Meshfree Approximation with MATLAB

Lecture V: "Optimal" Shape Parameters for RBF Approximation Methods

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Outline

Motivation

We saw earlier that the "correct" shape parameter ε plays a number of important roles:

- it determines the accuracy of the fit,
- it is important for numerical stability,
- it determines the speed of convergence,
- it is related to the saturation error of stationary approximation.

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In many applications the "best" ε is determined by "trial-and-error".

We now consider the use of cross validation.

Leave-One-Out Cross-Validation (LOOCV)

Proposed by [Rippa (1999)] (and already [Wahba (1990)] and [Dubrule '83]) for RBF interpolation systems $A\boldsymbol{c} = \boldsymbol{f}$

For a fixed $k = 1, \ldots, N$ and fixed ε, let

$$\mathcal{P}_f^{[k]}(\boldsymbol{x}, \varepsilon) = \sum_{\substack{j=1 \\ j \neq k}}^{N} c_j^{[k]} \Phi_\varepsilon(\boldsymbol{x}, \boldsymbol{x}_j)$$

be the RBF interpolant to training data $\{f_1, \ldots, f_{k-1}, f_{k+1}, \ldots, f_N\}$, i.e.,

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Let

$$e_k(\varepsilon) = f_k - \mathcal{P}_f^{[k]}(\boldsymbol{x}_k, \varepsilon)$$

be the error at the one validation point $\boldsymbol{x}_k$ not used to determine the interpolant.

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be the error at the one validation point $\boldsymbol{x}_k$ not used to determine the interpolant.
Find

$$\varepsilon_{opt} = \underset{\varepsilon}{\operatorname{argmin}} \|\boldsymbol{e}(\varepsilon)\|, \qquad \boldsymbol{e} = [e_1, \ldots, e_N]^T$$

Naive approach

- Add a loop over ε
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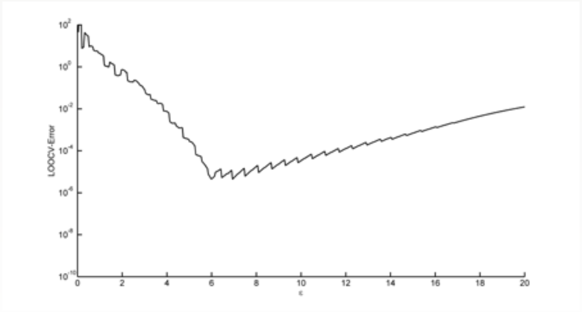

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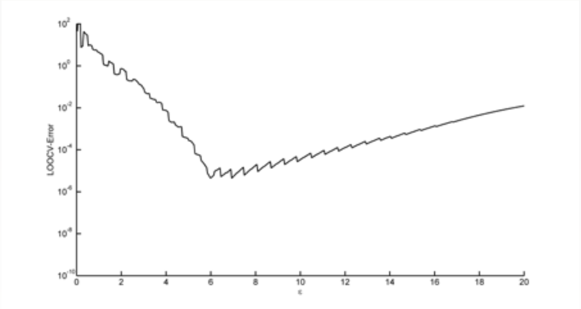

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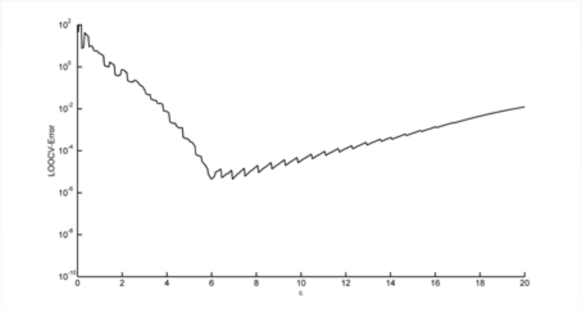

Problem: computationally very expensive, i.e., $\mathcal{O}(N^4)$ operations
Advantage: does not require knowledge of the solution

Does this work?

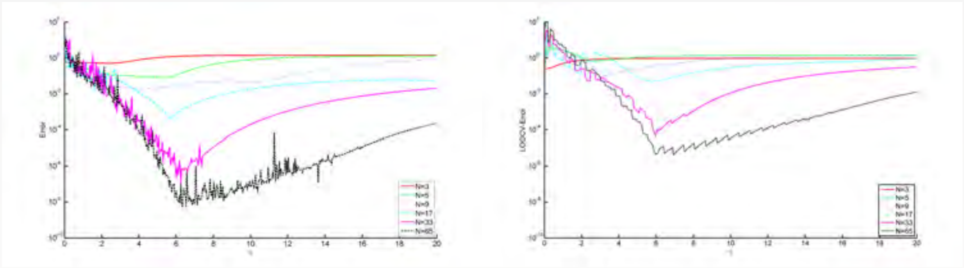

Figure: Optimal ε curves for trial and error (left) and for LOOCV (right) for 1D Gaussian interpolation.

N	3	5	9	17	33	65
trial-error	2.3246	5.1703	4.7695	5.6513	6.2525	6.5331
LOOCV	0.0401	0.0401	3.2064	5.7715	5.9319	6.9339

Table: Values of "optimal" ε.

A more efficient formula

Rippa (and also Wahba and Dubrule) showed that computation of the error components can be simplified to a single formula

$$e_k = \frac{c_k}{A_{kk}^{-1}},$$

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- *c_k and A^{-1} need to be computed only once for each value of ε, so we still have $\mathcal{O}(N^3)$ computational complexity.*
- *Can be vectorized in* MATLAB*:* `e = c./diag(inv(A))`*.*

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Program (CostEps.m)

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function ceps = CostEps(ep,r,rbf,rhs)
A = rbf(ep,r);
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Possible calling sequence for the cost function:

```
ep = fminbnd(@(ep) CostEps(ep,DM,rbf,rhs),mine,maxe);
```

Program (`RBFInterpolation_sDLOOCV.m`)

```
s = 2;  N = 289;  gridtype = 'h';  M = 500;
global rbf;  rbf_definition;  mine = 0; maxe = 20;
[dsites, N] = CreatePoints(N,s,gridtype);
ctrs = dsites;
epoints = CreatePoints(M,s,'r');
rhs = testfunctionsD(dsites);
DM = DistanceMatrix(dsites,ctrs);
ep = fminbnd(@(ep) CostEps(ep,DM,rbf,rhs),mine,maxe);
IM = rbf(ep,DM);
DM = DistanceMatrix(epoints,ctrs);
EM = rbf(ep,DM);
Pf = EM * (IM\rhs);
exact = testfunctionsD(epoints);
maxerr = norm(Pf-exact,inf)
rms_err = norm(Pf-exact)/sqrt(M)
```

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Simple (and cheap):
Vectorize Riley's algorithm so that it can handle multiple right-hand sides, i.e., solve

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In fact, the beauty of MATLAB is that the code for `Riley.m` does not change at all.

MATLAB Algorithm for Cost Function using Riley

```
function ceps = CostEps(ep,r,rbf,rhs)
A = rbf(ep,r);
invA = pinv(A);
errorvector = (invA*rhs)./diag(invA);
ceps = norm(errorvector);
```

Program (CostEpsRiley.m)

```
function ceps = CostEpsRiley(ep,r,rbf,rhs)
A = rbf(ep,r);
mu = 1e-11;
% find solution of Ax=b and A^-1
D = Riley(A,[rhs eye(size(A))],mu);
errorvector = D(:,1)./diag(D(:,2:end));
ceps = norm(errorvector);
```

Program (RBFInterpolation_sDLOOCVRiley.m)

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rhs = testfunctionsD(dsites);
DM = DistanceMatrix(dsites,ctrs);
ep = fminbnd(@(ep) CostEpsRiley(ep,DM,rbf,rhs,mu),...
     mine,maxe);
IM = rbf(ep,DM);
coef = Riley(IM,rhs,mu);
DM = DistanceMatrix(epoints,ctrs);
EM = rbf(ep,DM);
Pf = EM * coef;
exact = testfunctionsD(epoints);
maxerr = norm(Pf-exact,inf)
rms_err = norm(Pf-exact)/sqrt(M)
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Data	900 uniform	900 Halton	2500 uniform	2500 Halton
$\varepsilon_{opt,pinv}$	5.9725	7.0165	6.6974	6.1277
RMS-err	1.6918e-06	4.6326e-07	1.9132e-08	2.0648e-07
cond(A)	8.813772e+19	1.433673e+19	2.835625e+21	7.387674e+20
$\varepsilon_{opt,Riley}$	5.6536	5.9678	6.0635	5.6205
RMS-err	4.1367e-07	7.7984e-07	1.9433e-08	4.9515e-08
cond(A)	1.737214e+21	1.465283e+20	1.079238e+22	5.811212e+20

Table: Interpolation with Gaussians to 2D Franke function.

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Remark

- *LOOCV with Riley is much faster than with* `pinv` *and of similar accuracy.*
- *If we use backslash in* `CostEps`*, then results are less accurate than with* `pinv`

  e.g., $N = 900$ *uniform: RMS-err*$= 5.1521e\text{-}06$ *with* $\varepsilon = 7.5587$.

LOOCV for Iterated AMLS

Recall

$$\mathcal{Q}_f^{(n)}(\boldsymbol{x}) = \boldsymbol{\Phi}_\varepsilon^T(\boldsymbol{x}) \sum_{\ell=0}^{n} (I - A_\varepsilon)^\ell \boldsymbol{f}$$

Now we find both

- a good value of the shape parameter ε,
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In [F. & Zhang (2007b)] two algorithms were presented.
We discuss one of them.

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We showed earlier that

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where $\mathcal{Q}_{\boldsymbol{f}}^{(n)}$ is the IAMLS approximant evaluated on the data sites.
This is a linear system with system matrix A, but right-hand side vector $\mathcal{Q}_{\boldsymbol{f}}^{(n)}$. We want $\boldsymbol{f}$ on the right-hand side.

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Therefore, multiply both sides by

$$\left[\sum_{\ell=0}^{n} (I - A)^{\ell}\right]^{-1} A^{-1}$$

and obtain

$$\left[\sum_{\ell=0}^{n} (I - A)^{\ell}\right]^{-1} \left(\sum_{\ell=0}^{n} (I - A)^{\ell} \boldsymbol{f}\right) = \boldsymbol{f}.$$

Now

$$\left[\sum_{\ell=0}^{n}(I-A)^{\ell}\right]^{-1}\left(\sum_{\ell=0}^{n}(I-A)^{\ell}\boldsymbol{f}\right)=\boldsymbol{f}$$

is in the form of a standard interpolation system with

- system matrix $\left[\sum_{\ell=0}^{n}(I-A)^{\ell}\right]^{-1}$,
- coefficient vector $\sum_{\ell=0}^{n}(I-A)^{\ell}\boldsymbol{f}$,
- and the usual right-hand side $\boldsymbol{f}$.

Remark

The matrix $\sum_{\ell=0}^{n}(I-A)^{\ell}$ *is a truncated Neumann series approximation of* A^{-1}.

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Numerator and denominator can be accumulated iteratively.

Numerator: take k^{th} component of

$$\boldsymbol{v}^{(0)}=\boldsymbol{f},\qquad \boldsymbol{v}^{(n)}=\boldsymbol{f}+(I-A)\,\boldsymbol{v}^{(n-1)}$$

Denominator: take k^{th} diagonal element of

$$M^{(0)}=I,\qquad M^{(n)}=I+(I-A)\,M^{(n-1)}$$

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Need only diagonal elements of this. Since $M^{(n)}$ is diagonal this can be done efficiently as well.

Algorithm (for iterated AMLS with LOOCV)

```
Fix $\varepsilon$. Perform an eigen-decomposition
    $$I - A = X\Lambda X^{-1}$$
Initialize $\boldsymbol{v}^{(0)} = \boldsymbol{f}$ and $M^{(0)} = I$
For $n = 1, 2, \dots$
    Perform the updates
        $$\begin{aligned} \boldsymbol{v}^{(n)} &= \boldsymbol{f} + (I - A)\,\boldsymbol{v}^{(n-1)} \\ M^{(n)} &= I + \Lambda M^{(n-1)} \end{aligned}$$
    Compute the cost vector (using MATLAB notation)
        $$\boldsymbol{e}^{(n)} = \boldsymbol{v}^{(n)}./\mathrm{diag}(X * M^{(n)}/X)$$
    If $\left\|\boldsymbol{e}^{(n)}\right\| - \left\|\boldsymbol{e}^{(n-1)}\right\| < tol$
        Stop the iteration
    end
end
```

Also finds optimal stopping value for n

Ridge regression or smoothing splines

(see, e.g., [Kimeldorf & Wahba (1971)])

$$\min_{\boldsymbol{c}} \left\{ \boldsymbol{c}^T A \boldsymbol{c} + \gamma \sum_{j=1}^{N} \left(\mathcal{P}_f(\boldsymbol{x}_j) - f_j \right)^2 \right\},$$

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$$\left(A + \frac{1}{\gamma} I \right) \boldsymbol{c} = \boldsymbol{f}.$$

Just like before, so LOOCV error components given by

$$e_k = \frac{\left[\left(A + \frac{1}{\gamma} I \right)^{-1} \boldsymbol{f} \right]_k}{\left(A + \frac{1}{\gamma} I \right)^{-1}_{kk}}.$$

The "optimal" values of the shape parameter ε and the smoothing parameter γ are determined in a nested manner.
We now use a new cost function `CostEpsGamma`

Program (`CostEpsGamma.m`)

```
function ceg = CostEpsGamma(ep,gamma,r,rbf,rhs,ep)
A = rbf(ep,r);
A = A + eye(size(A))/gamma;
invA = pinv(A);
errorvector = (invA*rhs)./diag(invA);
ceg = norm(errorvector);
```

For a fixed initial ε we find the "optimal" γ followed by an optimization of `CostEpsGamma` over ε.
The algorithm terminates when the difference between to successive optimization runs is sufficiently small.

$N =$		9	25	81	289	1089
AMLS	RMSerr	4.80e-3	1.53e-3	6.42e-4	4.39e-4	2.48e-4
	ε	1.479865	1.268158	0.911530	0.652600	0.468866
	no. iter.	7	6	6	4	3
	time	0.2	0.4	1.0	5.7	254
Ridge	RMSerr	3.54e-3	1.62e-3	7.20e-4	4.57e-4	2.50e-4
	ε	2.083918	0.930143	0.704802	0.382683	0.181895
	γ	100.0	100.0	47.324909	26.614484	29.753487
	time	0.3	1.2	1.1	21.3	672

Table: Comparison of IAMLS and ridge regression using Gaussians for noisy data sampled at Halton points.

See [F. & Zhang (2007a)]

RBF-PS methods

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Instead of $A\boldsymbol{c} = \boldsymbol{f}$ with components of the cost vector determined by

$$e_k = \frac{c_k}{A^{-1}_{kk}}$$

we now have (due to the symmetry of A)

$$D = A_{\mathcal{L}} A^{-1} \quad \Longleftrightarrow \quad A D^T = (A_{\mathcal{L}})^T$$

RBF-PS methods

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Instead of $A\boldsymbol{c} = \boldsymbol{f}$ with components of the cost vector determined by

$$e_k = \frac{c_k}{A^{-1}_{kk}}$$

we now have (due to the symmetry of A)

$$D = A_{\mathcal{L}} A^{-1} \quad \Longleftrightarrow \quad AD^T = (A_{\mathcal{L}})^T$$

so that the components of the cost matrix are given by

$$E_{k\ell} = \frac{(D^T)_{k\ell}}{A^{-1}_{kk}}.$$

In MATLAB this can again be vectorized:

Program (CostEpsLRBF.m)

```
function ceps = CostEpsLRBF(ep,DM,rbf,Lrbf)
N = size(DM,2);
A = rbf(ep,DM);
rhs = Lrbf(ep,DM)';
invA = pinv(A);
errormatrix = (invA*rhs)./repmat(diag(invA),1,N);
ceps = norm(errormatrix(:));
```

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The function `Lrbf` creates the matrix $A_{\mathcal{L}}$. For the Gaussian RBF and the Laplacian differential operator this could look like

```
Lrbf = @(ep,r) 4*ep^2*exp(-(ep*r).^2).*((ep*r).^2-1);
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Remark

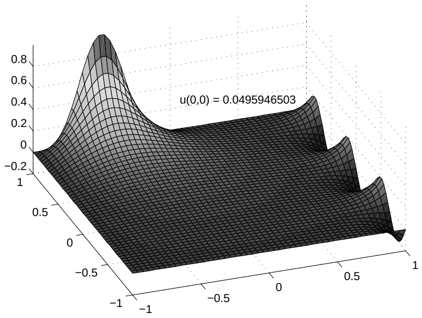
For differential operators of odd order one also needs difference matrices.

Example (2D Laplace equation, Program 36 of [Trefethen (2000)])

$$u_{xx} + u_{yy} = 0, \quad x, y \in (-1, 1)^2,$$

with piecewise defined boundary conditions

$$u(x,y) = \begin{cases} \sin^4(\pi x), & y = 1 \text{ and } -1 < x < 0, \\ \frac{1}{5}\sin(3\pi y), & x = 1, \\ 0, & \text{otherwise.} \end{cases}$$



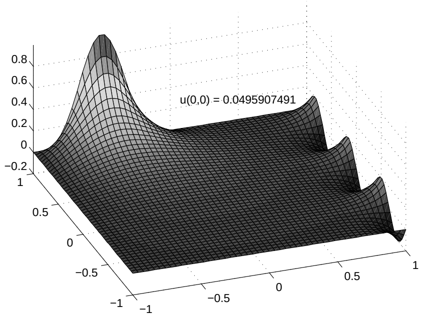


Figure: Solution of the Laplace equation using a Chebyshev PS approach (left) and cubic Matérn RBFs with $\varepsilon = 0.362752$ (right) with 625 collocation points.

Example (2D Helmholtz equation, Program 17 in [Trefethen (2000)])

$$u_{xx} + u_{yy} + k^2 u = f(x,y), \quad x, y \in (-1,1)^2,$$

with boundary condition $u = 0$ and

$$f(x,y) = \exp\left(-10\left[(y-1)^2 + (x-\frac{1}{2})^2\right]\right).$$

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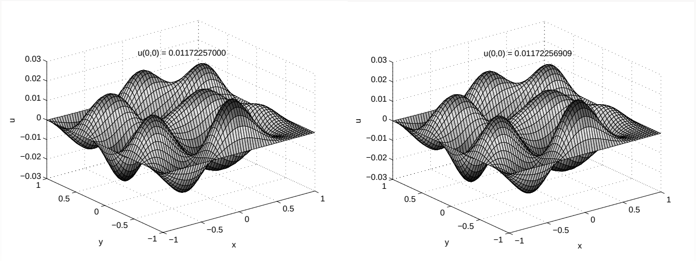


Figure: Solution of 2-D Helmholtz equation with 625 collocation points using the Chebyshev pseudospectral method (left) and Gaussians with $\varepsilon = 2.549243$ (right).

Example (Allen-Cahn equation, Program 35 in [Trefethen (2000)])

Most challenging for the RBF-PS method.

$$u_t = \mu u_{xx} + u - u^3, \qquad x \in (-1,1),\ t \geq 0,$$

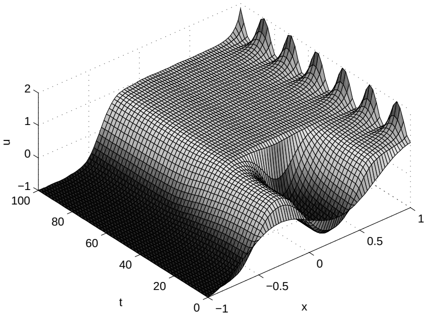
with parameter $\mu = 0.01$, initial condition

$$u(x,0) = 0.53x + 0.47\sin\left(-\frac{3}{2}\pi x\right), \qquad x \in [-1,1],$$

and non-homogeneous (time-dependent) boundary conditions

$$u(-1,t) = -1 \text{ and } u(1,t) = \sin^2(t/5).$$

The solution to this equation has three steady states ($u = -1, 0, 1$) with the two nonzero solutions being stable. The transition between these states is governed by the parameter μ.
The unstable state should vanish around $t = 30$.



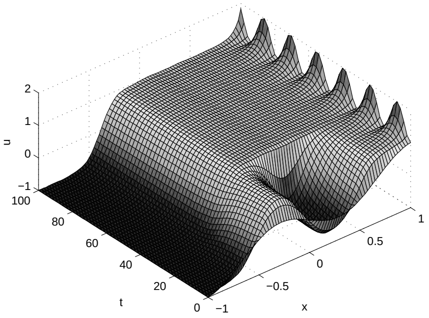


Figure: Solution of the Allen-Cahn equation using the Chebyshev pseudospectral method (left) and a cubic Matérn functions with $\varepsilon = 0.350920$ (right) with 21 Chebyshev points.

Summary

- Several applications of LOOCV:
  - RBF interpolation (with and without Riley),
  - IAMLS,
  - ridge regression,
  - RBF-PS
- Riley more efficient than `pinv`
- IAMLS method performs favorably when compared to ridge regression for noisy data (no dense linear systems solved)
- LOOCV algorithm for finding an “optimal” shape parameter for Kansa’s method in [Ferreira *et al.* (2007)]

Future work or work in progress:

- variable shape parameters (e.g., [Kansa & Carlson (1992), Fornberg and Zuev (2007)])
    - potential for improved accuracy and stability
    - challenging at the theoretical level
    - difficult multivariate optimization problem
- other criteria for “optimal” ε
    - compare Fourier transforms of kernels with data
    - maximum likelihood

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