Supplement to
"Robust Designs for 3D Shape Analysis with Spherical Harmonic Descriptors"
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Proof of Theorem 1. If $w \equiv 1$, $\eta_g^2 = 0$; $g_0 = 1$ $h(\cdot,\cdot) \equiv 0$ we have $k(\cdot) = m(\cdot)$ and as a consequence $\mathbf{C}_{w,g,m} = \mathbf{B}_m$. Therefore we obtain for the maximal integrated mean square errors

$$\max_{f\in\mathcal{F}} IMSE_{j,f,1,0}(\xi) = \begin{cases} \eta_f^2 ch_{\max}\left[\mathbf{B}_m^{-1}\mathbf{K}_m\mathbf{B}_m^{-1}\right] + \frac{\sigma_\varepsilon^2}{n} tr\left[\mathbf{B}_m^{-1}\right], & \text{if } j=1, \\ \eta_f^2 ch_{\max}\left[\mathbf{B}_m^{-1}\mathbf{K}_m\mathbf{B}_m^{-1}\right] + \frac{\sigma_\varepsilon^2}{n} tr\left[\mathbf{B}_m^{-1}\right] + \sigma_\varepsilon^2, & \text{if } j=2. \end{cases}$$

We now shows that both terms in this expression are minimized by the uniform distribution (1.2) on the unit sphere. For this first note that $tr\left[\mathbf{B}_m^{-1}\right]$ corresponds to Kiefer's A-optimality criterion, which was considered in Dette, Melas and Pepelyshev (2005) and is minimal for the uniform distribution (1.2) on the unit sphere. Secondly, note that $ch_{\max}\left[\mathbf{B}_m^{-1}\mathbf{K}_m\mathbf{B}_m^{-1}\right] - 1 = ch_{\max}\left[\mathbf{B}_m^{-1}\left(\mathbf{K}_m - \mathbf{B}_m^2\right)\mathbf{B}_m^{-1}\right]$. Moreover, for any vector $\mathbf{a}$ we have

$$\mathbf{a}^T\left(\mathbf{K}_m - \mathbf{B}_m^2\right)\mathbf{a} = \int_{\mathcal{S}}\left\{\mathbf{a}^T\left[\frac{m(\boldsymbol{\psi})}{\mu(\boldsymbol{\psi})}\mathbf{I} - \mathbf{B}_m\right]\mathbf{z}(\boldsymbol{\psi})\right\}^2 \mu(\boldsymbol{\psi})\, d\boldsymbol{\psi} \geq 0,$$

and consequently the matrix $\mathbf{K}_m - \mathbf{B}_m^2$ is non-negative definite, which implies $ch_{\max}\left[\mathbf{B}_m^{-1}\mathbf{K}_m\mathbf{B}_m^{-1}\right] \geq 1$. But this minimum value of 1 is attained by $m(\cdot) = \mu(\cdot)$, for which $\mathbf{K}_m = \mathbf{B}_m = \mathbf{I}$. ■

Proof of Proposition 2: For weight functions $w_0(\boldsymbol{\psi})$ and $w_1(\boldsymbol{\psi})$ and $t \in [0,1]$ define $w_t(\boldsymbol{\psi}) = (1-t)\, w_0(\boldsymbol{\psi}) + t w_1(\boldsymbol{\psi})$. In order that the function $w_0(\boldsymbol{\psi})$ minimize (2.2) subject to the normalizing conditions (2.3) it is sufficient that the function

$$\phi(t;\lambda) = \int_{\mathcal{S}} w_t(\boldsymbol{\psi})\, g_*(\boldsymbol{\psi})\, \mathbf{z}^T(\boldsymbol{\psi})\, \mathbf{B}_m^{-2}\mathbf{z}(\boldsymbol{\psi})\, m(\boldsymbol{\psi})\, d\boldsymbol{\psi} + \lambda\left[\int_{\mathcal{S}} \frac{m(\boldsymbol{\psi})}{w_t(\boldsymbol{\psi})} d\boldsymbol{\psi} - 1\right] \; (\lambda \geq 0)$$

be minimal at $t = 0$ for any $w_1(\cdot)$, and that $w_0(\cdot)$ satisfies (2.3). For this, since $\phi(t;\lambda)$ is a convex function of t, the first order condition is necessary and sufficient, i.e.

$$\phi'(0;\lambda) = \int_{\mathcal{S}} \left[w_1(\boldsymbol{\psi}) - w_0(\boldsymbol{\psi})\right]\left[g_*(\boldsymbol{\psi})\, \mathbf{z}^T(\boldsymbol{\psi})\, \mathbf{B}_m^{-2}\mathbf{z}(\boldsymbol{\psi})\, m(\boldsymbol{\psi}) - \lambda\frac{m(\boldsymbol{\psi})}{w_0^2(\boldsymbol{\psi})}\right] d\boldsymbol{\psi} \geq 0$$

for all $w_1(\cdot)$. This condition is satisfied if

$$w_0(\boldsymbol{\psi}) = \frac{\lambda}{\left\|\mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})\right\| \sqrt{g_*(\boldsymbol{\psi})}}$$

(on the support of $m(\cdot)$ - we can define $w_0(\boldsymbol{\psi})$ arbitrarily elsewhere), and it remains only to determine the constant λ to satisfy (2.3). ■

Proof of Theorem 2. From Proposition 2 we obtain

$$\min_w \max_{f,g} IMSE_{j,f,g,0}(\xi) = \begin{cases} \eta_f^2 ch_{\max}\left[\mathbf{B}_m^{-1}\mathbf{K}_m\mathbf{B}_m^{-1}\right] + \frac{\sigma_\varepsilon^2}{n}\gamma_m^2, & \text{if } j=1, \\ \eta_f^2 ch_{\max}\left[\mathbf{B}_m^{-1}\mathbf{K}_m\mathbf{B}_m^{-1}\right] + \frac{\sigma_\varepsilon^2}{n}\gamma_m^2 + \sigma_\varepsilon^2, & \text{if } j=2. \end{cases}$$

Because $g_0(\boldsymbol{\psi}) \equiv 1$, it follows that

$$\gamma_m = \sqrt{1+\eta_g^2}\int_{\mathcal{S}} \left\|\mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})\right\| m(\boldsymbol{\psi})\, d\boldsymbol{\psi}. \tag{A.1}$$

It was shown in the proof of Theorem 1 that the maximum eigenvalue $ch_{\max}\left[\mathbf{B}_m^{-1}\mathbf{K}_m\mathbf{B}_m^{-1}\right]$ is minimized by the uniform distribution on the sphere $\mu(\cdot)$, for which the corresponding minimax weights are, by Proposition 2, proportional to $\|\mathbf{z}(\boldsymbol{\psi})\|^{-1}$, hence by (1.7) are constant. If this choice of design can be shown to minimize (A.1) as well, then the assertion of the Proposition follows, i.e. $\mu(\cdot)$ minimizes (2.4). Showing this requires proving the inequality

$$\int_{\mathcal{S}} \left\|\mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})\right\| m(\boldsymbol{\psi})\, d\boldsymbol{\psi} \geq \int_{\mathcal{S}} \left\|\mathbf{B}_\mu^{-1}\mathbf{z}(\boldsymbol{\psi})\right\| \mu(\boldsymbol{\psi})\, d\boldsymbol{\psi} = d+1, \tag{A.2}$$

where we have used (1.7) and (1.6) for the last equality. However, the inequality in (A.2) is a direct consequence of the Cauchy-Schwarz inequality:

$$\left\|\mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})\right\| \geq \frac{\mathbf{z}^T(\boldsymbol{\psi})\,\mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})}{\|\mathbf{z}(\boldsymbol{\psi})\|} = \frac{\mathbf{z}^T(\boldsymbol{\psi})\,\mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})}{d+1};$$

this gives

$$\begin{aligned}\int_{\mathcal{S}} \left\|\mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})\right\| m(\boldsymbol{\psi})\, d\boldsymbol{\psi} &\geq \frac{1}{d+1}\int_{\mathcal{S}} \mathbf{z}^T(\boldsymbol{\psi})\,\mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})\, m(\boldsymbol{\psi})\, d\boldsymbol{\psi} \\ &= \frac{1}{d+1} tr\mathbf{B}_m^{-1}\int_{\mathcal{S}} \mathbf{z}(\boldsymbol{\psi})\,\mathbf{z}^T(\boldsymbol{\psi})\, m(\boldsymbol{\psi})\, d\boldsymbol{\psi} \\ &= \frac{1}{d+1} tr\mathbf{I}_{(d+1)^2} \;=\; d+1.\end{aligned}$$

■

Proof of Theorem 3: First take $j = 1$. From (2.7) and (2.6) we are to show that

$$\begin{aligned}
&\max_h \int_{\mathcal{S}} \int_{\mathcal{S}} h\left(\boldsymbol{\psi},\boldsymbol{\psi}'\right) \mathbf{z}^T\left(\boldsymbol{\psi}'\right) \mathbf{B}_m^{-2} \mathbf{z}\left(\boldsymbol{\psi}\right) m\left(\boldsymbol{\psi}\right) m\left(\boldsymbol{\psi}'\right) d\boldsymbol{\psi} d\boldsymbol{\psi}' \\
&= \eta_h^2 \int_{\mathcal{S}} \mathbf{z}^T\left(\boldsymbol{\psi}\right) \mathbf{B}_m^{-2} \mathbf{z}\left(\boldsymbol{\psi}\right) \frac{m^2\left(\boldsymbol{\psi}\right)}{\mu\left(\boldsymbol{\psi}\right)} d\boldsymbol{\psi} \\
&= \eta_h^2 \int_{\mathcal{S}} \left\| \mathbf{B}_m^{-1} \mathbf{z}\left(\boldsymbol{\psi}\right) \frac{m\left(\boldsymbol{\psi}\right)}{\mu\left(\boldsymbol{\psi}\right)} \right\|^2 \mu\left(\boldsymbol{\psi}\right) d\boldsymbol{\psi}
\end{aligned}$$

is minimized by $m(\cdot) = \mu(\cdot)$. By the Cauchy-Schwarz inequality and (A.2),

$$\begin{aligned}
\int_{\mathcal{S}} \left\| \mathbf{B}_m^{-1} \mathbf{z}\left(\boldsymbol{\psi}\right) \frac{m\left(\boldsymbol{\psi}\right)}{\mu\left(\boldsymbol{\psi}\right)} \right\|^2 \mu\left(\boldsymbol{\psi}\right) d\boldsymbol{\psi} &\geq \left\{ \int_{\mathcal{S}} \left\| \mathbf{B}_m^{-1} \mathbf{z}\left(\boldsymbol{\psi}\right) \frac{m\left(\boldsymbol{\psi}\right)}{\mu\left(\boldsymbol{\psi}\right)} \right\| \mu\left(\boldsymbol{\psi}\right) d\boldsymbol{\psi} \right\}^2 \\
&= \left\{ \int_{\mathcal{S}} \left\| \mathbf{B}_m^{-1} \mathbf{z}\left(\boldsymbol{\psi}\right) \right\| m\left(\boldsymbol{\psi}\right) d\boldsymbol{\psi} \right\}^2 \\
&\geq \ (d+1)^2 . \qquad \text{(A.3)}
\end{aligned}$$

But this lower bound $(d+1)^2$ is attained by $m(\cdot) = \mu(\cdot)$; this establishes Theorem 3 in the case $j = 1$.

For a proof of the result in the case $j = 2$ we recall (2.8) and consider the function

$$\begin{aligned}
\Phi(h;m) &= \int_{\mathcal{S}} \int_{\mathcal{S}} h\left(\boldsymbol{\psi},\boldsymbol{\psi}'\right) \mathbf{z}^T\left(\boldsymbol{\psi}'\right) \mathbf{B}_m^{-2} \mathbf{z}\left(\boldsymbol{\psi}\right) m\left(\boldsymbol{\psi}\right) m\left(\boldsymbol{\psi}'\right) d\boldsymbol{\psi} d\boldsymbol{\psi}' \\
&- 2 \int_{\mathcal{S}} \int_{\mathcal{S}} h\left(\boldsymbol{\psi},\boldsymbol{\psi}'\right) \mathbf{z}^T\left(\boldsymbol{\psi}'\right) \mathbf{B}_m^{-1} \mathbf{z}\left(\boldsymbol{\psi}\right) \mu\left(\boldsymbol{\psi}\right) m\left(\boldsymbol{\psi}'\right) d\boldsymbol{\psi} d\boldsymbol{\psi}' + \int_{\mathcal{S}} h\left(\boldsymbol{\psi},\boldsymbol{\psi}\right) \mu\left(\boldsymbol{\psi}\right) d\boldsymbol{\psi}.
\end{aligned}$$

We have to show that

$$\max_h \Phi(h;m) \geq \max_h \Phi(h;\mu) . \qquad \text{(A.4)}$$

To establish (A.4), it is clearly sufficient to show that for *any* function $h \in \mathcal{H}$,

$$0 \leq \Phi(h;m) - \Phi(h;\mu) \ \text{ for any } m(\cdot) . \qquad \text{(A.5)}$$

For this, note that

$$\begin{aligned}
\Phi(h;m)-\Phi(h;\mu) &= \int_{\mathcal{S}}\int_{\mathcal{S}} h(\boldsymbol{\psi},\boldsymbol{\psi}')\,\mathbf{z}^T(\boldsymbol{\psi}')\,\mathbf{B}_m^{-2}\mathbf{z}(\boldsymbol{\psi})\,m(\boldsymbol{\psi})\,m(\boldsymbol{\psi}')\,d\boldsymbol{\psi}d\boldsymbol{\psi}' \\
&\quad -2\int_{\mathcal{S}}\int_{\mathcal{S}} h(\boldsymbol{\psi},\boldsymbol{\psi}')\,\mathbf{z}^T(\boldsymbol{\psi}')\,\mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})\,\mu(\boldsymbol{\psi})\,m(\boldsymbol{\psi}')\,d\boldsymbol{\psi}d\boldsymbol{\psi}' \\
&\quad -\int_{\mathcal{S}}\int_{\mathcal{S}} h(\boldsymbol{\psi},\boldsymbol{\psi}')\,\mathbf{z}^T(\boldsymbol{\psi}')\,\mathbf{z}(\boldsymbol{\psi})\,\mu(\boldsymbol{\psi})\,\mu(\boldsymbol{\psi}')\,d\boldsymbol{\psi}d\boldsymbol{\psi}' \\
&\quad +2\int_{\mathcal{S}}\int_{\mathcal{S}} h(\boldsymbol{\psi},\boldsymbol{\psi}')\,\mathbf{z}^T(\boldsymbol{\psi}')\,\mathbf{z}(\boldsymbol{\psi})\,\mu(\boldsymbol{\psi})\,\mu(\boldsymbol{\psi}')\,d\boldsymbol{\psi}d\boldsymbol{\psi}' \\
&= \int_{\mathcal{S}}\int_{\mathcal{S}} h(\boldsymbol{\psi},\boldsymbol{\psi}')\,\mathbf{z}^T(\boldsymbol{\psi}')\,\mathbf{B}_m^{-2}\mathbf{z}(\boldsymbol{\psi})\,m(\boldsymbol{\psi})\,m(\boldsymbol{\psi}') \\
&\quad -2\mathbf{z}^T(\boldsymbol{\psi}')\,\mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})\,\mu(\boldsymbol{\psi})\,m(\boldsymbol{\psi}') \\
&\quad +\mathbf{z}^T(\boldsymbol{\psi}')\,\mathbf{z}(\boldsymbol{\psi})\,\mu(\boldsymbol{\psi})\,\mu(\boldsymbol{\psi}')\,d\boldsymbol{\psi}d\boldsymbol{\psi}' \\
&= \int_{\mathcal{S}}\int_{\mathcal{S}} h(\boldsymbol{\psi},\boldsymbol{\psi}')\,\mathbf{a}^T(\boldsymbol{\psi})\,\mathbf{a}(\boldsymbol{\psi}')\,d\boldsymbol{\psi}d\boldsymbol{\psi}',
\end{aligned}$$

with $\mathbf{a}(\boldsymbol{\psi}) = \mathbf{B}_m^{-1}\mathbf{z}(\boldsymbol{\psi})\,\mu(\boldsymbol{\psi}) - \mathbf{z}(\boldsymbol{\psi})\,m(\boldsymbol{\psi})$. Now (A.5) follows from the non-negative definiteness of the kernel $h(\cdot,\cdot)$, i.e. from the first inequality in (2.6). ■

Proof of Theorem 4: The constraint (3.1) on $\mathbf{f}$ is given by the equation $\mathbf{Z}^T\mathbf{P}\mathbf{f} = \mathbf{0}$. Equivalently, $\mathbf{Pf}$ lies in the orthogonal complement to the column space of $\mathbf{Z}$, so that $\mathbf{f} = \mathbf{P}^{-1}\tilde{\mathbf{Z}}\mathbf{c}$ for some vector $\mathbf{c}$. We have to maximize the expression

$$\mathbf{f}^T\mathbf{MQPQMf} + \mathbf{f}^T\mathbf{Pf} = \mathbf{c}^T\tilde{\mathbf{Z}}^T\mathbf{P}^{-1}\mathbf{MQPQMP}^{-1}\tilde{\mathbf{Z}}\mathbf{c} + \mathbf{c}^T\tilde{\mathbf{Z}}^T\mathbf{P}^{-1}\tilde{\mathbf{Z}}\mathbf{c}$$

subject to condition (3.2), which is $\mathbf{f}^T\mathbf{Pf} = \mathbf{c}^T\tilde{\mathbf{Z}}^T\mathbf{P}^{-1}\tilde{\mathbf{Z}}\mathbf{c} \le \eta_f^2$. Equivalently, with $\mathbf{e} = \left(\tilde{\mathbf{Z}}^T\mathbf{P}^{-1}\tilde{\mathbf{Z}}\right)^{1/2}\mathbf{c}/\eta_f$, we maximize

$$\mathbf{e}^T\left(\tilde{\mathbf{Z}}^T\mathbf{P}^{-1}\tilde{\mathbf{Z}}\right)^{-1/2}\tilde{\mathbf{Z}}^T\mathbf{P}^{-1}\mathbf{MQPQMP}^{-1}\tilde{\mathbf{Z}}\left(\tilde{\mathbf{Z}}^T\mathbf{P}^{-1}\tilde{\mathbf{Z}}\right)^{-1/2}\mathbf{e} + \mathbf{e}^T\mathbf{e}$$

subject to $\mathbf{e}^T\mathbf{e} \le 1$. This is a standard problem whose solution is as described in the Theorem. ■

Proof of Proposition 3: In light of Theorem 4 we have only to show that

(i) $\mathbf{r}^T\mathbf{g} = \sum r_i g(\boldsymbol{\psi}_i)$ and $\left(\boldsymbol{\mu} + \frac{1}{n}\mathbf{r}\right)^T = \sum\left(\mu_i + \frac{r_i}{n}\right)g(\boldsymbol{\psi}_i)$ are both maximized over $g \in \mathcal{G}_0$ by $g = g_*$;

(ii) $tr\left[\mathbf{QPQMHM}\right]$ and $tr\left[\left(\mathbf{QM}-\mathbf{I}\right)\mathbf{H}\left(\mathbf{MQ}-\mathbf{I}\right)\mathbf{P}\right]$ are both maximized over $h \in \mathcal{H}_0$ by $\mathbf{H} = \eta_h^2 \mathbf{P}^{-1}$.

The first of these is immediate from the definition of $\mathcal{G}_0$ and the fact that

$$r_i = \mathbf{z}^T\left(\boldsymbol{\psi}_i\right)\mathbf{B}_m^{-1}\mathbf{A}\mathbf{B}_m^{-1}\mathbf{z}\left(\boldsymbol{\psi}_i\right)m_i w_i = \left\|\mathbf{A}^{1/2}\mathbf{B}_m^{-1}\mathbf{z}\left(\boldsymbol{\psi}_i\right)\right\|^2 m_i w_i \geq 0.$$

The second follows from the fact that both traces are maximized by choosing $\mathbf{H}$ to be maximal with respect to the Loewner ordering. But from the definition of $\mathcal{H}_0$ it follows that $\mathbf{H} \leq \eta_h^2 \mathbf{P}^{-1}$ in this ordering. ■

Proof of Theorem 5. If $\eta_f^2 > 0$ then we are to minimize λ_m. But λ_m is minimized by $m = \mu$, with minimum value $\lambda_\mu = 0$. This is because for $m = \mu$ we have $\mathbf{M} = \mathbf{P}$, and consequently the matrix (3.3) contains a factor

$$\tilde{\mathbf{Z}}^T\mathbf{P}^{-1}\mathbf{MQ} = \tilde{\mathbf{Z}}^T\mathbf{Q} = \tilde{\mathbf{Z}}^T\mathbf{Z}\left(\mathbf{Z}^T\mathbf{PZ}\right)^{-1}\mathbf{Z}^T = \mathbf{0}.$$

If $\eta_g^2 > 0$ then we are to show that $\sum_{i=1}^N m_i \left\|\mathbf{B}_m^{-1}\mathbf{z}\left(\boldsymbol{\psi}_i\right)\right\|$ is also minimized by $m = \mu$. But this is merely the discrete analogue of (A.2), and is proven in an identical manner. That the minimax weights (3.5) are constant follows from (3.7), $\mathbf{B}_\mu = \mathbf{I}$ and the constancy of g_0.

It remains to show that the design $m = \mu$ is also optimal when $\eta_h^2 > 0$, i.e. that

$$tr\left[\mathbf{QPQMP}^{-1}\mathbf{M}\right] = \sum_{i=1}^N \left\|\mathbf{B}_m^{-1}\mathbf{z}\left(\boldsymbol{\psi}_i\right)\frac{m_i}{\mu_i}\right\|^2 \mu_i$$

and

$$tr\left[\left(\mathbf{QM}-\mathbf{I}\right)\mathbf{P}^{-1}\left(\mathbf{MQ}-\mathbf{I}\right)\mathbf{P}\right] = tr\left[\mathbf{QPQMP}^{-1}\mathbf{M}\right] + N - 2\left(d+1\right)^2.$$

are both minimized by $m = \mu$. The first of these is proven as at (A.3), and implies the second. ■