Solving Ill-Posed Cauchy Problems using Rational Krylov Methods

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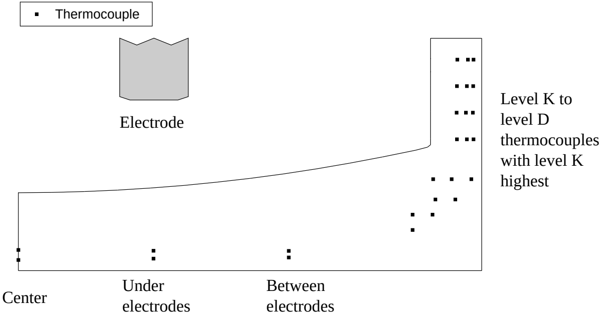
Outline

Motivating example: Ilmenite iron melting furnace

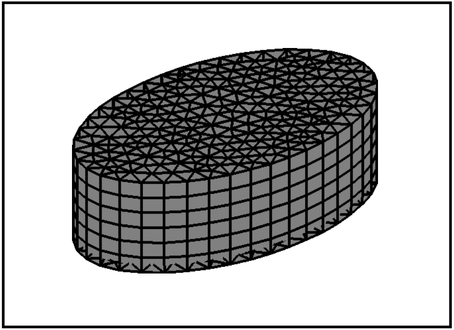


The furnace material properties are temperature dependent.
Problem: find the inner shape of the furnace.
Nonlinear, and (rather) complex geometry

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

Ill-Posed Cauchy Problem

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

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

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

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

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

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

then

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

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

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

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

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

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

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

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"**
  - $[Q_k, T_k] = \texttt{krylovstep}(L^{-1}, Q_{k-1}, T_{k-1})$
  - Compute $v_k(z) = Q_k F(z, S_k^c) Q_k^\top g_m$
- **end**
- Check residual $\|Kv_k - g_m\| < \epsilon$

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

How can we quantify "stable"?

Error Estimate for Krylov Procedure

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

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

Second term: Krylov approximation error for low frequency operator applied to the exact right hand side!

Heuristic

When the approximate solution does not change much between successive Krylov steps, then this error is small.

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

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

Test example 1: Laplace equation

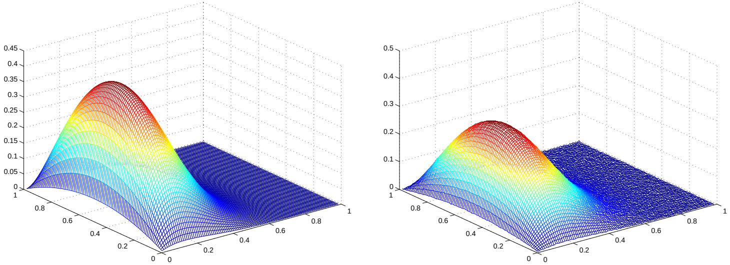
Ω: unit square

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

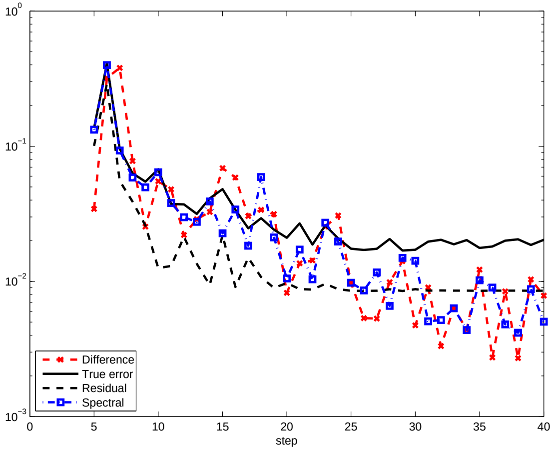
Determine the values at the upper boundary,
$f(x,y) = u(x,y,0.1),\ (x,y) \in \Omega.$

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

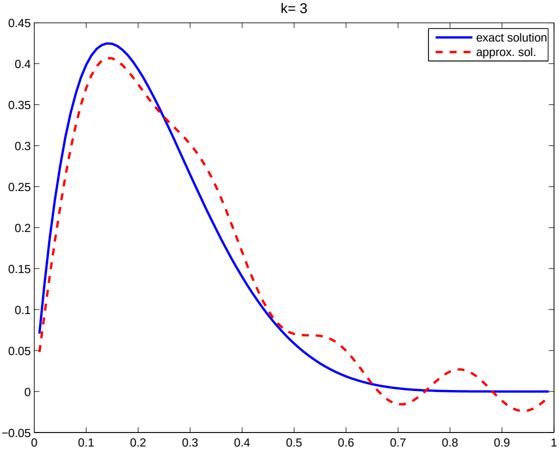
Solution and Exact Data



Convergence History ($0.75\lambda_c$)



Solutions as function of iteration index



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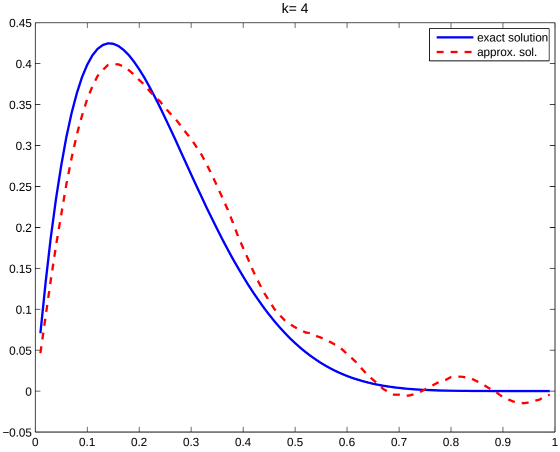

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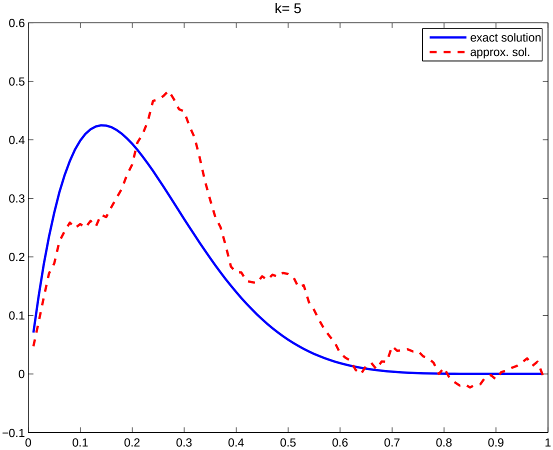

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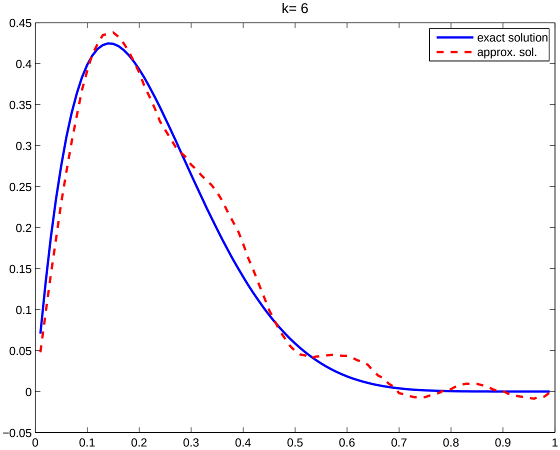

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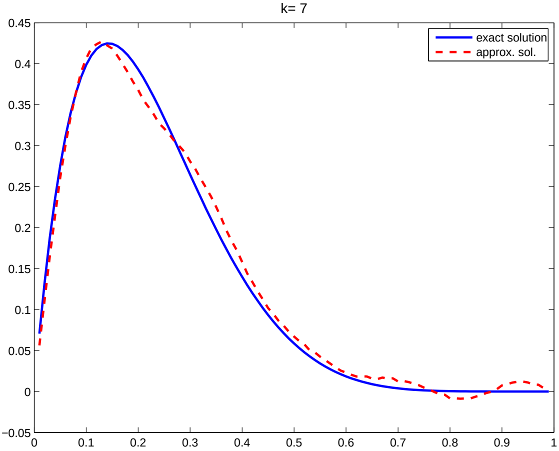

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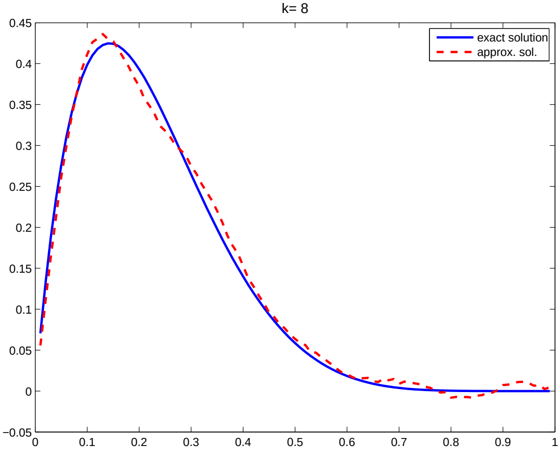

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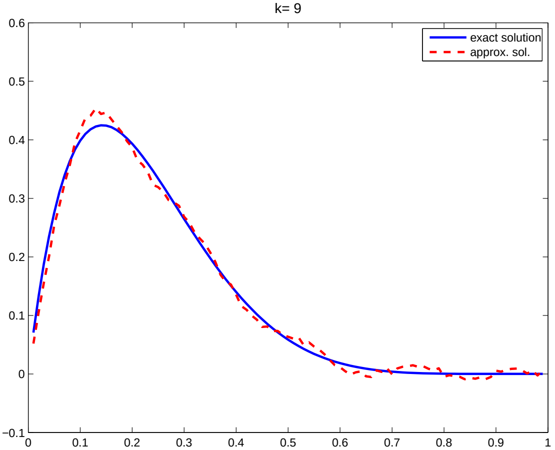

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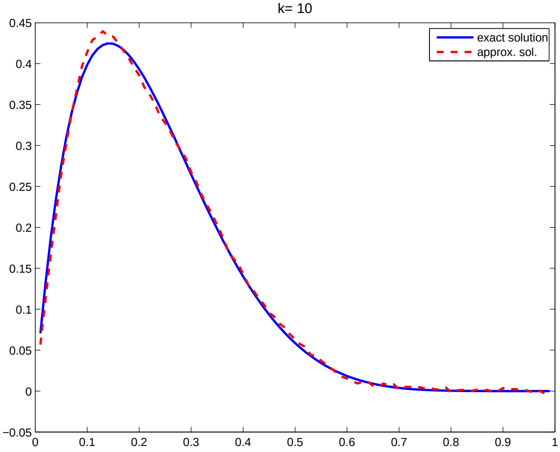

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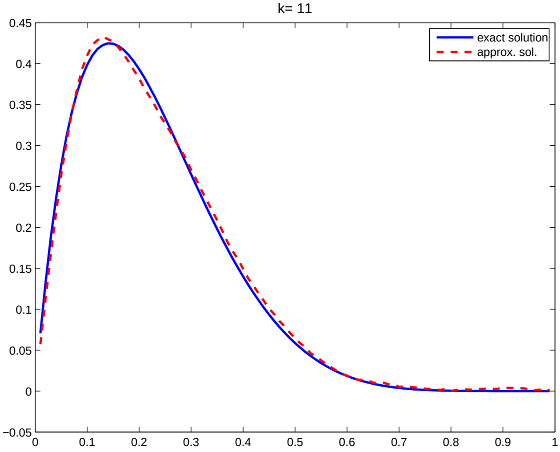

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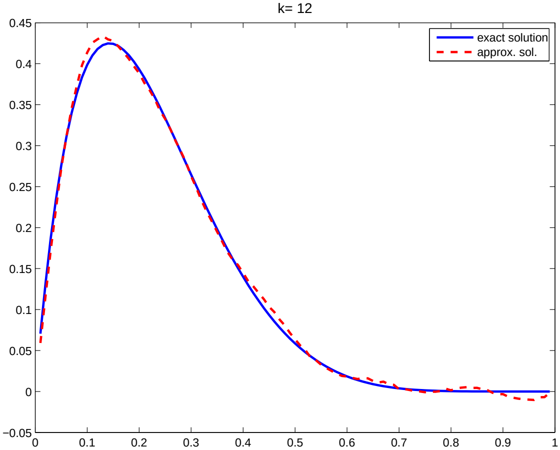

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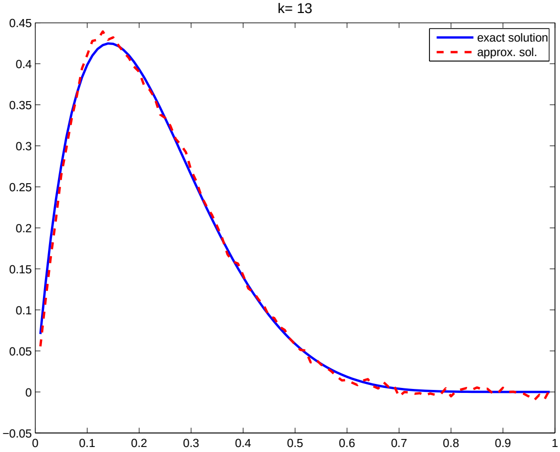

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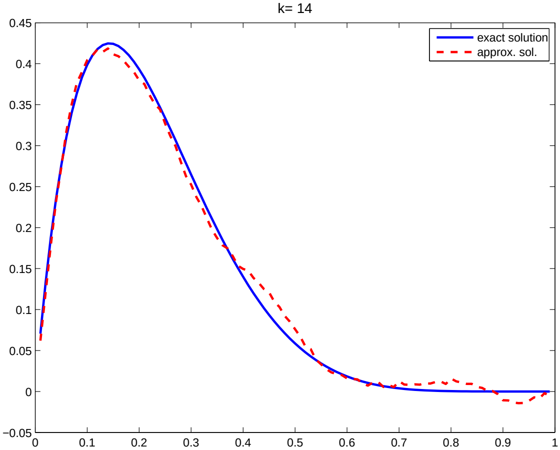

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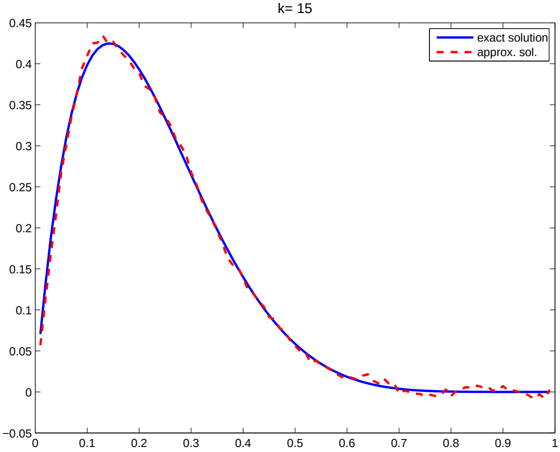

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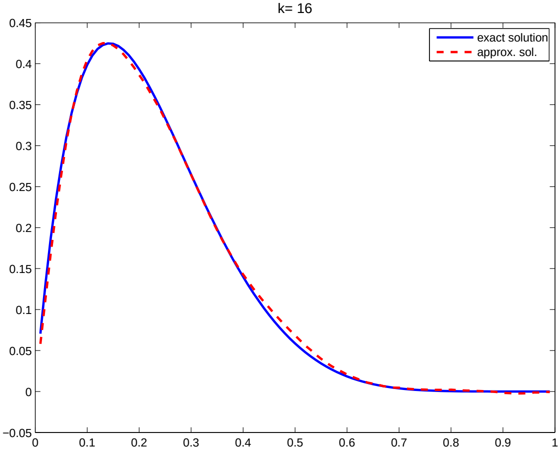

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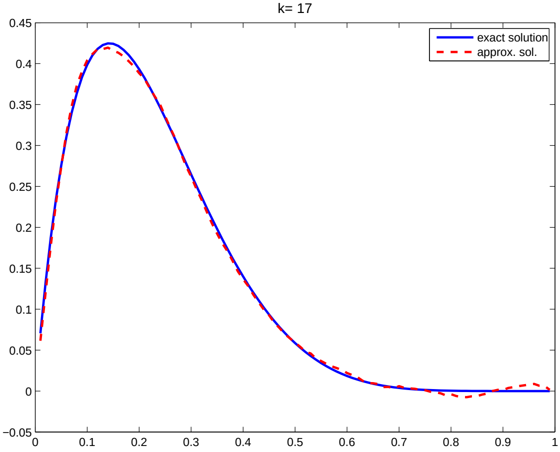

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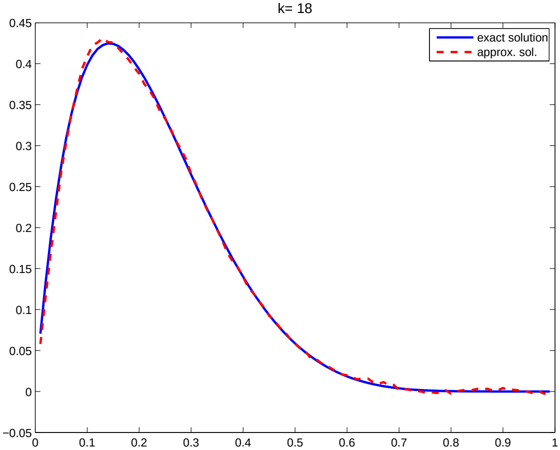

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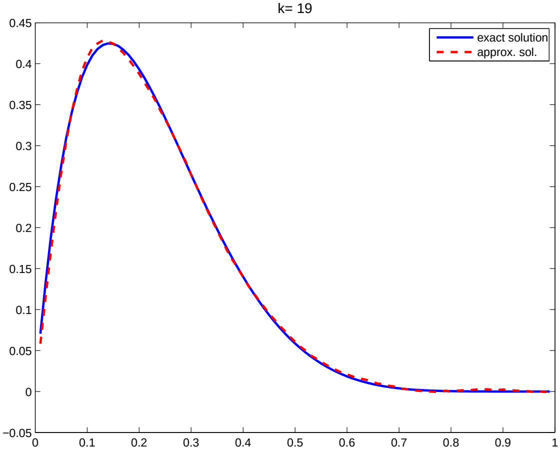

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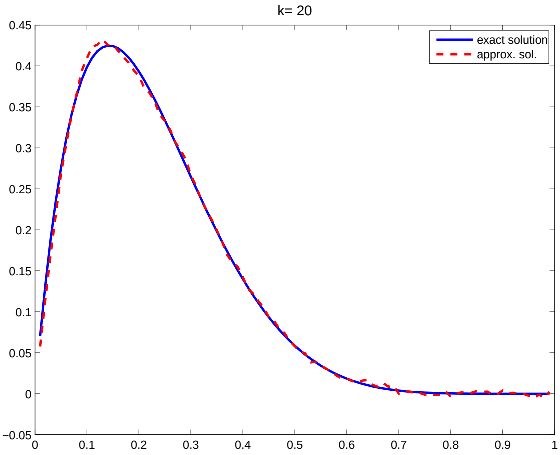

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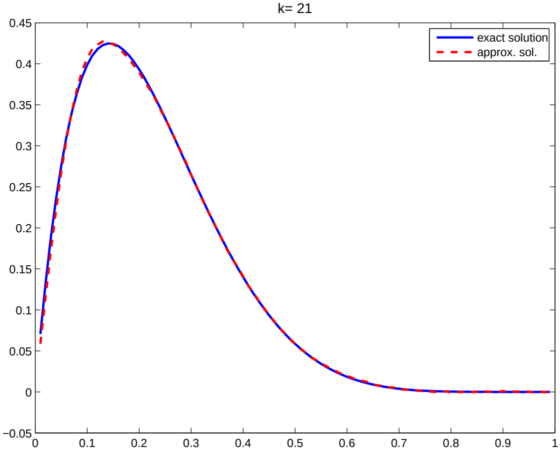

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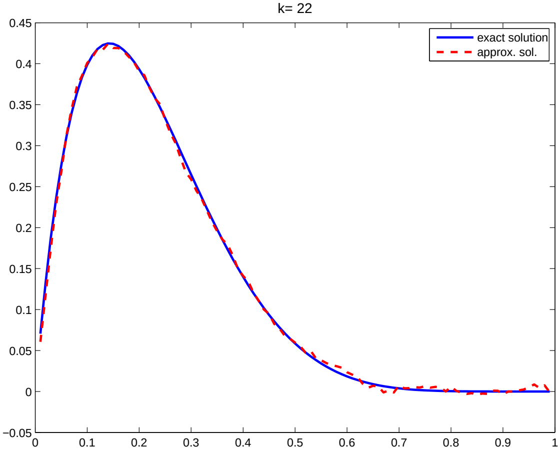

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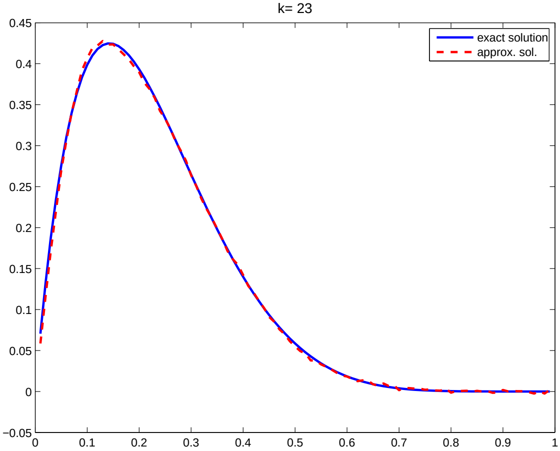

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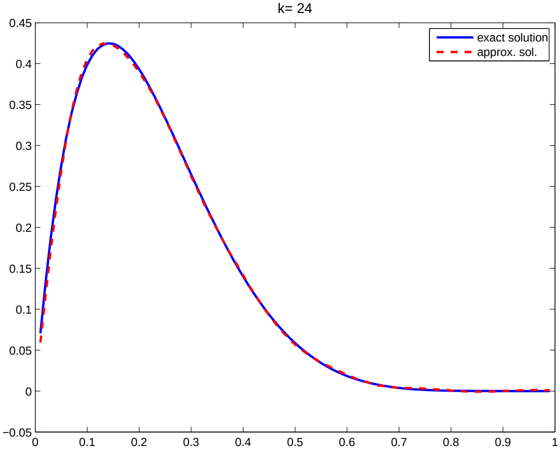
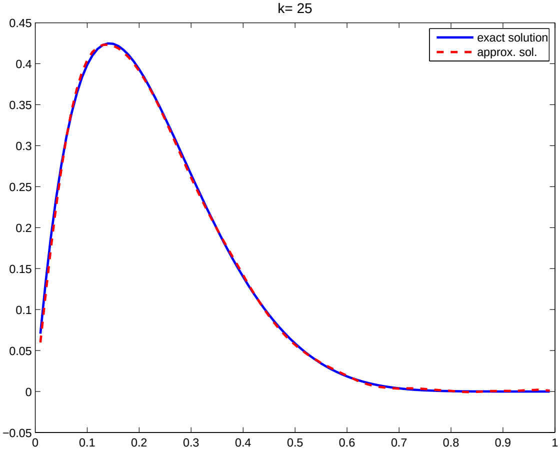


Stopping criterion satisfied here



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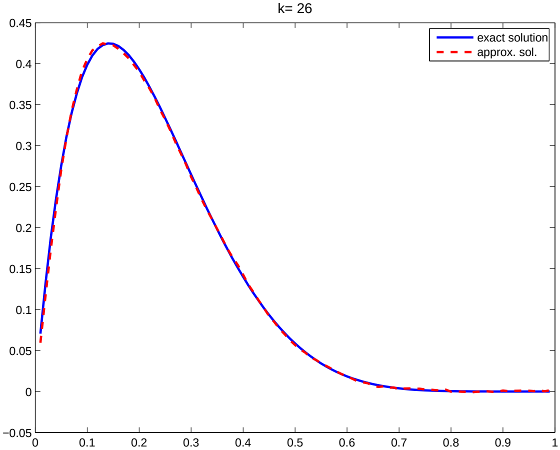

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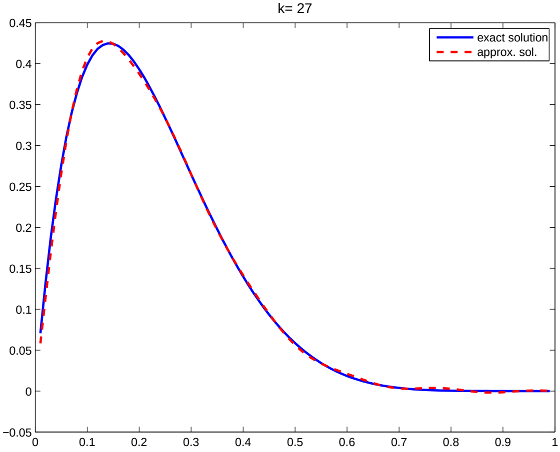

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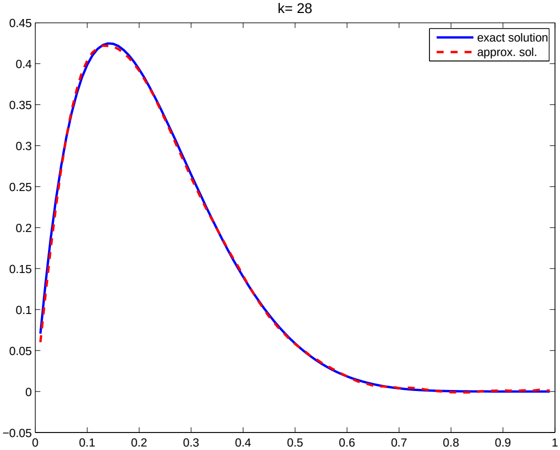

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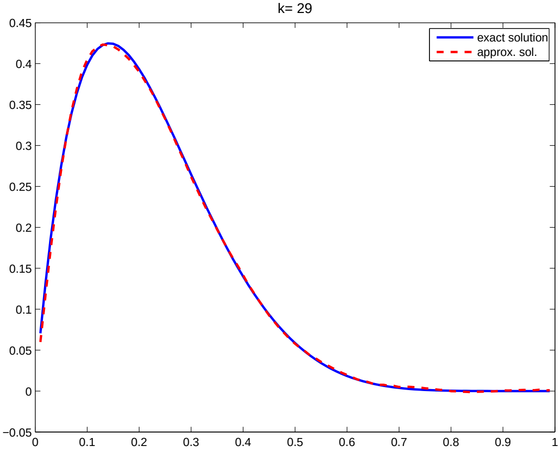

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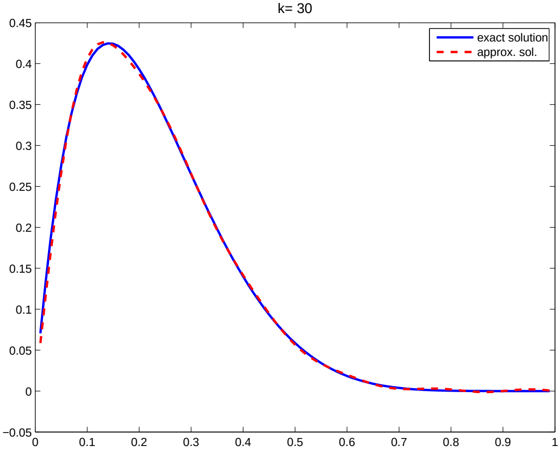


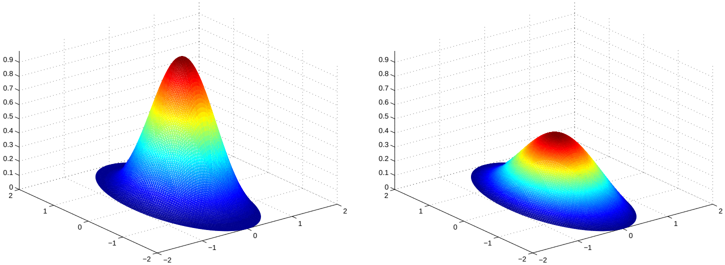
Example 2

Finite element discretization of L with variable coefficients on the ellipse

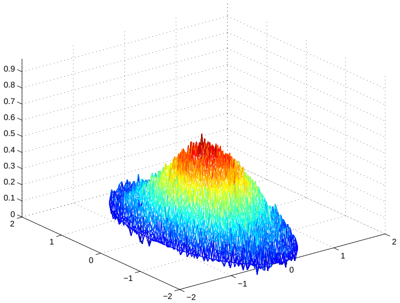
$$\Omega = \{(x, y, z) \mid x^2 + y^2/4 \leq 1, \ 0 \leq z \leq z_1 = 0.6\}.$$

The stiffness matrix has dimension 8065
Data perturbation: $\sim$ 1%

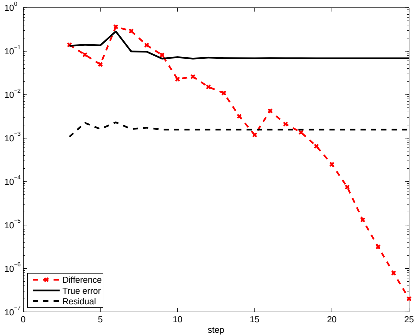
Solution and Exact Data

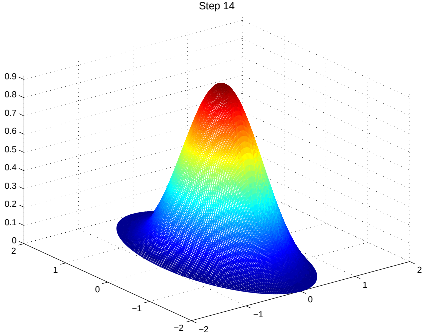


Perturbed Data



Convergence history ($0.5\lambda_c$). Solution after 14 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: Solution difference (cheap) $+$ 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: 25 solves
  - Highly accurate eigenvalues are not needed
  - The data influence the basis (projection) vectors

Remaining work

- Variable coefficients in z?
- Other Cauchy problems (parabolic, Helmholtz, transient electromagnetics)?

Talk and paper are available on my web page.