Numerical Solutions to PDEs

Lecture Notes #21
Elliptic Equations — Finite Difference Schemes

Peter Blomgren,
⟨blomgren.peter@gmail.com⟩

Department of Mathematics and Statistics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720

http://terminus.sdsu.edu/

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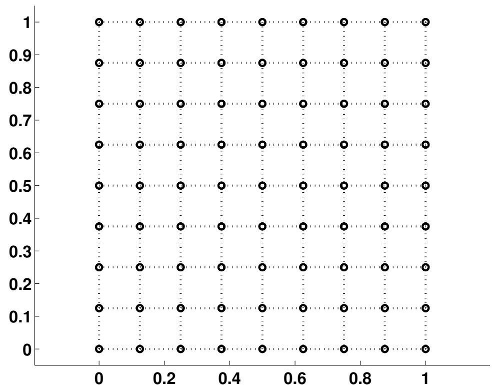
Outline

Finite Difference Schemes for Elliptic Problems

We start out by considering Poisson's equation

$$\nabla^2 u = f,$$

in the unit square. We lay in a grid with spacings $\Delta x = \Delta y = h$:



The Five-Point Laplacian

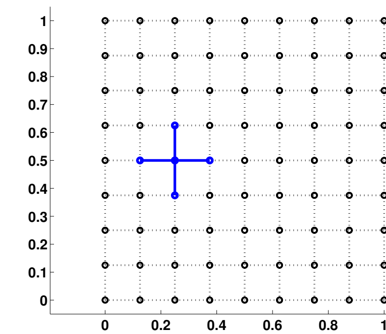
Here, we use standard centered second order finite difference approximations for the spatial derivatives

$$\delta_x^2 v_{\ell,m} + \delta_y^2 v_{\ell,m} = f_{\ell,m},$$

or, equivalently,

$$\frac{1}{h^2}\left(v_{\ell+1,m} + v_{\ell-1,m} + v_{\ell,m+1} + v_{\ell,m-1} - 4v_{\ell,m}\right) = f_{\ell,m}.$$

Figure: This difference operator is known as the five-point Laplacian, and the symbol ∇_h^2 is sometimes used. Applied at $(\ell, m) = (3, 5)$ we get the picture:



Discrete Maximum Principle

⇝ Uniqueness of Solutions...

Deriving a maximum principle for the discrete 5-point Laplacian analogous to the maximum principle for the PDE is quite straight-forward:

Theorem (Discrete Maximum Principle)

If $\nabla_h^2 v \geq 0$ on a region, then the maximum value of v on this region is attained on the boundary. Similarly if $\nabla_h^2 v \leq 0$, then the minimum value of v is attained on the boundary.

Further, for $\nabla_h^2 v = f$, it can be shown

Theorem

If $v_{\ell,m}$ is a discrete function defined on a grid on the unit square with $v_{\ell,m} = 0$ on the boundary, then

$$\|v\|_\infty \leq \frac{1}{8}\|\nabla_h^2 v\|_\infty = \frac{1}{8}\|f\|_\infty.$$

Error Estimate

The second theorem on slide 5 can be used to derive the following error estimate for the numerical solution

Theorem

Let $u(x, y)$ be the solution to $\nabla^2 u = f$ on the unit square with Dirichlet boundary conditions and let $v_{\ell,m}$ be the solution to $\nabla_h^2 v = f$ with $v_{\ell,m} = u(x_\ell, y_m)$ on the boundary. Then

$$\|u - v\|_\infty \leq ch^2\|\partial^4 u\|_\infty.$$

We see that we get second-order accuracy in the grid parameter h, and the constant depends on the maximal value of the fourth order derivatives of the exact solution.

The 9-Point Laplacian — 4th Order Accuracy — 1 of 2

Using Taylor expansions, it is quite easy* to identify what corrections need to be made to the 5-point Laplacian in order to cancel out the second order error terms; this procedure leads to the 4th order accurate scheme:

$$\nabla_h^2 v + \frac{1}{12}\left(\Delta x^2 + \Delta y^2\right)\delta_x^2\delta_y^2 v = f + \frac{1}{12}\left(\Delta x^2\delta_x^2 + \Delta y^2\delta_y^2\right) f.$$

In the case $\Delta x = \Delta y = h$ this breaks down to

$$\begin{aligned}
&\frac{1}{6}(v_{\ell+1,m+1} + v_{\ell+1,m-1} + v_{\ell-1,m+1} + v_{\ell-1,m-1}) \\
&\qquad + \frac{2}{3}(v_{\ell+1,m} + v_{\ell-1,m} + v_{\ell,m+1} + v_{\ell,m-1}) - \frac{10}{3}v_{\ell,m} \\
&\qquad\qquad = \frac{h^2}{12}(f_{\ell+1,m} + f_{\ell-1,m} + f_{\ell,m+1} + f_{\ell,m-1} + 8f_{\ell,m}).
\end{aligned}$$

* See *e.g.* Lecture #6.

The 9-Point Laplacian — 4th Order Accuracy — 2 of 2

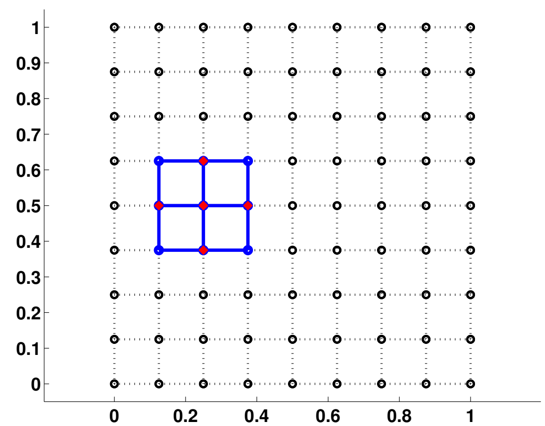


Figure: The 9-point Laplacian. The values of v at all nine points are involved in the expression, and the values of f at the five non-corners of the box are also involved. The scheme satisfies maximum principles and error estimates similar to the standard five-point Laplacian.

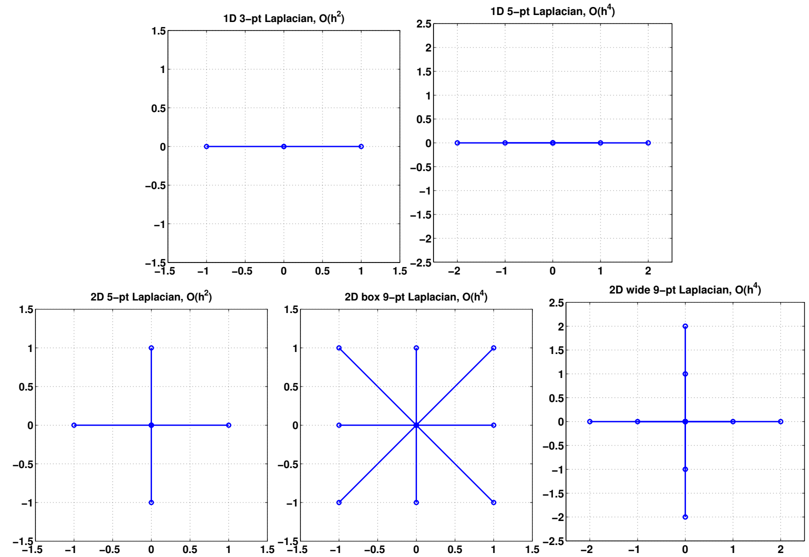
2D, 3D, nD...

In higher dimensions the second order (5-pt in 2D) and fourth order (9-pt in 2D) discrete Laplacians have even more points:

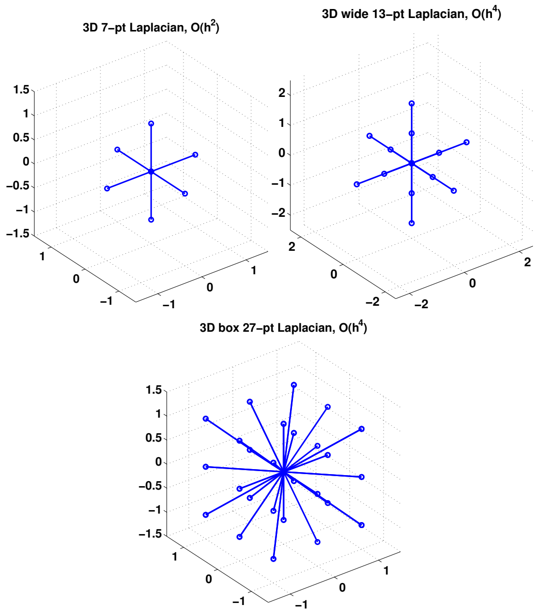
Dimensions	2nd Order	4th order
1	3-pt	5-pt
2	5-pt	9-pt
3	7-pt	13^{+} / $27^{\dagger}$-pt

$^{+}$ wide-stencil; † compact "box."

2D, 3D, nD...



2D, 3D, nD...



Regularity Estimates for Schemes

As for the PDE itself, it is possible to derive regularity estimates for finite difference schemes for elliptic problems. They essentially take the same form as the corresponding estimates for the PDE, *e.g.*

$$\|v\|^2_{h,s+2,\Omega_1} \leq C_s \left[\|f\|^2_{h,s,\Omega} + \|u\|^2_{h,0,\Omega} \right], \quad \Omega_1 \subset \Omega,$$

and the following can be shown:

Theorem

If the elliptic equation $Lu = f$ is approximated by the scheme $L_h v = R_h f$ on a domain Ω such that

$$\|L_h u - R_h L u\|_{h,s-2,\Omega} \leq c_0 h^r \|u\|_s, \text{ and } \|u - v\|_{h,0,\Omega} \leq c_1 h^r \|u\|_s$$

and $\Omega_1 \subset \Omega$, then $\|\delta_+^s \mathbf{u} - \delta_+^s \mathbf{v}\|_{h,0,\Omega_1} \leq \mathbf{c_2 h^r} \|\mathbf{u}\|_s$, where c_2 depends on the distance between Ω_1 and $\partial\Omega$.

Regularity Estimates for Schemes

The theorem (on slide 12) shows that if f is smooth enough, then the finite differences of v approximate the finite differences of the exact solution u to the same order that v itself approximates u.

In general, this is not true since

$$\frac{v_{\ell+1,m} - v_{\ell-1,m}}{2h} = \frac{\partial u(x_\ell, y_m)}{\partial x} + \mathcal{O}\left(h^{r-1}\right)$$

i.e. the division by $2h$ reduces divides the error by a factor of h.

However, the theorem states that when $v_{\ell,m}$ and u are solutions to elliptic problems, then the error term can be $\mathcal{O}\left(h^r\right)$. — **This is a significant result.**

Solving Finite Difference Schemes for Elliptic Problems

We now turn our attention to the important issue of how to find the (numerical) solutions to schemes for elliptic problems.

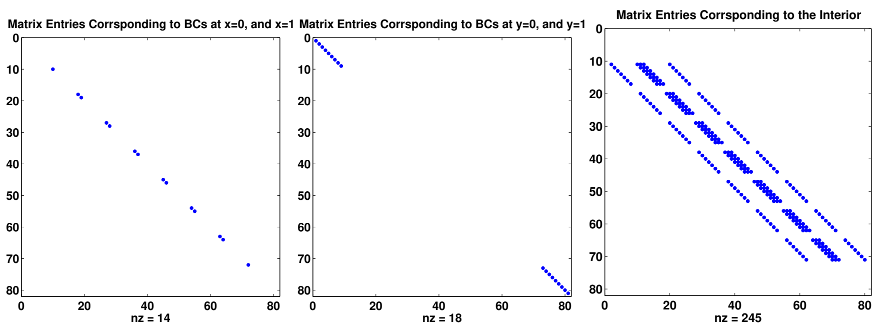
We consider Laplace's equation $\nabla^2 u = 0$ on the unit square, with Dirichlet boundary conditions. The 5-point Laplacian gives the relation

$$v_{\ell+1,m} + v_{\ell-1,m} + v_{\ell,m+1} + v_{\ell,m-1} - 4v_{\ell,m} = 0,$$

at the **interior points**. By mapping $k = \ell + (m-1)\cdot n_x$, where $h = 1/(n_x - 1) = 1/(n_y - 1)$ (n_x, n_y being the number of grid-points in the x- and y-directions respectively), and $w_k = v_{\ell,m}$ we get a linear system:

$$A\bar{\mathbf{w}} = \bar{\mathbf{b}}.$$

The Linear System $A\bar{\mathbf{w}} = \bar{\mathbf{b}}$



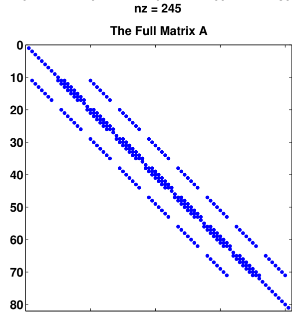


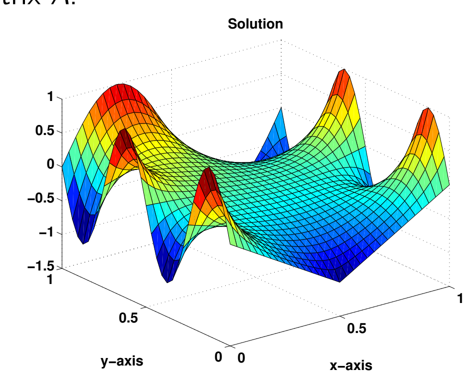
Illustration: The structure of the matrix A, the first panel show the diagonal entries, 1, corresponding to the boundary condition at $x = 0, 1$, $0 < y < 1$; the second panel to the diagonal entries for the BC at $y = 0, 1$, $0 \le x \le 1$; the third panel to the interior relations (the diagonal entry is -4 and the four off-diagonal entries are 1). The final panel shows the completed matrix.

The Linear System $A\bar{\mathbf{w}} = \bar{\mathbf{b}}$

The RIGHT-HAND-SIDE $\bar{\mathbf{b}}$ is zero, except in the entries corresponding to the boundary conditions; here we set (for $(x_\ell, y_m) \in \Gamma$)

$$b_{\ell+(m-1)n_x} = \sin(2\pi x_\ell) y_m + (1 - 2\,|x_\ell - 1/2|)(y_m - 1) + \sin(4\pi y_m),$$

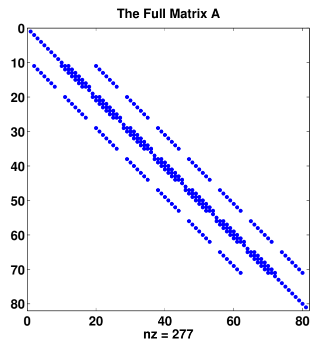
and get the solution; — here on a 33×33-grid, with a corresponding $1{,}089 \times 1{,}089$-matrix A:



Solving Elliptic Problems and $A\bar{\mathbf{w}} = \bar{\mathbf{b}}$

The numerical solution of elliptic problems invariably reduces to, hopefully efficiently, solving a linear system $A\bar{\mathbf{w}} = \bar{\mathbf{b}}$, where A is the discretization of the elliptic operator.

As we can see, the matrix A has a lot of "structure," in particular the majority of the entries are zeros (*i.e.* the matrix is **sparse**). Here, with the 5-point Laplacian, the "fill rate" is only $\sim 5/(n_x \cdot n_y) \sim 5h^2$. Taking full advantage of this structure is the key to efficient elliptic solvers.



As a benchmark, standard Gaussian Elimination applied to this problem requires $\mathcal{O}\left(n_x^3 n_y^3\right) \sim \mathcal{O}\left(h^{-6}\right)$ operations, this quickly grows out of control (in 3D the operation count grows as $\mathcal{O}\left(h^{-9}\right)$).

Linear Iterative Methods for $A\bar{\mathbf{w}} = \bar{\mathbf{b}}$

Directly inverting $A\bar{\mathbf{w}} = \bar{\mathbf{b}}$ by Gaussian elimination is usually out of the question for any problem of interesting size.

To get us thinking in the right direction, we look at three "classical" algorithms for approaching this problem:

- **the Jacobi method**,
- **the Gauss-Seidel method**, and
- **the SOR method**.

These methods are not particularly good, but serve as a starting point for our discussion.

Linear Iterative Methods for $A\bar{\mathbf{w}} = \bar{\mathbf{b}}$

The **Jacobi method** is given by the update formula

$$v_{\ell,m}^{k+1} = \frac{1}{4}\left(v_{\ell+1,m}^{k} + v_{\ell-1,m}^{k} + v_{\ell,m+1}^{k} + v_{\ell,m-1}^{k}\right),$$

applied to all interior points $\ell \in [2, n_x - 1]$, $m \in [2, n_y - 1]$. Once all the values $v_{\ell,m}^{k+1}$ are computed, we move on to compute $v_{\ell,m}^{k+2}$. Each iteration ("sweep") requires $\mathcal{O}\left(n_x n_y\right)$ operations/memory accesses. As long as this converges in less than $n_x^2 n_y^2$ iterations, this procedure will be faster than straight Gaussian elimination.

Storage Consideration: The Jacobi method requires (at least) two copies of the grid (time-level k, and $k+1$).

Linear Iterative Methods for $A\bar{\mathbf{w}} = \bar{\mathbf{b}}$

The Jacobi method converges very slowly (especially for large matrices), and it is quite easy to improve on it.

The **Gauss-Seidel method** converges twice as fast, and does not require extra storage to keep $v_{\ell,m}^{k}$ and the update $v_{\ell,m}^{k+1}$ simultaneously; the update formula is "Jacobi-style" but we use computed values as soon as we have them, *i.e.*

$$v_{\ell,m}^{k+1} = \frac{1}{4}\left(v_{\ell+1,m}^{k} + v_{\ell-1,m}^{\mathbf{k+1}} + v_{\ell,m+1}^{k} + v_{\ell,m-1}^{\mathbf{k+1}}\right),$$

Storage Consideration: The Gauss-Seidel method one requires one copy of the grid, since it is being over-written as the computation moves along.

The movies: `jacobi_update.mpg` and `gs_update.mpg` each illustrate the update sequence for one sweep.

Linear Iterative Methods for $A\bar{\mathbf{w}} = \bar{\mathbf{b}}$

The **Successive Over-relaxation (SOR)** method is an accelerated version of Gauss-Seidel

$$v_{\ell,m}^{k+1} = v_{\ell,m}^{k} + \omega\left[\frac{1}{4}\left(v_{\ell+1,m}^{k} + v_{\ell-1,m}^{\mathbf{k+1}} + v_{\ell,m+1}^{k} + v_{\ell,m-1}^{\mathbf{k+1}}\right) - v_{\ell,m}^{k}\right],$$

where $\omega \in (0,2)$. When $\omega = 1$ it reduces to Gauss-Seidel, and for the optimal choice* of ω is it significantly faster than the Gauss-Seidel iteration.

It turns out that (not so obviously)

$$\omega^* = \frac{2}{1 + \sin(\pi/(N-1))},$$

is the optimal choice for the 5-point Laplace operator on an $N \times N$ grid on the unit square.

Analysis of Linear Iterative Methods

We can only give the flavor of the analysis here, a full treatment requires the knowledge from **Math 543 – Numerical Matrix Analysis** and another semester course (643 – to be developed???) in iterative methods on top of that.

The following is an excellent reference:

[SAAD2003] Yousef Saad, **"Iterative Methods for Sparse Linear Systems,"** 2nd edition, Society for Industrial and Applied Mathematics (SIAM), 2003. ISBN 978-0-898715-34-7 (paperback), $117.00 ($81.90 member price).

Recently published:

[MS2015] Josef Málek and Zdenek Strakos, **"Preconditioning and the Conjugate Gradient Method in the Context of Solving PDEs,"** Society for Industrial and Applied Mathematics (SIAM), 2015. ISBN 978-1-611973-83-9 (paperback), $39.00 ($27.30 member price).

Analysis of Linear Iterative Methods

The iterative methods we have described are all aiming at solving a linear system

$$A\bar{\mathbf{x}} = \bar{\mathbf{b}},$$

and can be viewed as decomposing the matrix A by writing it as $A = B - C$ and then iteratively solving the system of equations

$$B\bar{\mathbf{x}}^{k+1} = C\bar{\mathbf{x}}^{k} + \bar{\mathbf{b}}.$$

In the Jacobi case B is the diagonal part of A, and in the Gauss-Seidel case it is the lower triangular part of A.

We always want to choose B so that the (iterative) linear system is easy (fast) to solve.

Since the exact solution satisfies $A\bar{\mathbf{x}} = \bar{\mathbf{b}}$ (and $B\bar{\mathbf{x}} = C\bar{\mathbf{x}} + \bar{\mathbf{b}}$), we get an iterative equation for the error, $\bar{\mathbf{e}}$:

$$\mathbf{B}\bar{\mathbf{e}}^{\mathbf{k+1}} = \mathbf{C}\bar{\mathbf{e}}^{\mathbf{k}}.$$

Analysis of Linear Iterative Methods

From $B\bar{\mathbf{e}}^{k+1} = C\bar{\mathbf{e}}^{k}$ we see that

$$\bar{\mathbf{e}}^{\mathbf{k+1}} = \mathbf{B}^{-1}\mathbf{C}\,\bar{\mathbf{e}}^{\mathbf{k}},$$

where the matrix $M = B^{-1}C$ is called the **iteration matrix** for the algorithm.

Clearly, we want the error to go to zero as fast as possible. The rate of convergence to zero is controlled by the **spectral radius**, ρ of the iteration matrix

$$\rho(M) = \max_i |\lambda_i|,$$

where λ_i, $i = 1, \ldots, N$ are the eigenvalues of M.

The spectral radius, $\rho(B^{-1}C)$, must be strictly bounded by 1 in order for the iterative scheme to be convergent.

Analysis of Linear Iterative Methods

After k iterations we have the following estimate for the error

$$\left\|\bar{\mathbf{e}}^k\right\| < \rho(B^{-1}C)^k \cdot \left\|\bar{\mathbf{e}}^0\right\|$$

Clearly, the smaller $\rho(B^{-1}C)$ is the faster we reach acceptable convergence $\left\|\bar{\mathbf{e}}^k\right\| \leq \epsilon_{\text{tol}}$.

For the 5-point Laplacian, the spectral radii for the Jacobi, Gauss-Seidel, and optimal SOR iteration matrices are

$$\begin{aligned} \rho_{\text{Jac}} &\sim 1 - \frac{\pi^2}{2N^2}, \\ \rho_{\text{GS}} &\sim 1 - \frac{\pi^2}{N^2}, \\ \rho^*_{\text{SOR}} &\sim 1 - \frac{2\pi}{N}. \end{aligned}$$

Analysis of Linear Iterative Methods

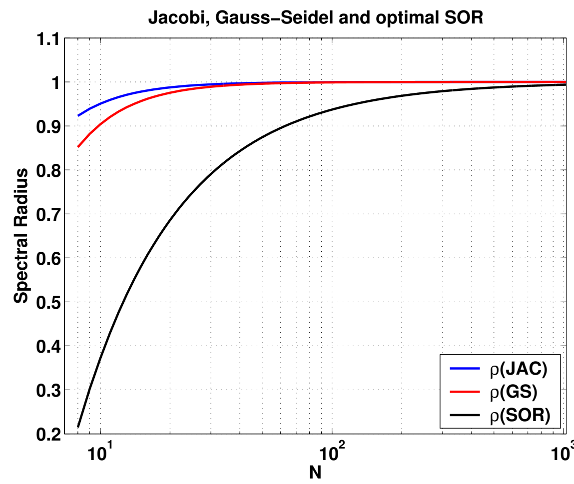


Figure: The spectral radii for the Jacobi, Gauss-Seidel, and SOR iteration matrices corresponding to the 5-point Laplacian. We see that all three approach one very rapidly.

Analysis of Linear Iterative Methods $\texttt{tol} = 10^{-8}$