Classical Multigrid Methods: Efficient for Diffusive Problems but Ineffective for Wave Propagation Problems

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July 2009

Classical Relaxation Methods

Hackbusch 1985: "For about one century the Jacobi and Gauss-Seidel method ('relaxation') were the only tools for solving small linear systems iteratively. A lot of interesting variations were proposed which were well-fitted for hand calculations."

For the linear system of equations $A\mathbf{u} = \mathbf{f}$ using the decomposition $A = L + D + U$, the classical Jacobi method is

$$\mathbf{u}^{n+1} = D^{-1}((-L - U)\mathbf{u}^n + \mathbf{f}) = \mathbf{u}^n + D^{-1}(\mathbf{f} - A\mathbf{u}^n)$$

and the classical Gauss Seidel Method is

$$\mathbf{u}^{n+1} = (L + D)^{-1}(-U\mathbf{u}^n + \mathbf{f}) = \mathbf{u}^n + (L + D)^{-1}(\mathbf{f} - A\mathbf{u}^n).$$

Example: For the Laplace equation in 2d, with the standard 5 point finite difference stencil $[-1, -1, 4, -1, -1]$, the Jacobi method is

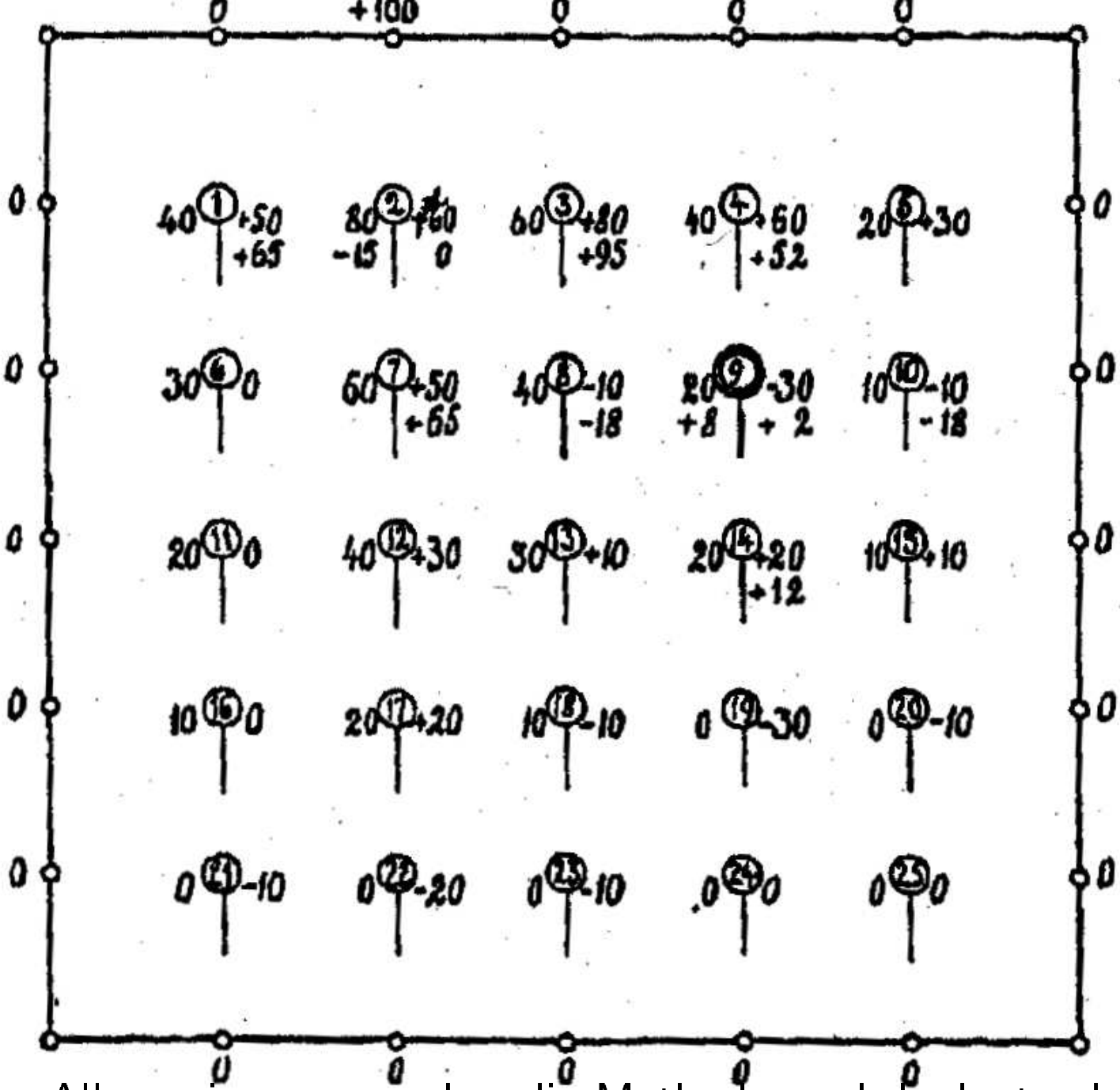
$$u_{j,i}^{n+1} = \frac{1}{4}(u_{i+1,j}^n + u_{i-1,j}^n + u_{i,j+1}^n + u_{i,j-1}^n)$$

Historical Purpose: Hand Relaxation

Stiefel 1952: Über einige Methoden der Relaxationsrechnung

"Ein geübter Rechner, der ein gewisses Gefühl für den Verlauf einer Potentialfunktion hat, kann im vorliegenden Beispiel von 25 Unbekannten mit diesem Einzelschrittverfahren durchkommen.

Links von jedem Gitterpunkt sind Funktionswerte oder Funktionsänderungen angeschrieben, rechts wird der jeweilige Stand der Residuen protokolliert"



"Im Allgemeinen muss aber die Methode noch bedeutend verfeinert werden"

General Idea of Relaxation (following Stiefel)

If A is symmetric and positive definite, we have

$$A\mathbf{u} = \mathbf{f} \quad \Longleftrightarrow \quad F(\mathbf{u}) := \frac{1}{2}\mathbf{u}^T A\mathbf{u} - \mathbf{f}^T\mathbf{u} \longrightarrow \min$$

To solve the minimization problem, a natural relaxation procedure is

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \alpha\mathbf{p}$$

where $\mathbf{p}$ is a search direction and α is the distance to go along this direction.

Example: The Jacobi method

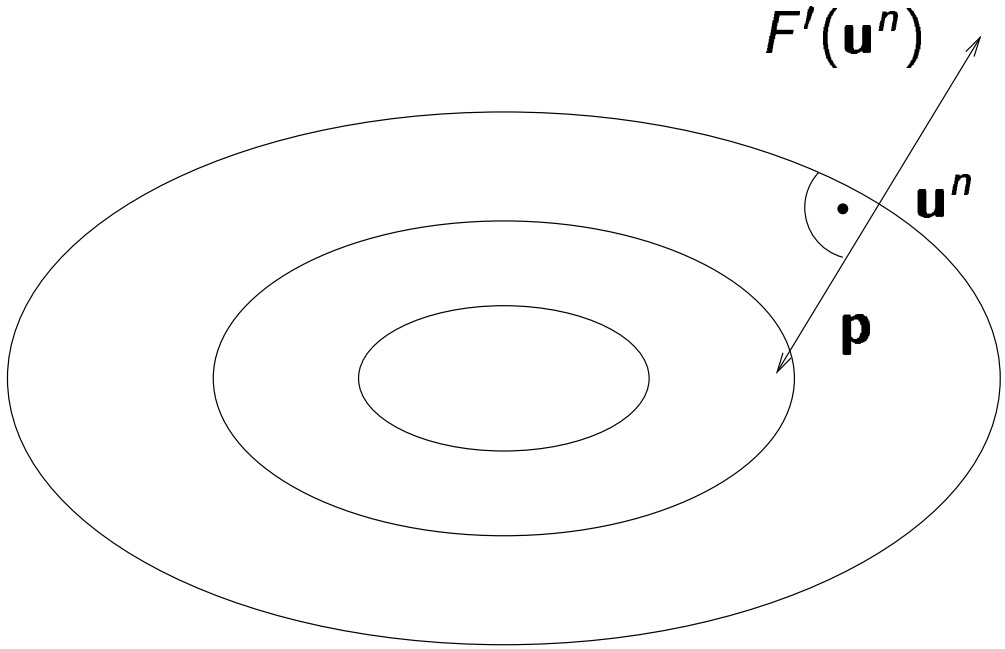
$$\mathbf{u}^{n+1} = \mathbf{u}^n + D^{-1}(\mathbf{f} - A\mathbf{u}^n)$$

for the five point finite difference Laplacian uses

$$\mathbf{p} := (\mathbf{f} - A\mathbf{u}^n) \quad \alpha = \frac{1}{4}.$$

Is the Jacobi Choice a Good One ?

The direction of Jacobi is $\mathbf{p} = (\mathbf{f} - A\mathbf{u}^n) = -F'(\mathbf{u}^n)$, and thus Jacobi goes into the direction of fastest decrease of F at $\mathbf{u}^n$:

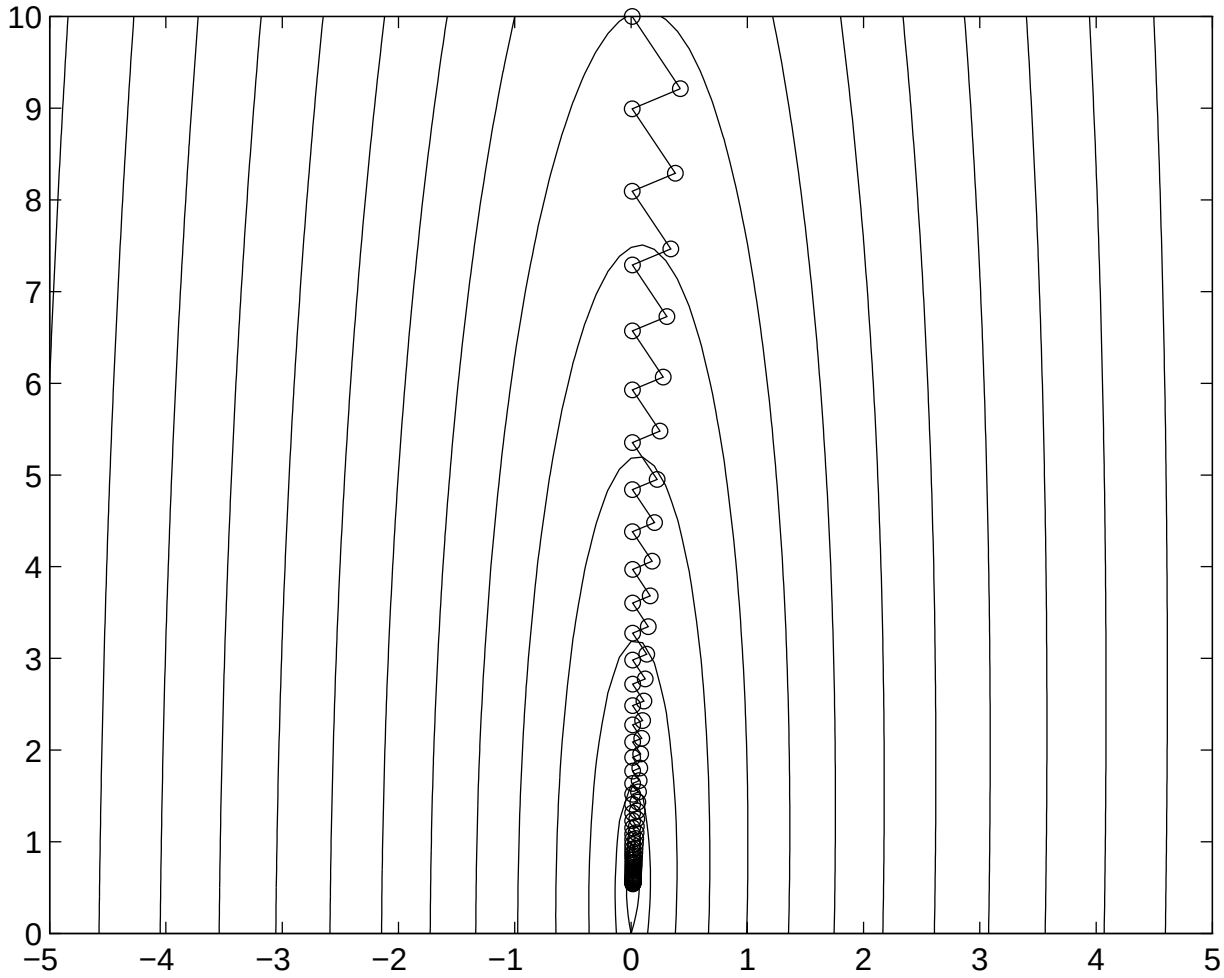


Hence the direction is a good choice, but the distance $\alpha = \frac{1}{4}$ might not be good.

"Ritzscher Gedanke (Stiefel)": Use α to minimize F along the direction $\mathbf{p}$, hence $\alpha = \alpha(n)$:

$$\Longrightarrow \textbf{Method of Steepest Descent.}$$

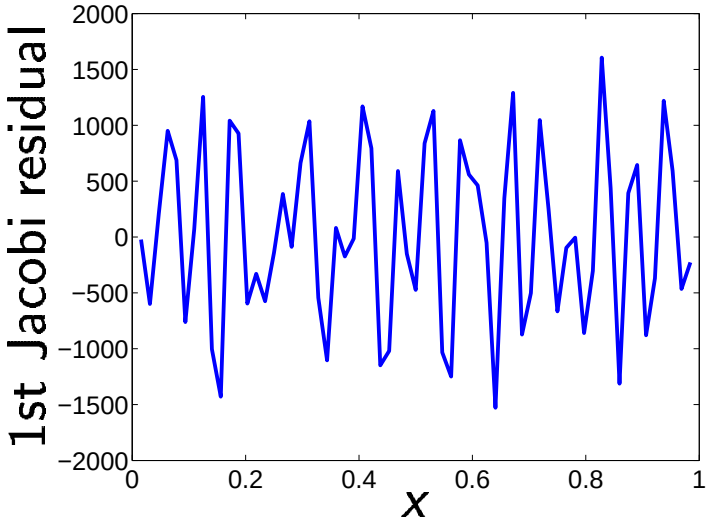
Problems of Steepest Descent: Prison Syndrome

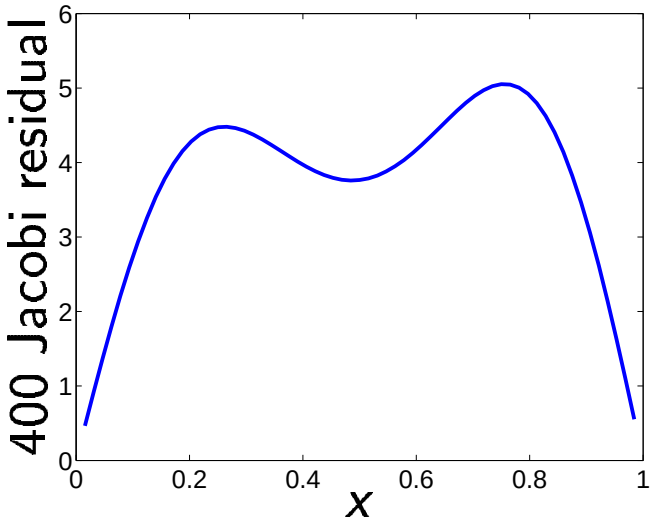


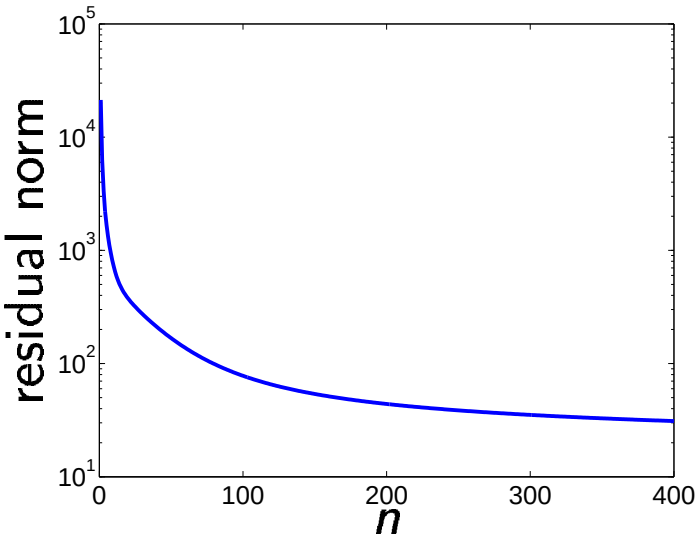
Stiefel 1952: "Das Auftreten von Käfigen ist eine allgemeine Erscheinung bei Relaxationsverfahren und sehr unerwünscht. Es bewirkt, dass eine Relaxation am Anfang flott vorwärts geht, aber dann immer weniger ausgiebig wird..."

General Prison Syndrome for Relaxation Methods

"... Es ist leicht festzustellen, wann man bei diesem Einzelschrittverfahren [Jacobi] des Dirichlet Problems in einem Käfig sitzt: Dies ist dann der Fall, wenn die Residuen in den inneren Punkten alle dieselben Vorzeichen haben."







"... so dass der positive Residualberg mit den Löffel statt mit einer Baggermaschine abgetragen wird !"

Remedies Proposed By Stiefel

- Block relaxation: simultaneous relaxation of several equations by the same averaged amount.
- "Scheibenrelaxation":
  1. either choosing search directions related to eigenfunctions on subdomains.
  2. or solving directly small subproblems for low modes by relaxation.

  "Es ist zweckmässig, für einen gegebenen Operator eine Sammlung von Scheiben anzulegen."

  These are precursors of **multigrid methods** and/or **domain decomposition**.
- Conjugate search directions: in that case, one can eliminate completely error components in the direction of each **p**, independent of the other directions.
- "Das n-Schritt Verfahren": the method of **conjugate gradients, (CG)**.

The Birth of Multigrid

Federenko (1961): A Relaxation Method for Solving Elliptic Difference Equations

The familiar iterative process [of Jacobi] is very slowly convergent. We shall try to use some special features of the convergence in order to speed it up...

We shall speak of the eigenfunctions as "good" and "bad"; the good ones include those that are smooth on the net and have few changes of sign in the domain; the bad ones often change sign and oscillate rapidly...

After a fairly small number of iterations, the error will consist of "good" eigenfunctions [...] We shall use the following method to annihilate the "good" components of the error. We introduce into the domain an auxiliary net, the step of which is q times greater than the step of the original net.

The Invention of Multigrid

Nicolaides 1975: On Multiple Grid and Related Techniques for Solving Discrete Elliptic Systems

Methods of multiple grid type: the general principle underlying this type of method was understood by pencil and paper relaxation users, and the method used by them and based on this principle was called "block relaxation."

For second-order elliptic equations in the plane [...] to reduce the error by a factor of 10^{-p} requires an amount of work proportional to the number of gridpoints n and p.

It must be said here that the implementation of a multiple grid method involves a high strategic component [...] programming a multiple grid method is a rather complex operation.

Hackbusch and Brandt

Two major competitors in the development of multigrid methods:

Brandt 1972: Multi-Level Adaptive Technique (MLAT) for Fast Numerical Solution to Boundary Value Problems

"The only disadvantage seems to be the complex programming involved"

Hackbusch 1976: A fast iterative method for solving Poisson's equation in a general region

"The basic idea – using auxiliary systems of difference equations corresponding to coarser grids – has been developed independently by the author, but it was already described by R. P. Federenko in 1961. Since then this idea has only been revived by N. S. Bakhvalov and A. Brandt."

Hackbusch and Brandt cont.

Brandt 1977: Multi-Level Adaptive Solutions to Boundary-Value Problems

"Multi-grid algorithms are not difficult to program, if the various grids are suitably organized."

"As soon as the residuals are smoothed out, convergence slows down. This is then exactly the point where relaxation sweeps should be discontinued and approximate solution of the (smoothed out) residual equations by coarser grids should be employed.".

"The basic tool is local mode (Fourier) analysis, applied to the locally linearized-frozen difference equations, ignoring boundaries."

Model Problem

We consider the classical model problem

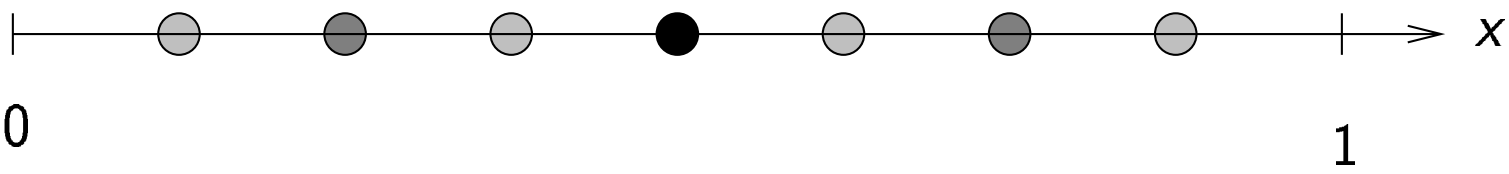
$$\eta u - \Delta u = f, \qquad \text{on } \Omega = (0,1),$$

with homogeneous Dirichlet boundary conditions.

Discretization by finite differences with $h = \frac{1}{M+1}$ on the mesh $x_m = mh$, $m = 1, 2, \ldots, M$, leads to the linear system

$$A\mathbf{u} := \frac{1}{h^2} \begin{bmatrix} 2 + h^2\eta & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & \end{bmatrix}_{M \times M} \mathbf{u} = \mathbf{f}.$$

The coarsest grid possible is $h = \frac{1}{2}$, with one grid point only.

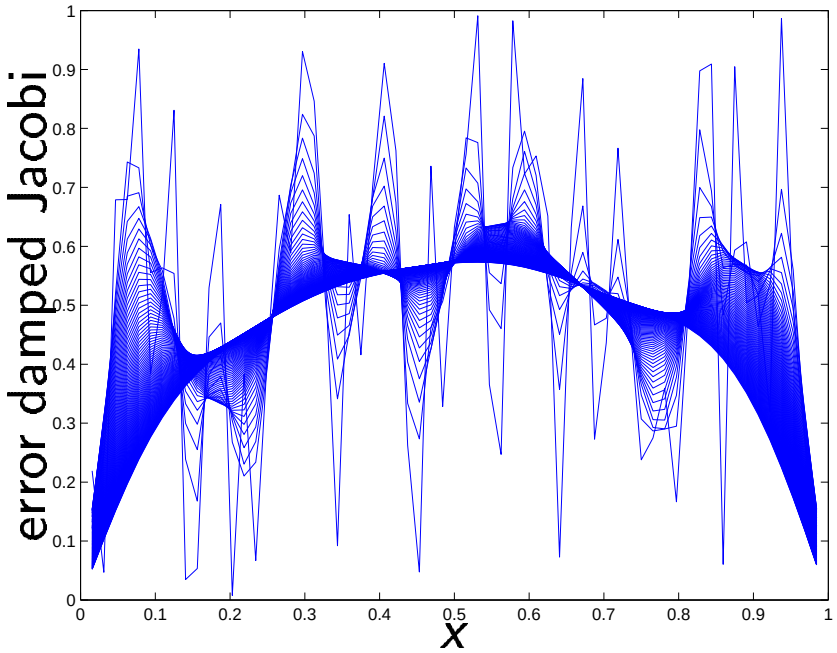


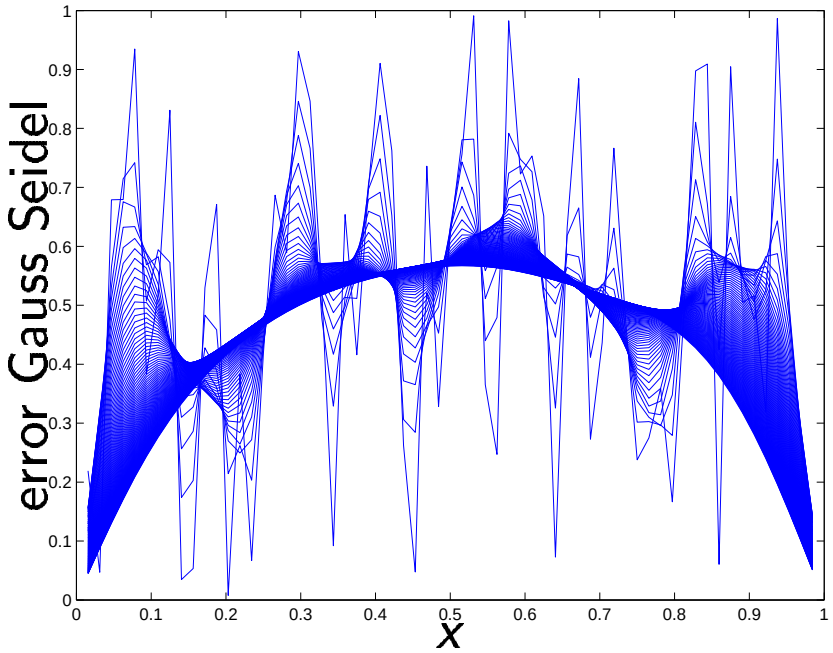
We consider only grids with $h = \frac{1}{2^{l+1}}$, $M = 2^{l+1} - 1$ and thus the coarsest level is $l = 0$, and there is always a mesh point in the center (M is odd).

Main Idea of Multigrid

Fact: Classical stationary iterative methods based on $A = L + D + U$ can be very effective for high frequency components of the error, but are not effective for low frequency components.

Examples: Damped Jacobi and Gauss Seidel for the model problem:





Damped Jacobi

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \omega D^{-1}(\mathbf{f} - A\mathbf{u}^n)$$

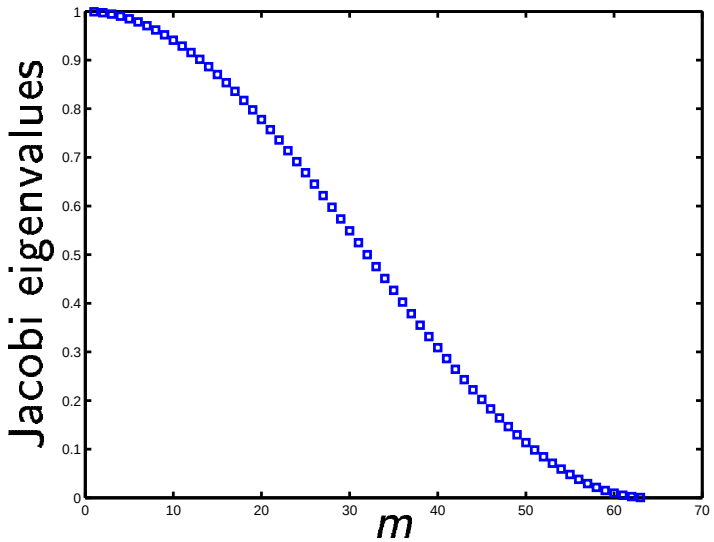
Gauss-Seidel

$$\mathbf{u}^{n+1} = \mathbf{u}^n + (L+D)^{-1}(\mathbf{f} - A\mathbf{u}^n)$$

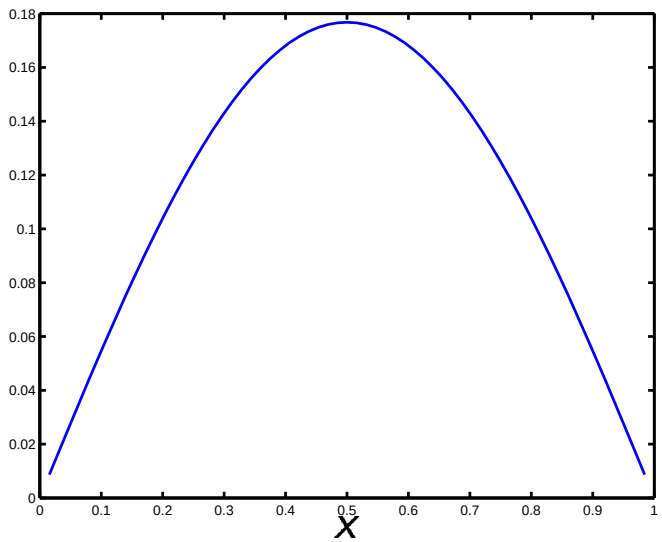
Spectra of the Iteration Operators

For the damped Jacobi iteration operator $I - \omega D^{-1} A$, $\omega = \frac{1}{2}$:

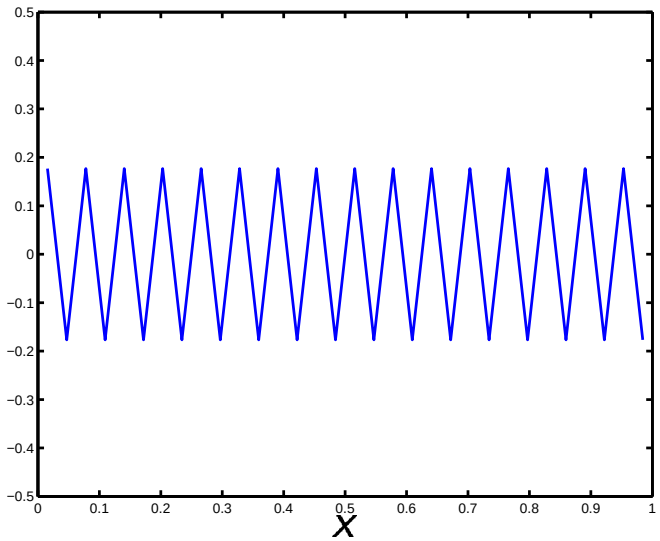
Spectrum



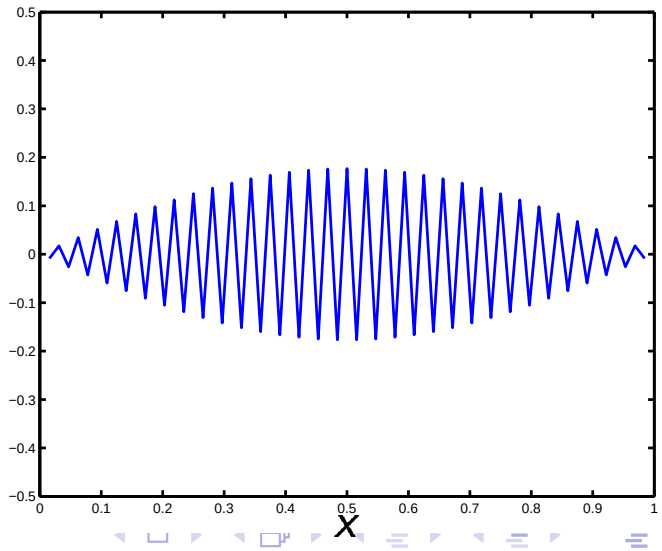
Lowest Mode



Intermediate Mode



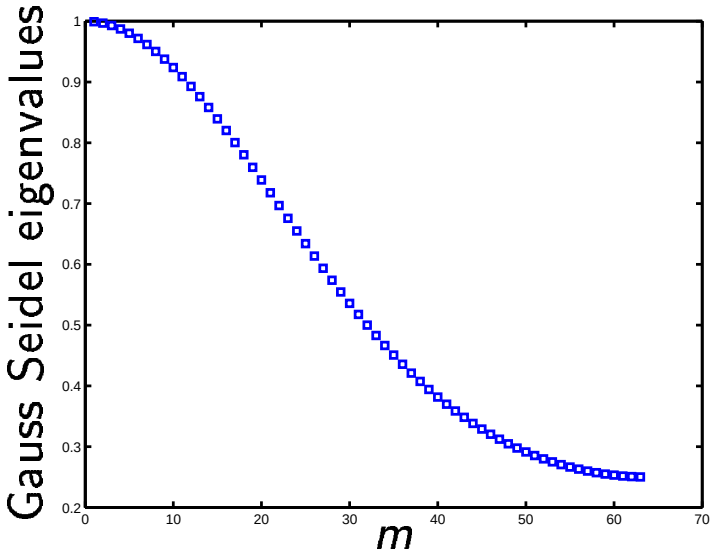
Highest Mode



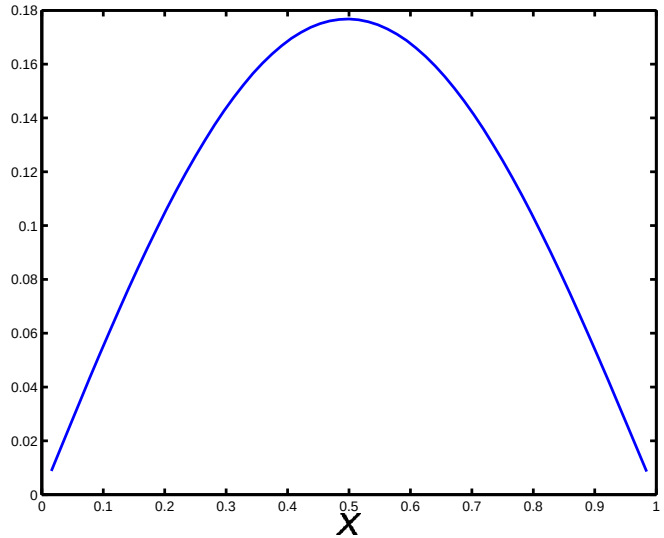
Spectra of the Iteration Operators

For the Gauss Seidel iteration operator $I - (D + L)^{-1}A$:

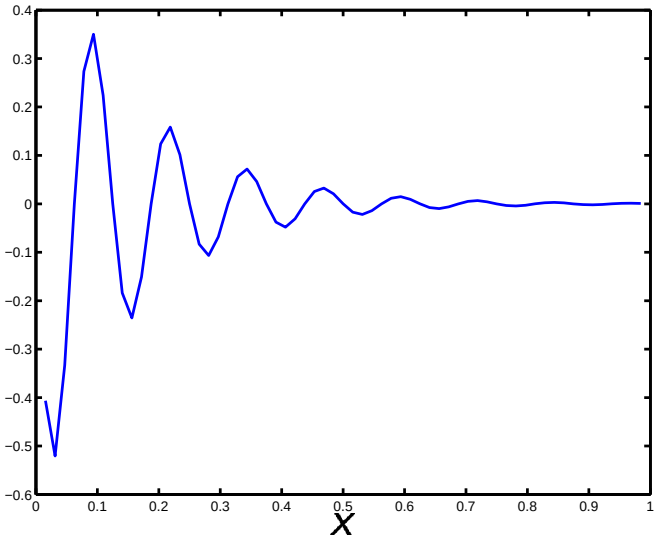
Spectrum



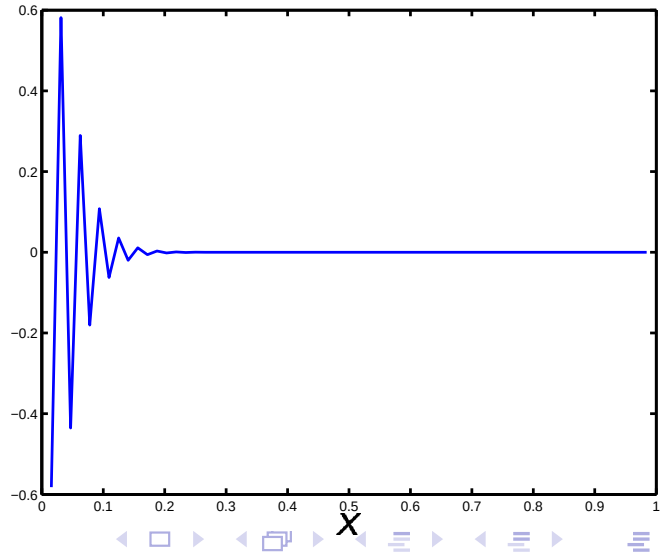
Lowest Mode



Intermediate Mode



Highest Mode



Analysis of Damped Jacobi

The eigenvalues and normalized eigenvectors for the model problem matrix

$$A = \frac{1}{h^2}\begin{bmatrix} 2+h^2\eta & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & \end{bmatrix}_{M\times M}$$

are given for $m = 1, 2, \ldots, M$ by the formulas

$$\lambda_m = \frac{4\sin^2(\frac{m\pi h}{2})}{h^2} + \eta, \quad \varphi_m(j) = \sqrt{2h}\sin(m\pi x_j),$$

Since the diagonal D is constant, the damped Jacobi iteration operator

$$I - \omega D^{-1} A$$

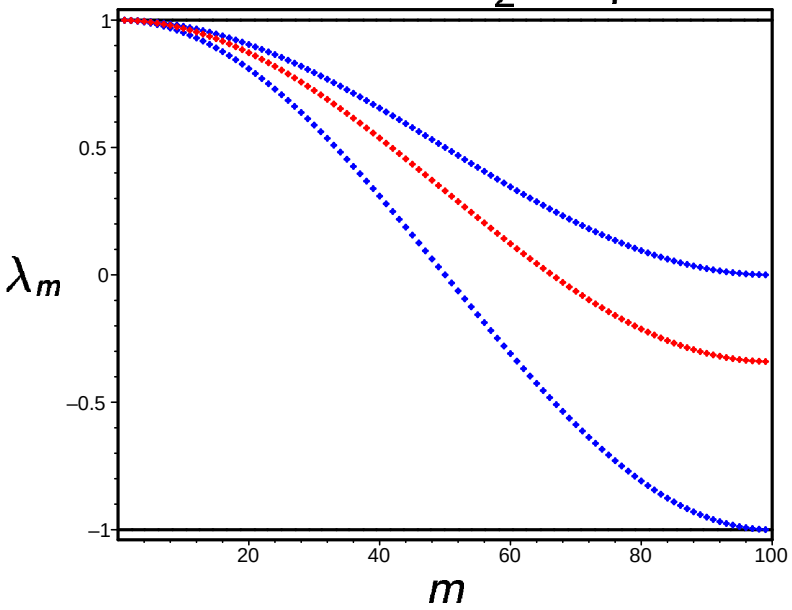
has the same eigenvectors, and the associated eigenvalues

$$\rho_m = 1 - \omega\frac{h^2}{2+h^2\eta}\lambda_m = 1 - \omega\frac{4\sin^2(\frac{m\pi h}{2}) + h^2\eta}{2+\eta h^2}.$$

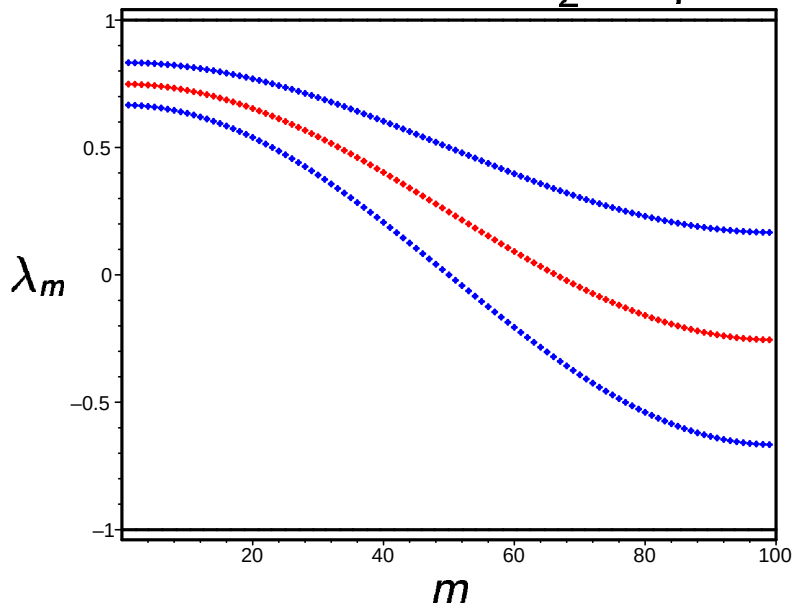
Hence each mode φ_m converges with factor ρ_m.

Choice of Relaxation Parameter

$\eta = 1$ and $\omega = \frac{1}{2}, \omega_{opt}, 1$



$\eta = 10000$ and $\omega = \frac{1}{2}, \omega_{opt}, 1$



Optimal choice of ω for convergence:

$$\min_{\omega} \max_{m \in 1,\ldots,M} |\rho_m| \Longrightarrow \omega^* \text{ solves } \rho_1(\omega) = -\rho_m(\omega)$$

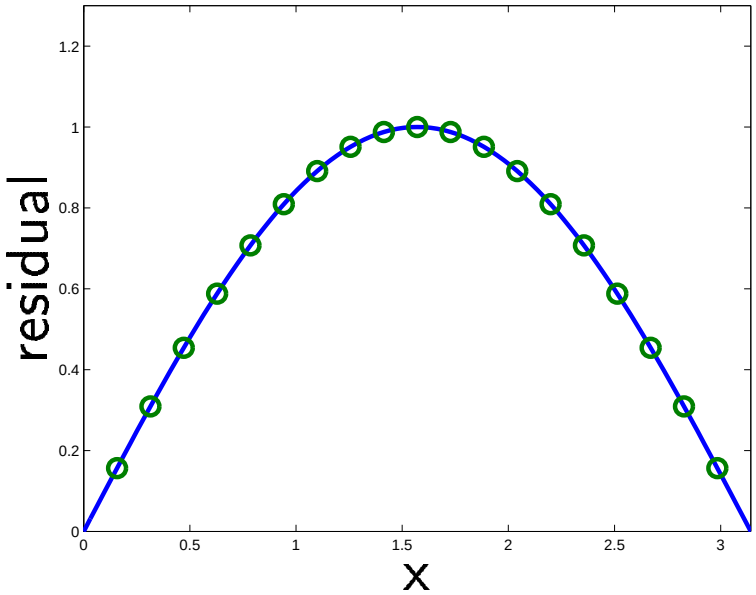
Optimal choice of ω for smoothing:

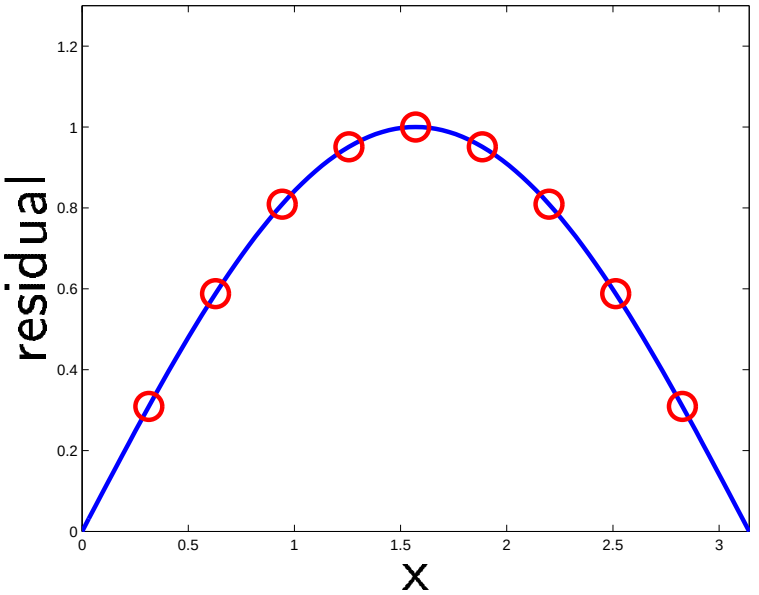
$$\min_{\omega} \max_{m \in \frac{M}{2},\ldots,M} |\rho_m| \Longrightarrow \omega^* \text{ solves } \rho_{\frac{M}{2}}(\omega) = -\rho_m(\omega)$$

which leads to $\omega_{opt} = \frac{2+h^2\eta}{2-\cos(\frac{M}{2}\pi h)+h^2\eta-\cos(M\pi h)} \approx \frac{2+h^2\eta}{3+h^2\eta}$

How to Treat Low Frequency Error?

Federenko (1961): "We introduce into the domain an auxiliary net, the step of which is q times greater than the step of the original net.





Need to transfer residual from a fine grid to a coarser grid, $r_H := I_h^H r_h$. Simplest possibility: injection

$$I_h^H = \begin{bmatrix} 0 & 1 & 0 & & & \\ & & 0 & 1 & 0 & \\ & & & & \ddots & \\ & & & & 0 & 1 & 0 \end{bmatrix}$$

"Restriction"

Interpolation Matrices

Also need to transfer residual from coarse grid back to the fine grid, $r_h = I_H^h r_H$: interpolation

$$I_H^h = \frac{1}{2}\begin{bmatrix} 1 & & & & \\ 2 & & & & \\ 1 & 1 & & & \\ & 2 & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & 2 & \\ & & & 1 & \end{bmatrix}$$

"**Prolongation**, **Extension**"

This gives an alternative for the restriction: full weighting

$$I_h^H = \frac{1}{2}(I_H^h)^T = \frac{1}{4}\begin{bmatrix} 1 & 2 & 1 & & & & \\ & & 1 & 2 & 1 & & \\ & & & & \ddots & & \\ & & & & & 1 & 2 & 1 \end{bmatrix}$$

The Coarse Grid Problem

There are two main possibilities to define a coarse grid problem:

1. Simply discretize the same problem on the coarser grid $H = 2h$:

$$A^H = \frac{1}{H^2} \begin{bmatrix} 2 + H^2\eta & -1 & & \\ -1 & \ddots & \ddots & \\ & & & \end{bmatrix}_{\frac{M+1}{2}-1 \times \frac{M+1}{2}-1}$$

2. Use the restriction and prolongation operators:

$$A^H = I_h^H A I_H^h.$$

Lemma

For the model problem and a FEM discretization, these two approaches give the same coarse problem A^H.

Proof:

The discretization of $(\eta - \Delta)u = f$ by finite elements leads to the discrete problem $(\eta M + K)\mathbf{u} = \mathbf{f}$, where the mass and stiffness matrices are

$$M = \frac{1}{6}\begin{bmatrix} 4 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 4 \end{bmatrix}_{M\times M} \qquad K = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}_{M\times M}$$

Now $M^H = I_h^H M I_H^h =$

$$= \frac{1}{4}\begin{bmatrix} 1 & 2 & 1 & & & \\ & & 1 & 2 & 1 & \\ & & & & \ddots & \end{bmatrix} \frac{1}{6}\begin{bmatrix} 4 & 1 & & \\ 1 & 4 & 1 & \\ & \ddots & \ddots & \ddots \end{bmatrix} \frac{1}{2}\begin{bmatrix} 1 & & & \\ 2 & & & \\ 1 & 1 & & \\ & 2 & & \\ & 1 & \ddots & \end{bmatrix}$$

$$= \frac{1}{48}\begin{bmatrix} 1 & 2 & 1 & & & \\ & & 1 & 2 & 1 & \\ & & & & & \ddots \end{bmatrix} \begin{bmatrix} 6 & 0 & \\ 10 & 1 & \\ & & \\ 6 & 6 & \ddots \\ 1 & 10 & \end{bmatrix} = \frac{1}{6}\begin{bmatrix} 4 & 1 & \\ 1 & 4 & 1 \\ & & \ddots \end{bmatrix}$$

Proof continued:

and for the stiffness matrix, we obtain $A^H = I_h^H A I_H^h =$

$$= \frac{1}{4}\begin{bmatrix} 1 & 2 & 1 & & \\ & & 1 & 2 & 1 \\ & & & & \ddots \end{bmatrix} \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & & \ddots & \end{bmatrix} \frac{1}{2}\begin{bmatrix} 1 & & \\ 2 & & \\ 1 & 1 & \\ & 2 & \\ & 1 & \ddots \end{bmatrix}$$

$$= \frac{1}{2(2h)^2}\begin{bmatrix} 1 & 2 & 1 & & \\ & & 1 & 2 & 1 \\ & & & & \ddots \end{bmatrix} \begin{bmatrix} 0 & 0 & \\ 2 & -1 & \\ 0 & 0 & \\ -1 & 2 & \\ & 0 & \ddots \\ & -1 & \end{bmatrix} = \frac{1}{H^2}\begin{bmatrix} 2 & -1 & \\ -1 & 2 & 1 \\ & & \ddots \end{bmatrix}$$

Note: The h^2 scaling on the stiffness matrix is unusual for FEM methods.

Two Grid Method

1. To solve $A\mathbf{u} = \mathbf{f}$, start with an initial guess $\mathbf{u}^0$
2. Apply ν_1 steps of damped Jacobi:
$$\mathbf{u}^{n+1} = \mathbf{u}^n + \omega D^{-1}(\mathbf{f} - A\mathbf{u}^n), \quad n = 0, 1, \ldots \nu_1 - 1$$
3. Compute the residual
$$\mathbf{r} = \mathbf{f} - A\mathbf{u}^{\nu_1}.$$
4. Instead of solving the residual equation for a correction, $A\mathbf{e} = \mathbf{r}$ ($\Longrightarrow A(\mathbf{u}^{\nu_1} + \mathbf{e}) = A\mathbf{u}^{\nu_1} + \mathbf{r} = \mathbf{f}$), solve this equation on a coarse grid:
$$A^H \mathbf{e}^H = I_h^H \mathbf{r}.$$
5. Extend this correction to the fine grid to correct the approximation:
$$\mathbf{u}^0 = \mathbf{u}^{\nu_1} + I_H^h \mathbf{e}^H$$
6. Apply ν_2 steps of damped Jacobi:
$$\mathbf{u}^{n+1} = \mathbf{u}^n + \omega D^{-1}(\mathbf{f} - A\mathbf{u}^n), \quad n = 0, 1, \ldots \nu_2 - 1$$

Convergence Analysis for Finite Differences

By linearity, it suffices to analyze the homogeneous problem and prove convergence to zero. The two grid iteration operator is then:

$$B := S^{\nu_2}(I - I_H^h (A^H)^{-1} I_h^H A) S^{\nu_1}$$

with the damped Jacobi smoothing step

$$S = I - \omega D^{-1} A$$

We know already that for an eigenvector $\varphi_m(j) = \sin(m\pi x_j)$ of the discretized model problem, ν damped Jacobi steps S^ν give

$$\rho_m^\nu = \left(1 - \omega \frac{4s_m^2 + \eta h^2}{2 + \eta h^2}\right)^\nu$$

where $s_m^2 := \sin^2(\frac{m\pi h}{2})$. Let also $c_m^2 := \cos^2(\frac{m\pi h}{2})$.

An Important Lemma

Lemma

Let $m = 1, 2, \ldots, \frac{M-1}{2}$ *and* $m' = M + 1 - m$. *Then*

$$c_{m'} = s_m, \qquad s_{m'} = c_m.$$

Proof: Using a trigonometric identity, we obtain

$$c_{m'} = \cos(\frac{m'\pi h}{2}) = \cos(\frac{(M+1-m)\pi h}{2}) = \cos(\frac{\pi}{2} - \frac{m\pi h}{2})$$

$$cos(A-B) = cos(A)cos(B) + sin(A)sin(B)$$

$$= \cos(\frac{\pi}{2})\cos(\frac{m\pi h}{2}) + \sin(\frac{\pi}{2})\sin(\frac{m\pi h}{2}) = \sin(\frac{m\pi h}{2}) = s_m.$$

The second identity then follows from
$s_{m'}^2 = 1 - c_{m'}^2 = 1 - s_m^2 = c_m^2$.

$$B = S^{\nu_2}(I - I_H^h (A^H)^{-1} I_h^H A) S^{\nu_1}$$

On a low frequency eigenmode φ_m, the operator A acts like

$$A\varphi_m = (\eta + \frac{4}{h^2} s_m^2)\varphi_m$$

and on a high frequency mode $\varphi_{m'}$, $m' = M + 1 - m$, it acts, using the Lemma, like

$$A\varphi_{m'} = (\eta + \frac{4}{h^2} c_m^2)\varphi_{m'}.$$

The coarse grid solver $(A^H)^{-1}$ acts on a coarse grid eigenvector $\varphi_m^H(j) = \sqrt{2H}\sin(m\pi jH)$, $j, m = 1, 2, \ldots \frac{M-1}{2}$:

$$(A^H)^{-1}\varphi_m^H = \frac{1}{\eta + \frac{4}{H^2}\sin^2\frac{m\pi H}{2}}\varphi_m^H = \frac{1}{\eta + \frac{4}{h^2}s_m^2 c_m^2}\varphi_m^H$$

since $\sin(2A) = 2sin(A)cos(A)$.

$$B = S^{\nu_2}(I - I_H^h (A^H)^{-1} I_h^H A) S^{\nu_1}$$

Applying the restriction to an eigenvector, we obtain

$$I_h^H \varphi_m = \frac{1}{4} \begin{bmatrix} 1 & 2 & 1 & & & \\ & & 1 & 2 & 1 & \\ & & & & & \ddots \end{bmatrix} \varphi_m$$

and hence for $j = 2, 4, \ldots, M$ we get the components

$$(I_h^H \varphi_m)(\frac{j}{2}) = \frac{\sqrt{2h}}{4}(\sin((j-1)m\pi h) + 2\sin(jm\pi h) + \sin((j+1)m\pi h))$$

$$\sin(A - B) = sin(A)cos(B) - cos(A)sin(B)$$

$$= \frac{\sqrt{2h}}{4}(\sin(jm\pi h)\cos(m\pi h) + 2\sin(jm\pi h) + \sin(jm\pi h)\cos(m\pi h))$$

$$= \frac{\sqrt{2h}}{4}(2 + 2\cos(m\pi h))\sin(\frac{j}{2}m\pi H),$$

$$\Longrightarrow I_h^H \varphi_m = \cos^2(m\pi h/2)\frac{1}{\sqrt{2}}\varphi_m^H = c_m^2 \frac{1}{\sqrt{2}}\varphi_m^H$$

But $I_h^H \varphi_m = c_m^2 \frac{1}{\sqrt{2}} \varphi_m^H$ is useful only for $m = 1, 2, \ldots \frac{M-1}{2}$.
If $m > \frac{M}{2}$, our last relation

$$(I_h^H \varphi_m)(\frac{j}{2}) = \sqrt{2h} c_m^2 \sin(\frac{j}{2} m\pi H)$$

gives for $m' = M + 1 - m$, $m = 1, 2, \ldots \frac{M-1}{2}$ using the Lemma

$$(I_h^H \varphi_{m'})(\frac{j}{2}) = \sqrt{2h} s_m^2 \sin(\frac{j}{2} m'\pi H)$$

and with $\sin(A - B) = sin(A)cos(B) - cos(A)sin(B)$

$$\sin(jm'\pi h) = \sin(j(M + 1 - m)\pi h) = \sin(j\pi - jm\pi h)$$

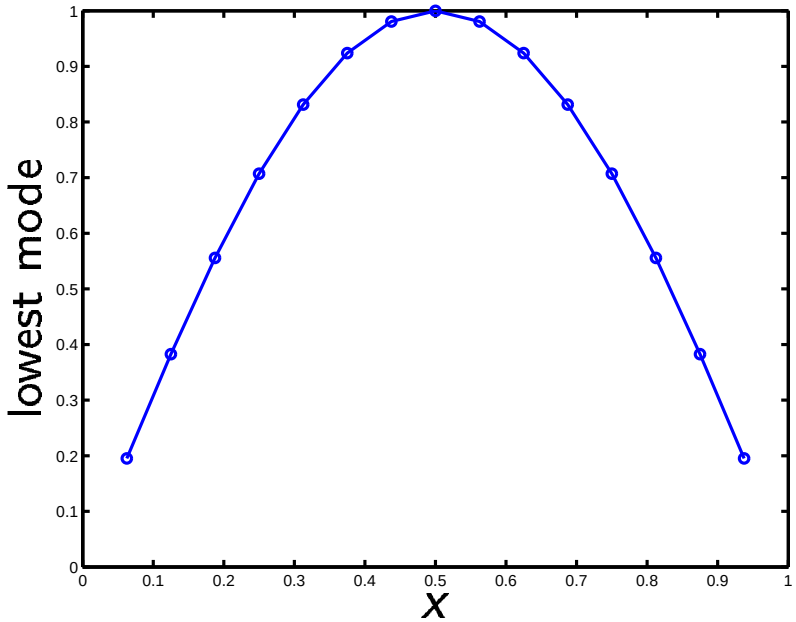
$$= \sin(j\pi)\cos(jm\pi h) - \cos(j\pi)\sin(jm\pi h)$$

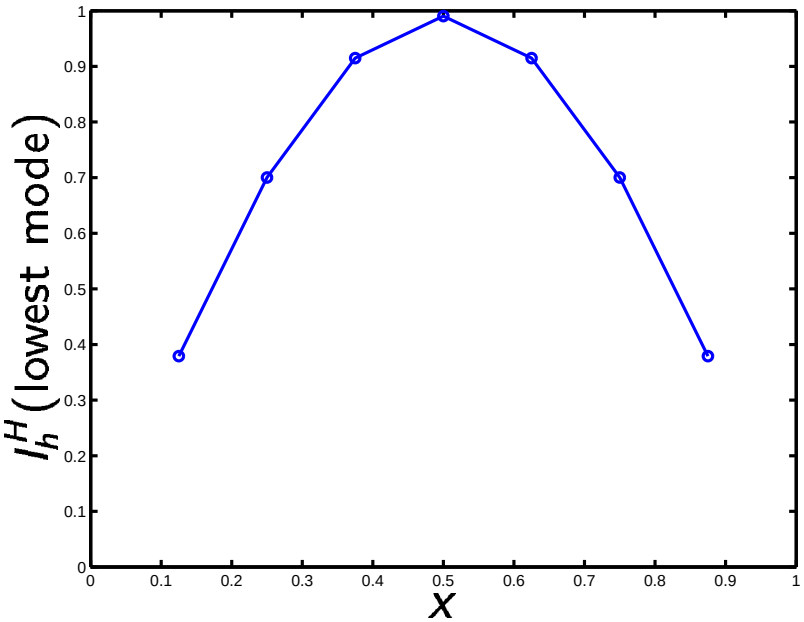
$$= -\sin(\frac{j}{2} m\pi H) \qquad \text{(remember } j \text{ is pair!)}$$

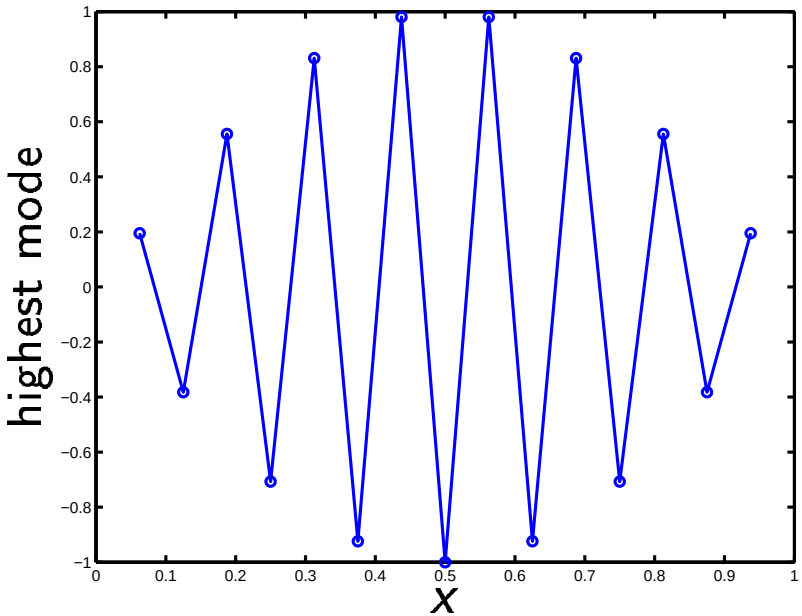
Hence, the restriction combines a low and high frequency mode:

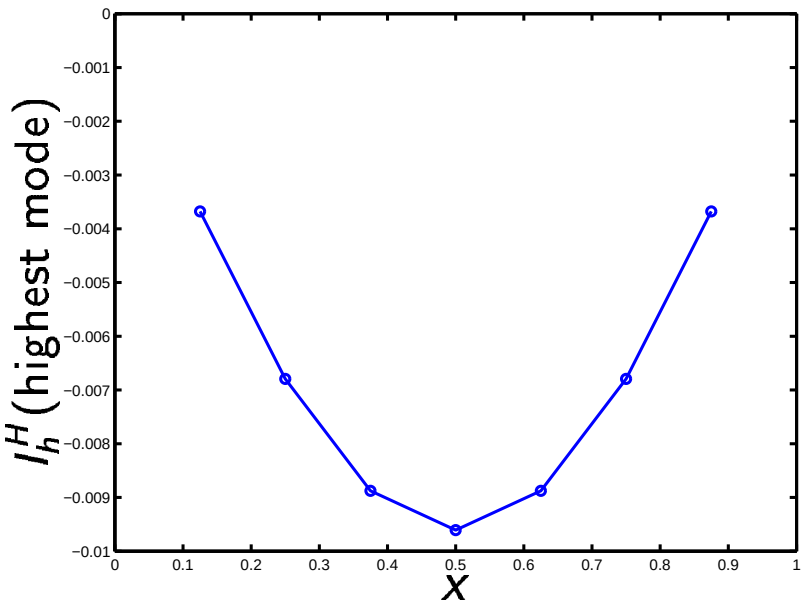
$$I_h^H \varphi_m = c_m^2 \frac{1}{\sqrt{2}} \varphi_m^H, \quad I_h^H \varphi_{m'} = -s_m^2 \frac{1}{\sqrt{2}} \varphi_m^H, \quad (I_h^H \varphi_{\frac{M+1}{2}} = 0).$$

Example: Lowest and Highest Mode

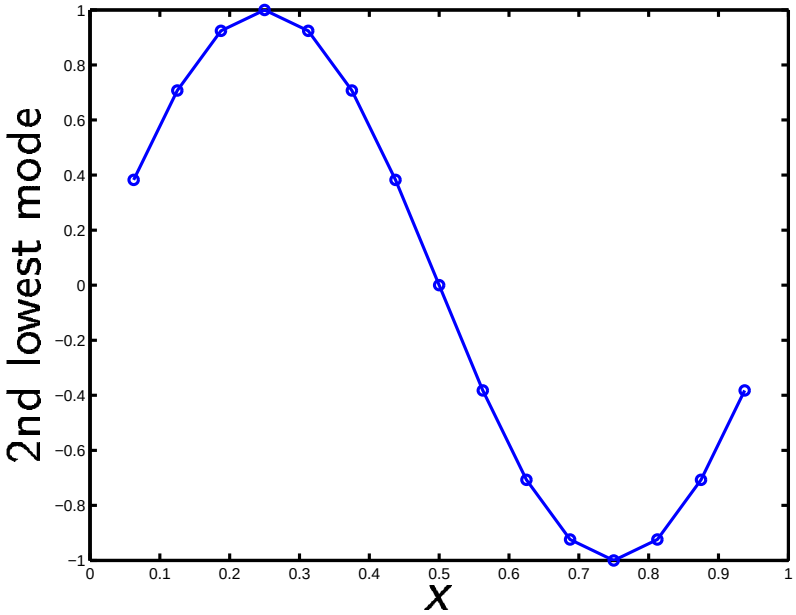


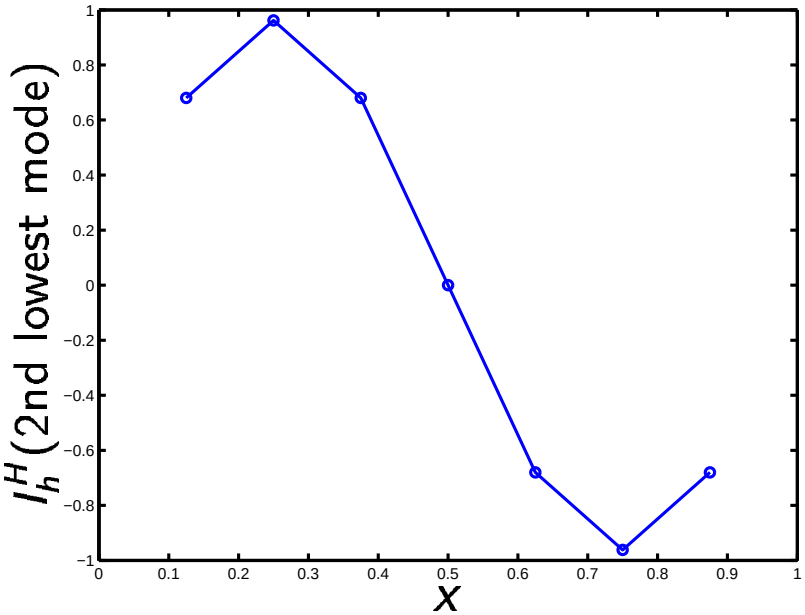


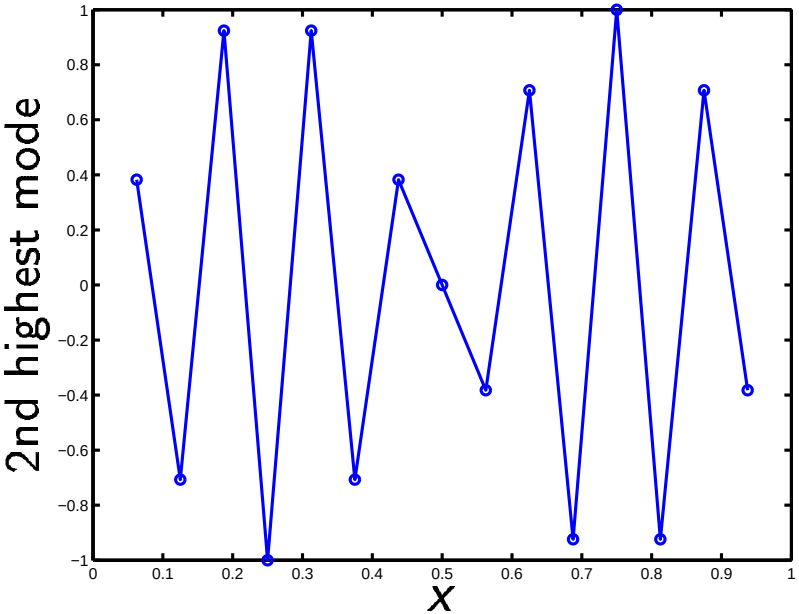


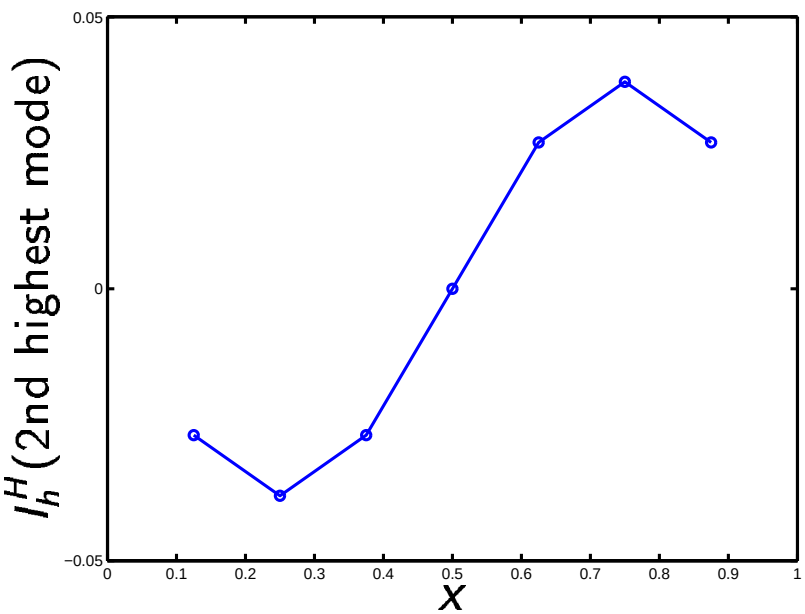


Second Lowest and Second Highest Mode









$$B = S^{\nu_2}(I - I_H^h (A^H)^{-1} I_h^H A) S^{\nu_1}$$

Using orthogonality and full weighting, $(I_h^H)^T = \frac{1}{2} I_H^h$, we obtain from the former relations on the one hand

$$(\varphi_m^H)^T I_h^H \varphi_m = c_m^2 \frac{1}{\sqrt{2}} (\varphi_m^H)^T \varphi_m^H = c_m^2 \frac{1}{\sqrt{2}}$$

and on the other hand

$$(\varphi_m^H)^T I_h^H \varphi_m = \left((\varphi_m^H)^T I_h^H \varphi_m \right)^T = \varphi_m^T (I_h^H)^T \varphi_m^H = \frac{1}{2} \varphi_m^T I_H^h \varphi_m^H$$

and thus the extension splits the low mode into the corresponding low mode on the fine grid

$$\varphi_m^T I_H^h \varphi_m^H = \sqrt{2} c_m^2$$

and similarly the corresponding high, "aliased" mode

$$\varphi_{m'}^T I_H^h \varphi_m^H = \sqrt{2} s_m^2.$$

Summary of the Convergence Analysis

Consider an error vector

$$\mathbf{e} = \alpha\varphi_m + \beta\varphi_{m'}$$

The two grid iteration operator

$$B := S^{\nu_2}(I - I_H^h (A^H)^{-1} I_h^H A) S^{\nu_1}$$

acts on the coefficients α and β of this vector as follows:

$$\begin{bmatrix} a & \\ & b \end{bmatrix}^{\nu_2} \left(I - \begin{bmatrix} c_m^2 \\ -s_m^2 \end{bmatrix} \frac{h^2}{4s_m^2 c_m^2 + \eta h^2} \begin{bmatrix} c_m^2, & -s_m^2 \end{bmatrix} \begin{bmatrix} \frac{4s_m^2}{h^2} + \eta & \\ & \frac{4c_m^2}{h^2} + \eta \end{bmatrix} \right) \begin{bmatrix} a & \\ & b \end{bmatrix}^{\nu_1}$$

where the smoothing coefficients are

$$a = 1 - \omega \frac{4s_m^2 + \eta h^2}{2 + \eta h^2}, \quad b = 1 - \omega \frac{4c_m^2 + \eta h^2}{2 + \eta h^2}.$$

On $\varphi_{\frac{M+1}{2}}$ only the smoother acts, with $b^{\nu_1+\nu_2}$.

Special Case of the Poisson Equation

If $\eta = 0$, and we choose $\omega = \frac{1}{2}$ as damping parameter in Jacobi, the action of the iteration operator B simplifies to

$$\begin{bmatrix} c_m^2 & \\ & s_m^2 \end{bmatrix}^{\nu_2} \begin{bmatrix} s_m^2 & c_m^2 \\ s_m^2 & c_m^2 \end{bmatrix} \begin{bmatrix} c_m^2 & \\ & s_m^2 \end{bmatrix}^{\nu_1}$$

and for $m = 1, 2, \ldots, \frac{M}{2}$, we have $0 < s_m^2 < \frac{1}{2}$ and $\frac{1}{2} < c_m^2 < 1$, and the complementarity of smoothing and coarse grid correction is evident.

Theorem (Convergence independent of h)

For $\nu_2 = 0$, the spectral radius of the iteration operator B is bounded by

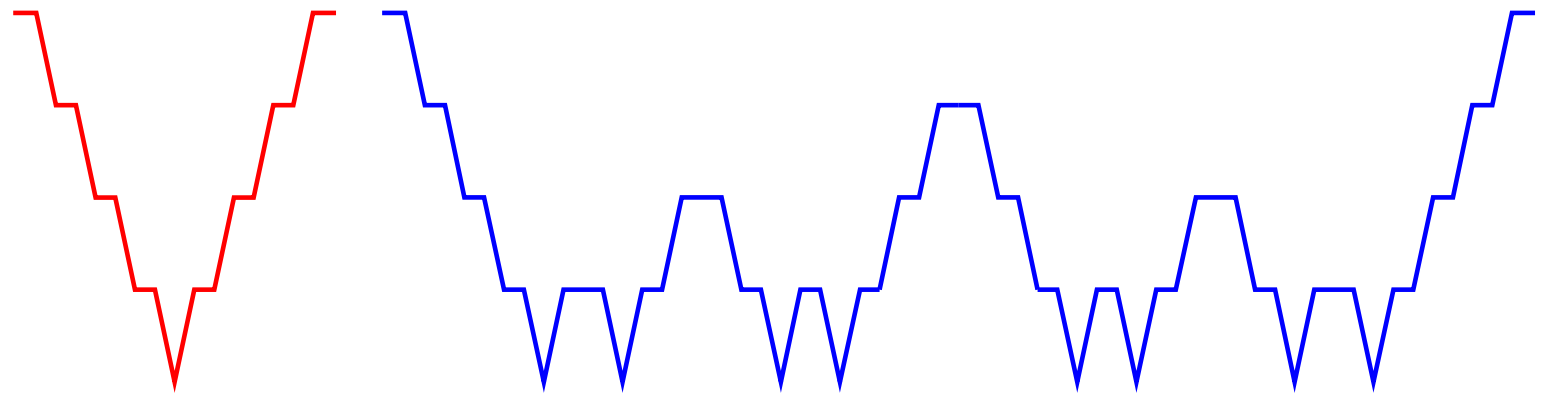
$$\max_{0 \le \xi \le \frac{1}{2}} \xi(1-\xi)^{\nu_1} + (1-\xi)\xi^{\nu_1} = [\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, 0.08333, \ldots, \sim \frac{1}{e\nu_1}]$$

Proof: The spectral radius of $\begin{bmatrix} s_m^2(c_m^2)^{\nu_1} & c_m^2(s_m^2)^{\nu_1} \\ s_m^2(c_m^2)^{\nu_1} & c_m^2(s_m^2)^{\nu_1} \end{bmatrix}$ is $s_m^2(c_m^2)^{\nu_1} + c_m^2(s_m^2)^{\nu_1}$. The dominant term is $\xi(1-\xi)^{\nu_1}$.

Classical Multigrid Cycle

Applying the same idea to the coarse problem, we get one multigrid cycle:

```
function u=Cycle(A,f,u0);
if isSmall(A) then u=A\f else
    u=Smooth1(A,f,u0);
    r=Restrict(f-Au);
    e=0; for i=1:n, e=Cycle(A^H,r,e); end;
    u=u+Extend(e);
    u=Smooth2(A,f,u);
end;
```



$n = 1$ V-cycle $n = 2$ W-cycle

Multigrid Algorithm Variants

Classical Multigrid Method:

```
u=u0;
for i=1:n, u=Cycle(A,f,u); end;
```

Full Multigrid Method:

```
u=A0\f0;
for j=1:l
    u=I_h^H u;
    for i=1:n, u=Cycle(Aj,f,u); end;
end;
```

Full Approximation Scheme: (nonlinear 2 grid cycle)

$$
\begin{aligned}
u &= \text{Smooth1}(A, f, u) \\
\text{solve } A^H(U) &= I_h^H(f - A^h(u)) + A^H(I_h^H u) \\
u &= u + I_H^h(U - I_h^H u) \\
u &= \text{Smooth2}(A, f, u)
\end{aligned}
$$

Wave Propagation Problems

We consider now the Helmholtz equation

$$\mathcal{L}u := -(\Delta + k^2)u = f, \quad \text{in } \Omega \subset \mathbb{R}^2$$

with appropriate boundary conditions.

This equation is very similar to the equation we considered before,

$$\mathcal{L}u := -(\Delta - \eta)u = f, \quad \text{in } \Omega \subset \mathbb{R}^2$$

and discretization leads again to a linear system

$$L\mathbf{u} = \mathbf{f},$$

but in the Helmholtz case, this system is indefinite, there are positive and negative eigenvalues.

How does this influence a multigrid method ?

A Very Early Reference

Bakhvalov 1965: On the Convergence of a Relaxation Method with Natural Constraints on the Elliptic Operator

For instance it is used in the case of the equation $\Delta u + \lambda u = f$ *with large positive* $\lambda(x_1, x_2)$. *Previously no methods of solving this equation with good asymptotics for the number of operations were known.*

... we carry out Abel's transformation and are convinced of the truth of the equality ...

In the case of the equation $\Delta u + \lambda u = f$ *with large positive* λ *we do not exclude the possibility that the evaluation of (3.21) may be attained in order. Then the increase in the number m in comparison with that calculated can lead to a deterioration in the discrepancy of the approximation.*

Problems for Helmholtz: from the Literature

Brandt and Livshits (1997):

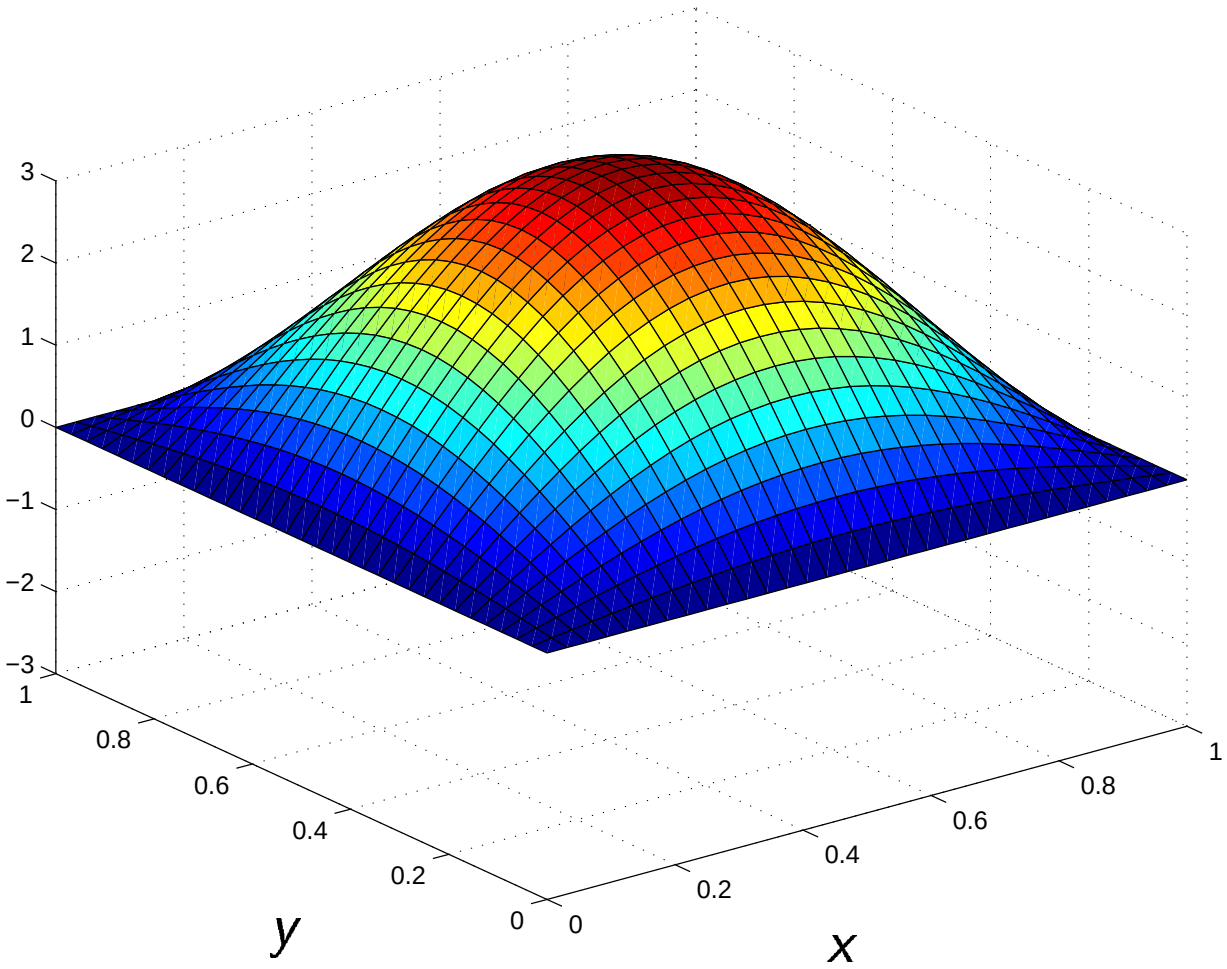
On the fine grids, where [the characteristic components] are accurately approximated by the discrete equations, they are invisible to any local relaxation, since their errors can have very small residuals. On the other hand, on coarser grids such components cannot be approximated, because the grid does not resolve their oscillations. Thus, there is a need for an alternative approach for reducing characteristic error components.

Lee, Manteuffel, McCormick and Ruge (2000):

Helmholtz problems tax multigrid methods by admitting certain highly oscillatory error components that yield relatively small residuals. Because these components are oscillatory, standard coarse grids cannot represent them well, so coarsening cannot eliminate them effectively. Because they yield small residuals, standard relaxation methods cannot effectively reduce them.

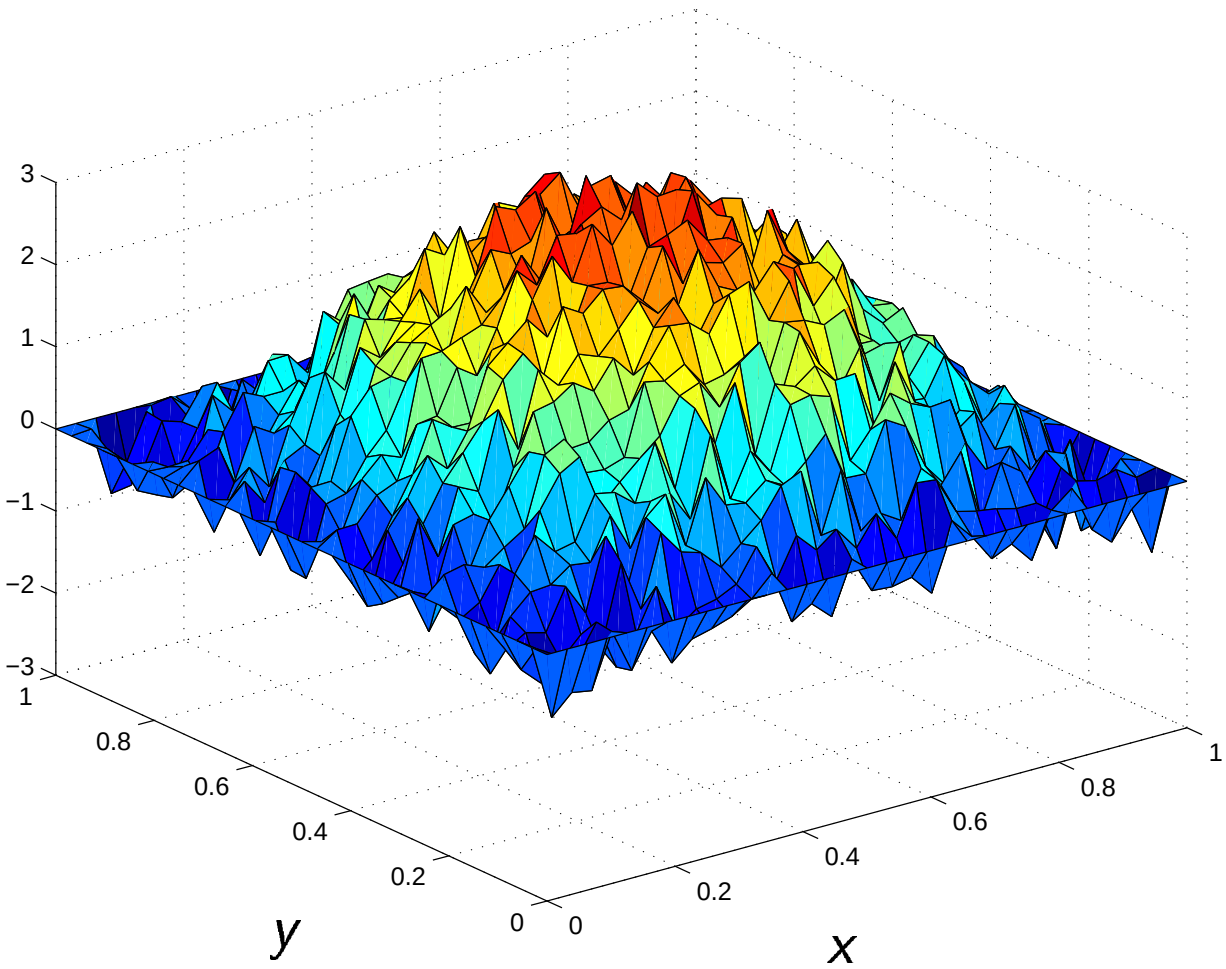
Problems of the Coarse Grid Correction

Example: solution we try to compute on $\Omega = (0,1) \times (0,1)$, $f = -\frac{1}{20}$, $h = \frac{1}{32}$, $k^2 = 19.7$ is

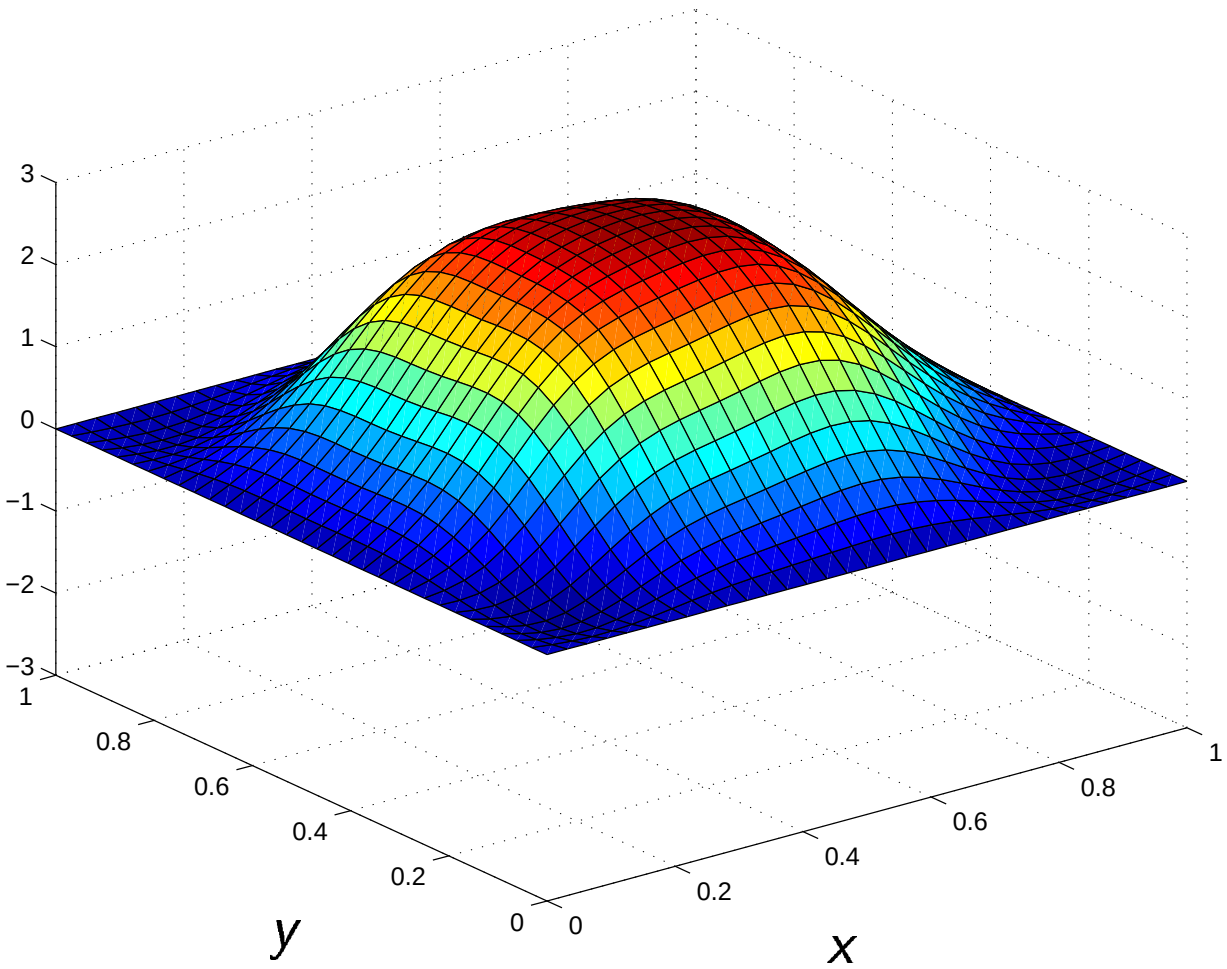


Random initial guess u_0, two grid cycle, Fourier smoothing (using the Boris Diskin principle)

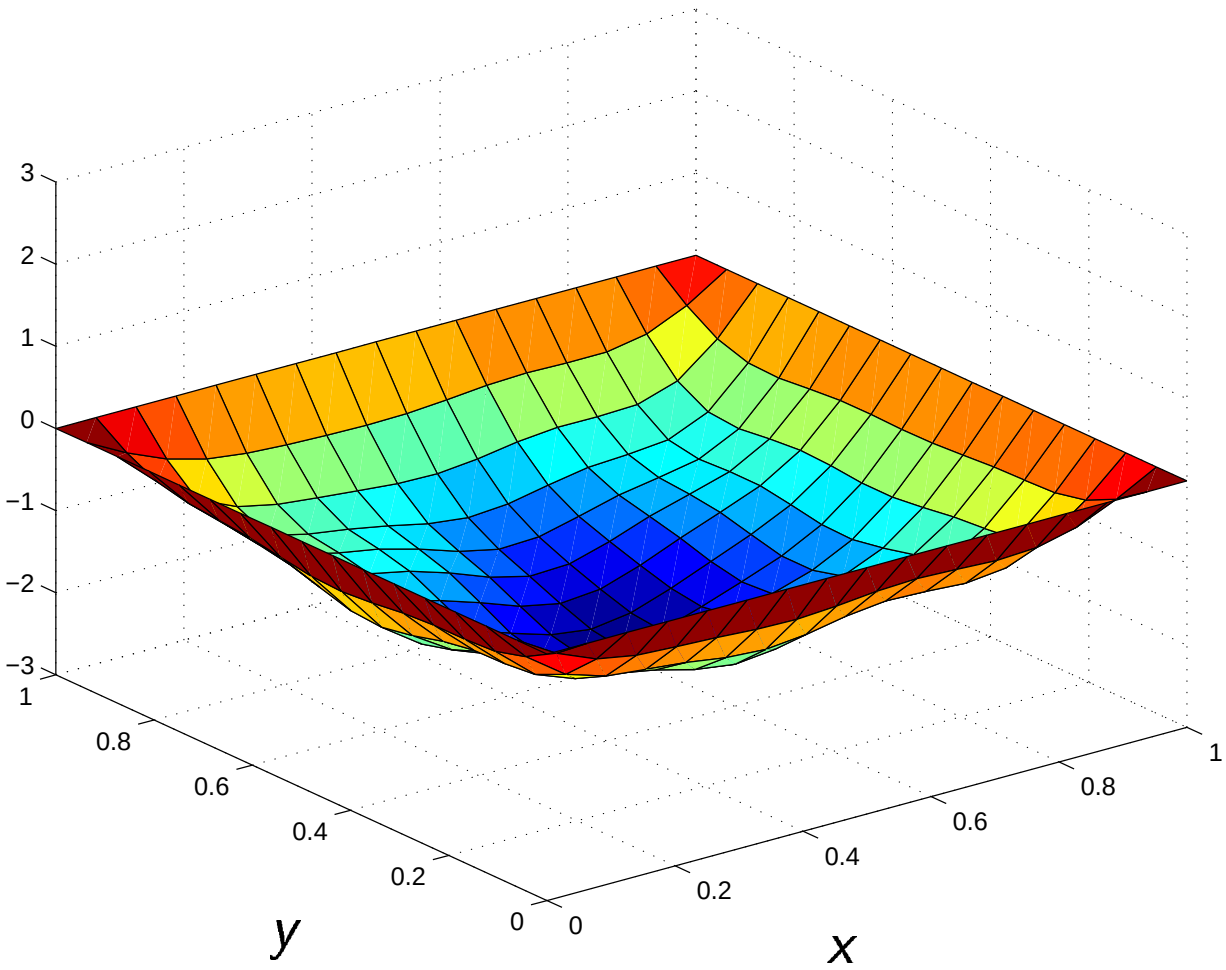
Iteration 1: error before presmoothing



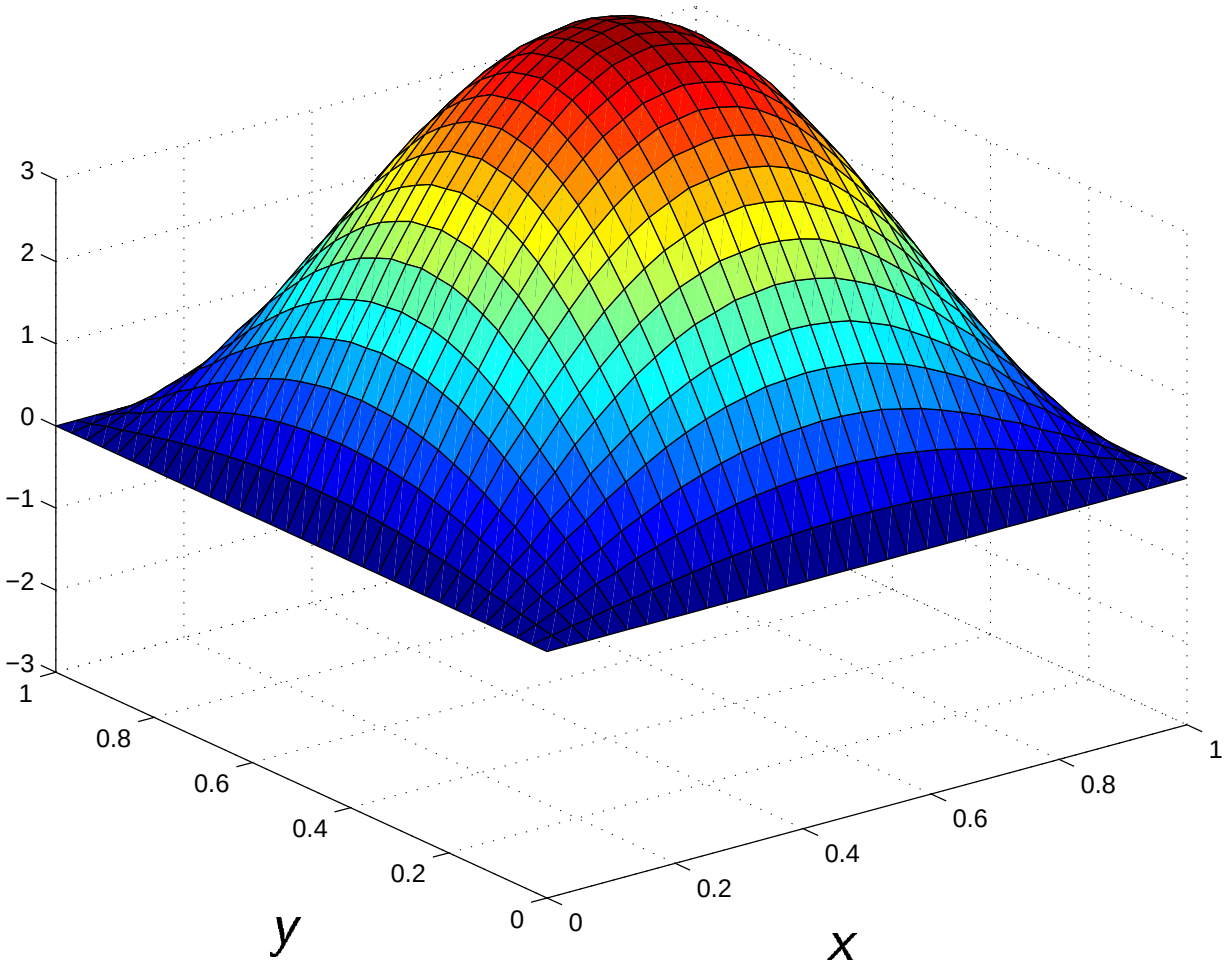
Iteration 1: error after presmoothing



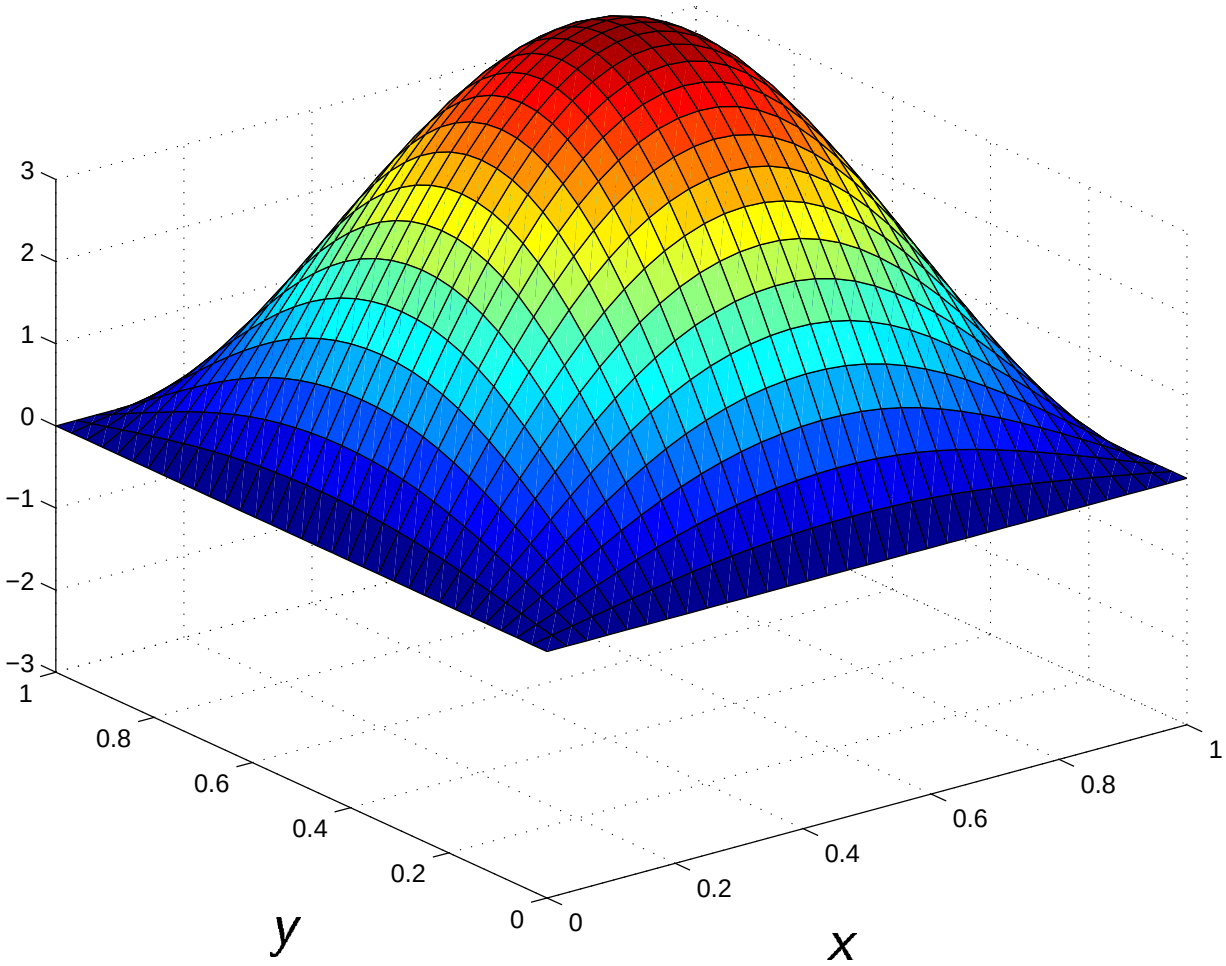
Iteration 1: error to remove from coarse grid correction



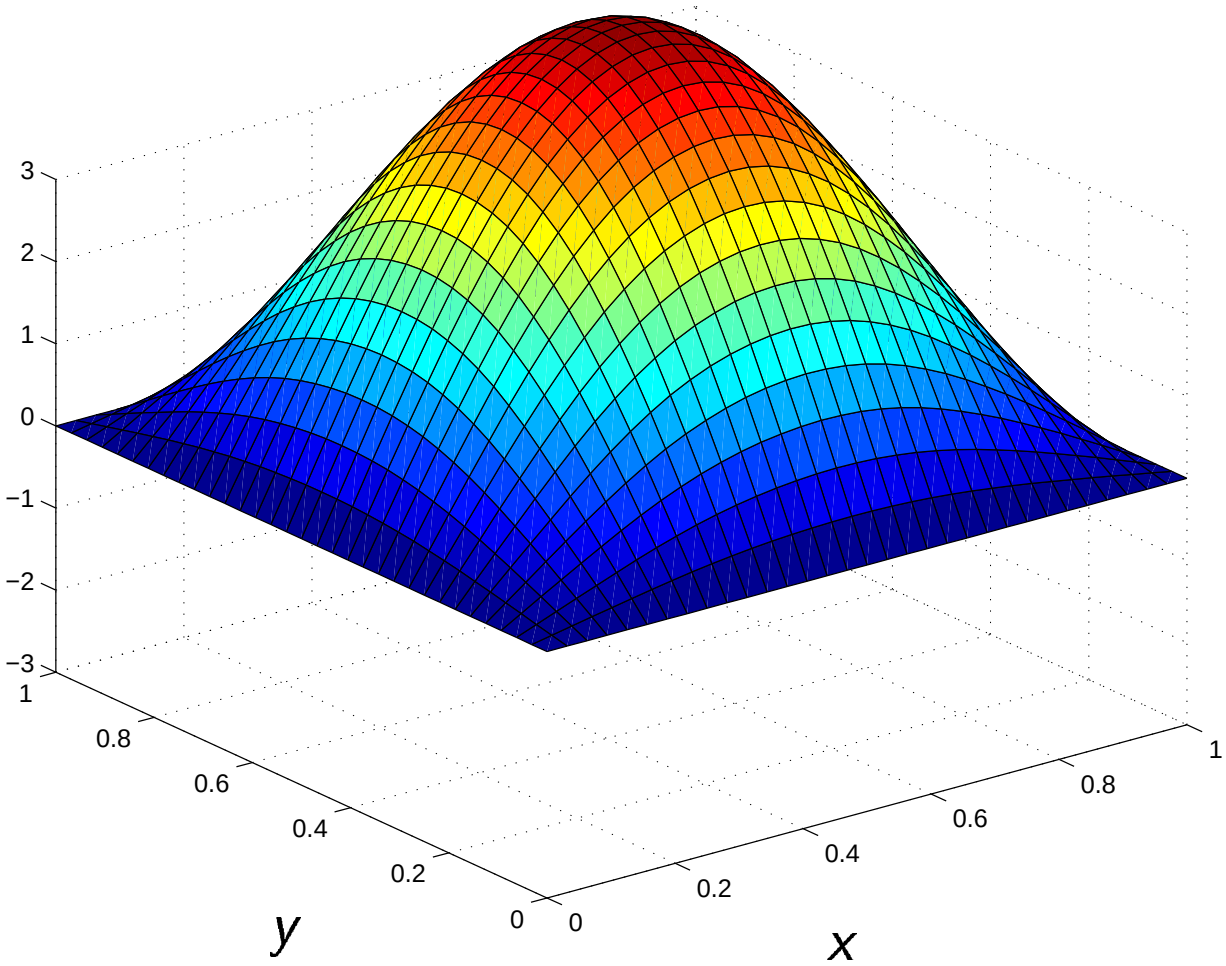
Iteration 1: error before postsmoothing



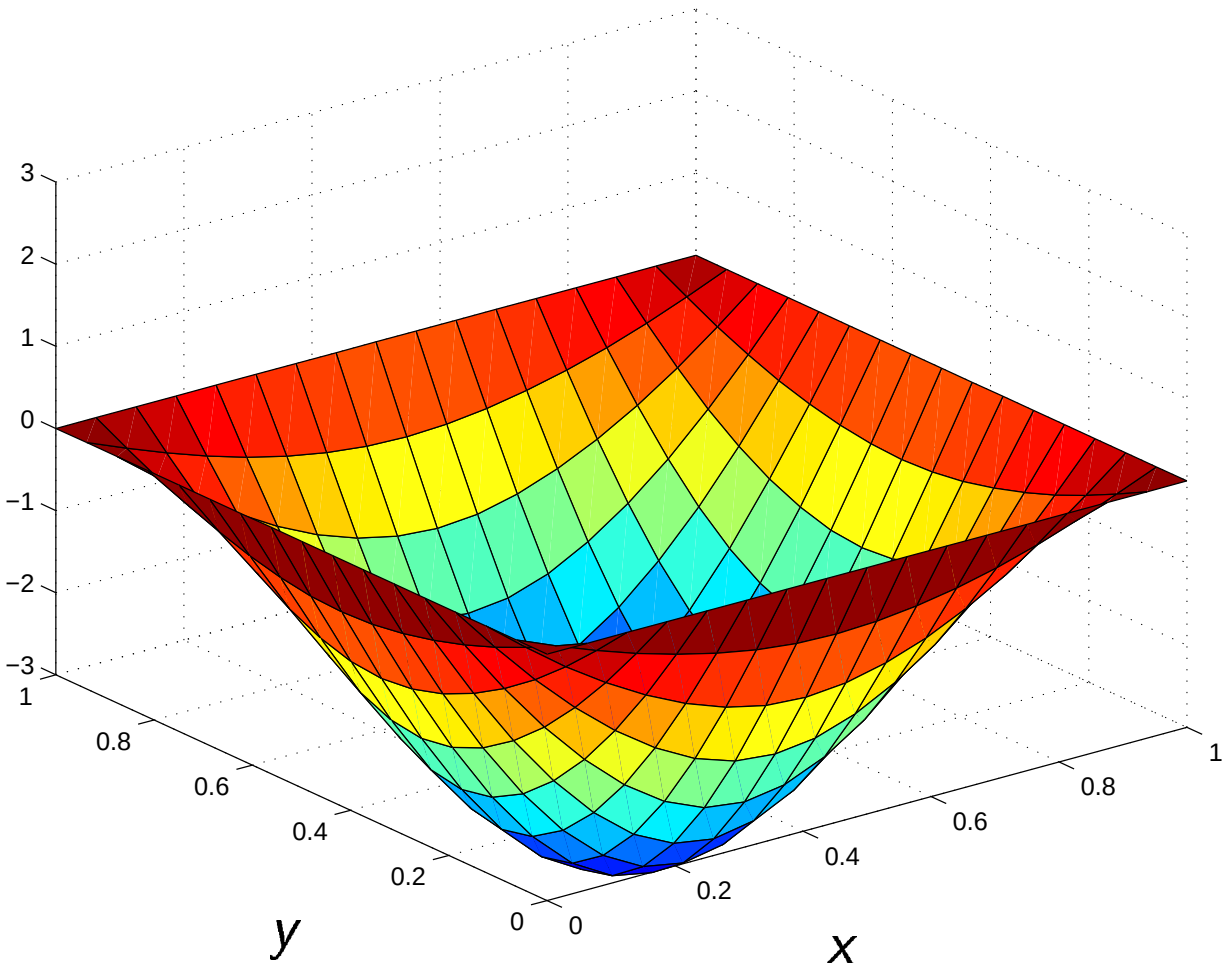
Iteration 1: error after postsmoothing



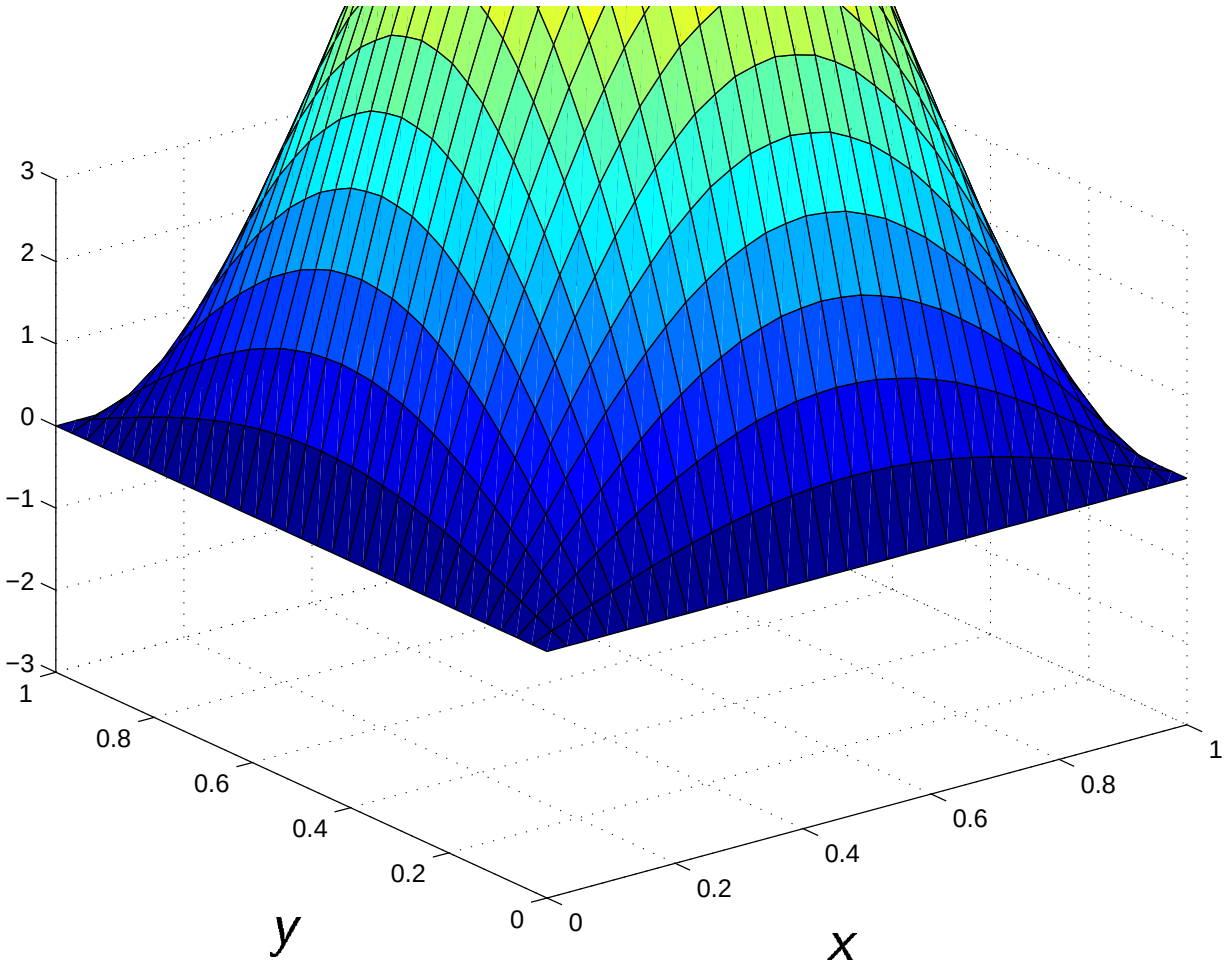
Iteration 2: error after presmoothing



Iteration 2: error to remove from coarse grid correction



Iteration 2: error before postsmoothing



Observation

- while the error on the coarse grid is well resolved, the correction calculated on the coarse grid is 100% incorrect, it has the wrong sign!
- the problem does not seem to be that certain high frequency components in the error are left to the coarse grid and can not be approximated accurately there.

Brandt and Ta'asan (1986):

Usual multigrid for indefinite problems is sometimes found to be very inefficient. A strong limitation exists on the coarsest grid to be used in the process. The limitation is not so much a result of the indefiniteness itself, but of the nearness to singularity, that is, the existence of nearly zero eigenvalues. These eigenvalues are badly approximated (e.g. they may even have a different sign) on coarse grids, hence the corresponding eigenfunctions, which are usually smooth ones, cannot efficiently converge.

Fourier Analysis of the Coarse Grid Correction

In order to explain, we consider the 1d case

$$-u_{xx} - k^2 u = f, \qquad \text{on } \Omega = (0,1),$$

with homogeneous Dirichlet conditions.

Discretization by finite differences with $h = \frac{1}{M+1}$ on the mesh $x_m = mh$, $m = 1, 2, \ldots, M$, leads to

$$L^h \mathbf{u}^h := \frac{1}{h^2} \begin{bmatrix} 2 - h^2 k^2 & -1 & & \\ & \ddots & \ddots & \\ & -1 & & \end{bmatrix} \mathbf{u}^h = \mathbf{f}^h.$$

The eigenvalues and eigenvectors of L^h are

$$\lambda_m^h = \frac{1}{h^2}(2 - 2\cos(m\pi h)) - k^2, \quad \varphi_m^h(l) = \sin(m\pi x_l),$$

for $m = 1, 2, \ldots, M$.

Fourier Analysis of the Coarse Grid Correction

Suppose on the fine grid, we have an error component $\varphi_1^h = \sin(\pi \mathbf{x})$. This function is very smooth and can be well approximated on the coarse grid. The fine grid residual of this error is

$$L^h \varphi_1^h = \lambda_1^h \varphi_1^h$$

and thus the coarse grid correction is solution of $(H = 2h)$

$$L^H \mathbf{v}^H = \lambda_1^h I_h^H \varphi_1^h.$$

Since the eigenfunction is smooth, $I_h^H \varphi_1^h$ is still approximately an eigenfunction of L^H with eigenvalue λ_1^H, and thus the coarse grid correction is

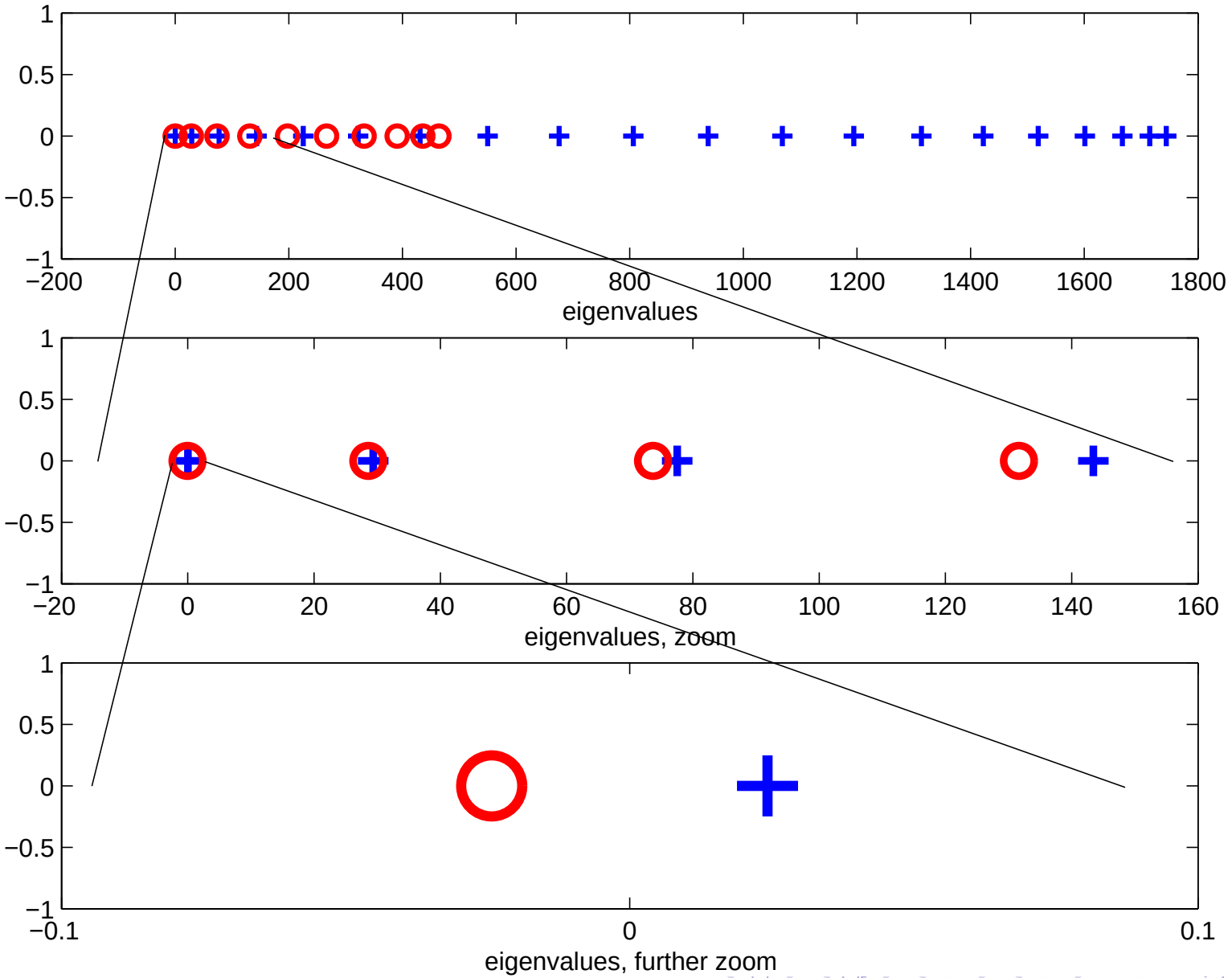
$$\mathbf{v}^H \approx \frac{\lambda_1^h}{\lambda_1^H} I_h^H \varphi_1^h$$

and the new error after correction is

$$\varphi_1^h - I_H^h \mathbf{v}^H \approx \left(1 - \frac{\lambda_1^h}{\lambda_1^H}\right) \varphi_1^h.$$

How Big Can the Error Be ?

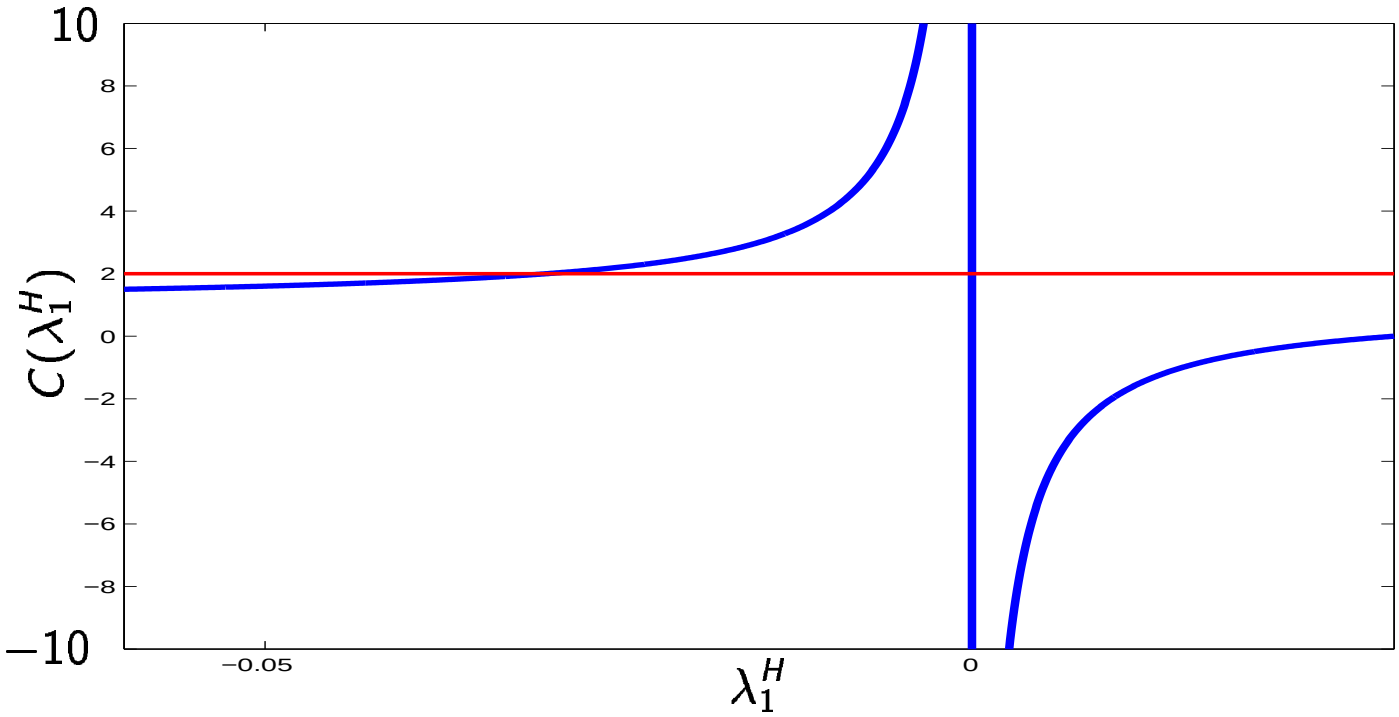
If $\lambda_1^H \approx \lambda_1^h$, then the error after correction is small. **BUT**



It Can Be Much More Than Just Double

Since λ_m^H can be arbitrarily close to zero if λ_m^h was close to zero, the error after the correction can be arbitrary large:

$$\varphi_1^h - I_H^h \mathbf{v}^H \approx \left(1 - \frac{\lambda_1^h}{\lambda_1^H}\right) \varphi_1^h = C(\lambda_1^H)\varphi_1^h$$

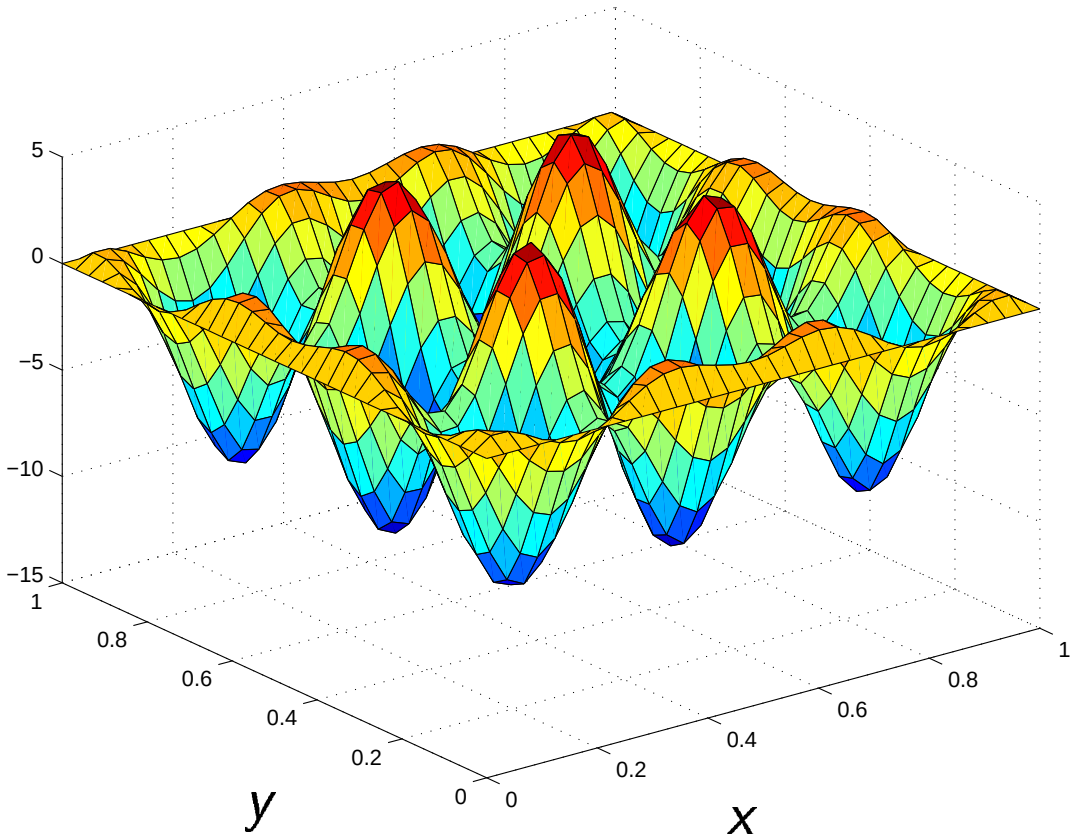


If $k = 0$, the positive definite case, we have

$$\lim_{H=\frac{1}{2}} C(\lambda_1^H) = -3 + 2\sqrt{2} \approx -0.1716.$$

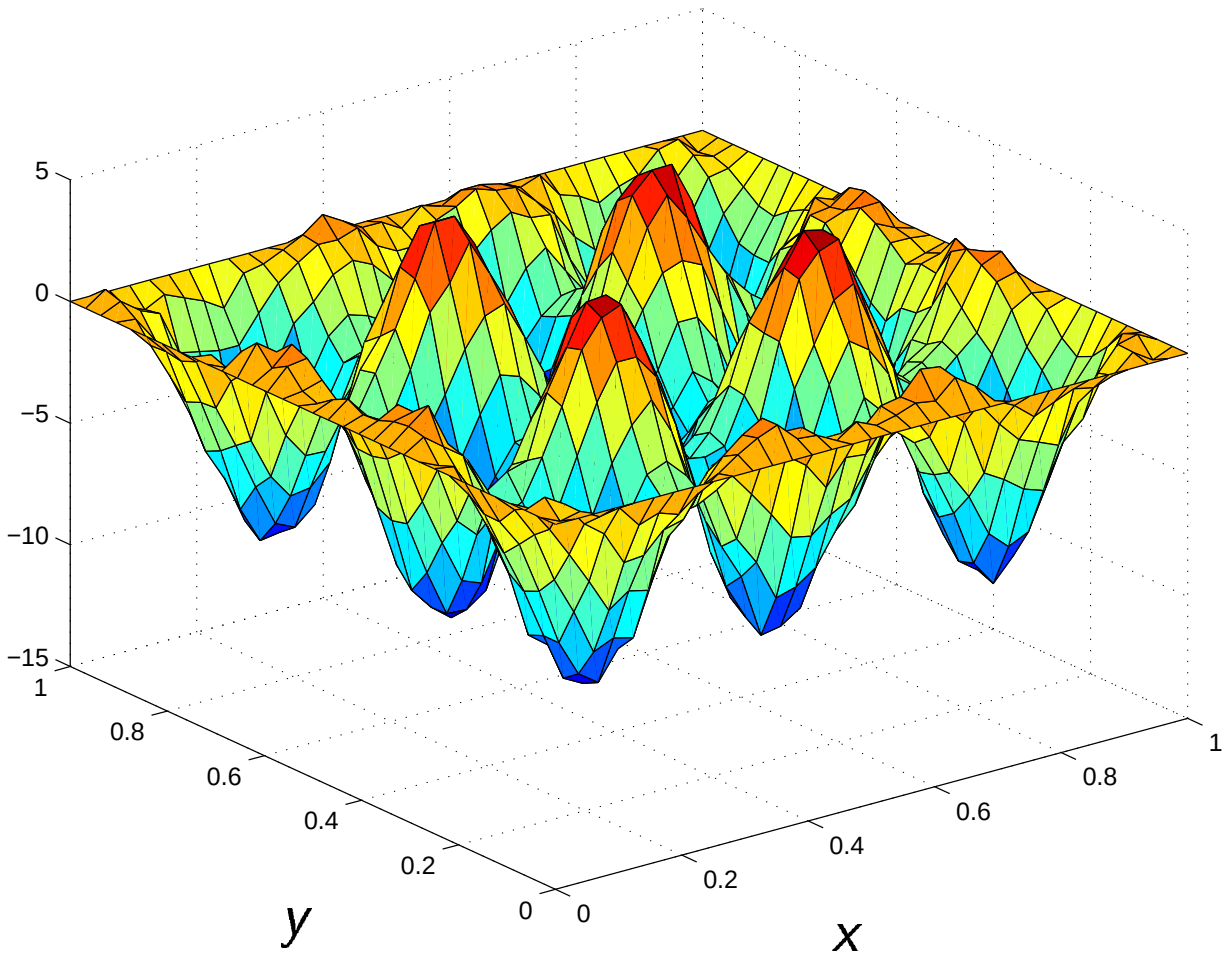
Problems of the Smoother

Example: solution we try to compute on $\Omega = (0,1) \times (0,1)$, $f = -1000$, $h = \frac{1}{32}$, $k^2 = 400$ is

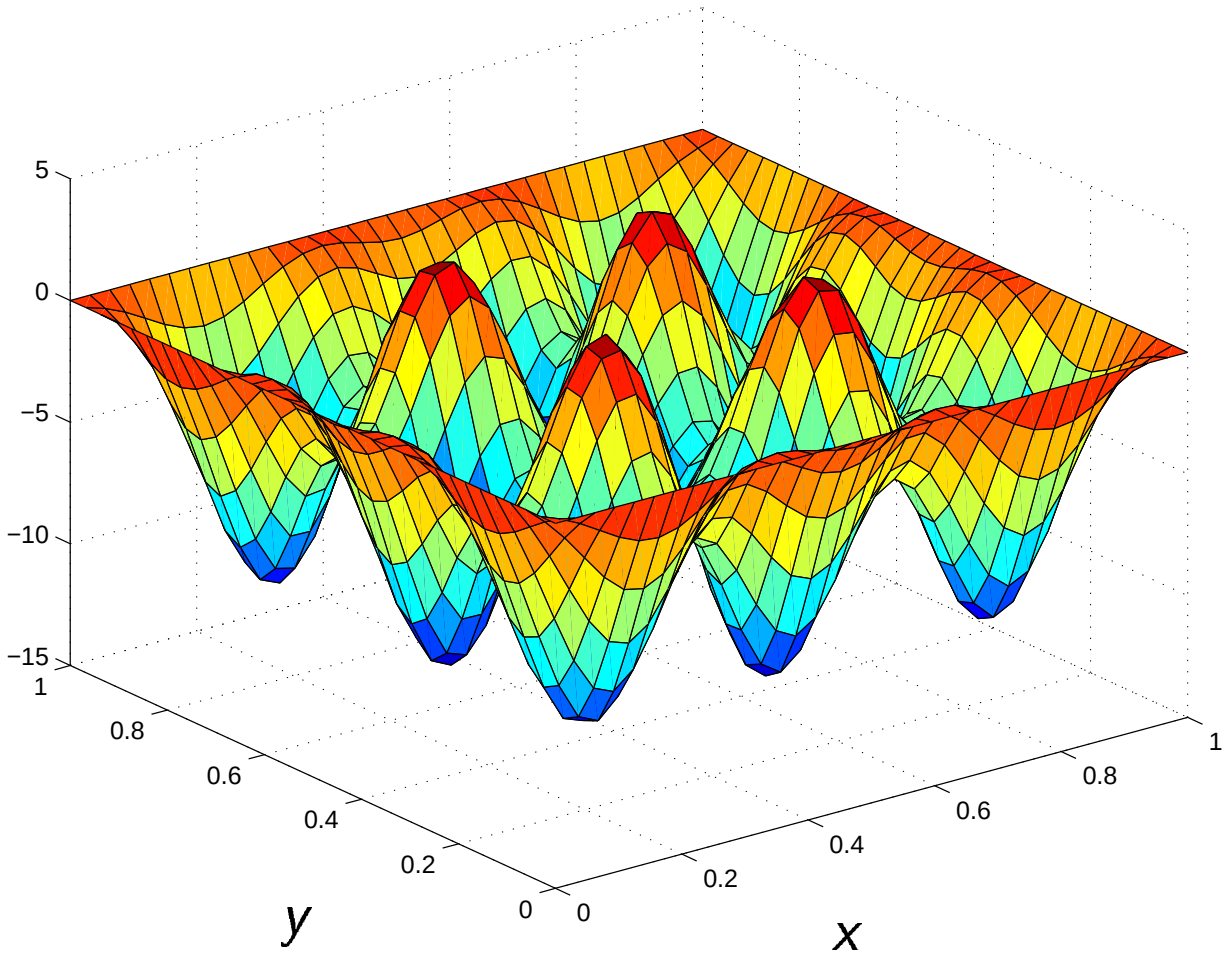


Random initial guess u_0, two grid cycle, exact coarse grid correction (the exact error on the fine grid, just restricted and extended), and an optimally relaxed Jacobi smoother.

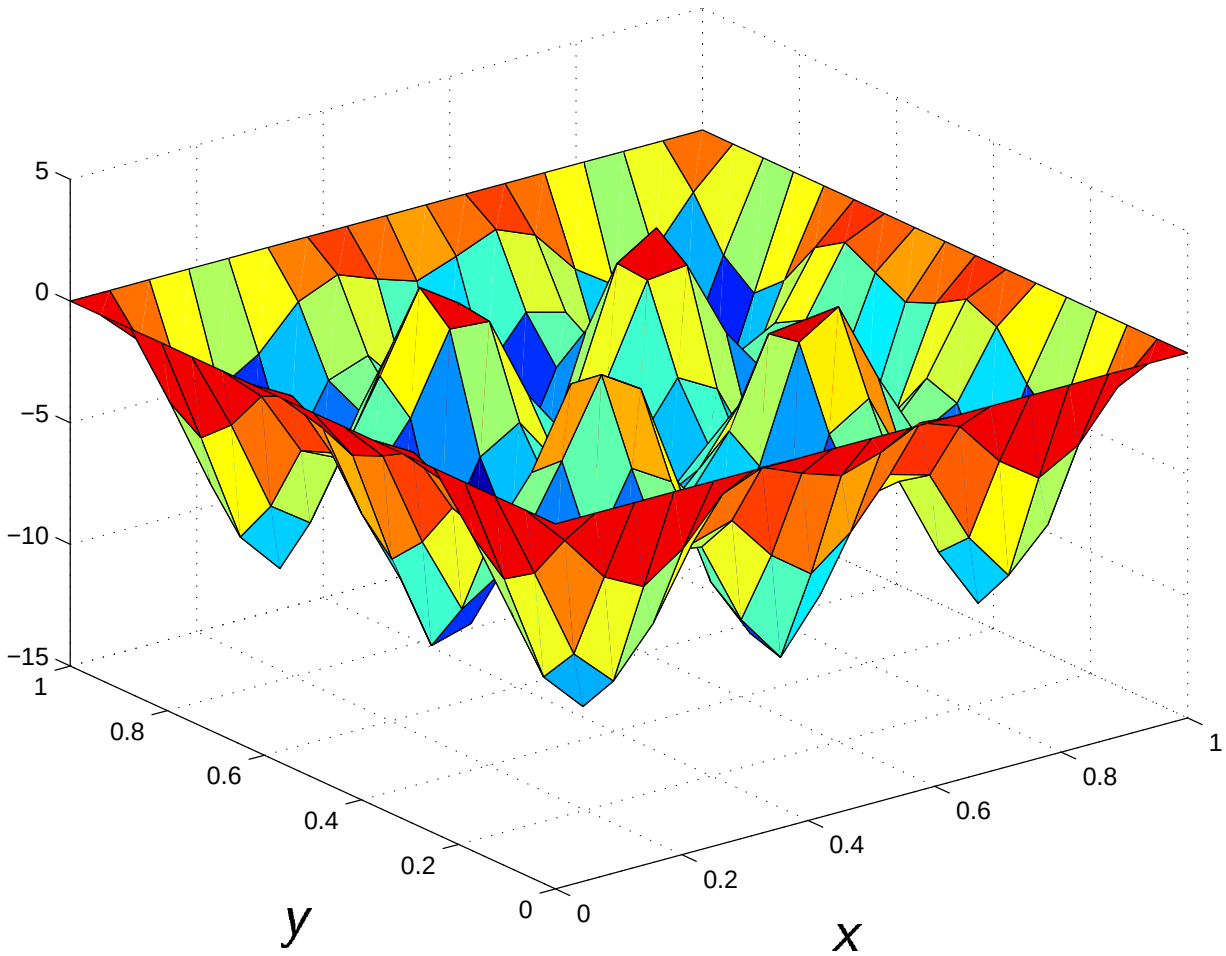
Iteration 1: error before presmoothing



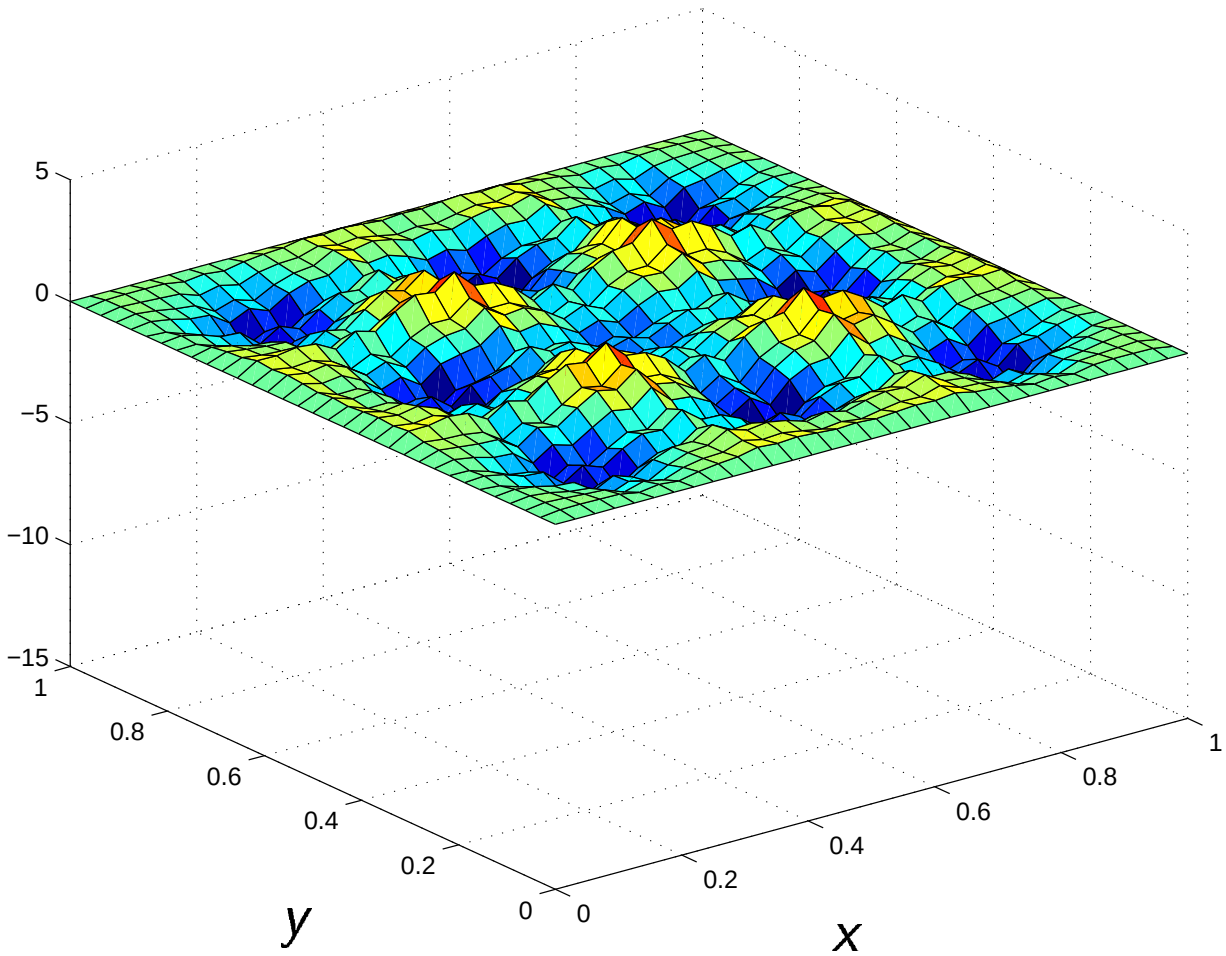
Iteration 1: error after presmoothing



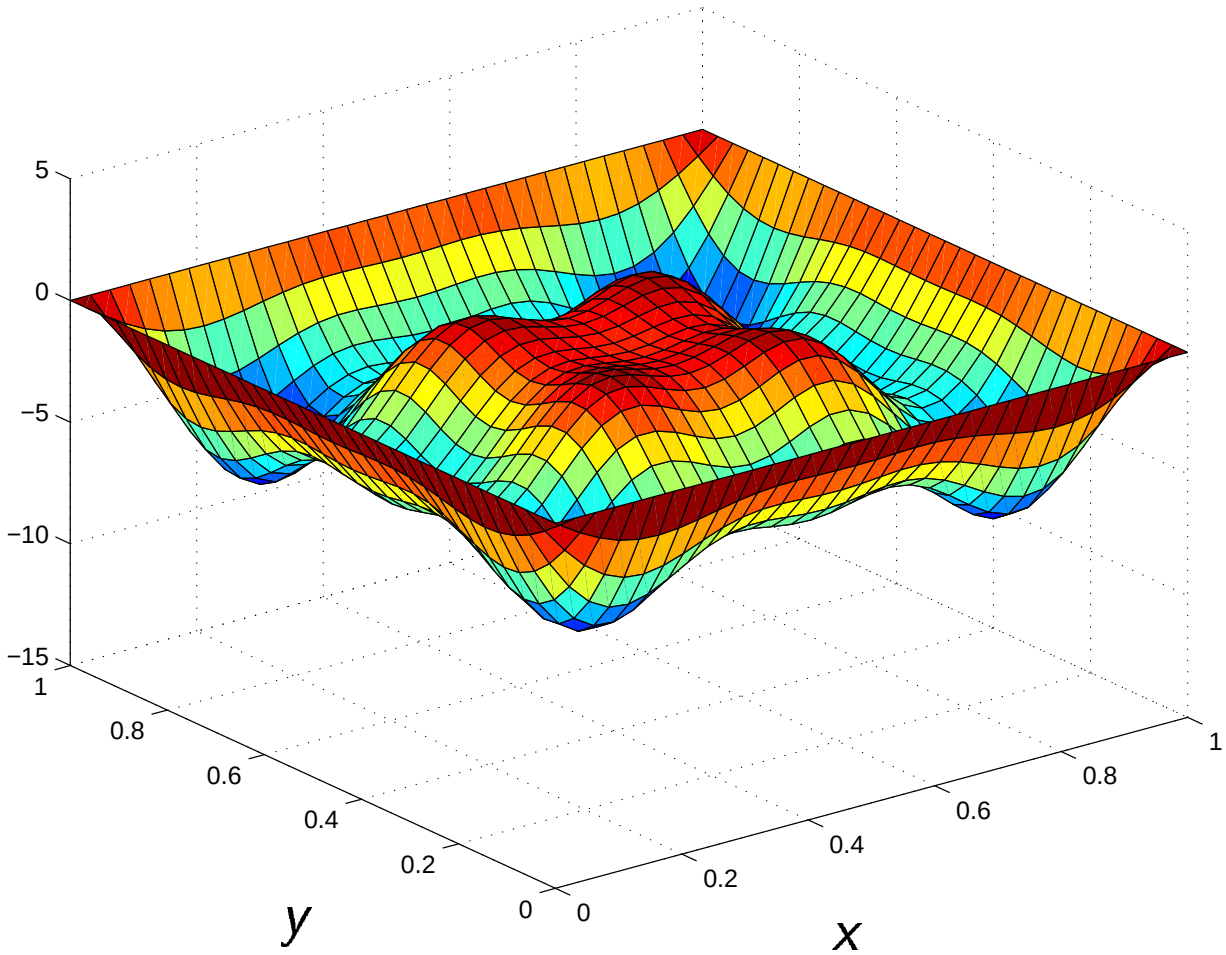
Iteration 1: error to remove from coarse grid correction



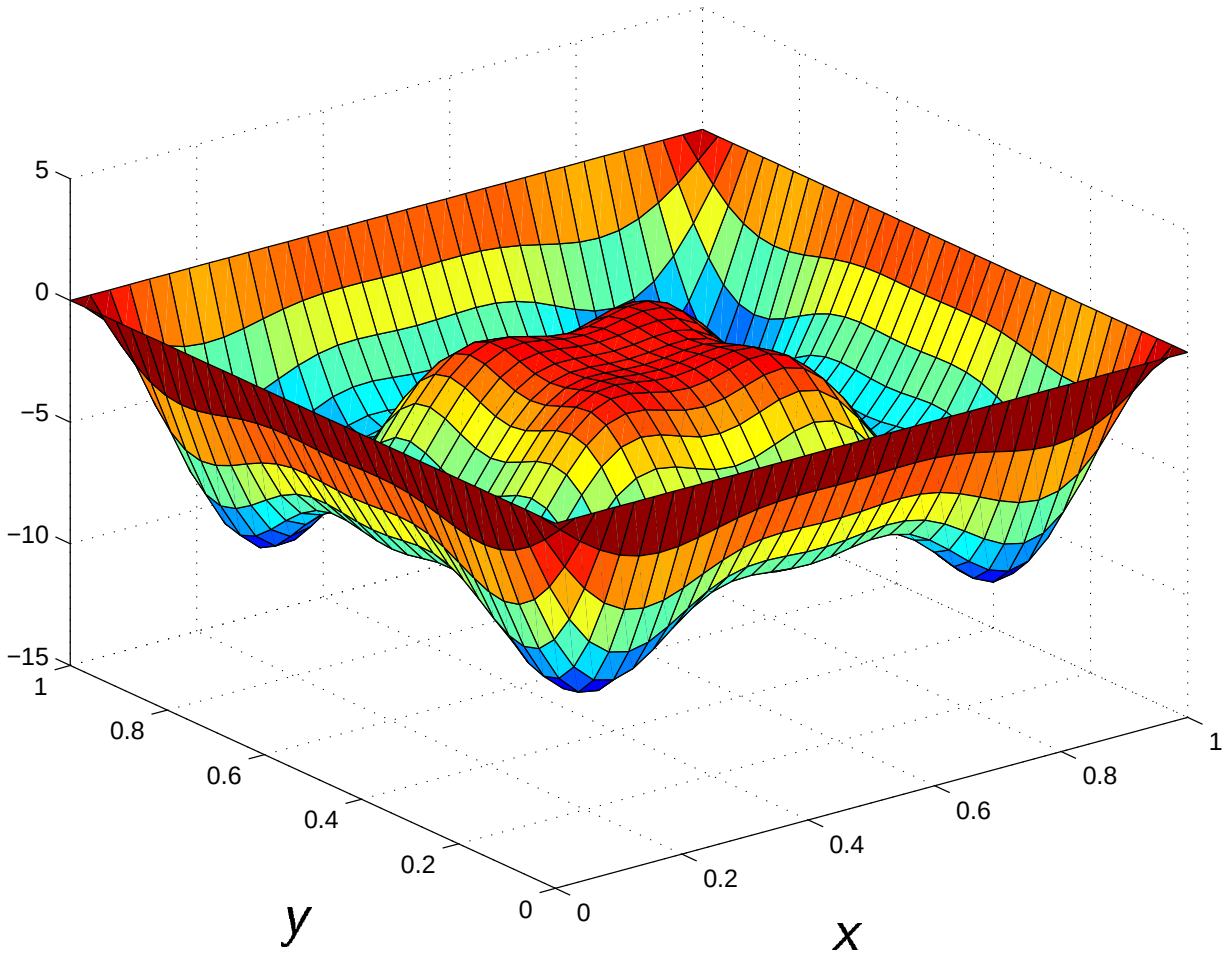
Iteration 1: error before postsmoothing



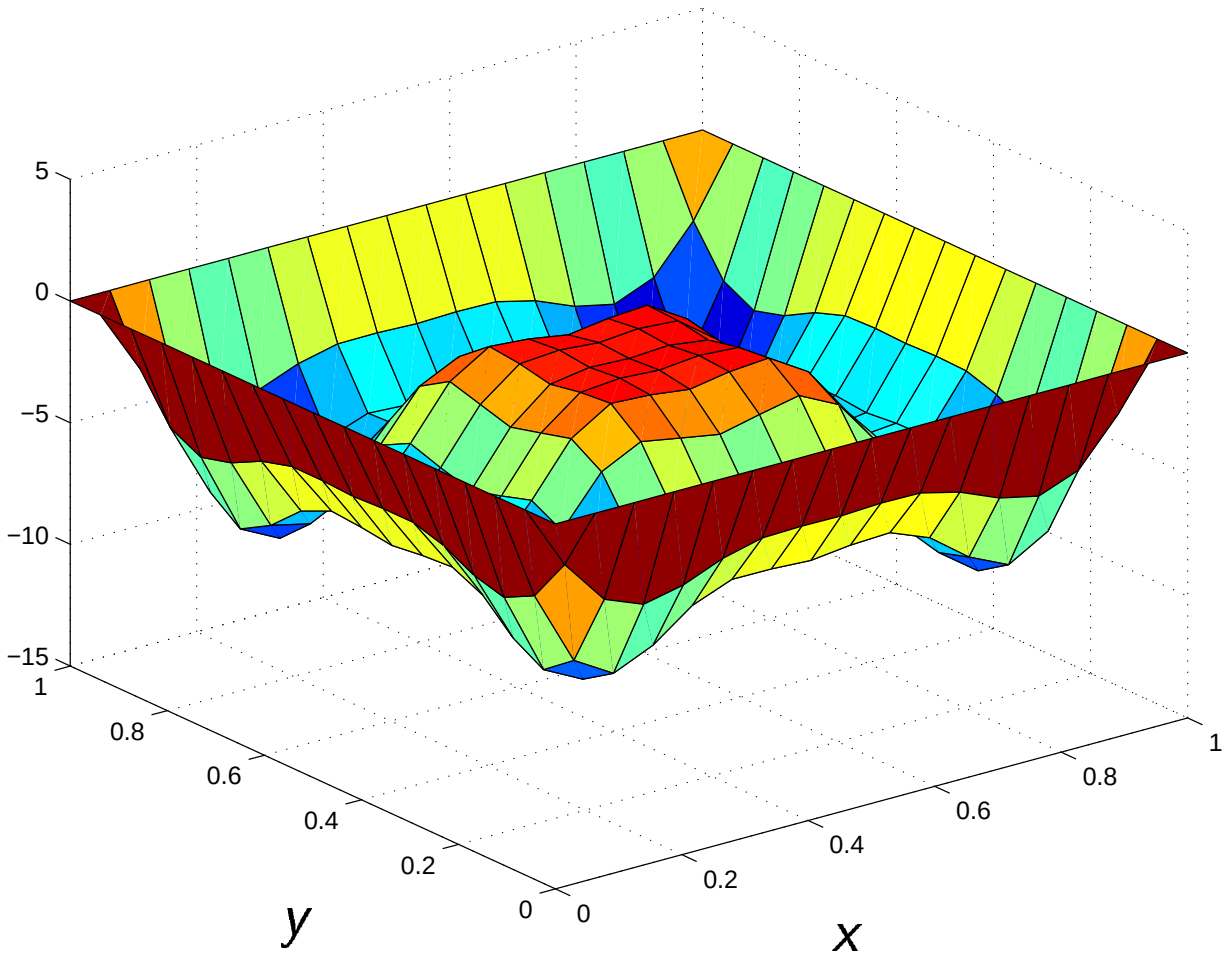
Iteration 1: error after postsmoothing



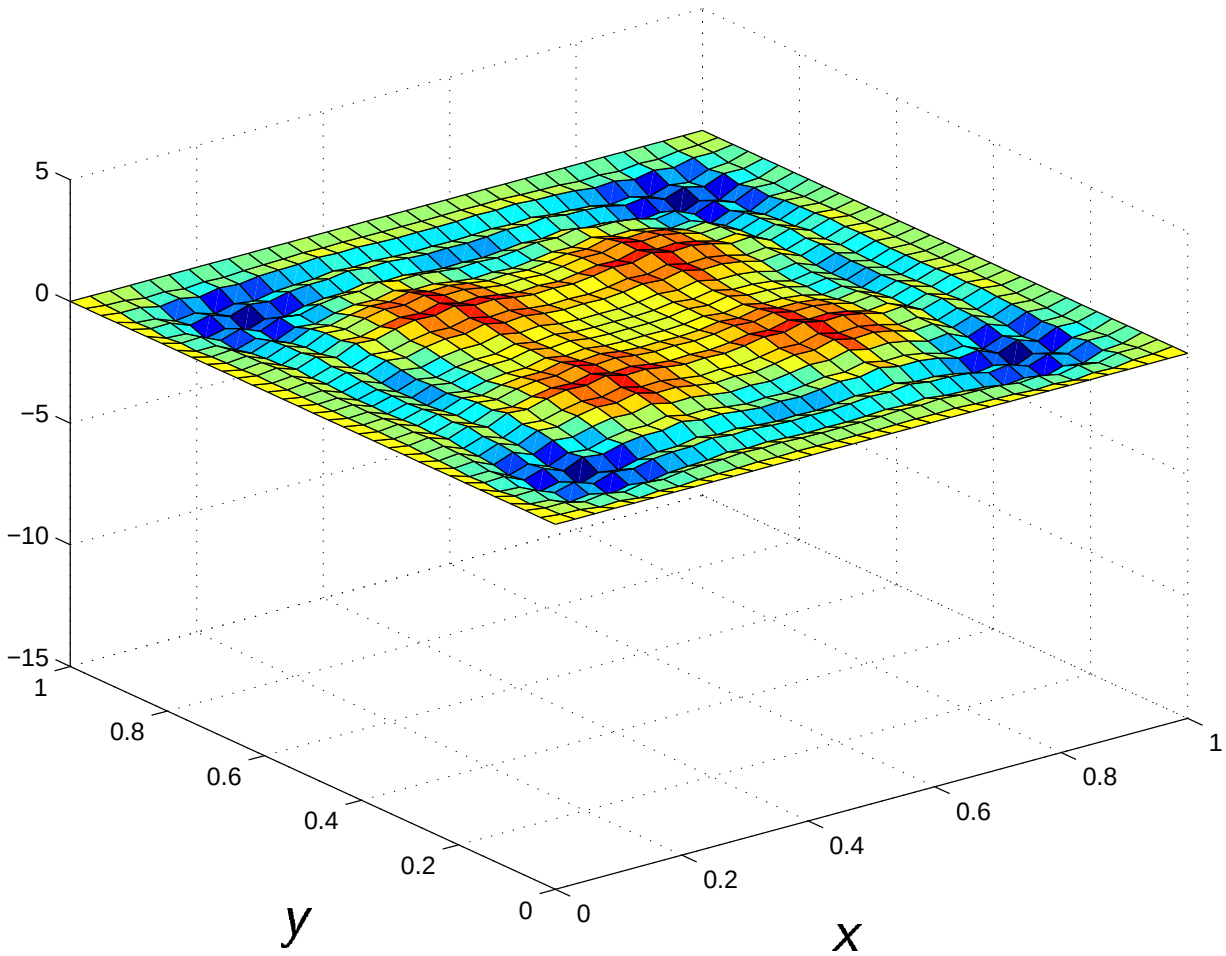
Iteration 2: error after presmoothing



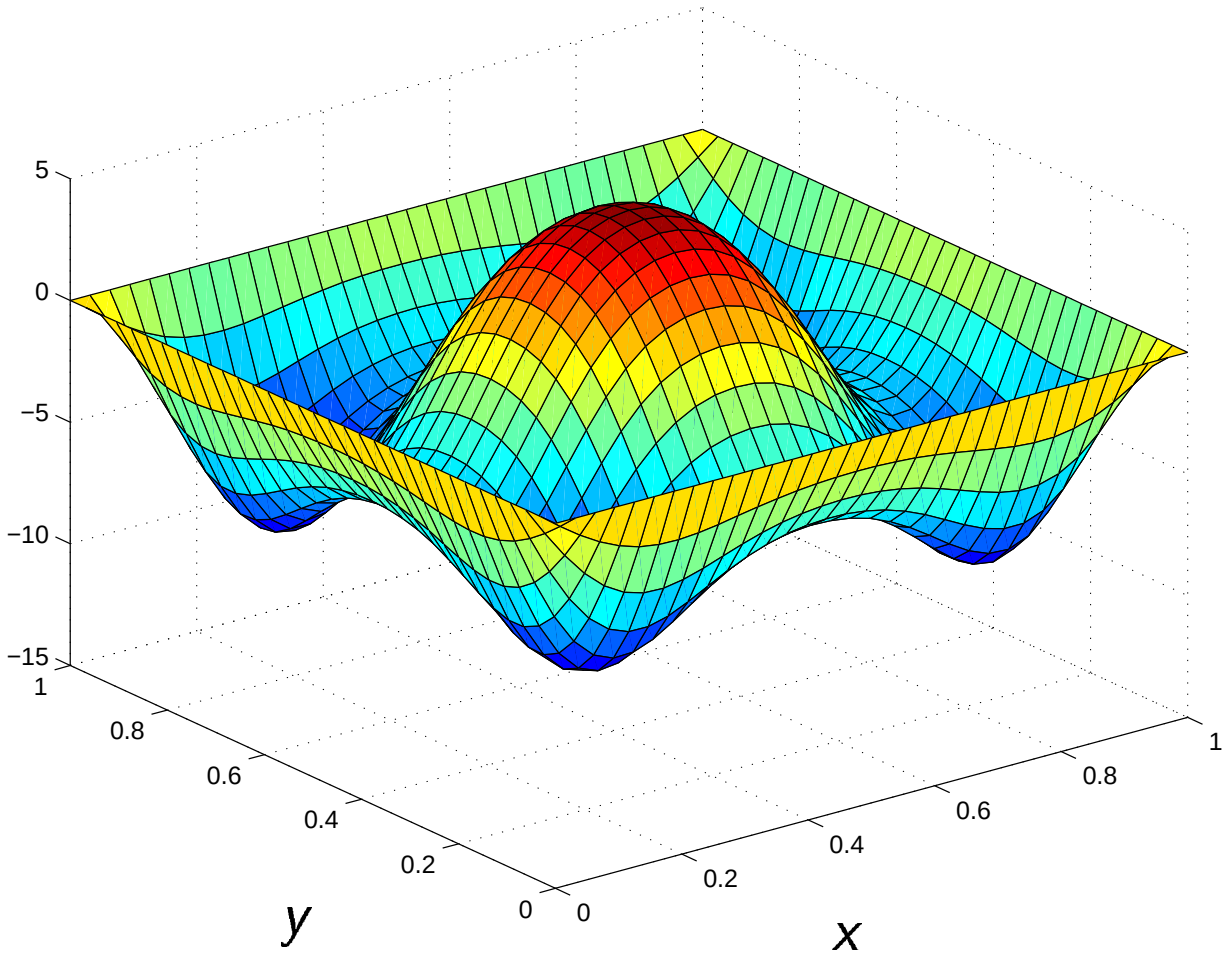
Iteration 2: error to remove from coarse grid correction



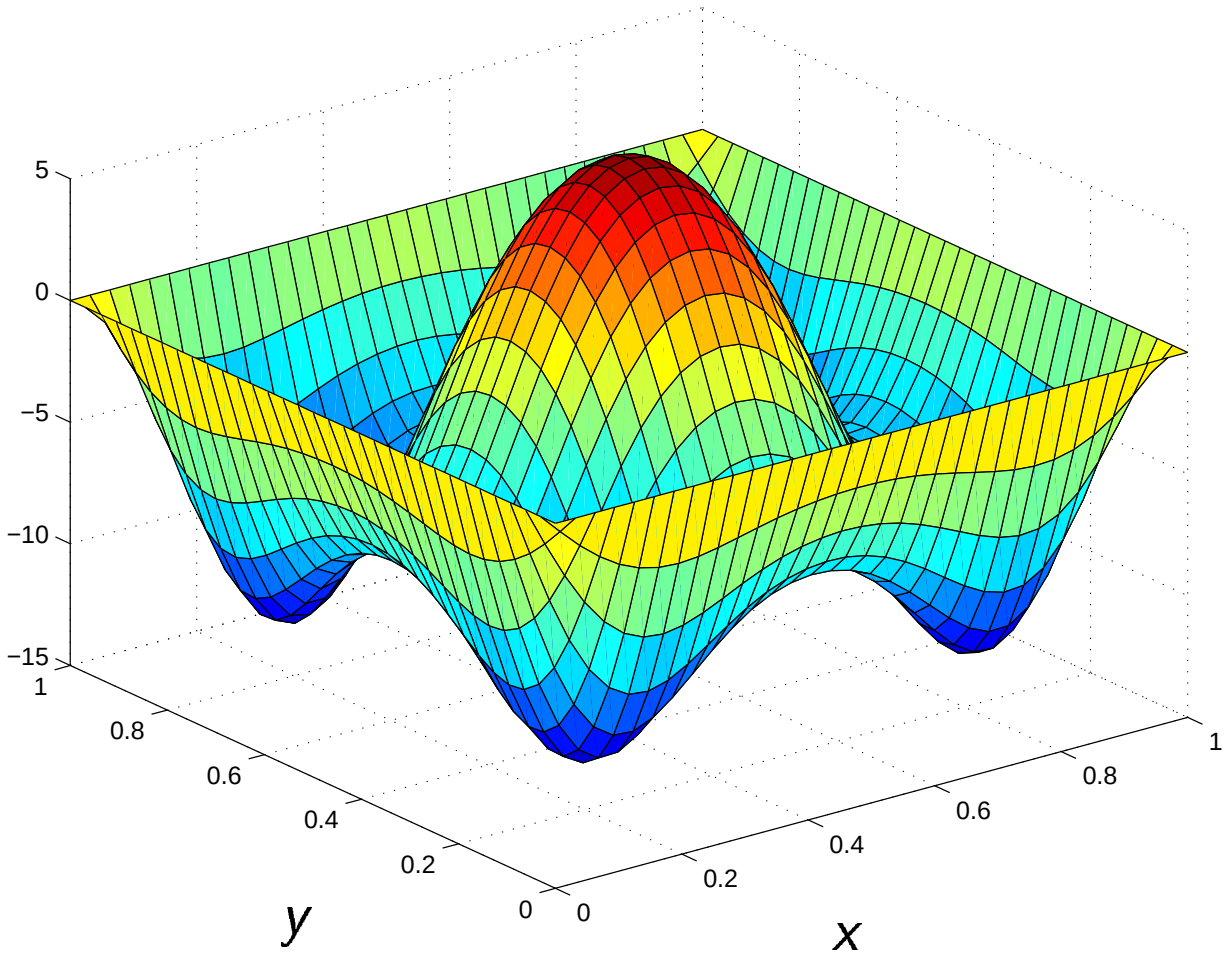
Iteration 2: error before postsmoothing



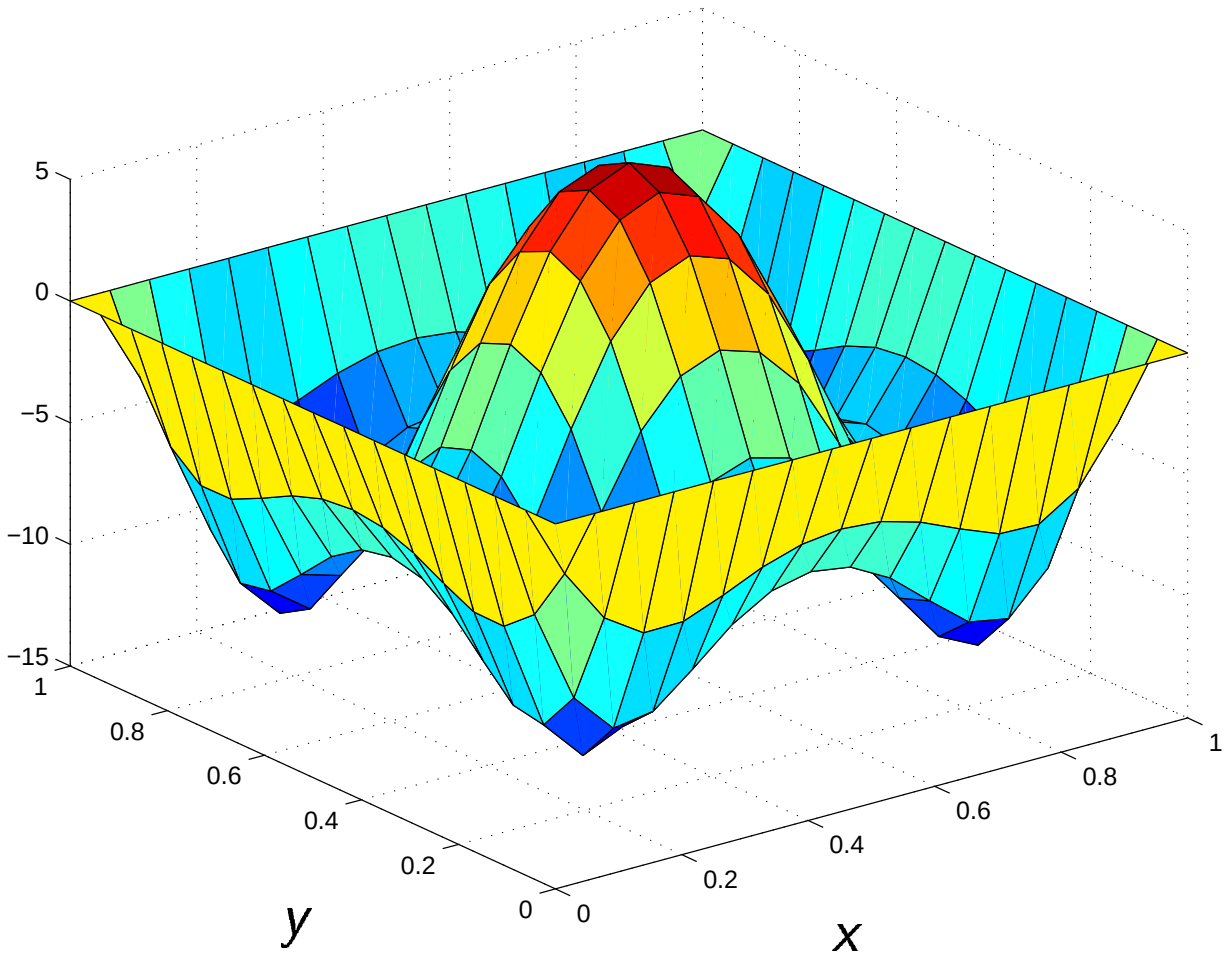
Iteration 2: error after postsmoothing



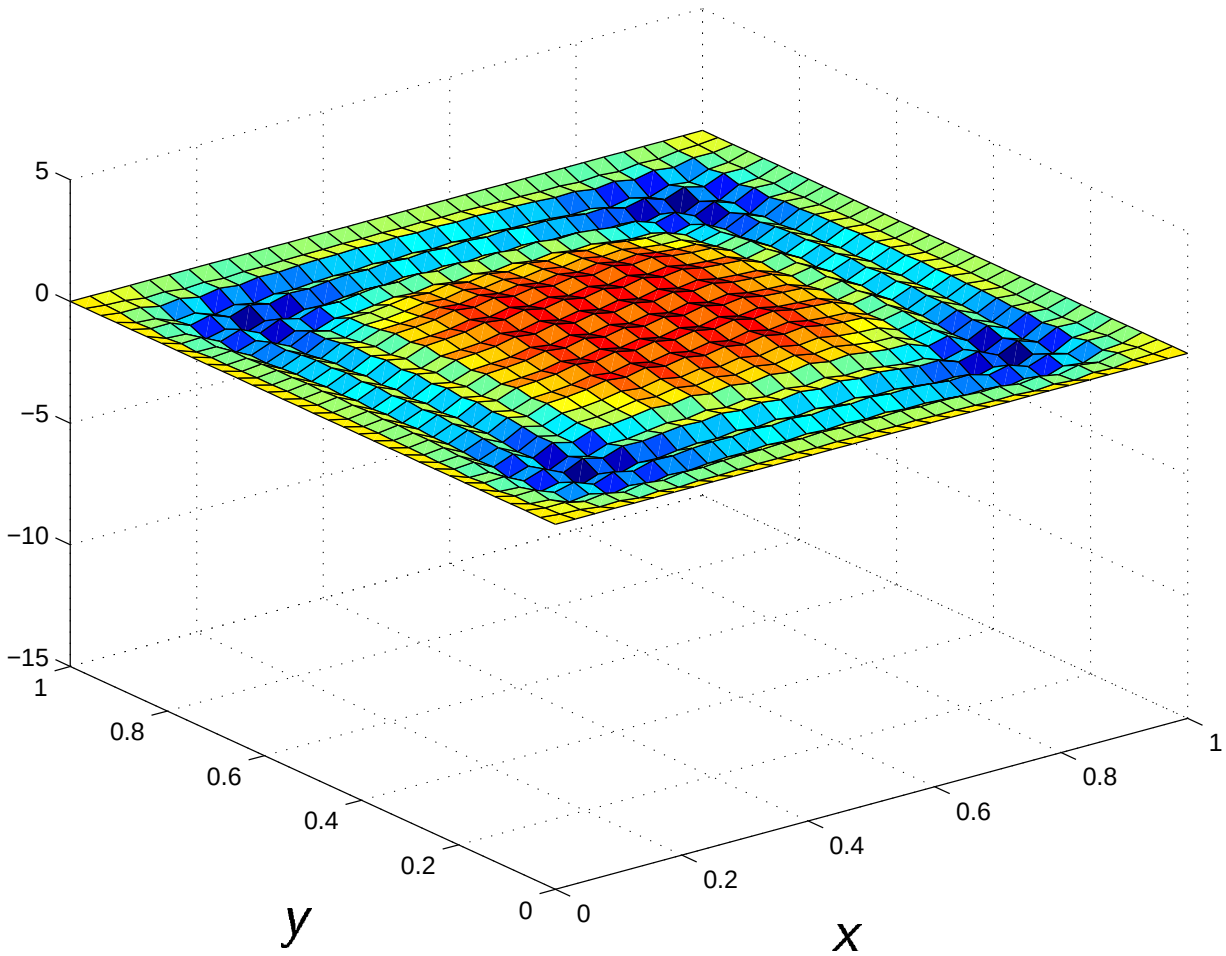
Iteration 3: error after presmoothing



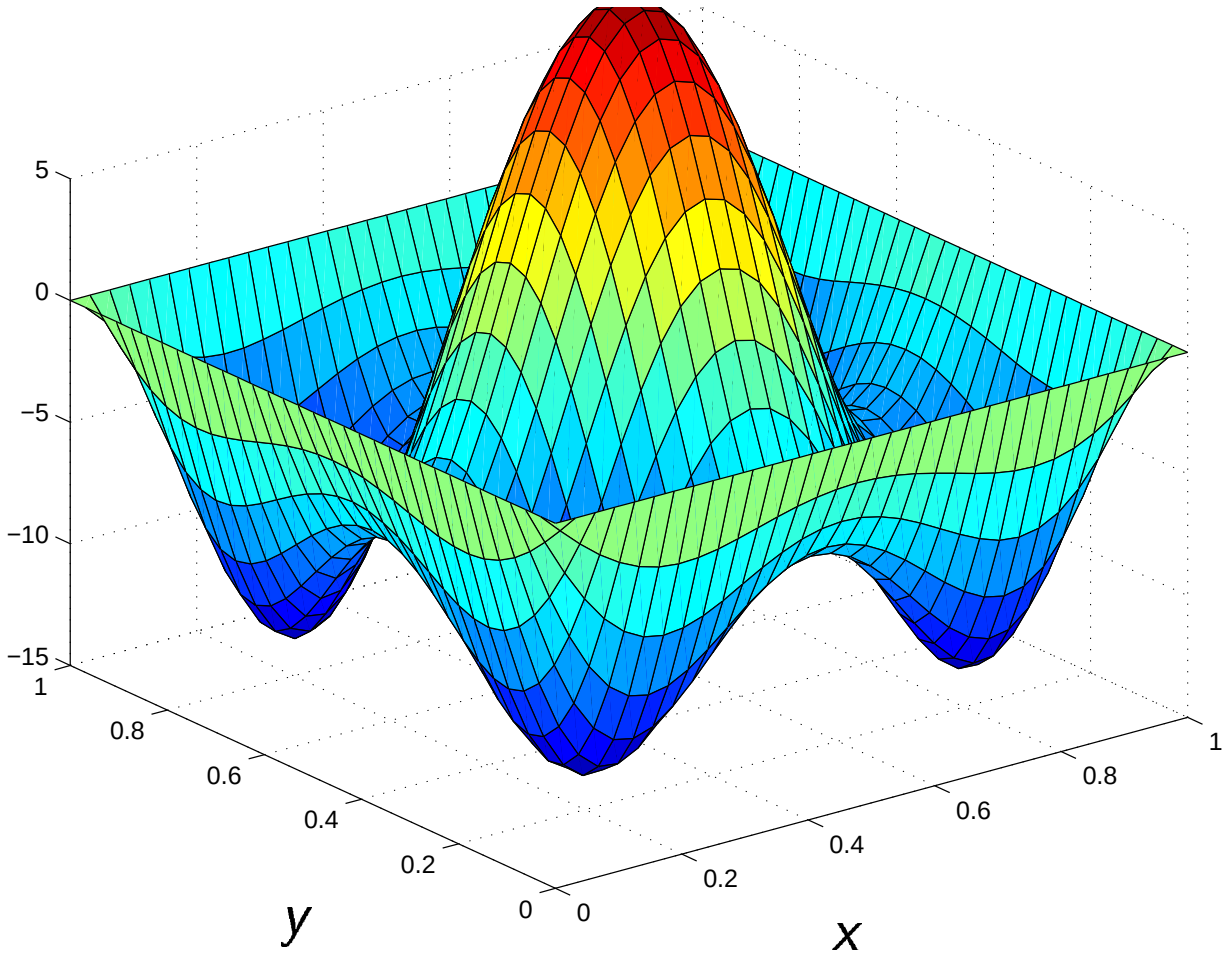
Iteration 3: error to remove from coarse grid correction



Iteration 3: error before postsmoothing



Iteration 3: error after postsmoothing



Fourier Analysis of the Smoother

In order to explain, we consider again the 1d example. Damped Jacobi for smoothing is

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \omega D^{-1}(\mathbf{b} - L\mathbf{u}^n).$$

Looking at each eigenfunction φ_m^h we obtain the corresponding contraction factor

$$\rho(m,\omega) = 1 - \omega\left(1 - \frac{2\cos(m\pi h)}{2 - h^2k^2}\right).$$

In order to obtain optimal damping for the higher half of the spectrum, one needs to choose $\omega = \omega^h$ such that

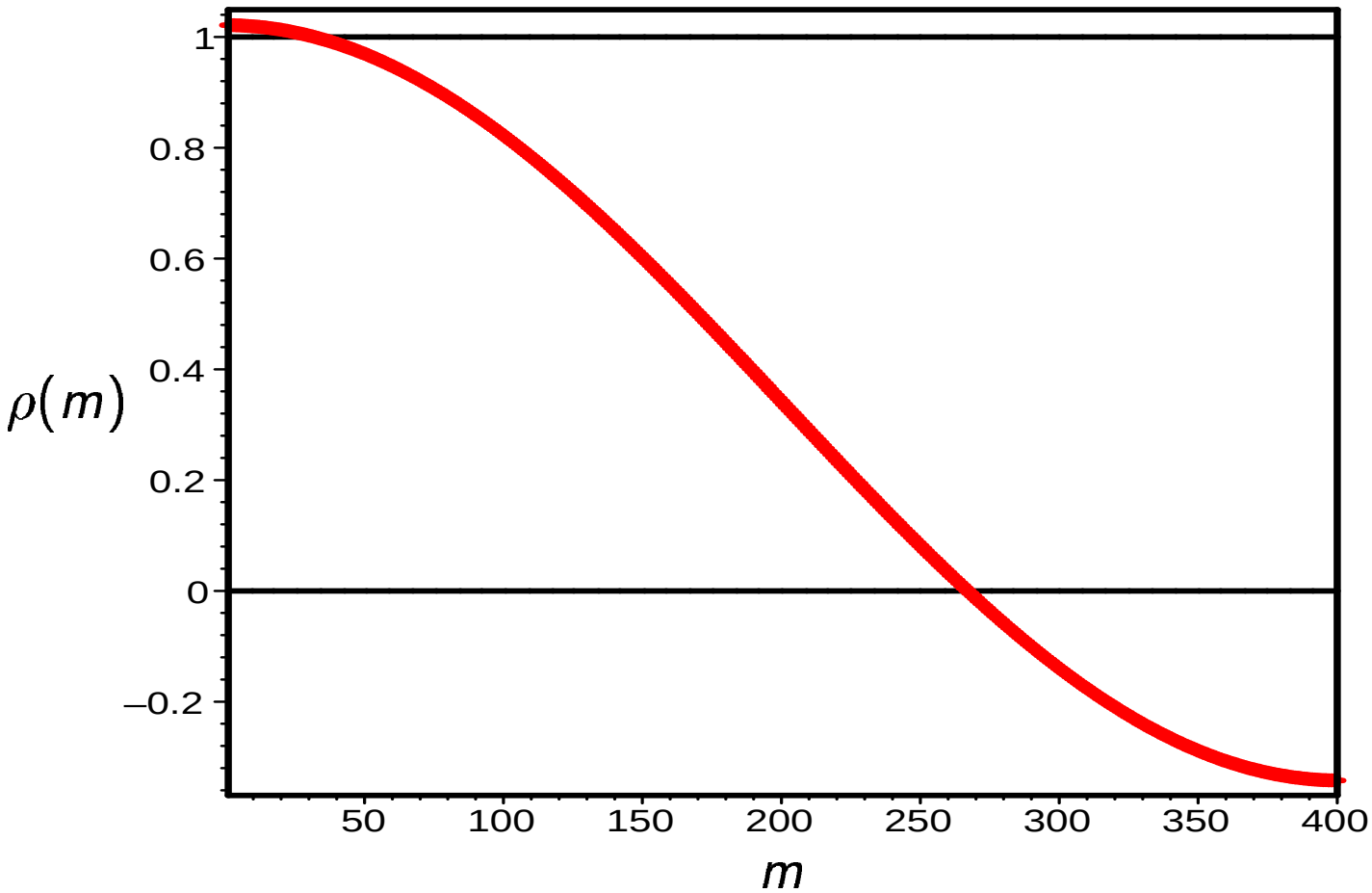
$$\omega^h = \text{argmin}_\omega \max_{m=\frac{M}{2}\ldots M} |\rho(m,\omega)|.$$

Note: If m_r solves $1 - \frac{2\cos(m_r\pi h)}{2-h^2k^2} = 0$, then for this mode $\rho(m_r,\omega) = 1$, and no contraction is possible, independent of ω^h.

Need to Consider Three Cases

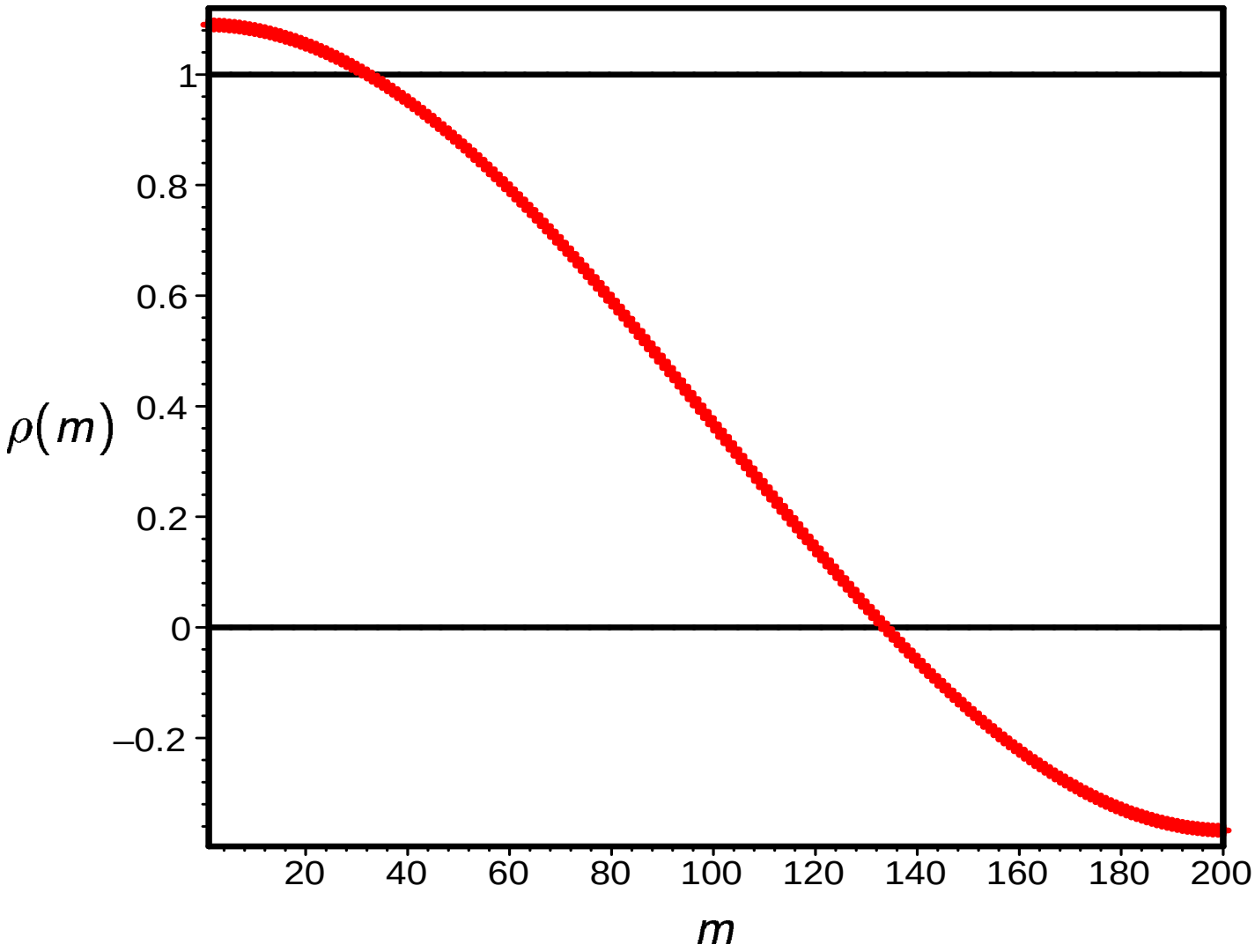
First case: $m_r < \frac{M}{2}$. Then equioscillation leads to the optimal relaxation parameter

$$\omega^h = \frac{h^2k^2 - 2}{h^2k^2 + \cos(m\pi h) + \cos(m\pi h/2) - 2} \approx \frac{h^2k^2 - 2}{h^2k^2 - 3}$$



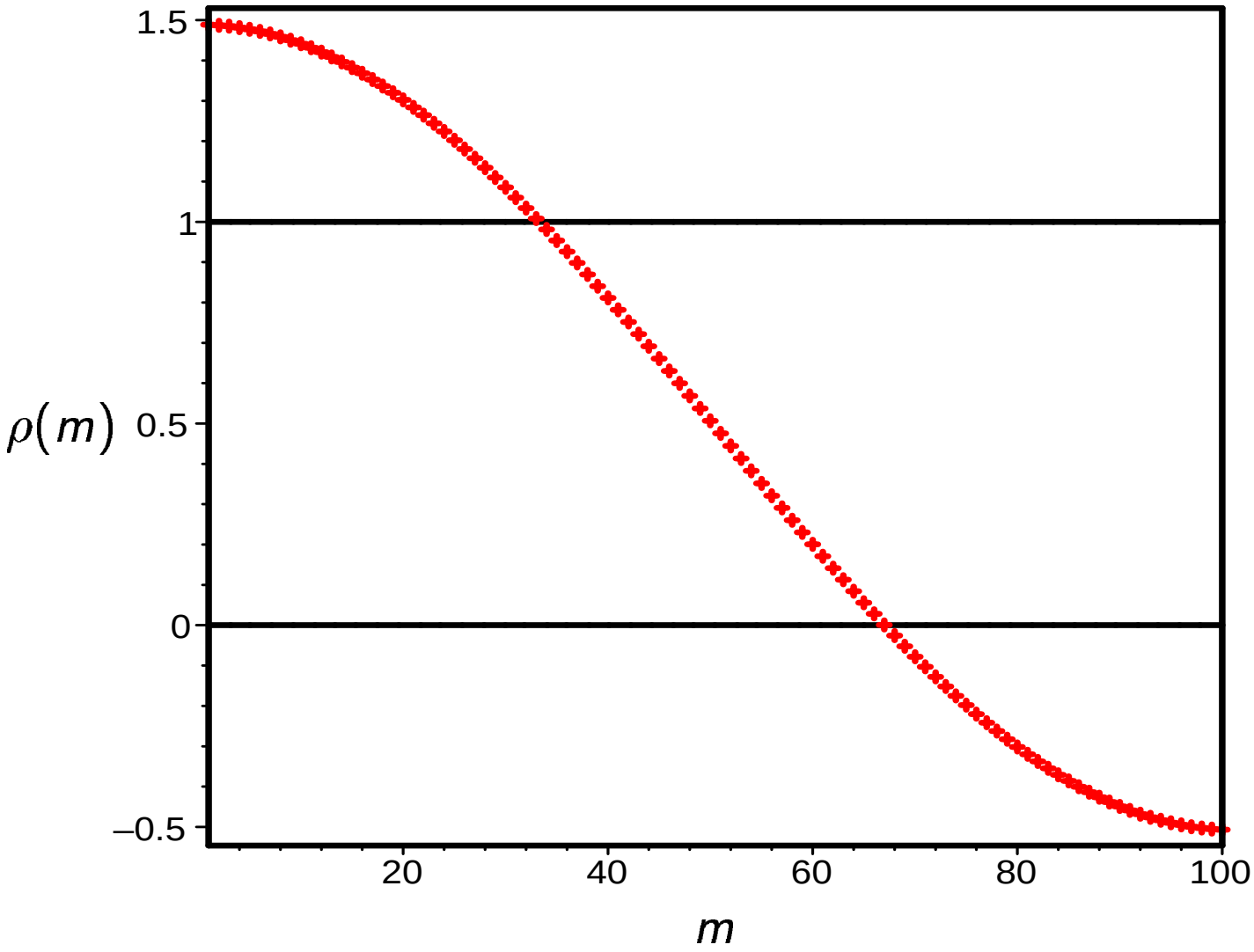
When the Grid Becomes Coarser

Still first case: $m_r < \frac{M}{2}$, but $h = 1/201$:



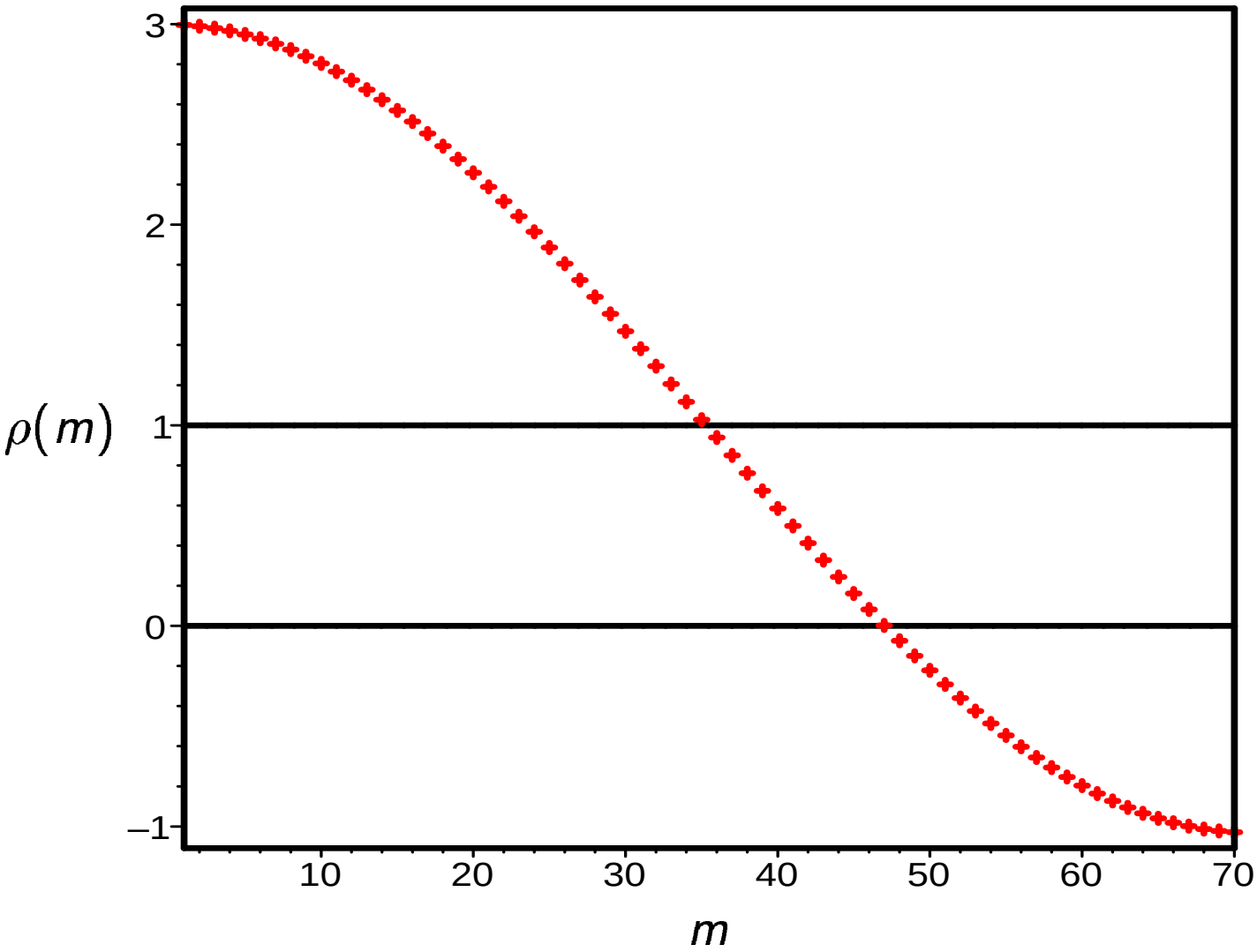
And Coarser ...

Still first case: $m_r < \frac{M}{2}$, but $h = 1/101$:



And Coarser ...

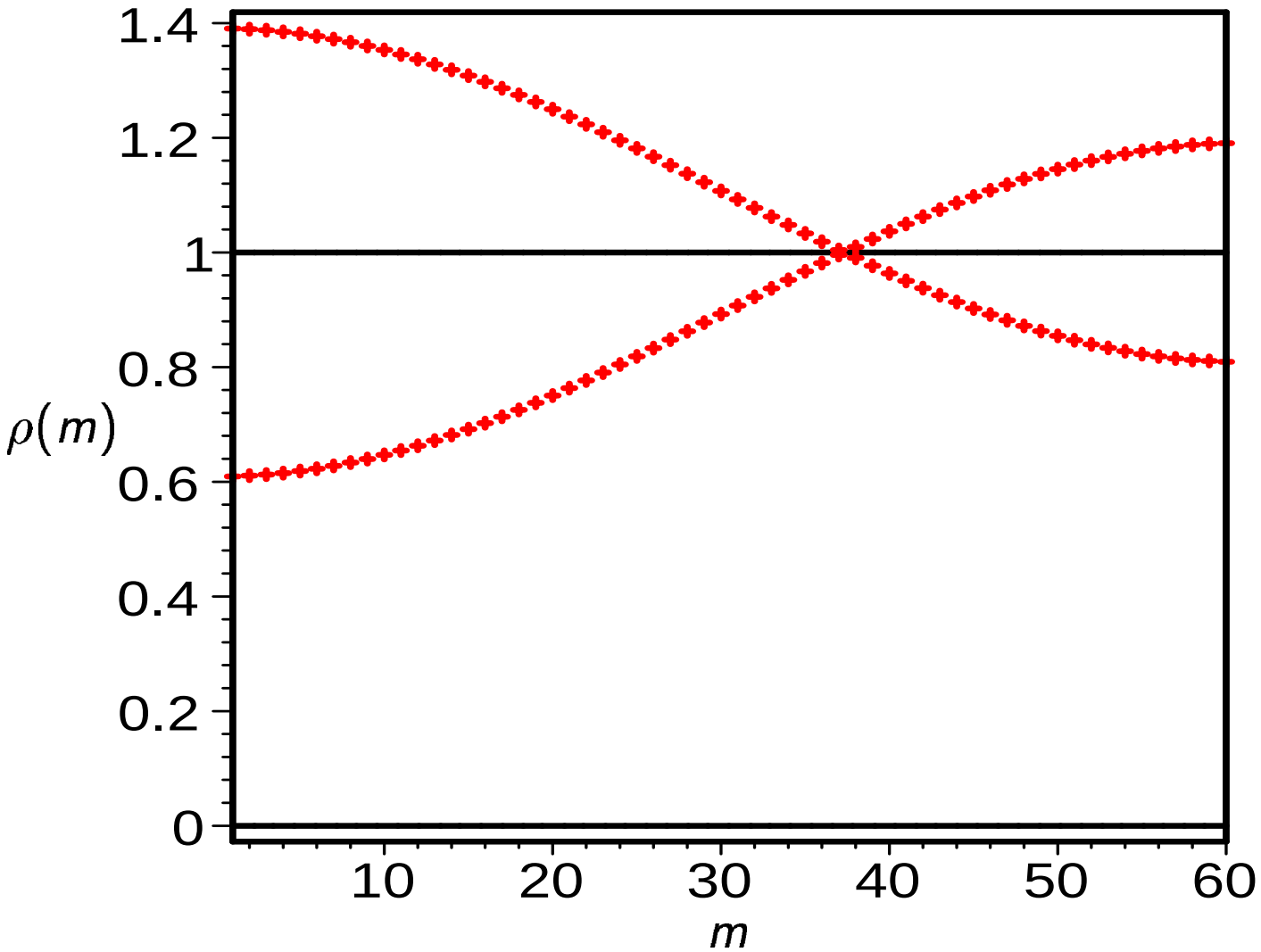
Still first case: $m_r < \frac{M}{2}$, but $h = 1/71$:



All low frequency modes are greatly amplified!

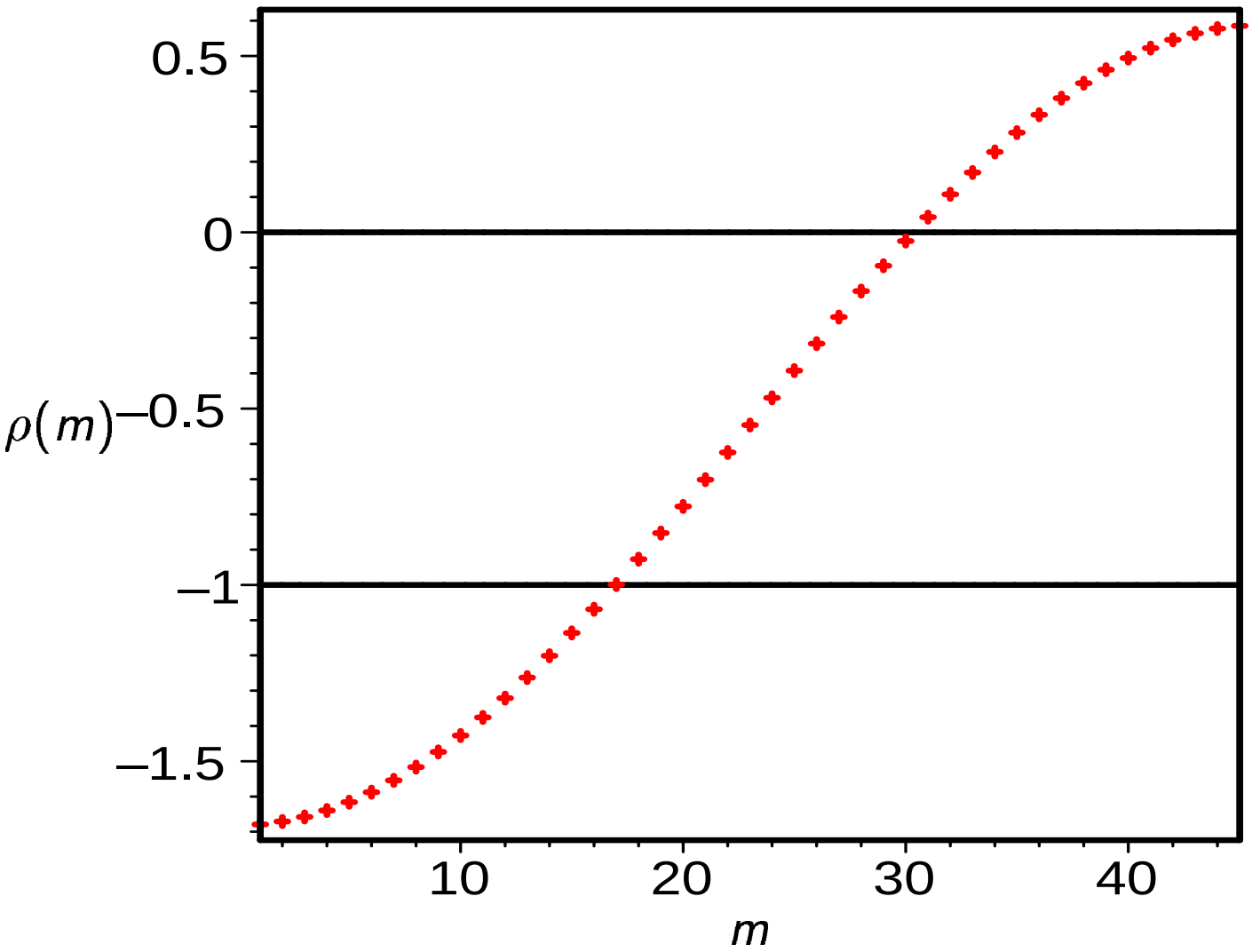
Second Case

Second case: $\frac{M}{2} < m_r < M$. In that case one can not use Jacobi for smoothing: for any choice of ω^h, high frequencies will be amplified



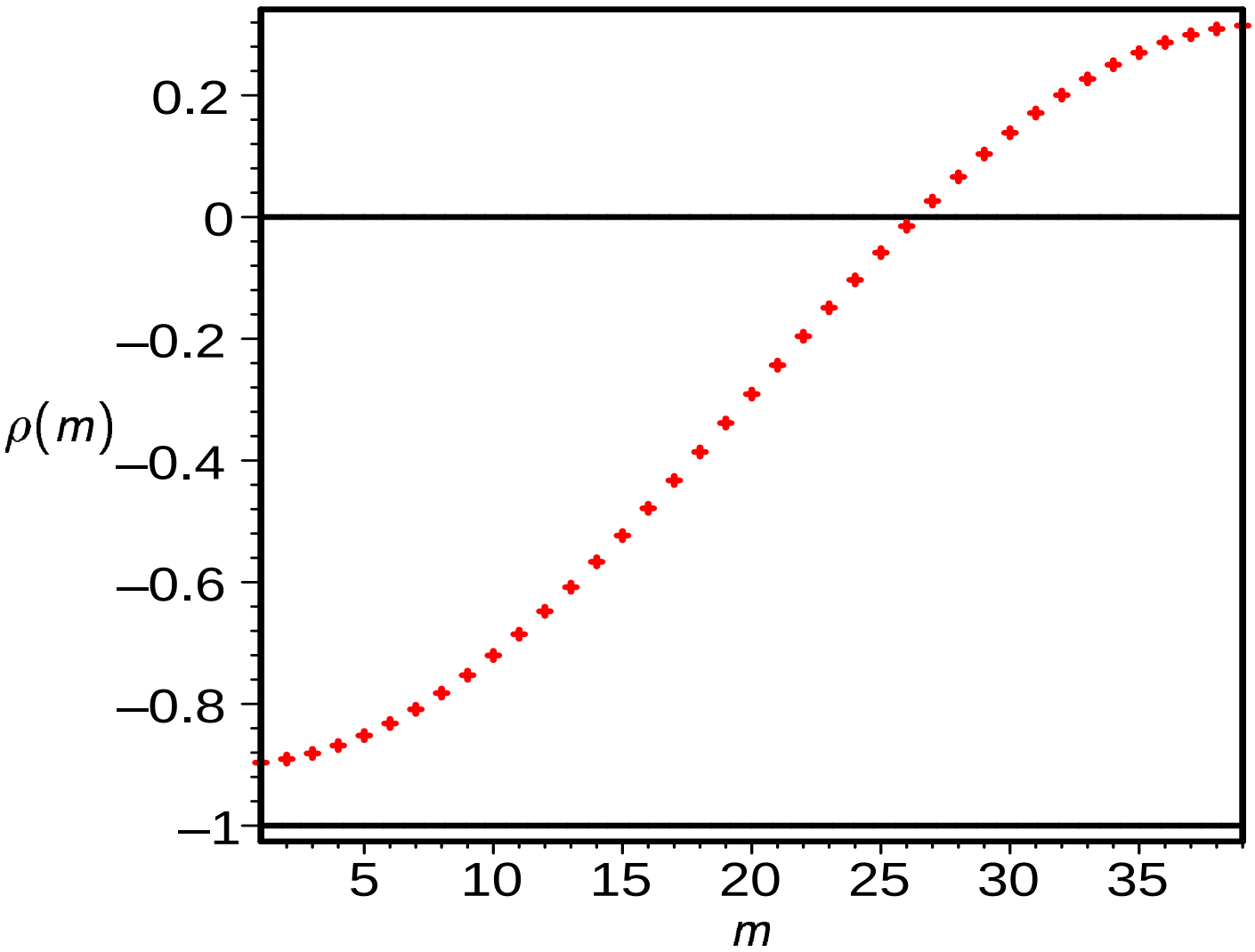
Last Case

Last case: $m_r > M$. Then equioscillation leads again to the same optimal relaxation parameter. For $h = 1/46$ we get



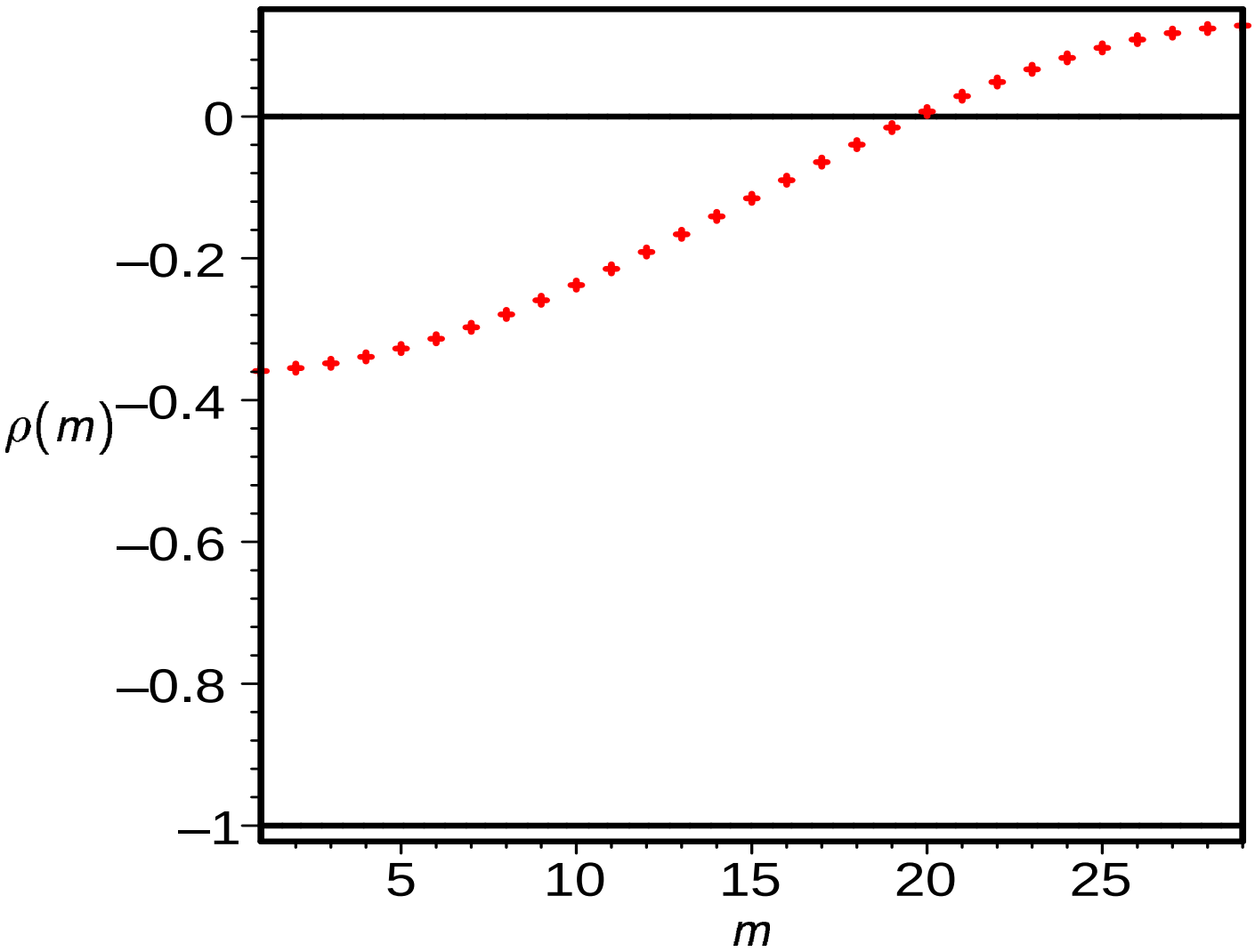
And Coarser ...

Last case: $m_r > M$, $h = 1/40$:



And Coarser ...

Last case: $m_r > M$, $h = 1/30$:



Solutions from the Literature: Coarse Grid

Brandt and Ta'asan (1986):

> *The trouble of the coarse-grid approximation has been resolved by introducing a modification to the usual coarse grid equations, based on the observation that there are just few smooth eigenfunctions which are not well represented on the coarse grid [in the slightly indefinite case].*

Modified Coarse Grid Equations

We use again the one dimensional model problem, and assume that just the first eigenmode φ_1^h is not corrected properly.

Suppose $\mathbf{u}^h$ is the exact solution on the fine grid,

$$L^h \mathbf{u}^h = \mathbf{f}^h.$$

Suppose that the current approximation $\tilde{\mathbf{u}}^h$ on the fine grid is missing η in the direction of φ_1^h,

$$(\mathbf{u}^h, \varphi_1^h) = (\tilde{\mathbf{u}}^h + \eta\varphi_1^h, \varphi_1^h).$$

If η was known, the approximation on the fine grid would be $\tilde{\mathbf{u}}^h + \eta\varphi_1^h$, and thus the coarse grid correction equation would be

$$L^H \mathbf{v}^H = I_h^H(\mathbf{f}^h - L^h\tilde{\mathbf{u}}^h - \eta L^h\varphi_1^h)$$

Modified Coarse Grid Equations

The coarse grid correction $\mathbf{v}^H$ obtained from this equation,

$$L^H \mathbf{v}^H = I_h^H (\mathbf{f}^h - L^h \tilde{\mathbf{u}}^h - \eta L^h \varphi_1^h)$$

computes an approximation to $\mathbf{v}^h := \mathbf{u}^h - \tilde{\mathbf{u}}^h - \eta \varphi_1^h$, which by the definition of η,

$$(\mathbf{u}^h, \varphi_1^h) = (\tilde{\mathbf{u}}^h + \eta \varphi_1^h, \varphi_1^h).$$

does not contain any component in the troublesome direction of φ_1^h, and thus the calculated correction is effective.

But η is not known, so we need an additional equation. A reasonable choice is (Brandt and Ta'asan 1986)

$$(\mathbf{v}^H, I_h^H \varphi_1^h) = 0.$$

Similar generalization to several problematic modes.

Solutions from the Literature: Smoother

Brandt and Ta'asan (1986):

> *Indeed, even though some smooth components diverge with this relaxation, on fine enough grids this divergence is slow and can, therefore, easily be corrected by the coarse-grid corrections. On coarser grids, however, the divergence of the smooth components in Gauss-Seidel relaxation is faster, hence, another relaxation scheme is needed. We have used for that purpose the Kaczmarz relaxation, which always converges.*

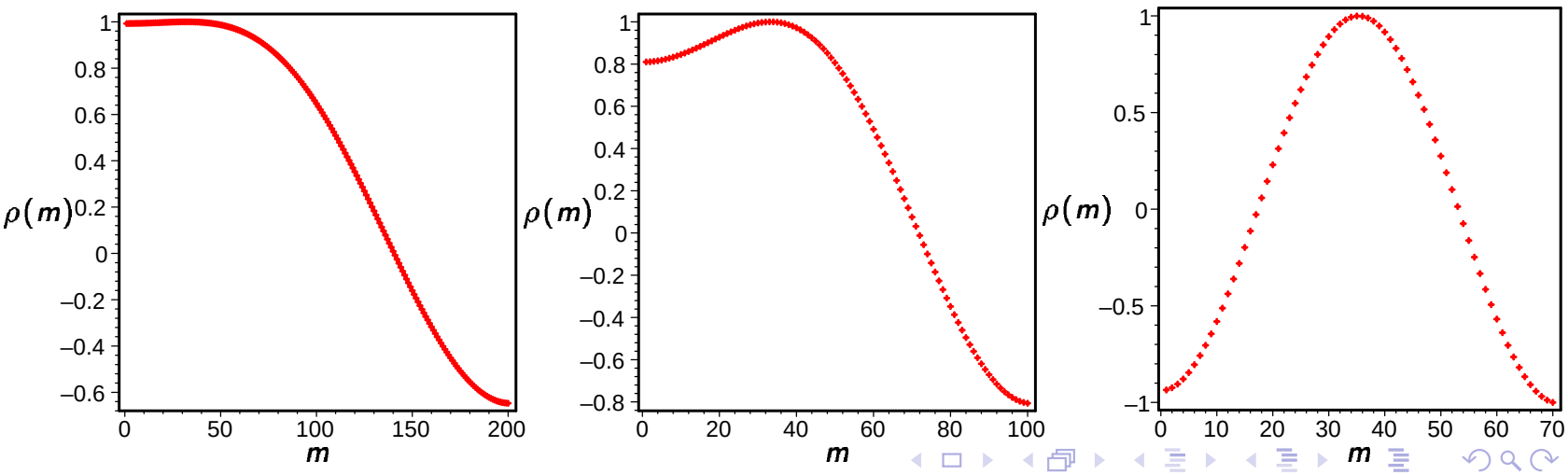
Kaczmarz Relaxation

Stefan Kaczmarz (1937): Przyblizone rozwiqzywanie ukladów równań liniowych.– Angenäherte Auflösung von Systemen linearer Gleichungen.

An iterative method for solving linear systems: "Gauss Seidel applied to the normal equations"

For our 1d Helmholtz model problem we get for the damped Jacobi variant (Cimmino 1938) the modal contraction factor

$$\rho(m,\omega) = 1 - \omega \frac{(2 - 2\cos(m\pi h) - k^2h^2)^2}{2 + (2 - h^2k^2)^2}.$$



The Wave Ray Multigrid Method

For large k, the detection of problematic modes and the modification of the coarse grid correction dominate the cost, and the algorithm is not optimal any more.

Idea of Wave Ray Multigrid: Brandt and Livshits (1997)

- Construct explicitly problematic modes using plane waves.
- On fine grids, where multigrid is effective, just use multigrid.
- On coarser grids, correct the error using a plane wave representation.

\+ Algorithm fully addresses all problems of multigrid for Helmholtz.

– Its implementation and use is not easy.

Using Krylov Methods

Ideas: Elmann, Ernst, O'Leary (2001)

- Since classical smoothers and Kazcmarz smoothing is not effective for problematic modes, replace in that case the smoother by a Krylov method. If GMRES is used, the method will minimize the residual, and thus will have to treat problematic modes.
- Since the overall convergence of the multigrid cycle is significantly worse than for the Poisson problem, use multigrid only as a preconditioner for an outer Krylov method: if the multigrid iteration computes

$$\mathbf{u}^{n+1} = \mathbf{u}^n + M_{MG}^{-1}(\mathbf{f} - L^h\mathbf{u}^n)$$

solve instead by GMRES the preconditioned system

$$M_{MG}^{-1}L^h\mathbf{u} = M_{MG}^{-1}\mathbf{f}.$$

\+ This algorithm is easy to use.

– It addresses only indirectly the problems of multigrid for Helmholtz.

New Ideas: Modified Discrete Equations

In 1d, the coarse grid correction equation can be modified to yield accurate corrections: instead of using

$$L^h \mathbf{u}^h := \frac{1}{h^2} \begin{bmatrix} 2 - h^2 k^2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & \end{bmatrix} \mathbf{u}^h = \mathbf{f}^h$$

we use

$$L^h \mathbf{u}^h := \frac{1}{h^2} \begin{bmatrix} 2 - h^2 k_h^2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & \end{bmatrix} \mathbf{u}^h = \mathbf{f}^h$$

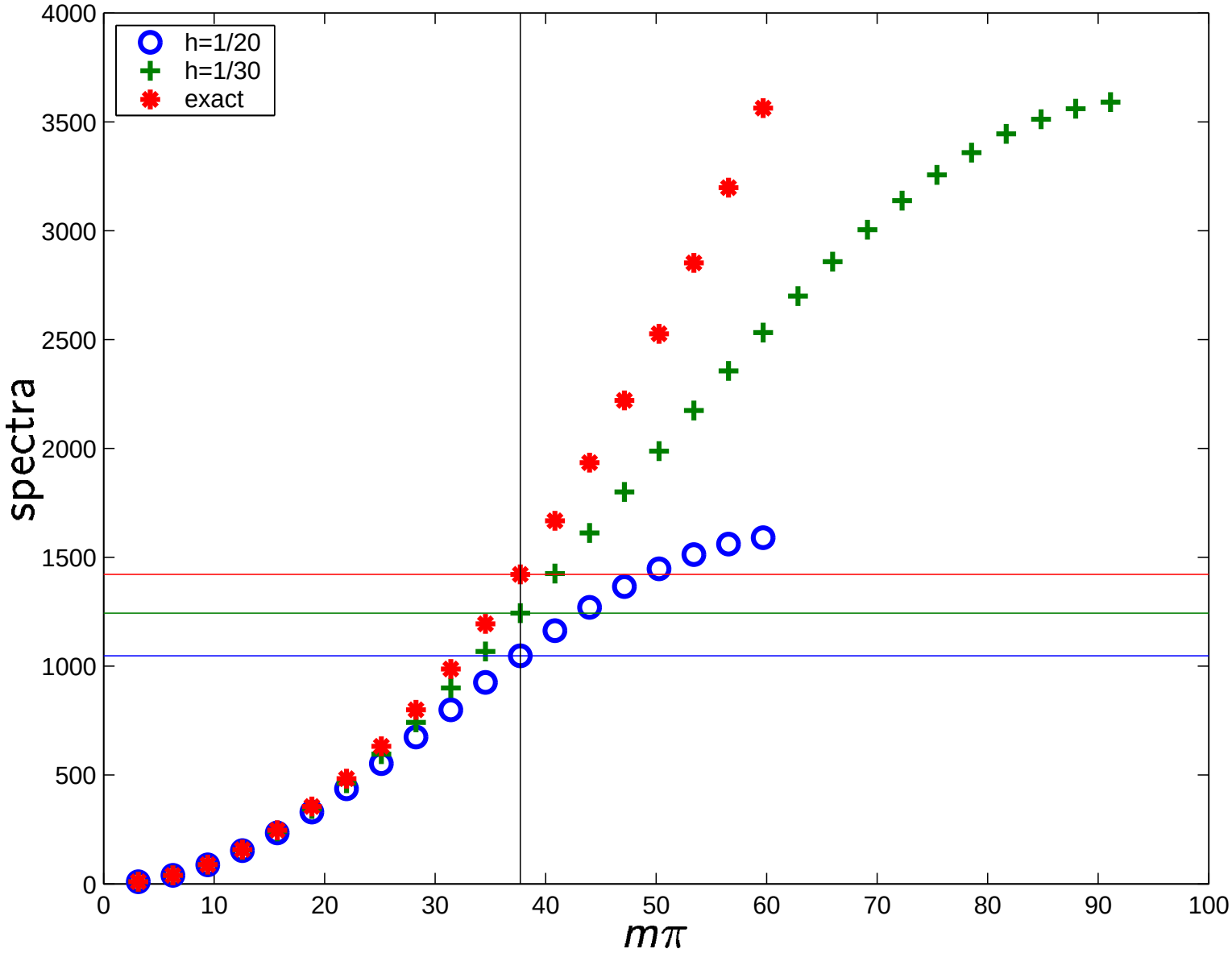
with

$$k_h^2 := \frac{1}{h^2}(2 - 2\cos(kh)).$$

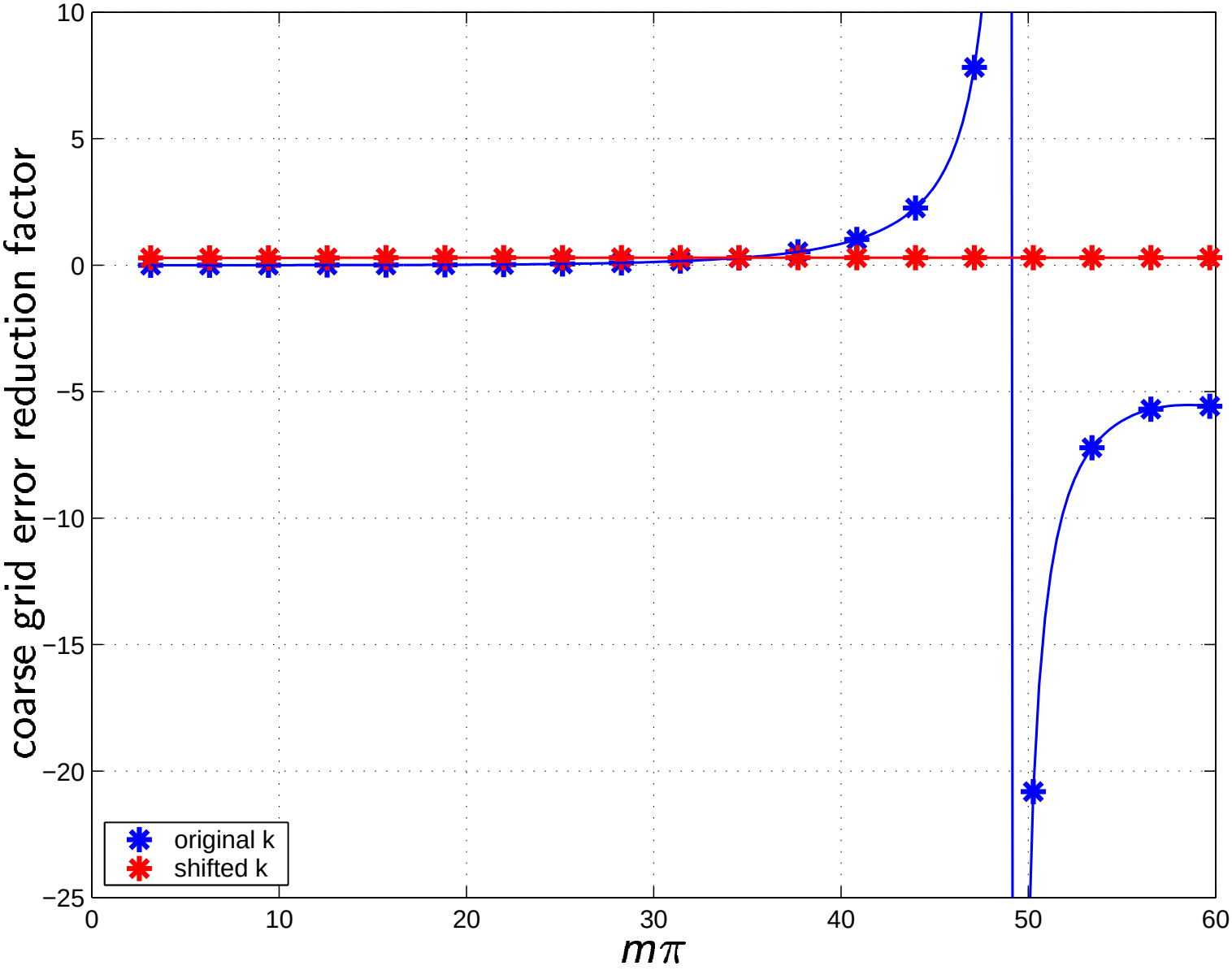
Thus the spectral shift due to the discretization is precisely compensated by a shift of the wave-number k_h, and the problematic modes are all correctly treated on any coarse grid,

$$\left(1 - \frac{\lambda_m^h}{\lambda_m^H}\right) \approx 0.$$

Spectral Shift with k_h

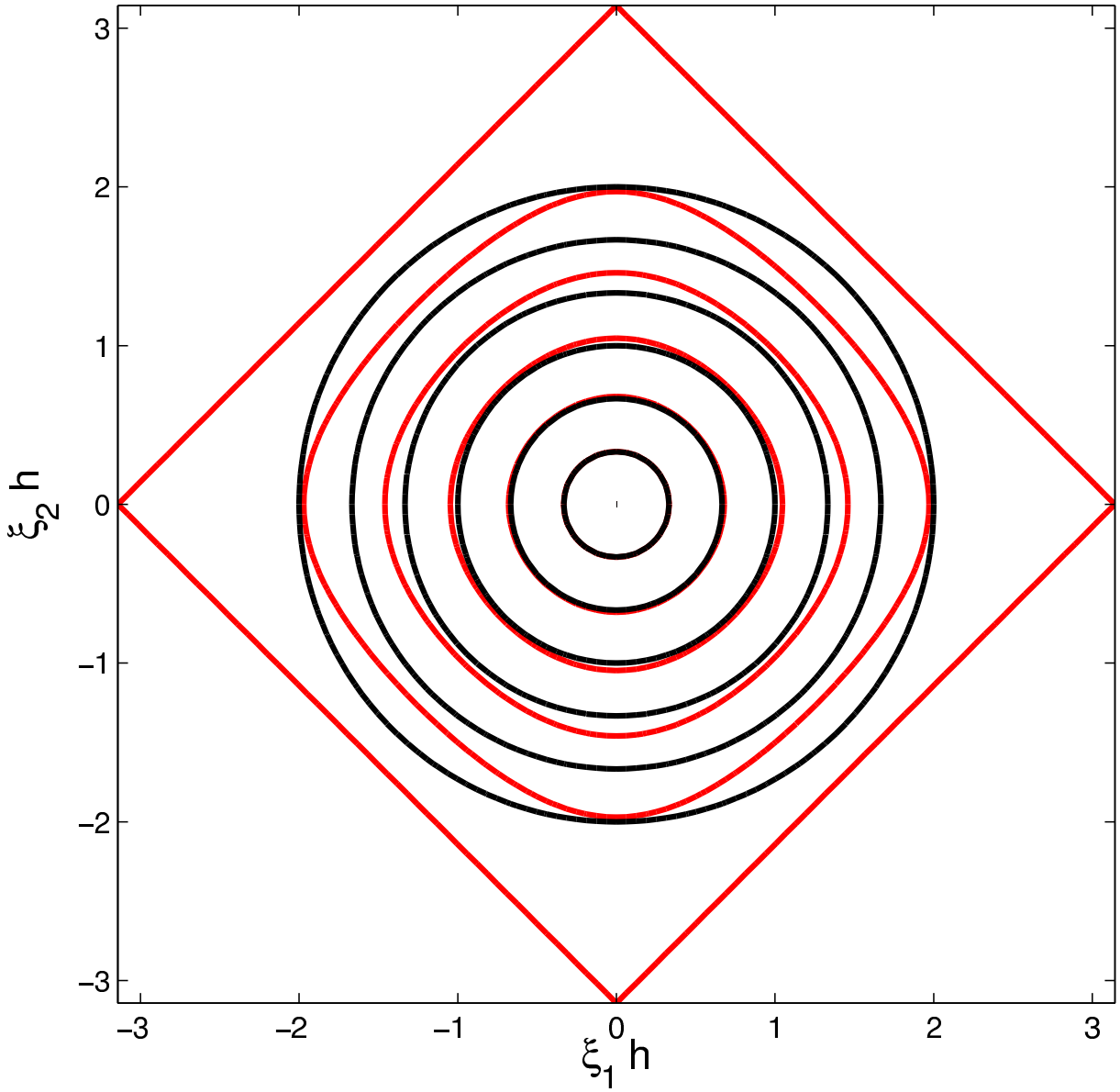


Coarse Grid Error Reduction Factor



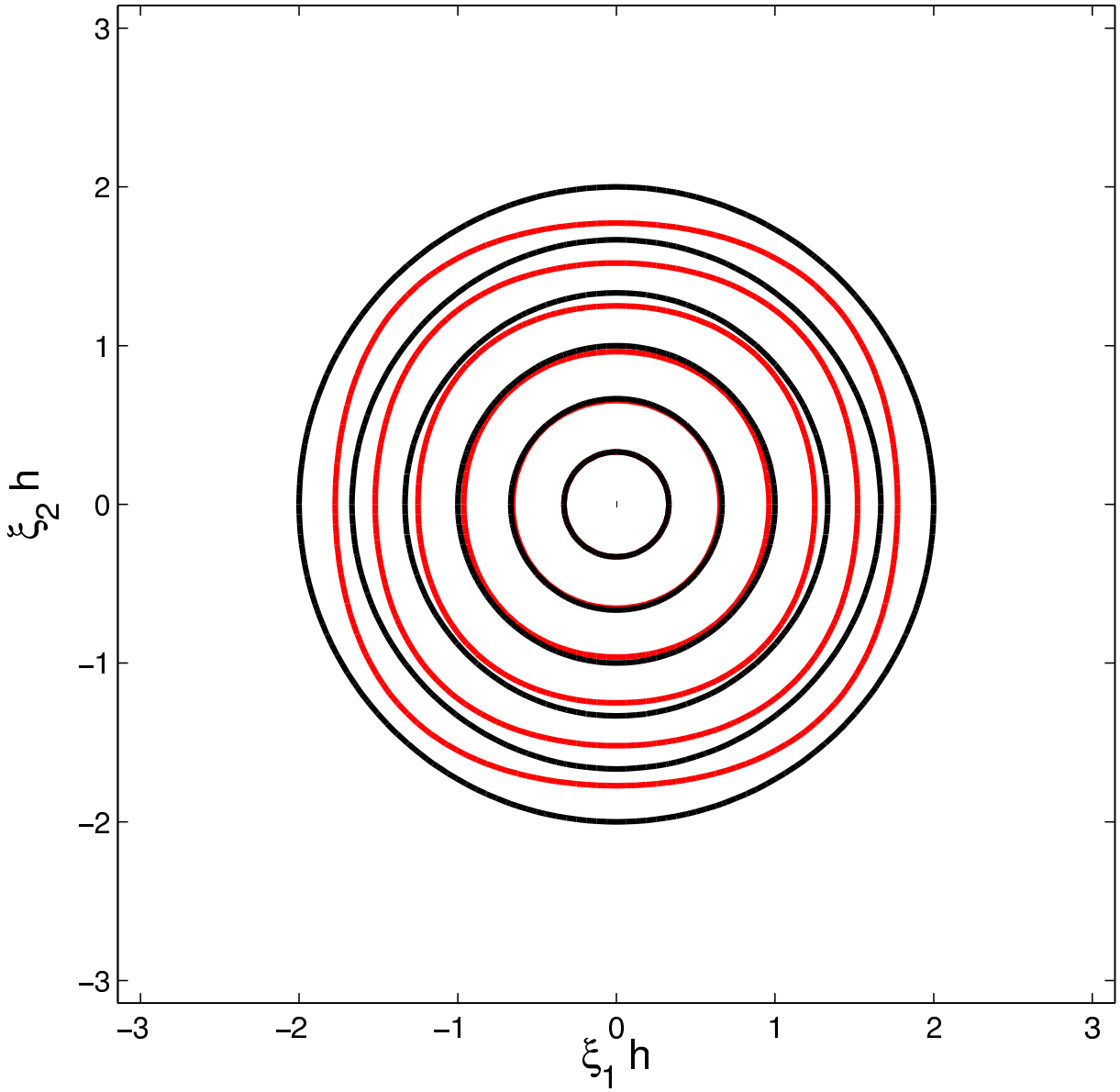
How About Higher Dimensions ?

Dispersion curves of a 5 point finite difference discretization



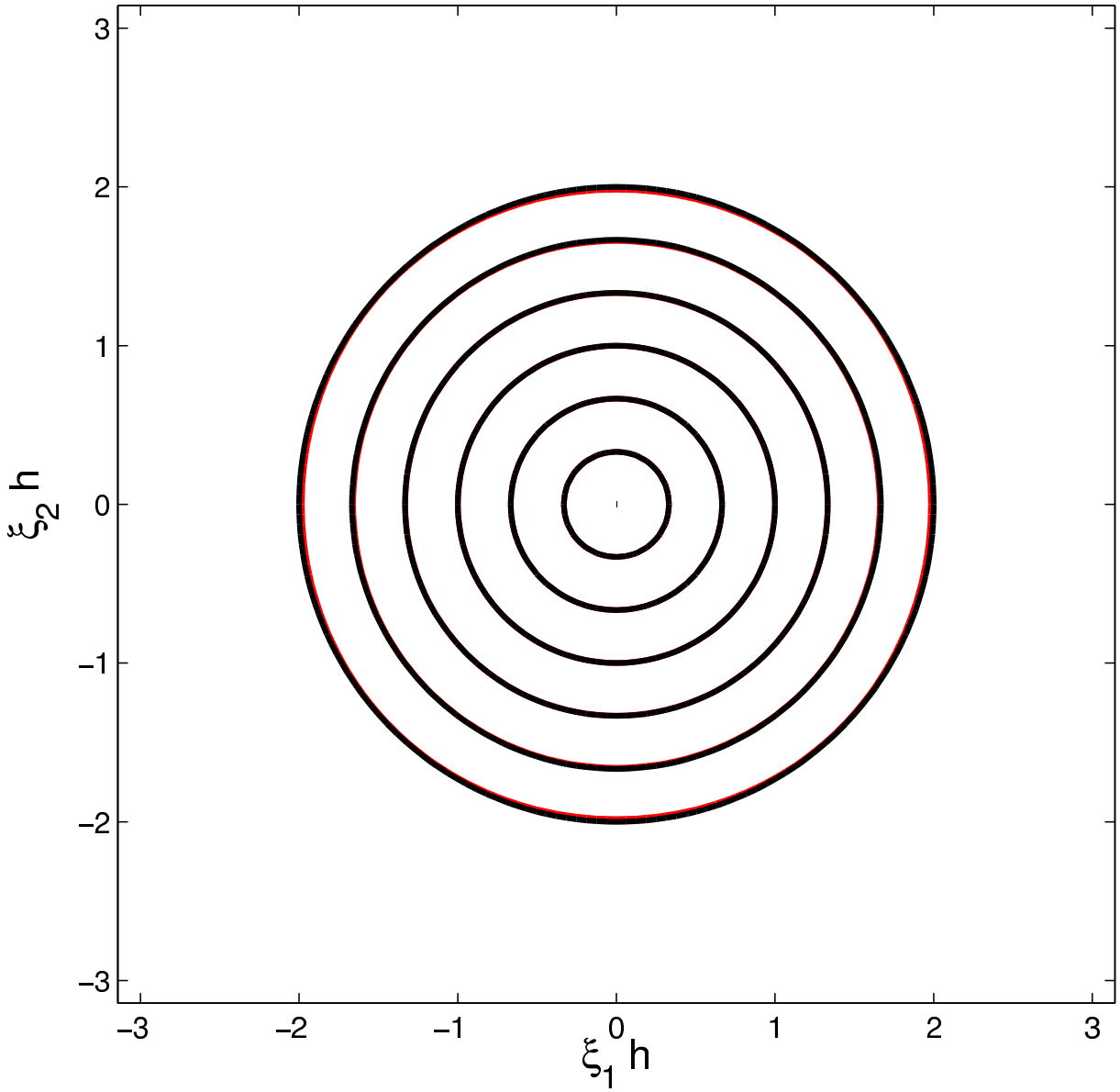
Further Dispersion Curves

Dispersion curves of a P1 finite element discretization



Further Dispersion Curves

Dispersion curves of a P2 finite element discretization



Multi Step Jacobi Smoother

A multi step Jacobi smoother performs several Jacobi steps with different damping parameter. For example for two steps:

$$\mathbf{u}^{n+1/2} = \mathbf{u}^n + \omega_1 D^{-1}(\mathbf{b} - L\mathbf{u}^n)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^{n+1/2} + \omega_2 D^{-1}(\mathbf{b} - L\mathbf{u}^{n+1/2})$$

The corresponding contraction factor for the 1d Helmholtz model problem is

$$\rho(m, \boldsymbol{\omega}) = \prod_{j=1}^{J} \left(1 - \omega_j \left(1 - \frac{2\cos(m\pi h)}{2 - h^2 k^2}\right)\right)$$

For this to be a good smoother, we need to satisfy two conditions:

1. $|\rho(m, \boldsymbol{\omega})| \leq 1$ for all $m = 1, 2, \ldots, M$.
2. $\boldsymbol{\omega} = \text{argmin}_{\boldsymbol{\omega}} \max_{m=\frac{M}{2}\ldots M} |\rho(m, \boldsymbol{\omega})|$

An interesting Best Approximation Problem

Note that the contraction factor is a polynomial of degree J:

$$R(x,\boldsymbol{\omega}) = \prod_{j=1}^{J}(1-\omega_j(1-x)), \quad x \in (x_{\min}, x_{\max})$$

which equals 1 at $x = 1$. Hence we have the polynomial best approximation problem

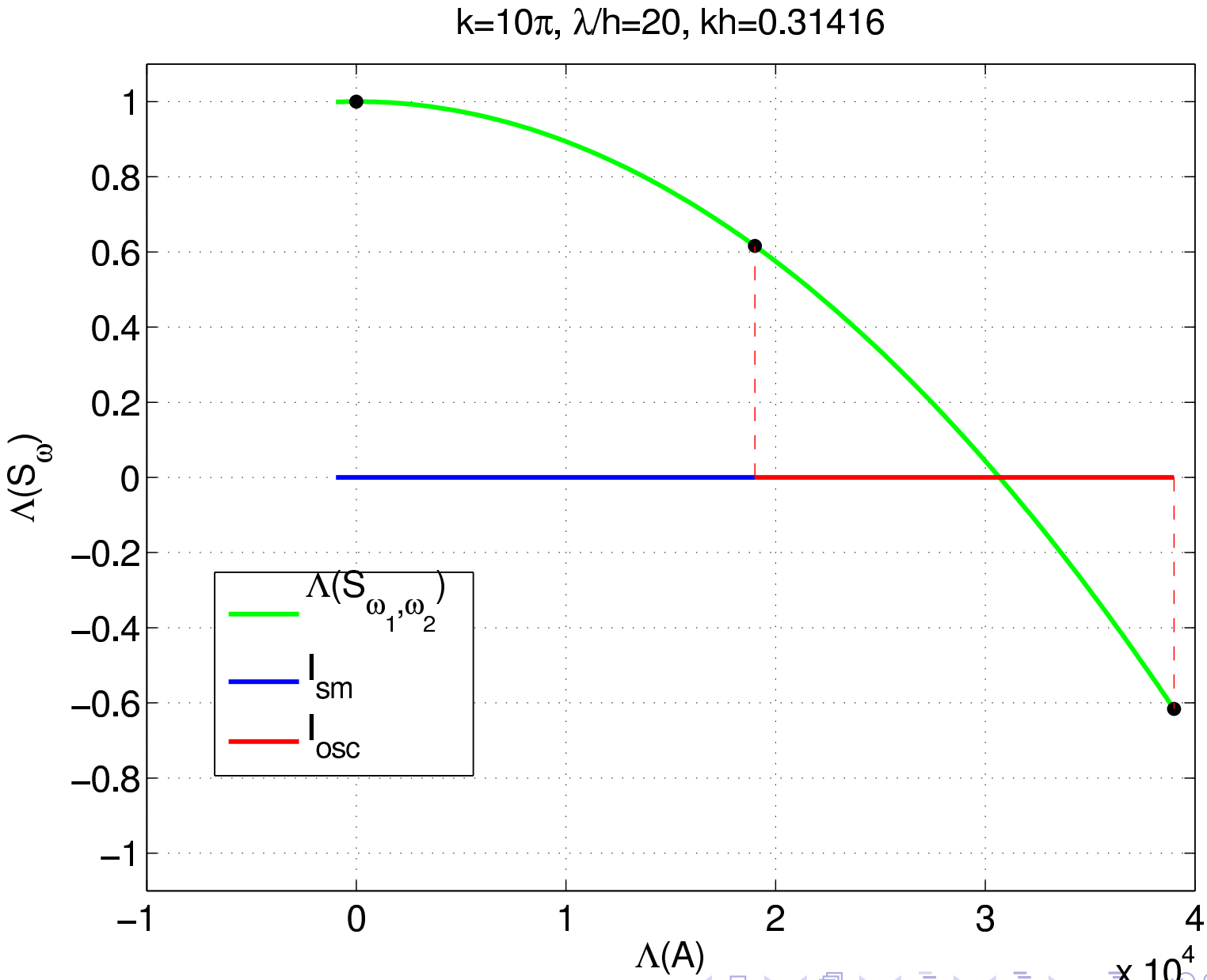
$$\min_{\boldsymbol{\omega}} \max_{x\in(x_m,x_{\max})} |R(x,\boldsymbol{\omega})|, \quad x_m := \frac{x_{\min}+x_{\max}}{2}$$

under the side constraint $|R(x,\boldsymbol{\omega})) \leq 1$. Need to distinguish again three cases:

1. $x_m > 1$: solution by equioscillation
2. $x_m < 1 < x_{\max}$: need to exclude resonance region in the best approximation problem.
3. $x_{\max} < 1$ solution by equioscillation

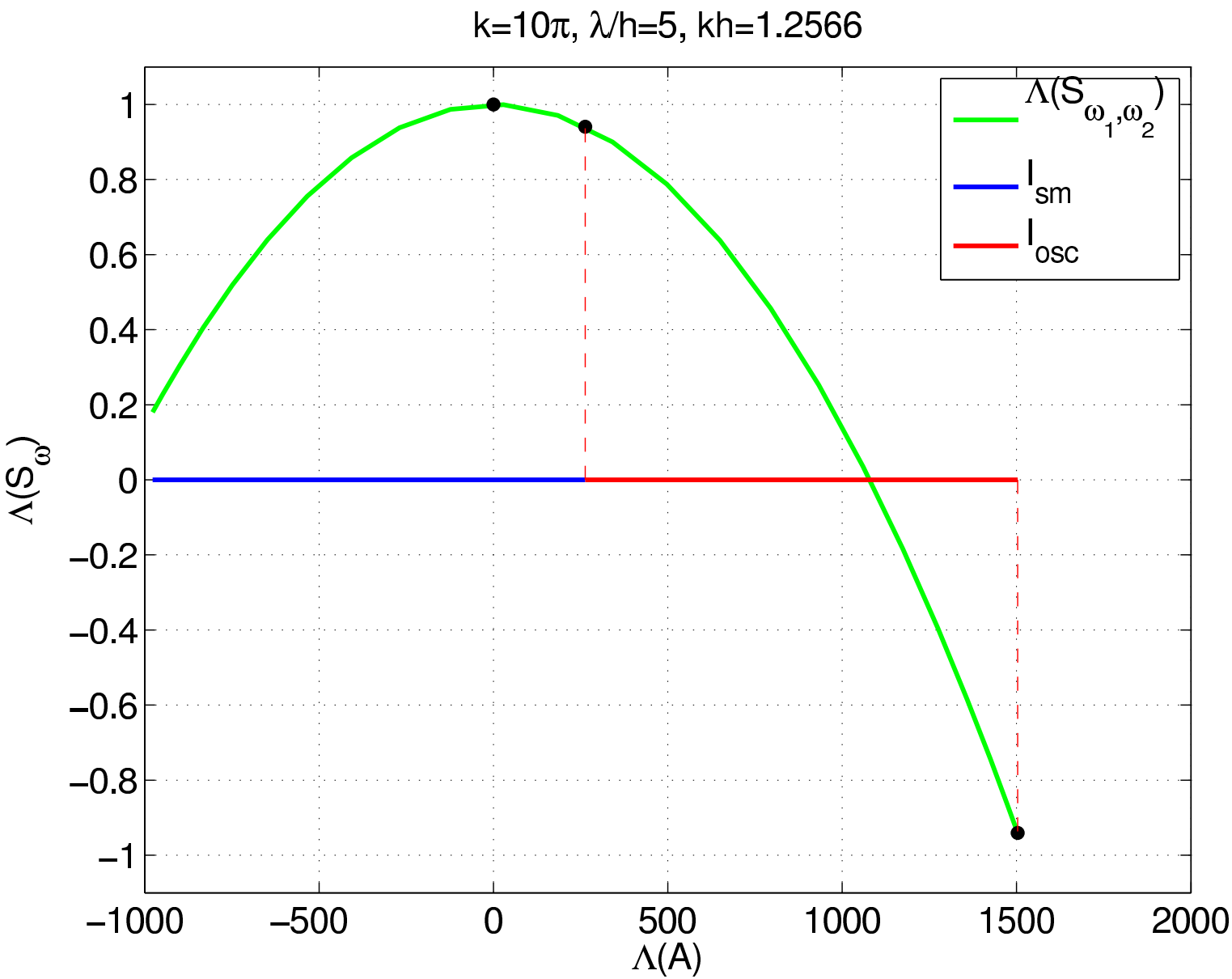
Example for a Two-Step Jacobi: Case 1

$x_m > 1$: solution by equioscillation



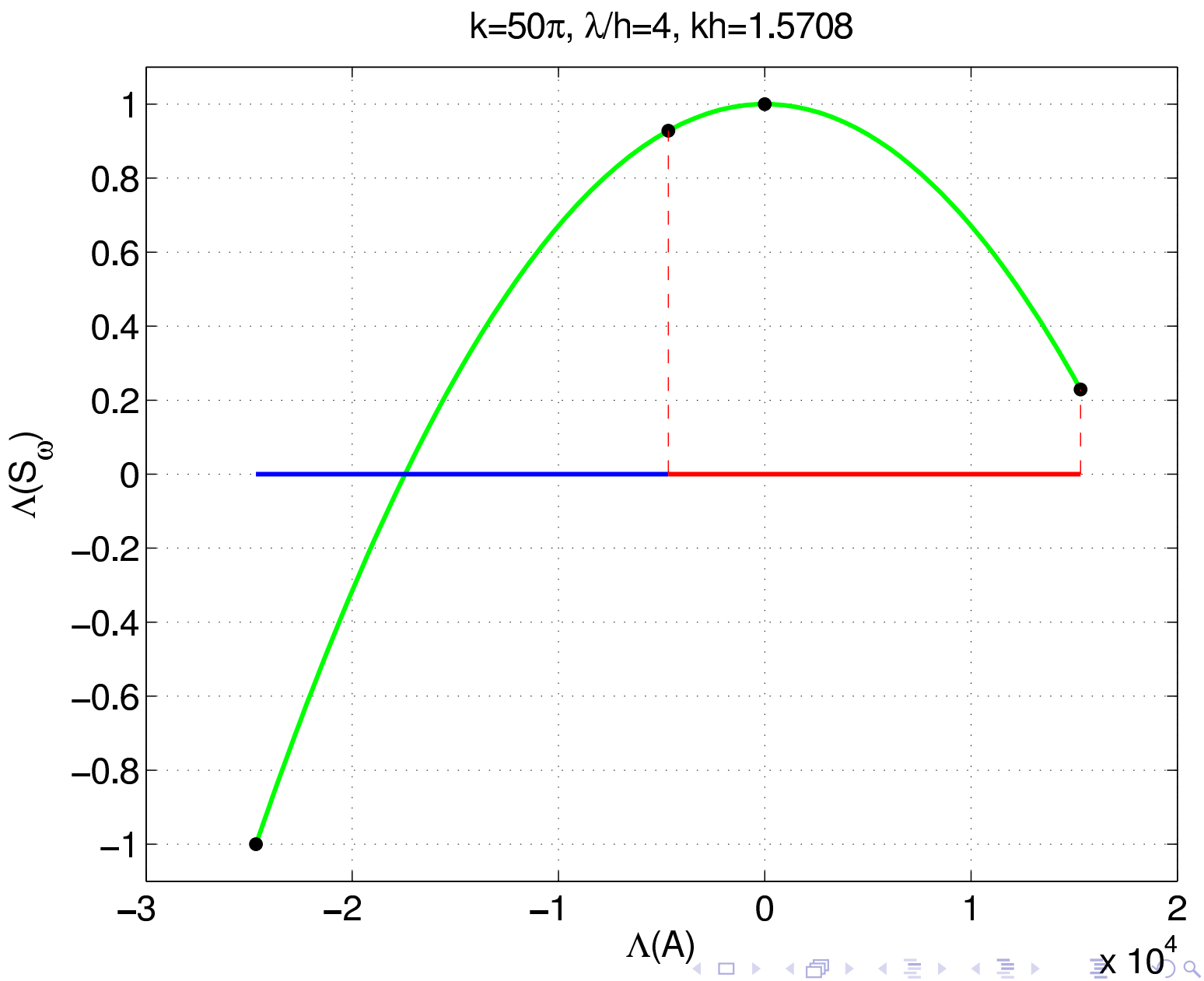
Example for a Two-Step Jacobi: Case 1

$x_m > 1$: solution by equioscillation



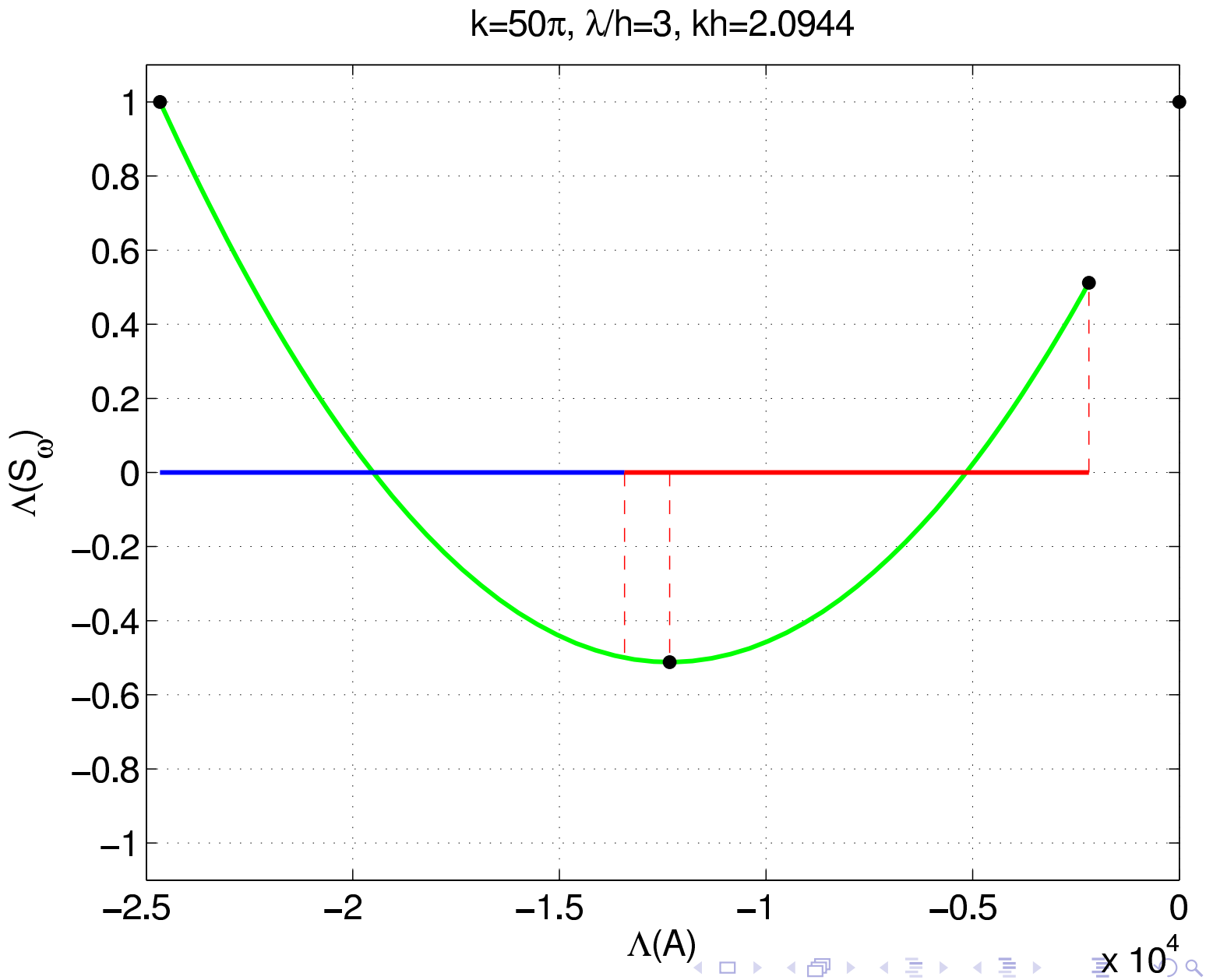
Example for a Two-Step Jacobi: Case 2

$x_m < 1 < x_{max}$: solution dominated by constraint



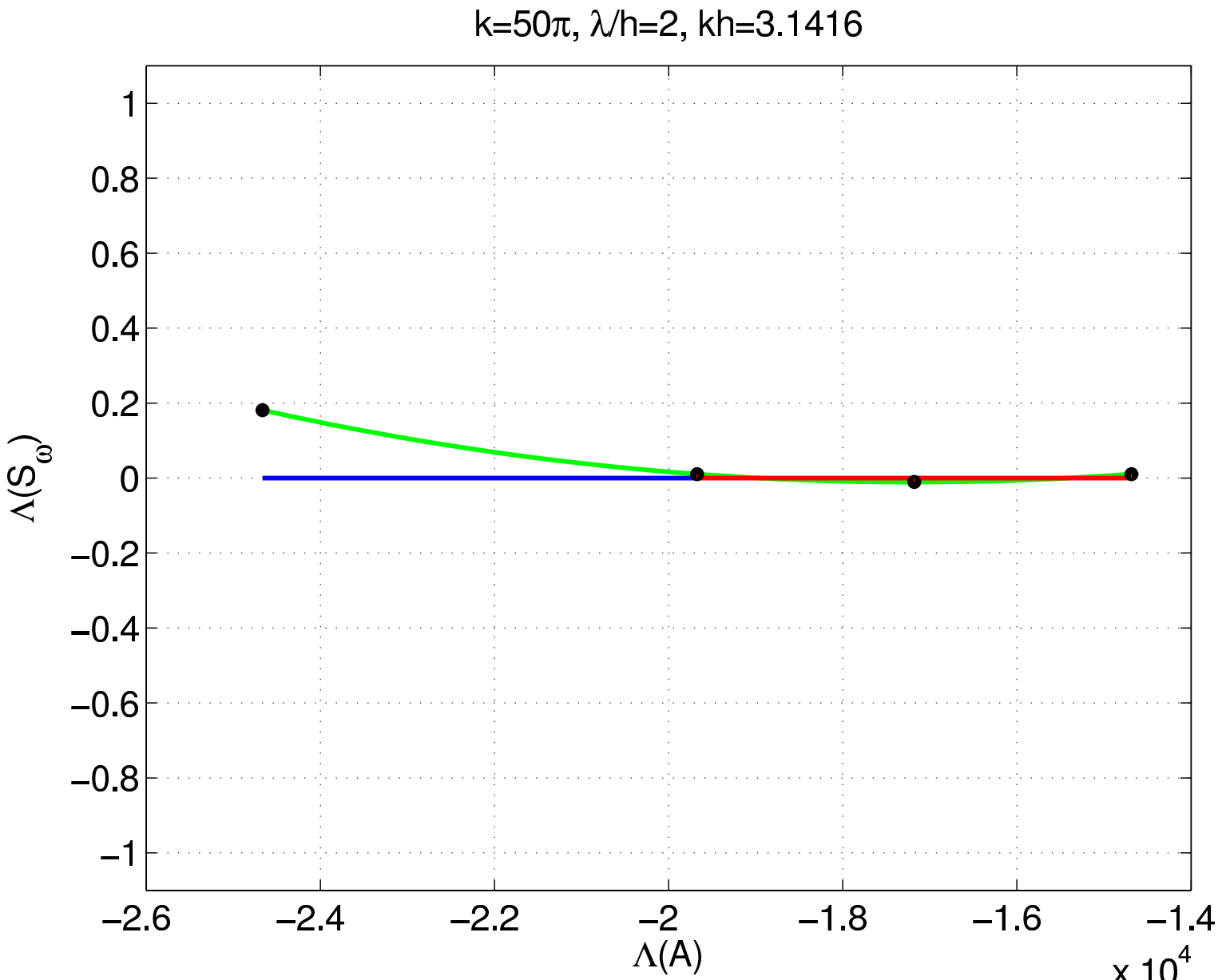
Example for a Two-Step Jacobi: Case 3

$x_{max} < 1$: solution by equioscillation and constraint



Example for a Two-Step Jacobi: Case 3

$x_{max} < 1$: solution by equioscillation



Theoretical Results

Theorem (Ernst and G (2009))

For the resonance case, $x_m < 1 < x_{\max}$, and an optimized but fixed J-step Jacobi smoother, one needs to perform $O(k^2)$ smoothing steps in order to obtain a multigrid algorithm that converges independently of k.

Theorem (Ernst and G (2009))

With a variable J-step Jacobi smoother (like the Chebyshev semi-iterative method), one only needs to perform $O(k)$ smoothing steps in order to obtain a multigrid algorithm that converges independently of k.

Corollary

If one uses a Krylov method for smoothing at the resonance level, $O(k)$ steps of the method suffice to obtain a multigrid algorithm which converges independently of k.

Numerical Results

1d Helmholtz equation with Dirichlet BC.

10 points per wavelength, 8 pre and post smoothing steps with spectral corrected coarse grid problem, optimized 2 step Jacobi, or Krylov smoother, relative residual reduction 10^{-6}

k	158.65	315.73	629.89	1258.21	2514.84
h	2^{-8}	2^{-9}	2^{-10}	2^{-11}	2^{-12}
levels	6	7	8	9	10
iter J	12	11	10	10	9
iter G	9	9	8	8	8

iter J: number of iterations when on the resonance level $O(k^2)$ 2-step optimized Jacobi steps are performed

iter G: number of iterations when on the resonance level $O(k)$ GMRES steps are performed.

Conclusions

- Multigrid methods are effective for symmetric positive definite problems because:
  1. The smoother is effectively removing high frequency components in the error
  2. The coarse grid correction is effectively removing low frequency components in the error

- It is difficult to solve Helmholtz problems by a multilevel method, because:
  1. Classical smoothers amplify smooth modes and are ineffective for modes close to resonance
  2. Classical coarse grid corrections can lead to arbitrarily bad corrections

- Any multilevel method for wave propagation problems will have to deal with the dispersion relation problem on coarser grids.