Entropy with Signed and Complex Measures

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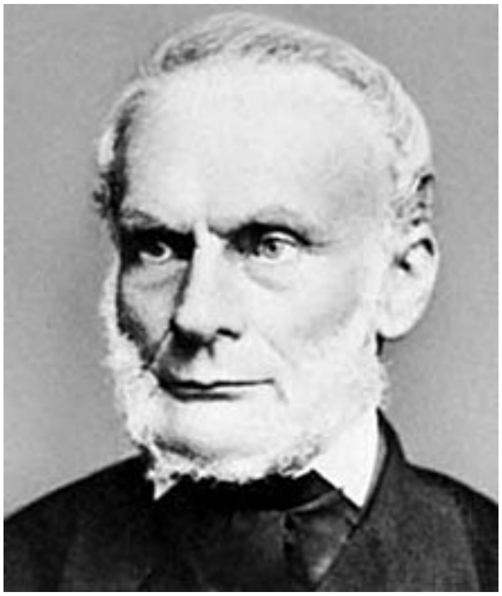
In the beginning ....

1865: Clausius invents ENTROPY in Thermodynamics



Rudolf Julius Emanuel Clausius

Clausius was thinking BIG !

Clausius proposes two Fundamental Laws of the Universe:

1) The energy (E) of the world remains constant.

2) The entropy (S) of the world tends toward its maximum.

Soon after ....

1872: Boltzmann's ENTROPY formula in Kinetic Gas Theory

Ludwig Eduard Boltzmann

Boltzmann's *H* functional and ENTROPY for a GAS

$$H_{\text{B}}(f) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3_s} f(s,p,t)\ln f(s,p,t)d^3p\,d^3s$$

$$S_{\text{B}}(f) = -Nk_{\text{B}}H(f)$$

$\uparrow$

k_{B} introduced by Planck $\approx$ 1900

Max Karl Ernst Ludwig Planck

Boltzmann's ENTROPY for Thermal Equilibrium

In the 1860s/70s Boltzmann proposes that in THERMAL EQUILIBRIUM:

$$S_{\text{B}}(E, N, V|U) = k_{\text{B}} \ln \int_{V^N \subset \mathbb{R}^{3N}} \int_{\mathbb{R}^{3N}_{\mathbf{q}}} \delta\left(H - E\right) d^{3N}p\, d^{3N}q$$

$$H(\mathbf{p}, \mathbf{q}) = \sum_{1 \leq k \leq N} \frac{|p_k|^2}{2m} + \sum_{1 \leq k < l \leq N} U(|q_k - q_l|)$$

with

$$U(r) = \frac{c^2}{r^4} \qquad (\textit{or such}!)$$

the pair interaction energy.

REMARK: for Neon, Argon, Krypton, Xenon, Radon

$$U_{\text{L-J}}(r) = A\left(\frac{R^{12}}{r^{12}} - \frac{R^6}{r^6}\right)$$ [Lennard-Jones (1924)]

The Boltzmann Maximum ENTROPY Principle

Boltzmann shows for the PERFECT GAS ($U \equiv 0$) that:

$$\lim_{N\to\infty} \frac{1}{N} S_{\mathrm{B}}(\varepsilon N, N, vN|0) = \max_{f} -k_{\mathrm{B}} H_{\mathrm{B}}(f)$$

where f is constrained by

$$f \geq 0;$$

$$\int_{v\subset\mathbb{R}^3} \int_{\mathbb{R}^3_s} f(s,p) d^3p\, d^3s = 1;$$

$$\int_{v\subset\mathbb{R}^3} \int_{\mathbb{R}^3_s} \tfrac{1}{2m}|p|^2 f(s,v) d^3p\, d^3s = \varepsilon.$$

Planck's formula for Boltzmann's equilibrium ENTROPY

Max Planck later epitomizes Boltzmann's entropy as:

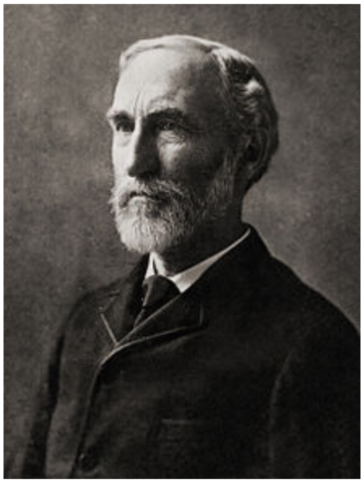
$$\boxed{S = k \log W}$$

Boltzmann's Tomb Stone in Vienna

Also around 1900 ...

Gibbs introduces his ensemble ENTROPY:

$$S_{\mathrm{G}}(F) = -k_{\mathrm{B}} \int_{\mathbb{R}^{3N}} \int_{\mathbb{R}^{3N}_{\mathbf{q}}} F(\mathbf{q}, \mathbf{p}, t) \ln F(\mathbf{q}, \mathbf{p}, t) d^{3N}p d^{3N}q$$



Josiah Willard Gibbs

The Gibbs Maximum ENTROPY Principle

Gibbs shows for “reasonable” $U(\neq 0)$ that:

$$\max_F S_{\rm F}(F) = \frac{E}{T} + k_{\rm B} \ln \int_{\mathbb{R}^{3N}} \int_{\mathbb{R}^{3N}_{\mathbf{q}}} e^{-\frac{1}{k_{\rm B}T} H(\mathbf{q},\mathbf{p})} d^{3N}p\, d^{3N}q;$$

here, F is constrained by

$$F \geq 0;$$

$$\int_{\mathbb{R}^{3N}} \int_{\mathbb{R}^{3N}_{\mathbf{q}}} F(\mathbf{q},\mathbf{p}) d^{3N}p\, d^{3N}q = 1;$$

$$\int_{\mathbb{R}^{3N}} \int_{\mathbb{R}^{3N}_{\mathbf{q}}} F(\mathbf{q},\mathbf{p}) H(\mathbf{q},\mathbf{p}) d^{3N}p\, d^{3N}q = E.$$

von Neumann's quantum ENTROPY:

$$S_{\mathrm{vN}}(\rho) = -k_{\mathrm{B}} Tr(\rho \ln \rho)$$

Shannon's Information ENTROPY:

$$H_{\mathrm{S}}(\{p\}) = -\sum_k p_k \log_2 p_k$$

Kullback-Leibler's DIVERGENCE (aka RELATIVE ENTROPY):

$$D_{\mathrm{KL}}(P\|Q) = \int_X \ln \frac{dP}{dQ} dP$$

N.B.: In the following, P is a probability measure,
while Q may be just a measure.

THM: *Let* $X = \mathbb{R}^{2N}$ *and* $dQ = e^{-H/N}\prod_{k=1}^{N} K(q_k)dq_k$*, with* $K(q)$ *a Schwartz function, and*

$$H(\mathbf{q}) = \sum_{1\leq k<l\leq N} \ln|q_k - q_l|.$$

Then

$$\lim_{N\to\infty}\frac{1}{N}\min_P \int_X \ln\frac{dP}{dQ}dP = \min_f \left[H_{\mathrm{B}}(f)+\frac{1}{2}\iint_{\mathbb{R}^2\times\mathbb{R}^2} f(s)f(s')\ln|s-s'|d^2s\, d^2s'\right]$$

where f *is a probability density. Moreover, defining*

$$-\int_{\mathbb{R}^2} f(s')\ln|s-s'|d^2s' =: 2u(s) + C$$

then C *can be chosen so that the maximizing* f *(viz.* u*) satisfies the*
PRESCRIBED GAUSS CURVATURE EQUATION

$$\boxed{-\Delta u(s) = K(s)e^{2u(s)}}$$

A question by Alice Chang (ca. 2000):

"Can you do this also for sign-changing Gauss curvatures?"

Let $z \in \mathbb{C}$, let $\sigma^2 > 0$ be a variance, $N \in \mathbb{N}$, and define the integrals

$$E_N(z;\sigma) = \begin{cases} \frac{1}{\sigma}\int_{\mathbb{R}} (x^2 + z^2) \frac{e^{-\frac{1}{2\sigma^2}x^2}}{\sqrt{2\pi}} dx \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{ if } N = 1, \\ \frac{1}{\sigma}\int_{\mathbb{R}^N} \prod\limits_{1\leq k<l\leq N} e^{-\frac{1}{2N}(1-\sigma^{-2})(x_k - x_l)^2} \prod\limits_{1\leq n\leq N} (x_n^2 + z^2) \frac{e^{-\frac{1}{2\sigma^2}x_n^2}}{\sqrt{2\pi}} dx_n \text{ if } N > 1. \end{cases}$$

These are expected values of the polynomials

$$P_N(z) = \textstyle\prod_{1\leq n\leq N}(X_n^2 + z^2)$$

whose $2N$ zeros $\{\pm iX_k\}_{k=1,\ldots,N}$ are generated by N identically distributed multi-variate mean-zero normal random variables $\{X_k\}_{k=1}^N$ with co-variance

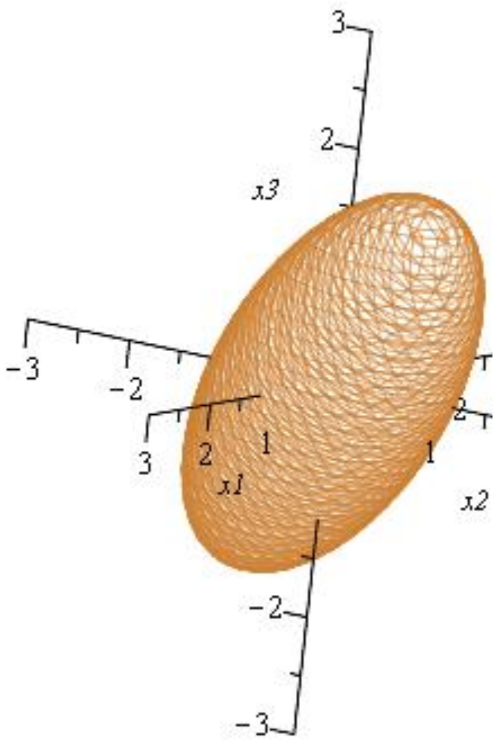
$$\mathrm{Cov}_N(X_k, X_l) = (1 + \tfrac{\sigma^2 - 1}{N})\delta_{k,l} + \tfrac{\sigma^2-1}{N}(1 - \delta_{k,l}).$$

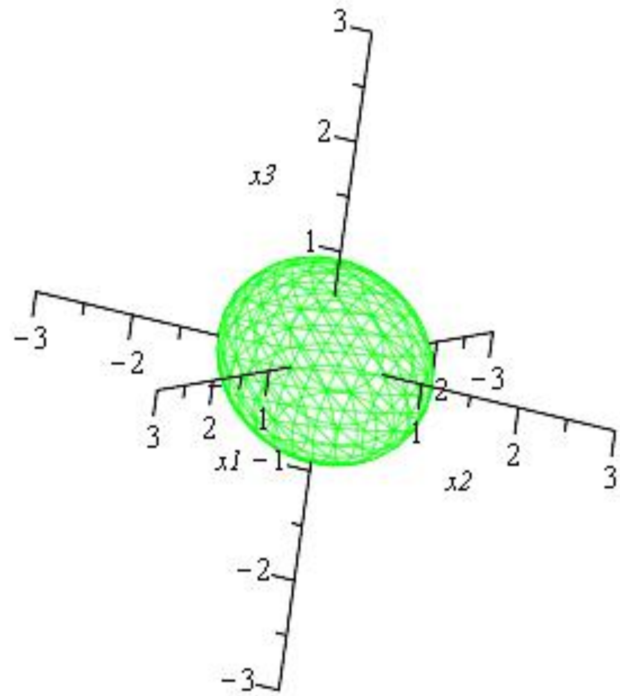
The $E_N(z;\sigma)$ are polynomials in z^2, explicitly computable for all N,

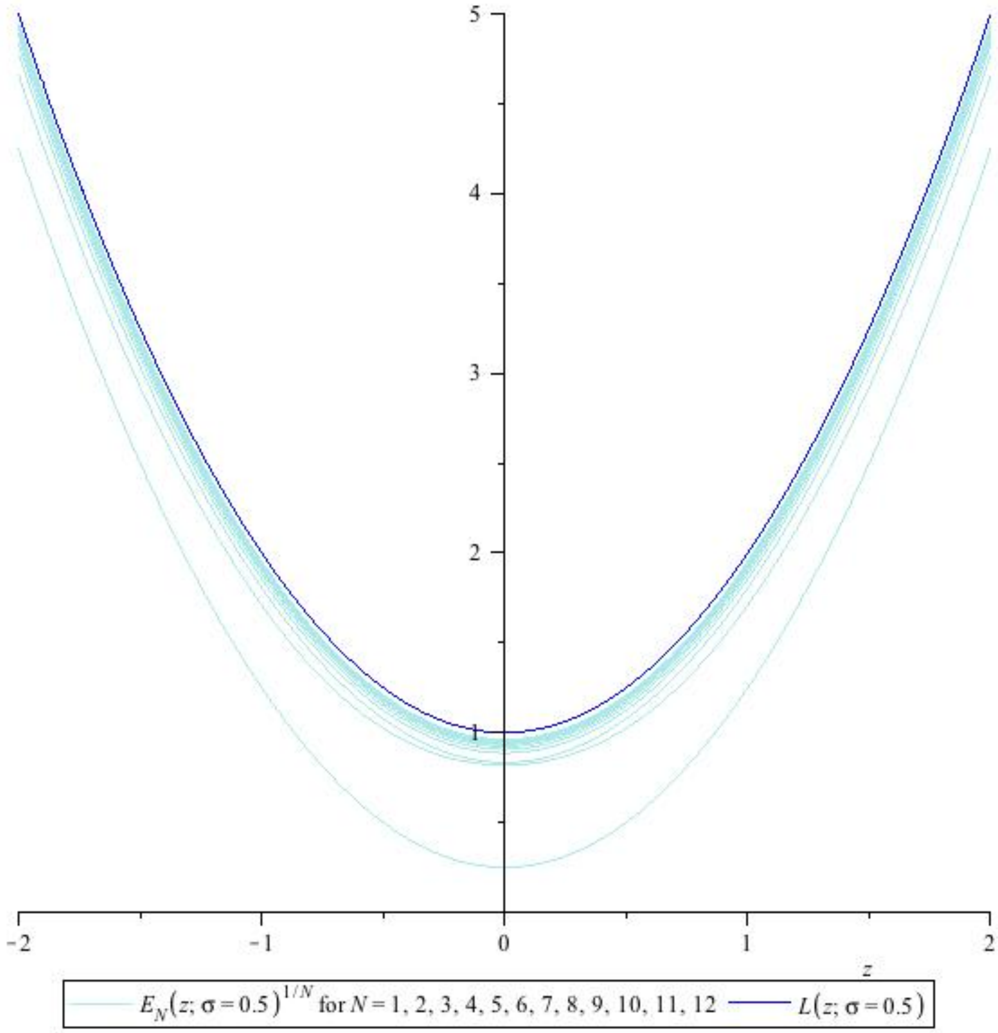
$$E_N(z;\sigma) = \sum_{j=0}^{N} z^{2j} \binom{N}{j} \sum_{k=0}^{N-j} \binom{N-j}{k} \frac{(2k)!}{2^k k!} \left(\frac{\sigma^2 - 1}{N}\right)^k \qquad (1)$$

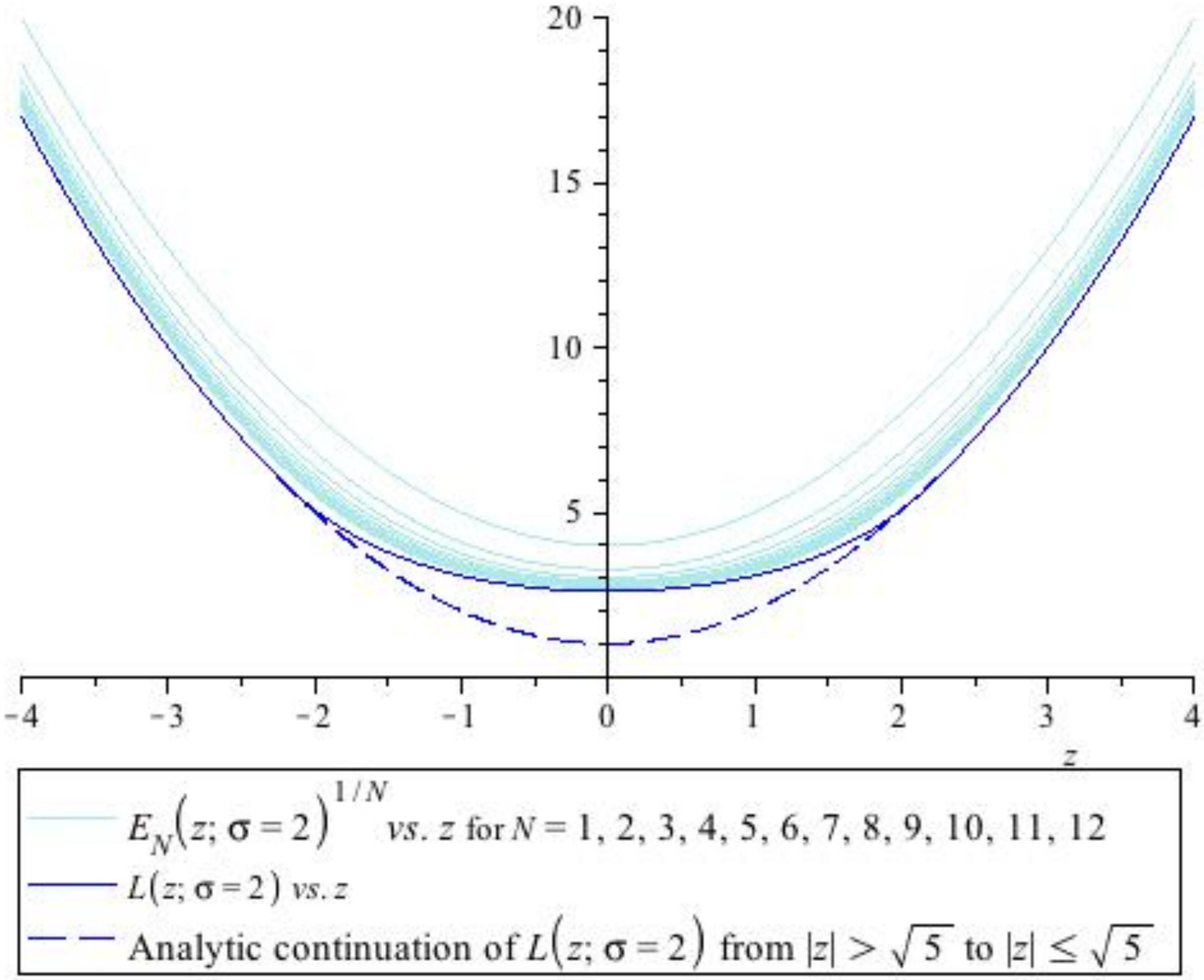
When $\sigma = 1$, then $E_N(z;1) = (1 + z^2)^N$ for all $z \in \mathbb{C}$ and $N \in \mathbb{N}$.

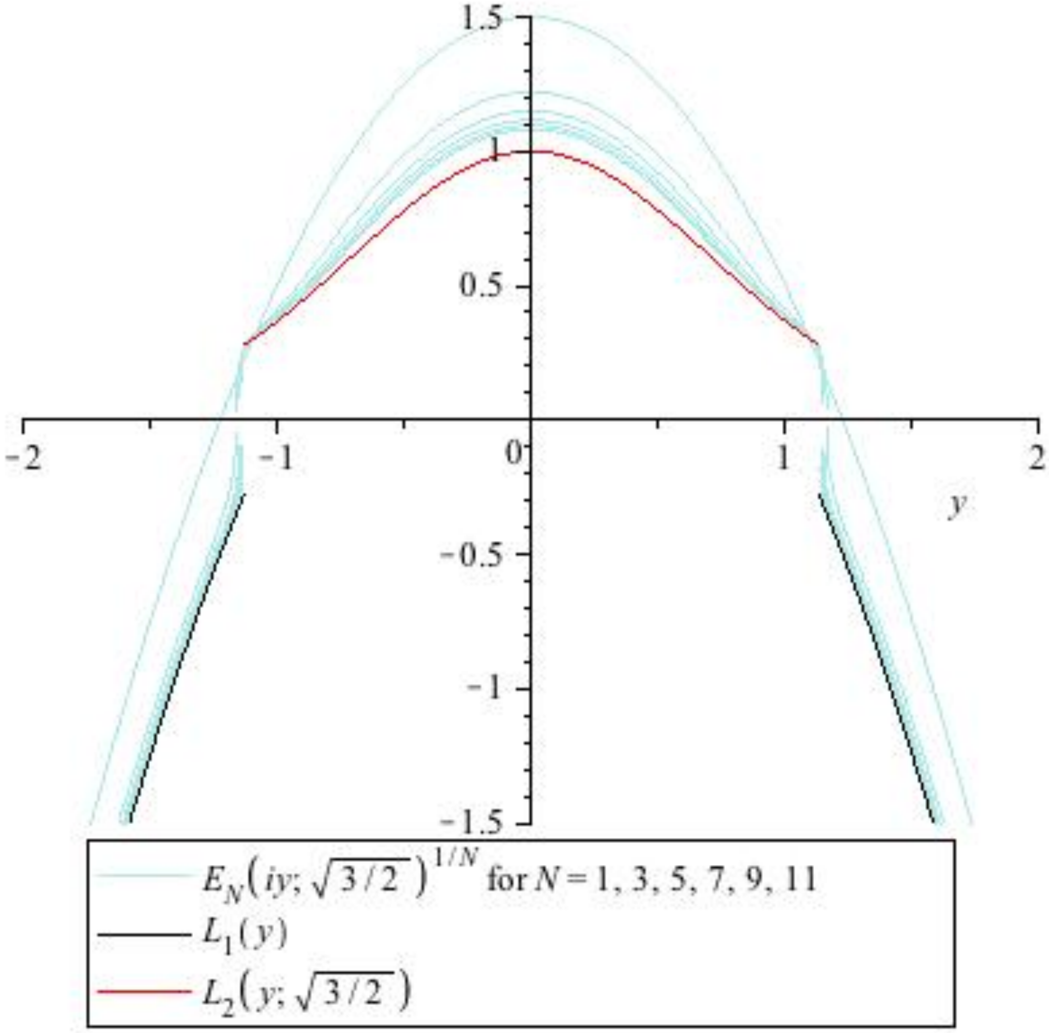
Multivariate Normal Level Surfaces: $\sigma > 1$ (left) and $0 < \sigma < 1$ (right)

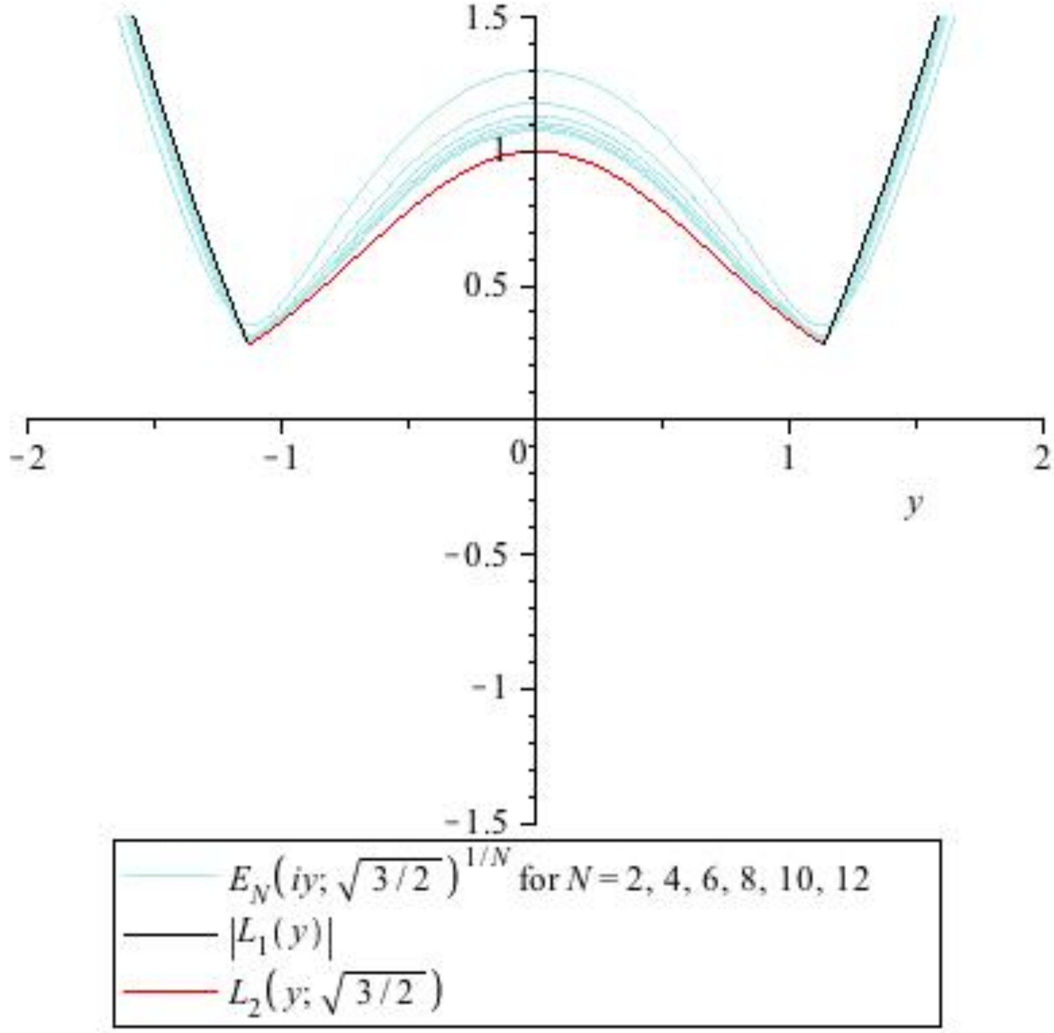


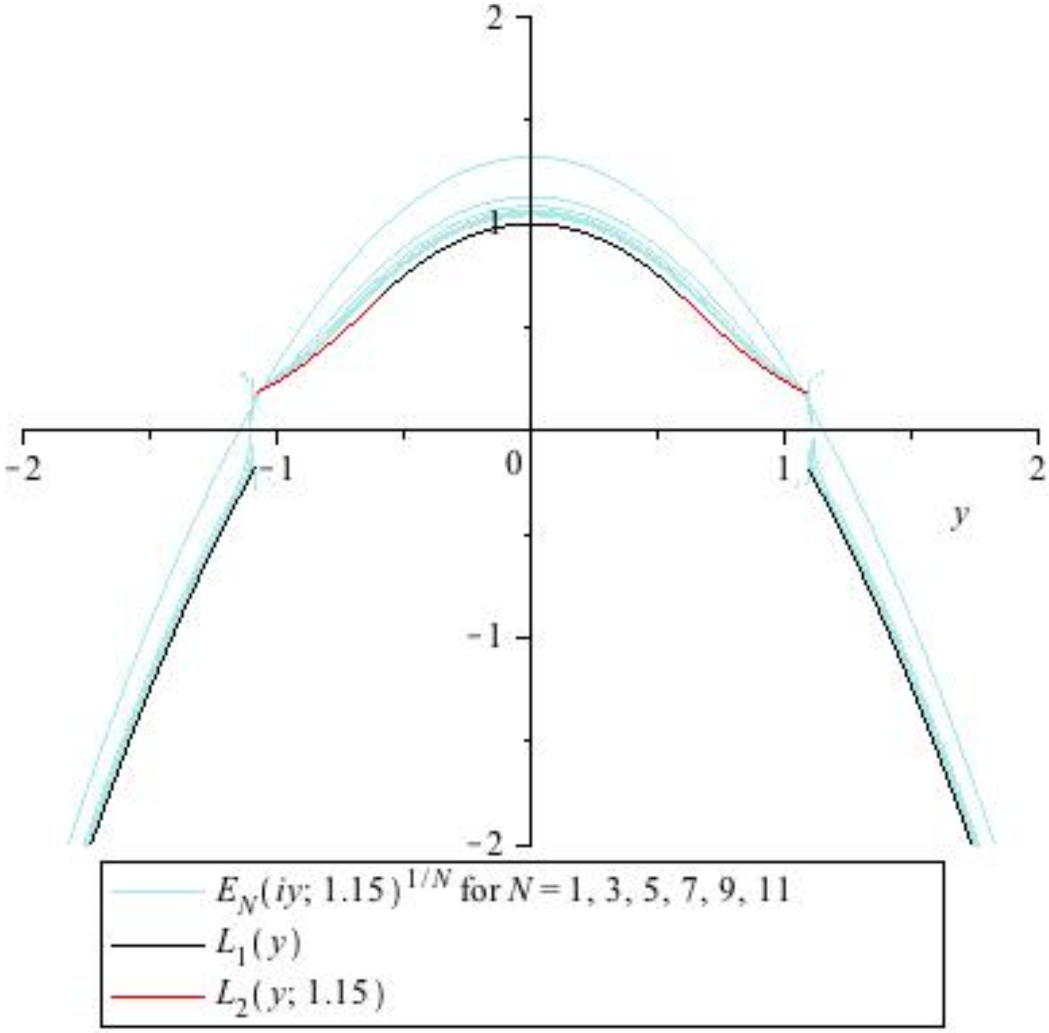



5
4
3
2
1
-2
-1
0
1
2
z
$E_N(z; \sigma = 0.5)^{1/N}$ for $N = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12$
$L(z; \sigma = 0.5)$

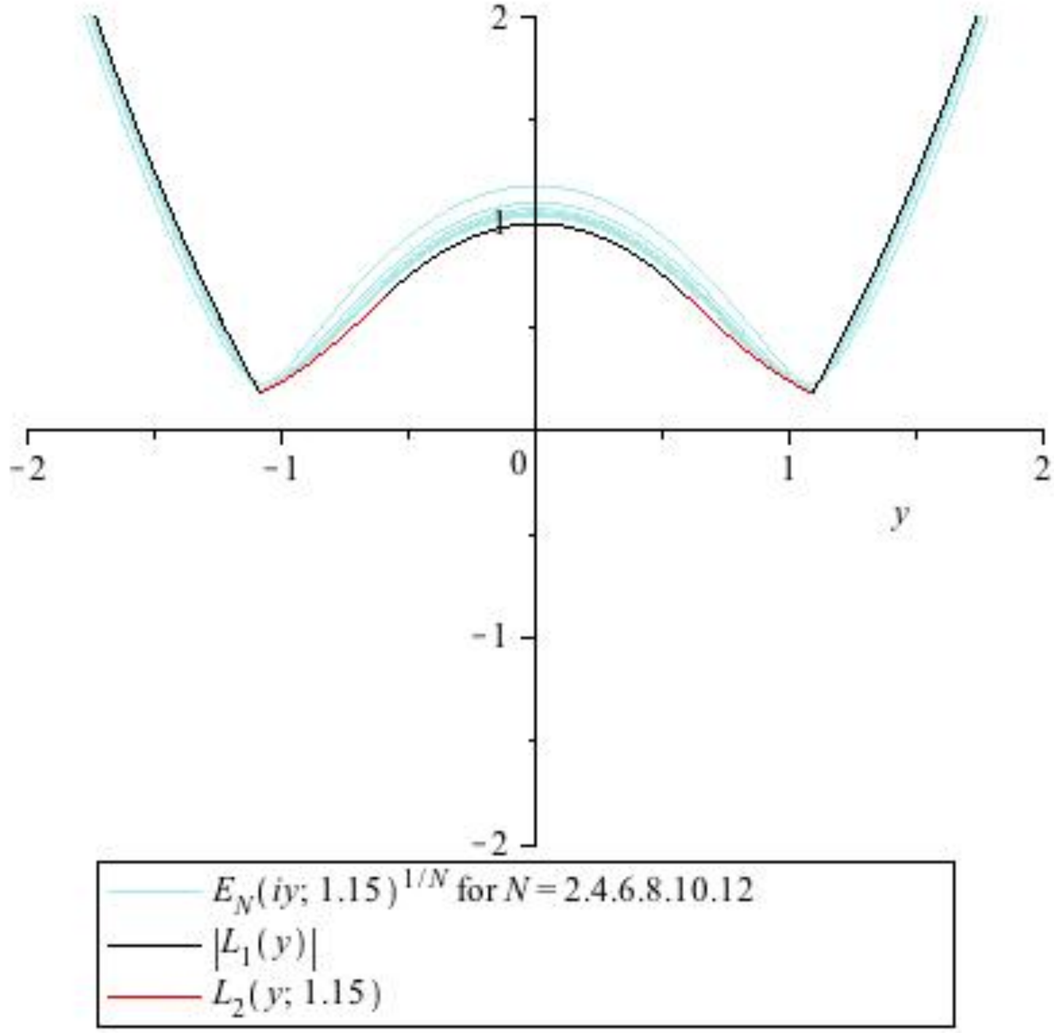

20
15
10
5
-4
-3
-2
-1
0
1
2
3
4
z
$E_N(z; \sigma = 2)^{1/N}$ vs. z for N = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
$L(z; \sigma = 2)$ vs. z
Analytic continuation of $L(z; \sigma = 2)$ from $|z| > \sqrt{5}$ to $|z| \leq \sqrt{5}$

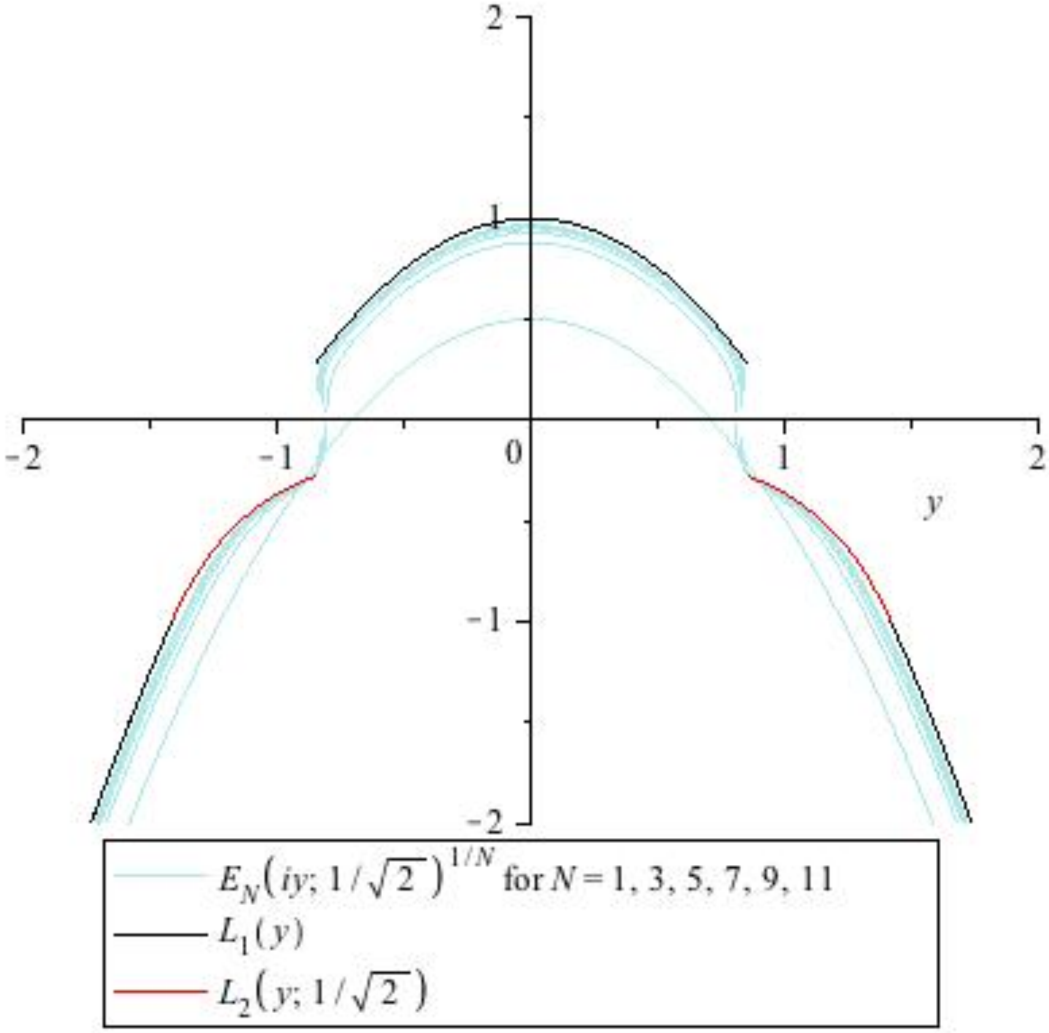

1.5
1
0.5
-0.5
-1
-1.5
-2
-1
0
1
2
y
$E_N\left(iy; \sqrt{3/2}\right)^{1/N}$ for $N = 1, 3, 5, 7, 9, 11$
$L_1(y)$
$L_2\left(y; \sqrt{3/2}\right)$

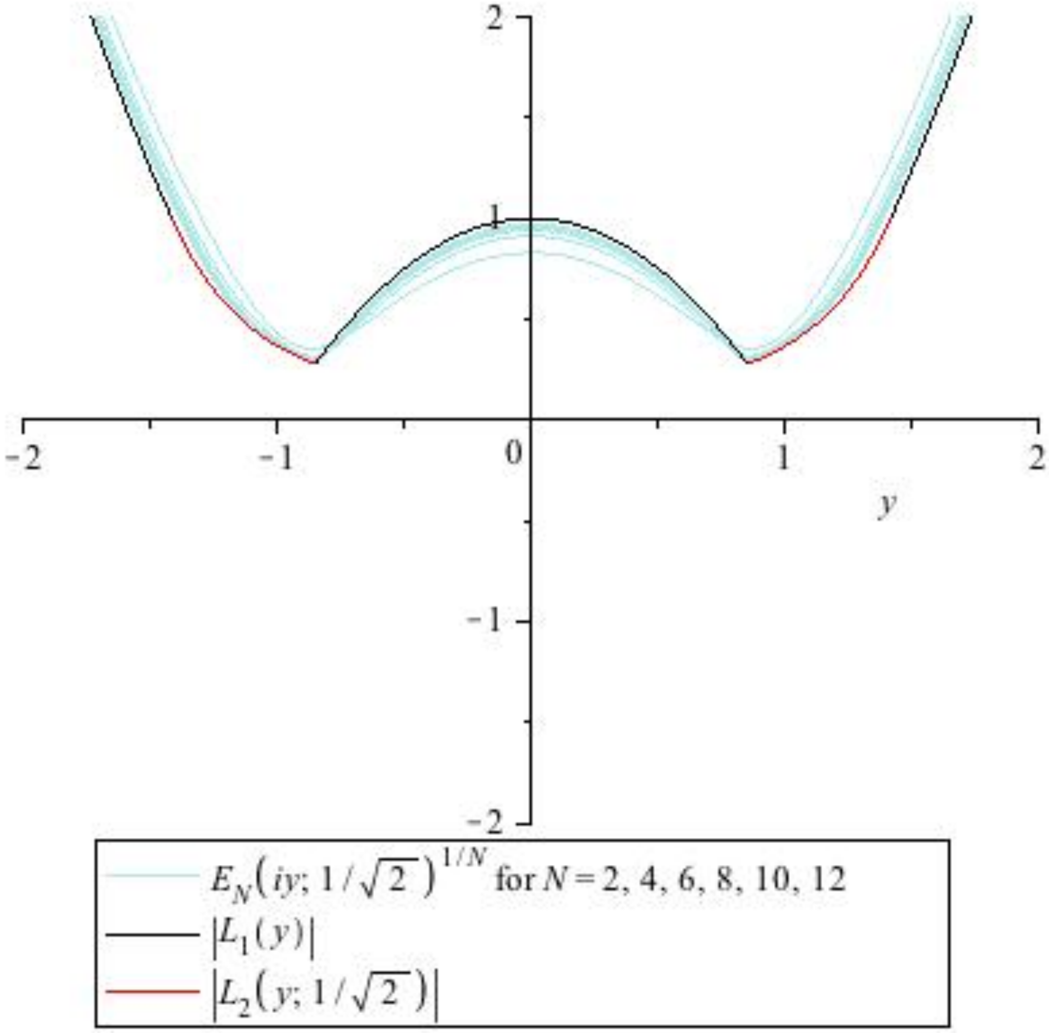

1.5
1
0.5
-0.5
-1
-1.5
-2
-1
0
1
2
y
$E_N(iy; \sqrt{3/2})^{1/N}$ for $N = 2, 4, 6, 8, 10, 12$
$|L_1(y)|$
$L_2(y; \sqrt{3/2})$

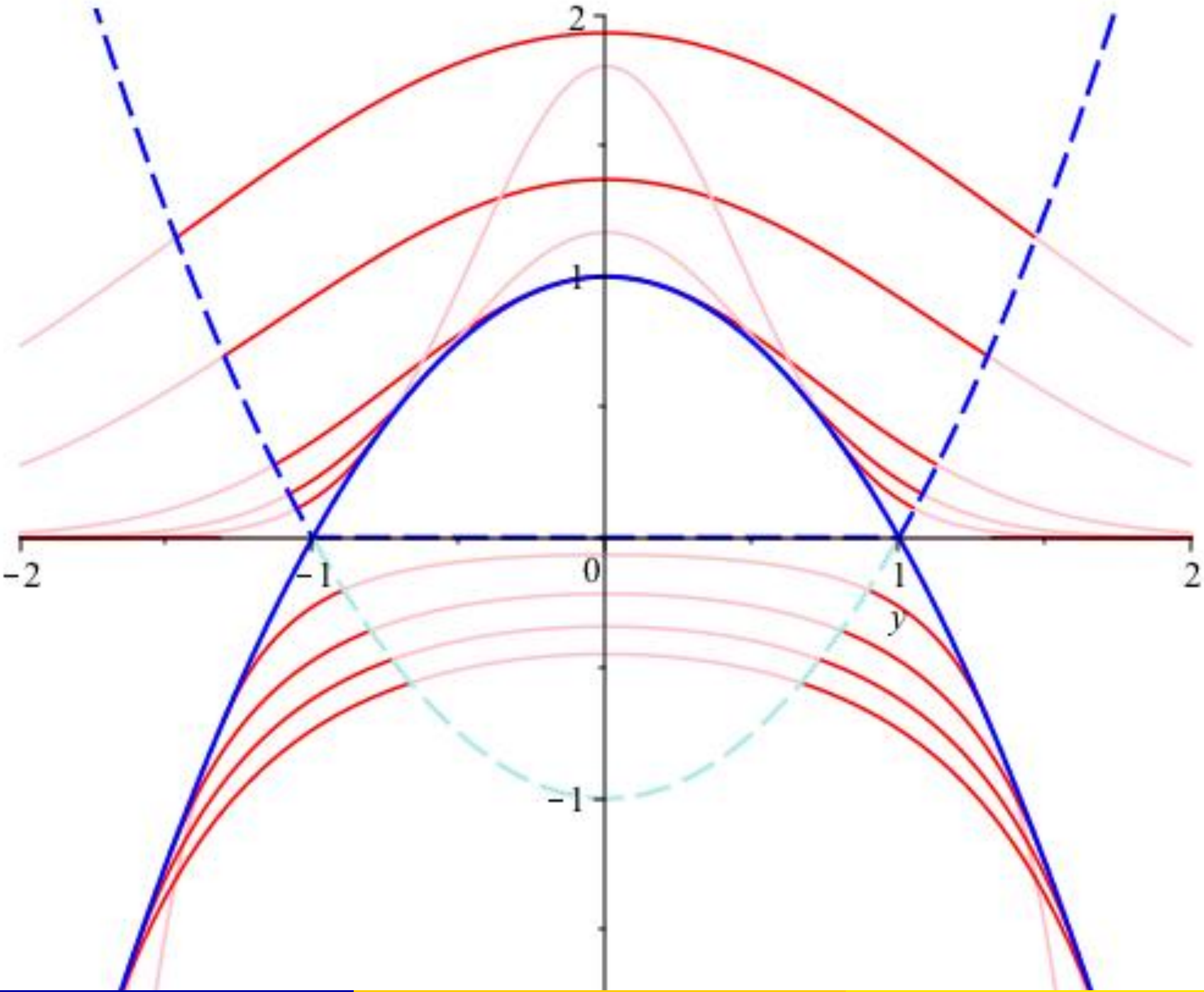


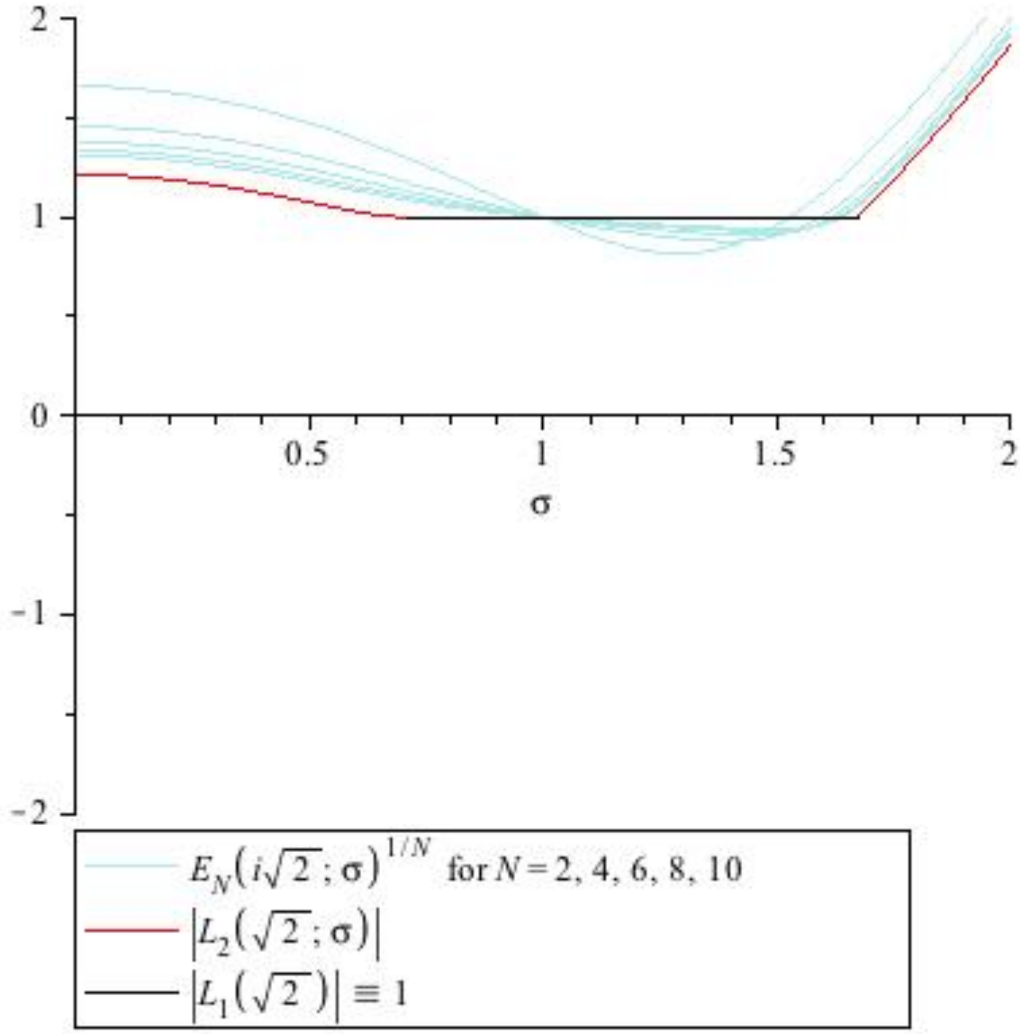
2
1
-2
-1
0
1
2
y
-1
-2
$E_N(iy; 1.15)^{1/N}$ for $N = 1, 3, 5, 7, 9, 11$
$L_1(y)$
$L_2(y; 1.15)$

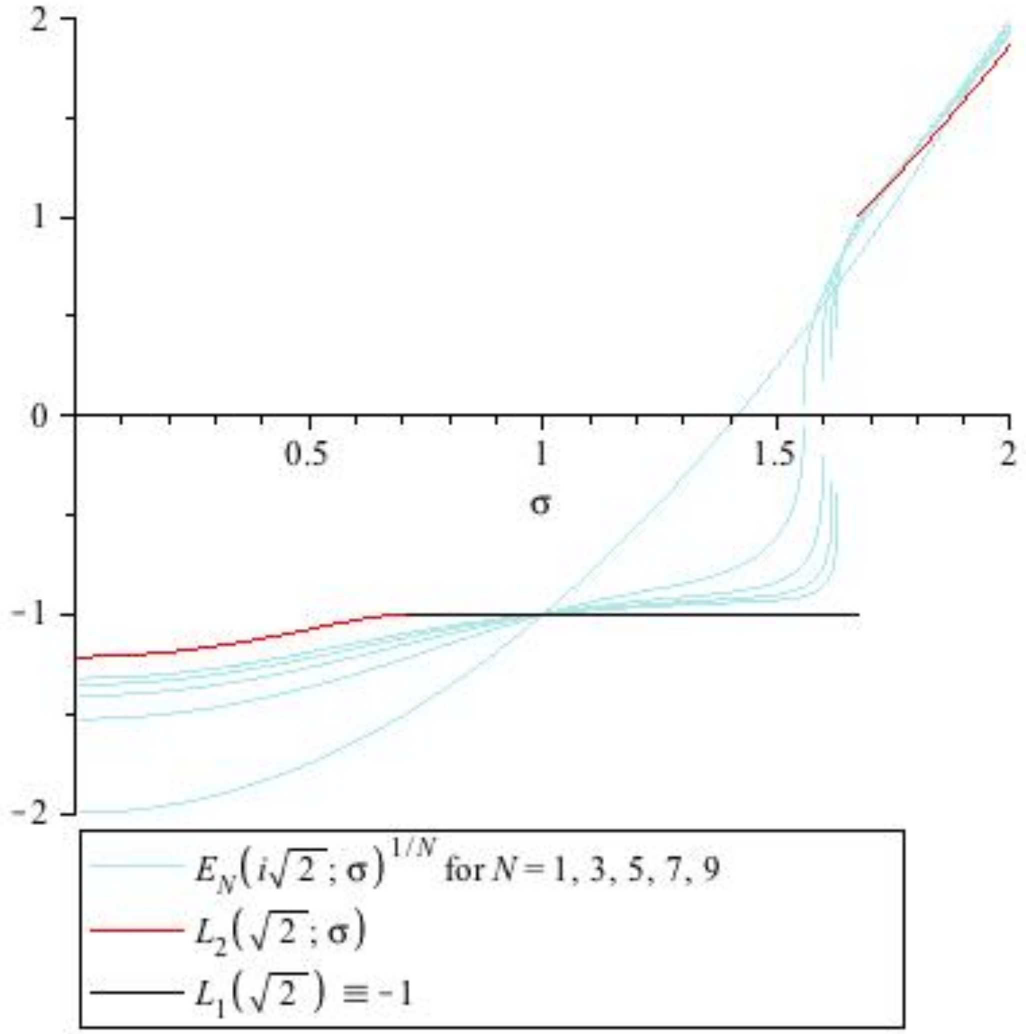

2
1
-1
-2
-2
-1
0
1
2
y
$E_N(iy; 1.15)^{1/N}$ for $N = 2.4.6.8.10.12$
$|L_1(y)|$
$L_2(y; 1.15)$


2
1
-2
-1
0
1
2
y
-1
-2
$E_N(iy; 1/\sqrt{2})^{1/N}$ for $N = 1, 3, 5, 7, 9, 11$
$L_1(y)$
$L_2(y; 1/\sqrt{2})$


2
1
0
-1
-2
-2
-1
1
2
y
$E_N(iy; 1/\sqrt{2})^{1/N}$ for $N = 2, 4, 6, 8, 10, 12$
$|L_1(y)|$
$|L_2(y; 1/\sqrt{2})|$


2
1
−2
−1
0
1
2
y
−1


2
1
0
-1
-2
0.5
1
1.5
2
σ
$E_N(i\sqrt{2};\sigma)^{1/N}$ for $N = 2, 4, 6, 8, 10$
$|L_2(\sqrt{2};\sigma)|$
$|L_1(\sqrt{2})| \equiv 1$


2
1
0
-1
-2
0.5
1
1.5
2
σ
$E_N(i\sqrt{2};\sigma)^{1/N}$ for $N = 1, 3, 5, 7, 9$
$L_2(\sqrt{2};\sigma)$
$L_1(\sqrt{2}) \equiv -1$

Further reading:

Heuristic Relative Entropy Principles with Complex Measures: Large-Degree Asymptotics of a Family of Multi-Variate Normal Random Polynomials
J. Stat. Phys. **169**:63–106 (2017).

THANK YOU FOR LISTENING!