Considered methods for solving elliptic equations

Poisson equation $$\nabla^2 u(\vec{r}) = -f(\vec{r})$$

Boundary conditions:

$$u(\vec{r})\big|_{\Gamma} = g(\vec{r})$$ (Dirichlet)

$$\left.\frac{\partial u(\vec{r})}{\partial n}\right|_{\Gamma} = g(\vec{r})$$ (Neumann)

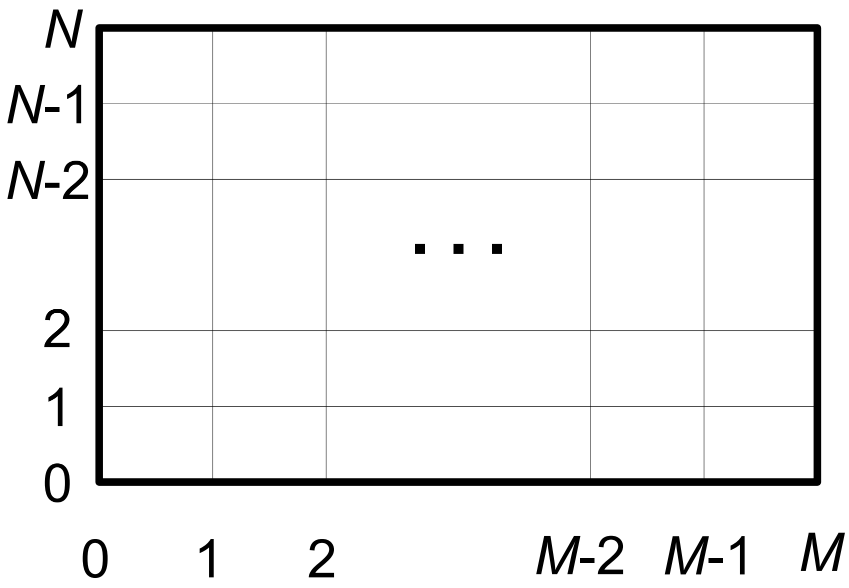
Electrostatics: $$\nabla^2 \phi(\vec{r}) = -\frac{4\pi\rho(\vec{r})}{\epsilon} \text{ (CGS)} \quad \text{or} \quad \nabla^2 \phi(\vec{r}) = -\frac{\rho(\vec{r})}{\epsilon_0 \epsilon} \text{ (SI)}$$

Stationary temperature distribution: $$\nabla^2 T(\vec{r}) = -\frac{f(\vec{r})}{\alpha}$$

Concentration of diffusing particles: $$\nabla^2 c(\vec{r}) = -\frac{f(\vec{r})}{D}$$

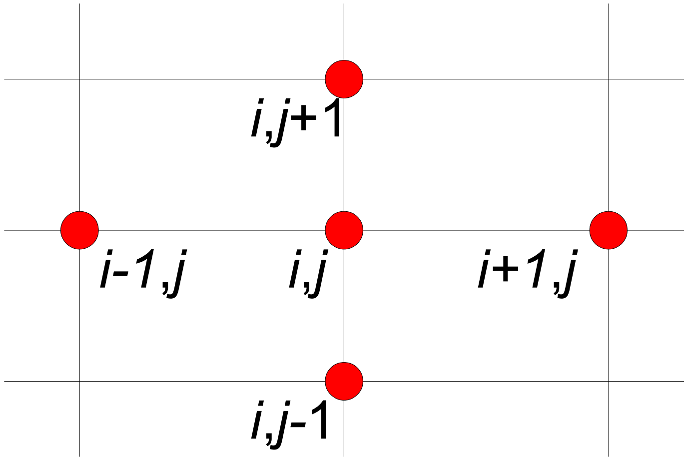
$$-\left(\frac{\partial^2 u(x,y)}{\partial x^2}+\frac{\partial^2 u(x,y)}{\partial y^2}\right)=f(x,y) \qquad u|_\Gamma=0$$

Finite difference method



Rectangular domain.

Introduce a grid.



Discretization

$$-\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{\Delta x^2}-\frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{\Delta y^2}\approx f_{ij}$$

5-point stencil

u's for boundary sites (i.e., $u_{0,j}$, $u_{M,j}$, $u_{i,0}$, and $u_{i,N}$) replaced with 0's

$$A\vec{u} = \vec{f}$$

$$A = \frac{1}{h^2}\left(\begin{array}{ccc|ccc|ccc}
4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\
\hline
-1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\
0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\
0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\
\hline
0 & 0 & 0 & -1 & 0 & 0 & 4 & -1 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4
\end{array}\right)$$

Block-tridiagonal matrix (block size is M-1) or band-diagonal with band width 2M-1

Symmetric positive definite.

Methods of solving the resulting linear system.

Take sparseness of the matrix into account.

Direct methods (Gauss elimination, Cholesky decomposition).

Iterative methods (Jacobi, Gauss-Seidel, SOR, alternating direction implicit, conjugate gradient).

Direct methods are exact in principle – but, of course, discretization itself is approximate and if the methods are so costly that only coarse discretization is possible, may not make sense to apply them.

Direct methods produce high accuracy, but take no advantage if only low accuracy is required.

Direct methods do not require an initial estimate, but do not make use of one of it is available.

Direct methods are more robust (no issue of slow convergence or non-convergence for “bad” systems). Do not rely on special properties of systems.

Generally, in 1D direct methods are definitely preferable – in the simplest case the matrix is tridiagonal.

In 2D, direct methods are competitive with at least the more straightforward iterative methods.

In 3D, iterative methods are generally preferable.

An interesting way to accelerate SOR.

$$x_i^{(k+1)} = (1-\omega)\, x_i^{(k)} + \frac{\omega}{a_{ii}}\left(-\sum_{j<i} a_{ij}\, x_j^{(k+1)} - \sum_{j>i} a_{ij}\, x_j^{(k)} + b_i\right)$$

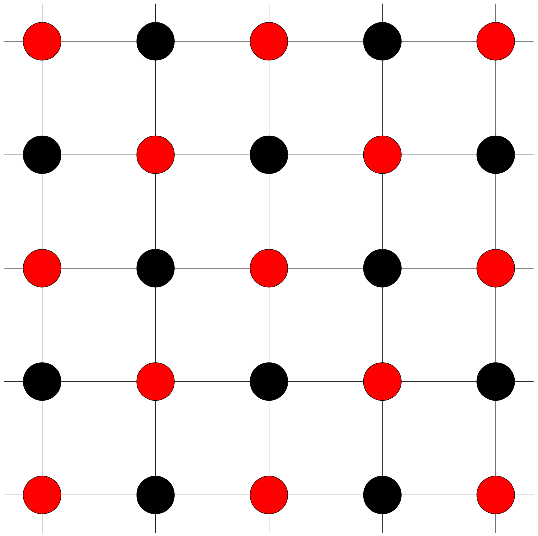
There is an optimal value of ω:

$$\omega_{\text{opt}} = \frac{2}{1+\sqrt{1-\lambda_J^2}}.$$

In our case, $\lambda_J = \dfrac{\cos(\pi/M) + \beta^2 \cos(\pi/N)}{1+\beta^2}$; $\beta = \Delta x/\Delta y$

λ_J is the spectral radius of the Jacobi iteration.

Turns out that ω_{opt} is only optimal asymptotically, after a large number of iterations.



Specifically for the red-black scheme, it is possible to improve initial convergence by varying ω:

$$\omega^{(0)} = 1 \qquad \omega^{(1)} = \frac{1}{1-\lambda_J^2/2}$$

$$\omega^{(n+1)} = \frac{1}{1-\lambda_J^2\, \omega^{(n)}/4}, \quad n = 1, 2, \ldots$$

$$\omega^{(\infty)} = \frac{1}{1-\lambda_J^2\, \omega^{(\infty)}/4} \Rightarrow \omega^{(\infty)} = \frac{2}{1\pm\sqrt{1-\lambda_J^2}}.$$

Only "+" is stable.

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There are some additional very fast methods that, however only work in special cases.

Fast Fourier Transform method

$$-\frac{u_{m+1,n}-2u_{m,n}+u_{m-1,n}}{\Delta x^2}-\frac{u_{m,n+1}-2u_{m,n}+u_{m,n-1}}{\Delta y^2}\approx f_{mn}$$

Assume periodic boundary conditions for now.

Inverse discrete Fourier transform

$$u_{m,n}=\frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1}\hat{u}_{k,l}e^{-2\pi imk/M}e^{-2\pi inl/N}$$

$$u_{m+1,n}=\frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1}\hat{u}_{k,l}e^{-2\pi imk/M}e^{-2\pi ik/M}e^{-2\pi inl/N}$$ etc.

$$f_{m,n}=\frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1}\hat{f}_{k,l}e^{-2\pi imk/M}e^{-2\pi inl/N}$$

$$\frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1}\hat{u}_{k,l}e^{-2\pi imk/M}e^{-2\pi inl/N}\left[-\frac{e^{-2\pi ik/M}-2+e^{2\pi ik/M}}{\Delta x^2}-\frac{e^{-2\pi il/N}-2+e^{2\pi il/N}}{\Delta y^2}\right]$$

$$=\frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1}\hat{f}_{k,l}e^{-2\pi imk/M}e^{-2\pi inl/N}$$

$$\frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1}\hat{u}_{k,l}e^{-2\pi imk/M}e^{-2\pi inl/N}\left[-\frac{e^{-2\pi ik/M}-2+e^{2\pi ik/M}}{\Delta x^2}-\frac{e^{-2\pi il/N}-2+e^{2\pi il/N}}{\Delta y^2}\right]$$

$$=\frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1}\hat{f}_{k,l}e^{-2\pi imk/M}e^{-2\pi inl/N}$$

Multiply by $e^{2\pi imr/M}e^{2\pi ins/N}$, sum over *m* and *n*, get factor $MN\,\delta_{kr}\,\delta_{ls}$

$$\hat{u}_{r,s}\left[-\frac{e^{-2\pi ik/M}-2+e^{2\pi ik/M}}{\Delta x^2}-\frac{e^{-2\pi il/N}-2+e^{2\pi il/N}}{\Delta y^2}\right]=\hat{f}_{r,s}$$

$$\hat{u}_{r,s}=\frac{\hat{f}_{r,s}/2}{\dfrac{1-\cos(2\pi k/M)}{\Delta x^2}+\dfrac{1-\cos(2\pi l/N)}{\Delta y^2}}$$

$$\Delta x=\Delta y=h \qquad \hat{u}_{r,s}=\frac{h^2\hat{f}_{r,s}/2}{2-\cos(2\pi k/M)-\cos(2\pi l/N)}$$

Do FFT of $f_{m,n}$, get $\hat{f}_{r,s}$, calculate $\hat{u}_{r,s}$, do inverse FFT to get $u_{m,n}$

For homogeneous Dirichlet conditions ($u|_{\Gamma}=0$), do discrete sine transform:

$$u_{m,n}=\frac{4}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1}\hat{u}_{k,l}\sin\frac{\pi mk}{M}\sin\frac{\pi nl}{N}$$

Satisfies boundary conditions automatically.

Fast sine transform is similar to FFT.

For inhomogeneous conditions, consider again the discretized equations:

$$-\frac{u_{m+1,n}-2u_{m,n}+u_{m-1,n}}{\Delta x^2}-\frac{u_{m,n+1}-2u_{m,n}+u_{m,n-1}}{\Delta y^2}\approx f_{mn}$$

For the homogeneous BC, *u*'s corresponding to boundary sites are fixed at zero. Now the only difference is they are fixed at some other value. Since this value is known, they can simply be moved to the right-hand side, and the left-hand side will be equivalent to the homogeneous case.

For homogeneous Neumann conditions ($\left.\frac{\partial u(\vec{r})}{\partial n}\right|_{\Gamma}=0$), do discrete cosine transform:

$$u_{m,n}=\frac{4}{MN}\sum{}'^{M}_{k=0}\sum{}'^{N}_{l=0}\hat{u}_{k,l}\cos\frac{\pi mk}{M}\cos\frac{\pi nl}{N}$$

“Prime” means that the first and last terms in the sums get multiplied by 1/2.

For inhomogeneous conditions ($\left.\frac{\partial u(\vec{r})}{\partial n}\right|_{\Gamma}=g(\vec{r})$), there are equations of the type

$$\frac{u_{1,n}-u_{-1,n}}{2\Delta x}=g_n$$

$$-\frac{u_{1,n}-2u_{0,n}+u_{-1,n}}{\Delta x^2}=-\frac{u_{1,n}-2u_{0,n}+u_{1,n}-2g_n\Delta x}{\Delta x^2}$$

So we have the same equation as in the homogeneous case, except we add

$2g_n/\Delta x$ to $f_{0,n}$.

The Fourier transform method is only applicable to the case of constant coefficients and rectangular boundaries.

Cyclic reduction

$$u_{xx}+u_{yy}+b(y)u_y+c(y)u=g(x,y)$$

This form arises, e.g., in polar coordinates.

$$\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{\Delta x^2}+\frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{\Delta y^2}+b_{i,j}\frac{u_{i,j+1}-u_{i,j-1}}{2\Delta y}+c_{i,j}u_{i,j}=g_{i,j}$$

$$\vec{u}_i=(u_{i,0},\dots,u_{i,N})^T \qquad \vec{g}_i=(g_{i,0},\dots,g_{i,N})^T \qquad \vec{u}_{i-1}+\boldsymbol{T}\cdot\vec{u}_i+\vec{u}_{i+1}=\vec{g}_i\Delta x^2$$

$\boldsymbol{T}=\boldsymbol{B}-2\boldsymbol{I}$ ***B*** and thus ***T*** are tridiagonal.

$$\vec{u}_{i-2}+\boldsymbol{T}\cdot\vec{u}_{i-1}+\vec{u}_i=\vec{g}_{i-1}\Delta x^2$$

$$\vec{u}_{i-1}+\boldsymbol{T}\cdot\vec{u}_i+\vec{u}_{i+1}=\vec{g}_i\Delta x^2$$

$$\vec{u}_i+\boldsymbol{T}\cdot\vec{u}_{i+1}+\vec{u}_{i+2}=\vec{g}_{i+1}\Delta x^2$$

Multiply the middle equation by ***-T***, add them up:

$$\vec{u}_{i-2}+(2\boldsymbol{I}-\boldsymbol{T}^2)\vec{u}_i+\vec{u}_{i+2}=(\vec{g}_{i-1}-\boldsymbol{T}\vec{g}_i+\vec{g}_{i+1})\Delta x^2$$

$$\vec{u}_{i-1}+\boldsymbol{T}\cdot\vec{u}_i+\vec{u}_{i+1}=\vec{g}_i\Delta x^2$$

$$\vec{u}_{i-2}+\left(2\boldsymbol{I}-\boldsymbol{T}^2\right)\vec{u}_i+\vec{u}_{i+2}=\left(\vec{g}_{i-1}-\boldsymbol{T}\vec{g}_i+\vec{g}_{i+1}\right)\Delta x^2$$

Have an equation of the same type, but on a mesh twice as coarse.

$$\boldsymbol{T}^{(1)}=2\boldsymbol{I}-T^2 \qquad \vec{g}_i^{(1)}=\vec{g}_{i-1}-\boldsymbol{T}\vec{g}_i+\vec{g}_{i+1}$$

If the number of mesh intervals along x, M = 2^{s+1}, then after *s* such transformations,

$$\vec{u}_0+\vec{T}^{(s)}\vec{u}_{M/2}+\vec{u}_M=\vec{g}_{M/2}^{(s)}\Delta x^2$$

$$\vec{T}^{(s)}\vec{u}_{M/2}=\vec{g}_{M/2}^{(s)}\Delta x^2-\vec{u}_0-\vec{u}_M$$

$\vec{u}_0$ and $\vec{u}_M$ are boundary conditions and thus are known. Tridiagonal system, can be solved quickly. Go back recursively, e.g.,

$$\vec{T}^{(s-1)}\vec{u}_{M/4}=\vec{g}_{M/4}^{(s)}\Delta x^2-\vec{u}_0-\vec{u}_{M/2} \qquad \vec{T}^{(s-1)}\vec{u}_{3M/4}=\vec{g}_{3M/4}^{(s)}\Delta x^2-\vec{u}_{M/2}-\vec{u}_M$$

Numerical stability issues.

Can combine with the Fourier transform in the y direction (FACR method).

Multigrid approach: if shorter-wavelength components relax faster than longer-wavelength components, then alternate between coarser and finer grids.

Method	2-D	3-D
Dense Cholesky	k^6	k^9
Jacobi	$k^4 \log k$	$k^5 \log k$
Gauss-Seidel	$k^4 \log k$	$k^5 \log k$
Band Cholesky	k^4	k^7
Optimal SOR	$k^3 \log k$	$k^4 \log k$
Sparse Cholesky	k^3	k^6
Conjugate gradient	k^3	k^4
Optimal SSOR	$k^{2.5} \log k$	$k^{3.5} \log k$
Preconditioned CG	$k^{2.5}$	$k^{3.5}$
Optimal ADI	$k^2 \log^2 k$	$k^3 \log^2 k$
Cyclic reduction	$k^2 \log k$	$k^3 \log k$
FFT	$k^2 \log k$	$k^3 \log k$
Multigrid V-cycle	$k^2 \log k$	$k^3 \log k$
FACR	$k^2 \log \log k$	$k^3 \log \log k$
Full Multigrid	k^2	k^3

M.T. Heath, Scientific Computing: An Introductory Survey, New York, McGraw-Hill, 1997.

k is the same as *M* or *N*.

Also considered Neumann and periodic boundary conditions, including other (e.g., first-order terms) in the equation. The eigenvalue problem:

$$-\nabla^2 u = \lambda u$$

$$-\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} - \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = \lambda u_{ij}$$

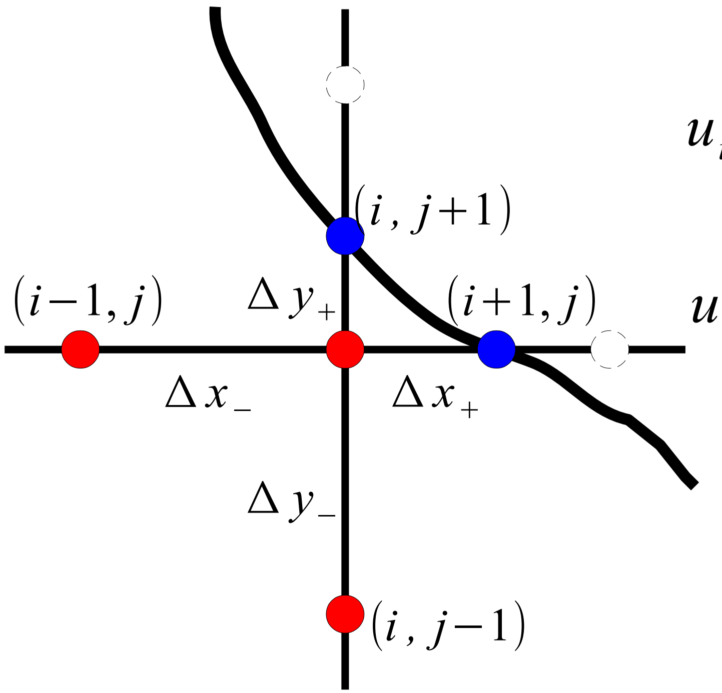
Algebraic eigenvalue problem

Non-rectangular domains.

Approximate the boundary crudely along grid lines. For instance: put $u_{i,j}$ = 0 for all sites on or outside the boundary.

There are more accurate options.

Nonuniform finite-difference approximations



$$u_{i+1,j} \approx u_{i,j} + u_x\big|_{i,j} \Delta x_+ + \frac{1}{2} u_{xx}\big|_{i,j} \Delta x_+^2 + \frac{1}{6} u_{xxx}\big|_{i,j} \Delta x_+^3$$

$$u_{i-1,j} \approx u_{i,j} - u_x\big|_{i,j} \Delta x_- + \frac{1}{2} u_{xx}\big|_{i,j} \Delta x_-^2 - \frac{1}{6} u_{xxx}\big|_{i,j} \Delta x_-^3$$

$$u_{i+1,j} \Delta x_- + u_{i-1,j} \Delta x_+ \approx (\Delta x_- + \Delta x_+) u_{i,j} + \frac{1}{2} u_{xx}\big|_{i,j} (\Delta x_+^2 \Delta x_- + \Delta x_-^2 \Delta x_+)$$
$$+ \frac{1}{6} u_{xxx}\big|_{i,j} (\Delta x_+^3 \Delta x_- - \Delta x_-^3 \Delta x_+)$$

$$u_{xx}\big|_{i,j} \approx 2 \frac{\Delta x_+ u_{i-1,j} - (\Delta x_- + \Delta x_+) u_{i,j} + \Delta x_- u_{i+1,j}}{\Delta x_- \Delta x_+^2 + \Delta x_+ \Delta x_-^2} - \frac{1}{3} (\Delta x_+ - \Delta x_-) u_{xxx}\big|_{i,j}$$

Without the last term, linear (quadratic only when $\Delta x_+ = \Delta x_-$).

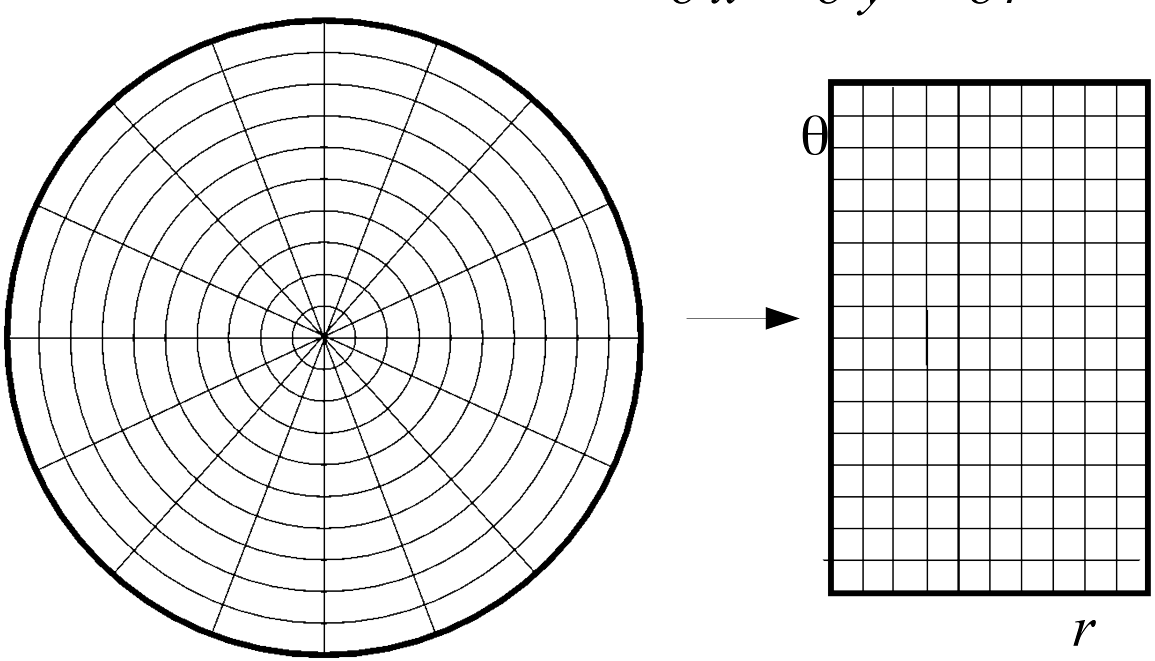
Another alternative: coordinate transformation

$(x, y) \rightarrow (\xi, \eta)$ such that the boundaries correspond to $\xi = \text{const},$ $\eta = \text{const}\,,$ or both.

Example: polar coordinates $x = r\cos\theta,\ y = r\sin\theta$

Convenient when the domain is a circle, a sector or a ring.

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}$$

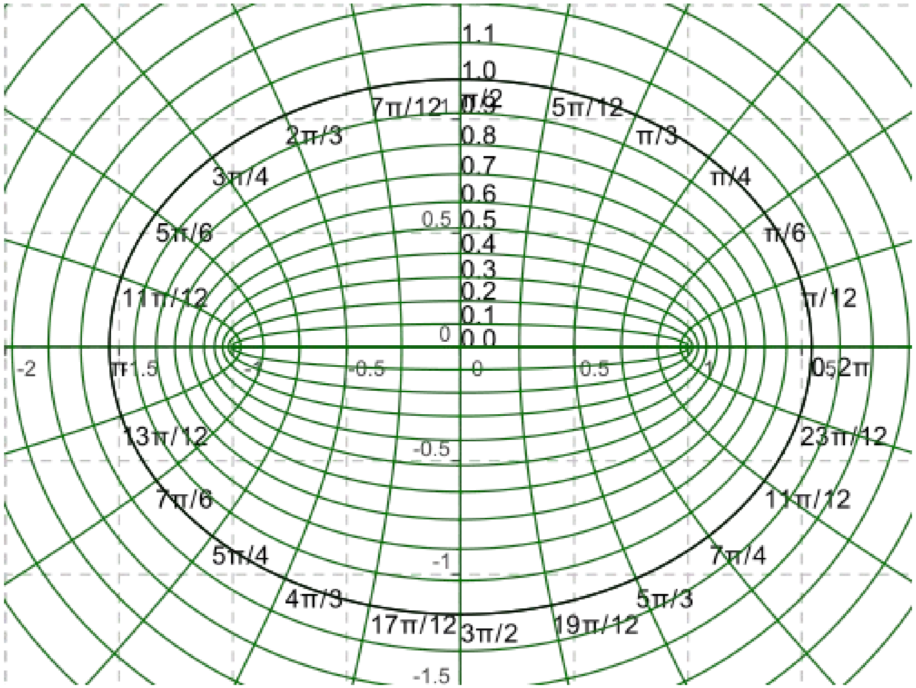


r=0 boundary merged into one point. Special treatment.

PBC in θ direction

For an ellipse: generalize polar coordinates: $x = ar\cos\theta;\; y = br\sin\theta$

Elliptic coordinates: $x = a\cosh\mu\cos\nu;\; y = a\sinh\mu\cos\nu$



$$(x, y) \to (\xi, \eta)$$

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial u}{\partial \eta}\frac{\partial \eta}{\partial x}$$

$$\frac{\partial u}{\partial y} = \frac{\partial u}{\partial \xi}\frac{\partial \xi}{\partial y} + \frac{\partial u}{\partial \eta}\frac{\partial \eta}{\partial y}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial \xi^2}\left(\frac{\partial \xi}{\partial x}\right)^2 + \frac{\partial u}{\partial \xi}\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 u}{\partial \eta^2}\left(\frac{\partial \eta}{\partial x}\right)^2 + \frac{\partial u}{\partial \eta}\frac{\partial^2 \eta}{\partial x^2} + 2\frac{\partial^2 u}{\partial \xi \partial \eta}\frac{\partial \xi}{\partial x}\frac{\partial \eta}{\partial x}$$

$$\frac{\partial^2 u}{\partial y^2} = \frac{\partial^2 u}{\partial \xi^2}\left(\frac{\partial \xi}{\partial y}\right)^2 + \frac{\partial u}{\partial \xi}\frac{\partial^2 \xi}{\partial y^2} + \frac{\partial^2 u}{\partial \eta^2}\left(\frac{\partial \eta}{\partial y}\right)^2 + \frac{\partial u}{\partial \eta}\frac{\partial^2 \eta}{\partial y^2} + 2\frac{\partial^2 u}{\partial \xi \partial \eta}\frac{\partial \xi}{\partial y}\frac{\partial \eta}{\partial y}$$

$$u_{xx} + u_{yy} = a(\xi, \eta)u_{\xi\xi} + b(\xi, \eta)u_{\xi\eta} + c(\xi, \eta)u_{\eta\eta} + d(\xi, \eta)u_{\xi} + e(\xi, \eta)u_{\eta}$$

It may also be convenient to start from

$$\frac{\partial u}{\partial \xi}=\frac{\partial u}{\partial x}\frac{\partial x}{\partial \xi}+\frac{\partial u}{\partial y}\frac{\partial y}{\partial \xi} \qquad \frac{\partial u}{\partial \eta}=\frac{\partial u}{\partial x}\frac{\partial x}{\partial \eta}+\frac{\partial u}{\partial y}\frac{\partial y}{\partial \eta}$$

Solve this system for $\frac{\partial u}{\partial x}$ and $\frac{\partial u}{\partial y}$.

$$\frac{\partial u}{\partial x}=\frac{1}{J}\left(\frac{\partial y}{\partial \eta}\frac{\partial u}{\partial \xi}-\frac{\partial y}{\partial \xi}\frac{\partial u}{\partial \eta}\right) \qquad \frac{\partial u}{\partial y}=\frac{1}{J}\left(-\frac{\partial x}{\partial \eta}\frac{\partial u}{\partial \xi}+\frac{\partial x}{\partial \xi}\frac{\partial u}{\partial \eta}\right)$$

$$J=\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta}-\frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi}$$

$$\frac{\partial^2 u}{\partial x^2}=\frac{\partial}{\partial x}\frac{\partial u}{\partial x}=\frac{1}{J}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi}-\frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\frac{\partial u}{\partial x}$$

Use $\frac{\partial u}{\partial x}$ above.

$$\frac{\partial^2 u}{\partial y^2}=\dots$$

Higher-order methods

1) 4th-order finite difference approximation of the 2[nd] derivative:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} \approx \frac{-u_{i-2,j}+16u_{i-1,j}-30u_{i,j}+16u_{i+1,j}-u_{i+2,j}}{12\Delta x^2}$$

Gives rise to a 9-point scheme. Cannot be used next to boundaries. Will need to use a lower-order scheme or an unsymmetrical scheme.

2) Compact 4th-order scheme for Laplace equation only: for $\Delta x = \Delta y = h$,

$$u_{i-1,j-1}+u_{i+1,j-1}+u_{i-1,j+1}+u_{i+1,j+1}+4\left(u_{i-1,j}+u_{i+1,j}+u_{i,j-1}+u_{i,j+1}\right)-20u_{i,j}=0$$

3) As always, Richardson extrapolation is possible (assuming no singularities).

For a method of order *n*, given two results, *y*1 for an original grid and *y*2 for a twice finer grid, $y \approx y_2 + (y_2 - y_1)/(2^n - 1)$. For *n* = 2,

$$y = (4/3)\,y_2 - (1/3)\,y_{1.}$$

Nonlinear equations

E.g., Poisson-Boltzmann eq. $\nabla^2 \phi = -4\pi \left[\rho + n_0 q \left\{ e^{-q\phi/k_B T} - e^{q\phi/k_B T} \right\} \right].$

1. Iteration. Discretize, obtain a set of nonlinear finite-difference equations.

$$\boldsymbol{A} \vec{u} = f(\vec{u})$$

$$\boldsymbol{A} \vec{u}^{(k+1)} = f(\vec{u}^{(k)})$$

$$\vec{u}^{(k+1)} = \boldsymbol{A}^{-1} f(\vec{u}^{(k)})$$

Underrelaxation can help convergence sometimes:

$$\vec{u}^{(k+1)} = (1-\omega)\vec{u}^{(k)} + \omega \boldsymbol{A}^{-1} f(\vec{u}^{(k)}), \;\; 0 < \omega < 1$$

2. Newton's method.

$$u(x, y) = U(x, y) + \delta u(x, y)$$

Linearize with respect to $\delta u(x, y)$, solve the linear system. Update

$$U^{(k+1)}(x, y) = U^{(k)}(x, y) + \delta u^{(k)}(x, y)$$

Both methods involve solving a linear system at each iteration. If this itself is done iteratively, no need to solve to convergence at early stages.

Finite differences is, of course, not the only way to solve elliptic PDEs.

$$\nabla^2 \phi(\vec{r}) = -4\pi\rho(\vec{r})$$

Coulomb's law $\phi = \int \frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} dV\,'$ in infinite space (no boundaries)

Green's function $\nabla^2 G(\vec{r},\vec{r}\,') = -\delta(\vec{r}-\vec{r}\,')$ $G(\vec{r},\vec{r}\,') = \frac{1}{4\pi|\vec{r}-\vec{r}\,'|}$

$$\nabla^2 \phi(\vec{r}) = -f(\vec{r}) \;\Rightarrow\; \phi = \int f(\vec{r}\,') G(\vec{r},\vec{r}\,') dV\,'$$

In 2D, $G(\vec{r},\vec{r}\,') = -\frac{1}{2\pi \ln|\vec{r}-\vec{r}\,'|}$ – the potential of an infinitely long thin wire

Suppose we have a charged surface somewhere inside our volume. If the charge density σ is known, the contribution to the potential is

$$\phi = \int \frac{\sigma(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} dS\,' = \int 4\pi\sigma(\vec{r}\,') G(\vec{r},\vec{r}\,') dS\,'$$

But suppose that the charge density is not known, but it is known that this is a conducting surface and its potential $\phi = \phi_0$ = const is known.

On the surface, $$\phi = \int 4\pi\sigma(\vec{r}\,')G(\vec{r},\vec{r}\,')dS' = \phi_0$$

This is an integral equation for σ. Discretize it by dividing the surface into *N* elements. Element *i* has position $\vec{r}_i$, charge density σ_i (assumed constant within the element), area ΔS_i.

$$\phi_i = \Sigma_{j \neq i} 4\pi\sigma_j G(\vec{r}_i, \vec{r}_j)\Delta S_j = \phi_0$$

Note $j \neq i$ – *G* diverges when its arguments coincide, although mildly enough that the integral should still converge.

This is a system of *N* equations for *N* unknowns σ_i. Once solved, we can in principle calculate the integral to find the potential everywhere.

This is the simplest variant of the boundary element method.

Let's get back to the problem of solving the Poisson equation in a finite domain with Dirichlet or Neumann boundary conditions.

Intuitively, we can think that to satisfy boundary conditions, we need to put some charge density on the surface.

$$\nabla^2 \phi = -4\pi\rho \qquad\qquad \nabla^2 G(\vec{r},\vec{r}\,') = -\delta(\vec{r}-\vec{r}\,')$$

$$\nabla \cdot [G(\vec{r}-\vec{r}\,')\nabla(\phi(\vec{r})) - \phi(\vec{r})\nabla(G(\vec{r}-\vec{r}\,'))] = -\phi(\vec{r})\nabla^2(G(\vec{r}-\vec{r}\,')) - 4\pi\rho(\vec{r})G(\vec{r}-\vec{r}\,')$$

Integrate over the whole volume, apply Gauss theorem:

$$\oint_\Gamma dS\left(G(\vec{r}-\vec{r}\,')\frac{\partial}{\partial n}(\phi(\vec{r})) - \phi(\vec{r})\frac{\partial}{\partial n}(G(\vec{r}-\vec{r}\,'))\right)$$

$$= -\int_V dV\,(\phi(\vec{r})\nabla^2(G(\vec{r}-\vec{r}\,')) + 4\pi\rho(\vec{r})G(\vec{r}-\vec{r}\,'))$$

$$= \phi(\vec{r}\,') - \int_V dV\, 4\pi\rho(\vec{r})G(\vec{r}-\vec{r}\,')\text{¿}.$$

$$\phi(\vec{r}\,')=\int_V dV\,4\pi\rho(\vec{r})G(\vec{r}-\vec{r}\,')$$
$$+\oint_\Gamma dS\left(G(\vec{r}-\vec{r}\,')\frac{\partial}{\partial n}(\phi(\vec{r}))-\phi(\vec{r})\frac{\partial}{\partial n}(G(\vec{r}-\vec{r}\,'))\right)$$

Physically, the first surface term does look like the contribution of some charge density, while the second looks like the contribution of a “double layer” of positive and negative charges.

The second term diverges when $\vec{r}\,'$ approaches the surface and should be considered carefully.

$$\int_{\Gamma_j}\phi(\vec{r})\frac{\partial}{\partial n}G(\vec{r}-\vec{r}\,')\,dS\rightarrow-(1/2)\phi(\vec{r}_j)+\mathrm{PV}\int_{\Gamma_j}\phi(\vec{r})\frac{\partial}{\partial n}G(\vec{r}-\vec{r}\,')\,dS$$

Then the integral can be discretized as before.

Boundary element method reduces the problem to a lower dimensionality problem. Smaller matrices, but normally dense! Makes sense when we need information about surfaces and only a few (if any) interior points. Also, much easier for the homogeneous problem ($\rho = 0$).