Interpolation Using Kernel Methods With Guaranteed Error Bounds

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Scattered Data Interpolation

- We want to approximate a real-valued function $f \in \mathcal{H}_d \subset L^2(\mathbb{R}^d, \rho_d)$, where $\mathcal{H}_d$ is a reproducing kernel Hilbert space with some symmetric positive definite kernel $K_d(x, t)$, $x, t \in \mathbb{R}^d$. and $\rho_d$ is some probability density function.

- Given the data $(x_i, y_i)$, $i = 1, \ldots, n$, where $y_i = f(x_i)$, The spline algorithm constructs the approximation as

$$ (A_n f)(x) = \sum_{i=1}^{n} c_i K(x, x_i) = k^T(x)c, $$

where $c = (c_i)_{i=1}^{n}$, $k(x) = (K(x, x_i))_{i=1}^{n}$. A good choice of $c$ is

$$ c = K^{-1}y, \quad \text{where } K = (K(x_i, x_j))_{i,j=1}^{n}, \quad y = (y_i)_{i=1}^{n}. $$
Following the power function approach, we have

\[
\sup_{0 \neq f \in \mathcal{H}} \frac{\|f - A_n f\|_{L_2}^2}{\|f\|_{\mathcal{H}}^2} \leq \int \sup_{0 \neq f \in \mathcal{H}} \frac{|f(x) - (A_n f)(x)|^2}{\|f\|_{\mathcal{H}}^2} \rho(x) dx \\
\leq \int \left( K(x, x) - k^T(x) K^{-1} k(x) \right) \rho(x) dx \\
= \int K(x, x) \rho(x) dx - \text{tr} \left( K^{-1} \tilde{K} \right) \\
=: h^2(n),
\]

where

\[
\tilde{K} = \int k(x) k^T(x) \rho(x) dx.
\]
Let $\| \cdot \|_{\tilde{H}}$ be a weaker norm defined by $\| f \|_{\tilde{H}} = \| Tf \|_{L^2}$, where $T : \mathcal{H} \to L^2(X, \rho)$ is a bounded linear operator and the linear functional $T_x : f \mapsto (Tf)(x)$ is also bounded. Then we can estimate the weaker norm by

$$
\tilde{H}^2_n(f) := \| T(A_n f) \|_{L^2}^2 = \| c^T \xi \|_{L^2}^2 = c^T \tilde{H} c,
$$

where

$$
\xi = (\xi(\cdot, x_i))_{i=1}^n = (TK(\cdot, x_i))_{i=1}^n,
$$

and

$$
\tilde{H} = \int_X \xi(x) \xi^T(x) \rho(x) dx.
$$
Functions in a Cone

Let $C_\tau = \{ f \in \mathcal{H} \mid \| f \|_\mathcal{H} \leq \tau \| f \|_\tilde{\mathcal{H}} \}$. Then for all $f \in C_\tau$,

$$\left| \| f \|_\tilde{\mathcal{H}} - \tilde{H}_n(f) \right| \leq \tilde{h}(n) \| f \|_\mathcal{H} \leq \tau \tilde{h}(n) \| f \|_\tilde{\mathcal{H}},$$

where

$$\tilde{h}^2(n) = \int_X T_x T_x \cdot K(\cdot, \cdot) \rho(x) dx - \text{tr} \left( K^{-1} \tilde{H} \right).$$

If $1 - \tau \tilde{h}(n) > 0$, this in turn gives an upper bound

$$\| f \|_\mathcal{H} \leq \frac{\tau \tilde{H}_n(f)}{1 - \tau \tilde{h}(n)}.$$
Problems With Power Function Estimation

Recall that the power function estimation is

$$|f(x) - (A_n f)(x)| \leq \sqrt{K(x, x) - k^T(x)K^{-1}k(x)}\|f\|_{\mathcal{H}}.$$  

- The matrices involved in the estimation of the error bound are often ill-conditioned.
- The estimated error bound is conservative in the sense that it does not converge as fast as the actual error.
- This approach only works for $\mathcal{L}_2$ error estimation.

It would be nice if we could find alternative error bounds that circumvent such limitations.
Error Estimates in Terms of the Fill Distance

Theorem (Wendland, 2005)

Suppose that $\Phi \in C^k_{\nu}(\mathbb{R}^d)$ is positive definite and that $\Omega \subseteq \mathbb{R}^d$ is bounded and satisfies an interior cone condition. For $\alpha \in \mathbb{N}^d_0$ with $|\alpha| \leq k/2$ and $X = \{x_1, \ldots, x_n\} \subseteq \Omega$ satisfying $h_{X,\Omega} \leq h_0$ we have the error bound

$$\|D^\alpha f - D^\alpha (A_nf)\|_{L^\infty(\Omega)} \leq Ch_{X,\Omega}^{(k+\nu)/2-|\alpha|} \|f\|_{\mathcal{H}}.$$ 

Theorem (Wendland, 2005)

Let $\Phi$ be one of the Gaussians. Suppose that $\Omega \subseteq \mathbb{R}^d$ is bounded and satisfies an interior cone condition. For every $\ell \in \mathbb{N}$ with $\ell \geq |\alpha|$ there exist constants $h_0(\ell)$, $C_\ell > 0$ such that

$$\|D^\alpha f - D^\alpha (A_nf)\|_{L^\infty(\Omega)} \leq C_{\alpha,\ell} h_{X,\Omega}^{\ell-|\alpha|} \|f\|_{\mathcal{H}}.$$ 

provided that $h_{X,\Omega} \leq h_0(\ell)$. 

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Spectral Convergence for Gaussians and (Inverse) Multiquadrics

Let \( W(x_0, R) := \{ x \in \mathbb{R}^d : \| x - x_0 \|_\infty \leq R \} \).

Theorem (Wendland, 2005)

Let \( \Omega = W(x_0, R) \) and let \( \Phi \) be one of the Gaussians. There exists a constant \( c \) such that

\[
\| f - A_n f \|_{\mathcal{L}_\infty(\Omega)} \leq e^{c \ln \frac{h_x,\Omega}{h_x,\Omega}} \| f \|_{\mathcal{H}}
\]

for all data sites \( X \) with sufficiently small \( h_x,\Omega \).

Question: What interior cone condition does \( W(x_0, R) \) satisfy?
Guaranteed Error Bounds for Gaussians

For Gaussians we obtain the same error bounds for any $1 \leq p < \infty$

$$\| f - A_n f \|_{L^p(X)} = \left( \int_X |f(x) - (A_n f)(x)|^p \rho(x) \, dx \right)^{1/p} \leq F(h_X, \Omega) \| f \|_{\mathcal{H}}.$$ 

Note that this result also holds for $p = \infty$. Similarly we obtain the bounds with the differential operator

$$\| Df - D(A_n f) \|_{L^p(X)} \leq C_{1, \ell} h_\Delta^{\ell-1} \| f \|_{\mathcal{H}}.$$ 

For $f \in \mathcal{C} := \{ g \in \mathcal{H} : Dg \in L^p(X), \| g \|_{\mathcal{H}} \leq \tau \| Dg \|_{L^p(X)} \}$, we have the guaranteed error bounds

$$\| f - A_n f \|_{L^p(X)} \leq \frac{\tau F(h_X, \Omega)}{1 - \tau C_{1, \ell} h_\Delta^{\ell-1}} \| D(A_n f) \|_{L^p(X)}.$$
Discussion

- There is a trade-off between the order of the convergence rates and the constants in front of them.
- For Gaussians the matrix $K$ often has a low rank when $n$ is large.

Thank you!