Supplementary Materials: Additive Gaussian Process for Computer Models With Qualitative and Quantitative Factors

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1 Proof of Theorem 1

Proof: When $q = 2$, the theorem follows by noting

$$\hat{y}_1(\mathbf{w}_0) = \hat{\mu} + \boldsymbol{\phi}_1^{\mathrm{T}}(\mathbf{w}_0)(\boldsymbol{\Phi}_1 + \boldsymbol{\Phi}_2)^{-1}(\mathbf{y} - \hat{\mu}\mathbf{1}),$$

and

$$\begin{aligned}
\hat{y}_2(\mathbf{w}_0) &= \boldsymbol{\phi}_2^{\mathrm{T}}(\mathbf{w}_0)\boldsymbol{\Phi}_2^{-1}(\mathbf{y} - \hat{\boldsymbol{y}}_1) \\
&= \boldsymbol{\phi}_2^{\mathrm{T}}(\mathbf{w}_0)\boldsymbol{\Phi}_2^{-1}[\mathbf{y} - \hat{\mu}\mathbf{1} - \boldsymbol{\Phi}_1(\boldsymbol{\Phi}_1 + \boldsymbol{\Phi}_2)^{-1}(\mathbf{y} - \hat{\mu}\mathbf{1})] \\
&= \boldsymbol{\phi}_2^{\mathrm{T}}(\mathbf{w}_0)\boldsymbol{\Phi}_2^{-1}[\mathbf{I} - \boldsymbol{\Phi}_1(\boldsymbol{\Phi}_1 + \boldsymbol{\Phi}_2)^{-1}](\mathbf{y} - \hat{\mu}\mathbf{1}) \\
&= \boldsymbol{\phi}_2^{\mathrm{T}}(\mathbf{w}_0)\boldsymbol{\Phi}_2^{-1}[(\boldsymbol{\Phi}_1 + \boldsymbol{\Phi}_2) - \boldsymbol{\Phi}_1](\boldsymbol{\Phi}_1 + \boldsymbol{\Phi}_2)^{-1}(\mathbf{y} - \hat{\mu}\mathbf{1}) \\
&= \boldsymbol{\phi}_2^{\mathrm{T}}(\mathbf{w}_0)(\boldsymbol{\Phi}_1 + \boldsymbol{\Phi}_2)^{-1}(\mathbf{y} - \hat{\mu}\mathbf{1}),
\end{aligned}$$

which leads to

$$\hat{y}_1(\mathbf{w}_0) + \hat{y}_2(\mathbf{w}_0) = \hat{\mu} + (\boldsymbol{\phi}_1(\mathbf{w}_0) + \boldsymbol{\phi}_2(\mathbf{w}_0))^{\mathrm{T}}(\boldsymbol{\Phi}_1 + \boldsymbol{\Phi}_2)^{-1}(\mathbf{y} - \hat{\mu}\mathbf{1}). \tag{1}$$

Now for a general $q \geq 3$, note that

$$\begin{aligned}
\hat{y}_{q-1}(\mathbf{w}_0) &= \boldsymbol{\phi}_{q-1}^{\mathrm{T}}(\mathbf{w}_0)(\boldsymbol{\Phi}_{q-1} + \boldsymbol{\Phi}_q)^{-1}\mathbf{e}_{q-2}, \\
\hat{y}_q(\mathbf{w}_0) &= \boldsymbol{\phi}_q^{\mathrm{T}}(\mathbf{w}_0)\boldsymbol{\Phi}_q^{-1}(\mathbf{e}_{q-2} - \hat{\boldsymbol{y}}_{q-1}).
\end{aligned}$$

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By applying the derivation and results in (1), we have

$$\begin{aligned}\hat{y}_{q-1}(\mathbf{w}_0) + \hat{y}_q(\mathbf{w}_0) &= (\boldsymbol{\phi}_{q-1}(\mathbf{w}_0) + \boldsymbol{\phi}_q(\mathbf{w}_0))^{\mathrm{T}}(\boldsymbol{\Phi}_{q-1} + \boldsymbol{\Phi}_q)^{-1}\mathbf{e}_{q-2} \\ &= (\boldsymbol{\phi}_{q-1}(\mathbf{w}_0) + \boldsymbol{\phi}_q(\mathbf{w}_0))^{\mathrm{T}}(\boldsymbol{\Phi}_{q-1} + \boldsymbol{\Phi}_q)^{-1}(\mathbf{e}_{q-3} - \hat{\boldsymbol{y}}_{q-2}). \qquad (2)\end{aligned}$$

We also note that

$$\hat{y}_{q-2}(\mathbf{w}_0) = \boldsymbol{\phi}_{q-2}^{\mathrm{T}}(\mathbf{w}_0)(\boldsymbol{\Phi}_{q-2} + \boldsymbol{\Phi}_{q-1} + \boldsymbol{\Phi}_q)^{-1}\mathbf{e}_{q-3}. \qquad (3)$$

Using (2) and (3), we can again apply the derivation and results in (1) to obtain

$$\hat{y}_{q-2}(\mathbf{w}_0) + \hat{y}_{q-1}(\mathbf{w}_0) + \hat{y}_q(\mathbf{w}_0) = (\boldsymbol{\phi}_{q-2}(\mathbf{w}_0) + \boldsymbol{\phi}_{q-1}(\mathbf{w}_0) + \boldsymbol{\phi}_q(\mathbf{w}_0))^{\mathrm{T}}(\boldsymbol{\Phi}_{q-2} + \boldsymbol{\Phi}_{q-1} + \boldsymbol{\Phi}_q)^{-1}\mathbf{e}_{q-3}.$$

Now we can continue this procedure recursively to $\hat{y}_2(\mathbf{w}_0)$, which gives

$$\hat{y}_2(\mathbf{w}_0) + \cdots + \hat{y}_q(\mathbf{w}_0) = (\boldsymbol{\phi}_2(\mathbf{w}_0) + \cdots + \boldsymbol{\phi}_q(\mathbf{w}_0))^{\mathrm{T}}(\boldsymbol{\Phi}_2 + \cdots + \boldsymbol{\Phi}_q)^{-1}\mathbf{e}_1.$$

Combing with $\hat{y}_1(\mathbf{w}_0) = \hat{\mu} + \boldsymbol{\phi}_1^{\mathrm{T}}(\mathbf{w}_0)(\sum_{j=1}^{q}\boldsymbol{\Phi}_j)^{-1}(\mathbf{y} - \hat{\mu}\mathbf{1})$, we have

$$\hat{y}_1(\mathbf{w}_0) + \hat{y}_2(\mathbf{w}_0) + \cdots + \hat{y}_q(\mathbf{w}_0) = (\boldsymbol{\phi}_1(\mathbf{w}_0) + \cdots + \boldsymbol{\phi}_q(\mathbf{w}_0))^{\mathrm{T}}(\boldsymbol{\Phi}_1 + \cdots + \boldsymbol{\Phi}_q)^{-1}(\mathbf{y} - \hat{\mu}\mathbf{1}).$$

This completes the proof. $\square$