Meshfree Approximation with MATLAB

Lecture III: Dealing with Ill-Conditioned RBF Systems

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Outline

Multivariate RBF Interpolation

Use data-dependent linear function space

$$\mathcal{P}_f(\boldsymbol{x}) = \sum_{j=1}^{N} c_j \Phi(\boldsymbol{x}, \boldsymbol{x}_j), \qquad \boldsymbol{x} \in \mathbb{R}^s$$

Here $\Phi : \mathbb{R}^s \times \mathbb{R}^s \to \mathbb{R}$ is strictly positive definite (reproducing) kernel

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To find c_j solve interpolation equations

$$\mathcal{P}_f(\boldsymbol{x}_i) = f(\boldsymbol{x}_i), \quad i = 1, \ldots, N$$

Leads to linear system $A\boldsymbol{c} = \boldsymbol{f}$ with symmetric positive definite — often ill-conditioned — system matrix

$$A_{ij} = \Phi(\boldsymbol{x}_i, \boldsymbol{x}_j), \quad i, j = 1, \ldots, N$$

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$$A\boldsymbol{c} = \boldsymbol{f}$$

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Standard textbook knowledge suggests:

1. Compute Cholesky factorization $A = LL^T$.
2. Solve the lower triangular system $L\boldsymbol{y} = \boldsymbol{f}$ for $\boldsymbol{y}$ by forward substitution.
3. Solve the upper triangular system $L^T\boldsymbol{c} = \boldsymbol{y}$ for $\boldsymbol{c}$ by back substitution.

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Problem: Doesn't work well if A is ill-conditioned.

The Basic Idea

Let P be a preconditioning matrix so that

$$\mathrm{cond}(PA) \ll \mathrm{cond}(A) \quad \text{or} \quad \mathrm{cond}(AP) \ll \mathrm{cond}(A)$$

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$$(PA)\boldsymbol{c} = P\boldsymbol{f} \Longleftrightarrow \boldsymbol{c} = (PA)^{-1}P\boldsymbol{f}$$

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$$(PA)\boldsymbol{c} = P\boldsymbol{f} \iff \boldsymbol{c} = (PA)^{-1}P\boldsymbol{f}$$

- Change only the left-hand-side (right preconditioning)

$$(AP)\widetilde{\boldsymbol{c}} = \boldsymbol{f} \iff \widetilde{\boldsymbol{c}} = (AP)^{-1}\boldsymbol{f} \qquad \widetilde{\boldsymbol{c}} = P^{-1}\boldsymbol{c}$$

We will use this approach

How to find *P*

- **Previous work on RBF preconditioning:**
  - Dyn and co-workers in the mid 1980s [Dyn (1987), Dyn *et al.* (1986)]: discretize associated differential operator (bi-Laplacian for TPSs)
  - more recent papers [Barba & Rossi (2008), Baxter (2002), Beatson *et al.* (1999), Brown *et al.* (2005), Ling & Kansa (2005)]: mostly with local approximate cardinal functions
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  - better basis of the approximation space [Beatson *et al.* (2000)]: use homogeneous kernel for TPSs
- **Our approach:**
  - use global approximate cardinal functions ([Zhang (2007)]) (related to polynomial preconditioners, e.g., [Dubois *et al.* (1979), Ashby *et al.* (1992)])

On polynomial preconditioners

From [Benzi (2002)]:

Preconditioning as a means of reducing the condition number in order to improve convergence of an iterative process seems to have been first considered by [Cesari (1937)]. Cesari's idea was to use a low degree polynomial $p(A)$ in A as a preconditioner for a Richardson-type iteration applied to the preconditioned system $p(A)A\boldsymbol{x} = p(A)\boldsymbol{b}$.

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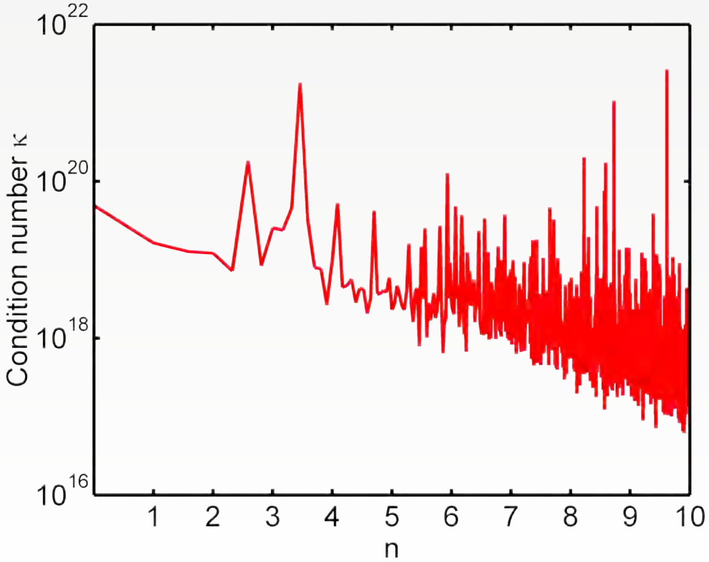
- Conclusion reported in [Ashby *et al.* (1992)]: $\deg(p) = 2$ "optimal"
- We may be providing new insight via acceleration

Condition number after $2^n - 1$ iterations



Theorem

Part I (without acceleration)

$$\mathcal{Q}_f^{(n)} = \boldsymbol{\Phi}^T \underbrace{\sum_{k=0}^{n} (I - A)^k}_{=P^{(n)}} \boldsymbol{f} =: \boldsymbol{\Phi}^{(n)T} \boldsymbol{f},$$

i.e., $\{\Phi^{(n)}(\cdot, \boldsymbol{x}_1), \ldots, \Phi^{(n)}(\cdot, \boldsymbol{x}_N)\}$ *provides new — approximately cardinal — basis for* $\mathrm{span}\{\Phi(\cdot, \boldsymbol{x}_1), \ldots, \Phi(\cdot, \boldsymbol{x}_N)\}$.

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Recursion for preconditioner

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

Right Preconditioning without Acceleration

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2. For $n = 1, 2, 3, \ldots$
$$P^{(n)} = I + P^{(n-1)}(I-A)$$
3. Solve $\left(AP^{(n)}\right)\boldsymbol{c} = \boldsymbol{f}$ for $\boldsymbol{c}$

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Evaluation on $\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_M\} \subset \mathbb{R}^s$:

$$\mathcal{P}_f(\boldsymbol{y}) = \left(BP^{(n)}\right)\boldsymbol{c}$$

with $B_{ij} = \Phi(\boldsymbol{y}_i, \boldsymbol{x}_j), \quad i = 1, \ldots, M, \; j = 1, \ldots, N.$

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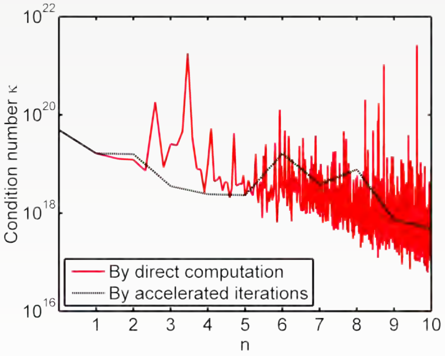

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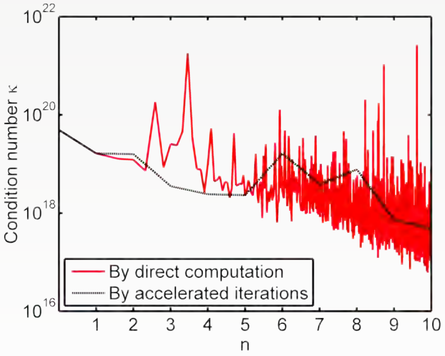

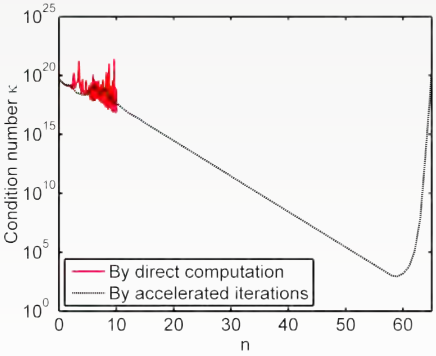

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Part II (with acceleration)

$$\widetilde{\mathcal{Q}}_f^{(n)} = \boldsymbol{\Phi}^T \underbrace{\left[\sum_{k=0}^{2^n-1} (I - A)^k\right]}_{=P^{(n)}} \boldsymbol{f} =: \boldsymbol{\Phi}^{(n)T} \boldsymbol{f},$$

i.e., $\{\Phi^{(n)}(\cdot, \boldsymbol{x}_1), \ldots, \Phi^{(n)}(\cdot, \boldsymbol{x}_N)\}$ *provides new — approximately cardinal — basis for* $\operatorname{span}\{\Phi(\cdot, \boldsymbol{x}_1), \ldots, \Phi(\cdot, \boldsymbol{x}_N)\}$.

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$$P^{(n+1)} = P^{(n)}\left[2I - AP^{(n)}\right], \qquad P^{(0)} = I.$$

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2. For $n = 1, 2, 3, \ldots$

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with $B_{ij} = \Phi(\boldsymbol{y}_i, \boldsymbol{x}_j), \quad i = 1, \ldots, M, \; j = 1, \ldots, N.$

Program (`IAMLSPrecond_sD.m`)

```
s = 2;  N = 289;  M = 500;  maxn = 50;
global rbf;  rbf_definition;  D = 2*s;
[dsites, N] = CreatePoints(N,s,'h');
ctrs = dsites;
epoints = CreatePoints(M,s,'r');
rhs = testfunctionsD(dsites);
h = 1/(nthroot(N,s)-1); ep = 1/(sqrt(D)*h);
DM_data = DistanceMatrix(dsites,ctrs);
IM = rbf(ep,DM_data)/(sqrt(pi*D)^s);
DM_eval = DistanceMatrix(epoints,ctrs);
EM = rbf(ep,DM_eval)/(sqrt(pi*D)^s);
P = eye(N);  AP = IM*P;
for n=1:maxn
    P = P*(2*eye(N)-AP);    AP = IM*P;
end
c = gmres(AP, rhs, [], 1e-10, 40);   % or use pcg
Pf = (EM*P) * c;
exact = testfunctionsD(epoints);
maxerr = norm(Pf-exact,inf)
rms_err = norm(Pf-exact)/sqrt(M)
```

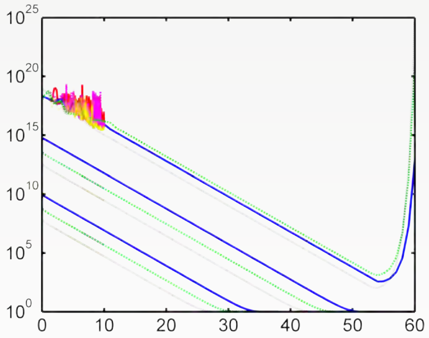
Comparison with [Beatson *et al.* (1999)]

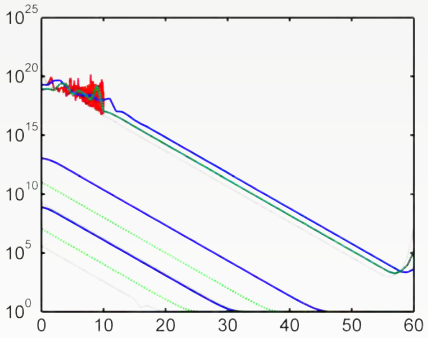
Cond. No.	289		1089		4225	
	no pre	pre	no pre	pre	no pre	pre
MQ BCM	1.506(8)	5.742(1)	2.154(9)	2.995(3)	3.734(10)	4.369(4)
TPS BCM	4.005(6)	3.330(0)	2.753(8)	1.411(2)	2.605(9)	2.025(3)
Gauss	8.796(9)	1.000(0)	6.849(10)	1.000(0)	7.632(10)	1.000(0)
IQ	1.186(8)	1.000(0)	4.284(8)	1.000(0)	1.082(9)	1.000(0)

No.	289		1089		4225	
GMRES iter.	no pre	pre	no pre	pre	no pre	pre
MQ BCM	145	8	>150	15	>150	28
TPS BCM	103	5	145	6	>150	9
Gauss	>150	2	>150	2	>150	2
IQ	>150	2	>150	2	>150	2

2D Halton points, $n = 40$, $\varepsilon_G = 6.4, 12.8, 25.6$, $\varepsilon_I = 3.2, 6.4, 12.8$

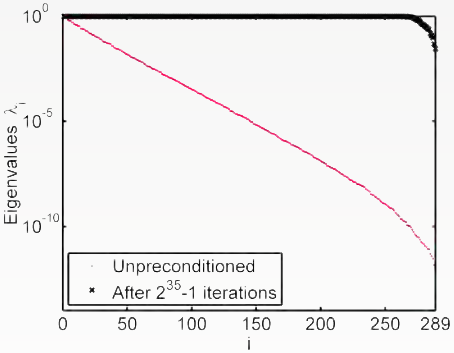
Condition number drop

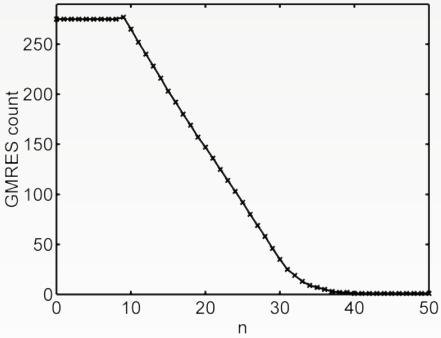




Laguerre-Gaussians (left, with $\varepsilon = 3.2, 4.8, 6.4$) and generalized IMQs (right, with $\varepsilon = 0.204, 2.04, 3.06$) for $d = 0, 1, 2$ and $N = 289$ Halton points

Eigenvalue distribution & GMRES convergence





Gaussian with $\varepsilon = 5.95$ and $N = 289$ Halton points

Summary of IAMLS Preconditioning

- Current implementation too slow to be useful (matrix-matrix product)
- Preconditioning with accelerated iterated AMLS very effective for “good” (i.e., reasonably conditioned) problems
- Preconditioner does not perform well for “bad” problems (cond(AP) can be made small, but P itself becomes ill-conditioned, so that evaluation unreliable)
- Automatic stopping criterion in [F. & Zhang (2008)]
- Accelerated iterated AMLS (as well as SVD) may be used to approximately solve “bad” problems or problems with noise
- Generalized inverse MQs and Laguerre-Gaussians seem to behave similarly

Our Latest Approach — Riley's Algorithm [Riley (1955)]

Instead of solving the ill-conditioned system

$$A\boldsymbol{x} = \boldsymbol{b}$$

we regularize, i.e., let

$$C = A + \mu I$$

and solve

$$C\boldsymbol{y} = \boldsymbol{b}.$$

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But this is not the end of Riley's algorithm.

Since $A = C - \mu I$ we can derive

$$A^{-1} = \frac{1}{\mu} \sum_{k=1}^{\infty} \left(\mu C^{-1}\right)^k \tag{1}$$

and therefore we get the solution to the original system as

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\end{aligned}$$

So

$$\boldsymbol{x}_{k+1} = \boldsymbol{y} + \mu C^{-1}\boldsymbol{x}_k, \qquad k = 0, 1, 2, \ldots, \qquad \boldsymbol{x}_0 = \boldsymbol{0} \qquad (2)$$

Alternative version of Riley's Algorithm

From above

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Compute product iteratively:

$$\begin{aligned} \boldsymbol{x}_0 &= \boldsymbol{0} \\ \boldsymbol{y}_0 &= C^{-1}\boldsymbol{b} \\ \boldsymbol{y}_{k+1} &= \mu C^{-1}\boldsymbol{y}_{k-1} \\ \boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + \boldsymbol{y}_k, \qquad k = 0, 1, 2, \ldots \end{aligned}$$

This is our main version of Riley's algorithm

Riley’s Algorithm in MATLAB

```
function x = Riley(A,b,mu)
    C = A + mu*eye(size(A));
    L = chol(C,'lower');
    z = L\b;
    y = L'\z;
    x = y;
    for k = 1:kend
        z = mu*(L\y);
        y = L'\z;
        x = x + y;
    end
end
```

Another Interpretation of Riley's Algorithm

Let $C = A + \mu I$ as before. Then

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Now split A and iterate

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where $\boldsymbol{x}_0 = \boldsymbol{0}$.

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This corresponds to

$$\boldsymbol{x}_{k+1} = \boldsymbol{y} + \mu C^{-1}\boldsymbol{x}_k, \qquad k = 0, 1, 2, \ldots, \quad \boldsymbol{x}_0 = \boldsymbol{0},\ \boldsymbol{y} = C^{-1}\boldsymbol{b}$$

which is the same as (2).

[Golub (1965)] showed this is equivalent to iterative improvement (see [Kincaid and Cheney (2002)]):

$$C\boldsymbol{e} = \boldsymbol{b} - A\boldsymbol{x}_k \tag{4}$$

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \boldsymbol{e} \tag{5}$$

also with $\boldsymbol{x}_0 = \boldsymbol{0}$.

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Verification of equivalence

$$\begin{aligned} C\boldsymbol{x}_{k+1} &\overset{(5)}{=} C\boldsymbol{x}_k + C\boldsymbol{e} \\ &\overset{(4)}{=} C\boldsymbol{x}_k + \boldsymbol{b} - A\boldsymbol{x}_k \end{aligned}$$

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$$\begin{aligned} C\boldsymbol{e} &= \boldsymbol{b} - A\boldsymbol{x}_k & (4) \\ \boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + \boldsymbol{e} & (5) \end{aligned}$$

also with $\boldsymbol{x}_0 = \boldsymbol{0}$.

Verification of equivalence

$$\begin{aligned} C\boldsymbol{x}_{k+1} &\overset{(5)}{=} C\boldsymbol{x}_k + C\boldsymbol{e} \\ &\overset{(4)}{=} C\boldsymbol{x}_k + \boldsymbol{b} - A\boldsymbol{x}_k \\ &\overset{C=A+\mu I}{=} \boldsymbol{b} + \mu I\boldsymbol{x}_k \end{aligned}$$

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Remark

[Neumaier (1998)] calls this method iterated Tikhonov regularization or preconditioned Landweber iteration (but attributes it to [Riley (1955)]).

Iterative Improvement Version of Riley's Algorithm in MATLAB

```
function x = Riley_Residuals(A,b,mu)
    C = A + mu*eye(size(A));
    L = chol(C,'lower');
    z = L\b;
    x = L'\z;
    for k=1:kend
        z = L\(b - A*x);
        x = x + L'\z;
    end
end
```

Major problem with Tikhonov regularization:

How should we choose μ?

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Usual approach: cross validation or maximum likelihood

Practical suggestion in [Riley (1955)]: choose μ small, i.e.,

$$\mu \approx 10^{-p+\alpha},$$

where p is desired precision, and $\alpha = 2$ or 3.

Convergence of the algorithm

The eigenvalues of μC^{-1} are $0 < \frac{\mu}{\lambda_i+\mu} < 1$, so the series

$$\boldsymbol{x} = \sum_{k=0}^{\infty} \left(\mu C^{-1}\right)^k \boldsymbol{y}$$

converges.

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The matrix C is better conditioned than A since

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Summary:

μ needs to be

- large enough to improve conditioning
- small enough to provide fast convergence

Recommended to use $\mu \approx \lambda_{\min}$ (we use $\mu = 10^{-11}$ when $\lambda_{\min} \approx 10^{-17}$)

SVD solution of $A\boldsymbol{x} = \boldsymbol{b}$:

$$\boldsymbol{x} = \sum_{j=1}^{r} \frac{\beta_j}{\sigma_j} \boldsymbol{v}_j,$$

where $A = U\Sigma V^T$ and $\beta = U^T\boldsymbol{b}$

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Riley:

$$\boldsymbol{x}_k = \sum_{j=1}^{r} \left[1 - \left(\frac{\mu}{\mu + \sigma_j}\right)^k\right] \frac{\beta_j}{\sigma_j} \boldsymbol{v}_j,$$

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- regularize by iteration (i.e., damping each mode)

Another look at the regularization parameters

Riley iteration: $$\boldsymbol{x}_k = \sum_{j=1}^{r} \left[1 - \left(\frac{\mu}{\mu + \sigma_j} \right)^k \right] \frac{\beta_j}{\sigma_j} \boldsymbol{v}_j$$

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Note: $1 - \left(\frac{\mu}{\mu+\sigma_j}\right)^k$, $j < r$ is even closer to 1

Obtaining a Stable Basis via SVD

Consider a stacked interpolation and evaluation system:

$$\begin{bmatrix} A \\ B \end{bmatrix} \boldsymbol{c} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{s} \end{bmatrix}$$

with $A_{ij} = \Phi(\boldsymbol{x}_i, \boldsymbol{x}_j)$, and $B_{kj} = \Phi(\boldsymbol{y}_k, \boldsymbol{x}_j)$, where $\boldsymbol{x}_i$ are centers = data sites, $\boldsymbol{y}_k$ are evaluation points

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$$\begin{aligned} \boldsymbol{s} &= B\boldsymbol{c} = U(\mathrm{N}{+}1{:}\mathrm{end}, 1{:}\mathrm{r})\boldsymbol{d} \\ &= U(\mathrm{N}{+}1{:}\mathrm{end}, 1{:}\mathrm{r})U^{\dagger}(1{:}\mathrm{N}, 1{:}\mathrm{r})\boldsymbol{f} \end{aligned}$$

The following quotes from [Golub (1965)] lead up to Riley's algorithm:

> . . . *results of an extensive calculation. The matrix consists of the first 5 columns of the inverse of the* 6×6 *Hilbert matrix.*

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The following quotes from [Golub (1965)] lead up to Riley's algorithm:

> *. . . results of an extensive calculation. The matrix consists of the first 5 columns of the inverse of the* 6×6 *Hilbert matrix.*
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> *For many problems, even with the use of orthogonal transformations it may be impossible to obtain an accurate solution.*

From the MathSciNet review of [Golub (1965)]:

> *This essentially consists in a more effective implementation of J. D. Riley's algorithm.*

In our experiments with $N = 900$ (either equally spaced or Halton) and $\mu = 10^{-11}$ we get

$$\frac{\mathrm{cond}(A)}{\mathrm{cond}(C)} \approx 10^6 - 10^8$$

for our ill-conditioned problems (i.e., with $\mathrm{cond}(A) \approx 10^{20}$).

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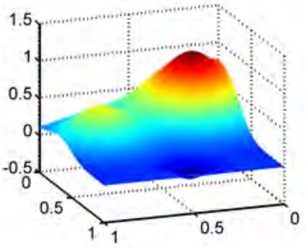
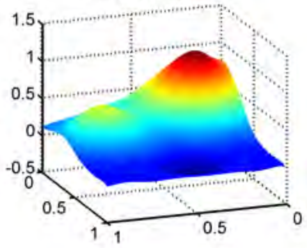
The timing for the Riley algorithm is only about 5% slower than standard `backslash` solver — and two orders of magnitude more accurate!

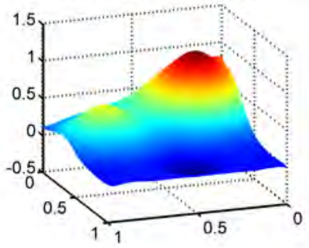
Franke test function



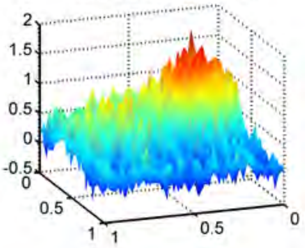
Riley approximation



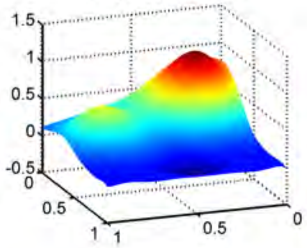
POD-SVD approximation



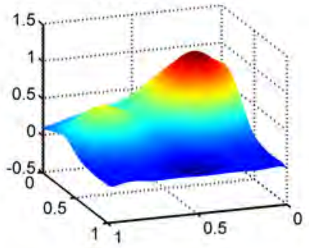
Standard approximation

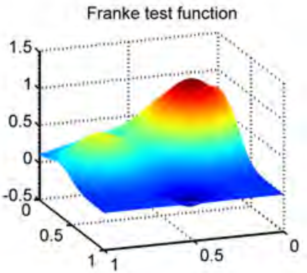


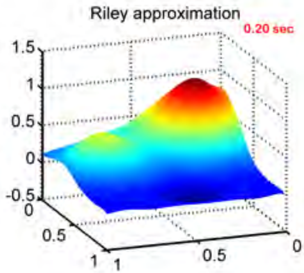
Riley2 approximation

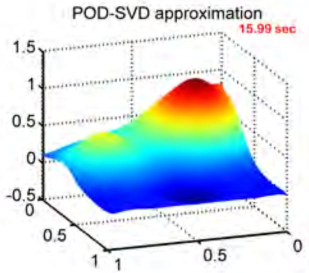


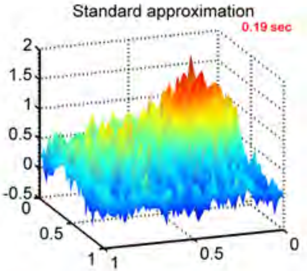
SVD approximation

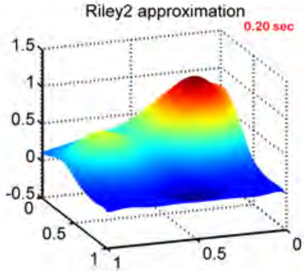


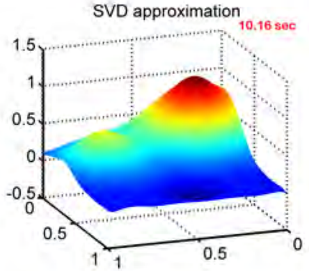

Franke test function
1.5
1
0.5
0
-0.5
0
0.5
1
1
0.5
0

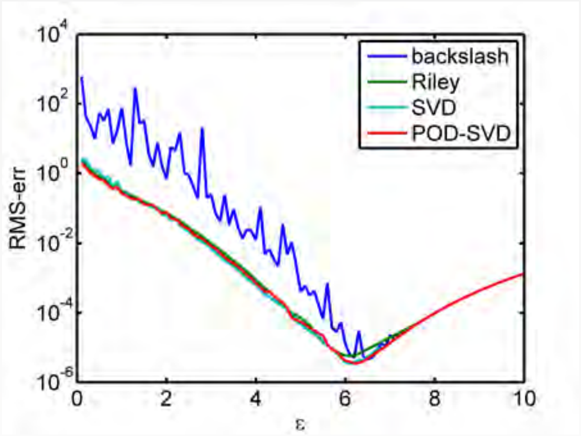

Riley approximation
0.20 sec
1.5
1
0.5
0
-0.5
0
0.5
1
1
0.5
0


POD-SVD approximation
15.99 sec
1.5
1
0.5
0
-0.5
0
0.5
1
1
0.5
0


Standard approximation
0.19 sec
2
1.5
1
0.5
0
-0.5
0
0.5
1
1
0.5
0

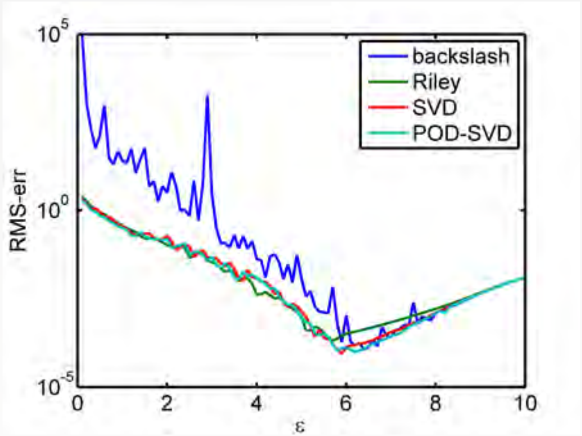

Riley2 approximation
0.20 sec
1.5
1
0.5
0
-0.5
0
0.5
1
1
0.5
0


SVD approximation
10.16 sec
1.5
1
0.5
0
-0.5
0
0.5
1
1
0.5
0



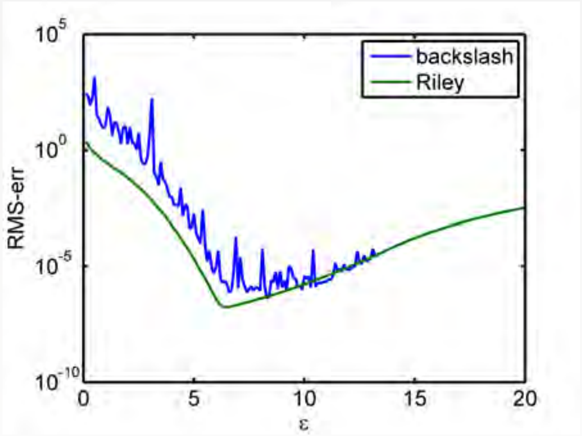
Method	backslash	Riley	SVD	POD-SVD
Time (sec)	24.1	26.0	710.0	1417.8

Table: Execution times for solution of 100 linear systems of size 900×900 (gridded data).



Method	backslash	Riley	SVD	POD-SVD
Time (sec)	24.0	26.7	739.1	1693.1

Table: Execution times for solution of 100 linear systems of size 900 $\times$ 900 (irregular data).



Method	backslash	Riley
Time (sec)	401.2	429.8

Table: Execution times for solution of 200 linear systems of size 2500×2500 (gridded data).

Summary

- Riley's paper seems largely forgotten/ignored
- Riley's algorithm seems to be superior to truncated SVD for ill-conditioned symmetric positive definite systems
- Riley's algorithm can be extended to
  - arbitrary (indefinite) square linear systems (use QR factorization of $C = A + \mu I$)
  - arbitrary non-square linear systems (use normal equations, and QR factorization of $C = A^T A + \mu I$)
  - sparse systems together with sparse Cholesky factorization (fast approximate sparse SVD)
- Riley's algorithm can be accelerated (e.g., by Aitken's method) — not yet done
- Need a strategy to find "optimal" regularization parameter μ

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