Improved Estimates for the Condition Number of Radial Basis Function Matrices

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Outline

Interpolation Matrix I

Let

$$\Phi : \mathbb{R}^d \to \mathbb{R}$$

be a positive definite function and

$$(\mathbf{x}_j, y_j)_{j=1,\dots,N} \in \mathbb{R}^d \times \mathbb{R} \quad \mathbf{x}_j \text{ pairwise distinct.}$$

Wishing to interpolate $(\mathbf{x}_j, y_j)$, i.e. finding $c_j \in \mathbb{R}$ with

$$f(\mathbf{x}_k) = \sum_{j=1}^{N} c_j \Phi(\mathbf{x}_k - \mathbf{x}_j) = y_k$$

we have to solve a linear system.

Interpolation Matrix II

Namely this one:

$$\mathbf{A}\mathbf{c} = \begin{pmatrix} \Phi(\mathbf{x}_1 - \mathbf{x}_1) & \dots & \Phi(\mathbf{x}_1 - \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ \Phi(\mathbf{x}_N - \mathbf{x}_1) & \dots & \Phi(\mathbf{x}_N - \mathbf{x}_N) \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix}$$

For this purpose, the condition number of **A** is of some interest.

$$\kappa = \kappa(\mathbf{A}) = \frac{\lambda_{\max}(\mathbf{A})}{\lambda_{\min}(\mathbf{A})} = \frac{\Lambda}{\lambda}.$$

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To avoid technical details, we will focus in this talk on

$$\Phi(\mathbf{x}) = e^{-\beta\|\mathbf{x}\|_2^2}.$$

Known Results

Smallest eigenvalue: Narcowich and Ward, Schaback proved an estimate like:

Bound on λ (Narcowich, Ward 92)

Let $q = 1/2 \min_{j \neq k} \|\mathbf{x}_j - \mathbf{x}_k\|_2$. Then

$$\lambda \gtrsim_d M^d \inf_{\|\mathbf{x}\|_2 \leq 2M} \hat{\Phi}(\mathbf{x})$$

for $M \geq 6.38d/q$.

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for $M \geq 6.38d/q$.

Note that the lower bound is uniform over the family of q-separated point sets X:

$$\inf_{X \ q\text{-separated}} \lambda(A_X) \gtrsim_d M^d \inf_{\|\mathbf{x}\|_2 \leq 2M} \hat{\Phi}(\mathbf{x}).$$

In particular, it is independent of $|X|$.

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for $M \geq 6.38d/q$.

We obtain for $q = 1/2$

$$\lambda \gtrsim_d \beta^{-d/2} e^{-160d^2/\beta}.$$

But numerical experiments (Boyd, Gildersleeve 2011) and theoretical results for gridded data (Baxter 1994) give

$$\lambda \sim_d \beta^{-d/2} e^{-d\pi^2/(4\beta)}$$

Known Results

Largest eigenvalue: In Wendland it is simply estimated by Gerschgorin circles (if possible):

$$\Lambda \leq \Phi(0) + \max_j \sum_{k \neq j} |\Phi(\mathbf{x}_j - \mathbf{x}_k)| \leq N\Phi(0) = N.$$

If Φ decays quickly, a more careful evaluation of this sum gives (Narcowich et al. 1993)

$$\Lambda \leq 1 + 3d \sum_{n=1}^{\infty} (n+2)^{d-1} e^{-\beta n^2/4}.$$

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For gridded data an optimal upper bound is known:

$$\Lambda \lesssim \beta^{-d/2} \sum_{k \in \mathbb{Z}^d} e^{-\|\pi k\|_2^2/\beta}.$$

Exponential Sums

Link to exponential sums:

$$\lambda_{min} = \min_{\|\mathbf{c}\|_2=1} \mathbf{c}^T \mathbf{A}\mathbf{c}$$

$$\begin{aligned}
\mathbf{c}^T \mathbf{A}\mathbf{c} &= \sum_{j,k} c_j c_k \Phi(\mathbf{x}_j - \mathbf{x}_k) = \sum_{j,k} c_j c_k (2\pi)^{-d} \int_{\mathbb{R}^d} e^{i(\mathbf{x}_j - \mathbf{x}_k)\cdot\mathbf{x}} \hat{\Phi}(\mathbf{x})\,d\mathbf{x} \\
&= (2\pi)^{-d} \int_{\mathbb{R}^d} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j\cdot\mathbf{x}} \right|^2 \hat{\Phi}(\mathbf{x})\,d\mathbf{x} \\
&\geq (2\pi)^{-d} \inf_{\mathbf{x}\in B_M} \hat{\Phi}(\mathbf{x}) \int_{B_M} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j\cdot\mathbf{x}} \right|^2 d\mathbf{x}
\end{aligned}$$

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$$\mathbf{c}^T \mathbf{A}\mathbf{c} = \sum_{j,k} c_j c_k \Phi(\mathbf{x}_j - \mathbf{x}_k) = \sum_{j,k} c_j c_k (2\pi)^{-d} \int_{\mathbb{R}^d} e^{i(\mathbf{x}_j - \mathbf{x}_k)\cdot \mathbf{x}} \hat{\Phi}(\mathbf{x})\, d\mathbf{x}$$

$$= (2\pi)^{-d} \int_{\mathbb{R}^d} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 \hat{\Phi}(\mathbf{x})\, d\mathbf{x}$$

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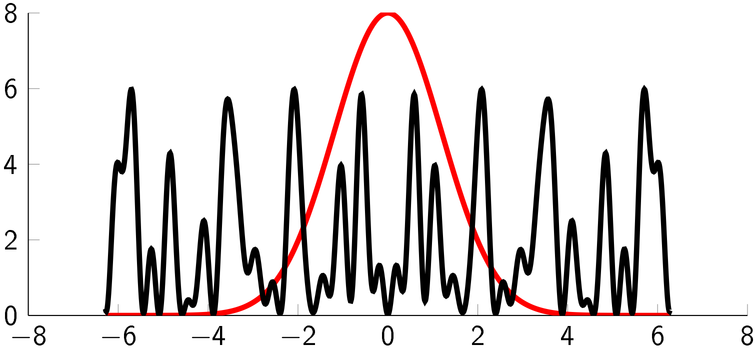
This estimate seems to be rather crude! How much do we loose?

How good is this estimate?

$$\int_{\mathbb{R}^d} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 \hat{\Phi}(\mathbf{x})\, d\mathbf{x} \geq \inf_{\mathbf{x} \in B_M} \hat{\Phi}(\mathbf{x}) \int_{B_M} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 d\mathbf{x}$$



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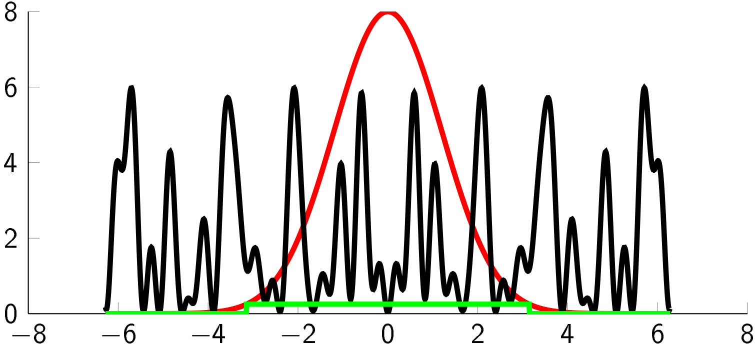

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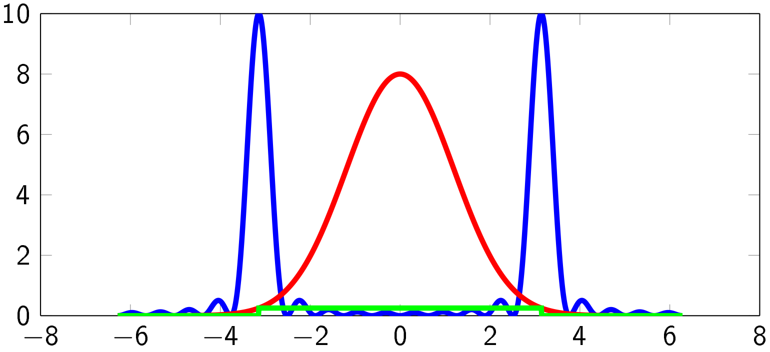
$$\int_{\mathbb{R}^d} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 \hat{\Phi}(\mathbf{x})\, d\mathbf{x} \geq \inf_{\mathbf{x} \in B_M} \hat{\Phi}(\mathbf{x}) \int_{B_M} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 d\mathbf{x}$$



Localization Estimates

Now we estimate

$$\int_{B_M} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 d\mathbf{x} \geq \int_{\mathbb{R}^d} \hat{\Psi}(\mathbf{x}) \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 d\mathbf{x}$$

where $\operatorname{supp} \hat{\Psi} \subset B_M$, $\hat{\Psi} \leq 1$.

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where $\operatorname{supp} \hat{\Psi} \subset B_M$, $\hat{\Psi} \leq 1$. Now as before

$$\int_{\mathbb{R}^d} \hat{\Psi}(\mathbf{x}) \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j\cdot\mathbf{x}} \right|^2 \, d\mathbf{x} = \sum_{j,k} c_j c_k \Psi(\mathbf{x}_j - \mathbf{x}_k) = \mathbf{c}^T \mathbf{B} \mathbf{c}$$

Then use Gerschgorin for $\mathbf{B}$. Hope: $\mathbf{B}$ is more diagonally dominant than $\mathbf{A}$.

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$$\int_{B_M} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 \mathrm{d}\mathbf{x} \geq \int_{\mathbb{R}^d} \hat{\Psi}(\mathbf{x}) \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 \mathrm{d}\mathbf{x}$$

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Then use Gerschgorin for $\mathbf{B}$. Hope: $\mathbf{B}$ is more diagonally dominant than $\mathbf{A}$.
In fact, only $\hat{\Psi} \leq \chi_{B_M}$ is necessary. Then it is possible that $\mathbf{B}$ is a diagonal matrix.

Results of Komornik and Loreti

Lower Bounds (Komornik and Loreti, 05)

Let $X \subset \mathbb{R}^d$ be a finite set with

$$q_\infty \geq 1/2 \min_{\mathbf{x} \neq \mathbf{y}} \|\mathbf{y} - \mathbf{x}\|_\infty.$$

If $M > \pi\sqrt{d}/(2q_\infty)$, then

$$\int_{B_M} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 \, \mathrm{d}\mathbf{x} \geq k_\infty(q, M) \|\mathbf{c}\|_2^2.$$

Here we can choose

$$k_\infty(q, M) = \left(1 - \frac{\pi^2 d}{4M^2 q_\infty^2}\right) \frac{\pi^{2d}}{4^{2d}} (2\pi)^d q_\infty^{-d}.$$

Bounds for λ

Recall

$$\mathbf{c}^T \mathbf{A} \mathbf{c} = \sum_{j,k} c_j c_k \Phi(\mathbf{x}_j - \mathbf{x}_k)$$

$$\geq (2\pi)^{-d} \inf_{\mathbf{x} \in B_M} \hat{\Phi}(\mathbf{x}) \int_{B_M} \left| \sum_{j=1}^{N} c_j e^{i \mathbf{x}_j \cdot \mathbf{x}} \right|^2 \, d\mathbf{x}$$

Applying the derived bound gives

Improved Bounds for λ

Let X have a ∞-separation radius of at least q_∞. Then

$$\lambda \geq \inf_{\mathbf{x} \in B_M} \hat{\Phi}(\mathbf{x}) \left(1 - \frac{\pi^2 d}{4 M^2 q_\infty^2} \right) \frac{\pi^{2d}}{4^{2d}} q_\infty^{-d}$$

for all $M > \pi\sqrt{d}/(2q_\infty)$.

The Gaussians

For our prototypical example $\Phi_\beta(\mathbf{x}) = e^{-\beta\|\mathbf{x}\|_2^2}$ we have that

$$\hat{\Phi}_\beta(\mathbf{w}) = \left(\frac{\pi}{\beta}\right)^{d/2} e^{-\|\mathbf{w}\|_2^2/(4\beta)}.$$

We again rescale X and β such that $q = 1/2$ and obtain

$$\begin{aligned} \lambda &\gtrsim_d \ \ \beta^{-d/2} e^{-\pi^2(d+1)/(4\beta)} \\ \lambda &\gtrsim_{d,\varepsilon} \beta^{-d/2} e^{-(\pi\sqrt{d}+\varepsilon)^2/(4\beta)}. \end{aligned}$$

Recall the optimal bound on regular grids:

$$\lambda \sim_d \beta^{-d/2} e^{-d\pi^2/(4\beta)}$$

Bounds on Λ

For the lower bound, we were able to use an estimate in Fourier space to obtain a better estimate. Is this here possible as well?

$$\mathbf{c}^T \mathbf{A} \mathbf{c} = (2\pi)^{-d} \int_{\mathbb{R}^d} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 \hat{\Phi}(\mathbf{x})\, d\mathbf{x}$$

We have to find reasonable upper bounds for integrals over exponential sums.

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Upper Bound of Selberg Type

Let $X \subset \mathbb{R}^d$ be a finite family of points with ∞-separation radius q_∞. Then

$$\int_{[-M,M]^d} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 d\mathbf{x} \leq \left(2M + \frac{\pi}{q_\infty} \right)^d \|\mathbf{c}\|_2^2.$$

Fourier-based Upper Bound

Upper Bounds for Λ (D., Iske 2016)

Let $\hat{\Phi} : \mathbb{R}^d \to \mathbb{R}$ be a function with $\hat{\Phi}(\mathbf{x}) = \varphi(\|\mathbf{x}\|_2)$ positive and decreasing. Then for X with ∞-separation radius q_∞ and any $M > 0$ we obtain

$$\int_{\mathbb{R}^d} \left| \sum_{j=1}^{N} c_j e^{i\mathbf{x}_j \cdot \mathbf{x}} \right|^2 \hat{\Phi}(\mathbf{x})\, d\mathbf{x} \leq 2^d \left(M + \frac{\pi}{q_\infty} \right)^d \sum_{\mathbf{k} \in \mathbb{Z}^d_{\geq 0}} \hat{\Phi}(M\mathbf{k}).$$

Proof: For any $\mathbf{k} \in \mathbb{Z}^d_{\geq 0}$ let

$$Q_{\mathbf{k}} = \{M\mathbf{k} + M(\alpha_1, \ldots \alpha_d)^T \mid \alpha_j \in [0,1)\}.$$

Then $\mathbb{R}^d_{\geq 0} = \cup Q_{\mathbf{k}}$ and we can cover $\mathbb{R}^d$ with blocks such that 2^d have minimal norm element $M\|\mathbf{k}\|_2$. Use the preceding lemma for each tile.

Gaussians

For our example, the Gaussians, we obtain

$$\Lambda \leq 4^d \left(\frac{\pi}{\beta}\right)^{d/2} \sum_{\mathbf{k}\in\mathbb{Z}^d_{\geq 0}} e^{-\|\pi\mathbf{k}\|_2^2/\beta}.$$

Baxter proved for $X \subset \mathbb{Z}^d$ that the best upper bound is given by

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Thus up to a constant we generalized this result to arbitrary grids.

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Thus up to a constant we generalized this result to arbitrary grids.

For the condition number we obtain for ∞-separation

$$\kappa = \frac{\Lambda}{\lambda} \leq 4^d \left(\sum_{\mathbf{k}\in\mathbb{Z}^d_{\geq 0}} e^{-\|\pi\mathbf{k}\|_2^2/\beta}\right) e^{(\pi\sqrt{d}+\varepsilon)^2/4\beta} C(\varepsilon, d)^{-1}.$$

Thank you for your attention!

Preprint:

B. Diederichs and A. Iske: Improved Estimates for Condition Numbers of Radial Basis Function Interpolation Matrices. *submitted, Preprint in Hamburger Beiträge*, 2016.