Iterative Methods and Multigrid

Part I: Introduction to Multigrid

Basic Iterative Methods (1)

Nonlinear equation: $f(x) = 0$
Rewrite as $x = F(x)$, and iterate $x_{i+1} = F(x_i)$ (fixed-point iteration)
Converges locally if $F'(x) < 1$ in neighborhood of solution

Linear system: $Ax = b$
Matrix splitting: $A = M - N$

$$(M - N)x = b \quad \Leftrightarrow \quad Mx = Nx + b \quad \Leftrightarrow$$
$$x = M^{-1}Nx + M^{-1}b$$

Iterate: $x_{k+1} = (I - P^{-1}A)x_k + P^{-1}b$ or Solve $Mx_{k+1} = Nx_k + b$
Converges iff (if and only if) $\rho(M^{-1}N) < 1$

Methods: Jacobi iteration, Gauss-Seidel, (S)SOR, ...

Fixed-point: $x = M^{-1}Nx + M^{-1}b \Leftrightarrow M^{-1}Ax = M^{-1}b$
Fixed-point is solution of the **preconditioned system**: $M^{-1}Ax = M^{-1}b$

Basic Iterative Methods (2)

$$x_{k+1} = M^{-1}Nx_k + M^{-1}b = M^{-1}(M - A)x_k + M^{-1}b$$
$$= x_k + M^{-1}b - M^{-1}Ax_k$$

Linear System: $Ax = b$ Prec. system: $M^{-1}Ax = M^{-1}b$

Residual: $r_k = b - Ax_k$ Prec. residual: $\tilde{r}_k = M^{-1}b - M^{-1}Ax_k$

$$x_{k+1} = x_k + \tilde{r}_k \quad \Rightarrow \quad x_{k+1} = x_0 + \tilde{r}_0 + \tilde{r}_1 + \cdots + \tilde{r}_k$$

Update: $x_{k+1} - x_0 = \tilde{r}_0 + \tilde{r}_1 + \cdots + \tilde{r}_k$

$$\tilde{r}_{k+1} = M^{-1}b - M^{-1}Ax_{k+1} = M^{-1}b - M^{-1}Ax_k - M^{-1}A\tilde{r}_k$$
$$= \tilde{r}_k - M^{-1}A\tilde{r}_k$$

$$\tilde{r}_{k+1} = (I - M^{-1}A)\tilde{r}_k \quad = \quad (M^{-1}N)^{k+1}\tilde{r}_0$$

Basic Iterative Methods (3)

Solution to $Ax = b$: $\hat{x}$ Error: $\varepsilon_k = \hat{x} - x_k$

Residual and error: $r_k = b - Ax_k = A\hat{x} - Ax_k = A\varepsilon_k \quad (\tilde{r}_k = M^{-1}A\varepsilon_k)$

Theorem: $\hat{x}$ is a fixed point of $x_{k+1} = M^{-1}Nx_k + M^{-1}b$ iff
$\hat{x}$ is the solution of $M^{-1}Ax = M^{-1}b \quad (\Leftrightarrow Ax = b)$

Proof: $x = (I - M^{-1}A)x + M^{-1}b = x - M^{-1}Ax + M^{-1}b \quad \Leftrightarrow$
$M^{-1}Ax = M^{-1}b$

$$\varepsilon_{k+1} = \hat{x} - x_{k+1} = M^{-1}N\hat{x} + M^{-1}b - M^{-1}Nx_k - M^{-1}b$$
$$= M^{-1}N\varepsilon_k$$

$\varepsilon_{k+1} = M^{-1}N\varepsilon_k = (M^{-1}N)^{k+1}\varepsilon_0$ and $\tilde{r}_{k+1} = (M^{-1}N)^{k+1}\tilde{r}_0$

Matrix Splittings (1)

Some well-known choices for M:

$$A = \begin{pmatrix} A_{11} & \cdots & A_{1p} \\ \vdots & \ddots & \vdots \\ A_{p1} & \cdots & A_{pp} \end{pmatrix}$$

$M = diag(A_{11}, A_{22}, \ldots, A_{pp})$ (point/block) Jacobi

$M = \begin{pmatrix} A_{11} & & \\ \vdots & \ddots & \\ A_{p1} & \cdots & A_{pp} \end{pmatrix}$ (point/block) Gauss-Seidel

$M = \begin{pmatrix} \omega^{-1} A_{11} & & \\ \vdots & \ddots & \\ A_{p1} & \cdots & \omega^{-1} A_{pp} \end{pmatrix}$ (point/block) SOR

$$x_{k+1}^{SOR} = \omega x_{k+1}^{GS} + (1-\omega) x_k^{SOR}$$

Review Basic Iterative Methods

Solving $Au = f$

Write $A = D - L - U$, where $-U$ is the strict upper triangular part, $-L$ is the strict lower triangular part, and D is the diagonal.

Jacobi iteration: $Du_{k+1} = (L + U)u_k + f$

Gauss-Seidel iteration: $(D - L)u_{k+1} = Uu_k + f$

Block versions possible.

Basic iteration: $u_{k+1} = P^{-1}(P - A)u_k + P^{-1}f = R_x u_k + P^{-1}f$
Convergence iff $\rho(R_x) < 1$ and asymptotic convergence rate: $\rho(R_x)$.

$R_J = D^{-1}(L + U)$
$R_{GS} = (D - L)^{-1}U$

Use of Relaxation Parameter

We can use a relaxation parameter to improve convergence:

Jacobi iteration: $\tilde{u}_k = D^{-1}(L+U)u_k + D^{-1}f$

$u_{k+1} = (1-\omega)u_k + \omega\tilde{u}_k$

Alternatively: $u_{k+1} = u_k + \omega\tilde{r}_k$ with $\tilde{r}_k = D^{-1}(f - Au_k)$

$$R_{J,\omega} = (1-\omega)I + \omega R_J$$

Gauss-Seidel iteration: $\tilde{u}_k = (D-L)^{-1}Uu_k + (D-L)^{-1}f$

$u_{k+1} = (1-\omega)u_k + \omega\tilde{u}_k$

Alternatively: $u_{k+1} = u_k + \omega\tilde{r}_k$ with $\tilde{r}_k = (D-L)^{-1}(f - Au_k)$

$$R_{GS,\omega} = (1-\omega)I + \omega R_{GS}$$

Model Problem

Consider the following model problem, $-u_{xx} = f$ for $x \in (0,1)$ with Dirichlet boundary conditions $u = 0$ for $x = 0$ and $x = 1$.

We discretize the problem (see Meurant 1.9) using $n+1$ grid points.
This gives $h = n^{-1}$ and $x_j = jh$ for $j = 0 \ldots n$.
We use the standard central finite difference discretization

$$u_{xx} = \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} + O(h^2).$$

This gives the matrix $A = tridiag\begin{pmatrix} & -1 & & -1 & & -1 & \\ 2 & & 2 & & 2 & & 2 \\ & -1 & & -1 & & -1 & \end{pmatrix}$.

This gives eigenvectors $u_j^{(k)} = \sin\frac{jk\pi}{n}$ and
eigenvalues $\lambda_k \equiv \lambda^{(k)} = 4\sin^2(\frac{k\pi}{2n})$. (see Meurant 1.10)

Model Problem (Jacobi)

Let's consider pointwise algorithm for model problem

$-u_{xx} + \sigma u = f$, for $0 < x < 1$, and $u(0) = u(1) = 0$

Equidistant grid points: $x_i = ih$ and $u_i = u(x_i)$. Initially $\sigma = 0$.

Centered finite differences:
$-u_{i-1} + 2u_i - u_{i+1} = h^2 f_i$ where $i = 1 \ldots n-1$.

Jacobi iteration: $u^{(k+1)} = D^{-1}(L+U)u^{(k)} + D^{-1}f$

Update at each point: $u_i^{(k+1)} = \frac{1}{2}\left(h^2 f_i + u_{i-1}^{(k)} + u_{i+1}^{(k)}\right) = u_i^{(k)} + \frac{1}{2} r_i^{(k)}$

Update can be done for all points at once (no dependencies).

With relaxation parameter ω: $u_i^{(k+1)} = u_i^{(k)} + \frac{1}{2}\omega\, r_i^{(k)}$

Model problem (Gauss-Seidel)

Let's consider pointwise algorithm for model problem

$-u_{xx} + \sigma u = f$, for $0 < x < 1$, and $u(0) = u(1) = 0$

Equidistant grid points: $x_i = ih$ and $u_i = u(x_i)$.
Centered finite differences:
$-u_{i-1} + 2u_i - u_{i+1} = h^2 f_i$ where $i = 1 \ldots n-1$.

Gauss-Seidel iteration: $u^{(k+1)} = (D-L)^{-1} U u^{(k)} + (D-L)^{-1} f$

Update at each point: $u_i^{(k+1)} = \frac{1}{2}\left(h^2 f_i + u_{i-1}^{(k+1)} + u_{i+1}^{(k)}\right) = u_i^{(k)} + \frac{1}{2} r_i^{(k)}$

where $r_i^{(k)} \equiv \left(h^2 f_i + u_{i-1}^{(k+1)} + u_{i+1}^{(k)} - 2u_i^{(k)}\right)$:
the residual evaluated after updating $u_{i-1} \to u_{i-1}^{(k+1)}$

With relaxation parameter ω: $u_i^{(k+1)} = u_i^{(k)} + \frac{1}{2}\omega\, r_i^{(k)}$

Point Jacobi for Model Problem

Now consider the rate of convergence of the point Jacobi iteration.

We take $M = 2I$, $N = M - A = 2I - A$, and $M^{-1}N = I - \frac{1}{2}A$.

The iteration matrix, $G \equiv M^{-1}N$, has the same eigenvectors as A.
For its eigenvalues we get $\lambda_G = 1 - \frac{1}{2}\lambda_A$.

We have $\lambda_{A,k} = 4\sin^2(k\frac{\pi}{2n}) = 4\sin^2(k\phi_n)$,
and so $\lambda_{G,k} = 1 - 2\sin^2(k\frac{\pi}{2n}) = 1 - 2\sin^2(k\phi_n)$

For $k = 1$ we get $\lambda_{G,1} = 1 - 2\sin^2(\phi_n) \approx 1 - 2\phi_n^2 = 1 - \frac{\pi^2}{2n^2}$

Likewise, we get $\lambda_{G,n-1} = 1 - 2\sin^2((n-1)\phi_n) \approx -1 + \frac{\pi^2}{2n^2}$

Clearly, for $n \to \infty$, $\rho(G) \to 1$ (and fairly rapidly so)

Error Smoothing

Convergence: $e^{(k)} = G^k e^{(0)}$, where G is iteration matrix

$G = (I - P^{-1}A)$.

$u^{(k+1)} = u^{(k)} + \omega P^{-1} r^{(k)} = u^{(k)} + \omega P^{-1}(f - Au^{(k)}) =$

$(I - \omega P^{-1}A)u^{(k)} + \omega P^{-1} f$

Jacobi iteration matrix: $(1-\omega)I + \omega R_J = (1-\omega)I + \omega D^{-1}(D - A)$
This gives: $I - \frac{\omega}{2}A$

Eigenvalues $I - \frac{\omega}{2}A$: $\lambda(I - \frac{\omega}{2}A) = 1 - \frac{\omega}{2}\lambda(A)$

Eigenvalues of A

Error Smoothing

Eigenvalues of A:

Assume eigenvector close to physical eigenvector: $v_k = \sin\frac{\pi k j}{n}$

Apply pointwise rule for Jacobi:

$$Av_{j,k} = -\sin\frac{\pi k(j-1)}{n} + 2\sin\frac{\pi kj}{n} - \sin\frac{\pi k(j+1)}{n} = 2\sin\frac{\pi kj}{n} - 2\sin\frac{\pi kj}{n}\cos\frac{\pi k}{n} =$$

$2\sin\frac{\pi kj}{n}\left(1-\cos\frac{\pi k}{n}\right)$ (so eigenvector indeed)

$$1-\cos\frac{\pi k}{n} = 1-\cos\frac{2\pi k}{2n} = 1-\left(1-2\sin^2\left(\frac{\pi k}{2n}\right)\right) = 2\sin^2\left(\frac{\pi k}{2n}\right)$$

$$2\sin\frac{\pi kj}{n}\left(1-\cos\frac{\pi k}{n}\right) = \sin\frac{\pi kj}{n} \bullet 4\sin^2\left(\frac{\pi k}{2n}\right)$$

This gives for the weighted Jacobi method: $I - \frac{\omega}{2}A$

$\lambda_{(R_{J,\omega})} = 1 - 2\omega\sin^2\left(\frac{\pi k}{2n}\right)$ where $0 < \omega \le 1$

Always converges. Poor convergence for which modes?

Point Gauss-Seidel for Model Problem

Next we consider the rate of convergence of the point Gauss-Seidel method (in natural ordering) for the model problem.

We solve $Ax = b$. Let $A = L + D + U$, where D is diagonal of A, and L and U are strictly lower and upper triangular part of A.

Take $M = L + D$ and $N = -U$. Iterate $Mx_{k+1} = Nx_k + b$.
Eigenvectors of $M^{-1}N$? $M^{-1}Nw = \lambda w \Leftrightarrow Nw = \lambda Mw$

Model problem: $2\lambda w_j - \lambda w_{j-1} = w_{j+1}$ with $w_0 = w_n = 0$.

Recurrence $w_{j+1} - 2\lambda w_j + \lambda w_{j-1} = 0$.
Substitute $w_j = z^j$; this gives $z^2 - 2\lambda z + \lambda = 0 \rightarrow z_{1,2} = \lambda \pm \sqrt{\lambda^2 - \lambda}$.

Real λ gives either strictly increasing or decreasing (or constant, i.e. zero).
So we need z complex, and therefore $0 < \lambda < 1$.

Point Gauss-Seidel for Model Problem

General solution $w_j = \alpha_1 z_1^j + \alpha_2 z_2^j$,
where $z_1 = \lambda + i\sqrt{\lambda - \lambda^2}$ and $z_2 = \lambda - i\sqrt{\lambda - \lambda^2}$

Note $|z_1| = \lambda^{1/2} \rightarrow z_{1,2} = \lambda^{1/2}\left(\lambda^{1/2} \pm i\lambda^{-1/2}\sqrt{\lambda - \lambda^2}\right) = \lambda^{1/2}e^{i\phi}$.
This gives $\lambda^{1/2} = \cos\phi$

$$w_0 = \alpha_1 + \alpha_2 = 0 \rightarrow \alpha_2 = -\alpha_1$$
$$w_n = \alpha_1 \cos^n\phi\, e^{in\phi} - \alpha_1 \cos^n\phi\, e^{-in\phi} = 2i\alpha_1 \cos^n\phi\, \sin n\phi = 0$$

So we must have $\phi = \phi_k = \frac{k\pi}{n}$ and we can take

$$w_{k,j} = \cos\frac{k\pi}{n} \sin\frac{jk\pi}{n} = \cos\phi_k \sin j\phi_k \text{ (why?)}$$

For the eigenvalue we therefore get $\lambda_k = \cos^2\phi_k$ for $k = 1 \ldots n-1$.
This gives $\rho = \lambda_1 = \cos^2\frac{\pi}{n} = 1 - \sin^2\frac{\pi}{n} \approx 1 - \frac{\pi^2}{n^2}$.
How does this relate to the convergence rate for Jacobi iteration?

Red-Black ordering for Gauss-Seidel

Gauss-Seidel depends on ordering.
Often-used special ordering: Red-Black ordering, where red unknowns reference only black unknowns and vice versa.
In this case, order *even grid points* first and then *odd grid points*

Red/Even update: $u_{2i}^{(k+1)} = \frac{1}{2}\left(h^2 f_{2i} + u_{2i-1}^{(k)} + u_{2i+1}^{(k)}\right) = u_{2i}^{(k)} + \frac{1}{2} r_{2i}^{(k)}$

where $r_{2i}^{(k)} \equiv \left(h^2 f_{2i} + u_{2i-1}^{(k)} + u_{2i+1}^{(k)} - 2u_{2i}^{(k)}\right)$

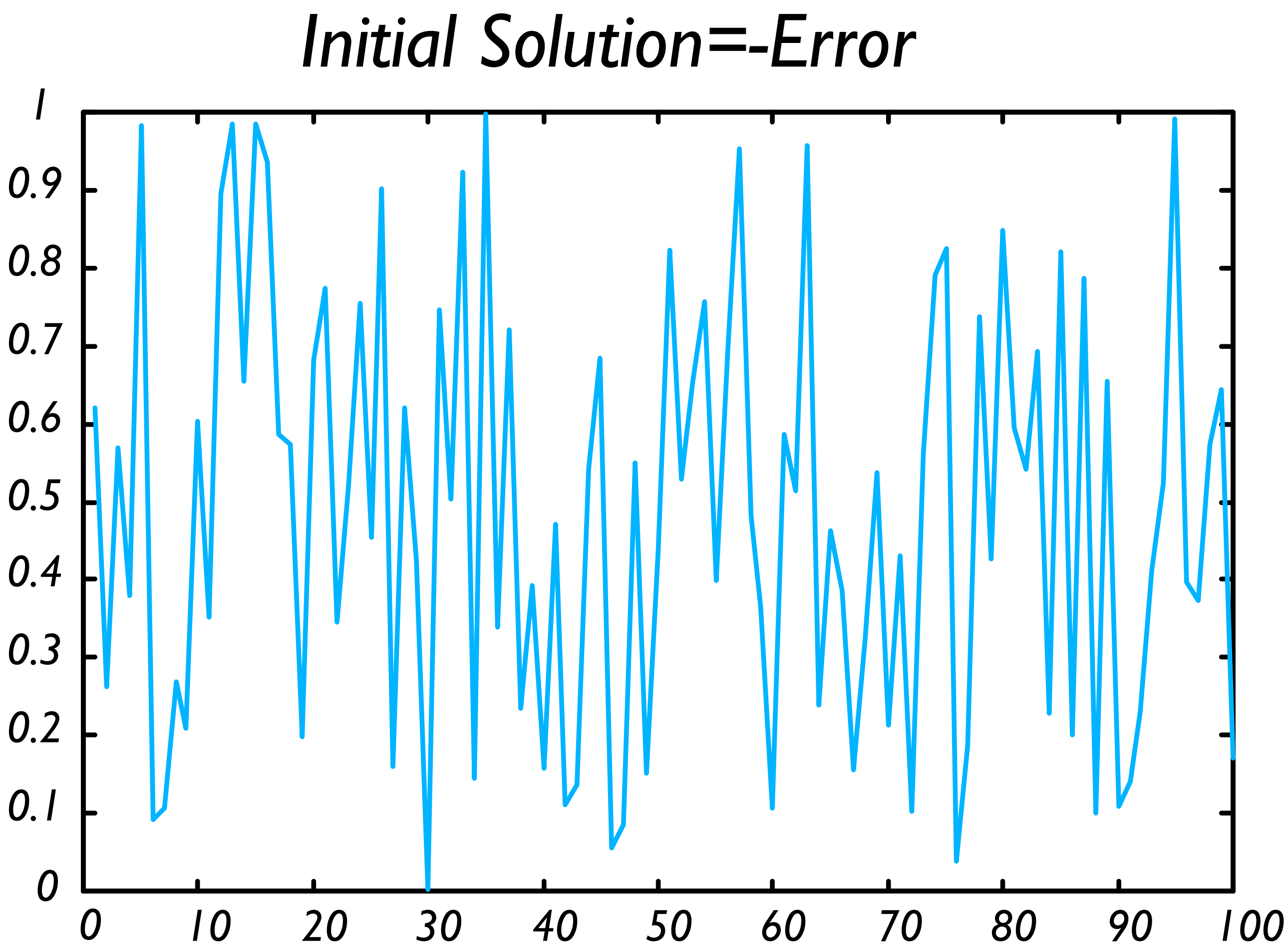
With relaxation parameter ω: $u_{2i}^{(k+1)} = u_{2i}^{(k)} + \frac{1}{2}\omega\, r_{2i}^{(k)}$

Black/Odd update: $u_{2i-1}^{(k+1)} = \frac{1}{2}\left(h^2 f_{2i-1} + u_{2i-2}^{(k+1)} + u_{2i+2}^{(k+1)}\right) = u_{2i-1}^{(k)} + \frac{1}{2} r_{2i-1}^{(k+1)}$

where $r_{2i-1}^{(k+1)} \equiv \left(h^2 f_{2i-1} + u_{2i-2}^{(k+1)} + u_{2i+2}^{(k+1)} - 2u_{2i-1}^{(k)}\right)$

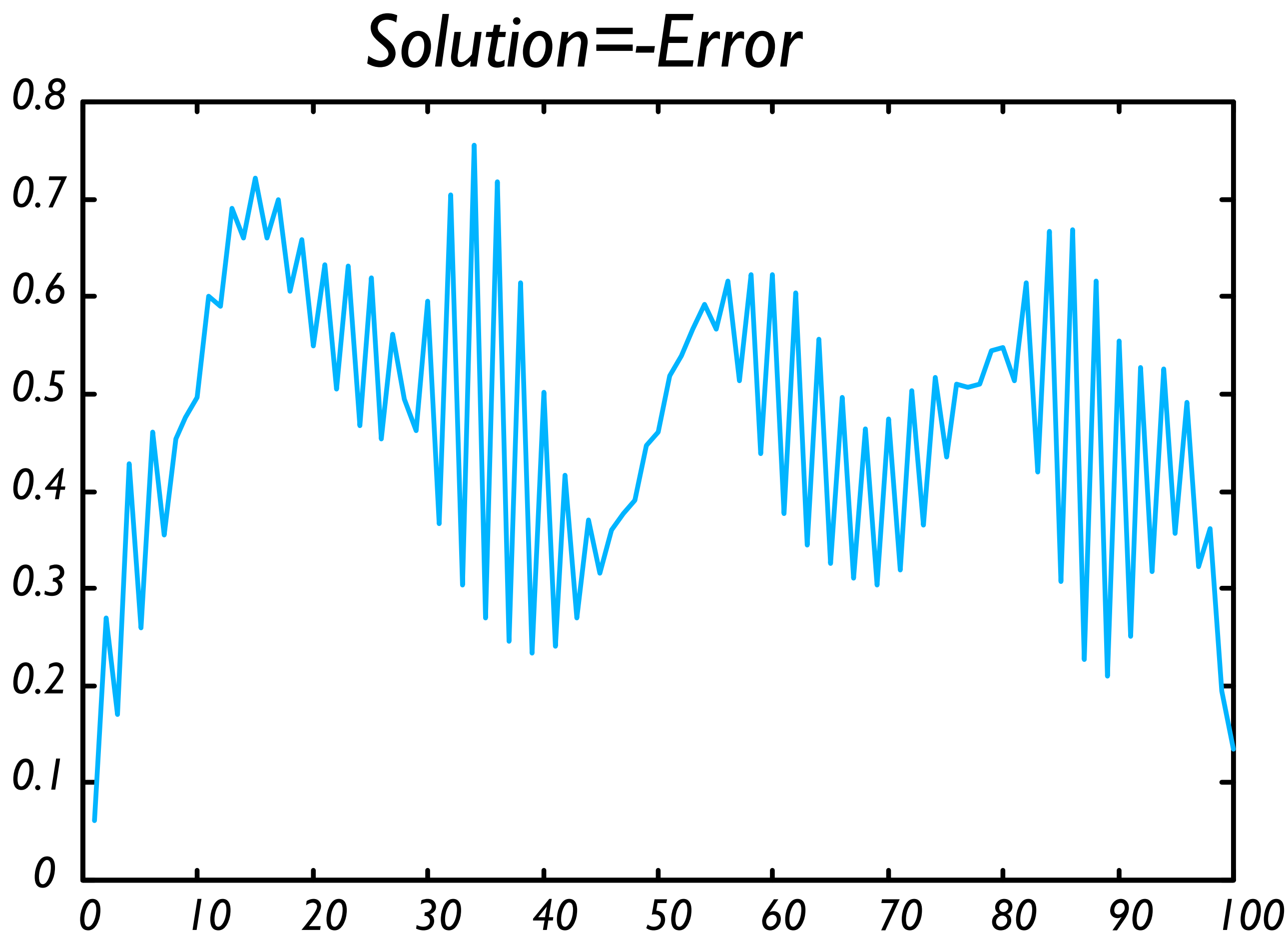
With relaxation parameter ω: $u_{2i-1}^{(k+1)} = u_{2i-1}^{(k)} + \frac{1}{2}\omega\, r_{2i-1}^{(k+1)}$

Error Smoothing



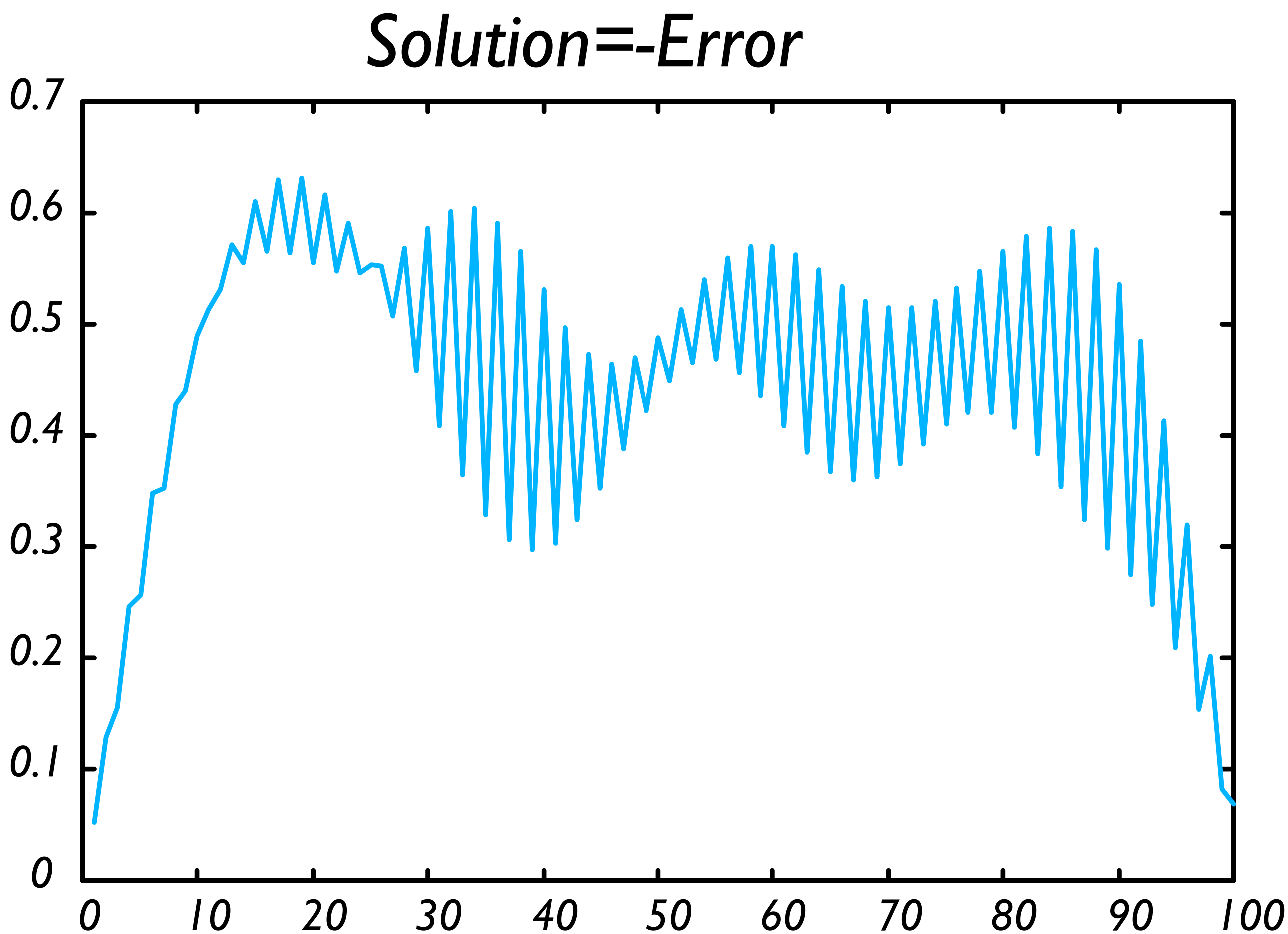
DCT: [4.9, 0.27, 0.16, 0.061, -2.4, ...], O(0.1) or O(0.2)

Error Smoothing



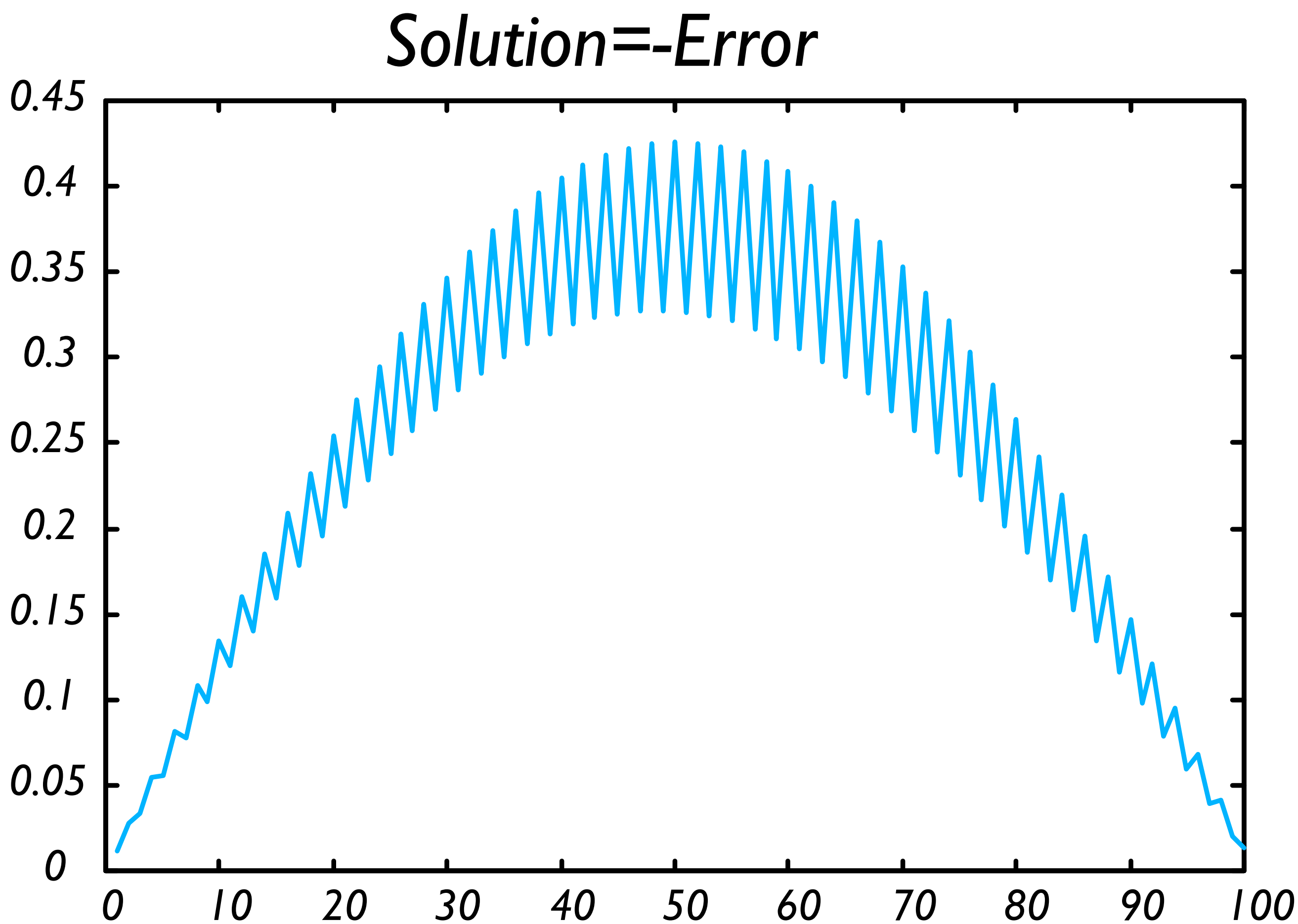
After 20 Jacobi iterations with $\omega=1$

Error Smoothing



After 50 Jacobi iterations with ω=1

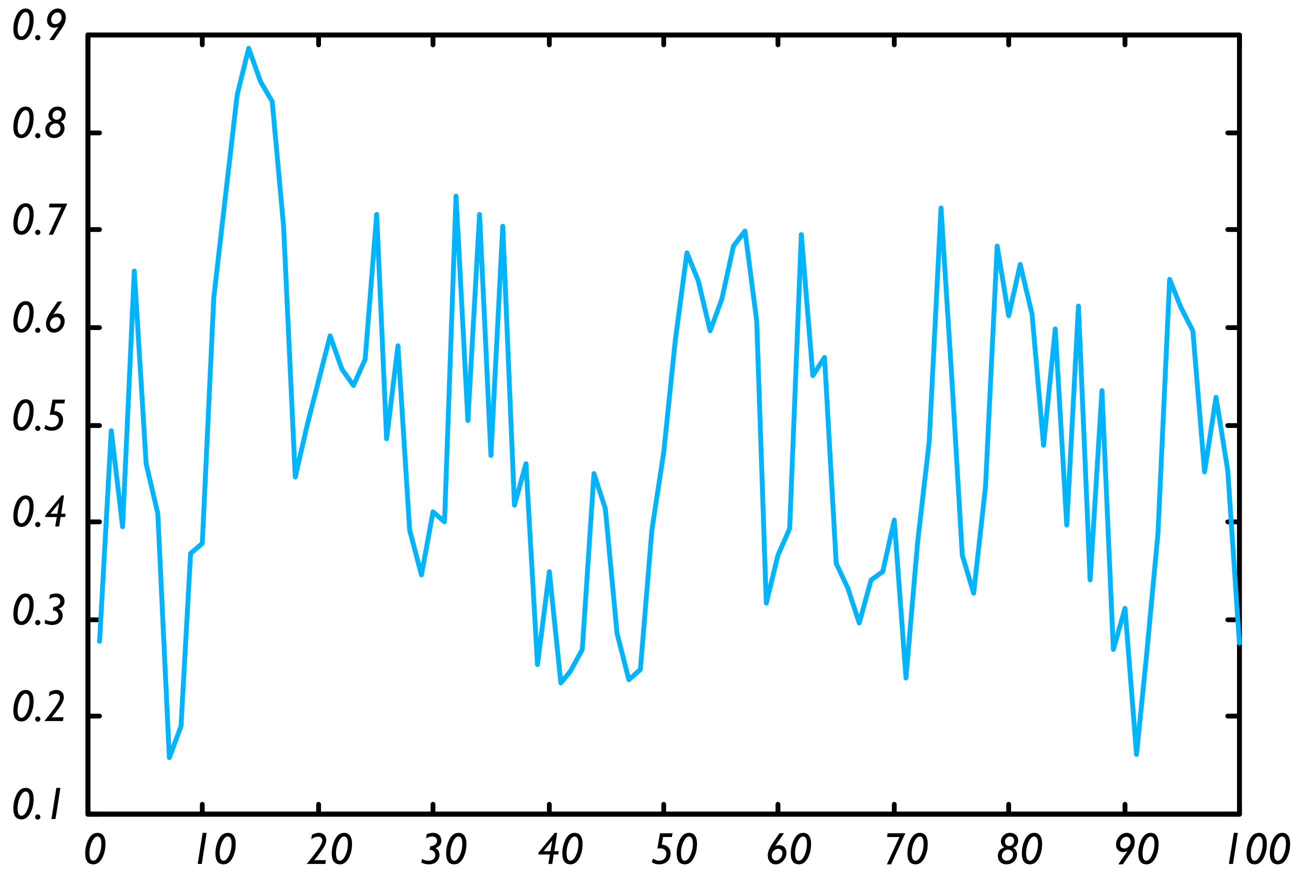
Error Smoothing



After 1000 Jacobi iterations with ω=1

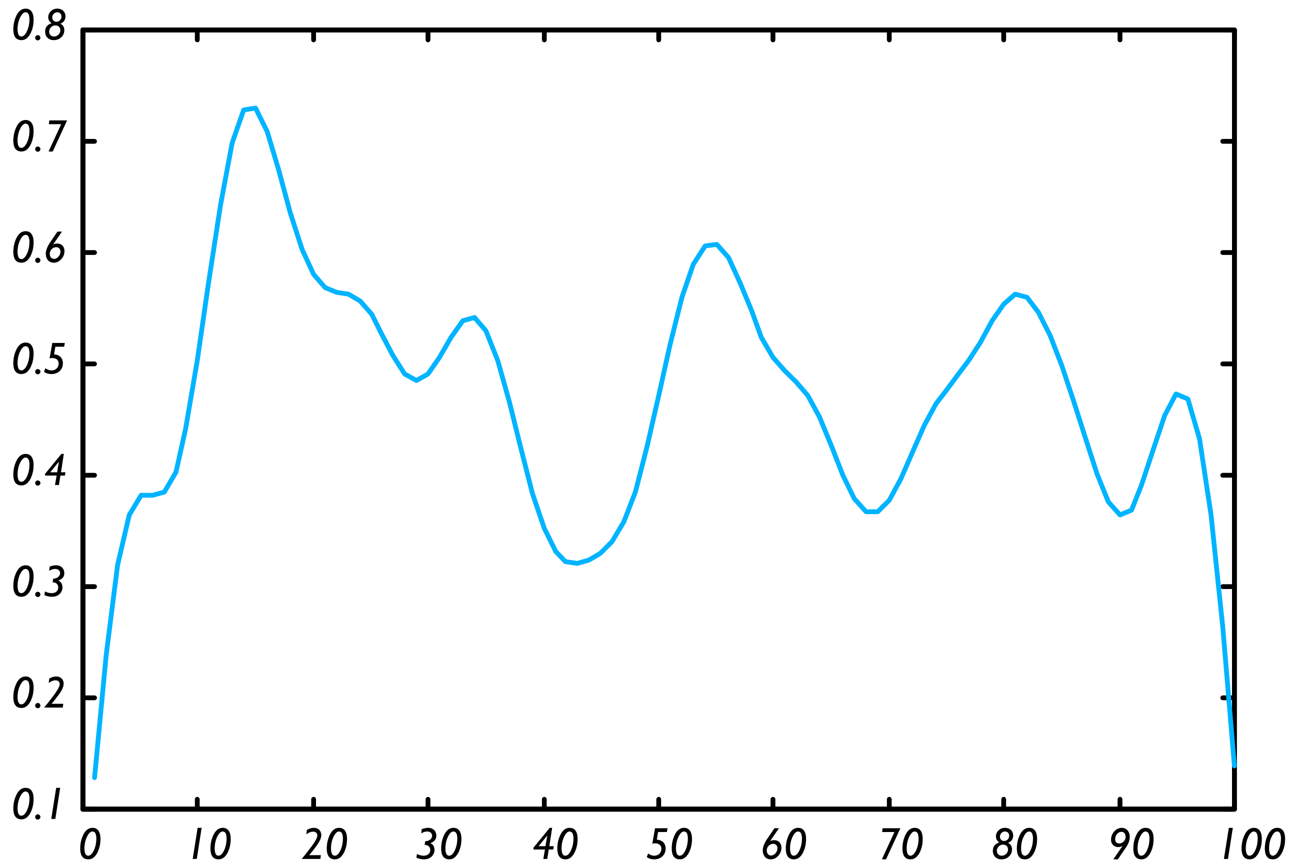
DCT: [2.4, ε, -1.1, ε, ... , ε, 0.35], ε=O(0.01), mainly O(1e-3)

Error Smoothing

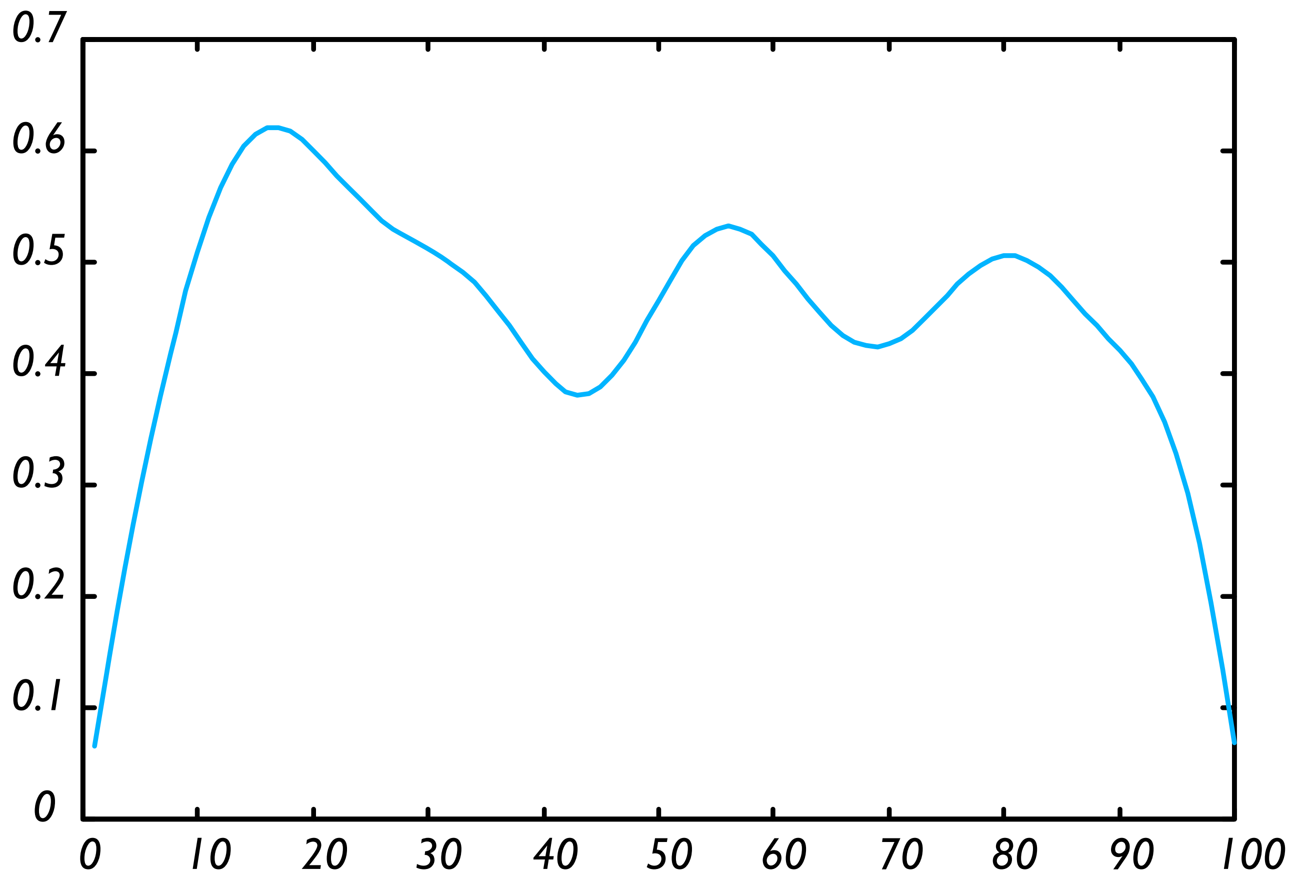


$\omega = 2/3$

Error Smoothing



Error Smoothing



Error Smoothing