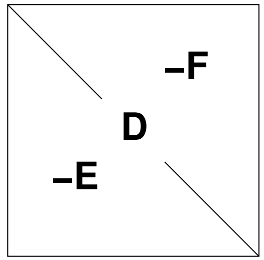
Iterative methods: Basic relaxation techniques

- Relaxation methods: Jacobi, Gauss-Seidel, SOR
- Basic convergence results
- Optimal relaxation parameter for SOR
- See Chapter 4 of text for details.

Basic relaxation schemes

➤ *Relaxation schemes:* methods that modify one component of current approximation at a time

➤ Based on the decomposition $A = D - E - F$ with: $D = \text{diag}(A)$, $-E$ = strict lower part of A and $-F$ = its strict upper part.



Gauss-Seidel iteration for solving $Ax = b$:

➤ corrects j-th component of current approximate solution, to zero the $j - th$ component of residual for $j = 1, 2, \cdots, n$.

➤ Gauss-Seidel iteration can be expressed as:

$$(D - E)x^{(k+1)} = Fx^{(k)} + b$$

Can also define a backward Gauss-Seidel Iteration:

$$(D - F)x^{(k+1)} = Ex^{(k)} + b$$

and a Symmetric Gauss-Seidel Iteration: forward sweep followed by backward sweep.

Over-relaxation is based on the splitting:

$$\omega A = (D - \omega E) - (\omega F + (1 - \omega)D)$$

$\rightarrow$ successive overrelaxation, (SOR):

$$(D - \omega E)x^{(k+1)} = [\omega F + (1 - \omega)D]x^{(k)} + \omega b$$

Iteration matrices

➤ Previous methods based on a splitting of A: $A = M - N \rightarrow$

$$Mx = Nx + b \quad \rightarrow \quad Mx^{(k+1)} = Nx^{(k)} + b \rightarrow$$

$$x^{(k+1)} = M^{-1}Nx^{(k)} + M^{-1}b \equiv Gx^{(k)} + f$$

Jacobi, Gauss-Seidel, SOR, & SSOR iterations are of the form

$$\begin{aligned} G_{Jac} &= D^{-1}(E + F) = I - D^{-1}A \\ G_{GS} &= (D - E)^{-1}F = I - (D - E)^{-1}A \\ G_{SOR} &= (D - \omega E)^{-1}(\omega F + (1 - \omega)D) \\ &= I - (\omega^{-1}D - E)^{-1}A \\ G_{SSOR} &= I - \omega(2 - \omega)(D - \omega F)^{-1}D(D - \omega E)^{-1}A \end{aligned}$$

General convergence result

Consider the iteration: $x^{(k+1)} = Gx^{(k)} + f$

(1) Assume that $\rho(G) < 1$. Then $I - G$ is non-singular and G has a fixed point. Iteration converges to a fixed point for any f and $x^{(0)}$.

(2) If iteration converges for any f and $x^{(0)}$ then $\rho(G) < 1$.

Example: Richardson's iteration

$$x^{(k+1)} = x^{(k)} + \alpha(b - Ax^{(k)})$$

✍1 Assume $\Lambda(A) \subset \mathbb{R}$. When does the iteration converge?

A few well-known results

- Jacobi and Gauss-Seidel converge for diagonal dominant matrices, i.e., matrices such that

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}|, i = 1, \cdots, n$$

- SOR converges for $0 < \omega < 2$ for SPD matrices
- The optimal ω is known in theory for an important class of matrices called 2-cyclic matrices or matrices with property A.

- A matrix has property A if it can be (symmetrically) permuted into a 2×2 block matrix whose diagonal blocks are diagonal.

$$PAP^T = \begin{bmatrix} D_1 & E \\ E^T & D_2 \end{bmatrix}$$

- Let A be a matrix which has property A. Then the eigenvalues λ of the SOR iteration matrix and the eigenvalues μ of the Jacobi iteration matrix are related by

$$(\lambda + \omega - 1)^2 = \lambda \omega^2 \mu^2$$

- The optimal ω for matrices with property A is given by

$$\omega_{opt} = \frac{2}{1 + \sqrt{1 - \rho(B)^2}}$$

where B is the Jacobi iteration matrix.

An observation — Introduction to Preconditioning

- The iteration $x^{(k+1)} = Gx^{(k)} + f$ is attempting to solve $(I - G)x = f$. Since G is of the form $G = M^{-1}[M - A]$ and $f = M^{-1}b$, this system becomes

$$M^{-1}Ax = M^{-1}b$$

where for SSOR, for example, we have

$$M_{SSOR} = (D - \omega E)D^{-1}(D - \omega F)$$

referred to as the SSOR 'preconditioning' matrix.

In other words:

Relaxation iter. $\Longleftrightarrow$ *Preconditioned Fixed Point Iter.*

Projection methods

- **Introduction to projection-type techniques**
- **Sample one-dimensional Projection methods**
- **Some theory and interpretation –**
- **See Chapter 5 of text for details.**

Projection Methods

➤ The main idea of projection methods is to extract an approximate solution from a subspace.

➤ We define a subspace of approximants of dimension m and a set of m conditions to extract the solution

➤ These conditions are typically expressed by orthogonality constraints.

➤ This defines one basic step which is repeated until convergence (alternatively the dimension of the subspace is increased until convergence).

Example: Each relaxation step in Gauss-Seidel can be viewed as a projection step

Background on projectors

➤ A projector is a linear operator that is idempotent: $P^2 = P$

A few properties:

- P is a projector iff $I - P$ is a projector
- $x \in \mathrm{Ran}(P)$ iff $x = Px$ iff $x \in \mathrm{Null}(I - P)$
- This means that : $\mathrm{Ran}(P) = \mathrm{Null}(I - P)$.
- Any $x \in \mathbb{R}^n$ can be written (uniquely) as $x = x_1 + x_2$, $x_1 = Px \in \mathrm{Ran}(P)$ $x_2 = (I - P)x \in \mathrm{Null}(P)$ - So:

$$\mathbb{R}^n = \mathrm{Ran}(P) \oplus \mathrm{Null}(P)$$

✍₂ Prove the above properties

Background on projectors (Continued)

➤ The decomposition $\mathbb{R}^n = K \oplus S$ defines a (unique) projector P:

- From $x = x_1 + x_2$, set $Px = x_1$.
- For this P: $\mathrm{Ran}(P) = K$ and $\mathrm{Null}(P) = S$.
- Note: $dim(K) = m$, $dim(S) = n - m$.

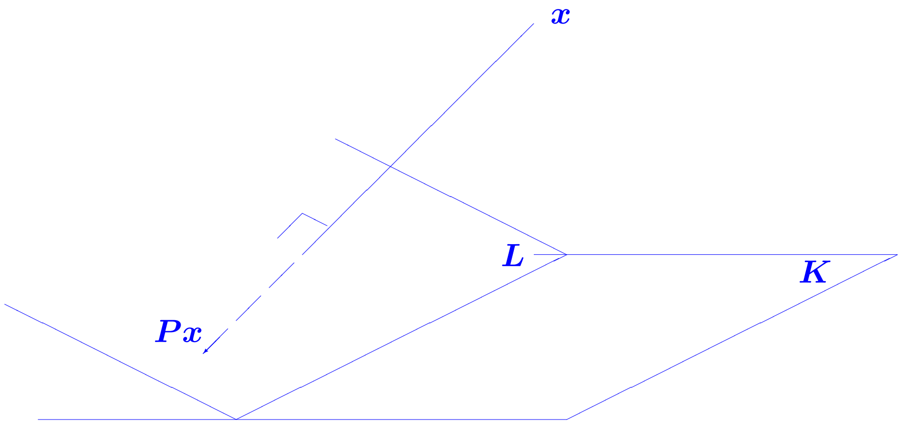
➤ Pb: express mapping $x \to u = Px$ in terms of K, S

➤ Note $u \in K$, $x - u \in S$

➤ Express 2nd part with m constraints: let $L = S^\perp$, then

$$u = Px \text{ iff } \begin{cases} u \in K \\ x - u \perp L \end{cases}$$

➤ Projection onto K and orthogonally to L



➤ Illustration: P projects onto K and orthogonally to L

➤ When $L = K$ projector is orthogonal.

➤ Note: $Px = 0$ iff $x \perp L$.

Projection methods

➤ Initial Problem: $b - Ax = 0$

Given two subspaces K and L of $\mathbb{R}^N$ define the approximate problem:

Find $\tilde{x} \in K$ such that $b - A\tilde{x} \perp L$

➤ Petrov-Galerkin condition

➤ m degrees of freedom (K) + m constraints (L) $\rightarrow$

➤ a small linear system ('projected problem')

➤ This is a basic projection step. Typically a sequence of such steps are applied

➤ With a nonzero initial guess x_0, approximate problem is

Find $\tilde{x} \in x_0 + K$ such that $b - A\tilde{x} \perp L$

Write $\tilde{x} = x_0 + \delta$ and $r_0 = b - Ax_0$. $\rightarrow$ system for δ:

Find $\delta \in K$ such that $r_0 - A\delta \perp L$

✍3 Formulate Gauss-Seidel as a projection method -

✍4 Generalize Gauss-Seidel by defining subspaces consisting of 'blocks' of coordinates $\text{span}\{e_i, e_{i+1}, ..., e_{i+p}\}$

Matrix representation:

Let
- $V = [v_1, \ldots, v_m]$ a basis of K &
- $W = [w_1, \ldots, w_m]$ a basis of L

➤ Write approximate solution as $\tilde{x} = x_0 + \delta \equiv x_0 + Vy$ where $y \in \mathbb{R}^m$. Then Petrov-Galerkin condition yields:

$$W^T(r_0 - AVy) = 0$$

➤ Therefore,

$$\tilde{x} = x_0 + V[W^TAV]^{-1}W^Tr_0$$

Remark: In practice W^TAV is known from algorithm and has a simple structure [tridiagonal, Hessenberg,..]

Prototype Projection Method

Until Convergence Do:

1. Select a pair of subspaces K, and L;

2. Choose bases: $V = [v_1, \dots, v_m]$ for K and $W = [w_1, \dots, w_m]$ for L.

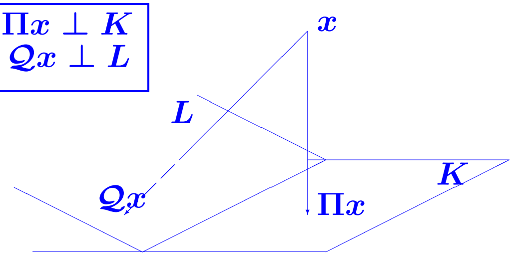
3. Compute :

$$r \leftarrow b - Ax,$$
$$y \leftarrow (W^T A V)^{-1} W^T r,$$
$$x \leftarrow x + V y.$$

Projection methods: Operator form representation

➤ Let Π = the orthogonal projector onto K and $\mathcal{Q}$ the (oblique) projector onto K and orthogonally to L.

$$\Pi x \in K, \quad x - \Pi x \perp K$$
$$\mathcal{Q} x \in K, \quad x - \mathcal{Q} x \perp L$$



Π and $\mathcal{Q}$ projectors

Assumption: no vector of K is $\perp$ to L

In the case $x_0 = 0$, approximate problem amounts to solving

$$\mathcal{Q}(b - Ax) = 0, \quad x \in K$$

or in operator form (solution is Πx)

$$\mathcal{Q}(b - A\Pi x) = 0$$

Question: what accuracy can one expect?

➤ Let x^* be the exact solution. Then

1) We cannot get better accuracy than $\|(I - \Pi)x^*\|_2$, i.e.,

$$\|\tilde{x} - x^*\|_2 \geq \|(I - \Pi)x^*\|_2$$

2) The residual of the exact solution for the approximate problem satisfies:

$$\|b - \mathcal{Q}A\Pi x^*\|_2 \leq \|\mathcal{Q}A(I - \Pi)\|_2 \|(I - \Pi)x^*\|_2$$

Two Important Particular Cases.

1. $L = K$

➤ When A is SPD then $\|x^* - \tilde{x}\|_A = \min_{z \in K} \|x^* - z\|_A$.

➤ Class of Galerkin or Orthogonal projection methods

➤ Important member of this class: Conjugate Gradient (CG) method

2. $L = AK$.

In this case $\|b - A\tilde{x}\|_2 = \min_{z \in K} \|b - Az\|_2$

➤ Class of Minimal Residual Methods: CR, GCR, ORTHOMIN, GMRES, CGNR, ...

One-dimensional projection processes

$K = span\{d\}$
and
$L = span\{e\}$

Then $\tilde{x} = x + \alpha d$. Condition $r - A\delta \perp e$ yields

$$\alpha = \frac{(r,e)}{(Ad,e)}$$

➤ Three popular choices:

(1) Steepest descent

(2) Minimal residual iteration

(3) Residual norm steepest descent

1. Steepest descent.

A is SPD. Take at each step $d = r$ and $e = r$.

Iteration:
$$r \leftarrow b - Ax,$$
$$\alpha \leftarrow (r, r)/(Ar, r)$$
$$x \leftarrow x + \alpha r$$

➤ Each step minimizes $f(x) = \|x - x^*\|_A^2 = (A(x - x^*), (x - x^*))$ in direction $-\nabla f$.

➤ Convergence guaranteed if A is SPD.

✍15 As is formulated, the above algorithm requires 2 'matvecs' per step. Reformulate it so only one is needed.

Convergence based on the Kantorovitch inequality: Let B be an SPD matrix, λ_{max}, λ_{min} its largest and smallest eigenvalues. Then,

$$\frac{(Bx, x)(B^{-1}x, x)}{(x, x)^2} \le \frac{(\lambda_{max} + \lambda_{min})^2}{4\ \lambda_{max}\lambda_{min}}, \quad \forall x \ne 0.$$

➤ This helps establish the convergence result

Let A an SPD matrix. Then, the A-norms of the error vectors $d_k = x_* - x_k$ generated by steepest descent satisfy:

$$\|d_{k+1}\|_A \le \frac{\lambda_{max} - \lambda_{min}}{\lambda_{max} + \lambda_{min}} \|d_k\|_A$$

➤ Algorithm converges for any initial guess x_0.

Proof: Observe $\|d_{k+1}\|_A^2 = (Ad_{k+1}, d_{k+1}) = (r_{k+1}, d_{k+1})$

- by substitution,

$$\|d_{k+1}\|_A^2 = (r_{k+1}, d_k - \alpha_k r_k)$$

- By construction $r_{k+1} \perp r_k$ so we get $\|d_{k+1}\|_A^2 = (r_{k+1}, d_k)$.

Now:

$$\begin{aligned}\|d_{k+1}\|_A^2 &= (r_k - \alpha_k A r_k, d_k) \\ &= (r_k, A^{-1} r_k) - \alpha_k (r_k, r_k) \\ &= \|d_k\|_A^2 \left(1 - \frac{(r_k, r_k)}{(r_k, Ar_k)} \times \frac{(r_k, r_k)}{(r_k, A^{-1} r_k)}\right).\end{aligned}$$

Result follows by applying the Kantorovich inequality. ■

2. Minimal residual iteration.

A positive definite ($A + A^T$ is SPD). Take at each step $d = r$ and $e = Ar$.

Iteration:
$$\begin{aligned} &r \leftarrow b - Ax, \\ &\alpha \leftarrow (Ar, r)/(Ar, Ar) \\ &x \leftarrow x + \alpha r \end{aligned}$$

- Each step minimizes $f(x) = \|b - Ax\|_2^2$ in direction r.
- Converges under the condition that $A + A^T$ is SPD.

✍6 As is formulated, the above algorithm would require 2 'matvecs' at each step. Reformulate it so that only one matvec is required

Convergence

Let A be a real positive definite matrix, and let

$$\mu = \lambda_{min}(A + A^T)/2, \quad \sigma = \|A\|_2.$$

Then the residual vectors generated by the Min. Res. Algorithm satisfy:

$$\|r_{k+1}\|_2 \le \left(1 - \frac{\mu^2}{\sigma^2}\right)^{1/2} \|r_k\|_2$$

- In this case Min. Res. converges for any initial guess x_0.

Proof: Similar to steepest descent. Start with

$$\begin{aligned}\|r_{k+1}\|_2^2 &= (r_k - \alpha_k A r_k, r_k - \alpha_k A r_k) \\ &= (r_k - \alpha_k A r_k, r_k) - \alpha_k (r_k - \alpha_k A r_k, A r_k).\end{aligned}$$

By construction, $r_{k+1} = r_k - \alpha_k A r_k$ is $\perp A r_k$. ➤ $\|r_{k+1}\|_2^2 = (r_k - \alpha_k A r_k, r_k)$. Then:

$$\begin{aligned}\|r_{k+1}\|_2^2 &= (r_k - \alpha_k A r_k, r_k) \\ &= (r_k, r_k) - \alpha_k (A r_k, r_k) \\ &= \|r_k\|_2^2 \left(1 - \frac{(Ar_k, r_k)}{(r_k, r_k)} \frac{(Ar_k, r_k)}{(Ar_k, Ar_k)}\right) \\ &= \|r_k\|_2^2 \left(1 - \frac{(Ar_k, r_k)^2}{(r_k, r_k)^2} \frac{\|r_k\|_2^2}{\|Ar_k\|_2^2}\right).\end{aligned}$$

Result follows from the inequalities $(Ax, x)/(x, x) \ge \mu > 0$ and $\|Ar_k\|_2 \le \|A\|_2 \, \|r_k\|_2$. ■

3. Residual norm steepest descent.

A is arbitrary (nonsingular). Take at each step $d = A^T r$ and $e = Ad$.

Iteration:
$$r \leftarrow b - Ax, d = A^T r$$
$$\alpha \leftarrow \|d\|_2^2 / \|Ad\|_2^2$$
$$x \leftarrow x + \alpha d$$

- Each step minimizes $f(x) = \|b - Ax\|_2^2$ in direction $-\nabla f$.
- Important Note: equivalent to usual steepest descent applied to normal equations $A^T A x = A^T b$.
- Converges under the condition that A is nonsingular.