Outline

1. Radial (Basis) Functions
2. Radial Basis Function Interpolation
Next goals

- Get a feel for more general kernels (in particular RBFs) before we study them in detail

- Want to overcome limitations of distance matrix interpolation, but keep overall structure:
  combine distance matrix with “good” basic functions
Example

The Gaussian

\[ \kappa(r) = e^{-(\varepsilon r)^2}, \quad r \in \mathbb{R}, \]

has a shape parameter \( \varepsilon \) related to the variance \( \sigma^2 \) of the normal distribution:

\[ \varepsilon^2 = 1/(2\sigma^2). \]

Compose the Gaussian with Euclidean distance function \( \| \cdot \|_2 \) and get

\[ K(x, z) = e^{-\varepsilon^2 \| x - z \|^2_2}, \quad x \in \mathbb{R}^d, \]

where \( z \in \mathbb{R}^d \) is some fixed center or knot.

Remark

Note that \( \kappa \) is univariate, but \( K \) is a multivariate kernel function such that

\[ B_j(x) = K(x, x_j) = \kappa(\| x - x_j \|^2_2) \quad \text{radial basis function (RBF)} \]
Definition

A multivariate function \( \tilde{K} : \mathbb{R}^d \to \mathbb{R} \) is called radial provided there exists a univariate function \( \kappa : [0, \infty) \to \mathbb{R} \) such that

\[
\tilde{K}(\mathbf{x}) = \kappa(r), \quad \text{where} \quad r = \|\mathbf{x}\|,
\]

and \( \| \cdot \| \) is some norm on \( \mathbb{R}^d \) — usually the Euclidean norm.

Thus, for a radial function

\[
\|\mathbf{x}_1\| = \|\mathbf{x}_2\| \implies \tilde{K}(\mathbf{x}_1) = \tilde{K}(\mathbf{x}_2), \quad \mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^d.
\]

Example

The Euclidean distance function \( \tilde{K}(\mathbf{x}) = \|\mathbf{x}\|_2 \) (or \( \kappa(r) = r \)) is a special case of a radial (basic) function.
Radial (Basis) Functions

Figure: Gaussian with $\varepsilon = 1$ (left) and $\varepsilon = 3$ (right) centered at the origin.

- A smaller value of $\varepsilon$ (i.e., larger variance) causes the function to become “flatter”, so it’s like an inverse length scale.
- Increasing $\varepsilon$ leads to a more peaked RBF.
- The choice of $\varepsilon$ influences both accuracy and numerical stability of the solution to our interpolation problem.
Instead of distance matrices we now use a radial basis function expansion to solve the scattered data interpolation problem by assuming

$$s(x) = \sum_{j=1}^{N} c_j \kappa (\|x - x_j\|_2), \quad x \in \mathbb{R}^d.$$  \hspace{1cm} (1)

Using the interpolation conditions $s(x_i) = f(x_i)$, $i = 1, \ldots, N$, we get $c_j$ from

$$
\begin{bmatrix}
    \kappa (\|x_1 - x_1\|_2) & \kappa (\|x_1 - x_2\|_2) & \cdots & \kappa (\|x_1 - x_N\|_2) \\
    \kappa (\|x_2 - x_1\|_2) & \kappa (\|x_2 - x_2\|_2) & \cdots & \kappa (\|x_2 - x_N\|_2) \\
    \vdots & \vdots & \ddots & \vdots \\
    \kappa (\|x_N - x_1\|_2) & \kappa (\|x_N - x_2\|_2) & \cdots & \kappa (\|x_N - x_N\|_2)
\end{bmatrix}
\begin{bmatrix}
    c_1 \\
    c_2 \\
    \vdots \\
    c_N
\end{bmatrix}
= 
\begin{bmatrix}
    f(x_1) \\
    f(x_2) \\
    \vdots \\
    f(x_N)
\end{bmatrix}.
$$

Question:

For what type of basic functions $\kappa$ is the system matrix non-singular?
Setup for Example

- Use $d = 2$
- Basic function: Gaussians or linear function $\kappa(r) = r$
- Code in `RBFInterpolation2D.m` written for 2D (can easily be generalized to $dD$), and uses `DistanceMatrix.m`.
- Use Franke’s function

$$f(x, y) = \frac{3}{4}e^{-1/4((9x-2)^2+(9y-2)^2)} + \frac{3}{4}e^{-(1/49)(9x+1)^2-(1/10)(9y+1)^2} + \frac{1}{2}e^{-1/4((9x-7)^2+(9y-3)^2)} - \frac{1}{5}e^{-(9x-4)^2-(9y-7)^2}$$

- Use Halton data sites (get others easily from `CreatePoints`)
- Compute errors on $40 \times 40$ uniform grid
Figure: Franke’s test function.
Program (RBFInterpolation2D.m)

1. `rbf = @(e,r) exp(-(e*r).^2); ep = 21.1;`
2. `f1 = @(x,y) 0.75*exp(-((9*x-2).^2+(9*y-2).^2)/4);`
3. `f2 = @(x,y) 0.75*exp(-((9*x+1).^2/49+(9*y+1).^2/10));`
4. `f3 = @(x,y) 0.5*exp(-((9*x-7).^2+(9*y-3).^2)/4);`
5. `f4 = @(x,y) 0.2*exp(-((9*x-4).^2+(9*y-7).^2));`
6. `testfunction = @(x,y) f1(x,y)+f2(x,y)+f3(x,y)-f4(x,y);`
7. `N = 1089; gridtype = 'h';`
8. `dsites = CreatePoints(N,2,gridtype);`
9. `ctrs = dsites;`
10. `neval = 40; M = neval^2;`
11. `epoints = CreatePoints(M,2,'u');`
12. `rhs = testfunction(dsites(:,1),dsites(:,2));`
13. `DM_data = DistanceMatrix(dsites,ctrs);`
14. `IM = rbf(ep,DM_data);`
15. `DM_eval = DistanceMatrix(epoints,ctrs);`
16. `EM = rbf(ep,DM_eval);`
17. `s = EM * (IM\rhs);`
18. `exact = testfunction(epoints(:,1),epoints(:,2));`
19. `maxerr = norm(s-exact,inf)`
20. `rms_err = norm(s-exact)/neval`
Remark

Note the conflicting use of the term stationary:

here vs. statistics = translation-invariant

We usually verify convergence of a method numerically by looking at a sequence of experiments with increasingly larger sets of data.

Non-stationary approximation: Use one fixed value of $\varepsilon$ for all of the experiments.

Stationary approximation: Scale the shape parameter $\varepsilon$ according to the fill distance (or meshsize) $h$ so that we end up using “peaked” basis functions for densely spaced data and “flat” basis functions for coarsely spaced data.

More details later
Fill distance

The fill distance (or covering radius) is usually defined as

\[ h = h_{\mathcal{X},\Omega} = \sup_{x \in \Omega} \min_{x_j \in \mathcal{X}} \| x - x_j \|_2. \]  

(2)

It indicates how well the data in the set \( \mathcal{X} \) fill out the domain \( \Omega \).

In MATLAB:

\[ h_{\mathcal{X}} = \max(\min(DM\_eval')) \]  

(3)

Remark

Since \( \min \) works along columns of a matrix, transposition of the non-symmetric evaluation matrix corresponds to finding — for each evaluation point — the distance to the corresponding closest data site, and then setting \( h_{\mathcal{X},\Omega} \) as the worst of those distances.
**Figure:** The fill distance for $N = 25$ Halton points ($h_{x,\Omega} \approx 0.2667$).

It’s the radius of the largest possible empty ball that can be placed among the data locations inside $\Omega$. 
Test of non-stationary interpolation

- **Fix** large $\varepsilon$ to prevent severe ill-conditioning with large $N$ (if $\varepsilon = 1$, then $N = 25$ already very ill-conditioned)
- **Consequence:** very localized basis functions that don’t capture enough information on small point sets (see left plot)

Figure: Gaussian RBF interpolant with $\varepsilon = 21.1$ at $N = 289$ (left) and at $N = 1089$ Halton points (right).
### Gaussian vs. Distance matrix

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<tr>
<th>$k$</th>
<th>$N$</th>
<th>RMS-error</th>
<th>max-error</th>
<th>RMS-error</th>
<th>max-error</th>
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</table>

**Table:** Non-stationary RBF interpolation to Franke’s function using Gaussians ($\varepsilon = 21.1$) and Euclidean distance matrices.

### Remark

- **Surprising observation in above example:** distance matrix fit more accurate than Gaussian.
- **Would expect Gaussian to be more accurate → find a better $\varepsilon$**
Same test function and Gaussians as before.

Figure: Maximum (blue) and RMS (red) errors vs. \( \varepsilon \) for 81 (top left), 289 (top right), 1089 (bottom left), and 4225 Halton points (bottom right).
What do we learn from the $\varepsilon$ error curves?

- Errors decrease with decreasing $\varepsilon$ (not the same as convergence for $h \to 0$).
- Error curves are not monotonic.
- Optimal value of $\varepsilon$ seems to exist which minimizes errors.
- For small enough values of $\varepsilon$ the computational results become unpredictable, and the error curves become erratic (ill-conditioning)
- We’ll consider $\varepsilon$ to be “safe” if we don’t get a MATLAB warning about ill-conditioning.
  - Note that for small $N$ optimal $\varepsilon$ is “safe”, but for larger $N$ not.
  - We obtain highly accurate solutions from severely ill-conditioned linear systems!
  - This is known as the uncertainty or trade-off principle.

- **Interesting problem**: how to compute optimal solution in a stable way. Later we will see how this can be done with the Hilbert–Schmidt SVD.
Best possible errors for Gaussian interpolation

<table>
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<tr>
<th>$k$</th>
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<th>max-error</th>
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</table>

Table: “Optimal” RBF interpolation to Franke’s function using Gaussians.

**Remark**

- **Errors for “safe” $\varepsilon$ now comparable (or smaller) than those for distance matrix interpolation.**
- **Much better for “optimal” $\varepsilon$. However, $\varepsilon = 6.2$ with $N = 1089$. Halton points yields $\text{RCOND} = 2.683527 \times 10^{-020}$.**
Avoiding the Uncertainty Principle With the Hilbert–Schmidt SVD

“Using the standard basis, one can’t have high accuracy and stability at the same time.”

[Sch95a, Sch95b]

Stable evaluation [FM12] inspired by [FP08, FLF11]
Summary

Remark

*If the data are not sampled from a known test function, then we will not be able to choose an “optimal” shape parameter by monitoring the RMS error.*

*New challenge: how to find “optimal” $\varepsilon$ based only on the data?*

We will study

- ill-conditioning and preconditioning,
- optimal shape parameter selection, and
- alternate stable evaluation methods via Hilbert–Schmidt SVD and eigenfunction expansions

later.
References I


