Supplementary Document on Using Moments to Represent Bounded Signals for Spectral Rendering

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A NEGATIVE RESULT ON LINEAR RECONSTRUCTIONS

Our bounded MESE reconstructs a bounded signal from trigonometric (0, 1)-moments in a non-linear fashion although the moments themselves depend on the signal linearly. In the paper we motivate this non-linear approach with a fundamental limitation of linear reconstructions: Binning is the only linear reconstruction that preserves non-negativity of signals. In the following, we formalize this statement and provide a proof. Our formulation focuses on non-negativity but if a constant function is part of the basis, it applies equally to all other lower or upper bounds.

To avoid technicalities of functional analysis, we only consider signals assigning a value to finitely many samples. With arbitrarily high sample counts, all well-behaved signals can be approximated to arbitrary accuracy, even those defined on a multi-dimensional domain. Therefore, this simplification does not limit the significance of our claim in practice.

Theorem A.1. *Let $\mathbb{D}$ be a finite set and denote the space of functions $f : \mathbb{D} \to \mathbb{R}$ by $\mathbb{F}$. Let $f_0, \ldots, f_{m-1} \in \mathbb{F}$ be a basis of a subspace of $\mathbb{F}$ and fix a weighting function $w \in \mathbb{F}$ with $w > 0$. Suppose that for all $f \in \mathbb{F}$ with $f \geq 0$, we also have $\sum_{j=0}^{m-1} y_j f_j \geq 0$ where the coefficients $y_0, \ldots, y_{m-1} \in \mathbb{R}$ minimize the weighted least-squares error*

$$\sum_{x \in \mathbb{D}} w(x) \left(f(x) - \sum_{j=0}^{m-1} y_j f_j(x) \right)^2 . \tag{A.1}$$

Then we can find a basis $g_0, \ldots, g_{m-1} \in \mathbb{F}$ spanning the same space as $f_0, \ldots, f_{m-1}$ using only non-negative functions $0 \leq g_0, \ldots, g_{m-1}$ with pairwise disjoint support.

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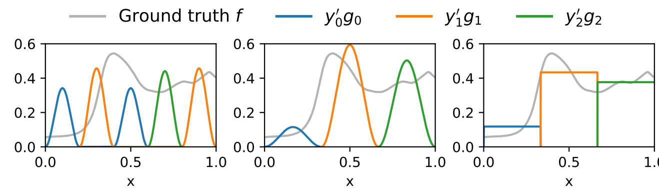

(a) Disconnected support (b) Differentiable basis (c) Classical binning

Fig. A.1. Least-squares fits of f using a few possible bases g_0, g_1, g_2.

In the modified basis, each function g_j corresponds to one bin and the weighted least-squares fit of $f \in \mathbb{F}$ takes a simple form:

$$\sum_{j=0}^{m-1} y_j f_j = \sum_{j=0}^{m-1} y_j' g_j \quad \text{with} \quad y_j' := \frac{\sum_{x \in \mathbb{D}} w(x) g_j(x) f(x)}{\sum_{x \in \mathbb{D}} w(x) g_j^2(x)}.$$

Disregarding the normalization factor, the optimal least-squares weight y_j' just accumulates the function f over the support of g_j, weighted by wg_j. Each basis function g_j is weighted by y_j' to obtain the least-squares fit. This procedure is a weighted form of binning. Although the computation to obtain the fit $\sum_{j=0}^{m-1} y_j f_j$ is different, the fit is the same and it suffers from the same drawbacks.

In theory, each basis function g_j may vary within its support and the support may be any set. Figure A.1 gives a few examples of what that means in practice. In Figure A.1a, g_0 and g_1 have disconnected support. Thus, the values of the fit at different locations become dependent in a way that is usually undesirable. Figure A.1b uses a differentiable basis but since the support of g_0, g_1, g_2 must be disjoint, this goal can only be accomplished by approaching zero at the boundary of the support. Therefore, the fit vanishes in locations determined by the basis, not by the signal f. If we want to avoid both issues, the natural choice is classical binning where g_0, g_1, g_2 are disjoint box functions covering the entire domain $\mathbb{D}$. Then the fit is piecewise constant as shown in Figure A.1c.

Theorem A.1 tells us that fits resulting from binning approaches are the only way to guarantee preservation of non-negativity. In other words, ringing artifacts are all but specific to the Fourier basis. Any basis that provides more sophisticated least-squares fits than binning must also suffer from ringing.

The proof interprets the least-squares fit as orthogonal projector with non-negative entries. Therefore, we prove two lemmata on such projectors before we prove the theorem itself.

Lemma A.2. *Let $Q = (q_{j,k})_{j,k=0}^{n-1} \in \mathbb{R}^{n\times n}$ be an orthogonal projector, i.e. $Q = Q^\mathsf{T} = Q^2$, with $q_{j,k} > 0$ for all $j, k \in \{0, \ldots, n-1\}$. Then Q has rank one.*

Proof. For all $k \in \{0, \ldots, n-1\}$ denote the k-th canonical basis vector by $e_k \in \mathbb{R}^n$. We consider a normalized column vector of Q:

$$r_k := \frac{1}{\sum_{j=0}^{n-1} q_{j,k}} Q e_k$$

Our goal is to prove that all r_k are equal. To this end, let

$$w_{l,k} := q_{l,k} \frac{\sum_{j=0}^{n-1} q_{j,l}}{\sum_{j=0}^{n-1} q_{j,k}} > 0$$

for all $l \in \{0, \ldots, n-1\}$. Since Q is a projector, we obtain

$$r_k = Q r_k = \sum_{l=0}^{n-1} Q e_l e_l^\mathsf{T} r_k = \sum_{l=0}^{n-1} \frac{q_{l,k}}{\sum_{j=0}^{n-1} q_{j,k}} Q e_l = \sum_{l=0}^{n-1} w_{l,k} r_l.$$

Furthermore, the weights sum to one:

$$\sum_{l=0}^{n-1} w_{l,k} = \frac{\sum_{j=0}^{n-1}\sum_{l=0}^{n-1} q_{j,l} q_{l,k}}{\sum_{j=0}^{n-1} q_{j,k}} = \frac{\sum_{j=0}^{n-1} q_{j,k}}{\sum_{j=0}^{n-1} q_{j,k}} = 1$$

In other words, r_k is a convex combination of $r_0, \ldots, r_{n-1}$ using positive weights only.

Let $v \in \mathbb{R}^n$ and let $j, k \in \{0, \ldots, n-1\}$ such that

$$v^\mathsf{T} r_j = \min_{l\in\{0,\ldots,n-1\}} v^\mathsf{T} r_l, \qquad v^\mathsf{T} r_k = \max_{l\in\{0,\ldots,n-1\}} v^\mathsf{T} r_l.$$

Then we find

$$\begin{aligned} v^\mathsf{T} r_k &= \sum_{l=0}^{n-1} w_{l,k} v^\mathsf{T} r_l = w_{j,k} v^\mathsf{T} r_j + \sum_{l=0, l\neq j}^{n-1} w_{l,k} v^\mathsf{T} r_l \\ &\leq w_{j,k} v^\mathsf{T} r_j + \sum_{l=0,l\neq j}^{n-1} w_{l,k} v^\mathsf{T} r_k = w_{j,k} v^\mathsf{T} r_j + (1 - w_{j,k}) v^\mathsf{T} r_k. \end{aligned}$$

The inequality implies $v^\mathsf{T} r_j \geq v^\mathsf{T} r_k$ and thus $v^\mathsf{T} r_j = v^\mathsf{T} r_k$. Since $v \in \mathbb{R}^n$ is arbitrary, we conclude that all r_k must be equal. □

Lemma A.3. *Let $P = (p_{j,k})_{j,k=0}^{n-1} \in \mathbb{R}^{n\times n}$ be an orthogonal projector with $p_{j,k} \geq 0$ for all $j, k \in \{0, \ldots, n-1\}$. Then any two columns of P are either linearly dependent or orthogonal.*

Proof. We define a relation on index pairs $j, k \in \{0, \ldots, n-1\}$:

$$j \sim k \quad :\Leftrightarrow \quad p_{j,k} > 0 \ \vee\ j = k$$

This relation is reflexive by definition and symmetric because P is symmetric. It is also transitive because for all pairwise different $j, t, k \in \{0, \ldots, n-1\}$:

$$j \sim t \ \wedge\ t \sim k \ \Rightarrow\ 0 < p_{j,t} p_{t,k} \leq \sum_{l=0}^{n-1} p_{j,l} p_{l,k} = p_{j,k} \ \Rightarrow\ j \sim k$$

In consequence, $\sim$ is an equivalence relation and as such it partitions $\{0, \ldots, n-1\}$ into equivalence classes. Without loss of generality, rows and columns of P are ordered such that the equivalence classes are $\{j_l, \ldots, j_{l+1}-1\}$ with a class index $l \in \{0, \ldots, m-1\}$ and starting indices $0 = j_0 < \ldots < j_m = n$. Then P is a block diagonal matrix

$$P = \begin{pmatrix} Q_0 & & \\ & \ddots & \\ & & Q_{m-1} \end{pmatrix}$$

with blocks $Q_l \in \mathbb{R}^{(j_{l+1}-j_l)\times(j_{l+1}-j_l)}$ because by definition of the equivalence relation, entries $p_{j,k}$ for non-equivalent index pairs $j, k \in \{0, \ldots, n-1\}$ must be zero. We distinguish two cases for each block.

Case 1, Q_l has a vanishing diagonal entry: Let $k \in \{0, \ldots, n-1\}$ be the column index of the vanishing diagonal entry $p_{k,k} = 0$. Then we know

$$0 = p_{k,k} = \sum_{j=0}^{n-1} p_{k,j} p_{j,k} = \sum_{j=0}^{n-1} p_{j,k}^2,$$

i.e. the whole column is zero. In particular, k is only equivalent to itself and we conclude $Q_l = 0 \in \mathbb{R}^{1\times 1}$.

Case 2, all diagonal entries of Q_l are non-zero: Since all indices within the equivalence class $\{j_l, \ldots, j_{l+1} - 1\}$ are equivalent, all entries of Q_l are positive. Furthermore, Q_l is still an orthogonal projector because

$$P = \begin{pmatrix} Q_0^\mathsf{T} & & \\ & \ddots & \\ & & Q_{m-1}^\mathsf{T} \end{pmatrix} = P^\mathsf{T} = P^2 = \begin{pmatrix} Q_0^2 & & \\ & \ddots & \\ & & Q_{m-1}^2 \end{pmatrix}.$$

Applying Lemma A.2, we find that Q_l has rank one.

Thus, two columns $j, k \in \{0, \ldots, n-1\}$ of P are linearly dependent if $j \sim k$ and orthogonal if they belong to two different classes. □

With these lemmata, we are prepared to prove the theorem.

Proof of Theorem A.1. Without loss of generality, the domain is $\mathbb{D} = \{0, \ldots, n-1\}$. We identify functions with weighted vectors through the vectorspace isomorphism

$$\begin{aligned} \psi :\ & \mathbb{F} \to \mathbb{R}^n \\ & f \mapsto (\sqrt{w(x)} f(x))_{x=0}^{n-1}. \end{aligned}$$

Through this identification, the weighted least-squares error in Equation (A.1) agrees with the squared 2-norm of $\mathbb{R}^n$. Then the solution of the least-squares system in Equation (A.1) is given by

$$(y_0, \ldots, y_{m-1})^\mathsf{T} = (A^\mathsf{T} A)^{-1} A^\mathsf{T} \psi(f) \quad \text{where} \quad A := (\psi(f_0), \ldots, \psi(f_{m-1})) \in \mathbb{R}^{n\times m}.$$

The matrix $P := A(A^\mathsf{T} A)^{-1} A^\mathsf{T} \in \mathbb{R}^{n\times n}$ is the orthogonal projector mapping the vector $\psi(f)$ to its least-squares fit $\psi(\sum_{j=0}^{m-1} y_j f_j)$. Let $k \in \{0, \ldots, n-1\}$ and consider the function $f \in \mathbb{F}$ with

$$f(x) := \begin{cases} \frac{1}{\sqrt{w(x)}} & \text{if } x = k, \\ 0 & \text{otherwise.} \end{cases}$$

By construction, $\psi(f) = e_k$ is the k-th canonical basis vector. Since $f \geq 0$, we know $\psi^{-1}(P e_k) \geq 0$. It follows that all entries of P are non-negative and therefore Lemma A.3 is applicable. If we pick a basis among $\psi^{-1}(P e_0), \ldots, \psi^{-1}(P e_{n-1})$, it spans the same space as

$f_0, \ldots, f_{m-1}$ and the basis functions are known to be pairwise orthogonal. Since they are also non-negative, they must have pairwise disjoint support. □

B THE BOUNDED MESE

Our explanation of the bounded maximum entropy spectral estimate (MESE) in the paper does not include proofs. We provide these in the following sections in the order in which they are mentioned in the paper.

B.1 The Fourier Coefficients of the Herglotz Kernel

The Herglotz transform is central to our derivation. To work with it, we first have to derive its Fourier series.

Proposition B.1. *The Fourier coefficients of the Herglotz kernel for all $j \in \mathbb{Z}$ and $z \in \mathbb{C}$ with $|z| < 1$ are*

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\exp(i\varphi)+z}{\exp(i\varphi)-z}\exp(-ij\varphi)\,\mathrm{d}\varphi = \begin{cases} 2z^{-j} & \text{if } j<0,\\ 1 & \text{if } j=0,\\ 0 & \text{if } j>0.\end{cases}$$

Proof. Let $\varphi \in \mathbb{R}$ and $w := \exp(i\varphi)$. Then the claimed Fourier series for the Herglotz kernel is:

$$\begin{aligned}1 + \sum_{j=-\infty}^{-1} 2z^{-j}w^j &= 1 + \sum_{j=1}^{\infty} 2\left(\frac{z}{w}\right)^j = -1 + 2\sum_{j=0}^{\infty}\left(\frac{z}{w}\right)^j\\ &= -1 + 2\frac{1}{1-\frac{z}{w}} = -1 + 2\frac{w}{w-z}\\ &= \frac{2w-(w-z)}{w-z} = \frac{w+z}{w-z} = \frac{\exp(i\varphi)+z}{\exp(i\varphi)-z}\end{aligned}$$

□

B.2 Reducing Bounded to Unbounded Problems

We show that for a continuous 2π-periodic function $g(\varphi) \in [0,1]$

$$\lim_{z\to\exp(i\varphi)} \Re\mathcal{H}[g](z) = g(\varphi). \tag{B.1}$$

Proof. For all $z \in \mathbb{C}$ with $|z| < 1$ and $\varphi \in \mathbb{R}$, the real part of the Herglotz kernel is a Poisson kernel:

$$\begin{aligned}\Re\frac{\exp(i\varphi)+z}{\exp(i\varphi)-z} &= \Re\frac{(\exp(i\varphi)+z)(\exp(-i\varphi)-\overline{z})}{|\exp(i\varphi)-z|^2}\\ &= \frac{\Re\left(1-\exp(i\varphi)\overline{z}+\exp(-i\varphi)z-|z|^2\right)}{|1-z\exp(-i\varphi)|^2}\\ &= \frac{1-|z|^2}{|1-z\exp(-i\varphi)|^2} = 2\pi P_z(\varphi)\end{aligned}$$

From Proposition B.1, it is evident that the Poisson kernel is normalized, i.e. $\int_{-\pi}^{\pi} P_z(\varphi)\,\mathrm{d}\varphi = 1$. It has its global maximum at $\varphi = \arg z$ and for $|z| \to 1$, it localizes all of its mass in this maximum. Thus

$$\lim_{z\to\exp(i\varphi)} \Re\mathcal{H}[g](z) = \lim_{z\to\exp(i\varphi)} \int_{-\pi}^{\pi} P_z(\psi)g(\psi)\,\mathrm{d}\psi = g(\varphi).$$

□

B.3 Exponential Moments

Next we prove the recurrence formula for exponential moments using a technique of Roger Barnard [Gustafsson and Putinar, 2017, p. 12].

Proof of Proposition 2. Let the Fourier coefficients $c_j, \gamma_j \in \mathbb{C}$ of the signals $g(\varphi) \in [0,1]$ and $d(\varphi) \geq 0$ be defined for all $j \in \mathbb{Z}$. The Herglotz transform is an inner product with the Herglotz kernel. Using Proposition B.1, we can rewrite it as an inner product of the Fourier transforms:

$$\begin{aligned}\mathcal{H}[g](z) &= c_0 + 2\sum_{j=-\infty}^{-1}\overline{c_j}z^{-j} = c_0 + 2\sum_{j=1}^{\infty}c_jz^j\\ \mathcal{H}[d](z) &= \gamma_0 + 2\sum_{j=1}^{\infty}\gamma_jz^j\end{aligned}$$

Thus, Equation (3) becomes

$$\exp\left(\pi i\left(c_0 - \frac{1}{2} + 2\sum_{j=1}^{\infty}c_jz^j\right)\right) = i\alpha + 2\pi\gamma_0 + 4\pi\sum_{j=1}^{\infty}\gamma_jz^j. \tag{B.2}$$

We define $\gamma_0' := \frac{i}{4\pi}\alpha + \frac{1}{2}\gamma_0$ and $\gamma_j' := \gamma_j$ for all $j \in \mathbb{N}$ to simplify the right-hand side to $4\pi\sum_{j=0}^{\infty}\gamma_j'z^j$.

Now we take the derivative with respect to z on both sides and rearrange terms:

$$\begin{aligned}&\frac{\partial}{\partial z}\exp\left(\pi i\left(c_0 - \frac{1}{2} + 2\sum_{k=1}^{\infty}c_kz^k\right)\right) = 4\pi\frac{\partial}{\partial z}\sum_{j=0}^{\infty}\gamma_j'z^j\\ \Leftrightarrow &\left(4\pi\sum_{j=0}^{\infty}\gamma_j'z^j\right)2\pi i\sum_{k=1}^{\infty}kc_kz^{k-1} = 4\pi\sum_{j=0}^{\infty}j\gamma_j'z^{j-1}\\ \Leftrightarrow &\, 2\pi i\sum_{j,k=0}^{\infty}k\gamma_j'c_kz^{j+k-1} = \sum_{j=0}^{\infty}j\gamma_j'z^{j-1}\\ \Leftrightarrow &\, 2\pi i\sum_{l=0}^{\infty}\left(\sum_{j=0}^{l-1}(l-j)\gamma_j'c_{l-j}\right)z^{l-1} = \sum_{j=0}^{\infty}j\gamma_j'z^{j-1}\end{aligned}$$

Hence, for all $l \in \mathbb{N}$

$$2\pi i\sum_{j=0}^{l-1}(l-j)\gamma_j'c_{l-j} = l\gamma_l,$$

which implies Equation (7).

To obtain γ_0', we set $z = 0$ in Equation (B.2):

$$\exp\left(\pi i\left(c_0 - \frac{1}{2}\right)\right) = i\alpha + 2\pi\gamma_0 \quad \Rightarrow \quad \gamma_0' = \frac{1}{4\pi}\exp\left(\pi i\left(c_0 - \frac{1}{2}\right)\right)$$

□

B.4 Trigonometric Moments of the MESE

In this Section, we introduce a novel linear recurrence to compute all trigonometric moments of the MESE. We begin by proving a Lemma that performs the first step of this recurrence:

Lemma B.2. *Let $\gamma \in \mathbb{C}^{m+1}$ such that $C(\gamma)$ is positive definite. Let $q := C^{-1}(\gamma)e_0$ and let*

$$\gamma_{m+1} := -\frac{1}{q_0}\sum_{j=1}^{m}\gamma_j q_{m+1-j}.$$

Then

$$C^{-1}\begin{pmatrix}\gamma\\ \gamma_{m+1}\end{pmatrix}e_0 = \begin{pmatrix}q\\ 0\end{pmatrix} \in \mathbb{C}^{m+2}.$$

Furthermore, if f is the MESE for γ,

$$\gamma_{m+1} = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\varphi)\exp(-i(m+1)\varphi)\,\mathrm{d}\varphi$$

is the first unconstrained moment of the MESE.

Proof. Let $v := \frac{1}{2\pi}(\gamma_{m+1},\dots,\gamma_1) \in \mathbb{C}^{1\times(m+1)}$. Then

$$C\begin{pmatrix}\gamma\\ \gamma_{m+1}\end{pmatrix}\begin{pmatrix}q\\ 0\end{pmatrix} = \begin{pmatrix}C(\gamma) & v^*\\ v & \frac{\gamma_0}{2\pi}\end{pmatrix}\begin{pmatrix}q\\ 0\end{pmatrix} = \begin{pmatrix}C(\gamma)q\\ vq\end{pmatrix}$$
$$= \begin{pmatrix}e_0\\ \frac{1}{2\pi}\left(q_0\gamma_{m+1} + \sum_{j=1}^{m}\gamma_j q_{m+1-j}\right)\end{pmatrix} = e_0 \in \mathbb{C}^{m+2}.$$

To prove that the extended Toeplitz matrix has full rank, we let $w := \frac{1}{2\pi}(\gamma_1,\dots,\gamma_{m+1})^\mathsf{T} \in \mathbb{C}^{m+1}$ and denote the k-th canonical basis vector by $e_k \in \mathbb{C}^{m+1}$. Then for all $k \in \{0,\dots,m\}$

$$C\begin{pmatrix}\gamma\\ \gamma_{m+1}\end{pmatrix}\begin{pmatrix}0\\ C^{-1}(\gamma)e_k\end{pmatrix} = \begin{pmatrix}\frac{\gamma_0}{2\pi} & w^*\\ w & C(\gamma)\end{pmatrix}\begin{pmatrix}0\\ C^{-1}(\gamma)e_k\end{pmatrix} = \begin{pmatrix}w^*C^{-1}(\gamma)e_k\\ e_k\end{pmatrix}.$$

Since e_0 is also in the column span, the matrix must be regular. It is even positive definite because by Cramer's rule

$$\frac{\det C(\gamma)}{\det C\begin{pmatrix}\gamma\\ \gamma_{m+1}\end{pmatrix}} = e_0^*C^{-1}\begin{pmatrix}\gamma\\ \gamma_{m+1}\end{pmatrix}e_0 = e_0^*\begin{pmatrix}q\\ 0\end{pmatrix} = q_0 = e_0^*C^{-1}(\gamma)e_0 > 0.$$

Now we consider the MESE for the moments $\gamma_0,\dots,\gamma_{m+1}$:

$$f_{m+1}(\varphi) := \frac{1}{2\pi}\frac{e_0^*C^{-1}\begin{pmatrix}\gamma\\ \gamma_{m+1}\end{pmatrix}e_0}{\left|e_0^*C^{-1}\begin{pmatrix}\gamma\\ \gamma_{m+1}\end{pmatrix}\begin{pmatrix}\mathbf{c}(\varphi)\\ \exp(i(m+1)\varphi)\end{pmatrix}\right|^2}$$
$$= \frac{1}{2\pi}\frac{q^*e_0}{|q^*\mathbf{c}(\varphi)|^2} = f(\varphi)$$

Thus, the MESE f_{m+1} for $\gamma_0,\dots,\gamma_{m+1}$ is identical to the MESE f for $\gamma_0,\dots,\gamma_m$. Since the $(m+1)$-th Fourier coefficient of f_{m+1} is γ_{m+1}, the same is true for f. □

Now we formulate and prove the actual recurrence for the trigonometric moments of the MESE f.

Proposition B.3. *Let $\gamma \in \mathbb{C}^{m+1}$ and f as in Theorem 4. For all $j \in \mathbb{N}$ with $j > m$ let*

$$\gamma_j := \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\varphi)\exp(-ij\varphi)\,\mathrm{d}\varphi.$$

Then for all $k \in \mathbb{N}_0$

$$\gamma_{m+1+k} = -\frac{1}{q_0}\sum_{j=1}^{m}\gamma_{j+k}q_{m+1-j} \tag{B.3}$$

and for the sequence defined in this manner

$$C^{-1}\begin{pmatrix}\gamma_0\\ \vdots\\ \gamma_{m+1+k}\end{pmatrix}e_0 = \begin{pmatrix}q\\ 0\end{pmatrix} \in \mathbb{C}^{m+2+k}.$$

Proof. We proceed by induction over k.
Induction start, $k = 0$: The claim is proven by Lemma B.2.
Induction hypothesis: The claim holds for $k-1$.
Induction step, $k-1 \to k$: According to the induction hypothesis

$$C^{-1}\begin{pmatrix}\gamma_0\\ \vdots\\ \gamma_{m+k}\end{pmatrix}e_0 = \begin{pmatrix}q\\ 0\end{pmatrix}.$$

Using this result with Lemma B.2, we have

$$\gamma_{m+1+k} = -\frac{1}{q_0}\sum_{j=k+1}^{m+k}\gamma_j q_{m+1+k-j} = -\frac{1}{q_0}\sum_{j=1}^{m}\gamma_{j+k}q_{m+1-j}.$$

Applying the other part of Lemma B.2 we find

$$C^{-1}\begin{pmatrix}\gamma_0\\ \vdots\\ \gamma_{m+1+k}\end{pmatrix}e_0 = \begin{pmatrix}C^{-1}\begin{pmatrix}\gamma_0\\ \vdots\\ \gamma_{m+k}\end{pmatrix}e_0\\ 0\end{pmatrix} = \begin{pmatrix}q\\ 0\end{pmatrix}.$$

□

B.5 The Herglotz Transform of the MESE

We are now prepared to derive our novel algorithm for computing the Herglotz transform of the MESE efficiently. First we derive a less efficient method. Then we prove its equivalence to Algorithm 1 and thus our efficient method to evaluate the bounded MESE.

Proposition B.4. *Let γ and f as in Theorem 4. Let I be the identity matrix and let*

$$U := -\frac{1}{q_0}\begin{pmatrix}0 & -q_0 I\\ q_m & q_{m-1}\cdots q_1\end{pmatrix} \in \mathbb{C}^{m\times m}.$$

Let $\gamma_j \in \mathbb{C}$ denote the j-th Fourier coefficient of f for all $j \in \mathbb{Z}$. Then for all $k \in \mathbb{N}_0$

$$(\gamma_{1+k},\dots,\gamma_{m+k})^\mathsf{T} = U^k(\gamma_1,\dots,\gamma_m)^\mathsf{T}. \tag{B.4}$$

Furthermore, for all $z \in \mathbb{C}$ with $|z| \leq 1$

$$\mathcal{H}[f](z) = \gamma_0 + 2e_0^*(z^{-1}I - U)^{-1}(\gamma_1,\dots,\gamma_m)^\mathsf{T}.$$

Proof. For $k = 1$, Equation (B.4) is merely a reformulation of Equation (B.3). For greater k, it follows by induction.

Since U is the transposed companion matrix of a polynomial [Golub and Van Loan, 2012, p. 382], its eigenvalues are solutions for $w \in \mathbb{C}$ of

$$\frac{1}{q_0}\sum_{j=0}^{m}q_{m-j}w^j = 0 \quad\Rightarrow\quad w^m = 0 \ \vee\ \sum_{j=0}^{m}q_j w^{-j} = 0.$$

The polynomial $\sum_{j=0}^{m}\overline{q_j}w^j$ only has roots with $|w| > 1$ [Peters et al., 2015, Lemma 1] and therefore all eigenvalues of U have magnitude less than one.

Hence, we can apply the geometric series for matrices to zU. Using Proposition B.1, we obtain:

$$\begin{aligned}\mathcal{H}[f](z) &= \gamma_0 + \sum_{j=-\infty}^{-1} \overline{\gamma_j} 2z^{-j} = \gamma_0 + 2z\sum_{k=0}^{\infty}\gamma_{k+1}z^k \\ &= \gamma_0 + 2z\sum_{k=0}^{\infty} e_0^* U^k (\gamma_1,\dots,\gamma_m)^\mathsf{T} z^k \\ &= \gamma_0 + 2ze_0^*\left(\sum_{k=0}^{\infty}(zU)^k\right)(\gamma_1,\dots,\gamma_m)^\mathsf{T} \\ &= \gamma_0 + 2ze_0^*(I-zU)^{-1}(\gamma_1,\dots,\gamma_m)^\mathsf{T} \\ &= \gamma_0 + 2e_0^*(z^{-1}I-U)^{-1}(\gamma_1,\dots,\gamma_m)^\mathsf{T}\end{aligned}$$

□

Proof of Theorem 5. For all $l \in \{0,\dots,m\}$, the variable p_l is a polynomial evaluated at z^{-1} using the Horner scheme:

$$p_l = \sum_{j=0}^{m-l} q_j z^{j+l-m} \in \mathbb{C}$$

Let

$$w := \frac{1}{p_0}\sum_{k=1}^{m} p_k\gamma_k \in \mathbb{C}, \quad v := \left(wz^{-l} - \sum_{k=1}^{l}\gamma_k z^{k-l}\right)_{l=0}^{m-1} \in \mathbb{C}^m.$$

Using notions from Proposition B.4, we want to prove that v solves

$$(z^{-1}I - U)v = (\gamma_1,\dots,\gamma_m)^\mathsf{T}. \tag{B.5}$$

Indeed, for all $l \in \{0,\dots,m-2\}$:

$$\begin{aligned}&e_l^*(z^{-1}I-U)v = z^{-1}v_l - v_{l+1} \\ =&wz^{-l-1} - \sum_{k=1}^{l}\gamma_k z^{k-l-1} - wz^{-l-1} + \sum_{k=1}^{l+1}\gamma_k z^{k-l-1} \\ =&\gamma_{l+1}z^{l+1-l-1} = \gamma_{l+1}\end{aligned}$$

Furthermore:

$$\begin{aligned}&e_{m-1}^*(z^{-1}I-U)v = z^{-1}v_{m-1} + \frac{1}{q_0}\sum_{j=1}^{m} v_{j-1}q_{m+1-j} \\ =&wz^{-m} - \sum_{k=1}^{m-1}\gamma_k z^{k-m} + \frac{1}{q_0}\sum_{j=1}^{m}\left(wz^{1-j} - \sum_{k=1}^{j-1}\gamma_k z^{1+k-j}\right)q_{m+1-j} \\ =&\gamma_m + \frac{1}{q_0}\sum_{j=1}^{m+1}\left(wz^{1-j} - \sum_{k=1}^{j-1}\gamma_k z^{1+k-j}\right)q_{m+1-j} \\ =&\gamma_m + \frac{w}{q_0}\sum_{j=1}^{m+1} q_{m+1-j}z^{1-j} - \frac{1}{q_0}\sum_{j=1}^{m+1}\sum_{k=1}^{j-1} q_{m+1-j}z^{1+k-j}\gamma_k \\ =&\gamma_m + \frac{w}{q_0}p_0 - \frac{1}{q_0}\sum_{j=1}^{m+1}\sum_{k=1}^{j-1} q_{m+1-j}z^{1+k-j}\gamma_k \\ =&\gamma_m + \frac{1}{q_0}\sum_{k=1}^{m}\sum_{j=0}^{m-k} q_j z^{j+k-m}\gamma_k - \frac{1}{q_0}\sum_{j=0}^{m}\sum_{k=1}^{m-j} q_j z^{j+k-m}\gamma_k \\ =&\gamma_m\end{aligned}$$

Thus, Equation (B.5) is proven. Using Proposition B.4, we conclude:

$$\begin{aligned}\mathcal{H}[f](z) &= \gamma_0 + 2e_0^*(z^{-1}I-U)^{-1}(\gamma_1,\dots,\gamma_m)^\mathsf{T} \\ &= \gamma_0 + 2e_0^* v = \gamma_0 + 2w = \gamma_0 + \frac{2}{p_0}\sum_{k=1}^{m}p_k\gamma_k\end{aligned}$$

Therefore, Algorithm 1 is correct.

Equation (5) gives us a density with the required properties, which equals $h(\varphi)$:

$$\begin{aligned}&\frac{1}{\pi}\arg\left(i\alpha + \lim_{z\to\exp(i\varphi)} 2\pi\mathcal{H}[f](z)\right) + \frac{1}{2} \\ =&\frac{1}{\pi}\arg\left(4\pi i\Im\gamma_0' + \lim_{z\to\exp(i\varphi)} 2\pi\mathcal{H}[f](z)\right) + \frac{1}{2} \\ =&\frac{1}{\pi}\arg\left(2i\Im\gamma_0' + \mathcal{H}[f](\exp(i\varphi))\right) + \frac{1}{2} = h(\varphi)\end{aligned}$$

Note that the correctness proof of Algorithm 1 covers the limit case $|z| = 1$. As an optimization, Algorithm 1 may exploit $z^{-1} = \overline{z}$.

To prove that the log sin entropy is maximized, we utilize Proposition 6. Let $\lambda_0,\dots,\lambda_m \in \mathbb{C}$ as in this Proposition. We observe that $\log\sin(\pi g)$ is a strictly concave function for all $g \in (0,1)$:

$$\begin{aligned}\frac{\partial}{\partial g}\log\sin(\pi g) &= \pi\frac{\cos(\pi g)}{\sin(\pi g)} = \pi\cot(\pi g) \\ \frac{\partial^2}{\partial g^2}\log\sin(\pi g) &= -\frac{\pi^2}{\sin^2(\pi g)} < 0\end{aligned}$$

Thus, the log sin entropy is strictly concave as well and any critical point constitutes a global maximum. Let $u(\varphi) \in \mathbb{R}$ be a 2π-periodic perturbation that leaves the Fourier coefficients unchanged, i.e.

$$\int_{-\pi}^{\pi} u(\varphi)\mathbf{c}(\varphi)\,\mathrm{d}\varphi = 0 \in \mathbb{C}^{m+1}.$$

Let $t \geq 0$ such that $h(\varphi) + tu(\varphi) \in (0,1)$ for all $\varphi \in \mathbb{R}$. We consider the change of the log sin entropy as a function of t:

$$\begin{aligned}&\left.\frac{\partial}{\partial t}\right|_{t=0}\int_{-\pi}^{\pi}\log\sin(\pi(h(\varphi)+tu(\varphi)))\,\mathrm{d}\varphi \\ =&\int_{-\pi}^{\pi}\left.\frac{\partial}{\partial t}\right|_{t=0}\log\sin(\pi(h(\varphi)+tu(\varphi)))\,\mathrm{d}\varphi \\ =&\int_{-\pi}^{\pi}\pi\cot(\pi(h(\varphi)))u(\varphi)\,\mathrm{d}\varphi \\ =&\int_{-\pi}^{\pi}\pi\cot\left(\arctan\left(\Re\lambda_0 + 2\Re\sum_{l=1}^{m}\lambda_l\exp(-il\varphi)\right)+\frac{\pi}{2}\right)u(\varphi)\,\mathrm{d}\varphi \\ =&\int_{-\pi}^{\pi}-\pi\left(\Re\lambda_0 + 2\Re\sum_{l=1}^{m}\lambda_l\exp(-il\varphi)\right)u(\varphi)\,\mathrm{d}\varphi = 0\end{aligned}$$

Thus, h must be a critical point and consequently a global maximum.

□

B.6 Computation of Lagrange Multipliers

We now derive novel formulas for the computation and use of Lagrange multipliers from the algorithm discussed in the previous section.

Proof of Proposition 6. Let $z := \exp(i\varphi)$. From the proof of Theorem 5, we know

$$\mathcal{H}[f](z) = \gamma_0 + \frac{2}{p_0}\sum_{k=1}^{m} p_k\gamma_k = \gamma_0 + 2\frac{\sum_{k=1}^{m}\sum_{j=0}^{m-k} q_j\gamma_k z^{j+k-m}}{\sum_{j=0}^{m} q_j z^{j-m}}$$
$$= \gamma_0 + \frac{\sum_{k=1}^{m}\sum_{j=0}^{m-k} q_j\gamma_k z^{j+k}}{\pi \mathbf{c}^*(\varphi)q}.$$

Using Equation (B.1), we rewrite $h(\varphi)$ as

$$\pi h(\varphi) - \frac{\pi}{2} = \arctan\frac{2\Im\gamma_0' + \Im\mathcal{H}[f](\exp(i\varphi))}{\Re\mathcal{H}[f](\exp(i\varphi))}$$
$$= \arctan\frac{2i\Im\gamma_0' + \mathcal{H}[f](\exp(i\varphi)) - \Re\mathcal{H}[f](\exp(i\varphi))}{i\Re\mathcal{H}[f](\exp(i\varphi))}$$
$$= \arctan\left(\frac{2i\Im\gamma_0' + \mathcal{H}[f](\exp(i\varphi))}{if(\varphi)} + i\right).$$

The MESE may be written as

$$f(\varphi) = \frac{1}{2\pi}\frac{q_0}{\mathbf{c}^*(\varphi)qq^*\mathbf{c}(\varphi)}.$$

As we combine the previous three equations, $\mathbf{c}^*(\varphi)q$ cancels out:

$$\pi h(\varphi) - \frac{\pi}{2}$$
$$= \arctan\left(\frac{2}{iq_0}\left(2\pi\gamma_0'\mathbf{c}^*(\varphi)q + \sum_{k=1}^{m}\sum_{j=0}^{m-k} q_j\gamma_k z^{j+k}\right)q^*\mathbf{c}(\varphi) + i\right)$$
$$= \arctan\left(\frac{2}{iq_0}\left(\sum_{j=0}^{m} q_j\gamma_0' z^j + \sum_{k=1}^{m}\sum_{j=0}^{m-k} q_j\gamma_k' z^{j+k}\right)q^*\mathbf{c}(\varphi) + i\right)$$
$$= \arctan\left(\frac{2}{iq_0}\sum_{k=0}^{m}\sum_{j=0}^{m-k} q_j\gamma_k' z^{j+k}q^*\mathbf{c}(\varphi) + i\right)$$
$$= \arctan\left(\frac{1}{\pi iq_0}\sum_{k=0}^{m}\sum_{j=0}^{m-k}\sum_{n=0}^{m}\gamma_k'\overline{q_n}q_j z^{j+k-n} + i\right)$$

The exponents on z range from $-m$ to m. Since the sum is real, we are dealing with a real Fourier series and it suffices to consider the coefficients for non-positive exponents on z. The sum of coefficients for z^{-l} with $l \in \{0, \dots, m\}$ is exactly

$$\frac{1}{\pi iq_0}\sum_{k=0}^{m-l}\sum_{j=0}^{m-k-l}\gamma_k'\overline{q_{j+k+l}}q_j = \lambda_l.$$

Hence, we have proven

$$\pi h(\varphi) - \frac{\pi}{2} = \arctan\left(\Re\lambda_0 + 2\Re\sum_{l=1}^{m}\lambda_l z^{-l}\right).$$

□

B.7 Uncertainty Bounds

Kovalishina and Potapov [1982] have devised an inequality that provides bounds on the Herglotz transform of a signal using solely

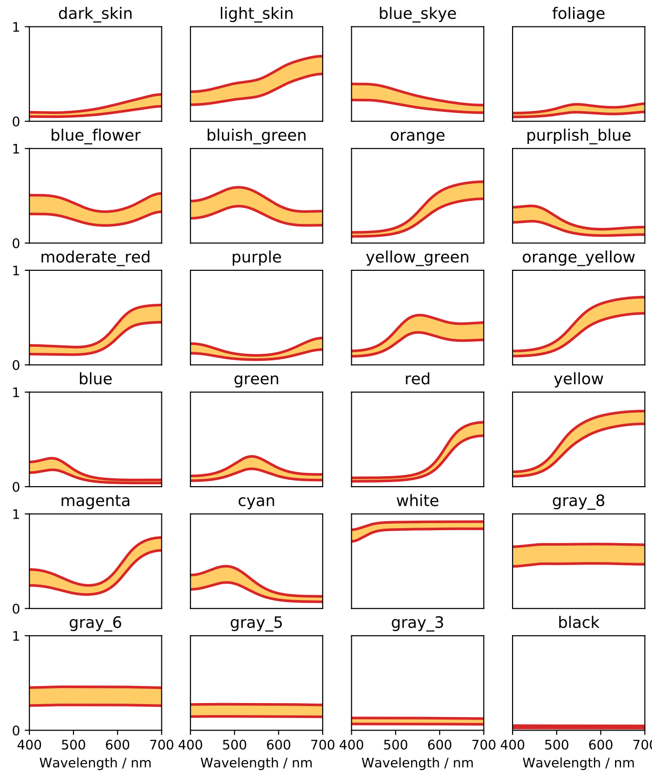

Fig. B.1. Uncertainty bounds for all spectra of the X-Rite color checker using $m = 7$, $r = 0.8$ and mirroring (Equation (12)). The bounds are particularly tight for spectra that are close to boundary cases, i.e. that use values near zero or one on long intervals.

knowledge of its trigonometric moments. In Section B.2, we have seen that the Poisson kernel and the Herglotz kernel are related by

$$P_z(\varphi) = \frac{1}{2\pi}\Re\frac{\exp(i\varphi) + z}{\exp(i\varphi) - z}. \tag{B.6}$$

Hence, we can use their result to compute bounds on a bounded density smoothed through convolution with a Poisson kernel. Figure B.1 shows some results.

Before we prove the uncertainty bounds themselves, we introduce a more general lemma on the Herglotz transform.

Lemma B.5. *Let $d(\varphi) \geq 0$ be a periodic density with trigonometric moments*

$$\gamma := \int_{-\pi}^{\pi} d(\varphi)\mathbf{c}(\varphi)\,\mathrm{d}\varphi.$$

Assume that $C(\gamma)$ is invertible. Let $z \in \mathbb{C} \setminus \{0\}$ with $|z| < 1$ and

$$\boldsymbol{a}(z) := \frac{1}{2\pi}(z^{-1-j})_{j=0}^{m}, \quad \boldsymbol{b}(z) := \frac{1}{2\pi}\left(z^{-1-j}\left(\gamma_0 + \sum_{k=1}^{j} 2\gamma_k z^k\right)\right)_{j=0}^{m},$$

$$p(z) := \frac{\frac{2}{1-|z|^2} + \boldsymbol{b}^*(z)C^{-1}(\gamma)\boldsymbol{a}(z)}{\boldsymbol{b}^*(z)C^{-1}(\gamma)\boldsymbol{b}(z)},$$

$$\rho(z) := |p(z)|^2 - \frac{\boldsymbol{a}^*(z)C^{-1}(\gamma)\boldsymbol{a}(z)}{\boldsymbol{b}^*(z)C^{-1}(\gamma)\boldsymbol{b}(z)}.$$

Then the Herglotz transform $\mathcal{H}[d](z)$ lies in the disk

$$|\mathcal{H}[d](z) - p(z)|^2 \leq \rho(z).$$

This bound is sharp in the sense that $\mathcal{H}[d](z)$ may be arbitrarily close to each point on the bounding circle.

Proof. The result is a special case of the fundamental matrix inequality [Kovalishina and Potapov, 1982, p. 19], which has been formulated by Karlsson and Georgiou [2013, Equation (22)]. □

Proposition B.6. *Let $g(\varphi) \in [0,1]$ be a bounded signal with trigonometric $(0,1)$-moments*

$$c := \int_{-\pi}^{\pi} g(\varphi)\mathbf{c}(\varphi)\,\mathrm{d}\varphi \in \mathbb{C}^{m+1}.$$

Let $\gamma \in \mathbb{C}^{m+1}$ and $\gamma_0' \in \mathbb{C}$ be as in Equations (6) and (7). Let $z := r\exp(i\varphi)$ for $r \in (0,1)$ and $p(z)$, $\rho(z)$ as in Lemma B.5. Then we obtain the following sharp bounds for the smoothed density $P_r * g$:

$$\left|P_r * g(\varphi) - \frac{1}{\pi}\arg(2i\Im\gamma_0' + p(z)) - \frac{1}{2}\right| \leq \frac{1}{\pi}\arcsin\frac{\sqrt{\rho(z)}}{|p(z)|} \quad \text{(B.7)}$$

Proof. Combining Equation (3) and Equation (B.6) yields

$$\Re\mathcal{H}[g](z) = -\frac{1}{\pi}\Re i\log\left(4\pi i\Im\gamma_0' + 2\pi\mathcal{H}[d](z)\right) + \frac{1}{2}$$
$$\Rightarrow P_r * g(\varphi) = -\frac{1}{\pi}\arg\left(2i\Im\gamma_0' + \mathcal{H}[d](z)\right) + \frac{1}{2}$$

By Lemma B.5, $2i\Im\gamma_0' + \mathcal{H}[d](z)$ lies anywhere in the disk with center $2i\Im\gamma_0' + p(z)$ and radius $\sqrt{\rho(z)}$. Basic trigonometry reveals that Equation (B.7) computes sharp bounds on the argument of points in this disk. □

C COMPUTATION OF MOMENTS

In the paper we point out that trigonometric $(0,1)$-moments must be computed in a way that is guaranteed to compute the integral of a signal bounded between zero and one. Considering that the spectral domain is usually sampled with a fairly low sample count, violating this rule may introduce significant errors. Therefore, we propose to use linear interpolation and to compute the moments exactly.

Suppose we are given phases $\varphi_0, \ldots, \varphi_{n-1} \in [-\pi, \pi]$ and corresponding reflectance values $g_0, \ldots, g_{n-1} \in [0,1]$. The phases are sorted and cover the entire range, i.e. $\varphi_0 = -\pi$ and $\varphi_{n-1} = 0$ if the signal is being mirrored and $\varphi_{n-1} = \pi$ otherwise. The linear interpolant is a piecewise linear function. For all $l \in \{0, \ldots, n-2\}$, we define the gradient and y-intercept

$$a_l := \frac{g_{l+1} - g_l}{\varphi_{l+1} - \varphi_l}, \qquad b_l := g_l - a_l\varphi_l.$$

Then the interpolated signal for $\varphi \in [\varphi_l, \varphi_{l+1}]$ is

$$g(\varphi) := a_l\varphi + b_l.$$

To compute trigonometric $(0,1)$-moments, we consider the following indefinite integrals for all $j \in \{1, \ldots, m\}$:

$$\int \exp(-ij\varphi)\,\mathrm{d}\varphi = \frac{i}{j}\exp(-ij\varphi) + C$$
$$\int \varphi\exp(-ij\varphi)\,\mathrm{d}\varphi = \frac{1 + ij\varphi}{j^2}\exp(-ij\varphi) + C$$

Substituting in the expression for $g(\varphi)$, we obtain:

$$\begin{aligned} c_j &:= \frac{1}{2\pi}\int_{-\pi}^{\pi} g(\varphi)\exp(-ij\varphi)\,\mathrm{d}\varphi \\ &= \frac{1}{2\pi}\sum_{l=0}^{n-2}\int_{\varphi_l}^{\varphi_{l+1}}(a_l\varphi + b_l)\exp(-ij\varphi)\,\mathrm{d}\varphi \\ &= \frac{1}{2\pi}\sum_{l=0}^{n-2}\left[\left(a_l\frac{1 + ij\varphi}{j^2} + b_l\frac{i}{j}\right)\exp(-ij\varphi)\right]_{\varphi_l}^{\varphi_{l+1}} \in \mathbb{C}\end{aligned}$$

For $j = 0$, the result is

$$c_0 := \frac{1}{2\pi}\sum_{l=0}^{n-2}\int_{\varphi_l}^{\varphi_{l+1}} a_l\varphi + b_l\,\mathrm{d}\varphi = \frac{1}{2\pi}\sum_{l=0}^{n-2}\left[\frac{a_l}{2}\varphi^2 + b_l\varphi\right]_{\varphi_l}^{\varphi_{l+1}} \in \mathbb{C}.$$

If the signal is being mirrored, the j-th real trigonometric $(0,1)$-moment is given by $2\Re c_j$.

When moments are computed for a whole texture, this formula should only be evaluated once per pair $j \in \{0, \ldots, m\}$ and $l \in \{0, \ldots, n-1\}$ with a spectrum where $g_l = 1$ and all other values are zero. The resulting $\mathbb{C}^{(m+1)\times n}$ matrix maps vectors of samples $(g_0, \ldots, g_{n-1})^\mathsf{T}$ to vectors of moments $c \in \mathbb{C}^{m+1}$.

For emission spectra, the same formulas may be used but a common discrete Fourier transform is an acceptable alternative since the spectral densities do not obey an upper bound.

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