2$ *and* $0 < \tau < \frac{\pi}{\sin(d)}$. *Then*

$$\big|\text{Im}\big(F(t+id)\big)\big| \leq f_I(t)$$

for all $t > 0$. *Furthermore,* $t \to f_I(t)$ *is a decreasing function for* $t > 0$.

Proof. From (3.1.2),

$$\big|\text{Im}\big(F(t+id)\big)\big| = \left|\frac{\sin\big(\tau\sin(d)\cosh(t)\big)}{\cosh\big(\tau\cos(d)\sinh(t)\big) + \cos\big(\tau\sin(d)\cosh(t)\big)}\right|,$$

If we define

$$a := \sin\big(\tau\sin(d)\cosh(t)\big)$$

and

$$b := \cosh\big(\tau\cos(d)\sinh(t)\big)$$

then $\cos\big(\tau\sin(d)\cosh(t)\big) = \pm\sqrt{1-a^2}$. Note that $|a| \leq 1$ and $b > 1$ (since $t \neq 0$). Then

$$\left|\frac{a}{b \pm \sqrt{1-a^2}}\right| \leq \frac{|a|}{b - \sqrt{1-a^2}} \leq \frac{1}{\sqrt{b^2-1}},$$

where in the last step we have omitted the elementary calculation of critical points showing that $a \to \frac{|a|}{b-\sqrt{1-a^2}}$ assumes its maximum for $|a| \leq 1$ precisely when $|a| = \sqrt{1-b^{-2}}$. But

$$\frac{1}{\sqrt{b^2-1}} = \frac{1}{\sqrt{\cosh^2\big(\tau\cos(d)\sinh(t)\big) - 1}} = \frac{1}{\big|\sinh\big(\tau\cos(d)\sinh(t)\big)\big|} = f_I(t),$$

and f_I is obviously a decreasing function. □

Proposition 3.1.6. *Let*

$$\omega = \omega_d = \{t \geq 0 : \ \cosh(t) < \pi/(\tau \sin(d))\},$$

and assume $0 < d < \pi/2$ *and* $0 < \tau < \frac{\pi}{\sin(d)}$. *Let* $g_I = g_{I,d} : \omega \to \mathbb{R}$ *be*

$$g_I(t) = \tan\left(\tfrac{\tau}{2} \sin(d) \cosh(t)\right).$$

Then,

$$\left|\mathrm{Im}\left(F(t+id)\right)\right| \leq |g_I(t)|$$

for $t \in \omega$. *Furthermore,* $t \to g_I(t)$ *is an increasing function for* $t \in \omega$.

Proof. From (3.1.2),

$$\left|\mathrm{Im}\left(F(t+id)\right)\right| = \left|\frac{\sin\left(\tau \sin(d) \cosh(t)\right)}{\cosh\left(\tau \cos(d) \sinh(t)\right) + \cos\left(\tau \sin(d) \cosh(t)\right)}\right|.$$

But

$$\cosh\left(\tau \cos(d) \sinh(t)\right) + \cos\left(\tau \sin(d) \cosh(t)\right) \geq 1 + \cos\left(\tau \sin(d) \cosh(t)\right),$$

and $\cos\left(\tau \sin(d) \cosh(t)\right) \neq -1$ if $t \in \omega$. Therefore,

$$\left|\mathrm{Im}\left(F(t+id)\right)\right| \leq \left|\frac{\sin\left(\tau \sin(d) \cosh(t)\right)}{1 + \cos\left(\tau \sin(d) \cosh(t)\right)}\right| = \left|\tan\left(\tfrac{\tau}{2} \sin(d) \cosh(t)\right)\right| = |g_I(t)|,$$

where we used the elementary identity $\sin(y)/\left(1 + \cos(y)\right) = \tan(y/2)$. Again, g_I is obviously increasing, being a composition of increasing functions. □

The statement and proof of the next Proposition are entirely analogous to that of Proposition 3.1.4, so we omit the proof.

Proposition 3.1.7. *Let* $f_I = f_{I,d}$ *and* $g_I = g_{I,d}$ *be the functions defined in Propositions 3.1.5 and 3.1.6. Then for any* $0 < d < \frac{\pi}{2}$ *and* $0 < \tau < \frac{\pi}{\sin(d)}$ *there exists a unique* y_1 *such that* $1 \leq \cosh(y_1) < \pi/\left(\tau \sin(d)\right)$ *and* $g_I(y_1) = f_I(y_1)$. *Moreover, if* $y_0 > 0$ *and* $g_I(y_0) \leq f_I(y_0)$, *then for all* w *in the closure of the strip*

$$D_d = \{w \in \mathbb{C} | \ |\mathrm{Im}(w)| < d\}$$

we have $\left|\mathrm{Im}\left(F(w)\right)\right| \leq f_I(y_0)$.

Figure 3.4 illustrates the Proposition when $d = \pi/3$ and $\tau = 2d$.

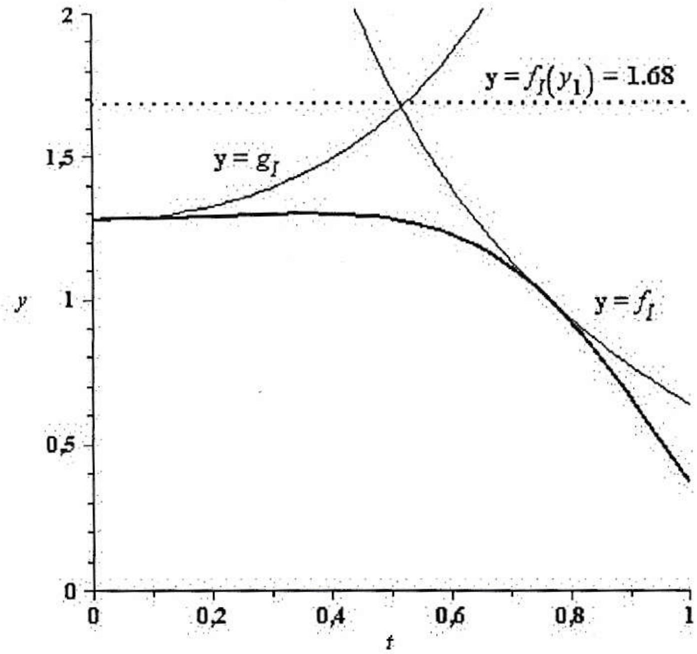

Figure 3.4 Why for $d = \pi/3$ and $\tau = 2d$ we have $|\mathrm{Im}(F(x+id))| < 1.68$.

3.2 Estimating the sum and integral

In the next Proposition we introduce a new free variable A, which we will presently choose depending on n and d so as to optimize the bound.

Proposition 3.2.1. *Let* $F(t) = \tanh\left(\frac{\tau}{2}\sinh(t)\right)$, *and suppose* $0 < d < \pi/2$, $0 < \tau < \pi/\sin(d)$. *Let A satisfy* $\tau - \frac{1}{2} < A < \tau$ *and take* $h > 0$ *and any integer* $n \geq 0$. *Then*

$$h \sum_{|k|>n} F'(hk) < \frac{8\tau\, \mathrm{e}^{-\frac{1}{2}} \exp(A\mathrm{e}^{-hn}/2) \exp(-A\mathrm{e}^{hn}/2)}{A(\tau - A)\, \mathrm{e}^{hn}}.$$

Proof. A short calculation gives

$$F'(t) = \tau \cosh(t) / \left(\cosh(\tau \sinh(t)) + 1\right),$$

an even function of t. Letting $u = \sinh(t)$ for short, we can write

$$F'(t) = \frac{\tau\sqrt{1+u^2}}{\cosh(\tau u) + 1} = \frac{2\tau\sqrt{1+u^2}}{e^{\tau u} + e^{-\tau u} + 2} < \frac{2\tau\sqrt{1+u^2}}{e^{\tau u}} = \frac{2\tau}{e^{Au}} \cdot \frac{\sqrt{1+u^2}}{e^{(\tau - A)u}}. \qquad (3.2.3)$$

Since $A < \tau$, the function $g(u) = \sqrt{1+u^2}/e^{(\tau-A)u}$ is bounded for $u \geq 0$. Now, letting $j = \tau - A$ for short,

$$g'(u) = \frac{ue^{-ju}}{\sqrt{1+u^2}} - \sqrt{1+u^2}e^{-ju}j = \frac{e^{ju}(u - j(1+u^2))}{\sqrt{1+u^2}\,\mathrm{e}^{2ju}}.$$

At a critical point u_0 we have $ju_0^2 - u_0 + j = 0$, which has a real solution if $|j| \leq \frac{1}{2}$, which holds in our case as we assumed $\tau - \frac{1}{2} < A < \tau$. Solving the above equation for u_0 we find

$$u_0 = \frac{1 \pm \sqrt{1-4j^2}}{2j},$$

and the local maximum occurs with the + sign as g tends to 0 at ∞. Since $1 + u_0^2 = u_0/j$,

$$g^2(u_0) = \frac{u_0}{j}\,\mathrm{e}^{-2ju_0} = \frac{(1+\sqrt{1-4j^2}\,)\,\mathrm{e}^{-\left(1+\sqrt{1-4j^2}\right)}}{2j^2} < \frac{1}{j^2}\,\mathrm{e}^{-1},$$

Since $g(0) = 1$ we have

$$g(u) \leq g(u_0) < \frac{1}{j}\,\mathrm{e}^{-\frac{1}{2}} = \frac{1}{\tau - A}\,\mathrm{e}^{-\frac{1}{2}}.$$

Using (3.2.3) we obtain for $k \geq n+1 \geq 0$ and $u = \sinh(hk)$,

$$\begin{aligned} F'(hk) &= \frac{\tau\cosh(hk)}{\cosh(\tau\sinh(hk)) + 1} < \frac{2\tau}{\mathrm{e}^{Au}} \cdot \frac{\mathrm{e}^{-\frac{1}{2}}}{(\tau - A)} = \frac{2\tau\,\mathrm{e}^{-\frac{1}{2}}\,\mathrm{e}^{-A\sinh(hk)}}{(\tau-A)} \\ &= \frac{2\tau\,\mathrm{e}^{-\frac{1}{2}}\,\exp\left((-A\mathrm{e}^{hk} + A\mathrm{e}^{-hk})/2\right)}{\tau - A} < \frac{2\tau\,\mathrm{e}^{-\frac{1}{2}}}{\tau - A}\exp(A\mathrm{e}^{-hn}/2)\,\exp(-A\mathrm{e}^{hk}/2). \end{aligned}$$

Thus,

$$h\sum_{|k|>n} F'(hk) = 2h\sum_{k=n+1}^{\infty} F'(hk) < \frac{4h\tau\,\mathrm{e}^{-\frac{1}{2}}}{\tau - A}\exp(A\mathrm{e}^{-hn}/2)\sum_{k=n+1}^{\infty}\exp(-A\mathrm{e}^{hk}/2),$$

which we can estimate by an integral as follows.

$$\begin{aligned} \sum_{k=n+1}^{\infty}\exp(-A\mathrm{e}^{hk}/2) &\leq \int_n^{\infty}\exp(-A\mathrm{e}^{hx}/2)dx \leq \frac{1}{\mathrm{e}^{hn}}\int_n^{\infty}\exp(-A\mathrm{e}^{hx}/2)\mathrm{e}^{hx}dx \\ &= \frac{2}{hA\mathrm{e}^{hn}}\int_{A\mathrm{e}^{hn}/2}^{\infty}\mathrm{e}^{-u}du = \frac{2}{hA\mathrm{e}^{hn}}\exp(-A\mathrm{e}^{hn}/2). \end{aligned}$$

Hence,

$$h\sum_{|k|>n} F'(hk) < \frac{8\tau\,\mathrm{e}^{-\frac{1}{2}}\,\exp(A\mathrm{e}^{-hn}/2)\,\exp(-A\mathrm{e}^{hn}/2)}{A(\tau - A)\,\mathrm{e}^{hn}}.$$

□

We now estimate the integral in Theorem 1.0.4. It again proves useful to introduce a new parameter, which we call C.

Proposition 3.2.2. *Let* $F(w) = \tanh\left(\frac{\tau}{2}\sinh(w)\right)$, $0 < d < \pi/2$, $0 < \tau < \pi/\sin(d)$ *and* $0 < C < \sqrt{\left(\frac{\pi}{\sin(d)\tau}\right)^2 - 1}$. *Then*

$$\int_{-\infty}^{\infty} \left(|F'(t+id)| + |F'(t-id)|\right) dt \le \frac{4\tau C}{\cos(\alpha\sqrt{1+C^2})+1} + \frac{4\left(\coth(\beta C/2)-1\right)}{\cos(d)},$$

with $\alpha = \tau\sin(d)$ *and* $\beta = \tau\cos(d)$.

Proof. We already found at the beginning of the proof of the previous Proposition that

$$\left|F'(t \pm id)\right| = \tau\left|\frac{\cosh(w)}{\cosh\left(\tau\sinh(w)\right)+1}\right|, \qquad (w = t+id).$$

But

$$\left|\cosh(w)\right|^2 = \cos^2(d)\cosh^2(t) + \sin^2(d)\sinh^2(t) = \cos^2(d) + \sinh^2(t).$$

Abbreviating

$$a := \tau\sin(d)\cosh(t), \qquad b := \tau\cos(d)\sinh(t),$$

we calculate

$$\begin{aligned}
\left|\cosh\left(\tau\sinh(w)\right)+1\right|^2 &= \left|\cos(a)\cosh(b) + i\sin(a)\sinh(b) + 1\right|^2 \\
&= \cos^2(a)\cosh^2(b) + 2\cos(a)\cosh(b) + 1 + \sin^2(a)\sinh^2(b) \\
&= \cos^2(a) + \cos^2(a)\sinh^2(b) + 2\cos(a)\cosh(b) + 1 + \sin^2(a)\sinh^2(b) \\
&= \cos^2(a) + \sinh^2(b) + 2\cos(a)\cosh(b) + 1 = \left(\cos(a)+\cosh(b)\right)^2.
\end{aligned}$$

Substituting back for a and b into the last expression gives us

$$\left|\cosh\left(\tau\sinh(w)\right)+1\right| = \cos\left(\tau\sin(d)\cosh(t)\right) + \cosh\left(\tau\cos(d)\sinh(t)\right).$$

Thus

$$\left|F'(w)\right| = \frac{\tau\sqrt{\cos^2(d)+\sinh^2(t)}}{\cos\left(\tau\sin(d)\cosh(t)\right) + \cosh\left(\tau\cos(d)\sinh(t)\right)}. \tag{3.2.4}$$

Since $F'(w)$ is even,

$$\begin{aligned}
I = \int_{-\infty}^{\infty} \left(|F'(t+id)| + |F'(t-id)|\right) dt &= 4\int_0^{\infty} |F'(t+id)|\, dt \\
&= 4\int_0^{\infty} \frac{\tau\sqrt{\cos^2(d)+\sinh^2(t)}}{\cos\left(\tau\sin(d)\cosh(t)\right) + \cosh\left(\tau\cos(d)\sinh(t)\right)}\, dt \\
&= 4\int_0^{\infty} \frac{\tau\sqrt{(\beta/\tau)^2+\sinh^2(t)}}{\cos\left(\alpha\cosh(t)\right) + \cosh\left(\beta\sinh(t)\right)}\, dt.
\end{aligned}$$

Considering the change of variable $s = \sinh(t)$, we have

$$\begin{aligned} I &= 4\int_0^\infty \tau\sqrt{\frac{(\beta/\tau)^2+s^2}{1+s^2}}\frac{1}{\cos\big(\alpha\sqrt{1+s^2}\big)+\cosh(\beta s)}\,ds. \\ &\le 4\tau\int_0^\infty \frac{ds}{\cos\big(\alpha\sqrt{1+s^2}\big)+\cosh(\beta s)}, \end{aligned}$$

because $0 < \frac{\beta}{\tau} = \cos(d) < 1$.

The above integral we write as

$$\underbrace{\int_0^C \frac{ds}{\cos\big(\alpha\sqrt{1+s^2}\big)+\cosh(\beta s)}}_{I_1} + \underbrace{\int_C^\infty \frac{ds}{\cos\big(\alpha\sqrt{1+s^2}\big)+\cosh(\beta s)}}_{I_2}.$$

But the function $1/\big(\cos(\alpha\sqrt{1+s^2})+1\big)$ is increasing for $0 < s < C$ provided

$$0 < \alpha\sqrt{1+C^2} < \pi,$$

i.e. $C < \sqrt{\left(\frac{\pi}{\sin(d)\tau}\right)^2 - 1}$, which we have assumed. Hence,

$$I_1 \le \int_0^C \frac{ds}{\cos\big(\alpha\sqrt{1+s^2}\big)+1} \le \frac{C}{\cos(\alpha\sqrt{1+C^2})+1}.$$

For the integral I_2, we see that

$$I_2 \le \int_C^\infty \frac{ds}{\cosh(\beta s)-1} = \frac{1}{2}\int_C^\infty \frac{ds}{\sinh^2(\beta s/2)} = \frac{\coth(\beta C/2)-1}{\beta}.$$

Thus, since $\tau/\beta = 1/\cos(d)$,

$$I = 4\tau(I_1+I_2) \le \frac{4\tau C}{\cos(\alpha\sqrt{1+C^2})+1} + \frac{4\big(\coth(\beta C/2)-1\big)}{\cos(d)}$$

□

3.3 Error bound for the double exponential case

We begin with an error bound with still many free variables that collects the results of the previous sections.

Theorem 3.3.1. *Let $0 < d < \pi/2$ and $0 < \tau < \frac{\pi}{\sin(d)}$, and let $a = f_{R,d}(x_1)$ and $b = f_{I,d}(y_1)$ be as defined in Propositions 3.1.4 and 3.1.7. Suppose f is analytic and bounded in the interior of the rectangle*

$$\{z \in \mathbb{C} : |\mathrm{Re}(z)| \le a,\ |\mathrm{Im}(z)| \le b\}.$$

Then, for $h > 0$, $0 < C < \sqrt{\left(\frac{\pi}{\sin(d)\tau}\right)^2 - 1}$, $\tau - \frac{1}{2} < A < \tau$ *and* $n \in \mathbb{N}$ *we have*

$$\left|\int_{-1}^{1} f(x)\,dx - h\sum_{k=-n}^{n} g(hk)\right|$$
$$< M_{a,b}(f)\cdot\left(\frac{B_d\,\mathrm{e}^{-2\pi d/h}}{1-\mathrm{e}^{-2\pi d/h}} + \frac{8\tau\,\mathrm{e}^{-\frac{1}{2}}\exp(A\mathrm{e}^{-hn}/2)\exp(-A\mathrm{e}^{hn}/2)}{A(\tau - A)\,\mathrm{e}^{hn}}\right),$$

where $M_{a,b}$ *is the supremum of* $|f(z)|$ *on the rectangle, and*

$$g(t) = \tfrac{\tau}{2} f\big(\tanh(\tau\sinh(t)/2)\big)\cosh(t)/\cosh^2(\tau\sinh(t)/2),$$
$$B_d = \frac{4\tau C}{\cos(\alpha\sqrt{1+C^2})+1} + \frac{4\big(\coth(\beta C/2)-1\big)}{\cos(d)},$$

with $\alpha = \tau\sin(d)$, $\beta = \tau\cos(d)$.

Proof. $F(t) = \tanh\big(\frac{\tau}{2}\sinh(t)\big)$ is strictly increasing on $\mathbb{R}$, being the composition of strictly increasing functions, and maps $\mathbb{R}$ to $(-1,1)$. We saw at the beginning of §3.1 that F is analytic on the strip $|\mathrm{Im}(z)| < \pi/2$. As we have assumed $0 < d < \pi/2$, to check that all the hypotheses of Theorem 1.0.4 are satisfied we must only prove

$$\int_{-d}^{d} |F'(\pm M + it)|dt = o(1) \qquad \text{as } M \to \infty. \tag{3.3.5}$$

Using (3.2.4) we bound for $|t| \le d$,

$$\big|F'(M+it)\big| = \frac{\tau\sqrt{\cos^2(t)+\sinh^2(M)}}{\cos\big(\tau\sin(t)\cosh(M)\big)+\cosh\big(\tau\cos(t)\sinh(M)\big)}$$
$$\le \frac{\tau\sqrt{1+\sinh^2(M)}}{\cosh\big(\tau\cos(d)\sinh(M)\big)-1} = \frac{\tau\cosh(M)}{\cosh\big(\tau\cos(d)\sinh(M)\big)-1},$$

from which (3.3.5) follows. Now the Theorem follows directly from Theorem 1.0.4 and Propositions 3.1.4, 3.1.7, 3.2.1 and 3.2.2. □

In the next bound we make the following choices for the parameters in Theorem 3.3.1.

$$\tau = 2d, \qquad C = \frac{1}{2}\sqrt{\left(\frac{\pi}{2d\sin(d)}\right)^2 - 1}, \qquad A = 2d - \frac{1}{n}\log(n),$$

and step size

$$h = \frac{\log\Big(4\pi d n^2/\big(2dn - \log(n)\big)\Big) - \log\big(\log(n)\big)}{n}.$$

Corollary 3.3.1. *Under the hypotheses of Theorem 3.3.1 and with parameters as shown above, we have for any $n > 1$ the bound*

$$\left|\int_{-1}^{1} f(x)dx - h\sum_{k=-n}^{n} g(hk)\right| < M_{a,b}(f)\cdot\left(\mathrm{e}^{-2\pi dn/\log(n)} + \frac{B_d\,\mathrm{e}^{-2\pi dn/\log(\frac{4\pi dn^2}{(2dn-\log(n))\log(n)})}}{1-\mathrm{e}^{-2\pi dn/\log(\frac{4\pi dn^2}{(2dn-\log(n))\log(n)})}}\right).$$

Proof. One easily verifies that the above choice of parameters places them in the ranges required in Theorem 3.3.1. Substituting the chosen value of h into the terms in the bound given in Theorem 3.3.1 we find

$$\begin{aligned}
\mathrm{e}^{-2\pi d/h} &= \mathrm{e}^{-2\pi dn/\log\left(\frac{4\pi dn^2}{(2dn-\log(n))\log(n)}\right)},\\
\mathrm{e}^{hn} &= \frac{4\pi dn}{A\log(n)} = \frac{4\pi dn^2}{(2dn-\log(n))\log(n)},\\
\exp(-A\mathrm{e}^{hn}/2) &= \mathrm{e}^{-2\pi dn/\log(n)},\\
\exp(A\mathrm{e}^{-hn}/2) &= \exp\big(A^2\log(n)/(8\pi dn)\big) < \exp\big(d\log(n)/(2\pi n)\big) \quad (\text{since } A < \tau = 2d)\\
&< \exp\big(\log(n)/(4n)\big) \qquad (\text{since } d < \pi/2)\\
&< \exp(\log(3)/12) < 1.1\,.
\end{aligned}$$

Substituting these into our bound gives

$$\begin{aligned}
&\left|\int_{-1}^{1} f(x)dx - h\sum_{k=-n}^{n} g(hk)\right|\\
&\quad< M_{a,b}(f)\cdot\left(\frac{B_d\,\mathrm{e}^{-2\pi dn/\log\left(\frac{4\pi dn^2}{(2dn-\log(n))\log(n)}\right)}}{1-\mathrm{e}^{-2\pi dn/\log\left(\frac{4\pi dn^2}{(2dn-\log(n))\log(n)}\right)}} + \frac{4\cdot(1.1)\,\mathrm{e}^{-2\pi dn/\log(n)}}{\pi\,\mathrm{e}^{\frac{1}{2}}}\right).
\end{aligned}$$

The Corollary follows on noting that $\frac{4\cdot(1.1)}{\pi\,\mathrm{e}^{\frac{1}{2}}} < 1$. □

The bound in the above Corollary simplifies if we assume in addition that n is not too small. Let N_d be any positive integer satisfying

$$\frac{1}{4\pi d} > \frac{N_d}{(2dN_d - \log(N_d))\log(N_d)}.$$

Corollary 3.3.2. *Let $0 < d < \pi/2$ be such that for $a = f_{R,d}(x_1)$ and $b = f_{I,d}(y_1)$ (as defined in Propositions 3.1.4 and 3.1.7 and tabulated in Table 3.1). Assume f is analytic and bounded in the interior of the rectangle*

$$\{z \in \mathbb{C} : |\mathrm{Re}(z)| \le a,\ |\mathrm{Im}(z)| \le b\}.$$

Then, we have for $n \ge N_d$ the error bound

$$\left|\int_{-1}^{1} f(x)dx - h\sum_{k=-n}^{n} g(hk)\right| < M_{a,b}(f)\cdot B(d)\cdot \mathrm{e}^{-2\pi dn/\log(n)}, \tag{3.3.6}$$

where $M_{a,b}$ is the supremum of $|f(z)|$ on the rectangle, and

$$\begin{aligned} g(t) &= d \cdot f\big(\tanh\big(d\sinh(t)\big)\big)\cosh(t)/\cosh^2\big(d\sinh(t)\big), \\ B(d) &= \frac{B_d}{1 - e^{-2\pi d N_d/\log(N_d)}} + 1, \\ B_d &= \frac{8dC}{\cos(2d\sin(d)\sqrt{1+C^2})+1} + \frac{4\big(\coth(d\cos(d)C)-1\big)}{\cos(d)}, \\ C &= \frac{1}{2}\sqrt{\Big(\frac{\pi}{2d\sin(d)}\Big)^2 - 1}. \end{aligned}$$

Proof. From the hypothesis on n we directly obtain

$$2\pi dn/\log\Big(\frac{4\pi dn^2}{(2dn - \log(n))\log(n)}\Big) > 2\pi dn/\log(n).$$

Since $t \to e^{-t}/(1-e^{-t})$ is decreasing for $t > 0$, Corollary 3.3.1 now yields the desired bound. □

In Table 3.1 below we tabulate for d between $d = .1$ and $d = 1.5$ the values of a, b, $B(d)$ and N_d. For example, the result quoted in the Introduction follows on taking $d = .5$, , obtaining $a = 1.51$, $b = 0.49$, $B(\frac{1}{2}) = 15.28$ and $N_{\frac{1}{2}} = 575$.

The columns labeled d, x_1, a, y_1, b, N_d and $B(d)$ in Table 3.1 are defined in Corollary 3.3.2. The columns a_o and b_o are the graphically observed (but not rigorously proved) optimal values of a and b, respectively.

d	x_1	a	$a_\circ$	y_1	b	$b_\circ$	N_d	$B(d)$
.1	2.88	1.42	1.1	3.3	.14	.05	723	63.95
.2	2.20	1.43	1.1	2.42	.23	.1	632	32.67
.3	1.81	1.44	1.1	1.91	.31	.15	600	22.41
$\pi/8$	1.57	1.47	1.1	1.56	.39	.21	586	17.89
.4	1.55	1.48	1.1	1.54	.4	.22	586	17.68
.5	1.35	1.51	1.1	1.28	.49	.3	575	15.28
$\pi/6$	1.32	1.53	1.1	1.22	.52	.32	573	14.94
.6	1.2	1.58	1.1	1.07	.61	.39	569	14.26
.7	1.07	1.68	1.11	.9	.75	.52	564	14.56
$\pi/4$	.97	1.8	1.2	.78	.9	.65	561	15.69
.8	.96	1.82	1.2	.76	.93	.67	561	15.98
.9	.85	2.05	1.33	.66	1.14	.87	558	19.48
1	.76	2.37	1.56	.56	1.47	1.12	556	25.81
$\pi/3$	.71	2.61	1.71	.51	1.68	1.28	555	30.68
1.1	.66	2.95	1.94	.48	1.93	1.50	554	38.43
1.2	.57	3.92	2.64	.41	2.67	2.06	552	66.58
1.3	.48	5.83	4.09	.35	3.99	3.19	551	137.63
1.4	.38	10.82	8.02	.28	7.38	5.44	550	420.01
1.5	.25	37.32	29.91	.2	23.4	19.15	549	3587.33

Table 3.1: Table for Corollary 3.3.2

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