Solving Ill-Posed Cauchy Problems in Three Space Dimensions using Krylov Methods

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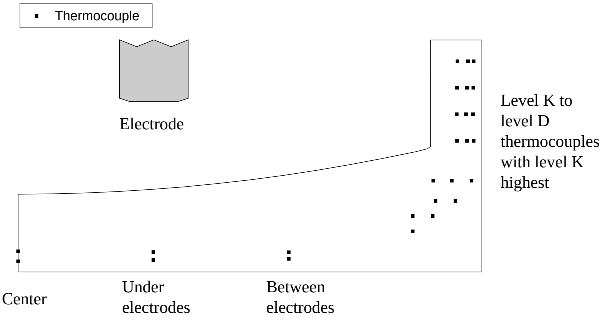
Motivating example: Ilmenite iron melting furnace

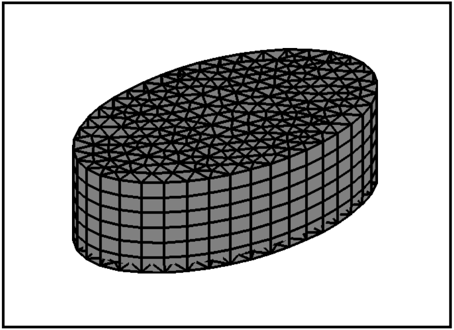


The furnace material properties are temperature dependent.
Problem: find the inner shape of the furnace.
Nonlinear, and (rather) complex geometry

PhD thesis: I M Skaar, Monitoring the Lining of a Melting Furnace, NTNU, Trondheim, 2001

Inverse Heat Conduction Problem

Steady state heat conduction problem:



The upper boundary is unavailable for measurements

3D problem!

See also Egger et al., Inverse Problems, 2009

Outline

1. Cauchy Problem
   - Regularization
   - Error Estimate
2. Rational Krylov method
   - Krylov/Regularization
3. Numerical Examples
   - Example 1
   - Animation
   - Example 2
4. Conclusions
   - Future work

Ill-Posed Cauchy Problem

Ω: connected in $\mathbb{R}^2$ with smooth boundary $\partial\Omega$
L: linear, self-adjoint, positive definite elliptic in Ω.

$$\begin{aligned}
u_{zz} - Lu &= 0, && (x,y) \in \Omega, \quad z \in [0, z_1], \\
u(x,y,z) &= 0, && (x,y) \in \partial\Omega, \quad z \in [0, z_1], \\
u(x,y,0) &= g(x,y), && (x,y) \in \Omega, \\
u_z(x,y,0) &= 0, && (x,y) \in \Omega.
\end{aligned}$$

Sought: $f(x,y) = u(x,y,z_1)$, $(x,y) \in \Omega$.

Formal solution

$u(x,y,z) = \cosh(z\sqrt{L})g$

BUT: L is a pos. def. unbounded operator $\Rightarrow$ ILL-POSED!

Standard Iterative Procedure

Guess $f^{(1)}$

1. for $k = 1, 2, \ldots$ until convergence
    1. Solve

$$\begin{aligned} u_{zz} - Lu &= 0, & (x,y) \in \Omega, \quad & z \in [0, z_1], \\ u(x,y,z) &= 0, & (x,y) \in \partial\Omega, \quad & z \in [0, z_1], \\ u(x,y,z_1) &= f^{(k)}, & (x,y) \in \Omega, & \\ u_z(x,y,0) &= 0, & (x,y) \in \Omega. & \end{aligned}$$

       giving $u^{(k)}$
    2. Evaluate $\|g(\cdot,\cdot) - u^{(k)}(\cdot,\cdot,0)\|$ and adjust $f^{(k)} \longrightarrow f^{(k+1)}$

In every iteration: Solve a 3D well-posed problem
Often slow convergence.

Other possible methods?

- Tikhonov regularization?
  Impossible, because we do not know the integral operator for equations with variable coefficients and/or complicated geometry.
- Replace unbounded L by a bounded approximation?
  Possible in connection with finite difference approximation, but more difficult with finite elements.
  BUT: Krylov method!

Regularization

Formal solution

$u(x, y, z) = \cosh(z\sqrt{L})g$

BUT: L is a pos. def. unbounded operator $\Rightarrow$ ILL-POSED!

High frequency perturbations in g are blown up

Regularization

Replace unbounded operator by a bounded one!

Cut Off High Frequencies

Eigenvalues of L: $\lambda_j^2, j = 1, 2, \ldots$ and $\lambda_j \to +\infty$ as $j \to \infty$

General approach: Compute the k eigenvalues of smallest modulus:

$$LX_k = X_k D_k,$$

where X_k holds orthonormal eigenvectors

Approximate by projection

$$\cosh(z\sqrt{L})g \approx \cosh(z\sqrt{L})X_k X_k^\top g = X_k \cosh(z\sqrt{D_k})X_k^\top g$$

Eigenvalues of L

L is *large and sparse* (of the order $10^4 - 10^5$, say)

Compute the smallest eigenvalues

$$\Downarrow$$

Operate with L^{-1}

$$\Downarrow$$

Solve many standard 2D elliptic problems

$$-Lw = v$$

Error Estimate

$L_2(\Omega)$ setting, u is an "exact solution"
v is an approximate solution with perturbed data g_m

Theorem

Assume that $\|u(\cdot,\cdot,1)\| \leq M$ and that the data perturbation satisfies $\|g - g_m\| \leq \epsilon$. Then if v is computed by projection using the eigenvalues satisfying $\lambda_j \leq \lambda_c$, where

$$\lambda_c = (1/z_1)\log(M/\epsilon)$$

then

$$\|u(\cdot,\cdot,z) - v(\cdot,\cdot,z)\| \leq 3\epsilon^{1-z/z_1} M^{z/z_1}, \qquad 0 \leq z \leq z_1.$$

Optimal error bound

Eigenvalue method

- Is it necessary to compute the eigenvalues and eigenvectors accurately?
- Do we need all the information that we get in the eigenvalues?
- Can we take advantage of the fact that we want to compute an approximation of

$$\cosh(z\sqrt{L})g$$

for this particular vector?

Eigenvalue method

- Is it necessary to compute the eigenvalues and eigenvectors accurately? NO!
- Do we need all the information that we get in the eigenvalues? NO!
- Can we take advantage of the fact that we want to compute an approximation of

$$\cosh(z\sqrt{L})g$$

  for this particular vector? YES!

Lanczos tridiagonalization

Choose q_1 and iterate

$$L^{-1}q_k = q_{k-1}\beta_{k-1} + q_k\alpha_k + q_{k+1}\beta_k, \quad k = 1, 2, \ldots,$$

with $\alpha_k = q_k^\top L^{-1}q_k$ and $\beta_k = q_{k+1}^\top L^{-1}q_k$;

One matrix-vector multiply $L^{-1}q_k$ per step

One standard 2D elliptic solve (black box) per step

$$-Lw = q_k$$

Lanczos properties

- Initial convergence influenced by starting vector v_1. Choose $q_1 = 1/\beta \, g_m, \quad \beta = \|g_m\|$
- Faster for largest eigenvalues of L^{-1} $\Rightarrow$ Fast convergence for some of the smallest eigenvalues of L
- Optional: To get faster convergence for eigenvalues in $[0, \lambda_c]$ operate with $(L - \tau I)^{-1}$, where $\tau = \lambda_c/2$

Lanczos reduction

$$L^{-1}Q_k = Q_k T_k + \beta_{k+1} q_{k+1} e_{k+1}^\top \approx Q_k T_k$$

Approximation

$$\cosh(z\sqrt{L})g \approx Q_k \cosh(zT_k^{-1/2})Q_k^\top g$$

Problem: We cannot prevent T_k from approximating large eigenvalues!

Solution: Regularize T_k: cut off large eigenvalues[1]

[1] Krylov+regularization: O'Leary & Simmons (1981), Björck, Grimme & Van Dooren (1994)

Projected and Truncated Approximation

Let

$$((\theta_j^{(k)})^2, y_j^{(k)}), j = 1, \ldots, k$$

be the eigenpairs of T_k^{-1}

Define $F(z, \lambda) = \cosh(z\lambda^{1/2})$ and $S_k = T_k^{-1}$

Truncated approximation:

$$\begin{aligned} v_k(z) &= Q_k F(z, S_k^c) Q_k^\top g_m \\ &:= Q_k \sum_{\theta_j^{(k)} \leq \lambda_c} y_j^{(k)} \cosh(z\theta_j^{(k)})(y_j^{(k)})^\top e_1 \|g_m\|. \end{aligned}$$

Error Estimate

Recall $F(z,\lambda) = \cosh(z\lambda^{1/2})$ and $S_k = T_k^{-1}$

Theorem

Let u be the "exact solution" and

$$v_k(z) = Q_k F(z, S_k^c) Q_k^\top g_m$$

Under the same hypotheses as earlier,

$$\begin{aligned} \|u(z) - v_k(z)\| &\leq 3\epsilon^{1-z/z_1} M^{z/z_1} \\ &+ 2\|[F(z, L^c) - Q_k F(z, S_k^c) Q_k^\top] g\|. \end{aligned}$$

Krylov/Regularization, First version

- Starting vector $q_1 = 1/\beta\, g_m$
- **for** $k = 2, 3, \ldots$ **until "stable"**
  - $[Q_k, T_k] = \mathtt{krylovstep}(L^{-1}, Q_{k-1}, T_{k-1})$
  - Compute $v_k(z) = Q_k F(z, S_k^c) Q_k^\top g_m$
- **end**
- Check residual $\|Kv_k - g_m\| < \epsilon$

Kv_k is the solution of the 3D problem with $u = v_k$ at the upper boundary and $u_z = 0$ at the lower. Expensive!

Residual: $\|Kv_k - g_m\| < \epsilon$

Solve 3D problem (denote solution u_k)

$$
\begin{aligned}
u_{zz} - Lu &= 0, \qquad (x,y) \in \Omega, \quad z \in [0, z_1], \\
u(x,y,z) &= 0, \qquad (x,y) \in \partial\Omega, \quad z \in [0, z_1], \\
u(x,y,1) &= v_k(x,y), \qquad (x,y) \in \Omega, \\
u_z(x,y,0) &= 0, \qquad (x,y) \in \Omega.
\end{aligned}
$$

Well-posed but expensive!

$$Kv_k = u_k(x,y,0)$$

We only want to compute this when we are sure that $\|Kv_k - g_m\| < \epsilon$

Krylov/Regularization: "stable"

- Starting vector $q_1 = 1/\beta\, g_m$
- **for** $k = 1, 2, \ldots$ **until "stable"**
  - $[Q_k, T_k] = \texttt{krylovstep}(L^{-1}, Q_{k-1}, T_{k-1})$
  - Compute $v_k(z) = Q_k F(z, S_k^c) Q_k^\top g_m$
- **end**
- Check residual $\|K v_k - g_m\| < \epsilon$

How can we quantify "stable"?

Recall $F(z,\lambda) = \cosh(z\lambda^{1/2})$ and $S_k = T_k^{-1}$

Cheap (2D) approximate residual: $r_k^{(k+p)}$

- Starting vector $q_1 = 1/\beta\, g_m$
- **for** $k = 1, 2, \ldots$ **maxit**
    - $[Q_k, T_k] = \mathtt{krylovstep}(L^{-1}, Q_{k-1}, T_{k-1})$
    - Compute $w_k(z) = F(z, S_k^c) Q_k^\top g_m$
    - **if** $\left| \|r_k^{(k+p)}\| - \|r_{k-1}^{(k-1+p)}\| \right| / \|r_k^{(k+p)}\| < tol$ **then**
        - **if** $\|Kv_k - g_m\| < \epsilon$ **then stop iterating**
    - **endif**
- **end**
- Compute $v_k = Q_k w_k$

Test example 1: Laplace equation

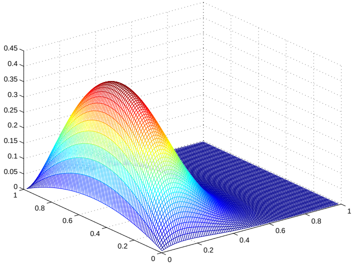
Ω: unit square

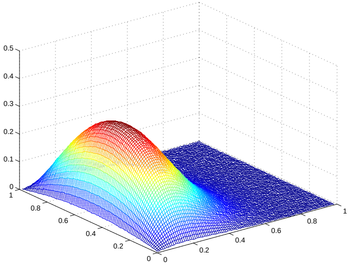
$$\begin{aligned} u_{zz} + \Delta u &= 0, \qquad (x,y,z) \in \Omega \times [0, 0.1], \\ u(x,y,z) &= 0, \qquad (x,y,z) \in \partial\Omega \times [0, 0.1], \\ u(x,y,0) &= g(x,y), \qquad (x,y) \in \Omega, \\ u_z(x,y,0) &= 0, \qquad (x,y) \in \Omega. \end{aligned}$$

Determine the values at the upper boundary,
$f(x,y) = u(x,y,0.1)$, $(x,y) \in \Omega$.

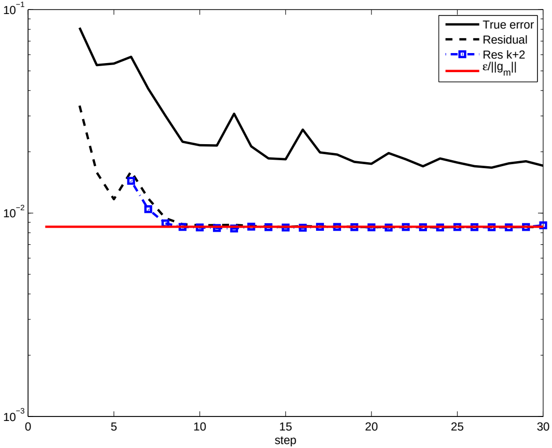
Data perturbation: $\|g - g_m\| / \|g\| \approx 0.0085$
98 eigenvalues are smaller than the tolerance
`eigs` performs approximately 300 2D elliptic solves.

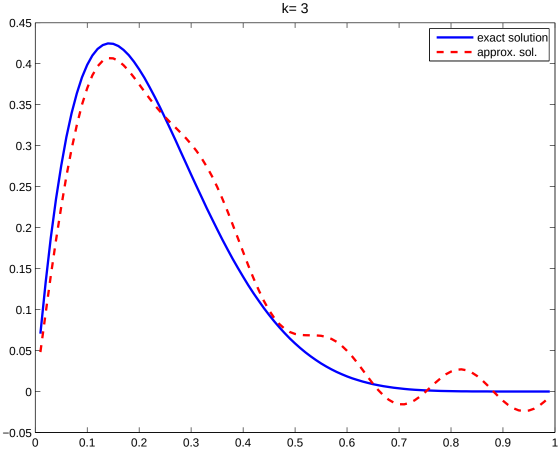
Solution and Exact Data



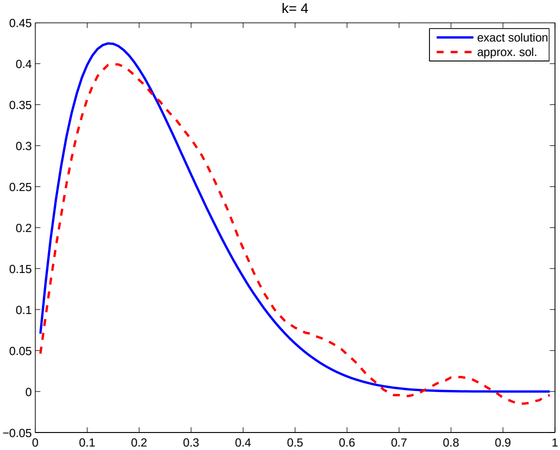


Convergence History ($0.8\lambda_c$)




k= 3
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
−0.05
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
exact solution
approx. sol.

Solutions as function of iteration index



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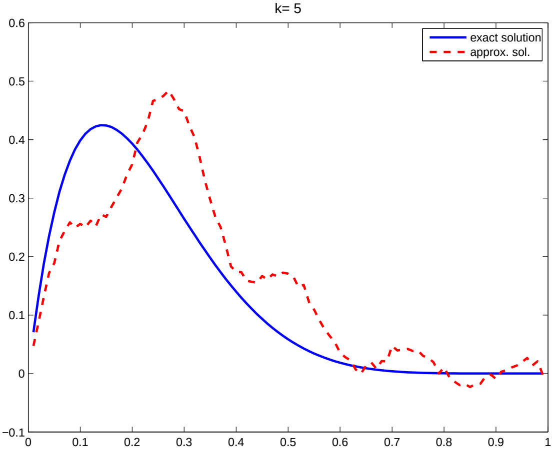

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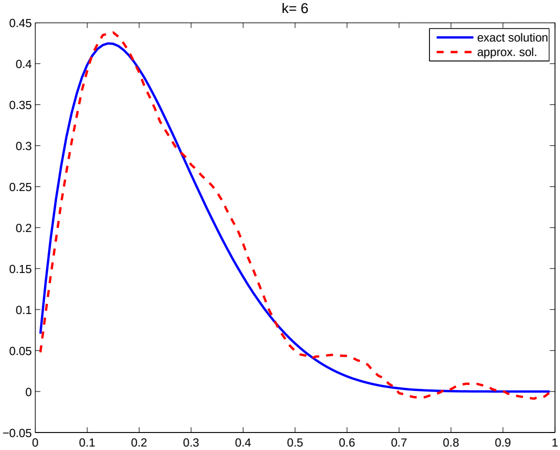

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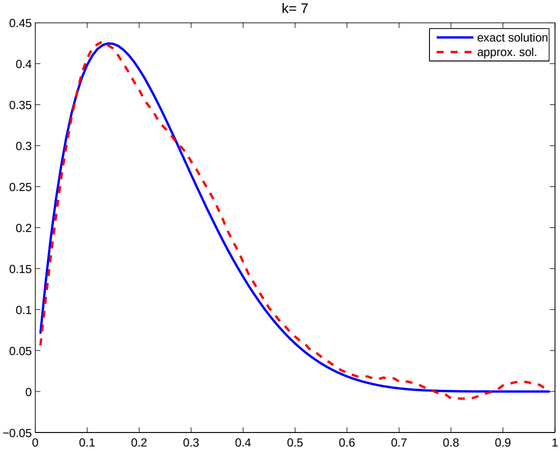

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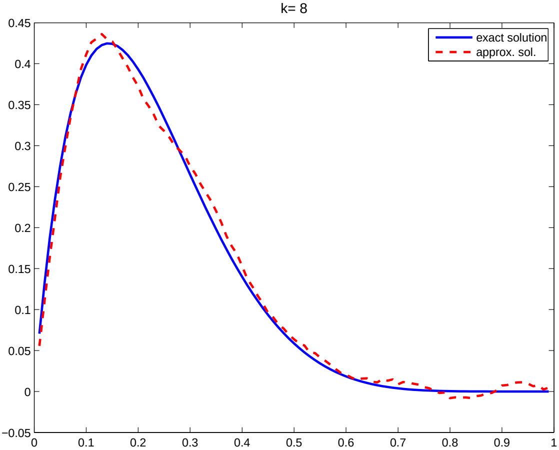

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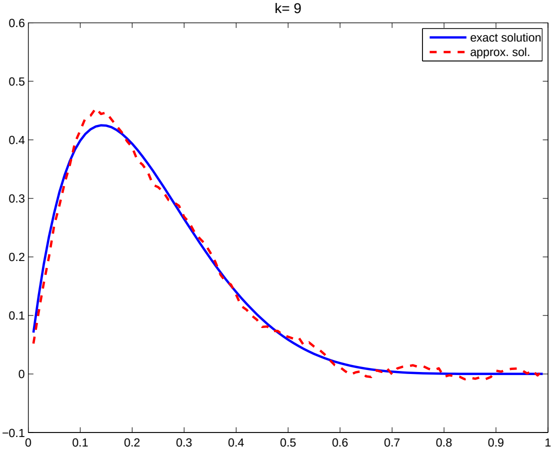

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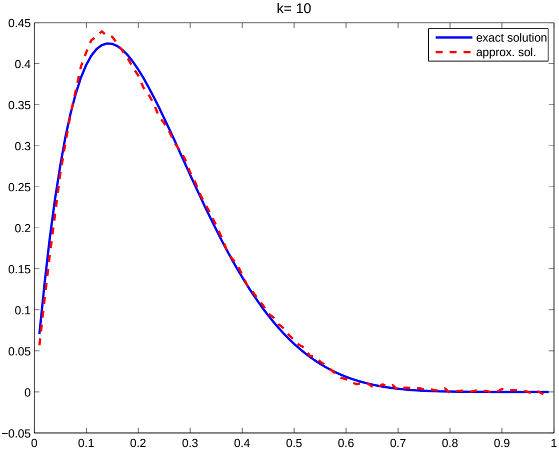

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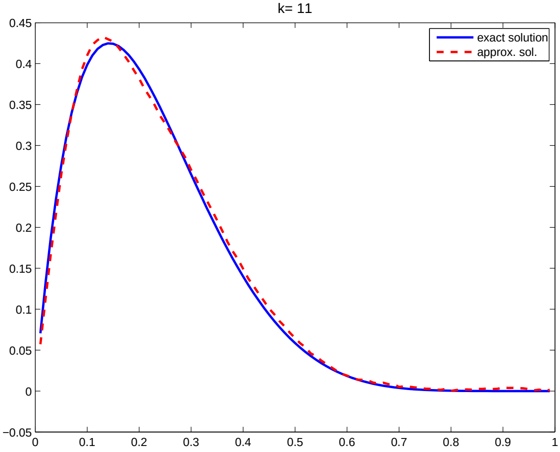

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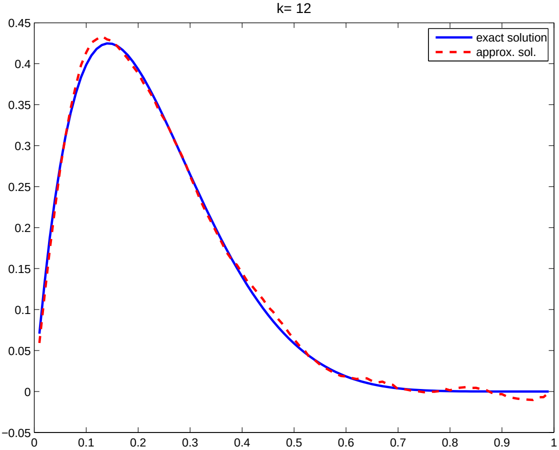

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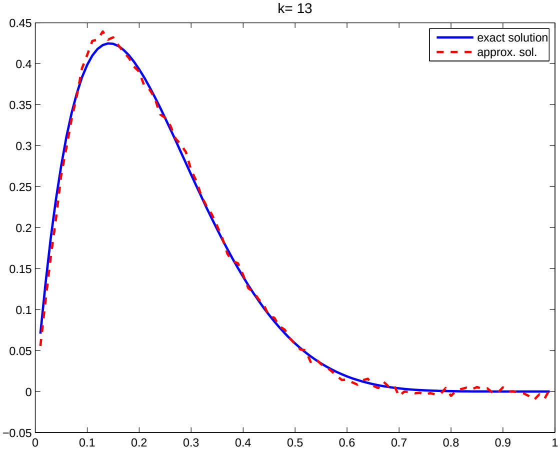

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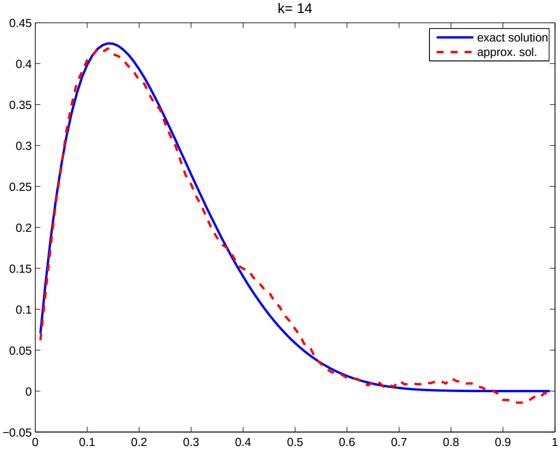

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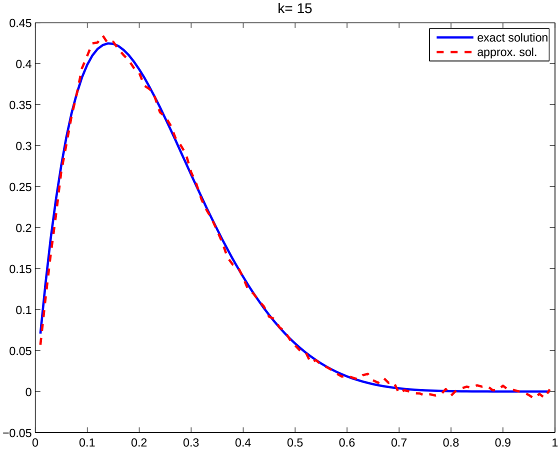

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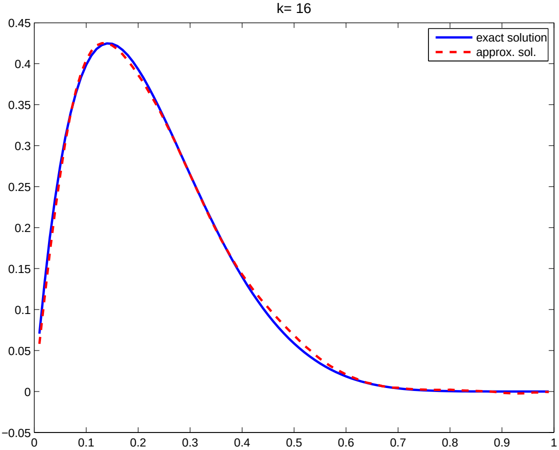

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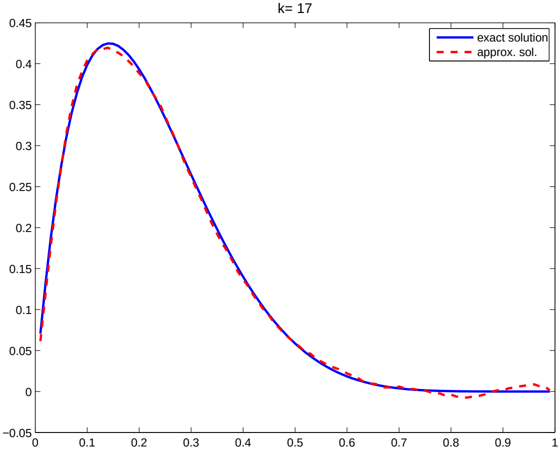

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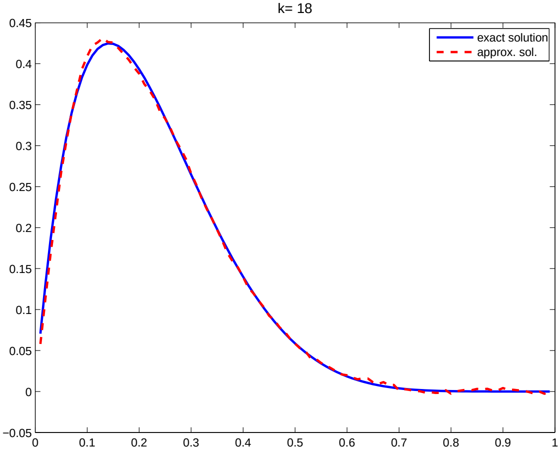

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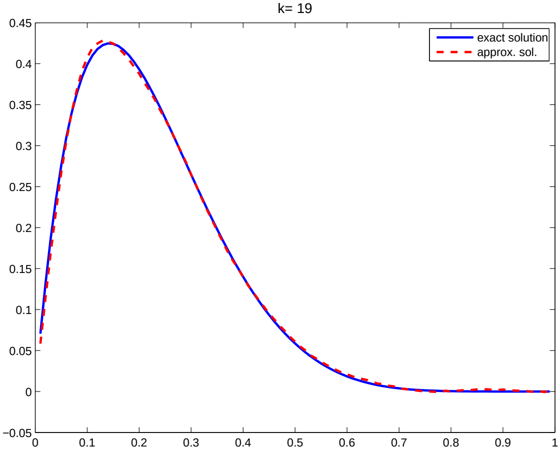

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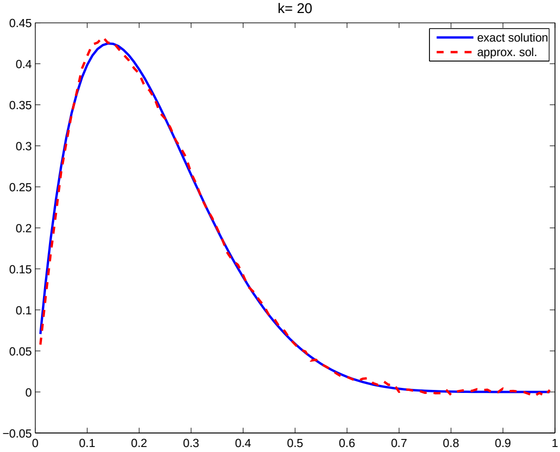

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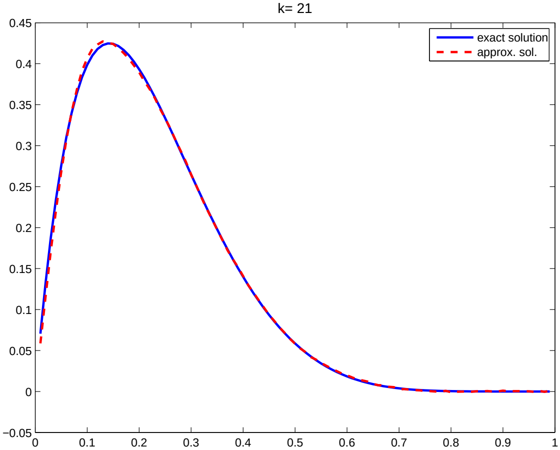

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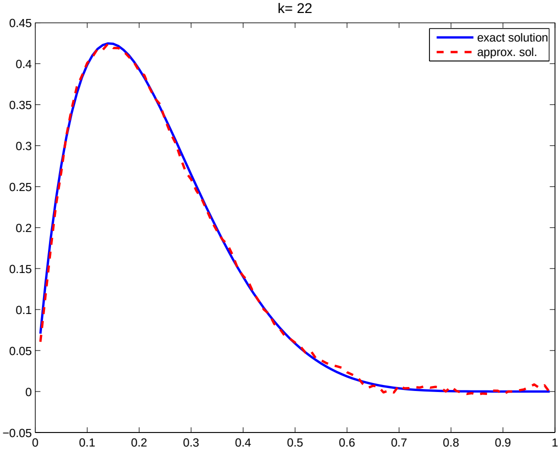

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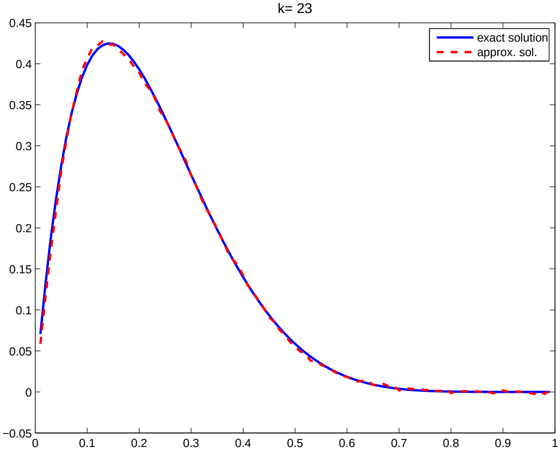

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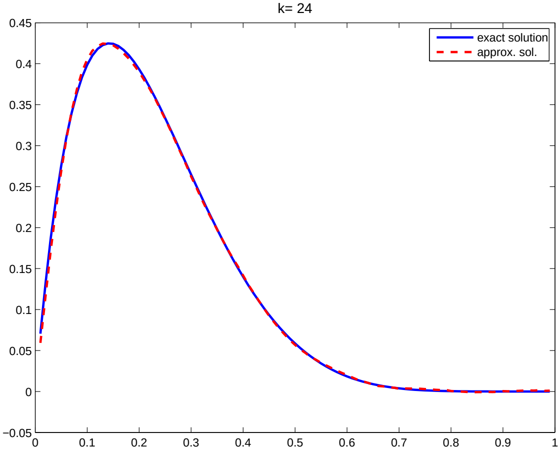
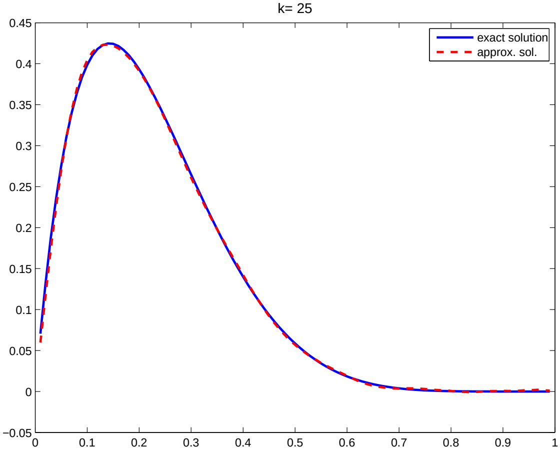


Stopping criterion satisfied here



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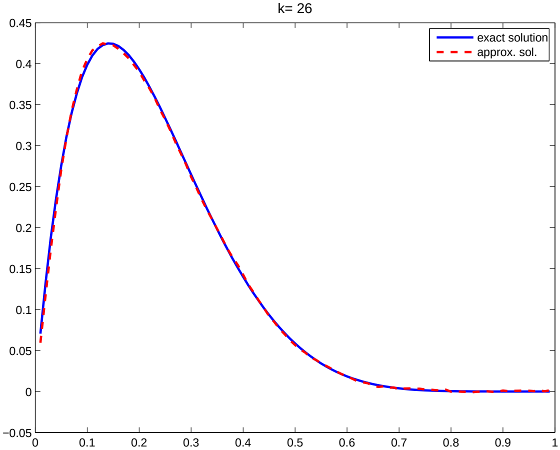

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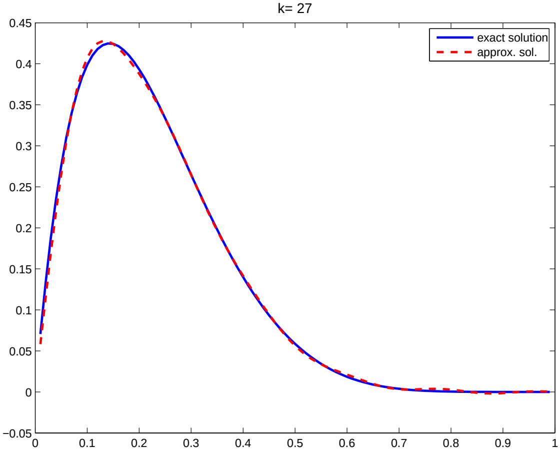

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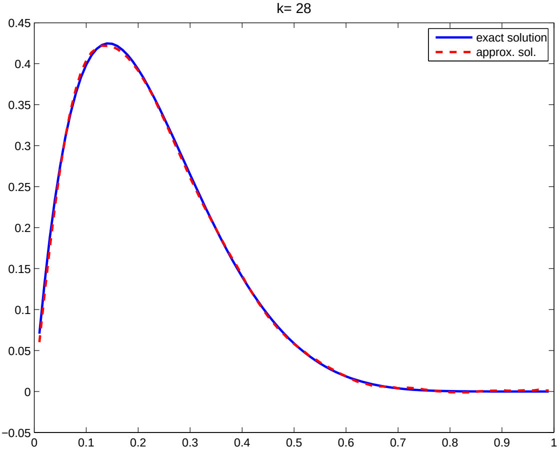

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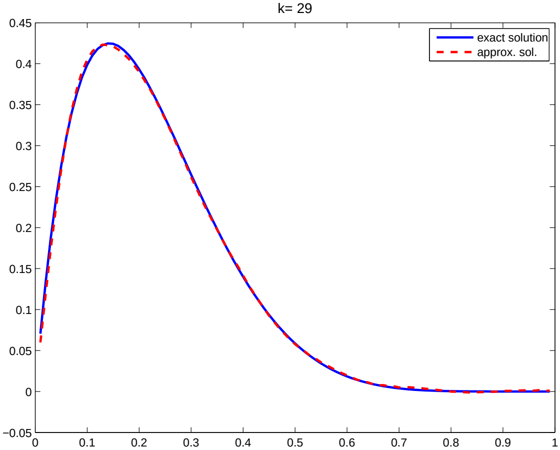

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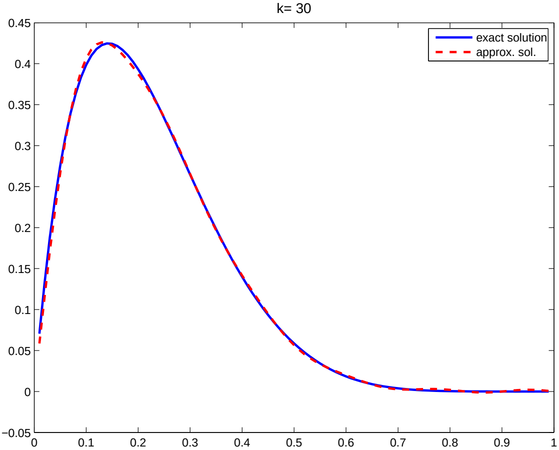


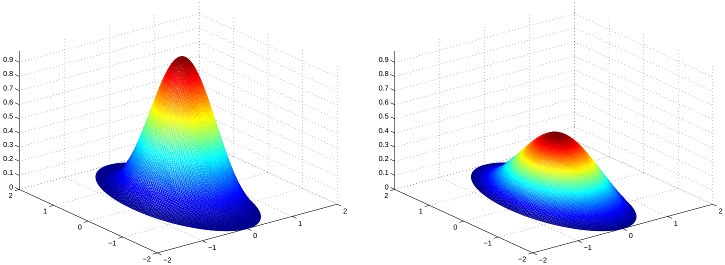
Example 2

Finite element discretization of L with variable coefficients on the ellipse

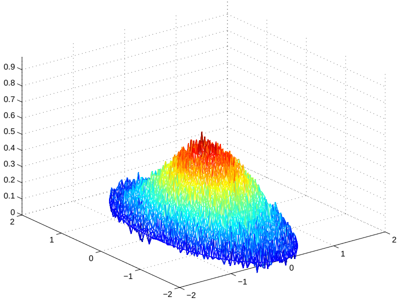
$$\Omega = \{(x, y, z) \mid x^2 + y^2/4 \leq 1,\ 0 \leq z \leq z_1 = 0.6\}.$$

The stiffness matrix has dimension 8065
Data perturbation: $\sim 3\%$

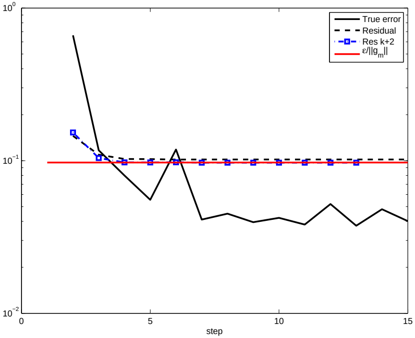
Solution and Exact Data

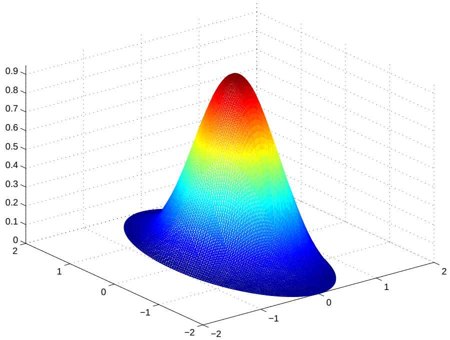


Perturbed Data



Convergence history ($0.6\lambda_c$). Solution after 9 steps





Conclusions

- 3D Cauchy problem: complex 2D geometry $+$ cylinder in z
- Krylov method $+$ black box 2D elliptic solver
- Stability theory $\Longrightarrow$ recipe for cut-off level
- Exponential of small matrix is computed (cheap)
- Safe-guarded stopping criterion:
  Approximate residual (cheap) $+$ True residual (rather expensive)
- Much fewer 2D elliptic solves than eigenvalue computation: 98 eigenvalues were smaller than the tolerance.
  MATLAB's `eigs`: 300 2D solves
  Krylov: 18 solves
  - Highly accurate eigenvalues are not needed
  - The data influence the basis (projection) vectors

Extensions

- Variable coefficients in z?
- Other Cauchy problems:
  - parabolic: Zohreh Ranjbar's thesis
  - Helmholtz, transient electromagnetics?

Paper: Inverse Problems 2009