

Supplementary Materials of “The Reconstruction Approach: From Interpolation to Regression”

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Abstract All proofs are given in the Supplementary Materials.

Appendix: Proofs

Proof of Theorem 1. We have

$$\begin{aligned} \text{MSE}(\hat{f}(\mathbf{x}_0)) &= E\left(\hat{f}(\mathbf{x}_0) - f(\mathbf{x}_0)\right)^2 = E\left(\sum_{j=1}^m b_j(\mathbf{x}_0)\hat{\gamma}_j - f(\mathbf{x}_0)\right)^2 \\ &\leq E\left(\sum_{j=1}^m [\hat{\gamma}_j - f(\mathbf{a}_j)] b_j(\mathbf{x}_0)\right)^2 / 2 + \left(\sum_{j=1}^m b_j(\mathbf{x}_0)f(\mathbf{a}_j) - f(\mathbf{x}_0)\right)^2 / 2 \\ &\leq E \sup_{j=1, \dots, m} |\hat{\gamma}_j - f(\mathbf{a}_j)|^2 \left(\sum_{j=1}^m |b_j(\mathbf{x}_0)|\right)^2 / 2 + \delta_m^2 / 2 = O(\delta_m^2 + \epsilon_n), \end{aligned}$$

which completes the proof. \square

Proof of (11). Let $b_j(x) = \prod_{1 \leq k \leq m, k \neq j} (x - a_k) / (a_j - a_k)$. We have

$$\begin{aligned} E\hat{f}(x_0) - f(x_0) &= \sum_{j=1}^m b_j(x_0)E\hat{\gamma}_j - f(x_0) = \sum_{j=1}^m b_j(x_0)f(a_j) - f(x_0); \\ \text{Var}(\hat{f}(x_0)) &= \sum_{j=1}^m b_j^2(x_0)\text{Var}(\hat{\gamma}_j) = \sigma^2 \|\mathbf{b}(x_0)\|^2 / l. \end{aligned}$$

By the theoretical results on the Chebyshev nodes-based polynomial interpolation (Stewart

1996), the convergence rate $\delta_m = \max_{t \in [0,1]} |f^{(m)}(t)|/2^{2m-1}m!$ and $\|\mathbf{b}(x_0)\| \leq 1$. Therefore,

$$\text{MSE}(\hat{f}(x_0)) \leq \delta_m^2 + m\sigma^2/n = \left[\frac{1}{2^{2m-1}m!} \max_{t \in [0,1]} |f^{(m)}(t)| \right]^2 + m\sigma^2/n.$$

(i) Assume that $\max_{t \in [0,1]} |f^{(m)}(t)| = O(m!)$. Take $m = C \log(n/\log(n))$ with constant $C \in (0, 1/2]$. We have

$$\frac{1}{2^{2m-1}m!} \max_{t \in [0,1]} |f^{(m)}(t)| = O\left(\frac{1}{4^m}\right) = o\left(\frac{1}{e^m}\right) = o\left(\sqrt{\frac{\log(n)}{n}}\right),$$

which implies

$$\text{MSE}(\hat{f}(x_0)) = o\left(\sqrt{\frac{\log(n)}{n}}\right) + m\sigma^2/n = O\left(\frac{\log(n)}{n}\right).$$

(ii) Assume that $\max_{t \in [0,1]} |f^{(m)}(t)| = O((4/e)^m m)$ and $m\sqrt{\log(m)} = C \log(n)$ with constant $C > 0$. By Stirling's formula, we have

$$\begin{aligned} & \frac{1}{2^{2m-1}m!} \max_{t \in [0,1]} |f^{(m)}(t)| \cdot \sqrt{\frac{n}{\log(n)}} = O\left(\frac{m\sqrt{n}}{\sqrt{m}m^m\sqrt{\log(n)}}\right) \\ & = O\left(\frac{\exp(m\sqrt{\log(m)}/C)}{\exp(m \log(m))(\log(m))^{1/4}}\right) = o(1), \end{aligned}$$

which implies

$$\text{MSE}(\hat{f}(x_0)) = o\left(\sqrt{\frac{\log(n)}{n}}\right) + m\sigma^2/n = o\left(\frac{\log(n)}{n}\right). \quad \square$$

Proof of (13). Assume $f \in C^4([0,1])$. Since the convergence rate of the cubic spline interpolator is $1/m^4$ (Stewart 1996), similar to the proof of (11), we have

$$\text{MSE}(\hat{f}(x_0)) \leq (m^{-4})^2 + O(m/n).$$

With $m \sim n^{1/9}$,

$$\text{MSE} \left(\hat{f}(x_0) \right) = O \left(n^{-8/9} \right). \quad \square$$

Let \tilde{f} denote the solution to the general KRR problem (26) in Section 4.2. Recall that \hat{f} is defined in (25). We now prove $\tilde{f} = \hat{f}$.

Proof. For simplicity, let \mathbf{R} , \mathbf{G} , and $\mathbf{r}(\mathbf{x})$ denote $\mathbf{R}_{\mathcal{X}}$, $\mathbf{G}_{\mathcal{X}}$, and $\mathbf{r}_{\mathcal{X}}(\mathbf{x})$, respectively.

By (25),

$$\hat{f}(\mathbf{x}) = \mathbf{y}'(\mathbf{I}_n + n\lambda \mathbf{V} \mathbf{R} \mathbf{V}')^{-1} \mathbf{b}(\mathbf{x}) = \mathbf{y}'(\mathbf{I}_n + n\lambda \mathbf{V} \mathbf{R} \mathbf{V}')^{-1} \{ \mathbf{U} \mathbf{g}(\mathbf{x}) + \mathbf{V} \mathbf{r}(\mathbf{x}) \}.$$

By (26) and the representer theorem (Schölkopf, Herbrich, and Smola 2001),

$$\tilde{f}(\mathbf{x}) = \mathbf{y}'(\mathbf{R} \ \mathbf{G}) \begin{pmatrix} \mathbf{R}^2 + n\lambda \mathbf{R} & \mathbf{R} \mathbf{G} \\ \mathbf{G}' \mathbf{R} & \mathbf{G}' \mathbf{G} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{r}(\mathbf{x}) \\ \mathbf{g}(\mathbf{x}) \end{pmatrix}.$$

It suffices to prove

$$(\mathbf{R} \ \mathbf{G}) \begin{pmatrix} \mathbf{R}^2 + n\lambda \mathbf{R} & \mathbf{R} \mathbf{G} \\ \mathbf{G}' \mathbf{R} & \mathbf{G}' \mathbf{G} \end{pmatrix}^{-1} = (\mathbf{I}_n + n\lambda \mathbf{V} \mathbf{R} \mathbf{V}')^{-1} (\mathbf{V} \ \mathbf{U}),$$

which is implied by

$$(\mathbf{V} \ \mathbf{U}) \begin{pmatrix} \mathbf{R}^2 + n\lambda \mathbf{R} & \mathbf{R} \mathbf{G} \\ \mathbf{G}' \mathbf{R} & \mathbf{G}' \mathbf{G} \end{pmatrix} = (\mathbf{I}_n + n\lambda \mathbf{V} \mathbf{R} \mathbf{V}') (\mathbf{R} \ \mathbf{G}). \quad (0.1)$$

Recall $\mathbf{U} = \mathbf{R}^{-1} \mathbf{G} (\mathbf{G}' \mathbf{R}^{-1} \mathbf{G})^{-1}$ and $\mathbf{V} = [\mathbf{I}_n - \mathbf{R}^{-1} \mathbf{G} (\mathbf{G}' \mathbf{R}^{-1} \mathbf{G})^{-1} \mathbf{G}'] \mathbf{R}^{-1}$. We have

$$\begin{aligned} \mathbf{V} \mathbf{R} \mathbf{V}' \mathbf{R} &= [\mathbf{I}_n - \mathbf{R}^{-1} \mathbf{G} (\mathbf{G}' \mathbf{R}^{-1} \mathbf{G})^{-1} \mathbf{G}'] \mathbf{R}^{-1} [\mathbf{R} - \mathbf{G} (\mathbf{G}' \mathbf{R}^{-1} \mathbf{G})^{-1} \mathbf{G}'] \\ &= \mathbf{I}_n - \mathbf{R}^{-1} \mathbf{G} (\mathbf{G}' \mathbf{R}^{-1} \mathbf{G})^{-1} \mathbf{G}' = \mathbf{V} \mathbf{R}. \end{aligned}$$

Therefore,

$$\begin{aligned} & [\mathbf{V}(\mathbf{R}^2 + n\lambda\mathbf{R}) + \mathbf{U}\mathbf{G}'\mathbf{R}] - [\mathbf{R} + n\lambda\mathbf{V}\mathbf{R}\mathbf{V}'\mathbf{R}] = \mathbf{V}\mathbf{R}^2 + \mathbf{U}\mathbf{G}'\mathbf{R} - \mathbf{R} + n\lambda(\mathbf{V}\mathbf{R} - \mathbf{V}\mathbf{R}\mathbf{V}'\mathbf{R}) \\ & = \mathbf{R} - \mathbf{R}^{-1}\mathbf{G}(\mathbf{G}'\mathbf{R}^{-1}\mathbf{G})^{-1}\mathbf{G}'\mathbf{R} + \mathbf{R}^{-1}\mathbf{G}(\mathbf{G}'\mathbf{R}^{-1}\mathbf{G})^{-1}\mathbf{G}'\mathbf{R} - \mathbf{R} = \mathbf{0}. \end{aligned} \quad (0.2)$$

On the other hand, we have

$$\mathbf{V}'\mathbf{G} = \mathbf{R}^{-1} [\mathbf{I} - \mathbf{G}(\mathbf{G}'\mathbf{R}^{-1}\mathbf{G})^{-1}\mathbf{G}'\mathbf{R}^{-1}] \mathbf{G} = \mathbf{0}.$$

Therefore,

$$\begin{aligned} & [\mathbf{V}\mathbf{R}\mathbf{G} + \mathbf{U}\mathbf{G}'\mathbf{G}] - [\mathbf{G} + n\lambda\mathbf{V}\mathbf{R}\mathbf{V}'\mathbf{G}] = \mathbf{V}\mathbf{R}\mathbf{G} + \mathbf{U}\mathbf{G}'\mathbf{G} - \mathbf{G} \\ & = [\mathbf{I}_n - \mathbf{R}^{-1}\mathbf{G}(\mathbf{G}'\mathbf{R}^{-1}\mathbf{G})^{-1}\mathbf{G}'] \mathbf{G} + \mathbf{R}^{-1}\mathbf{G}(\mathbf{G}'\mathbf{R}^{-1}\mathbf{G})^{-1}\mathbf{G}'\mathbf{G} - \mathbf{G} = \mathbf{0}. \end{aligned} \quad (0.3)$$

Obviously (0.1) follows from (0.2) and (0.3). \square

References

- Stewart, G. W. (1996). *Afternotes on Numerical Analysis*, Society for Industrial and Applied Mathematics.
- Schölkopf, B., Herbrich, R., and Smola, A. J. (2001). A generalized representer theorem. In *International Conference on Computational Learning Theory*, 416–426, Springer.